Phase transitions: on a crossroads of probability and analysis

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Abstract. Contour methods first emerged in the probabilistic proofs of long range order for lattice models. With help of cluster expansions, they turned into a powerful tool for investigation of phase transitions for a large class of models that allows to study various phenomena involving coexisting phases (interfaces, equilibrium crystal shapes) as well as the behaviour in finite volume including the asymptotics of the phase transition points as well as the determination of asymptotic location of zeros of partition functions. The aim of the talk, presented at the "Young Researchers Symposium", was to introduce contour methods and, trying to avoid technicalities in this rather technical subject, show some of their applications.

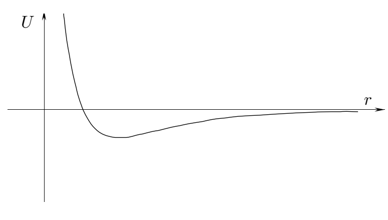
Problem of phase transitions

Phase transitions are in the core of Statistical Physics—they describe collective emergent phenomena not immediately apparent directly from the properties of constituting molecules.

Even though it was conceptually clear already to Gibbs how to microscopically describe, say, liquid-vapour transition, the rigorous proof of the occurrence of the transition starting only from first principles is still an important and, in addition, easily formulated open problem. The goal is to prove that there indeed occurs a discontinuity in the density for a system of interacting particles with Hamiltonian

$$H_N(\vec{p}_1, \dots, \vec{p}_N, \vec{r}_1, \dots, \vec{r}_N) = \sum_{i=1}^{N} \frac{\vec{p}_i^{\,2}}{2m} + \sum_{i,j=1}^{N} U(|\vec{r}_i - \vec{r}_j|), \qquad (1)$$

where U is a suitable pair potential (for realistic gases it might be something like the Lenard-Jones potential, $U(r) \sim -\left(\frac{\alpha}{r}\right)^6 + \left(\frac{\alpha}{r}\right)^{12}$, with strong short range repulsion and long range attraction, as shown in the figure). Here, the density ρ



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is given by $\rho = \mathfrak{z}\frac{\partial}{\partial \mathfrak{z}}\big(\lim_{V\nearrow\mathbb{R}^3}\frac{1}{|V|}\log Z_G(\beta,\mathfrak{z},V)\big)$, where the *grandcanonical partition function* is

$$Z_G(\beta,\mathfrak{z},V) = \sum_N \frac{\mathfrak{z}^N}{N!}\int_{\mathbb{R}^{3N}\times V^N} e^{-\beta H_N}\frac{\prod d^3\vec{p}_i \prod d^3\vec{r}_i}{h^{3N}} = \\ = \sum_N \frac{\mathfrak{z}^N}{N!}\Big(\frac{2\pi m}{\beta h^2}\Big)^{\frac{3}{2}N}\int_{V^N} e^{-\beta\sum_{i,j}U(|\vec{r}_i-\vec{r}_j|)}\prod d^3\vec{r}_i. \tag{2}$$

The open problem is:

Prove that, for suitable range of β's (sufficiently large), there exists $\mathfrak{z}_t(\beta)$ such that the function $\rho(\beta,\mathfrak{z})$ has a discontinuity at $\mathfrak{z}=\mathfrak{z}_t(\beta)$.

The first steps done recently in this direction for genuinely continuous systems are presented in the plenary talk of Errico Pressutti [**Pr**].

The idea that a phase transitions can be described by a theory based only on a unique underlying Hamiltonian that does not *a priori* distinguish the phases, did not come easily[1]. In finite volume, the function $\rho_V(\beta,\mathfrak{z}) = \mathfrak{z}\frac{1}{|V|}\frac{\partial}{\partial\mathfrak{z}}\log Z_G(\beta,\mathfrak{z},V)$ is clearly a real analytic function of its variables β and $\mathfrak{z}$. In particular, it has no discontinuity—it is just very steep in the neighbourhood of $\mathfrak{z}_t$. It would be difficult, however, to introduce phase transitions as points at which the function ρ_V is growing "very rapidly". Conceptually much simpler is to consider a mathematical idealization: to go to infinite volume (thermodynamic limit), $V\to\mathbb{R}^3$, and instead of rapid change to look for real discontinuities.

Two roads to phase transitions

There are two alternative ways how to detect the first order phase transitions in the thermodynamic limit:

- as an *existence of nonanalyticities* in a thermodynamic potential;
- as *instabilities of the probability distribution* with respect to boundary conditions.

We will explain these two roads to phase transitions on the example of the Ising model; the simplest case for which we have a full understanding of all involved subtleties.

In the same time, this will allow us to introduce the contour method—the central topic of the talk—whose use is actually based on a subtle entanglement of probability and analysis. The contour method is, in its full generality, a powerful approach to the phase transitions with a lot of applications. Actually, for the results described in two plenary talks at this Congress [**Pr, Sh**], this technique plays a decisive role.

[1] Serious doubts existed for long time. This was witnessed by an anecdotal ballot at the van der Waals Centenary Conference in 1937. The question was *"does the partition function contain the information necessary to describe a sharp phase transition?"* The outcome of the vote was not very conclusive.

To set the stage, let us consider the Ising model on the lattice $\mathbb{Z}^d$, $d \geq 2$. Its configurations are $\boldsymbol{\sigma} = \{\sigma_x; x \in \mathbb{Z}^d\}$ with spins σ_x taking values ± 1, $\sigma_x \in \{-1, 1\}$. For any finite $\Lambda \subset \mathbb{Z}^d$, we define the energy of a configuration $\boldsymbol{\sigma}_\Lambda$ in Λ under the boundary conditions $\overline{\boldsymbol{\sigma}}$ by

$$H_\Lambda(\boldsymbol{\sigma}_\Lambda \mid \overline{\boldsymbol{\sigma}}) = -J \sum_{\substack{\langle x,y\rangle \\ x,y\in\Lambda}} (\sigma_x\sigma_y - 1) - J \sum_{\substack{\langle x,y\rangle \\ x\in\Lambda, y\in\Lambda^c}} (\sigma_x\overline{\sigma}_y - 1) - h\sum_{x\in\Lambda}\sigma_x \quad (3)$$

with $\langle x, y\rangle$ denoting (unordered) pairs of nearest neighbours and J a coupling (supposed to be positive when playing the role of a model of ferromagnets).

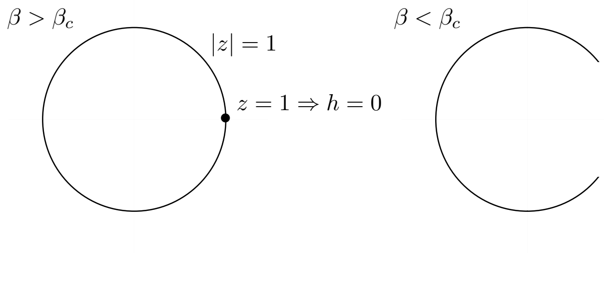
Passing to the thermodynamic limit, it is easy to show that the *free energy*

$$f(\beta, h) = -\frac{1}{\beta} \lim_{\Lambda_n \nearrow \mathbb{Z}^d} \frac{1}{|\Lambda_n|} \log Z^{\overline{\boldsymbol{\sigma}}}_{\Lambda_n}, \quad (4)$$

where $Z^{\overline{\boldsymbol{\sigma}}}_\Lambda$ is the partition function $Z^{\overline{\boldsymbol{\sigma}}}_\Lambda = \sum_{\boldsymbol{\sigma}_\Lambda} e^{-\beta H_\Lambda(\boldsymbol{\sigma}_\Lambda|\overline{\boldsymbol{\sigma}})}$, exists for any sequence Λ_n such that $|\Lambda_n| \to \infty$, $\frac{|\partial\Lambda_n|}{|\Lambda_n|} \to 0$ (convergence in the van Hove sense) and that it does not depend on $\overline{\boldsymbol{\sigma}}$ and on the particular sequence Λ_n.

The *analysis road* to the phase transitions for the Ising model thus consists in studying nonanalyticities[2] of the free energy $f(\beta, h)$.

Given that the finite volume partition functions $Z^{\overline{\boldsymbol{\sigma}}}_\Lambda$ are actually analytic functions of parameters β and h , the only points that can cause trouble (can lead to a nonanalyticity of $f(\beta, h)$) are zeros of the partition functions or, rather, accumulation points of the sequences of zeros for $Z^{\overline{\boldsymbol{\sigma}}}_{\Lambda_n}$. Based on this fact, Lee and Yang [**LY, YL**] proposed a program of analyzing the phase transitions in terms of zeros of partition function. In particular, they studied the zeros of the Ising model partition function Z_{T_N} with periodic boundary conditions. Here, the partition function Z_{T_N} is defined in terms the Hamiltonian $H_{T_N}(\boldsymbol{\sigma}_{T_N})$ on the torus $T_N = \mathbb{Z}^d/(N\mathbb{Z})^d$ with $|T_N| = N^d$ sites. The partition function $Z_{T_N}(z)$, viewed as a function of the complex variable $z = e^{-2\beta h}$ with the complex magnetic field h, is a polynomial of the order N^d. In addition to showing that there is no phase transition for any real z whose neighbourhood (in the complex z plane) is free of zeros of the partition functions $Z_{T_N}(z)$ for large N,



[2]We will restrict our attention to first order phase transitions where a first derivative is discontinuous as opposed to other points of nonanalyticities referred to as continuous phase transitions.

they have proven the remarkable result that all zeros of $Z_{T_N}(z)$, for any N, necessarily lie on the unit circle, $|z| = 1$. This implies that there are no phase transitions for any $h \neq 0$. For sufficiently small temperatures (β large), there is an accumulation point of zeros on real axis at $z = 1$, while for high temperatures, $\beta < \beta_c$, there is a gap with no zeros in a neighbourhood of real z.

On the other hand, we can take the *probabilistic road* and record a nonuniqueness of the limiting Gibbs states μ defined by

$$\mu(\cdot) = \lim_{\Lambda_n \nearrow \mathbb{Z}^d} \mu_{\Lambda_n}(\cdot \mid \overline{\boldsymbol{\sigma}}) \tag{5}$$

with the limit over finite volume Gibbs states under fixed boundary conditions,

$$\mu_\Lambda(\boldsymbol{\sigma}_\Lambda \mid \overline{\boldsymbol{\sigma}}) = \frac{e^{-\beta H_\Lambda(\boldsymbol{\sigma}_\Lambda | \overline{\boldsymbol{\sigma}})}}{Z_\Lambda^{\overline{\boldsymbol{\sigma}}}}. \tag{6}$$

More precisely, (5) defines a measure on $\{-1,1\}^{\mathbb{Z}^d}$ by the weak limit

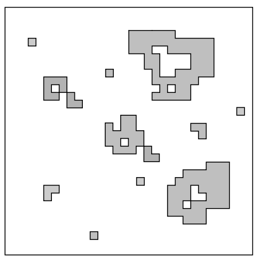
$$\mu(\varphi) = \lim_{\Lambda_n \nearrow \mathbb{Z}^d} \mu_{\Lambda_n}(\varphi \mid \overline{\boldsymbol{\sigma}}) \tag{7}$$

for cylindric functions φ on $\{-1,1\}^{\mathbb{Z}^d}$ (functions depending only on the values of $\boldsymbol{\sigma}$ in a finite subset of $\mathbb{Z}^d$). A phase transition of the first order occurs whenever the limiting Gibbs state is not unique, revealing certain instability with respect to boundary conditions—a small change on the boundary may lead to a dramatic change in the limiting measure on $\{-1,1\}^{\mathbb{Z}^d}$.

In particular, for the Ising model it can be shown that, at $h = 0$ and for β sufficiently large, there is a phase transition since the measures $\mu_+(\cdot) = \lim_{\Lambda_n \nearrow \mathbb{Z}^d} \mu_{\Lambda_n}(\cdot \mid \boldsymbol{\sigma}^+)$ and $\mu_-(\cdot) = \lim_{\Lambda_n \nearrow \mathbb{Z}^d} \mu_{\Lambda_n}(\cdot \mid \boldsymbol{\sigma}^-)$ differ. Here, $\boldsymbol{\sigma}^+$ and $\boldsymbol{\sigma}^-$ are *plus* and *minus* boundary conditions, $\sigma_x^\pm = \pm 1$, $x \in \mathbb{Z}^d$. At the transition, the variables σ_x are strongly dependent—the typical configurations of $\mu_\pm$ do not differ too much from the corresponding *ground configurations* $\boldsymbol{\sigma}^\pm$.

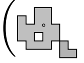
Contour language

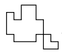
That this is indeed the case, can be shown with the help of the famous *Peierls argument.* The configurations $\boldsymbol{\sigma}_\Lambda$ in Λ, under the boundary condition $\boldsymbol{\sigma}^+$, are in one-to-one correspondence with collections $\partial = \{\gamma\}$ of disjoint contours—connected components of the set of the boundary lines between regions of *plus* and *minus* spins. In the figure on the right, the regions of minuses are shaded and the contours form their boundary. The probability that the spin σ_0 at the origin is *minus* (as it is the case for the



configuration on the figure) is then bounded as follows:

$$P_\Lambda(\sigma_0 = -1 \mid \boldsymbol{\sigma}^+) \leq \sum_{\gamma \circledcirc 0} P_\Lambda\Big(\quad\Big) \leq \sum_{\gamma \circledcirc 0} e^{-2\beta|\gamma|} \leq \sum_{n=2d}^{\infty} e^{-2\beta n} K^n \leq \varepsilon. \tag{8}$$



Namely, one evaluates the probability that $\sigma_0 = -1$ by the probability that there exists a contour γ surrounding the origin, $\gamma \circledcirc 0$. The probability that a particular contour γ is present, here $\gamma \equiv$ , is then estimated in terms of its length $|\gamma|$ by $e^{-2\beta|\gamma|}$. Here we are using the fact that, after the contour γ has been extracted, all terms remaining in the sum over all collections of contours that are mutually compatible and, in the same time, compatible with γ can be found in the normalizing factor—the partition function

$$Z_\Lambda^{\boldsymbol{\sigma}^+} = \sum_{\partial \text{ in } \Lambda} \prod_{\gamma \in \partial} e^{-2\beta|\gamma|}, \tag{9}$$

where the sum is over all collections ∂ of mutually compatible contours in Λ. Finally, we notice that the length of the shortest contour is $2d$ and that the number of contours of length n surrounding origin is at most K^n with a suitable constant K. As a result, we get the uniform bound ε by taking β large enough. Hence, even for the limiting measure μ_+, the spin σ_0 very likely equals $+1$. On the other hand, for μ_-, by symmetry, it very likely equals -1; the measures μ_+ and μ_- differ. We say that, at $h = 0$ and for β large, both *plus* and *minus* phases are *stable*—the corresponding boundary conditions lead to distinct states with majority of spins agreeing with the boundary.

There are two important ingredients in the argument above. First, *compatibility* of contours is defined pairwise by a sort of "hard core repulsion". Namely, two contours are compatible whenever they are disjoint. In particular, any configuration with a particular contour taken away is again a legal contour configuration (corresponding to a well defined spin configuration). Second, long contours are *suppressed*; the factor $e^{-2\beta|\gamma|}$ decays exponentially with the size of the contour. Both this facts allow us to view the system as a *hard core gas of contours* with small fugacity. However, small fugacity means low density, allowing a good control of the probability $\mu^+(\sigma_0 = -1)$ as a perturbation of the "empty system" corresponding to the pure ground configuration $\boldsymbol{\sigma}^+$ with no minuses (no contours).

Cluster expansions

Small fugacity contour gas perturbations can be used not only for a discussion of the instabilities, with respect to boundary conditions, of the probability distributions; in addition, it yields a tool for a detailed analysis of analytic properties of the partition functions. This concerns even more general situations: in fact, any model whose partition functions can be reformulated in terms of contours as

$$Z_\Lambda(w) = \sum_{\partial \text{ in } \Lambda} \prod_{\gamma\in\partial} w(\gamma), \tag{10}$$

where $w(\gamma)$ are some, sufficiently decaying, weights. The compatibility must be defined pairwise, but it can be more general than the condition of disjointness occurring for the contours of the Ising model.

Actually, one can formulate very strong claims, coming under the heading *cluster expansions*, that form a basic building block for more involved applications. It is useful to state the standard cluster expansion results in an abstract setting [**KP**] and, as recently stressed by Sokal [**So**], the simplest formulation is in terms of graphs. Consider thus a graph G with (possibly infinite countable) set of vertices V and set of edges E. In the situation of the contour model above, V is the set of all contours and any pair of contours that are not mutually compatible is joined by an edge. The partition function Z_Λ is well defined by (10) for any map $w : V \to \mathbb{C}$ and any[3] finite $\Lambda \subset V$. In the graph theory language, the collections ∂ of compatible contours become *independent sets* of vertices $\partial \subset \Lambda$—the graph induced on ∂ by G contains no edges.

A condition on smallness of fugacities $w(\gamma)$ can, in this abstract setting, be given in the following way:

there exists a function $b : V \to (0,\infty)$ *such that, for each* $\gamma \in V$,

$$|w(\gamma)| \le (1 - e^{-b(\gamma)}) \exp\{\sum_{\bar\gamma:(\bar\gamma,\gamma)\in E} b(\bar\gamma)\}. \tag{11}$$

This condition (extending slightly that one from [**KP**]) was formulated by Dobrushin who used it in an elegant and simple complex analysis proof of the cluster expansion results [**Do1**]. Even though it might seem to be a bit indirect way of evaluating the decay of w's, it is actually very natural—it pops out exactly as formulated here in the inductive proof. In the case of standard contours (like those for Ising model) it follows directly from the assumption of exponential decay of contour weights: $|w(\gamma)| \le e^{-\tau_0|\gamma|}$ for any contour γ, with a suitably chosen factor τ_0 (depending on the constant K in the bound K^n on the number of contours of length n containing a fixed site).

Let $\mathcal{X}$ be the set of all multiindices $X : V \to \{0, 1, \dots\}$ such that $\sum_{\gamma\in V} X(\gamma) < \infty$, let $\mathcal{X}(\Lambda) = \{X \in \mathcal{X} \colon \gamma \notin \Lambda \Rightarrow X(\gamma) = 0\}$, $w^X = \prod_\gamma w(\gamma)^{X(\gamma)}$ and, finally, let $\operatorname{supp} X = \{\gamma \in V : X(\gamma) \neq 0\}$. With this notation, we can summarize [**Do1, M-S**] the cluster expansion claims in the following way:

[3] It is natural to identify lattice volumes with the sets of all contours contained in it. However, it turns out to be very useful to consider a generalization [**KP**] by taking for Λ any finite subset of V. Such an extension prepares ground for surprisingly easy and straightforward induction proofs.

Cluster expansion. *There exists a function* $\phi : \mathcal{X} \to \mathbb{R}$ *that is nonvanishing only on* clusters *(i.e.* $\phi(X) = 0$ *if the graph induced by* G *on the set of vertices* $\operatorname{supp} X$ *is not connected), so that for any contour weight* $w : V \to \mathbb{C}$ *satisfying* (11)*:*

(i) *for every finite* $\Lambda \subset V$ *one has* $Z_\Lambda(w) \neq 0$ *and*

$$\log Z_\Lambda(w) = \sum_{X \in \mathcal{X}(\Lambda)} \phi(X) w^X,$$

(ii) $\sum_{X \in \mathcal{X}: \operatorname{supp} X \ni \gamma} |\phi(X)||w|^X \leq b(\gamma)$.

This theorem has important, less or more direct, implications in the particular case of the contour reformulation of the Ising model. The main point is that using the claim (i) above, we have a very explicit expression for the logarithm of the partition function in terms of local contributions (with a good control of their decay by (ii)) allowing not only an explicit expression for the free energy in (12) below, but also explicit expressions for the surface terms that are useful when discussing interfaces between coexisting stable phases.

Let us, very briefly, outline some most important applications:

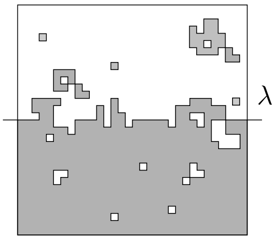
Analyticity of the free energy. Directly from (i) above, we get an explicit formula

$$f(\beta, h = 0) = -d - \frac{1}{\beta} \sum_{X: A(X) \ni 0} \frac{\phi(X) w^X}{|A(X)|}. \tag{12}$$

Here, $A(X)$ is the set of sites attached to contours from $\operatorname{supp} X$, $A(X) = \{x \in \mathbb{Z}^d \mid \exists \gamma \in \operatorname{supp} X \text{ such that } \operatorname{dist}(x, \gamma) \leq 1/2\}$. Notice that due to symmetry of the Ising model, the cluster expansions corresponding to $+$ and $-$ phase are identical. As a consequence of the fact that (12) is, for large β, an absolutely convergent sum of analytic terms $\phi(X) w^X$ (considered as functions of β), the function $f(\beta, h = 0)$ is, for large β, analytic in β. This is a precursor of many similar results proven with help of the cluster expansion.

Existence of a Gibbs state with interface. The existence of a Gibbs state (for the Ising model with $d \geq 3$ and $h = 0$) whose typical configuration exhibits an interface, was first proven by Dobrushin [**Do2**]. Enforcing the state by an appropriate boundary conditions $\boldsymbol{\sigma}^{\mathrm{I}}$ (for example, $\sigma^{\mathrm{I}}_x = +1$ for $x = (x_1, \dots, x_d)$ with $x_1 \geq 0$ and $\sigma^{\mathrm{I}}_x = -1$ otherwise) one evaluates the probability that the interface λ does not differ too much from the plane[4] corresponding to the boundary conditions. To this end, it is useful to replace, with help of the cluster expansion, the partition functions in the regions $\Lambda^{\mathrm{up}}_\lambda$

[4]In spite of showing an illustration for $d = 2$, we have in mind here the case $d = 3$. Actually, for $d = 2$ the interface does not exist (is not stable in the thermodynamic limit) [**Ga**].



above λ and $\Lambda_\lambda^{\rm down}$ below of it, as well as inside of "pockets" $\Lambda_{\lambda,1}^{\rm int}$, $\Lambda_{\lambda,2}^{\rm int}$,... enclosed by λ. Using a shorthand $\Phi(X) = \phi(X)w^X$ and taking into account that $\Lambda_\lambda^{\rm up}$, $\Lambda_\lambda^{\rm down}$, as well as each connected "pocket" $\Lambda_{\lambda,\alpha}^{\rm int}$ is surrounded by either *plus* or *minus* spins (it has a fixed boundary condition $\boldsymbol{\sigma}^+$ or $\boldsymbol{\sigma}^-$) and noticing that all contributing contours are compatible with λ, we get[5], up to a normalization,

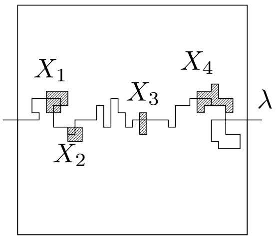
$$P_\Lambda(\lambda \mid \boldsymbol{\sigma}^\pm) \sim e^{-2\beta|\lambda|} Z^{\boldsymbol{\sigma}^+}(\Lambda_\lambda^{\rm up}) Z^{\boldsymbol{\sigma}^-}(\Lambda_\lambda^{\rm down}) \prod_\alpha Z^{\boldsymbol{\sigma}^\pm}(\Lambda_{\lambda,\alpha}^{\rm int}) \sim$$

$$\sim e^{-2\beta|\lambda|} \exp\Big\{ \sum_{\substack{X:\, \text{supp}\, X \subset \Lambda \\ X \text{ not compatible with } \lambda}} \Phi(X) \Big\}. \qquad (13)$$

Expanding

$$\prod_X \big\{1 + e^{\Phi(X)} - 1\big\} = \sum_{\{X_i\}} \prod_i \big(e^{\Phi(X)} - 1\big), \qquad (14)$$

we are getting the probability distribution of interfaces λ in terms of weight factors depending on these interfaces decorated by a collection of cluster terms.

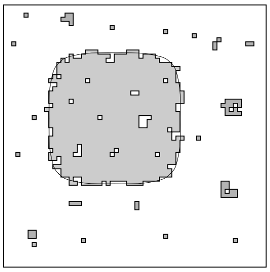


The statistics of decorated interfaces can then be discussed, following Dobrushin, by splitting them into collection of independent *walls* (all connected portions of decorated interface that are locally not identical to a shifted ideal plane). What we are getting here, is a *gas of walls* that can be again treated by cluster expansions. This way of rewriting the probability of the original interface is especially useful in more general situations, when we have no symmetry of the Ising model and we want study the interface between two stable phases controlled with the help of Pirogov-Sinai theory discussed below. Even though the case of the horizontal interface was studied in full generality [**HKZ1, ČK**], including models featuring several competing ideal interfaces [**HKZ2**], the case of an interface with a general inclination angle has been discussed only for particular models [**DKS, HK**] and its description in a general situation remains to be an important open problem.

Wulff shape. With a good understanding of the statistics of interfaces, which essentially amounts to a good control of the interface free energy (surface tension), one can address the problem of typical

[5] Here, the configurations in $\Lambda_\lambda^{\rm up}$ contributing to $Z^{\boldsymbol{\sigma}^\pm}(\Lambda_\lambda^{\rm up})$ have to contain only contours compatible with λ. The partition function $Z^{\boldsymbol{\sigma}^\pm}(\Lambda_\lambda^{\rm up})$ (so called *diluted partition function*) thus slightly differs from $Z^{\boldsymbol{\sigma}^\pm}_{\Lambda_\lambda^{\rm up}}$. Similarly for $\Lambda_\lambda^{\rm down}$ and $\Lambda_{\lambda,\alpha}^{\rm int}$.

configurations under the condition of a fixed magnetization. This is the problem of the equilibrium droplet in the Ising model (mimicking an equilibrium crystal shape). It turns out that typical configurations feature a big contour whose shape is very close to the Wulff shape obtained by optimalization of the macroscopic surface tension under the condition of a fixed volume of the droplet. This claim has been first proven in the two-dimensional case (and at low temperatures) in [**DKS**] by a strategy based on the use of cluster expansion techniques. There was a remarkable development recently that lead to a solution of an analog of this problem for the three-dimensional percolation [**Ce**] and later also the three-dimensional Ising model [**CP**],[**Bo1**], see also the contribution [**Bo2**] in this volume. An extension to the situation of coexistence of nonsymmetric phases is, however, an open problem.



Out of the coexistence line

Up to now, we discussed the case $h = 0$.

What happens when $h \neq 0$? Of course, we know from the spin-flip symmetry that the transition occurs exactly at $h = 0$. The problem is that for a more general system with no analogous symmetry (even in the Ising model, it is easy to imagine an addition of small interacting terms to the Hamiltonian that would break the symmetry $h \to -h$), the value $h_t(\beta)$ at which the transition occurs is *a priori* not known. Having this fact in mind, it is useful to treat the case $h \neq 0$ of the Ising model pretending, if possible, that we do not know where the transition actually occurs[6].

We can still write the partition function in terms of contours. This time, however, the formula (9) is replaced by

$$Z_\Lambda^{\boldsymbol{\sigma}^+} = \sum_{\partial \text{ in } \Lambda} e^{-\beta e_+ |\Lambda_+(\partial)| - \beta e_- |\Lambda_-(\partial)|} \prod_{\gamma \in \partial} e^{-2\beta|\gamma|}. \tag{15}$$

Here, $e_\pm = \mp h$ is the energy (per site) of the ground configuration $\boldsymbol{\sigma}^\pm$ and $\Lambda_\pm(\partial)$ is the set of sites in $\Lambda(\partial)$ occupied by $\pm$ spins. Notice that now a contour cannot be erased without changing all configuration ($\Lambda_\pm(\partial)$ has to be changed). Moreover, in a more general case with asymmetric interaction, one should also take into account that the contour weight $e^{-2\beta|\gamma|}$ can be replaced by a weight $\rho(\gamma)$ that explicitly distinguishes the sign of spins surrounding the contour, say, $\rho(\ {}^{-}_{+}\ ) \neq \rho(\ {}^{+}_{-}\ )$. In any case, we are losing the principal property—the fact that

[6] This pedagogic trick was suggested by C. Borgs.

compatibility of contours is defined pairwise. In general, one cannot erase a contour from a configuration without changing the weight of remaining contours!

Can we still apply the powerful cluster expansions here? The answer is yes, after some work: there is a way how to recover contour independence and come back to, even though somewhat artificial, hard core contour gas. Let us define two different weights corresponding to plus and minus boundary conditions. Namely,

$$w_+(\gamma) = \rho(\gamma)\frac{Z^{\boldsymbol{\sigma}^-}(\operatorname{Int}\gamma)}{Z^{\boldsymbol{\sigma}^+}(\operatorname{Int}\gamma)} \tag{16}$$

for contours with outer spin *plus* and

$$w_-(\gamma) = \rho(\gamma)\frac{Z^{\boldsymbol{\sigma}^+}(\operatorname{Int}\gamma)}{Z^{\boldsymbol{\sigma}^-}(\operatorname{Int}\gamma)} \tag{17}$$

for those with outer spin *minus*. Here, $\operatorname{Int}\gamma$ is the set of sites inside γ (union of finite components of $\mathbb{Z}^d \cap (\mathbb{R}^d \setminus \gamma)$) and the configurations in $\operatorname{Int}\gamma$ contributing to $Z^{\boldsymbol{\sigma}^\pm}(\operatorname{Int}\gamma)$ are supposed to contain only[7] contours compatible with γ. It is easy to show by induction in $|\Lambda|$ that

$$Z_\Lambda^{\boldsymbol{\sigma}^+} = e^{-\beta e_+|\Lambda|}\sum_{\partial \text{ in } \Lambda}\prod_{\gamma\in\partial} w_+(\gamma) = e^{-\beta e_+|\Lambda|}Z_\Lambda(w_+) \tag{18}$$

and

$$Z_\Lambda^{\boldsymbol{\sigma}^-} = e^{-\beta e_-|\Lambda|}\sum_{\partial \text{ in } \Lambda}\prod_{\gamma\in\partial} w_-(\gamma) = e^{-\beta e_-|\Lambda|}Z_\Lambda(w_-). \tag{19}$$

We thus succeeded to rewrite $Z_\Lambda^{\boldsymbol{\sigma}^\pm}$ in terms of contour model partition functions defined by (10); but do the weights w_+ and w_- satisfy (11), to enable the use of cluster expansions? Since they yield a correct evaluation of the probability of outer contours (under $\mu_\Lambda(\cdot \mid \boldsymbol{\sigma}^+)$ and $\mu_\Lambda(\cdot \mid \boldsymbol{\sigma}^-)$), one would then be able to use them for a proof of the fact that the corresponding phase is stable: typical configurations contain only small contours. One can interpret, say, $w_+(\gamma)$ as "the cost of erasing the contour γ" including the replacement of $Z^{\boldsymbol{\sigma}^-}(\operatorname{Int}\gamma)$ in its interior by $Z^{\boldsymbol{\sigma}^+}(\operatorname{Int}\gamma)$. Then it is not surprising that one can actually prove that $w_+(\gamma)$ satisfies the bound (11) in the region of the stability of the plus phase (i.e. for all $h \geq 0$ in the case of the Ising model). In addition, and this is a crucial fact, the weight $w_+(\gamma)$ satisfies (11) even for $h < 0$ for contours γ that are not too large. Indeed, if a contour γ is so small (in dependence on $|h|$) that $2|h||\operatorname{Int}\gamma| < |\gamma|$, we have

$$\left|\frac{Z^{\boldsymbol{\sigma}^\mp}(\operatorname{Int}\gamma)}{Z^{\boldsymbol{\sigma}^\pm}(\operatorname{Int}\gamma)}\right| \leq e^{\beta|h|2|\operatorname{Int}\gamma|} \leq e^{\beta|\gamma|} \tag{20}$$

[7] Again (as explained in the footnote 5), the partition function $Z^{\boldsymbol{\sigma}^\pm}(\operatorname{Int}\gamma)$ slightly differs from $Z^{\boldsymbol{\sigma}^\pm}_{\operatorname{Int}\gamma}$.

and thus

$$|w_+(\gamma)| \le e^{-\beta|\gamma|}. \tag{21}$$

On the other hand, sufficiently large contours are not suppressed as we are actually loosing by their erasure; *plus* being an unstable phase (recall, $h < 0$), it is profitable to flip over a long contour into a stable *minus* phase gaining a volume term proportional to $|h||\mathrm{Int}\,\gamma|$. The smaller is $|h|$, the larger is the class of contours with decaying weight $w_+(\gamma)$. Nevertheless, to deal only with contours whose weights are well decaying, we can simply disregard those for which this is not the case by defining new weights $\overline{w}_+(\gamma)$ that equal to $w_+(\gamma)$ once (21) is satisfied and setting $\overline{w}_+(\gamma) = 0$ otherwise[8]. The weights $\overline{w}_+$ constitute some sort of well decaying "creeping approximation" of w_+: in the region of stability of plus phase ($h \ge 0$) we have an exact identity, $\overline{w}_+ \equiv w_+$, while in the region of instability they coincide on bigger and bigger class of contours as we are coming closer and closer to the transition line. Similarly we define also $\overline{w}_-$.

The weights $\overline{w}_\pm$ are somehow artificially defined, but have an important property—they are sufficiently suppressed so that we can use cluster expansions for them. In particular, we can use the claim (i) from the cluster expansion theorem to write explicitly the limit

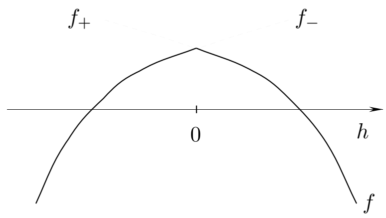
$$\lim \frac{\log Z_\Lambda(\overline{w}_+)}{\Lambda} = \sum_{X:A(X)\ni 0} \frac{\phi(X)\overline{w}_+{}^X}{|A(X)|} \tag{22}$$

and *define*

$$f_+ = e_+ - \frac{1}{\beta} \sum_{X:A(X)\ni 0} \frac{\phi(X)\overline{w}_+{}^X}{|A(X)|} \tag{23}$$

and, similarly,

$$f_- = e_- - \frac{1}{\beta} \sum_{X:A(X)\ni 0} \frac{\phi(X)\overline{w}_-{}^X}{|A(X)|}. \tag{24}$$



The functions $f_\pm(\beta, h)$ (referred to, with a slight terminological abuse, as to *metastable free energies*) have remarkable properties: they intersect *exactly* at the transition point $h = 0$ and their minimum is, again *exactly*, the actual free energy $f(\beta, h)$ defined by (4), $f(\beta, h) = \min(f_+(\beta, h), f_-(\beta, h))$. Given the equalities (18) and (19), this fact follows from the claims $\overline{w}_+ \equiv w_+$ for $h \ge 0$ and $\overline{w}_- \equiv w_-$ for $h \le 0$.

In a general nonsymmetric case, however, the logic has to be reversed. Think, for simplicity, about the Ising model with a small local interaction added that breaks the $\pm$ symmetry. In this case, we do

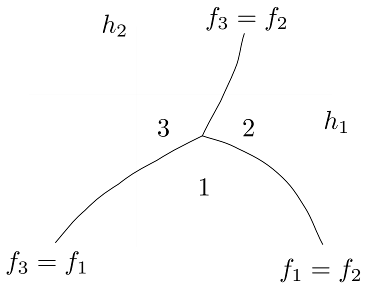
[8] This is a version [**BI**] of the definition introduced originally in [**Za**].

not know the value of the transition point h_t any more. Nevertheless, we can still introduce the *creeping approximation weights* $\overline{w}_\pm$. Using them to define the metastable free energies $f_\pm$, we first *define* $h_t(\beta)$ as the solution of the equation $f_+(\beta, h) = f_-(\beta, h)$ and then *prove*, by induction in $\operatorname{Int}\gamma$, that $\overline{w}_+ \equiv w_+$ and thus the *plus phase is stable for* $h \geq h_t$, while $\overline{w}_- \equiv w_-$ and the *minus phase is stable for* $h \leq h_t$. In particular, for $h = h_t$ we have the simultaneous stability of both phases; each of them can be chosen by fixing the corresponding boundary conditions—there is a phase transition exactly at $h = h_t$!

Without going into details of this rather complex induction process, we only notice that the crucial point is the fact that $\bar{w}_\pm$ are, indeed, creeping approximation weights: the closer to the (unknown) transition point, the larger contours have the weight satisfying the bound (21). This claim can be actually proven by induction. In this way we are ensured that the solution of the equation $f_+(\beta, h) = f_-(\beta, h)$ is *exactly* the transition point. Notice, finally, that even though the definition of the functions $f_\pm$ is unambiguous in terms of $\overline{w}_\pm$, there is some freedom in the definition of $\overline{w}_\pm$ (without changing either $\min(f_+(\beta, h), f_-(\beta, h))$ or h_t). This freedom allows a smoother definition of the weights $\overline{w}_\pm$, the possibility that is crucial for some applications mentioned further.

Pirogov-Sinai theory

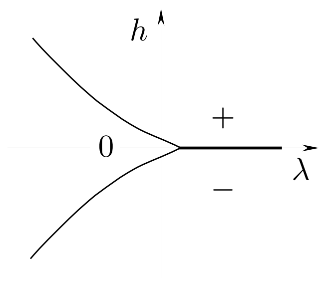
The strategy described above is the quintessence of the contemporary version [**Za, BI, BoKo**] of the Pirogov-Sinai theory [**PS**]. It actually works for a quite general class of lattice models. One has just to assume (but extensions exist) that there is a finite number of periodic ground states that could enter the competition for stable phases, that in any configuration one pays for any boundary between two ground states by an energy contribution proportional to the size of the boundary (so called Peierls condition; in the case of Ising model this is responsible for the weight $e^{-2\beta|\gamma|}$), and that the temperature is sufficiently small. The crucial point is that one can again constructively define a *metastable free energy* f_m for each of the ground states coming into consideration. The line of coexistence of the phases m and q in the phase diagram (in terms of suitable driving fields parametrizing the Hamiltonian; here h_1 and h_2) is then given by the equality $f_m = f_q$. Inside the region corresponding to the phase m, there is a unique Gibbs state characterized by the fact that its typical configuration consists of a "sea" of the ground configuration m with separated islands of different configurations.



A popular example [**BS**] to illustrate the construction of the phase diagram in the Pirogov-Sinai theory and to show the role of entropic contributions, is the Blume-Capel model. Considering the spins $\sigma_x \in \{-1, 0, 1\}$, its Hamiltonian is

$$H_\Lambda(\boldsymbol{\sigma}) = -J \sum_{\langle x,y \rangle} (\sigma_x - \sigma_y)^2 - -\lambda \sum_{x \in \Lambda} \sigma_x^2 - h \sum_{x \in \Lambda} \sigma_x. \tag{25}$$

Taking only the lowest order excitations into account, we get:
$\tilde{f}_\pm = -\lambda \mp h - \frac{1}{\beta} e^{-\beta(2d - \lambda \pm h)}$ (a single spin flip $\pm \to 0$) and
$\tilde{f}_0 = -\frac{1}{\beta} e^{-\beta(2d+\lambda)} \big(e^{\beta h} + e^{-\beta h} \big)$ (a single spin flip either $0 \to +$ or $0 \to -$). Since these functions differ from full metastable free energies $f_\pm$, f_0 by terms of higher order ($\sim e^{-(4d-2)\beta}$), the real phase diagram differs in this order from that one constructed with the help of $\tilde{f}_\pm$, $\tilde{f}_0$. Schematically, we get (for a fixed, sufficiently small, temperature) the coexistence lines as shown in the figure. In particular, notice that at the origin, $\lambda = h = 0$, it is the phase 0 that is stable at all small temperatures since $f_0 \sim -\frac{2}{\beta} e^{-\beta 2d} < f_\pm \sim -\frac{1}{\beta} e^{-\beta 2d}$. The only reason why the phase 0 is favoured at this point with respect to phases $+$ and $-$, is that there are *two* excitations of order $e^{-2d\beta}$ for the phase 0, while there is only *one* such excitation for $+$ or $-$. The entropy of the lowest order contribution to f_0 is overweighting the entropy of the contribution to $f_\pm$ of the same order.



The basic statement of the Pirogov-Sinai theory yielding the construction of the full phase diagram has been extended to a big class of models. Let us, without any pretension on completeness, mention at least few of them:

- continuous spins [**DZ, BW**] ...
- Potts model [**Ma, BKL, KLMR, LMMRS**] ...
- ANNNI model, microemulsions [**DS, DM, KLMM**]
- random field Ising model [**BrKu**] (using a *renormalization group version* of the Pirogov-Sinai theory first formulated in [**GKK**])
- quantum models [**DFF, DFFR, BKU**]...
- continuous systems [**LMP**].

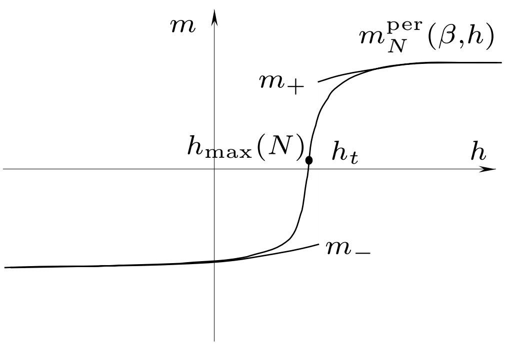
Several applications, stemming from the Pirogov-Sinai theory, are based on the fact that, due to the cluster expansion, we have quite accurate description of the model in finite volume. Considering the simplest example of the periodic boundary conditions, for a model with r competing phases, the partition function $Z_{T_N}(\beta, h)$ can be, with the help of the cluster expansion, explicitly and very accurately evaluated,

$$\Big| Z_{T_N} - \sum_{m=1}^{r} e^{-\beta f_m N^d} \Big| \le \exp\{-\beta f N^d - b\beta N\}, \tag{26}$$

with a fixed constant b. We will see that this remarkable formula (and its generalization to the case of complex external fields) allows to harvest various results concerning the behaviour of the model in finite volumes. In the remaining sections we will mention two of them.

Finite-size effects

Considering, for illustration, a perturbation of the Ising model, so that it has no more the $\pm$ symmetry (and the transition point $h_t(\beta)$ is not known), we can pose a natural question that has an importance for correct interpretation of simulation data. Namely, what is the asymptotic behaviour of the magnetization $m_N^{\text{per}}(\beta,h) = \langle\sum_{i\in\Lambda}\sigma_i\rangle_{T_N}$ in a finite cube, $|\Lambda| = N^d$, under periodic boundary conditions? In the thermodynamic limit, the magnetization $m_\infty^{\text{per}}(\beta,h)$ displays, as a function of h, a discontinuity at $h = h_t(\beta)$. For finite N, the jump is smoothed; we get a *rounding* of the discontinuity as on the attached illustration. What is the shift of a naturally chosen finite volume transition point $h_t(N)$ with respect to the limiting value h_t? The clue to a systematic description of the rounding lies in two facts. First, with the help of (26), we can approximate $Z_{T_N}(\beta,h)$ by the sum $e^{-\beta f_+ N^d} + e^{-\beta f_- N^d}$. In the same time, the freedom in the definition of the "metastable free energies" $f_+(\beta,h)$ and $f_-(\beta,h)$ can be used to replace them by a sufficiently smooth version [**BoKo**], so that the functions $f_\pm$ above can be approximated by their Taylor expansion around limiting point h_t.



As a result, it turns out that, in spite of the asymmetry of the model, the finite volume magnetization $m_N^{\text{per}}(\beta,h)$ has a universal behaviour in the neighbourhood of the transition point h_t. Considering a fixed (sufficiently large) β and using $m_\pm = \lim_{h\to h_t\pm} m_\infty^{\text{per}}(\beta,h)$, $m_0 = \frac{1}{2}(m_+ + m_-)$, and $m = \frac{1}{2}(m_+ - m_-)$, we have

$$m_N^{\text{per}}(\beta,h) = m_0 + m\tanh\bigl\{N^d\beta m(h-h_t)\bigr\} + R(h,N). \tag{27}$$

The error[9] can be bounded by $|R(h,N)| \le e^{-b\beta N} + K(h-h_t)^2$.

Another direct consequence of (26) concerns the asymptotic behaviour of different variants of the finite volume approximations of the transition point. A natural choice for the transition point is the inflection point $h_{\max}(N)$ of $m_N^{\text{per}}(\beta,h)$.

[9]For h far from h_t there are more accurate approximations in terms of $m_\pm(\beta,h)$.

Its asymptotic behaviour can be precisely described. Namely, it can be proven [**BoKo**] that

$$h_{\max}(N) = h_t + \frac{3\chi}{2\beta^2 m^3} N^{-2d} + O(N^{-3d}). \tag{28}$$

Moreover, as a result of the corresponding analysis, it turns out that there are also other, more accurate, choices of the finite volume transition point. For example, the value $h_0(N)$ defined as the solution of $m_N^{\text{per}}(\beta, h) = m_0$ is asymptotically exponentially close to h_t, $h_0(N) = h_t + O(e^{-b_0 \beta N})$.

For the Potts model that, for $d \geq 2$ and the number of spin values q large enough, features a discontinuity in the mean energy as a function of temperature [**KS**], the rounding is also under control [**BKM**]. Namely,

$$E_N^{\text{per}}(\beta) \approx E_0 + E \tanh\Big\{E(\beta - \beta_t)N^d + \tfrac{1}{2}\log q\Big\}. \tag{29}$$

The inverse temperature $\beta_{\max}(L)$ where the slope of $E_N^{\text{per}}(\beta)$ is maximal is shifted by

$$\beta_{\max}(N) - \beta_t = -\frac{\log q}{2E} N^{-d} + O(N^{-2d}). \tag{30}$$

We see clearly the origin of the difference between the asymptotic behaviour of the shift of the inflection point for the perturbed Ising model and the Potts model (it was a source of certain controversy in the literature—see [**BoKo**] for references and a detailed discussion). The fact that the shift for the Potts model is of the order N^{-d} can be traced down to the term $\log q$ in the argument of tanh, i.e., to the fact that at β_t we have coexistence of q low temperature phases with one high temperature phase. Perturbed Ising model corresponds in this sense to $q = 1$ (coexistence of one phase for $h \leq h_t$ with one phase for $h \geq h_t$) and the term of the order N^{-d} multiplied by the factor $\log q$ vanishes, leaving the next term of the order N^{-2d} to lead the asymptotic behaviour.

General Lee-Yang zeros

The full strength of the formula (26) is revealed when studying the zeros of the partition function $Z_{T_N}(z)$ as a polynomial in the complex parameter z. Again, we consider a lattice system with r competing phases. After some effort it turns out [**BBCKK**] that the definitions of the metastable free energies go through even for complex values of z. It should be stressed that the construction goes still through yielding, this time genuinely complex, contour models $w_\pm$ with the help of an inductive procedure. No analytic continuation is involved. In addition, an analog of (26) is still valid,

$$\Big|Z_{T_N}(z) - \sum_{m=1}^{r} e^{-\beta f_m N^d}\Big| \le \exp\{-\beta f N^d - b\beta N\}. \tag{31}$$

Only, this time the function $f(z)$ in the error term is *defined* as $f(z) = \min_m \mathfrak{Re} f_m(z)$. The stability of the m^{th} phase is characterized by the condition $\mathfrak{Re} f_m = f$; the function f_m for stable m equals the free energy of the system with boundary condition m (in complex case, the free energy in general depends on the boundary conditions).

It is not difficult to convince oneself that the loci of zeros can be traced down to the phase coexistence lines. Indeed, on the line of the coexistence of two phases[10] $\mathfrak{Re} f_m = \mathfrak{Re} f_n = f$ and $\mathfrak{Re} f_\ell > f$ for $\ell \notin \{m,n\}$, The partition function $Z_{T_N}(z)$ is approximated by $e^{-\beta f N^d}\big(e^{-\beta \mathfrak{Im} f_m N^d} + e^{-\beta \mathfrak{Im} f_n N^d}\big)$. The zeros of this approximation are thus given by the equations

$$\begin{aligned} &\mathfrak{Re} f_m = \mathfrak{Re} f_n < \mathfrak{Re} f_\ell \ \text{ for all } \ell \ne m,n,\\ &\beta N^d(\mathfrak{Im} f_m - \mathfrak{Im} f_n) = \pi \bmod 2\pi. \end{aligned} \tag{32}$$

The zeros of the full partition function $Z_{T_N}(z)$ can be proven to be exponentially close, up to a shift of order $\mathcal{O}(e^{-\beta b N})$, to those of the discussed approximation.

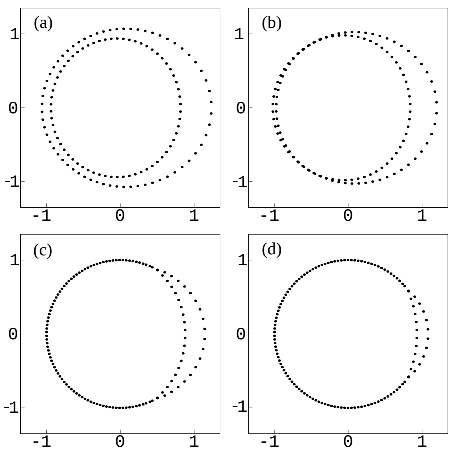
Briefly, *the zeros of $Z_{T_N}(z)$ asymptotically concentrate on the phase coexistence curves with the density* $\frac{1}{2\pi}\beta N^d|(d/dz)(f_m - f_n)|$.

Finally, let us illustrate this general analysis on a simple example where it yields rather unexpected picture for the zeros location. Namely, let us consider, again, the case of the Blume-Capel model with a fixed parameter λ and a complex $z = e^{-\beta h}$. First, we notice that, in analogy with the real case, the large β expansions of the free energies (in the case $d = 2$, for simplicity) can be easily computed [**BBCKK**],

$$\begin{aligned} e^{-\beta f_+} &= z e^{\beta\lambda} \exp\left\{\tfrac{1}{z} e^{-\beta(\lambda+4)} + 2\tfrac{1}{z^2} e^{-\beta(2\lambda+6)} + \mathcal{O}(e^{-8\beta})\right\}\\ e^{-\beta f_-} &= \tfrac{1}{z} e^{\beta\lambda} \exp\left\{z e^{-\beta(\lambda+4)} + 2z^2 e^{-\beta(2\lambda+6)} + \mathcal{O}(e^{-8\beta})\right\}\\ e^{-\beta f_0} &= \exp\left\{(z+\tfrac{1}{z}) e^{\beta(\lambda-4)} + 2(z^2+\tfrac{1}{z^2}) e^{\beta(2\lambda-6)} + \mathcal{O}(e^{-8\beta})\right\}. \end{aligned}$$

The zeros for different values of λ are shown on the left (the figure is taken from [**BBCKK**]). Notice that the zeros have a non-uniform distribution, they form curves of non-circular shape, and for λ in a certain interval $(\lambda_c^-, \lambda_c^+)$, a bifurcation occurs. All these facts can be rigorously established with help of the general analysis discussed above.

[10] A neighborhood of size $\delta_N \sim N^{-(d-1)}$ of the finite-volume triple or higher coexistence points has to be excluded from the following simple reasoning. In these neighbourhoods the argument is more involved and, actually, suitable conditions on the dependence of the ground state energies on z have to be assumed.



On the attached figure taken from [**BBCKK**], there are 128 zeros corresponding to $N = 8$; we put $e^{-4\beta} = 1/16$ and $e^{\beta\lambda} =$ (a) 0.9, (b) 0.94, (c) 1, (d) 1.07. For $\lambda < \lambda_c^- \approx -e^{-4J}$, the outer region of the $+$ phase is separated from the inner $-$ phase by an annular region of the 0 phase (a); asymptotically, the zeros lie on the boundaries of these regions. As λ increases through λ_c^-, the two boundaries coalesce on the left hand side, leading to bifurcation for $\lambda > \lambda_c^-$. The common boundary grows (c,d) and, eventually, at $\lambda = \lambda_c^+ \approx e^{-4J}$, the region of the 0 phase disappears. For $\lambda > \lambda_c^+$, all zeros lie on the unit circle.

Notice that for $\lambda = 0$ (the figure (c)), the phase 0 is stable at $z = 1$, while it is unstable at $z = -1$. We already established the former claim corresponding to the origin $\lambda = h = 0$; it stems from the fact that the phase 0 is favoured by having more lowest order excitations then phases $+$ and $-$. However, this is actually also the reason for the latter claim! For $z = -1$ the sign of the corresponding contribution to the free energy changes and thus the phase 0 is suppressed.

For $\beta < \beta_c$ a gap around real axis will open (as it was in the case of the Ising model). A challenging open problem (also for the Ising model) is to prove the convergence of the corresponding cluster expansion for $z = -1$. The fact that z is negative should lead to a suppression of whole classes of contours in spite of the fact that the decay $e^{-2\beta|\gamma|}$ is not sufficiently strong.

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