GEOMETRIC REPRESENTATION OF LATTICE MODELS AND LARGE VOLUME ASYMPTOTICS

ROMAN KOTECKÝ*
Centre for Theoretical Study
Charles University
Celetná 20
116 36 Praha 1
Czech Republic
e-mail: kotecky@cspuni12.bitnet

Abstract. The finite volume asymptotics of lattice models near first-order phase transitions is discussed. The tool for the description of finite size effects is (a version of) the Pirogov–Sinai theory. Its main ideas are reviewed and illustrated on simple models.

Key words: Lattice models, phase transitions, finite size effects, Pirogov–Sinai theory.

1. Introduction

There is a vast inventory of lattice models providing examples of first-order phase transitions and coexistence of phases. It became clear already from the first proof of existence of such a transition for the Ising model by the Peierls argument [P, G, D1] that a convenient tool for a study of the coexistence of phases is a representation in terms of probabilities of configurations of geometric objects — contours. This approach has been systematically developed in Pirogov–Sinai theory [PS, S]. At present it is the main technique for the study of phase transitions for models with no symmetry between coexisting phases. Here, I will discuss its use for the derivation of the asymptotic behaviour, as the size of the system grows, in the region of the first-order phase transitions [BK1, BK2, BKM, BI1–3].

Even though the original papers by Pirogov and Sinai were published almost twenty years ago, the theory is not widely known outside a rather restricted group of mathematical physicists. Thus, my first aim in this lecture is to present a simple-minded introduction to the Pirogov–Sinai theory taking into account some latest developments. I will not attempt to develop the theory in its full generality. Instead, only the main principles will be explained and the theory will be ilustrated on the simplest examples of models that still capture the general features.

As a starting point, let us recall a couple of banal facts about the standard ferromagnetic Ising model. The probability of a configuration $\sigma_\Lambda \equiv \{\sigma_i\}_{i\in\Lambda}$, $\sigma_i \in \{-1,+1\}$, on a finite lattice $\Lambda \subset \mathbb{Z}^d$, $d \geq 2$, and under the boundary conditions

*Also in the Department of Theoretical Physics, Charles University.

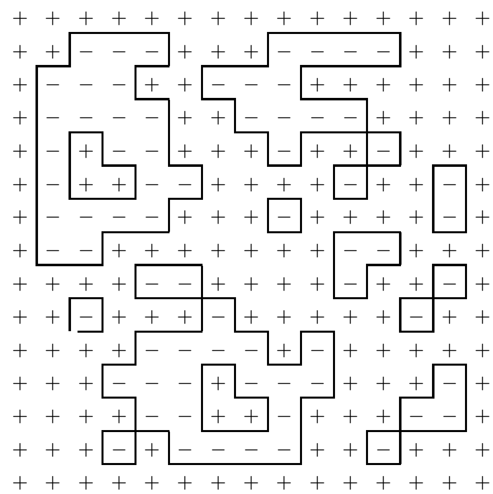

Fig. 1

$\overline{\sigma}_{\Lambda^c} = \{\overline{\sigma}_i\}_{i \in \mathbb{Z}^d \setminus \Lambda}$, is given by

$$\mu_\Lambda(\sigma_\Lambda \,|\, \overline{\sigma}_{\Lambda^c}) = \frac{e^{-\beta H_\Lambda(\sigma_\Lambda \,|\, \overline{\sigma}_{\Lambda^c})}}{Z_\Lambda(\overline{\sigma}_{\Lambda^c})}, \tag{1}$$

where the energy is[1]

$$H_\Lambda(\sigma_\Lambda \,|\, \overline{\sigma}_{\Lambda^c}) = -\sum_{\substack{\langle i,j \rangle \\ i,j \in \Lambda}} (\sigma_i \sigma_j - 1) - \sum_{\substack{\langle i,j \rangle \\ i \in \Lambda, j \in \Lambda^c}} (\sigma_i \overline{\sigma}_j - 1) - h \sum_{i \in \Lambda} \sigma_i \tag{2}$$

with the sum over pairs of nearest neighbours, and the normalizing partition function is

$$Z_\Lambda(\overline{\sigma}_{\Lambda^c}) = \sum_{\sigma_\Lambda} e^{-\beta H_\Lambda(\sigma_\Lambda \,|\, \overline{\sigma}_{\Lambda^c})}. \tag{3}$$

At high temperatures, β small, the random variables σ_i are ‘almost independent’ and as a result, for $\Lambda \nearrow \mathbb{Z}^d$, there is a unique weak limit μ of (1) independent of boundary conditions (or sequence of boundary conditions $\{\overline{\sigma}_{\Lambda^c}\}_\Lambda$).

On the other hand, at low temperatures, β large, the variables σ_i are strongly dependent — a first-order phase transition occurs that reveals itself in the fact that, for $h = 0$, the particular boundary conditions corresponding to the ground configurations $\overline{\sigma}_{\Lambda^c} = +\underline{1}$, $\overline{\sigma}_i = +1$ for all $i \in \Lambda^c$, and $\overline{\sigma}_{\Lambda^c} = -\underline{1}$, lead for vanishing external field, $h = 0$, to different limiting measures μ_+ and μ_-.

The proof of this fact by the famous Peierls argument is based on a reformulation of the model (with $h = 0$) in terms of probabilities of particular spatial patterns

[1]A constant has been added to the Hamiltonian, so that the energy of ground configurations in the case without external field, $h = 0$, vanishes.

in the configurations. Namely, one considers configurations $\partial = \{\Gamma\}$ of contours Γ introduced for a spin configuration σ as components of the boundaries between areas of pluses and minuses (see Fig. 1)[2]. For a fixed boundary condition (say $+\underline{1}$) the correspondence between spin configurations and collections ∂ of mutually disjoint contours is one to one and the probability of a contour configuration ∂ under the measure $\mu_\Lambda(\cdot\,|+\underline{1})$ (with $h=0$) is

$$\mu_\Lambda(\partial\,|+\underline{1}) = \frac{1}{\mathcal{Z}(\Lambda)} \prod_{\Gamma\in\partial} e^{-2\beta|\Gamma|}. \tag{4}$$

Here

$$\mathcal{Z}(\Lambda) = \sum_{\partial\in\Lambda} \prod_{\Gamma\in\partial} e^{-2\beta|\Gamma|} \tag{5}$$

with the sum over collections of mutually disjoint contours in Λ. It differs from $Z_\Lambda(+\underline{1})$ ($\equiv Z_\Lambda(-\underline{1})$) by the factor that equals the contribution of the configuration $+\underline{1}$ to $Z_\Lambda(+\underline{1})$.

The typical configurations σ of the measure μ_+ obtained as the limit of $\mu_\Lambda(\,\cdot\,|+\underline{1})$ can be characterized by proving that, in the limiting probability obtained from (4), the typical contour configurations ∂ are such that for every $\Gamma\in\partial$ there exists the most external contour surrounding it. (No infinite 'cascades' of contours exist.) This fact is proven, with the help of the Borel–Cantelli lemma, by evaluating the probability of every contour surrounding a fixed site in such a way that the sum of these probabilities can be shown to converge. As a result, one characterizes the typical configurations σ of the measure μ_+ as consisting of a connected sea of pluses containing finite islands of minuses. Or, in other words, in a typical configuration of μ_+ the pluses percolate (and minuses do not). This situation can be described as a *stability* of plus phase. By the same reasoning we can show that also the minus phase is stable and characterize the measure μ_- as supported by configurations with percolating minuses. The measures μ_+ and μ_- thus differ – we say that two different phases coexist for $h=0$ and β large or that phase transition of the first order occurs for $h=0$.

The trick that allows one to describe the typical configurations, in spite of the fact that the variables σ_i are actually strongly dependent, is based on replacing them by 'contour variables' and viewing their probability distribution (4) as a perturbation of a contour-free (empty) configuration that corresponds to the ground spin state $+\underline{1}$ in the case of μ_+. The crucial fact for the Ising model is its plus-minus symmetry. It follows not only that the phase transition should be expected to occur for vanishing external field, $h=0$, but also that the contours distributed by (4) are *essentially independent*. We use this term to refer to the fact that the weight factor in (4) is multiplicative; once the contours in ∂ are pairwise compatible – every two contours Γ and $\overline{\Gamma}$ from ∂ are disjoint – they contribute independently.

A configuration with a particular contour skipped is again a possible configuration (under fixed boundary conditions $+\underline{1}$ there exists a uniquely defined corresponding

[2]We are illustrating the two-dimensional case here, with contours characterized as connected sets consisting of edges of the dual lattice $(\mathbb{Z}^2)^* \equiv \mathbb{Z}^2 + (\frac{1}{2},\frac{1}{2})$ such that every vertex of $(\mathbb{Z}^2)^*$ is contained in even number (0, 2, or 4) of its edges.

spin configuration in Λ) and the weights of remaining contours do not change. The second main ingredient is the fact that the long contours are sufficiently *damped* — the weight factor of a given contour Γ (in our case $e^{-2\beta|\Gamma|}$) decreases quickly with its length $|\Gamma|$; namely, it can be bounded by $e^{-\tau|\Gamma|}$ with a sufficiently large τ (to achieve this in our case one simply takes β large enough). This is a direct consequence of the fact that the difference of the energy of a configuration and the ground state configuration (say $+\underline{1}$) is proportional to the length of its contours (Peierls condition).

It is the fulfilment of these two conditions, essential independence and damping, that allows us to use any form of standard *cluster expansion* for a study of properties of the contour probability distribution. In the next section we summarize the properties of such contour models in a form to be used later. Unfortunately, even a small perturbation to the Ising Hamiltonian (2) may break the essential independence of contours. Instead, one is getting a model with 'labeled contours' with 'long-range matching conditions'. In Section 3 we explain this notion by representing a simple perturbation of the Ising model in terms of such a *labeled contour model*. The perturbed Ising model, in spite of its simplicity, actually contains all the ingredients of the general case and we will simplify the presentation of the main ideas by formulating and proving the results just in this case. Our first step is to recover the essential independence – to find contour models, one for each phase, that yield information about the original model with the corresponding boundary conditions. Before showing, in Section 5, how to achieve this, we discuss in Section 4 the Potts model – our aim there is to illustrate how a model of quite different type also naturaly leads to a labeled contour model. The main step of Pirogov–Sinai theory in the present setting is to show that a transition point $h_t(\beta)$ exists such that (for large β) both contour models constructed in Section 5 are damped and thus both phases are stable for $h = h_t$. For some models (such as the unperturbed Ising ferromagnet) the value h_t can be guessed from the symmetry. In Section 6 we discuss the case of Ising antiferromagnet that can be considered to be 'half way' to the general case. Even though the transition point can be guessed from the symmetry, the real proof of stability of both concerned phases is a good illustration of inductive procedure used also in less symetric cases. The perturbed Ising model, as a representative of the general case, is discussed in Section 7. In a finite volume, say a cube $\Lambda = L \times L \times \cdots \times L$, the transition reveals itself as a rapid change, as the function of h, of the magnetization defined as the mean value $\left\langle \sum_{i\in\Lambda} \sigma_i \right\rangle_\Lambda^{\text{per}}$ under the periodic boundary conditions. The final Section 8 is devoted to an application of the results of Section 7 to the discussion of universal behaviour of the magnetization in the neighbourhood of the transition point and the asymptotic dependence of the finite volume transition point $h_t(L)$ defined, say, as the inflexion point of the finite volume magnetization curve.

2. Contour Models

Let us suppose that a weight factor z assigning a real non-negative number $z(\Gamma)$ to every contour Γ is given[3]. A collection ∂ of contours of contours in Λ is called *compatible* if they are mutually disjoint. The *contour model*, satisfying the condition of essential independence, with the weight factor z is defined by specifying the probability of any compatible collection ∂ of contours in Λ by

$$\mu_\Lambda(\partial; z) = \frac{1}{\mathcal{Z}(\Lambda; z)} \prod_{\Gamma \in \partial} z(\Gamma) \tag{6}$$

with the partition function (we reserve script $\mathcal{Z}$ for partition functions of contour models)

$$\mathcal{Z}(\Lambda; z) = \sum_{\partial \in \Lambda} \prod_{\Gamma \in \partial} z(\Gamma). \tag{7}$$

The contribution of the empty configuration $\partial = \emptyset$ is taken to be 1 by definition.

We are not going to discuss the details of the cluster expansion here; let us only formulate its main assertion [GK, Se, KP2, DKS] that can be for our case translated into the following statement.

Proposition 1. *For a contour model with a damped weight factor z, satisfying, for sufficiently large τ and for every contour Γ, the (damping) bound*

$$z(\Gamma) \leq e^{-\tau|\Gamma|}, \tag{8}$$

there exists a mapping Φ assigning real numbers to finite connected (in the connection by paths whose edges are pairs of nearest neighbour sites) subsets of $\mathbb{Z}^d$, such that

$$\log \mathcal{Z}(\Lambda; z) = \sum_{C \subset \Lambda} \Phi(C) \tag{9}$$

for every finite Λ. Moreover, the contributions $\Phi(C)$ are damped,

$$|\Phi(C)| \leq e^{-\tau d(C)/2}, \tag{10}$$

where $d(C)$ is the minimal summary length (area) of a set of contours such that the union of their interiors equals C. Actually, there is an explicit formula for $\Phi(C)$,

$$\Phi(C) = \sum_{A: A \subset C} (-1)^{|C \setminus A|} \log \mathcal{Z}(A; z). \tag{11}$$

[3] Here we have in mind the contours as introduced above, but sometimes (e.g., when studying interfaces [HKZ1, HKZ2]) it is useful to consider slightly more complicated structures — standard contours 'decorated' by some additional sets etc. The present formulation of the contour model can be easily reformulated in a more abstract way [KP2] covering these situations. In particular, the condition of compatibility may differ from simple disjointness. However, an important feature that has to be valid is that compatibility is defined pairwise — a collection ∂ is compatible if all pairs of contours from ∂ are compatible.

Also, the weight $z(\Gamma)$ may be in general complex. To assume that it is real non-negative suffices in our case and it simplifies the formulation.

If the contour model is translation invariant[4]*, there exists the 'free energy'* $g(z) = -\beta^{-1} \lim\{\Lambda^{-1} \log \mathcal{Z}(\Lambda; z)\}$*, given by*

$$g(z) = \sum_{C: i \in C} \frac{\Phi(C)}{|C|}. \tag{12}$$

Here the sum is over all finite sets containing a given fixed site and $|C|$ *denotes the number of points in* C*. The free energy is bounded by*

$$g(z) \le e^{-\tau/2}. \tag{13}$$

3. Perturbed Ising Model

In the case of the Ising ferromagnet with vanishing external field we were fortunate to get immediately the representation (4) in terms of a contour model. This is not at all obvious. Actually, even a small perturbation to the Hamiltonian (2) may introduce a 'long-distance dependence' among contours. To see what I mean by that, consider a simple plus-minus symmetry breaking term, say,

$$-\kappa \sum_{(i,j,k)} \sigma_i \sigma_j \sigma_k, \tag{14}$$

added to the Hamiltonian (2). Here the sum is over all triangles consisting of a site j and two its nearest neighbours i and k such that the edges (ij) and (jk) are orthogonal. We consider all triplets with at least one of the sites i, j, k in Λ; σ for those sites that are outside Λ is to be interpreted as the corresponding boundary condition $\overline{\sigma}$ (say $+\underline{1}$). Rewriting the model in terms of contours we obtain

$$\mu_\Lambda(\partial \,|\, +\underline{1}) = \frac{1}{Z_\Lambda(+\underline{1})} \prod_{\gamma \in \partial} \rho(\gamma) e^{-\beta e_+ |V_\Lambda^+(\partial)| - \beta e_- |V_\Lambda^-(\partial)|} . \tag{15}$$

Here $V_\Lambda^+(\partial)$ (resp. $V_\Lambda^-(\partial)$ is the number of sites in Λ occupied, for the configuration corresponding to ∂, by pluses (resp. minuses), cf. Fig. 1, and $e_+ = -h - \kappa 2d(d-1)$ (resp. $e_- = h + \kappa 2d(d-1)$) is the average energy per site of the configuration $+\underline{1}$ (resp. $-\underline{1}$). Notice that the weights $\rho(\gamma)$ actually depend not only on the geometrical form of the contour, but also on whether γ is surrounded from outside by pluses or minuses. For example for the contour suronding a single plus spin immersed in minuses we obtain $\rho(\gamma) = e^{-\beta(8+8\kappa d)}$, while for the contour surrounding a single minus spin immersed in pluses we obtain $\rho(\gamma) = e^{-\beta(8-8\kappa d)}$. As a result we have to label the contours by the signature of the spins surrounding it from outside (in (15) we anticipated it and introduced labeled contours $\gamma = (\Gamma, \varepsilon)$ consisting of a geometrical shape Γ labeled by $\varepsilon = \pm 1$ of the outer spins). In (15) we obtained

[4] I.e., $z(\Gamma) = z(\Gamma + i)$ for any contour Γ and any shift i. A correspondingly modified statement is true for contour model satisfying some condition of periodicity.

again the representation in terms of contours with the weights ρ damped (for κ and h small), however, the condition of essential independence has been lost. The order of labeled contours matters — if a plus-contour is surrounded by another plus-contour, there must be a minus-contour immersed between them (in the configuration shown in Fig. 1 there are minus-contours that, in view of plus boundary conditions, have to be surrounded by plus contours). Unlike in unperturbed case, this matching condition introduces certain 'long-range hard core' — a minus-contour γ surrounded by a disjoint plus-contour $\overline{\gamma}$ 'knows' about its presence. Erasing $\overline{\gamma}$ would turn γ into plus-contour and thereby change its weight $\rho(\gamma)$.

4. Potts Model

The representation of a lattice model in terms of a probability distribution of matching collections of labeled contours, see (15), is not restricted to our simple perturbed Ising model. There exists a large class of models that naturally yield such a representation which is actually the starting point of Pirogov–Sinai theory. Before discussing how to recover essential independence and to transform this representation into a contour model, let us consider an example of slightly different type – the Potts model – that leads to a similar representation as (15).

The Potts model is discussed in detail in other lectures in this volume [Gr, N] and thus I will abstain from introducing it here and start directly from its random cluster formulation to get its contour representation. Contours were used already in the original proof of existence of first-order phase transitions [KS] for this model. However, their probability was controlled there with the help of chessboard estimates. A treatment by the Pirogov–Sinai theory has been presented, among others, in [KLMR, BKL] and [M]. A simplification based on the Fortuin–Kasteleyn representation was suggested in [LMMRS] and here I will use the reformulation from [BKM].

Let us begin from the Fortuin–Kasteleyn random cluster representation [FK] with the weight of a set ω of bonds (a subset of the set B_Λ of all bonds intersecting Λ) given by

$$p^{|\omega|}(1-p)^{|\backslash\omega|}q^{c(\omega,b)}. \tag{16}$$

Here $|\omega|$ is the number of bonds in ω, $\backslash\omega \equiv B_\Lambda \setminus \omega$ denotes the complementary set of bonds and $c(\omega,b)$ is the number of components[5] of the set ω under the boundary conditions b (for example, $b=f$, the free boundary conditions when all sites outside Λ are considered to be disjoint; or $b=w$, the wired boundary conditions with all sites outside Λ connected). Up to a factor depending on Λ, the partition function is

$$Z_\Lambda(b) = \sum_\omega (e^\beta - 1)^{|\omega|} q^{c(\omega,b)}, \tag{17}$$

where the temperature factor $1-e^{-\beta}=p$ has been reintroduced. For every set of bonds ω we can introduce contours in the following way: consider first the closed set $\overline{\omega}$ consisting of the union of all bonds from ω with all unit squares whose all four

[5]Each site not touched by ω is counted as one additional component.

Fig. 2. Contours for a configuration of occupied bonds ω in the random cluster representation of the Potts model under the wired boundary conditions. Thick lines correspond to the bonds from ω. Plain thin lines denote the ordered contours (ω from outside), while dashed thin lines denote the disordered contours (ω from inside).

sides belong to ω, all unit cubes whose all twelve edges belong to ω etc. Taking now the $\frac{1}{4}$-neighbourhood $U_{1/4}(\overline{\omega})$ of $\overline{\omega}$ we define the contours as connected components of the boundary of $U_{1/4}(\overline{\omega})$. This procedure is illustrated in Fig. 2. The contours are boundaries between regions occupied by ω (*ordered* regions) and empty (*disordered*) regions whose each site contributes by the factor q to the partition function (17) (it represents the component attributed to a site unattached to ω). Denoting by V_Λ^0 the set of bonds in the former and V_Λ^d in the latter, we get

$$Z_\Lambda(b) = \sum_{\partial} (e^\beta - 1)^{|V_\Lambda^0(\partial)|} q^{|V_\Lambda^d(\partial)|/d} \prod_{\gamma \in \partial} \rho(\gamma). \tag{18}$$

Here the weights of contours $\rho(\gamma)$ depend on the surrounding regions — if γ is surrounded by the order (i.e., ω) from outside (plain thin lines in Fig. 2), we have

$$\rho(\gamma) = q^{-|\gamma|/(2d)}, \tag{19}$$

while for γ surrounded by the disorder from outside (dashed lines in Fig. 2) we have

$$\rho(\gamma) = q^{-|\gamma|/(2d)+1}. \tag{20}$$

Again, in (18) we have a similar representation as in (15). Taking q large enough allows to get sufficiently small weights ρ above. Notice also that the role of the ground state energies $e_\pm$ is played by the free energies (per bond) $\log(e^\beta - 1)$ and $d^{-1} \log q$ of the ordered and entirely disordered states, respectively.

5. Recovering Essential Independence

In any case, as already mentioned, it is the representation of the form (15) (or (18)) that is a starting point for the Pirogov–Sinai representation. An important fact is that we cannot directly apply standard cluster expansions — we first have to get rid off the above described long-range dependence of labeled contours. However, this is rather easy to achieve [PS, Z, KP1]. Namely, one introduces two contour weight factors $z_+(\Gamma)$ and $z_-(\Gamma)$ (by using the notation Γ for the contour here we want to stress that, unlike for $\rho(\gamma)$, the dependence will be only on the shape of the contour (the label being delegated to the subscript of z))

$$z_+(\Gamma) = \rho((\Gamma,+))e^{-\beta(e_- - e_+)|\partial_{\mathrm{I}}\Gamma|}\frac{Z_{\mathrm{Int}\,\Gamma}(-\underline{1})}{Z_{\mathrm{Int}\,\Gamma}(+\underline{1})} \tag{21}$$

and

$$z_-(\Gamma) = \rho((\Gamma,-))e^{-\beta(e_+ - e_-)|\partial_{\mathrm{I}}\Gamma|}\frac{Z_{\mathrm{Int}\,\Gamma}(+\underline{1})}{Z_{\mathrm{Int}\,\Gamma}(-\underline{1})}. \tag{22}$$

Here $\partial_{\mathrm{I}}\Gamma$ denotes the set of all sites attached from inside to the contour Γ (those sites from $\mathbb{Z}^d$ inside Γ whose distance from Γ in the maximum metric equals $\frac{1}{2}$) and $\mathrm{Int}\,\Gamma$ is the set of all sites from $\mathbb{Z}^d$ inside Γ that are not contained in $\partial_{\mathrm{I}}\Gamma$.

With the help of these weights, we get the original partition functions in terms of a contour model.

Lemma 1. *For every finite Λ one has*

$$Z_\Lambda(+\underline{1}) = e^{-\beta e_+|\Lambda|}\sum_{\partial\subset\Lambda}\prod_{\Gamma\in\partial} z_+(\Gamma) \tag{23}$$

and

$$Z_\Lambda(-\underline{1}) = e^{-\beta e_-|\Lambda|}\sum_{\partial\subset\Lambda}\prod_{\Gamma\in\partial} z_-(\Gamma). \tag{24}$$

Proof. Indeed, resumming in the expression (cf. (15))

$$Z_\Lambda(+\underline{1}) = \sum_{\partial\subset\Lambda}\prod_{\gamma\in\partial}\rho(\gamma)e^{-\beta e_+|V_\Lambda^+(\partial)|-\beta e_-|V_\Lambda^-(\partial)|} \tag{25}$$

over all ∂ with a fixed collection ϑ of all most external (plus-)contours, we get

$$Z_\Lambda(+\underline{1}) = \sum_{\vartheta\subset\Lambda} e^{-\beta e_+|\,\mathrm{Ext}_\Lambda(\vartheta)|}\prod_{(\Gamma,+)\in\vartheta}\rho((\Gamma,+))e^{-\beta e_-|\partial_{\mathrm{I}}\Gamma|}Z_{\mathrm{Int}\,\Gamma}(-\underline{1}). \tag{26}$$

Here, we use $\mathrm{Ext}_\Lambda(\vartheta)$ to denote the set of all lattice sites in Λ that are outside every contour Γ of ϑ. Notice that the partition function $Z_{\mathrm{Int}\,\Gamma}(-\underline{1})$ has the fixed minus boundary condition on $\partial_{\mathrm{I}}\Gamma$ and every contour contributing to it is disjoint from Γ. Multiplying each term on the right-hand side of (26) by $\exp(-\beta e_+|\partial_{\mathrm{I}}\Gamma| + \beta e_+|\partial_{\mathrm{I}}\Gamma|)$ $Z_{\mathrm{Int}\,\Gamma}(+\underline{1})/Z_{\mathrm{Int}\,\Gamma}(+\underline{1})$, using the definition (21), and proceeding in proving (23) and (24) by induction in the number of sites in Λ, we use (23) for $Z_{\mathrm{Int}\,\Gamma}(+\underline{1})$ on the right-hand side valid by induction hypothesis ($\operatorname{Int}\Gamma \subsetneq \Lambda$) and obtain thus (23) for the full volume Λ. □

As a result, in (23) and (24) we succeeded in rewriting the partition functions $Z_\Lambda(+\underline{1})$ and $Z_\Lambda(-\underline{1})$ in terms of partition functions $\mathcal{Z}(\Lambda; z_+)$ and $\mathcal{Z}(\Lambda; z_-)$ of contour models z_+ and z_-. These are contour models according to our definition from Section 2 with the condition of essential independence fulfilled.

Two questions may now arise. First, in the formulas (23) and (24) we rewrote only the partition functions. Moreover, we did so in terms of rather artificial contour model (formally speaking, we suppose that inside a plus contour there are again only plus contours). Thus, even if we have the corresponding contour models under control, will it suffice to say something, for example, about typical configurations of the measures μ_+ and μ_-? The answer is positive. Namely, it is clear that the contour models z_+ and z_- introduced above, not only lead to the same (up to a factor) partition functions as the original model, but also yield exactly the same probabilities that a given set ϑ of external contours is present,

$$\mu_\Lambda(\vartheta \mid \pm\underline{1}) = \frac{1}{\mathcal{Z}(\Lambda; z_\pm)} \prod_{\Gamma\in\vartheta} z_\pm(\Gamma)\mathcal{Z}(\operatorname{Int}\Gamma; z_\pm). \tag{27}$$

Once we know that the corresponding contour model, say z_+, is damped (satisfies the bound (8)), we can control the limit $\Lambda \nearrow \mathbb{Z}^d$ and with the help of the equality (27), show that there are no infinite cascades of contours in the limiting measure μ_+ and the plus phase is stable.

However, and this is the second question, it is not clear that, even though the original weights ρ were damped, the newly defined weights z_+ and z_- are also damped. The answer depends on the values of the parameters β and h. It turns out that for a fixed (sufficiently large) β there exists a value $h_t \equiv h_t(\beta)$ such that for $h = h_t$ both z_+ and z_- are damped and thus both plus and minus phases are stable, while for $h > h_t$ only z_+ is damped and for $h < h_t$ only z_- is damped.

The description of this *transition point* $h_t(\beta)$ actually yields the *phase diagram* in the case of the perturbed Ising model[6].

Our next task thus will be to find the transition point with the above formulated properties. Sometimes, in presence of a symmetry, the value of the transition point can be guessed. For example, for the unperturbed Ising model we expected $h_t = 0$. Indeed, for $h = 0$ we got $e_+ = e_- = 0$, $Z_\Lambda^+ = Z_\Lambda^-$, and thus directly

$$z_+(\Gamma) = z_-(\Gamma) = e^{-2\beta|\Gamma|}.$$

Before turning to the general situation, when h_t is *a priori* unknown, let us consider another case for which the value of the transition point can be guessed.

[6]The 'tuning parameter' (driving field) here was the external field h. For the Potts model, one can closely follow our treatment of the perturbed Ising model. The role of 'tuning parameter' is played by the (inverse) temperature β and, to get damped weight $\rho(\gamma)$, we have to suppose that q is large enough.

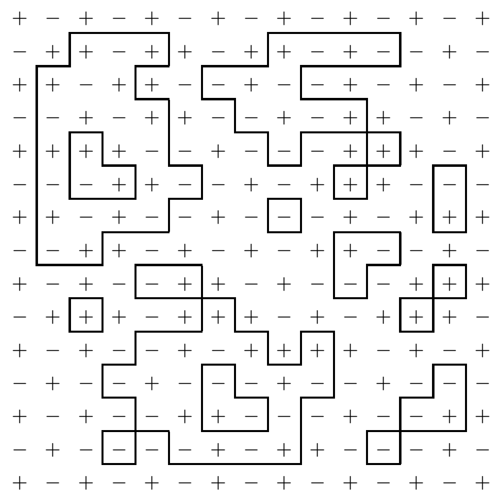

Fig. 3

6. Ising Antiferromagnet

The model I have in mind here is the Ising antiferromagnet with the Hamiltonian

$$H_\Lambda(\sigma_\Lambda \,|\, \overline{\sigma}_{\Lambda^c}) = \sum_{\substack{\langle i,j\rangle \\ i,j\in\Lambda}} (\sigma_i\sigma_j + 1) + \sum_{\substack{\langle i,j\rangle \\ i\in\Lambda, j\in\Lambda^c}} (\sigma_i\overline{\sigma}_j + 1) - h\sum_{i\in\Lambda}\sigma_i. \tag{28}$$

It is known [D2] that for sufficiently small temperatures and small external field h, there exist two antiferromagnetic phases corresponding to two ground configurations. Namely, the configuration with pluses on even lattice sites ($i = (i_1, i_2, \ldots, i_d)$ such that $\|i\| = |i_1| + |i_2| + \cdots + |i_d|$ is even) and minuses on odd sites, let us call it the *even* ground configuration (and use the subscript 'e' to refer to it), and the same configuration shifted by a unit vector the *odd* ground configuration (the subscript 'o').

Let us prove that, indeed, both phases are stable once, for β large enough, the external field h is sufficiently small. In spite of its simplicity, there are two reasons for including this model here. The proof that contour weights for both coexisting phases are really damped is not immediate and it actually involves an important ingredient of the general case. Moreover, a similar reasoning might be useful also in other, more complex, situations — actually, recently we had an occasion to use it for a description of phase transitions in diluted spin systems [CKS] and in a discussion of renormalization group transformations for large external field [EFK].

Let us take, say, the odd ground configuration as the boundary condition. To introduce contours, we again consider the boundaries between regions with even and odd ground configurations. However, this time we take as belonging to the same contour all components whose distance, in maximum metric, is one. Thus, for the configuration on Fig. 3 we have just one contour[7]. Again, under fixed boundary

[7] The configuration in Fig. 3 is deliberately chosen so that the set of all boundary lines is

conditions we have a one-to-one correspondence between spin configurations and collections of contours. Notice that even though we consider, in general, a non-vanishing h, the energies of the ground configuration are (contrary to the case of Ising ferromagnet) equal, $e_o = e_e = 0$.

Thus we have a particularly simple form of labeled contour model with

$$Z_\Lambda(e) = \sum_{\partial\subset\Lambda}\prod_{\gamma\in\partial}\rho(\gamma). \tag{29}$$

Even though this formula is reminiscent of that for the ferromagnet with vanishing field (cf. (5)), here the weights of labeled contours γ depend on the label (which ground configuration surrounds it from outside). To compute the weight $\rho(\gamma)$, one has to compute the energy of the configuration σ for which γ is the single contour. Consider, for the configuration σ, all pairs i, j of nearest neighbour sites such that $j = i + (1, 0, \dots, 0)$ ($j_1 = i_1 + 1,\ j_k = i_k,\ k = 2, \dots, d$) and $\sigma_i = 1,\ \sigma_j = -1$. The remaining unpaired sites are necessarily attached to the contour. Denoting $S(\gamma) = \sum \sigma_i$, with the sum over all these unpaired sites, we clearly have

$$\rho(\gamma) = e^{-2\beta|\gamma| - \beta h S(\gamma)}. \tag{30}$$

The reason for gluing together different components[8] of the boundary between ground configurations was that otherwise these unpaired sites might be shared by different contours. Had we chosen the standard definition of contour, the weight $\rho(\gamma)$ would depend on whether the contour γ is isolated or there are other contours around whose distance from γ is 1 and they share some unpaired sites. Notice, for future use, that the complement of a contour, say an even contour $\gamma = (\Gamma, e)$, may have several components (cf. Fig. 3). We take for the interior of Γ, $\operatorname{Int}\Gamma$, only those sites that are in the configuration σ (the configuration whose single contour is γ) occupied by the odd ground configuration and whose distance, again in maximum metric, from Γ is larger than $\frac{3}{2}$. Notice also that the weight of a labeled contour γ equals the weight of the contour shifted by a unit vector but labeled by the other ground configuration,

$$\rho((\Gamma, e)) = \rho((\Gamma + (1, 0, \dots, 0), o)). \tag{31}$$

We can again use the strategy of the preceding section and introduce the weights

$$z_e(\Gamma) = \rho((\Gamma, e))\frac{Z_{\operatorname{Int}\Gamma}(o)}{Z_{\operatorname{Int}\Gamma}(e)} \tag{32}$$

and

$$z_o(\Gamma) = \rho((\Gamma, o))\frac{Z_{\operatorname{Int}\Gamma}(e)}{Z_{\operatorname{Int}\Gamma}(o)}, \tag{33}$$

identical to that in Fig. 1. While in Fig. 1 we have 11 contours, in Fig. 3 all of them are glued together to a single contour.

[8]The idea of gluing together different connected components is in the general Pirogov–Sinai approach automatically carried out by considering ‘thick contours’ that would consist, for the present case, of components of the union of all those $2\times 2\times\cdots\times 2$ cubes for which the configuration σ restricted to it differs from both ground configurations.

for which

$$Z_\Lambda(e) = \mathcal{Z}(\Lambda; z_e), \quad Z_\Lambda(o) = \mathcal{Z}(\Lambda; z_o). \tag{34}$$

Showing now that both z_e and z_o are damped, we will prove that both phases are stable[9].

Proposition 2. *Let $h < 2$ and β be sufficiently large (depending on h). Then both z_e and z_o are damped and both phases are stable.*

Proof. We will prove the bound (8) for z_e and z_o simultaneously by induction on $\operatorname{diam}\Gamma$. Let us suppose that both z_e and z_o satisfy (8) for all $\overline{\Gamma}$ such that $\operatorname{diam}\overline{\Gamma} < n$. Considering now Γ with $\operatorname{diam}\Gamma = n$, we apply (34) for $Z_{\operatorname{Int}\Gamma}(e)$ and $Z_{\operatorname{Int}\Gamma}(o)$. By the induction hypothesis we can use the cluster expansion (9) for $\mathcal{Z}(\operatorname{Int}\Gamma; z_e)$ and $\mathcal{Z}(\operatorname{Int}\Gamma; z_o)$ yielding

$$\frac{\mathcal{Z}(\operatorname{Int}\Gamma; z_e)}{\mathcal{Z}(\operatorname{Int}\Gamma; z_o)} = \exp\left\{\sum_{C\subset \operatorname{Int}\Gamma} (\Phi_e(C) - \Phi_o(C))\right\}. \tag{35}$$

Observing first that $\Phi_e(C) = \Phi_o(C + (1, 0, \ldots, 0))$ as the direct consequence (by the explicit expression (11)) of the equality $Z_A(e) = Z_{A+(1,0,\ldots,0)}(o)$ implied by (31), the terms in the exponent on the right hand side of (35) with C not too near to the boundary of $\operatorname{Int}\Gamma$ will be cancelled. To bound the remaining terms we notice that since to $\Phi_e(C)$ and $\Phi_o(C)$ in (35) only contours $\overline{\Gamma}$ with $\operatorname{diam}\overline{\Gamma} < n$ contribute, the bound (10) is satisfied[10] by the induction hypothesis. As a consequence we obtain

$$\exp\{-\varepsilon|\Gamma|\} \le \frac{\mathcal{Z}(\operatorname{Int}\Gamma; z_e)}{\mathcal{Z}(\operatorname{Int}\Gamma; z_o)} \le \exp\{\varepsilon|\Gamma|\} \tag{36}$$

with ε of the order $e^{-\tau/2}$. Taking into acount that, clearly, $|S(\gamma)| \le |\gamma|$, we get the bound (8) once $h < 2$. □

7. Transition Point

Finally, we consider the perturbed Ising model as a representative of the general case for which the value of the transition point h_t is not known.

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[9] This is true for a range of values of the field h — the field h does not break the symmetry between the phases. For a 'tuning parameter' that is able to discriminate between these two phases one has to introduce an additional field, for example a *staggered field* in the form of the term $g\sum(-1)^{\|i\|}\sigma_i$ added to the Hamiltonian. Here we are actually taking the transition value $g_t = 0$.

[10] Formally, we may consider $z^{(n)}_{e(o)}$ defined by

$$z^{(n)}_{e(o)}(\overline{\Gamma}) = \begin{cases} z_{e(o)}(\overline{\Gamma}) & \text{if } \operatorname{diam}\overline{\Gamma} < n \\ 0 & \text{otherwise,} \end{cases}$$

notice that $\mathcal{Z}\left(A; z^{(n)}_{e(o)}\right) = \mathcal{Z}(A; z_{e(o)})$ for every A such that $\operatorname{diam} A < n$ by the induction hypothesis, and that in view of (11) only those A contribute to $\Phi_e(C)$ and $\Phi_o(C)$ in (35).

The task is to decide, for given values of parameters h, κ, and β, which of the phases is stable, or in other words, which of the contour weights z_+ or z_- is damped. Following the reformulation of Pirogov–Sinai theory by Zahradník [Z] (or, rather, the version by Borgs and Imbrie [BI1]) we introduce *metastable states* by suppresing all contours whose weights are not damped. Putting thus

$$\overline{z}_\pm(\Gamma) = \begin{cases} z_\pm(\Gamma) & \text{if } |z_\pm(\Gamma)| \le e^{-\tau(\Gamma)}, \\ 0 & \text{otherwise,} \end{cases} \tag{37}$$

we define

$$\overline{Z}_\Lambda(\pm\underline{1}) = e^{-\beta e_\pm |\Lambda|} \mathcal{Z}(\Lambda; \overline{z}_\pm). \tag{38}$$

Notice that both weights $\overline{z}_+$ and $\overline{z}_-$ are automatically damped, and it follows that the cluster expansion can be employed to control the limit $g(\overline{z}_\pm) = -\beta^{-1} \lim\bigl\{|\Lambda|^{-1} \log \mathcal{Z}(\Lambda; \overline{z}_\pm)\bigr\}$ (see (12)). Comparing the explicit expressions (9) and (12), we get $\log \mathcal{Z}(\Lambda; \overline{z}_\pm) = -\beta|\Lambda| g(\overline{z}_\pm) + \varepsilon|\partial\Lambda|$ with ε (as well as βg) of the order $e^{-\tau/2}$ and thus

$$\overline{Z}_\Lambda(\pm\underline{1}) = \exp\{-\beta f_\pm |\Lambda| + \varepsilon|\partial\Lambda|\} \tag{39}$$

with

$$f_\pm = e_\pm + g(\overline{z}_\pm). \tag{40}$$

The *metastable free energies* defined by the equality (40) play an important role in determining which phase is stable — it turns out that the stable phase is characterized by having the minimal metastable free energy. Namely, defining

$$a_\pm = \beta\bigl(f_\pm - \min(f_+, f_-)\bigr), \tag{41}$$

we claim that z_+ is damped once $a_+ = 0$ (and similarly for the minus phase). To prove this assertion we prove by induction on n the following.

Lemma 2 [Z, BI1]**.** *Let κ and h be such that $2|\kappa|(d^2-1) + |h| < 1$ and let $a_+ = 0$. Then, for sufficiently large β, for every n:*

(i) *if* $\operatorname{diam}\Lambda \le n$ *and* $a_- \operatorname{diam}\Lambda \le 1$*, then* $z_-(\Gamma) \le e^{-\tau|\Gamma|}$ *for every* Γ *in* Λ*,*
(ii) $z_+(\Gamma) \le e^{-\tau|\Gamma|}$ *for every* Γ *with* $\operatorname{diam}\Gamma \le n$*.*

Remarks. (1) Notice that, by definition, $\min(a_+, a_-) = 0$. Thus, by this lemma, always at least one of the phases is stable (the plus phase above). Moreover, by (ii) one actually has $\overline{z}_+ \equiv z_+$ and $\overline{Z}_\Lambda(+\underline{1}) = Z_\Lambda(+\underline{1})$. Thus

$$f_+ = -\beta^{-1} \lim\bigl\{|\Lambda|^{-1} \log Z_\Lambda(+\underline{1})\bigr\} \equiv f;$$

the metastable free energy of the stable phase equals the standard free energy of the original model (which, actually, does not depend on the boundary conditions).
(2) The transition point h_t is characterized by the equation $a_+ = a_- = 0$. The parameter $\max(a_+, a_-)$ can be viewed as a measure of distance from the transition point. For sufficiently large volumes is the unstable phase suppressed — the system with unstable (minus) boundary conditions prefers to flip to the plus phase over a long contour encircling large part of the volume Λ. Even though the energy cost of such

a large contour is of the order $|\partial\Lambda|$, there is a volume gain $a_-|\Lambda|$. The statement (i) of Lemma 2 then says that for 'small volumes' ($a_- \operatorname{diam}\Lambda \le 1$) the system prefers to stay in the minus phase. The closer to the transition point (i.e., the smaller is the parameter a_-) the larger volumes are able to support the unstable phase. Very close to the transition point, both phases seem to be stable from the point of view of small volumes (we are saying that the unstable phase (minus) is metastable in small volumes) and, only coming to large volumes, the system is able to distinguish which phase is really stable.

Proof. (i) By the induction hypothesis we can replace $Z_{\operatorname{Int}\Gamma}(\pm\underline{1})$ by $\overline{Z}_{\operatorname{Int}\Gamma}(\pm\underline{1})$. Applying then the equality (39) in the definition (22), we get

$$\begin{aligned}\frac{Z_{\operatorname{Int}\Gamma}(+\underline{1})}{Z_{\operatorname{Int}\Gamma}(-\underline{1})} = \frac{\overline{Z}_{\operatorname{Int}\Gamma}(+\underline{1})}{\overline{Z}_{\operatorname{Int}\Gamma}(-\underline{1})} &\le \exp\{-\beta(f_+ - f_-)|\operatorname{Int}\Gamma| + 2\varepsilon|\Gamma|\} \\ &= \exp\{a_-|\operatorname{Int}\Gamma| + 2\varepsilon|\Gamma|\} \le \exp\{(1+2\varepsilon)|\Gamma|\} \qquad (42)\end{aligned}$$

with ε of the order $e^{-\tau/2}$. In the last inequality we used the inequality $|\operatorname{Int}\Gamma| \le |\Gamma| \operatorname{diam}\Gamma$ and the assumption $a_- \operatorname{diam}\Lambda \le 1$. Taking into account that

$$\rho(\gamma) \le \exp\{-2\beta(1 - 2|\kappa|(d-1))|\gamma|\}, \qquad (43)$$

we get (8) for $z_+(\Gamma)$ once $2|\kappa|(d^2-1) + |h| < 1$ and β is large enough.
(ii) Let us call *small* those contours that satisfy the condition $a_- \operatorname{diam}\Gamma \le 1$. The remaining contours will be called *large*. Resumming in (25) over all collections ∂ of contours with a fixed set ϑ of large external contours and using the induction hypothesis, we get

$$\begin{aligned}\frac{Z_{\operatorname{Int}\Gamma}(-\underline{1})}{Z_{\operatorname{Int}\Gamma}(+\underline{1})} &= \sum_{\substack{\vartheta \text{ large} \\ \vartheta\subset\operatorname{Int}\Gamma}} \frac{Z^{\text{small}}_{\operatorname{Ext}_{\operatorname{Int}\Gamma}(\vartheta)}(-\underline{1}) \prod_{\overline{\gamma}\in\vartheta} \rho(\overline{\gamma}) e^{-\beta e_+|\partial_{\mathrm{I}}\overline{\gamma}|} \overline{Z}_{\operatorname{Int}\overline{\gamma}}(+\underline{1})}{\overline{Z}_{\operatorname{Int}\Gamma}(+\underline{1})} \\ &\le e^{2\varepsilon|\Gamma|} \sum_{\substack{\vartheta \text{large} \\ \vartheta\subset\operatorname{Int}\Gamma}} \exp\Big\{-|\operatorname{Ext}_{\operatorname{Int}\Gamma}(\vartheta)|\beta(f_-^{\text{small}} - f_+)\Big\} \prod_{\overline{\gamma}\in\vartheta} \rho(\overline{\gamma}) e^{3\varepsilon|\overline{\gamma}|}. \qquad (44)\end{aligned}$$

(One $\varepsilon|\overline{\gamma}|$ in the last term comes from the bound on $\beta|e_+ - f_+||\partial_{\mathrm{I}}\overline{\gamma}|$.) In this equation, $Z^{\text{small}}_{\operatorname{Ext}_\Lambda(\vartheta)}(-\underline{1})$ is the partition function with sum taken only over small contours and f_-^{small} is the corresponding metastable free energy. Consider an auxiliary contour model with the weight

$$\tilde{z}(\overline{\Gamma}) = \begin{cases} \big\{\rho((\overline{\Gamma},+)) + \rho((\overline{\Gamma},-))\big\} e^{|\Gamma|} & \text{if } \overline{\Gamma} \text{ is large} \\ 0 & \text{otherwise.} \end{cases}$$

Taking into account the bound (43), we can show that

$$\mathcal{Z}(\Lambda;\tilde{z}) = \exp\{-\beta\tilde{f}|\Lambda| + \varepsilon|\partial\Lambda|\} \qquad (45)$$

(cf. (39)) with ε and $\beta\tilde{f}$ of the order $\exp\{-\tau/(2a_-)\}$ (only large contours for which $|\Gamma| \geq \operatorname{diam}\Gamma \geq (a_-)^{-1}$ contribute). On the other side,

$$\beta|f_- - f_-^{\text{small}}| \leq \sum_{\substack{C \ni i \\ \operatorname{diam} C \geq (a_-)^{-1}}} \frac{\overline{\Phi}_-(C)}{|C|} \leq \exp\left\{-\frac{\tau}{2a_-}\right\} \tag{46}$$

and thus

$$\beta(f_-^{\text{small}} - f_+) \geq a_- - \exp\{-\tau/(2a_-)\}.$$

Since $2\exp\{-\tau/(2a_-)\} \leq 2(2a_-)/\tau \leq a_-$, we have

$$-\beta\tilde{f} = \beta|\tilde{f}| \leq \exp\left\{-\frac{\tau}{2a_-}\right\} \leq a_- - \exp\left\{-\frac{\tau}{2a_-}\right\} \leq \beta\big(f_-^{\text{small}} - f_+\big). \tag{47}$$

Multiplying now the right-hand side of (44) by $e^{\beta\tilde{f}|\operatorname{Int}\Gamma| - \beta\tilde{f}|\operatorname{Int}\Gamma|}$ and using (47) we get the bound

$$e^{2\varepsilon|\Gamma|} e^{\beta\tilde{f}|\operatorname{Int}\Gamma|} \sum_{\substack{\vartheta \text{large} \\ \vartheta \subset \Lambda}} \prod_{\overline{\gamma} \in \vartheta} \rho(\overline{\gamma}) e^{4\varepsilon|\overline{\gamma}|} e^{-\beta\tilde{f}|\operatorname{Int}\overline{\gamma}|}. \tag{48}$$

Applying twice the approximation (45) we get

$$e^{2\varepsilon|\Gamma|} e^{\beta\tilde{f}|\operatorname{Int}\Gamma|} \sum_{\substack{\vartheta \text{large} \\ \vartheta \subset \operatorname{Int}\Gamma}} \prod_{\overline{\gamma} \in \vartheta} \rho(\overline{\gamma}) \mathcal{Z}(\operatorname{Int}\overline{\gamma}; \tilde{z}) \cdot e^{5\varepsilon|\overline{\gamma}|}$$
$$\leq e^{2\varepsilon|\Gamma|} e^{\tilde{f}|\operatorname{Int}\Gamma|} \mathcal{Z}(\operatorname{Int}\Gamma; \tilde{z}) \leq e^{\beta\tilde{f}|\operatorname{Int}\Gamma| - \beta\tilde{f}|\operatorname{Int}\Gamma| + 3\varepsilon|\Gamma|}. \tag{49}$$

Thus, referring again to the bound (43) and the definition (21), we conclude that $z_+(\Gamma)$ satisfies the bound (8). □

The free energies $f_\pm$ are, in view of the equality (40), close to the ground configuration energies $e_\pm$; the difference $\beta g(z_\pm)$ is of the order $e^{-\tau/2}$ (cf. (13)). Moreover, while the ground state energies $e_\pm$ are linear in h, the functions $\beta g(\overline{z}_\pm)$ can be shown to be Lipschitz with the Lipschitz constant of the order $e^{-\tau}$. The free energies $f_\pm$ are, in view of the equality (40), close to the ground configuration energies $e_\pm$; the difference $\beta g(z_\pm)$ is of the order $e^{-\tau/2}$ (cf. (13)). Moreover, while the ground state energies $e_\pm$ are linear in h, the functions $\beta g(\overline{z}_\pm)$ can be shown to be Lipschitz with the Lipschitz constant of the order $e^{-\tau}$. Indeed, using the definition (7), the (one sided) derivative $\frac{d}{dh} g(\overline{z}_\pm)$ can be expressed as the sum, over all contours Γ passing through a given site, of the product of the probability of the appearance of Γ (bounded by $e^{-\tau|\Gamma|}$) and the term $\frac{d}{dh}\log\overline{z}_\pm(\Gamma)$ (whenever $\overline{z}_\pm(\Gamma) \neq 0$). The latter can be bounded by $3|\Gamma| + 2|\operatorname{Int}\Gamma|$ as follows directly from the definition (21, 22). To get the bound

$$\left|\frac{d}{dh}\log\frac{Z_{\operatorname{Int}\Gamma}(\pm\underline{1})}{Z_{\operatorname{Int}\Gamma}(\mp\underline{1})}\right| \leq 2|\operatorname{Int}\Gamma|,$$

one takes into account the explicit expressions (3) and (2) (see [Z] for details).

Since the energies $e_\pm$ are linear in h, $e_\pm = \mp h \mp \kappa 2d(d-1)$, we infer that the free energies $f_\pm$ are 'almost linear' in h. As a result, there exists a unique solution h_t of the equation $f_+ = f_-$ and the value h_t differs from the value determined by equality of the ground configuration energies, $e_+ = e_-$, by at most $e^{-\tau}$ (remember that $e^{-\tau}$ can be taken to be of the order, say $e^{-\beta}$)[11]. This fact can be stated in a more general form:

The phase diagram for large β is a deformation, of the order $e^{-\beta}$, of the phase diagram at vanishing temperature ($\beta = \infty$).

This statement remains true also when there are r different ground configurations and one needs $(r-1)$ external fields to discriminate between them. The general statement of Pirogov–Sinai theory actually claims the above assertion for this case.

Having insufficient space here to discuss various existing extensions of the original Pirogov–Sinai theory, we only mention two of them. One is the work of Bricmont and Slawny [BS, Sl] whose approach allowed to study some systems with degenerated ground states. For example, it turned useful for a discussion of ANNNI model [DS] or lattice models of micro-emulsions [DM, KLMM].

An alternative approach to Pirogov–Sinai theory is based on an idea of renormalization group transformations applied to labeled contour models (cf. (15)–(18)) [GKK]. Combining these ideas with the Imry–Ma argument, Bricmont and Kupiainen were able to prove the existence of phase transition for the three-dimensional random field Ising model [BKu].

8. Finite Volume Asymptotics

Sticking to our ilustrative perturbed Ising model, the issue is to find the asymptotic behaviour of the magnetization $m_L^{\mathrm{per}}(\beta, h) = \langle \sum_{i\in\Lambda} \sigma_i \rangle_L^{\mathrm{per}}$ in a finite cube, $|\Lambda| = L^d$, under periodic boundary conditions. The cubic geometry and periodic boundary conditions are considered here as a simplest case and in view of the fact that it is this situation that is most often studied by computer simulations. We will comment on other cases later.

In the limit $L \to \infty$, the magnetization $m_\infty^{\mathrm{per}}(\beta, h)$ displays, as a function of h, a discontinuity at $h = h_t(\beta)$. For finite L, the jump is smoothed into a steep increase in a neighbourhood of h_t. It is this *rounding* and its asymptotic behaviour that is our concern here. The magnetization $m_L^{\mathrm{per}}(\beta, h)$ is, in terms of the corresponding partition function $Z_L^{\mathrm{per}}(\beta, h)$, given by

$$m_L^{\mathrm{per}}(\beta, h) = -\frac{1}{\beta L^d} \frac{d}{dh} \log Z_L^{\mathrm{per}}(\beta, h). \tag{50}$$

We start from a representation of the partition function $Z_L^{\mathrm{per}}(\beta, h)$ in terms of a labeled contour model analogous to (15) and prove the validity of the following crucial approximation involving a smooth variant of metastable free energies.

[11]For the Potts model, the transition point β_t can be claimed, for q large, to be close (in the order $q^{-1/d}$) to the value yielded by the equation $(e^\beta - 1) = q^{1/d}$.

Lemma 3 [BK1]**.** *For every $A \in (0,1)$ there exist constants b and c and functions $\overline{f}_+(\beta,h)$ and $\overline{f}_-(\beta,h)$ that are four times differentiable in h such that*[12]

$$\min(\overline{f}_+,\overline{f}_-) = f = -\frac{1}{\beta}\lim\left\{\frac{1}{L^d}\log Z_L^{\mathrm{per}}(\beta,h)\right\}, \tag{51}$$

$$\overline{f}_\pm - f \geq \pm c(h-h_t), \tag{52}$$

and

$$\left|Z_L^{\mathrm{per}}(\beta,h) - \exp\{-\beta\overline{f}_+L^d\} - \exp\{-\beta\overline{f}_-L^d\}\right| \leq \exp\{-\beta f L^d - b\beta L\} \tag{53}$$

whenever $2|\kappa|(d^2-1)+|h| < A$ and β is large enough.

Remarks. (1) There is an amusing immediate consequence of this Lemma [BI1, BK1]. Namely, the limit

$$\lim_{L\to\infty}\frac{Z_L^{\mathrm{per}}(\beta,h)}{\exp\{-\beta f L^d\}} = N(\beta,h) \tag{54}$$

exists and yields an integer that equals the number of phases. This implies that $N(\beta,h)=1$ for $h\neq h_t$ and $N(\beta,h)=2$ for $h=h_t$. A similar claim is valid also in the general Pirogov–Sinai situation. In particular, for the Potts model the limit $N(\beta)$ equals

$$N(\beta) = \begin{cases} q & \text{for } \beta > \beta_t, \\ q+1 & \text{for } \beta = \beta_t, \\ 1 & \text{for } \beta < \beta_t. \end{cases}$$

(2) The fact that we are proving differentiability of $\overline{f}_\pm$ up to the fourth order is a purely technical matter. We needed the error term of this order in the Taylor expansion of $\overline{f}_\pm$ to evaluate the location of the maximum of susceptibility (see Proposition 4 below). Even though we needed larger β for higher orders, one can suppose that an optimization of the present methods would lead to bounds for all orders.

Main ideas of proof of Lemma 3. Suppressing all contours wrapped around the torus[13], at the cost of an error of the order $\exp\{-\beta f L^d - b\beta L\}$, we can approximate $Z_L^{\mathrm{per}}(\beta,h)$ by the sum of two terms — contributions of all configurations with plus or minus external contours, respectively,

$$Z_L^{\mathrm{per}}(\beta,h) \approx Z_L^{\mathrm{per},+}(\beta,h) + Z_L^{\mathrm{per},-}(\beta,h). \tag{55}$$

For h close to h_t, so that $\max(a_-,a_+)L \leq \tau/4$, both phases can be treated as stable in Λ (in Lemma 2 we can clearly get the same statement with the damping weakened

[12] The function f is the standard free energy (cf. Remark 1 after Lemma 2).

[13] These are simply configurations for which we might be in doubt whether to classify them as belonging to the plus or minus phase, and for which the notion of external contours might not be well defined.

to $e^{-\tau|\Gamma|/2}$ and with the bound $a_-\operatorname{diam}\Lambda \le 1$ replaced by $a_-\operatorname{diam}\Lambda \le \tau/4$). The right-hand side of (55) then equals

$$\overline{Z}_L^{\mathrm{per},+}(\beta,h)+\overline{Z}_L^{\mathrm{per},-}(\beta,h) = \exp\{-\beta e_+ L^d\}\mathcal{Z}^{\mathrm{per}}(L^d;\overline{z}_+)+\exp\{-\beta e_- L^d\}\mathcal{Z}^{\mathrm{per}}(L^d;\overline{z}_-). \quad (56)$$

Here $\mathcal{Z}^{\mathrm{per}}(L^d;\overline{z}_\pm)$ are the contour model partition functions defined by (7) with collections of contours *on the torus* without any contour wrapped around it. Being defined on the torus, their approximation by $\exp\{-\beta g(\overline{z}_\pm)L^d\}$ is very accurate. Namely, the first clusters C in which the cluster expressions for $-\beta g(\overline{z}_\pm)L^d$ and $\log\mathcal{Z}^{\mathrm{per}}(L^d;\overline{z}_\pm)$ differ are the clusters wrapped around the torus. In particular, unlike in (39), there is no surface term proportional to L^{d-1} and we have

$$\left|\log\overline{Z}_L^{\mathrm{per},\pm}(\beta,h)+\beta f_\pm L^d\right| \le e^{-\tau L}. \quad (57)$$

On the other side, if say $a_- L \ge \tau/4$, then

$$Z_L^{\mathrm{per},-}(\beta,h)e^{\beta f L^d} \le e^{-a_- L^d/2}+e^{-\tau b'' L^{d-1}}. \quad (58)$$

Namely, one is either losing the bulk term of the order a_- or there is a long contour along which the configuration flips from minuses to pluses.

Thus we obtain the expression of the form (53) with the metastable free energies $f_\pm$. Even though the weights $z_\pm$ defined by (21) and (22) are smooth functions of h (and of β), the definition (37) is rather discontinuous. However, it turns out that there is actually some freedom in the definition of $\overline{z}_\pm$ that allows us to modify the definition of the metastable free energies to make them smooth.

Namely, the only property really needed is that the weights $\overline{z}_\pm$ are damped and that $\overline{z}_\pm = z_\pm$ in the metastable situation, (i.e., when $\max(a_+,a_-)\operatorname{diam}\Gamma \le \tau/4$). To avoid a reference to a_+ and a_- defined in the limit $\Lambda\to\mathbb{Z}^d$, we have chosen in [BK1] (see also [HKZ2]) the inductive definition

$$\overline{z}_+(\Gamma) = \rho((\Gamma,+))e^{-\beta(e_- - e_+)|\partial_{\mathrm{I}}\Gamma|}\frac{Z_{\mathrm{Int}\,\Gamma}(-\underline{1})}{\overline{Z}_{\mathrm{Int}\,\Gamma}(+\underline{1})}\Theta_{+,\Gamma} \quad (59)$$

(and a similar definition for $\overline{z}_-(\Gamma)$). Here $\Theta_{+,\Gamma}$ is an indicator function (defined also in an inductive way) that interpolates smoothly between 0 and 1 (in the metastable region):

$$\Theta_{+,\Gamma} = \begin{cases} 0 & \text{whenever } (h \text{ is such that}) \ \overline{Z}_{\mathrm{Int}\,\Gamma}(+\underline{1}) \le \exp\{-\frac{1}{4}\tau|\Gamma|-1\}\overline{Z}_{\mathrm{Int}\,\Gamma}(-\underline{1}) \\ 1 & \text{whenever } \overline{Z}_{\mathrm{Int}\,\Gamma}(+\underline{1}) \ge \exp\{-\frac{1}{4}\tau|\Gamma|+1\}\overline{Z}_{\mathrm{Int}\,\Gamma}(-\underline{1}). \end{cases} \quad (60)$$

Following the method of the proof of Lemma 2, it is easy to verify that these weights meet the above formulated conditions. Indeed, proceding by induction in $\operatorname{diam}\Gamma = n$, in the metastable region we have $\Theta_{\pm,\Gamma}=1$ and $\overline{Z}_{\mathrm{Int}\,\Gamma}(\pm\underline{1}) = Z_{\mathrm{Int}\,\Gamma}(\pm\underline{1})$. On the other side, introducing $\overline{z}_\pm^{(n)}$ by taking $\overline{z}_\pm$ as already defined for $\overline{\Gamma}$ with $\operatorname{diam}\overline{\Gamma} < n$

and setting $\overline{z}_{\pm}^{(n)}(\overline{\Gamma}) = 0$ otherwise, and denoting $f_{\pm}^{(n)}$ the corresponding free energy and $a_{\pm}^{(n)} = \beta\big(f_{\pm}^{(n)} - \min(f_{+}^{(n)}, f_{-}^{(n)})\big)$, we prove by induction that

$$Z_{\operatorname{Int}\Gamma}(\pm\underline{1}) \le \exp\Big\{-\beta\min(f_{+}^{(n)}, f_{-}^{(n)})|\operatorname{Int}\Gamma| + |\Gamma|\Big\}.$$

Thus,

$$\begin{aligned}\frac{Z_{\operatorname{Int}\Gamma}(\mp\underline{1})}{\overline{Z}_{\operatorname{Int}\Gamma}(\pm\underline{1})} &\le \exp\Big\{|\Gamma| - \beta\min(f_{+}^{(n)}, f_{-}^{(n)})\operatorname{Int}\Gamma + \beta f_{\pm}^{(n)}|\operatorname{Int}\Gamma|\Big\}\\ &\le \frac{\overline{Z}_{\operatorname{Int}\Gamma}(\mp\underline{1})}{\overline{Z}_{\operatorname{Int}\Gamma}(\pm\underline{1})}\exp\{2|\Gamma|\},\end{aligned}$$

and by (60) the indicator $\Theta_{\pm,\Gamma} = 0$ whenever the ratio

$$\frac{Z_{\operatorname{Int}\Gamma}(\mp\underline{1})}{\overline{Z}_{\operatorname{Int}\Gamma}(\pm\underline{1})} \le \frac{\overline{Z}_{\operatorname{Int}\Gamma}(\mp\underline{1})}{\overline{Z}_{\operatorname{Int}\Gamma}(\pm\underline{1})}e^{2|\Gamma|}$$

is too large. The new weights $\overline{z}_{\pm}(\Gamma)$ redefined in this way yield the metastable free energies $\overline{f}_{\pm} = \lim_{n\to\infty} f_{\pm}^{(n)}$ and $\overline{a}_{\pm} = \lim_{n\to\infty} a_{\pm}^{(n)}$. These parameters might slightly differ from $a_{\pm}$ in Lemma 2 – they vanish, however, for the same set of external fields h and yield the same h_t (as they should).

Moreover, the new metastable free energies $\overline{f}_{\pm}$ are smooth. Namely, in the essentially same way as when proving Lemma 2 we can bound also the derivatives of $\overline{z}_{\pm}(\Gamma)$. An inductive step for that are bounds of the type (42) and (44) with (49) for the derivatives of the left-hand sides of (42) and (44). See [BK1] for details. □

The magnetization $m_{\infty}^{\text{per}}(\beta, h)$ as well as the susceptibility $\chi_{\infty}^{\text{per}}(\beta, h)$ (recall that the perturbed Ising model does not have the plus-minus symmetry) may have a discontinuity at $h = h_t$. Let us introduce the spontaneous magnetizations and susceptibilities

$$m_{\pm} = \lim_{h\to h_t\pm} m_{\infty}^{\text{per}}(\beta, h), m_0 = \tfrac{1}{2}(m_+ + m_-), m = \tfrac{1}{2}(m_+ - m_-),$$

$$\chi_{\pm} = \frac{\partial m_{\infty}^{\text{per}}(\beta, h)}{\partial h\pm}, \chi_0 = \tfrac{1}{2}(\chi_+ + \chi_-), \chi = \tfrac{1}{2}(\chi_+ - \chi_-).$$

It turns out that, in spite of the asymmetry of the model, the finite volume magnetization $m_L^{\text{per}}(\beta, h)$ has a universal behaviour in the neighbourhood of the transition point h_t. Expanding the metastable free energies in (53) into a Taylor expansion around h_t, we get the following proposition in a rather straightforward manner (again, see [BK1] for the proof).

Proposition 3 [BK1]. *For any $A \in (0, 1)$ there exist constants K and b such that the approximation*

$$\begin{aligned}m_L^{\text{per}}(\beta, h) &= m_0 + \chi_0(h - h_t)\\ &\quad + (m + \chi(h - h_t))\tanh\Big\{L^d\beta\big[m(h - h_t) + \tfrac{1}{2}\chi(h - h_t)^2\big]\Big\} + R(h, L)\end{aligned}$$

with the error bound $|R(h,L)| \le e^{-b\beta L} + K(h-h_t)^2$ *is valid whenever* $2|\kappa|(d^2-1)+|h| < A$ *and* β *is large enough.*

Having now a good control over the behaviour of $m_L^{\text{per}}(\beta,h)$ in the transition region, we can evaluate the asymptotic behaviour of different variants of the finite volume approximations of the transition point. This is important for the interpretation of computer simulations. In particular, comparison with theoretically predicted asymptotic behaviour is used to settle the question whether an unknown transition is continuous or first-order. When only finite size data are available, a natural choice for the transition point is the value $h_{\max}(L)$ for which the susceptibility $\partial m_L^{\text{per}}(\beta,h)/\partial h$ attains its maximum (the inflection point of $m_L^{\text{per}}(\beta,h)$). Other possible definitions: the point $h_0(L)$ for which $m_L^{\text{per}}(\beta,h) = m_0$ or the point $h_t(L)$ for which an approximation to (54), say

$$N_L(\beta,h) = \left[\frac{Z_L^{\text{per}}(\beta,h)^{2^d}}{Z_{2L}^{\text{per}}(\beta,h)}\right]^{\frac{1}{2^d-1}},$$

attains its maximum. In fact, the latter is exactly the point for which $m_L^{\text{per}}(\beta,h) = m_{2L}^{\text{per}}(\beta,h)$. With the help of Proposition 3 we get:

Proposition 4 [BK1]. *For a fixed constant* δ, $2|\kappa|(d^2-1)+|h| < 1$, *and* β *large enough, one has*

(i) $h_{\max}(L) = h_t + \dfrac{3\chi}{2\beta^2 m^3} L^{-2d} + O(L^{-3d})$,

(ii) *in the interval* $[h_t-\delta,\ h_t+\delta]$, *there exists a unique* $h_0(L)$ *for which* $m_L^{\text{per}}(\beta,h) = m_0$; *for this* $h_0(L)$ *one has* $h_0(L) = h_t + O(e^{-b_0\beta L})$, *and*

(iii) $h_t(L) = h_t + O(e^{-b_0\beta L})$.

A popular testing ground for discussion of finite size simulation data is the Potts model (see, e.g., [CLB, BJ, BLM, LK]). Similar results as above can be proved [BKM] for the Potts model with $d \ge 2$ and q large enough. In this case, the mean energy can be approximated by

$$E_L^{\text{per}}(\beta) \approx E_0 + E\tanh\Big\{E(\beta-\beta_t)L^d + \tfrac{1}{2}\log q\Big\}. \tag{61}$$

As a consequence, the inverse temperature $\beta_{\max}(L)$ where the slope of $E_L^{\text{per}}(\beta)$ is maximal is shifted by

$$\beta_{\max}(L) - \beta_t = -\frac{\log q}{2E} L^{-d} + O(L^{-2d}), \tag{62}$$

while the inverse temperature $\beta_t(L)$ for which $N_L(\beta)$ is maximal again differs from β_t only by an exponentially small error $O(q^{-bL})$.

It seems that the value $h_t(L)$ (resp. $\beta_t(L)$) with an exponentially small shift might be particulary useful in determining the transition point. For further discussion illustrated by computer simulations see [BKa, BJ].

Notice that the difference between the asymptotic behaviour of the shift in Proposition 4(i) for the perturbed Ising model and (62) for the Potts model. Proposition

4(i) actually settled a controversy [BL, CLB] about the order of the shift. The proof that the shift is of the order L^{-2d} follows by showing that $\frac{\partial \chi_L^{\text{per}}(\beta,h)}{\partial h}\big|_{h=h_t}$ is of the order L^d and $\left|\frac{\partial^2 \chi_L^{\text{per}}(\beta,h)}{\partial h^2}\right|$ does not exceed L^{3d} in the interval $(h_t - \text{const.}L^{-d}, h_t + \text{const.}L^{-d})$. The fact that the shift for the Potts model is of the order L^{-d} can be traced down to the term $\log q$ in the argument of tanh in (62), 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 L^{-d} multiplied by the factor $\log q$ vanishes.

Two final remarks: similarly, as in the last section, the theory can be extended to cover more general situations with several coexisting phases. See [BK1] for a discussion of such cases.

Secondly, as already mentioned, asymptotic behaviour for other geometries as well as other boundary conditions was also studied. In the case of cylinder geometry, $\Lambda = M \times \cdots \times M \times L$ with L much larger than M, one obtains an effective one-dimensional model and the asymptotics can be studied with the help of the method of transfer matrix [BI2, B]. Another interesting case concerns surface induced shifts (in cubic geometry) driven by the free boundary conditions with possible addition of boundary fields. The shift of transition point is of the order L^{-1} and can be explicitely computed in terms of (cluster expansions of) surface free energies [BK3].

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