PIROGOV-SINAI THEORY

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Pirogov-Sinai theory is a method developed to study phase diagrams of lattice models at low temperatures. The general claim is that, under appropriate conditions, the phase diagram of a lattice model is, at low temperatures, a small perturbation of the zero temperature phase diagram designed by ground states. The treatment can be generalised to cover temperature driven transitions with coexistence of ordered and disordered phases.

1. Formulation of the main result

1.1 Setting.

Refraining first from full generality, we formulate the result for a standard class of lattice models with finite spin state and finite range interaction. We will mention different generalisations later.

We consider *classical lattice models* on the d-dimensional hypercubic lattice $\mathbb{Z}^d$ with $d \geq 2$. A *spin configuration* $\sigma = (\sigma_x)_{x \in \mathbb{Z}^d}$ is an assignment of a spin with values in a finite set S to each lattice site $x \in \mathbb{Z}^d$; the configuration space is $\Omega = S^{\mathbb{Z}^d}$. For $\sigma \in \Omega$ and $\Lambda \subset \mathbb{Z}^d$, we use $\sigma_\Lambda \in \Omega_\Lambda = S^\Lambda$ to denote the restriction $\sigma_\Lambda = \{\sigma_x; x \in \Lambda\}$.

The Hamiltonian is given in terms of a collection of interaction potentials (Φ_A), where Φ_A are real functions on Ω, depending only on σ_x with $x \in A$, and A runs over all finite subsets of $\mathbb{Z}^d$. We assume that the potential is *periodic* with *finite range of interactions*. Namely, $\Phi_{A'}(\sigma') = \Phi_A(\sigma)$ whenever A and σ are related to A' and σ' by a translation from $(a\mathbb{Z})^d$ for some fixed integer a and there exists $R \geq 1$ such that $\Phi_A \equiv 0$ for all A with diameter exceeding R.

Without loss of generality (possibly multiplying the number a by an integer and increasing R) we may assume that $R = a$.

The Hamiltonian $H_\Lambda(\sigma|\eta)$ in Λ with boundary conditions $\eta \in \Omega$ is then given by

$$H_\Lambda(\sigma|\eta) = \sum_{A \cap \Lambda \neq \emptyset} \Phi_A(\sigma_\Lambda \vee \eta_{\Lambda^c}), \tag{1}$$

where $\sigma_\Lambda \vee \eta_{\Lambda^c} \in \Omega$ is the configuration σ_Λ extended by η_{Λ^c} on Λ^c. The *Gibbs state in* Λ *under a boundary conditions* $\eta \in \Omega$ (and with Hamiltonian H) is the probability $\mu_\Lambda(\cdot|\eta)$ on Ω_Λ defined by

$$\mu_\Lambda(\{\sigma_\Lambda\}|\eta) = \frac{\exp\{-\beta H_\Lambda(\sigma|\eta)\}}{Z(\Lambda|\eta)} \tag{2}$$

with the *partition function*

$$Z(\Lambda|\eta) = \sum_{\sigma_\Lambda} \exp\{-\beta H_\Lambda(\sigma|\eta)\}. \tag{3}$$

We use $\mathcal{G}(H)$ to denote the set of all *periodic Gibbs states with Hamiltonian* H defined on Ω by means of the Dobrushin-Lanford-Ruelle (DLR) equations.

1.2 Ground state phase diagram and the removal of degeneracy.

A periodic configuration $\sigma \in \Omega$ is called a *(periodic) ground state* of a Hamiltonian $H = (\Phi_A)$ if

$$H(\tilde{\sigma};\sigma) = \sum_A (\Phi_A(\tilde{\sigma}) - \Phi_A(\sigma)) \geq 0 \tag{4}$$

for every finite perturbation $\tilde{\sigma} \neq \sigma$ of σ ($\tilde{\sigma}$ differs from σ at a finite number of lattice sites). We use $g(H)$ to denote the set of all periodic ground states of H. For every configuration $\sigma \in g(H)$, we define the *specific energy* $e_\sigma(H)$ by

$$e_\sigma(H) = \lim_{n\to\infty} \frac{1}{|V_n|} \sum_{A\cap V_n \neq \emptyset} \Phi_A(\sigma) \tag{5}$$

(with V_n denoting a cube consisting of n^d lattice sites).

To investigate the phase diagram, we will consider a parametric class of Hamiltonians around a fixed Hamiltonian $H^{(0)}$ with a finite set of periodic ground states $g(H^{(0)}) = \{\sigma_1, \ldots, \sigma_r\}$. Namely, let $H^{(0)}, H^{(1)}, \ldots,$ and $H^{(r-1)}$ be Hamiltonians determined by potentials $\Phi^{(0)}, \Phi^{(1)}, \ldots,$ and $\Phi^{(r-1)}$, respectively, and consider the $(r-1)$-parametric set of Hamiltonians $H_{\boldsymbol{t}} = H^{(0)} + \sum_{\ell=1}^{r-1} t_\ell H^{(\ell)}$ with $\boldsymbol{t} = (t_1, \ldots, t_{r-1}) \in \mathbb{R}^{r-1}$. Using a shorthand $e_m(H) = e_{\sigma_m}(H)$, and introducing the vectors $\boldsymbol{e}(H) = (e_1(H), \ldots, e_r(H))$ and $\boldsymbol{h}(\boldsymbol{t}) = \boldsymbol{e}(H_{\boldsymbol{t}}) - \min_m e_m(H_{\boldsymbol{t}})$, we notice that for each $\boldsymbol{t} \in \mathbb{R}^{r-1}$, the vector $\boldsymbol{h}(\boldsymbol{t}) \in \partial Q_r$, the boundary of the positive octant in $\mathbb{R}^r$. A crucial assumption for such a parametrisation $H_{\boldsymbol{t}}$ to yield a meaningful phase diagram is the *condition of removal of degeneracy*: we assume that $g(H^{(0)} + H^{(\ell)}) \subsetneqq g(H^{(0)})$, $\ell = 1, \ldots, r-1$, and that the vectors $\boldsymbol{e}(H^{(\ell)}), \ell = 1, \ldots, r-1$, are linearly independent.

In particular, its immediate consequence is that the mapping $R^{r-1} \ni \boldsymbol{t} \mapsto \boldsymbol{h}(\boldsymbol{t}) \in \partial Q_r$ is a bijection. This fact has a straightforward interpretation in terms of *ground state phase diagram*. Viewing the phase diagram (at zero temperature) as a partition of the parameter space into regions K_g with a given set $g \subset g(H^{(0)})$ of ground states—"coexistence of zero temperature phases from g"—the above bijection means that the region K_g is the preimage of the set

$$Q_g = \{\boldsymbol{h} \in \partial Q_r | h_m = 0 \text{ for } \sigma_m \in g \text{ and } h_m > 0 \text{ otherwise } \}. \tag{6}$$

The partition of the set ∂Q_r has a natural hierarchical structure implied by the fact that $\overline{Q_{g_1}} \cap \overline{Q_{g_2}} = \overline{Q_{g_1 \cup g_2}}$ ($\overline{Q_g}$ is the closure of Q_g). Namely, the origin $\{0\} = Q_{g(H^{(0)})}$ is the intersection of r positive coordinate axes $\overline{Q_{\{\sigma_{\bar{m}}, \bar{m}\neq m\}}}, m = 1, \ldots, r$; each of those halflines is an intersection of $(r-1)$ two-dimensional quarter-planes with boundaries on positive coordinate axes, etc., up to $(r-1)$-dimensional planes $\overline{Q_{\{\sigma_m\}}}, m = 1, \ldots, r$. This hierarchical structure is thus inherited by the partition of the parameter space $\mathbb{R}^{r-1}$ into the regions K_g. The phase diagrams with such regular structure are sometimes said to satisfy the Gibbs phase rule.

We can thus summarise in a rather trivial conclusion that the condition of removal of degeneracy implies that ground state phase diagram obeys the Gibbs phase rule. The task of the Pirogov-Sinai theory is to provide means for proving that this remains to be true, at least in a neighbourhood of the origin of parameter space, also for small nonzero temperatures. To achieve this we need an effective control of excitation energies.

1.3 Peierls condition.

A crucial assumption for the validity of the Pirogov-Sinai theory is a lower bound on energy of excitations of ground states—the Peierls condition.

In spite of the fact that for a study of phase diagram we consider a parametric set of Hamiltonians whose set of ground states may differ, it is useful to introduce the Peierls condition with respect to a single fixed collection G of *reference configurations* (eventually, it will be identified with the ground states of the Hamiltonian $H^{(0)}$). Let thus a fixed set G of periodic configurations $\{\sigma_1, \dots, \sigma_r\}$ be given. Again, without loss of generality we may assume that the periodicity of all configurations $\sigma_m \in G$ is R.

Before formulating the Peierls condition, we have to introduce the notion of contours. Consider the set of all *sampling cubes* $C(x) = \{y \in \mathbb{Z}^d \| y_i - x_i| \leq R \text{ for } 1 \leq i \leq d\}$, $x \in \mathbb{Z}^d$. A *bad cube* of a configuration $\sigma \in \Omega$ is a sampling cube C for which σ_C differs from σ_m restricted to C for every $\sigma_m \in G$. The *boundary* $B(\sigma)$ of σ is the union of all bad cubes of σ. If $\sigma_m \in G$ and σ is its finite perturbation (differing from σ_m on a finite set of lattice sites), then, necessarily, $B(\sigma)$ is finite. A *contour* of σ is a pair $\gamma = (\Gamma, \sigma_\Gamma)$ where Γ(the *support* of the contour γ) is a connected component of $B(\sigma)$ (and σ_Γ is the restriction of σ on Γ). Here, the connectedness of Γ means that it cannot be split into two parts whose (Euclidean) distance is larger than 1. We use $\partial(\sigma)$ to denote the set of all contours of σ, $B(\sigma) = \bigcup_{\gamma \in \partial(\sigma)} \Gamma$.

Consider a configuration σ^γ such that γ is its unique contour. The set $\mathbb{Z}^d \setminus \Gamma$ has one infinite component to be denoted $\operatorname{Ext}\gamma$ and a finite number of finite components whose union will be denoted $\operatorname{Int}\gamma$. Observing that the configuration σ^γ coincides with one of the states $\sigma_m \in G$ on every component of $\mathbb{Z}^d \setminus B(\sigma)$, each of those components can be labelled by the corresponding m. Let q be the label of $\operatorname{Ext}\gamma$, we say that γ is a q-contour, and let $\operatorname{Int}_m \gamma$ be the union of all components of $\operatorname{Int}\gamma$ labelled by m, $m = 1, \dots, r$.

Defining the "energy" $\Psi(\gamma)$ of a q-contour γ by the equation

$$\Psi(\gamma) = H(\sigma^\gamma; \sigma_q) + e_q(H)|\Gamma| - \sum_{m=1}^{r} (e_m(H) - e_q(H))|\operatorname{Int}_m \gamma|, \tag{7}$$

the *Peierls condition* with respect to the set G of reference configurations is an assumption of the existence of $\rho > 0$ such that

$$\Psi(\gamma) \geq (\rho + \min_m e_m(H))|\Gamma| \tag{8}$$

for any contour of any configuration σ that is a finite perturbation of $\sigma_q \in G$.

Notice that if $G = g(H)$, the sum on the right hand side of (7) vanishes.

1.4 Phase diagram.

The main claim of the Pirogov-Sinai theory provides, for β sufficiently large, a construction of regions $\mathcal{K}_g(\beta)$ of the parameter space characterized by coexistence of phases labeled by configurations $\sigma_m \in g$. This is done similarly as for the ground state phase diagram discussed in Section 1.2 by constructing a homeomorphism $\boldsymbol{t} \mapsto$

$\boldsymbol{a}(\boldsymbol{t})$ from a neighbourhood of the origin of the parameter space to a neighbourhood of the origin of ∂Q_r that provides the phase diagram (actually, the function $\boldsymbol{a}(\boldsymbol{t})$ will turn out to be just a perturbation of $\boldsymbol{h}(\boldsymbol{t})$ with errors of order $e^{-\beta}$).

Before stating the result, however, we have to clarify what exactly is meant by existence of phase m for a given Hamiltonian H. Roughly speaking, it is the existence of a periodic extremal Gibbs state $\mu_m \in \mathcal{G}(H)$, whose typical configurations do not differ too much from the ground state configuration σ_m. In a more technical terms, the existence of such state is provided once we prove a suitable bound, for the finite-volume Gibbs state $\mu_\Lambda(\{\sigma_\Lambda\}|\sigma_m)$ under the boundary conditions σ_m, on the the probability that a fixed point in Λ is encircled by a contour from $\partial\sigma$. If this is a case, we say that the *phase m is stable*. It turns out that such a bound is actually an integral part of the construction of metastable free energies $f_m(\boldsymbol{t})$ yielding the homeomorphism $\boldsymbol{t} \mapsto \boldsymbol{a}(\boldsymbol{t})$. In this way, we get the main claim formulated as follows:

Theorem 1.1. *Consider a parametric set of Hamiltonians $H_{\boldsymbol{t}} = H^{(0)} + \sum_{\ell=1}^{r-1} t_\ell H^{(\ell)}$ with periodic finite range interactions satisfying the condition of removal of degeneracy as well as the Peierls condition with respect to the reference set $G = g(H^{(0)})$. Let $d \geq 2$ and let β be sufficiently large. Then there exists a homeomorphism $\boldsymbol{t} \mapsto \boldsymbol{a}(\boldsymbol{t})$ of a neighbourhood V_β of the origin of the parameter space R^{r-1} onto a neighbourhood U_β of the origin of ∂Q_r such that, for any $\boldsymbol{t} \in V_\beta$, the set of all stable phases is $\big\{m \in \{1, \ldots, r\} | a_m(\boldsymbol{t}) = 0\big\}$.*

The Peierls condition can be actually assumed only for the Hamiltonian $H^{(0)}$ inferring its validity for $H_{\boldsymbol{t}}$ on a sufficiently small neighbourhood V_β.

Notice also that the result can be actually stated not as a claim about phase diagram in a space of parameters, but as a statement about stable phases of a fixed Hamiltonian H. Namely, for a Hamiltonian H satisfying Peierls condition with respect to a reference set G, one can assure existence of parameters a_m labelled by elements from G such that the set of extremal periodic Gibbs states of H consists of all those m-phases for which $a_m = 0$.

1.5 Construction of metastable free energies.

An important part of the Pirogov-Sinai theory is an actual construction of the *metastable free energies*—a set of functions $f_m(\boldsymbol{t}), m = 1, \ldots, r$ that provide the homeomorphism $\boldsymbol{a}(\boldsymbol{t})$ by taking $a_m(\boldsymbol{t}) = f_m(\boldsymbol{t}) - \min_{\bar{m}} f_{\bar{m}}(\boldsymbol{t})$.

We start with a *contour representation of partition function* $Z(\Lambda|\sigma_q)$. Considering, for each contributing configuration σ, the collection $\partial(\sigma)$ of its contours, we notice that, in addition to the fact that different contours $\gamma, \gamma' \in \partial(\sigma)$ have disjoint supports, $\Gamma \cap \Gamma' = \emptyset$, the contours from $\partial(\sigma)$ have to satisfy the *matching conditions*: if C is a connected component of $\mathbb{Z}^d \setminus \bigcup_{\gamma\in\partial} \Gamma$, then the restrictions of the spin configurations σ^γ to C are the same for all contours $\gamma \in \partial(\sigma)$ with $\operatorname{dist}(\Gamma, C) = 1$. In other words, the contours touching C induce the same label on C. Let us observe that there is actually one to one correspondence between configurations σ that coincide with σ_q on Λ^c and collections $\mathcal{M}(\Lambda, q)$ of contours ∂ in Λ satisfying the matching condition and such that the external among them are q-contours. Here, a contour $\gamma \in \partial$ is called an *external contour in* ∂ if $\Gamma \subset \operatorname{Ext}\gamma'$ for all $\gamma' \in \partial$ different from γ.

With this observation and using $\Lambda_m(\partial)$ to denote the union of all components of $\Lambda \setminus \bigcup_{\gamma\in\partial} \Gamma$ with label m, we get

$$Z(\Lambda|\sigma_q) = \sum_{\partial\in\mathcal{M}(\Lambda,q)} \prod_m e^{-\beta e_m(H)|\Lambda_m(\gamma)|} \prod_{\gamma\in\partial} e^{-\beta\Psi(\gamma)}. \tag{9}$$

A usefulness of such contour representation stems from an expectation that, for a stable phase q, contours should constitute a suppressed excitation and one should be able to use cluster expansions to evaluate the behaviour of the Gibbs state μ_q. However, the direct use of the cluster expansion on (9) is trammelled by the presence of the energy terms $e^{-\beta e_m(H)|\Lambda_m(\partial)|}$ and, more seriously, by the requirement that the contour labels match.

Nevertheless, one can rewrite the partition function in a form that does not involve any matching condition. Namely, considering first a sum over mutually external contours ∂^{ext} and resumming over collections of contours which are contained in their interiors without touching the boundary (being thus prevented to "glue" with external contours), we get

$$Z(\Lambda|\sigma_q) = \sum_{\partial^{\text{ext}}} e^{-\beta e_q(H)|\operatorname{Ext}|} \prod_{\gamma\in\partial^{\text{ext}}} \Bigl\{ e^{-\beta\Psi(\gamma)} \prod_m Z^{\text{dil}}(\operatorname{Int}_m \gamma|\sigma_m)\Bigr\}. \tag{10}$$

Here, the sum goes over all collections of compatible external q-contours in Λ, $\operatorname{Ext} = \operatorname{Ext}_\Lambda(\partial^{\text{ext}}) = \bigcap_{\gamma\in\partial^{\text{ext}}}(\operatorname{Ext}\gamma \cap \Lambda)$, and the partition function $Z^{\text{dil}}(\Lambda|\sigma_q)$ is defined by (9) with $\mathcal{M}(\Lambda, q)$ replaced by $\mathcal{M}^{\text{dil}}(\Lambda, q) \subset \mathcal{M}(\Lambda, q)$, the set of all those collections whose external contours γ are such that $\operatorname{dist}(\Gamma, \Lambda^c) > 1$. Multiplying now each term by

$$1 = \prod_{\gamma\in\partial^{\text{ext}}} \prod_m \frac{Z^{\text{dil}}(\operatorname{Int}_m \gamma|\sigma_q)}{Z^{\text{dil}}(\operatorname{Int}_m \gamma|\sigma_q)}, \tag{11}$$

we get

$$Z(\Lambda|\sigma_q) = \sum_{\partial^{\text{ext}}} e^{-\beta e_q(H)|\operatorname{Ext}|} \prod_{\gamma\in\partial^{\text{ext}}} \Bigl(e^{-\beta e_q(H)|\Gamma|} w_q(\gamma) Z^{\text{dil}}(\operatorname{Int}\gamma|\sigma_q)\Bigr), \tag{12}$$

where $w_q(\gamma)$ is given by

$$w_q(\gamma) = e^{-\beta\Psi(\gamma)}\, e^{\beta e_q(H)|\Gamma|} \prod_m \frac{Z^{\text{dil}}(\operatorname{Int}_m \gamma|\sigma_m)}{Z^{\text{dil}}(\operatorname{Int}_m \gamma|\sigma_q)}. \tag{13}$$

Observing that a similar expression is valid for $Z^{\text{dil}}(\Lambda|\sigma_q)$ (with an appropriate restriction on the sum over external contours ∂^{ext}) and proceeding by induction, we eventually get the representation

$$Z(\Lambda|\sigma_q) = e^{-\beta e_q(H)|\Lambda|} \sum_{\partial\in\mathcal{C}(\Lambda,q)} \prod_{\gamma\in\partial} w_q(\gamma), \tag{14}$$

where $\mathcal{C}(\Lambda, q)$ denotes the set of all collections of non-overlapping q-contours in Λ. Clearly, the sum on the right hand side is exactly of the form needed to apply cluster expansion, provided the contour weights satisfy the necessary convergence assumptions.

Even though this is not necessarily the case, there is a way to use this representation. Namely, one can artificially change the weights to satisfy the needed bound, for example, by modifying them to the form

$$w'_q(\gamma) = \min\bigl(w_q(\gamma), e^{-\tau|\Gamma|}\bigr) \tag{15}$$

with a suitable constant τ. The modified partition function

$$Z'(\Lambda|\sigma_q) = e^{-\beta e_q(H)|\Lambda|} \sum_{\partial \in \mathcal{C}(\Lambda,q)} \prod_{\gamma\in\partial} w'_q(\gamma) \tag{16}$$

can then be controlled by cluster expansion allowing to *define*

$$f_q(H) = -\frac{1}{\beta} \lim_{|\Lambda|\to\infty} \frac{1}{|\Lambda|} \log Z'(\Lambda|\sigma_q). \tag{17}$$

This is the *metastable free energy* corresponding to the phase q. Applying the cluster expansion to the logarithm of the sum in (16), we get $|f_q(H)-e_q(H)| \le e^{-\frac{\tau}{2}}$. The metastable free energy corresponds to taking of the ground state σ_q and its excitations as long as they are sufficiently suppressed. Once $w_q(\gamma)$ exceeds the weight $e^{-\tau|\Gamma|}$ (and the contour would have been actually preferred), we suppress it "by hand". The point is that if the phase q is stable, this never happens and $w'_q(\gamma) = w_q(\gamma)$ for *all* q-contours γ. This is the idea behind the use the function $f_q(H)$ as an indicator of the stability of the phase q by taking

$$a_q(\boldsymbol{t}) = f_q(H_{\boldsymbol{t}}) - \min_m f_m(H_{\boldsymbol{t}}). \tag{18}$$

Of course, the difficult point is to actually prove that stability of phase q (i.e. the fact that $a_q(\boldsymbol{t}) = 0$) indeed implies $w'_q(\gamma) = w_q(\gamma)$ for all γ. The crucial step is to prove, by induction on the diameter of Λ and γ, the following three claims (with $\epsilon = 2e^{-\frac{\tau}{2}}$):

(i) *If γ is a q-contour with $a_q(\boldsymbol{t}) \operatorname{diam}\Gamma \le \frac{\tau}{4}$, then $w'_q(\gamma) = w_q(\gamma)$.*
(ii) *If $a_q(\boldsymbol{t}) \operatorname{diam}\Lambda \le \frac{\tau}{4}$, then $Z(\Lambda|\sigma_q) = Z'(\Lambda|\sigma_q) \ne 0$ and*

$$|Z(\Lambda|\sigma_q)| \ge e^{-f_q(H_{\boldsymbol{t}})|\Lambda| - \epsilon|\partial\Lambda|}. \tag{19}$$

(iii) *If $m \in G$, then*

$$|Z(\Lambda|\sigma_m)| \le e^{-\min_q f_q(H_{\boldsymbol{t}})|\Lambda|} e^{\epsilon|\partial\Lambda|}. \tag{20}$$

A standard example illuminating the perturbative construction of the metastable free energies and showing the role of entropic contributions, is the Blume- Capel model. It is defined by the Hamiltonian

$$H_\Lambda(\sigma) = -J \sum_{\langle x,y\rangle} (\sigma_x - \sigma_y)^2 - \lambda \sum_{x\in\Lambda} \sigma_x^2 - h \sum_{x\in\Lambda} \sigma_x \tag{21}$$

with spins $\sigma_x \in \{-1, 0, 1\}$. Taking into account only the lowest order excitations, we get:
$\tilde{f}_\pm(\lambda, h) = -\lambda \mp h - \frac{1}{\beta} e^{-\beta(2d-\lambda\pm h)}$ (sea of pluses or minuses with a single spin flip $\pm \to 0$) and
$\tilde{f}_0(\lambda, h) = -\frac{1}{\beta} e^{-\beta(2d+\lambda)}\big(e^{\beta h} + e^{-\beta h}\big)$ (sea of zeros with a single spin flip either $0 \to +$ or $0 \to -$). Since these functions differ from full metastable free energies $f_\pm(\lambda, h)$, $f_0(\lambda, h)$ by terms of higher order ($\sim e^{-(4d-2)\beta}$), the real phase diagram differs in this order from that one constructed by equating the functions $\tilde{f}_\pm(\lambda, h)$ and $\tilde{f}_0(\lambda, h)$. Particularly interesting is to inspect the origin, $\lambda = h = 0$. It is only the phase 0 that is stable there at all small temperatures since

$$f_0(0,0) \sim -\frac{2}{\beta} e^{-\beta 2d} < f_\pm(0,0) \sim -\frac{1}{\beta} e^{-\beta 2d}. \tag{22}$$

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 $f_0(0,0)$ is overweighting the entropy of the contribution to $f_\pm(0,0)$ of the same order.

2. Applications

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.

One class of applications concerns various problems featuring interfaces between coexisting phases. To be able to transform the problem into study of random boundary line separating the two phases, one needs a precise cluster expansion formula for partition functions in volumes occupied by those phases. In the situation with no symmetry between the phases, the use of the Pirogov-Sinai theory is indispensable.

Another interesting class of applications concerns behaviour of the system with periodic boundary conditions. It is based on the fact that the partition function Z_{T_N} on a torus T_N consisting of N^d sites can be, again with the help of the cluster expansions, explicitly and very accurately evaluated in terms of metastable free energies,

$$\bigl|Z_{T_N} - \sum_{q=1}^{r} e^{-\beta f_q(H) N^d}\bigr| \le \exp\{-\beta \min_m f_m(H) N^d - b\beta N\}, \tag{23}$$

with a fixed constant b. This formula (and its generalization to the case of complex parameters) allows to obtain various results concerning the behaviour of the model in finite volumes.

2.1 Finite-size effects.

Considering, as an illustration, a perturbation of the Ising model, so that it has not the $\pm$ symmetry any more (and the value $h_t(\beta)$ of external field at which the phase transition between plus and minus phase occurs 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 $m_N^{\rm per}(\beta,h) = \mu_{T_N}\bigl(\frac{1}{|\Lambda|}\sum_{x\in\Lambda}\sigma_x\bigr)$ on a torus? In the thermodynamic limit, the magnetization $m_\infty^{\rm per}(\beta,h)$ displays, as a function of h, a discontinuity at $h = h_t(\beta)$. For finite N we get a *rounding* of the discontinuity—the jump is smoothed. What is the shift of a naturally chosen finite volume transition point $h_t(N)$ with respect to the limiting value h_t? The answer can be obtained with help of (23) once sufficient care is taken to use the freedom in the definition of the metastable free energies $f_+(h)$ and $f_-(h)$ to replace them with a sufficiently smooth version allowing an approximation of the functions $f_\pm(h)$ around limiting point h_t in terms of their Taylor expansion.

As a result, in spite of the asymmetry of the model, the finite volume magnetization $m_N^{\rm per}(\beta,h)$ has a universal behaviour in the neighbourhood of the transition point h_t. With suitable constants m and m_0, we have

$$m_N^{\rm per}(\beta,h) \sim m_0 + m\tanh\bigl\{N^d\beta m(h-h_t)\bigr\}. \tag{24}$$

Choosing the inflection point $h_{\max}(N)$ of $m_N^{\mathrm{per}}(\beta, h)$ as a natural finite volume indicator of the occurence of the transition, one can show that

$$h_{\max}(N) = h_t + \frac{3\chi}{2\beta^2 m^3} N^{-2d} + O(N^{-3d}). \tag{25}$$

2.2 Zeros of partition functions.

The full strength of the formula (23) is revealed when studying the zeros of the partition function $Z_{T_N}(z)$ as a polynomial in a complex parameter z entering the Hamiltonian of the model. To be able to use the theory in this case, one has to extend the definitions of the metastable free energies to complex values of z. Indeed, the construction goes still through yielding, this time genuinely complex, contour models $w_\pm$ with the help of an inductive procedure. Notice that no analytic continuation is involved. An analog of (23) is still valid,

$$\bigl|Z_{T_N}(z) - \sum_{m=1}^{r} e^{-\beta f_m(z) N^d}\bigr| \le \exp\{-\beta \min_m \mathfrak{Re} f_m(z) N^d - b\beta N\}. \tag{26}$$

Using (26), 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 $\mathfrak{Re} f_m = \mathfrak{Re} f_q$ the partition function $Z_{T_N}(z)$ is approximated by $e^{-\beta f N^d}\bigl(e^{-\beta \mathfrak{Im} f_m N^d} + e^{-\beta \mathfrak{Im} f_n N^d}\bigr)$. The zeros of this approximation are thus given by the equations

$$\begin{aligned} &\mathfrak{Re} f_m = \mathfrak{Re} f_n < \mathfrak{Re} f_\ell \ \text{ for all } \ell \ne m, n, \\ &\beta N^d(\mathfrak{Im} f_m - \mathfrak{Im} f_n) = \pi \bmod 2\pi. \end{aligned} \tag{27}$$

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 $\frac{1}{2\pi}\beta N^d |(d/dz)(f_m - f_n)|$.

3. Bibliographical remarks and generalisations

The original works [PS75, PS76, Sin] were introducing an analog of the weights $w'_q(\gamma)$ and parameters $a_q(H)$ as a fixed point of a suitable mapping on a Banach space. The inductive definition used here was introduced in [KP] and [Zah]. The *completeness of phase diagram*—the fact that the stable phases exhaust the set of all periodic extremal Gibbs states was first proven in [Zah]. Extension to complex parameters was first considered in Gawędzki *et al.* (1987) and Borgs and Imbrie (1989). For a review of standard Pirogov-Sinai theory see [Sin, Sl].

Application of Pirogov-Sinai theory for finite size effects was studied in [BoKo] and general theory of zeros of partition functions is presented in [BBCK].

The basic statement of the Pirogov-Sinai theory yielding the construction of the full phase diagram has been extended to a large class of models. Let us mention just few of them (with rather incomplete references):

Continuous spins. The main difficulty in these models is that one has to deal with contours immersed in a sea of fluctuating spins (Dobrushin and Zahradník 1986, Borgs and Waxler 1989).

Potts model. An example of a system with a transition in temperature with coexistence of the low temperature ordered and the high temperature disordered phases.

Contour reformulation is employing contours between ordered and disordered regions [BKL, KLMR]. The treatment is simplified with help of Fortuin-Kasteleyn representation [LMMRS].
Models with competing interactions. ANNNI model, microemulsions. Systems with a rich phase structure [DS].
Disordered systems. An example is a proof of existence of the phase transition for the 3-dimensional random field Ising model [BrKu] using a *renormalization group version* of the Pirogov-Sinai theory first formulated in [GKK].
Quantum lattice models. A class of quantum models that can be viewed as a quantum perturbation of a classical model. With help of Feynman-Kac formula are rewritten as a $(d+1)$-dimensional classical model that is, in its turn, treated by standard Pirogov-Sinai theory (Datta *et al* 1996, Borgs *et al* 1996).
Continuous systems. Gas of particles in continuum interacting with a particular potential of Kac type. Pirogov-Sinai theory is used for a proof of existence of the phase transitions after a suitable discretisation [LMP].

See also:. Equilibrium statistical mechanics, Cluster expansion, Phase transitions in continuum systems, Quantum spin systems

References

[BBCK] M. Biskup, C. Borgs, J. T. Chayes, and R. Kotecký. *Partition function zeros at first-order phase transitions: Pirogov-Sinai theory.* Jour. Stat. Phys. **116** (2004) 97–155.

[BI] C. Borgs and J.Z. Imbrie, *A unified approach to phase diagrams in field theory and statistical mechanics*, Commun. Math. Phys. **123** (1989) 305–328.

[BK] C. Borgs and R. Kotecký, *A rigorous theory of finite-size scaling at first-order phase transitions*, J. Statist. Phys. **61** (1990) 79–119.

[BW] C. Borgs and R. Waxler, *First Order Phase Transitions in Unbounded Spin Systems: Construction of the Phase Diagram*, Commun. Math. Phys. **126** (1989) 291–324.

[BKL] J. Bricmont, T. Kuroda, J. Lebowitz, *First order phase transitions in lattice and continuum systems: Extension of Pirogov–Sinai theory.* Commun. Math. Phys. **101** (1985), 501–538.

[BKU] C. Borgs, R. Kotecký, D. Ueltschi, *Low temperature phase diagrams for quantum perturbations of classical spin systems.* Commun. Math. Phys. **181** (1996), 409–446.

[BoKo] C. Borgs, R. Kotecký, *A rigorous theory of finite-size scaling at first-order phase transitions.* Journal of Statistical Physics **61** (1990), 79–119.

[BrKu] J. Bricmont, A. Kupiainen, *Lower critical dimensions for the random field Ising model.* Physical Review Letters **59** (1987), 1829–1832; *Phase transition in the 3d random field Ising model.* Commun. Math. Phys. **116** (1988), 539–572.

[DFF] N. Datta, R. Fernández, J. Fröhlich, *Low-temperature phase diagrams of quantum lattice systems. I. Stability for quantum perturbations of classical systems with finitely-many ground states* Jour. Stat. Phys. **84** (1996), 455–534.

[DS] E. L. Dinaburg, Ya. G. Sinaï, *An analysis of ANNNI model by Peierls contour method.* Commun. Math. Phys. **98** (1985), 119–144.

[DZ] R. L. Dobrushin, M. Zahradník, *Phase Diagrams of Continuous Lattice Systems.* Math. Problems of Stat. Physics and Dynamics (ed. R. L. Dobrushin), Reidel, Dordrecht 1986, pp. 1–123.

[GKK] K. Gawędzki, R. Kotecký, A. Kupiainen, *Coarse-graining approach to first-order phase transitions.* Journal of Statistical Physics **47** (1987), 701–724.

[KLMR] R. Kotecký, L. Laanait, A. Messager, J. Ruiz, *The q-state Potts model in the standard Pirogov–Sinai theory: surface tensions and Wilson loops.* Journal of Statistical Physics **58** (1990), 199–248.

[KP] R. Kotecký and D. Preiss, *An inductive approach to PS theory*, Proc. Winter School on Abstract Analysis, Suppl. ai Rend. del Mat. di Palermo (1983).

[LMP] J.L. Lebowitz, A. Mazel, E. Presutti, *Liquid-vapor phase transitions for systems with finite range interactions.* Journal of Statistical Physics **94** (1999), 955–1025.

[LMMRS] L. Laanait, A. Messager, S. Miracle-Solé, J. Ruiz, S. B. Shlosman, *Interfaces in the Potts model I: Pirogov-Sinai theory of the Fortuin-Kasteleyn representation.* Commun. Math. Phys. **140** (1991), 81–91.

[PS75] S.A Pirogov and Ya.G. Sinai, *Phase diagrams of classical lattice systems* (Russian), Theor. Math. Phys. **25** (1975) no. 3, 358–369.

[PS76] S.A Pirogov and Ya.G. Sinai, *Phase diagrams of classical lattice systems. Continuation* (Russian), Theor. Math. Phys. **26** (1976), no. 1, 61–76.

[Sin] Ya.G. Sinai, *Theory of Phase Transitions: Rigorous Results*, Pergamon Press, New York, 1982.

[Sl] J. Slawny, *Low temperature properties of classical lattice systems: Phase transitions and phase diagrams.* Phase Transitions and Critical Phenomena, vol. 11, eds. C. Domb, J. L. Lebowitz, Academic Press, New York, 1987, pp. 127–205.

[Zah] M. Zahradník, *An alternate version of Pirogov-Sinai theory*, Commun. Math. Phys. **93** (1984) 559–581.