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Surface Tension and Phase Coexistence for General Lattice Systems[1]

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We investigate the surface tension between coexisting phases of general discrete lattice systems. In particular the different phases need not be connected by any symmetry. We prove the positivity of the surface tension in the low-temperature regime where the Pirogov–Sinai theory of first-order phase transitions is valid: finite-range Hamiltonian having a finite number of periodic ground states. We give a brief description (with some extensions) of this theory.

KEY WORDS: Surface tension; low temperature phase diagrams; alloys; Gibbs measure.

1. INTRODUCTION

The properties of an equilibrium macroscopic system are determined by its temperature and the chemical potentials of its constituents. These are the system's thermodynamic parameters. For certain values of these parameters, comprising lower-dimensional surfaces in the parameter space, the system can exist in more than one pure phase, e.g., gas or liquid. It is generally found that there is a positive surface tension between these phases, i.e., when two such phases are in physical contact the free energy of the system exceeds, by a term proportional to the surface area of contact,

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the sum of the free energies of the pure phases. In this paper, we give a rigorous mathematical proof of this fact for fairly general lattice systems at low temperatures.

There are several microscopic definitions of the surface tension (see Refs. 1, 2, 4, 6, 11, 15), all of which coincide where they can be computed exactly, e.g., in the two-dimensional Ising model.[1,2,15] We shall use the following definition: given thermodynamic parameters such that we have two phases, say, 1 and 2, we take a rectangular box V, of cross section L^2, and height M, $|V| = L^2M$, and impose boundary conditions which lead to the presence of phase 1 in the top half of the box and phase 2 in the bottom half. The surface tension per unit area is then defined as

$$\tau_{12} = \lim_{L\to\infty} \lim_{M\to\infty} \frac{1}{L^2} \left[\psi_V^{(12)} - \left(\frac{\psi_V^{(1)} + \psi_V^{(2)}}{2} \right) \right] \tag{1.1}$$

$\psi_V^{(12)}$ is the free energy in V with the mixed boundary conditions described above while $\psi_V^{(j)}$ is the corresponding free energy with homogeneous boundary conditions, $j = 1, 2$; i.e. boundary conditions which produce a system in one of the pure phases.

We expect that $\tau_{12} > 0$ when 1 and 2 are indeed different phases and $\tau_{12} = 0$ otherwise, e.g., for parameter values at which the system has only one pure phase τ_{12} should be zero whatever the boundary conditions 1 and 2 are. These expectations are certainly consistent with the known results about the surface tension defined according to (1.1). These are as follows.

For the Ising model with general ferromagnetic pair interactions in any dimension, where 1 and 2 are the plus and minus magnetization states, τ_{12} is known[13,14] to be nonzero above β_c and zero below, where β_c is the inverse critical temperature defined by the onset of the spontaneous magnetization. In particular, for the two-dimensional Ising model with nearest-neighbor ferromagnetic interactions J, we have[2, 15]

$$\beta\tau_{12} = \begin{cases} 2\beta J + \log(\tanh \beta J), & \beta > \beta_c \\ 0, & \beta \leqslant \beta_c \end{cases} \tag{1.2}$$

For a broader class of discrete ferromagnetic spin systems possessing high-temperature–low-temperature duality one knows that the limit defining τ_{12} exists and that τ_{12} is monotone in the interactions and strictly positive at low temperatures.[7,11]

In all cases $\tau_{12} = 0$ at sufficiently high temperatures.[7]

This definition of surface tension therefore seems appropriate for systems with discrete phases. For systems with continuous symmetry the situation may however be different. Thus for the plane rotator model $\tau_{12} = 0$ at all temperatures.[8] Another definition of surface tension is therefore necessary for such systems (see Ref. 8).

An important feature of all models for which a nonvanishing surface tension has been proven is that the ground states, and therefore the phases, are related by a symmetry of the Hamiltonian like the + and − phases of the usual Ising model. If we want to study the surface tension in more general systems, e.g., between the liquid and the vapor in continuum fluids, we need a theory that does not use explicitly this symmetry since it does not occur in general. A general theory of first-order phase transitions at low temperatures has been constructed by Pirogov and Sinai for discrete spin systems with finite-range interactions having a finite number of ground states, not necessarily with any symmetry.[16] (It has been extended to quantum field theory[13] and to continuous spins[5] with a finite number of ground states). As examples of such systems we have the antiferromagnet in a (weak) external field or a general mixture of particles on a crystal lattice with arbitrary short-range interactions. In this paper, we show that there is a nonzero surface tension between any two phases constructed by the method of Pirogov and Sinai. It already follows from Ref. 7 that for these systems $\tau_{12} = 0$ at high temperatures.

Our result however still leaves open the problem of a direct and general relation between the surface tension and the coexistence of several phases: i.e., is $\tau_{12} > 0$ equivalent to the fact that the boundary conditions 1 and 2 lead to different thermodynamic phases? We know the answer only for the ferromagnet Ising model[3,4] with pair interactions where it is true (and also that it cannot be the case for rotators[8]).

The outline of this paper is as follows: In Section 2, we summarize the theory of Pirogov and Sinai. The models that we consider explicitly are slightly more restricted than those of Pirogov and Sinai. Their extension is discussed in the Appendix using ideas of Holsztynski and Slawny.[12] In Section 3 we state our results and give the proofs. They are somewhat similar to those of Ref. 7 but we do not use a duality transformation; we rely on some estimates on partition functions whose importance was emphasized by Imbrie.[13]

2. PHASE TRANSITIONS AT LOW TEMPERATURE: PIROGOV–SINAI THEORY

The main problem in the theory of phase transitions is to describe the set of pure phases, represented by indecomposable, infinite-volume, Gibbs measures. These are obtained by taking the limit of finite-volume Gibbs measures with different boundary conditions.[17,18] We expect that, at least at low temperatures, the homogeneous pure phases will be simply related to the ground states of the Hamiltonian, i.e, it should be possible to describe them as a "dilute gas of excitations" of a particular ground state configura-

tion. Pirogov and Sinai[16,17] take this picture as their motivation and make it into a precise mathematical theory of first-order phase transitions at low temperatures for a certain general class of lattice systems: in particular they do not require any symmetry between the different ground states which is essential for all other proofs of phase transitions.

In the Pirogov–Sinai theory we consider a regular lattice $\mathbb{Z}^d$. We associate to each site $x \in \mathbb{Z}^d$ the spin variable S_x which can take on n values, $S_x \in \{1, \ldots, n\}$, n finite. We consider systems whose Hamiltonian H has finite-range interactions with a finite number of periodic ground states and satisfies the Peierls condition. The latter means that the cost in energy required to embed a finite piece of one ground state configuration into another ground state extending over the rest of the lattice is bounded below by the "surface area" between the two different regions. Since the number of values, n, which S can take at each site is arbitrary, there is no loss in generality in assuming that each site x really stands for a whole cell, and that the ground states are the constant configurations given, say, by $S_x = i$ for all $x \in \mathbb{Z}^d$, $i \in \{1, \ldots, r\}$ $1 \leqslant r \leqslant n$.

A wide class of Hamiltonians of this type (see Appendix on how to extend this to the general case) can be written in the following form. (For simplicity we consider explicitly the case $d = 2$ but the results are valid for all $d \geqslant 2$.)

We denote the elementary square of $\mathbb{Z}^2$ consisting of four nearest-neighbor sites by p. For each spin configurations S_p in p we consider the interaction $G(S_p)$. This includes all two-, three- and four-body interactions. We also consider single site energies $F(S_x)$.

For a finite subset V of $\mathbb{Z}^2$ with an area $|V|$, we define the interaction energy for spin configurations $S_V = \{S_x : x \in V\}$ by

$$H_V(S_V) = \sum_{p \subset V} G(S_p) + \sum_{x \in V} F(S_x) \tag{2.1}$$

where the first sum runs over all elementary squares in V.

We assume the following conditions on F and G:

$$(A-1)\begin{cases} F(S) = 0, & \text{if } S \in \{1, \ldots, r\} \\ F(S) \geqslant c > 0, & \text{if } S \in \{r+1, \ldots, n\} \end{cases}$$

for some r, $1 \leqslant r \leqslant n$, and

$$(A-2)\begin{cases} G(S_p) \geqslant 0, & \\ G(S_p) = 0, & \text{if } S_p = i \text{ for some } i \in \{1, 2, \ldots, r\}, \\ & \text{i.e., } S_x = i \text{ for all } x \in p \\ G(S_p) \geqslant c > 0, & \text{if each } S_x \in \{1, 2, \ldots, r\} \text{ but } S_{x_1} \neq S_{x_2} \\ & \text{for some } x_1 \text{ and } x_2 \in p \end{cases}$$

Pirogov and Sinai now study the low-temperature pure phases which naturally go over into the ground states, $S^{(i)}$, where $S_x^{(i)} = i$, all x, $i \in \{1, \ldots, r,\}$, as the temperature goes to zero. To do this let $E(\cdot)$ be a function on $S = \{1, \ldots, n\}$ satisfying the condition

$$E(l) - \min_{1 \leqslant k \leqslant n} E(k) \leqslant c/8 \qquad \text{for each} \quad l \in \{1, \ldots, r\} \tag{2.2}$$

We may assume, without loss of generality, that $\min E(l) = 0$ for $l \in \{1, \ldots, r\}$, and set $\mu = (\mu_1, \ldots, \mu_r)$

$$\mu_i = E(i), \qquad i \in \{1, \ldots, r\} \tag{2.3}$$

Define now a perturbed Hamiltonian H^{μ}:

$$\begin{aligned} H_V^{\mu}(S_V) &= H_V(S_V) + \sum_{x \in V} E(S_x) \\ &= H_V(S_V) + \sum_{i=1}^{r} \mu_i N_i(S_V) + \sum_{i=r+1}^{n} E(i) N_i(S_V) \end{aligned} \tag{2.4}$$

where $N_i(S_V) = \#\{x \in V;\ S_x = i\}$. Condition (2.2) assures that any configuration other than the ground states, $S_x^{(i)} = i$, $i \in \{1, \ldots, r\}$, for all $x \in \mathbb{Z}^2$, has a higher energy, even for the perturbed Hamiltonian (2.4).

Consider now the space of parameters

$$G = \left\{ \mu = (\mu_1, \ldots, \mu_r): \min_{1 \leqslant i \leqslant r} \mu_i = 0 \text{ and } |\mu| \equiv \max_{1 \leqslant k \leqslant r} |\mu_i| < \epsilon \right\}$$

The theory of Pirogov and Sinai gives the following picture of the phase diagram for some small value of ϵ and sufficiently large β. Let p_{μ}^{q} be the infinite-volume Gibbs state of the system with Hamiltonian (2.4), obtained by taking the thermodynamic limit with q-boundary conditions. We then have the following:

(i) There exists a point $\bar{\mu} \in G$ such that the limiting Gibbs states $P_{\bar{\mu}}^{q} = (q \in \{1, \ldots, r\})$ are all distinct pure phases;

(ii) there exists an orbit γ_u in G starting from $\bar{\mu}$ such that the limiting Gibbs states P_{μ}^{q} $(q \in \{1, \ldots, r\} \backslash \{u\})$ are all distinct pure phases for each $\mu \in \gamma_u$, i.e., there are $n - 1$ pure phases on γ_u;

(iii) there exists a two-dimensional finite surface γ_{uv} whose boundaries are given by γ_u and γ_v such that the limiting Gibbs states P_{μ}^{q} $(q \in \{1, \ldots, \} \backslash \{u, v\})$ are all distinct pure phases for each $\mu \in \gamma_{uv}$.

In general

(iv) there exists a k-dimensional finite surface γ_A whose boundaries are given by $\gamma_{A \backslash \{u\}}$ $(u \in A)$ such that the limiting Gibbs states P_{μ}^{q} $(q \in \{1, \ldots, r\} \backslash A)$ are all distinct pure phases for each $\mu \in \gamma_A$, where $k = \#(A)$.

Also we have $G = \bigcup_{A \subset \{1, \ldots, r\}} \gamma_A$.

In order to explain the result of Pirogov and Sinai in a bit more detail we need some definitions. For a given configuration we call an elementary square p *regular* if all S_x, $x \in p$ are equal and belong to $\{1, 2, \ldots, r\}$. Otherwise the square is called irregular. Note that

$$G(S_p) + \sum_{x \in p} F(s_x) \begin{cases} = 0, & \text{if } p \text{ is regular} \\ \geqslant c, & \text{if } p \text{ is irregular} \end{cases} \tag{2.5}$$

We decompose the set of irregular squares of a configuration into connected components. A *contour* Γ is defined as a pair; a connected component and a configuration on it. This definition is a generalization of the Ising model contour. To each contour we associate the ground state configuration in the complement of the contour with infinite volume. We call such a configuration (necessarily in $\{1, 2, \ldots, r\}$) the boundary condition of the contour.

Now we introduce contour models. A family of contours is called *compatible* if they are mutually disjoint. We denote by $D_q(V)$ the set of compatible families of contours in V with q-boundary conditions. We write Γ^q to indicate that Γ has q-boundary conditions.

Note that a real configuration does not always correspond to a family of contours in $D_q(V)$ since the latter all have q-boundary conditions. A function F_q on the set of contours with q-boundary conditions is called a τ functional if it satisfies

$$\text{(i)} \qquad F_q(\Gamma^q) \geqslant \tau |\Gamma^q| \tag{2.6}$$

and

$$\text{(ii)} \qquad F_q \text{ is translation invariant} \tag{2.7}$$

where $|\Gamma^q|$ is the number of squares in Γ^q.

A *contour model* is a probability measure on $D_q(V)$ given by

$$P_V(\partial) = \Omega^0(V : F_q)^{-1} \exp\left[- \sum_{s=1}^{m} F_q(\Gamma_s^q) \right]$$

where

$$\partial = (\Gamma_1^q, \ldots, \Gamma_m^q) \in D_q(V)$$

and Ω^0 is a normalization factor

$$\Omega^0(V : F_q) = \sum_{\{\Gamma_s^q\}_{s=1}^m \in D_q(V)} \exp\left[- \sum_{s=1}^{m} F_q(\Gamma_s^q) \right]$$

For τ sufficiently large one can prove the following lemma. Let C be the set of maps from contours with q-boundary conditions into $\mathbb{N}$, and F be the set of functions from C into $\mathbb{R}$. When ψ_1 and $\psi_2 \in F$, their product

$\psi_1 \cdot \psi_2$ is defined by

$$(\psi_1 \cdot \psi_2)(x) = \sum_{\substack{(x_1, x_2) \\ x_1 + x_2 = x}} \psi_1(x_1)\psi_2(x_2), \qquad x \in C$$

where the addition $x_1 + x_2$ is defined pointwise. For each $\psi \in F$ such that $\psi(0) = 1$ we define

$$\psi^T(x) = (\log \psi)(x) = \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} \psi_0^n(x)$$

where

$$\psi_0(x) = \begin{cases} \psi(x), & \text{if } x \neq 0 \\ 0, & \text{if } x = 0 \end{cases}$$

Let $\phi \in F$ be defined by

$$\phi(x) = \begin{cases} \exp\left[-\sum_{s=1}^{m} F(\Gamma_s^q) \right], & \text{if } x \text{ satisfies:} \\ & x(\Gamma) = \begin{cases} 1, & \text{if } \Gamma \in \{\Gamma_1^q, \ldots, \Gamma_m^q\} \\ 0, & \text{otherwise} \end{cases} \\ & \text{for some compatible } \{\Gamma_1^q, \ldots, \Gamma_m^q\} \\ 0, & \text{otherwise} \end{cases}$$

Then we have the following:

Lemma 1 (see Ref. 10). For sufficiently large τ the following estimates hold:

(1) $$\sum_{x \ni 0} |\phi^T(x)| \leqslant \exp(-c\tau)$$

where $x \ni 0$ means $x(\Gamma) \neq 0$ for some Γ containing a given square (called 0);

(2) $$\Omega^0(V : Fq) = \exp\left[\sum_{x \subset V} \phi^T(x) \right]$$

where $x \subset V$ means $x(\Gamma) = 0$ unless $\Gamma \subset V$;

(3) $$S(Fq) = \lim_{V \uparrow \mathbb{Z}^d} \frac{1}{|V|} \ln \Omega^0(V : Fq)$$

exists when the limit is taken in the sense of Van Hove. $S(F_q)$ is the thermodynamic limit of the free energy per unit volume of the contour model.

(4) Moreover,

$$|\Delta(V : F_q)| \leqslant \exp(-c\tau)|\partial V|$$

where

$$\Delta(V : F_q) \equiv \log \Omega^0(V : F_q) - S(F_q)|V|$$

Next we introduce the *parametric contour statistical sum* as follows:

$$\Omega^a(V : Fq) = \sum_{\{\Gamma_s^q\}_{s=1}^m \in D_q(V)} \prod_{s=1}^m e^{-F(\Gamma_s^q)} \exp\left\{ a \left| \bigcup_s \operatorname{Int} \Gamma_s^q \right| \right\}$$

where $\operatorname{Int}\Gamma_s^q$ is the union of the finite connected components of the complement of Γ_s^q. It is easy to see that

$$\Omega^a(V : Fq) \leqslant \exp(a|V|)\Omega^0(V : Fq) \tag{2.8}$$

We define the partition function in V with q-boundary conditions:

$$Z^q(V) = \sum_{S_x} \exp(-\beta H_{V,q}^{\mu}(S_V)) \tag{2.9}$$

$$H_{V,q}^{\mu}(S_V) = H_V^{\mu}(S_v) + \sum_{P \cap \partial V \neq \phi} G(S_p) \tag{2.10}$$

where the sum in (2.9) is over all S_x, $x \in V$, and the one in (2.10) is over the squares that intersect both V and V^c and where $S_x = q$ for each $x \in V^c$. Put

$$\tilde{Z}^q(V) = \exp(\beta E(q)|V|)Z^q(V) \tag{2.11}$$

Then we have the following relations between the parametric contour model and the original one.

Proposition 1 (See Lemma 4.1 in Ref. 16 and Proposition 2.6 in Ref. 17). There exists $\epsilon > 0$ and $\beta_0 < \infty$ such that for any μ with $|\mu| \leqslant \epsilon$ and $\beta \geqslant \beta_0$, there exists a family of functions $F_\mu = (F_1, \ldots, F_r)$ satisfying (2.6) and (2.7) with τ proportional to β such that for each $q \in \{1, \ldots, r\}$

$$\tilde{Z}^q(V) = \Omega^{a^q}(V : F_q) \tag{2.12}$$

$$a^q(F_q) = \beta E(q) - S(F_q) + \alpha \tag{2.13}$$

where α is determined by $\inf a^q(F_q) = 0$.

Corollary (see Ref. 13). If $a^q(F_q) = 0$ then for all $p \in \{1, \ldots, r\}$,

$$\frac{Z^p(V)}{Z^q(V)} \leqslant \exp(c|\partial V|)$$

where c does not depend on β.

Proof of the Corollary. Using definition (2.11) and Proposition 1, we have

$$\frac{Z^p(V)}{Z^q(V)} = e^{-\beta(E_p - E_q)|V|}\frac{\tilde{Z}^p(V)}{\tilde{Z}^q(V)}$$

$$= e^{-\beta(E_p - E_q)|V|}\frac{\Omega^{a^p}(V : F_p)}{\Omega^0(V : F_q)}$$

and by (2.8)

$$\leqslant \exp\{[-\beta(E_p - E_q)]|V| + a^p(F_p)|V|\}\frac{\Omega^0(V : F_p)}{\Omega^0(V : F_q)} \tag{2.14}$$

By (2.13) the right-hand side of (2.14) is equal to

$$\exp[S(F_q) - S(F_p)]|V|)\frac{\Omega^0(V : F_p)}{\Omega^0(V : F_q)} \tag{2.15}$$

since $a^q(F_q) = 0$.

Hence we have from Lemma 1.4,

$$\frac{Z^p(V)}{Z^q(V)} \leqslant \exp\{\Delta(V : F_p) - \Delta(V : F_q)\}$$

$$\leqslant \exp(e^{-c\tau})|\partial V| \quad \blacksquare \tag{2.16}$$

The main conclusion of the Proposition and of its Corollary is that for the ground states satisfying $a^q(F_q) = 0$, one can construct thermodynamic Gibbs states having those ground states as typical configurations (see Ref. 16).

We call a ground state q *dominant* for a given β and μ if $a^q(F_q) = 0$.

3. SURFACE TENSION

Assume that for a given μ and β there is more than one dominant ground state. We shall study the surface tension between two phases corresponding to two of these ground states; call them 1 and 2.

Take a box

$$V_{L,M} = \{x \in Z^2 \,|\, |x_1| \leqslant M, |x_2| \leqslant L\}$$

and put as boundary conditions on $V_{L,M}$ either all $S_x = 1$ or all $S_x = 2$ or $S_x = 1$ if $x_1 \geqslant 0$ and $S_x = 2$ if $x_1 < 0$. Z_V^1, Z_V^2, and $Z_V^{1,2}$ are the correspond-

ing partition functions (see Ref. 11). Define

$$\beta\tau_{1,2}(L,M) = -\frac{1}{2L+1}\log\frac{Z_V^{1,2}}{(Z^1Z^2)^{1/2}} \tag{3.1}$$

The *surface tension* τ_{12} is defined as the limit (if it exists)

$$\tau_{12} = \lim_{L\to\infty}\lim_{M\to\infty}\tau_{1,2}(L,M)$$

We shall not discuss the existence of the limit (for ferromagnetic systems, it was proven in Ref. 11 but only give a lower bound, uniform in L and M.

Theorem 1. There exists a $k > 0$ such that, for all, β, μ to which Proposition 1 applies and such that the ground states 1 and 2 are dominant for β, μ,

$$\tau_{1,2}(L,M) \geqslant k$$

uniformly in L, M.

The proof of the theorem is rather simple: we show that in each configuration contributing to $Z_{12}(L,M)$ there is a contour, called the

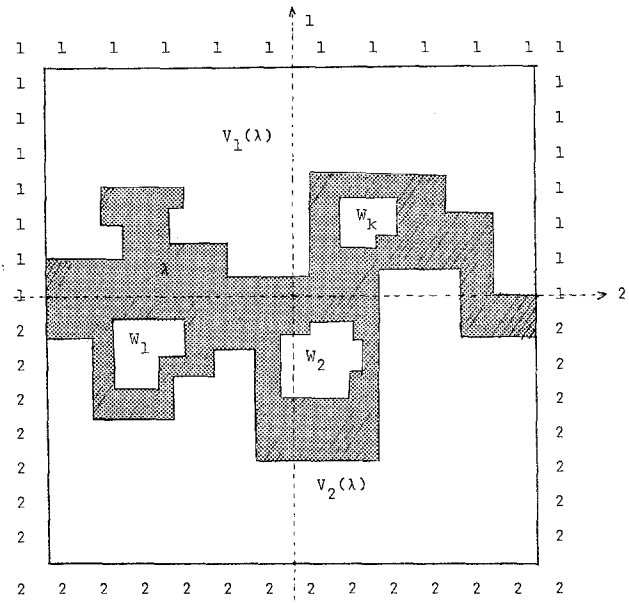

Fig. 1. The shaded area is the interface λ.

interface, separating the two phases. Then we show that this contour has a sufficiently small weight.

First of all, we remark that, if a square is irregular there must be another irregular square adjacent to it. Moreover, in the (1,2) boundary conditions, we know that there are two irregular squares intersecting both V and V^c the one containing the points of coordinates $(0, -L)$, $(0, -L-1)$, $(-1, -L)$ $(-1, -L-1)$ and the one obtained by symmetry with respect to the axis $x_2 = 0$.

For any configuration with the (1,2) boundary conditions, we define the *interface* as the connected set of irregular squares containing these two squares. For any interface λ we let $\bar{\lambda}$ be the union of the squares in λ and of those adjacent to them. The complement of $\bar{\lambda}$ in $V_{L,M}$ is divided into several connected components; one is connected to the part of the boundary with boundary conditions $S_x = 1$, it is called the *upper region* (one takes x_1 in the vertical direction). The component connected to the boundary with $S_x = 2$ is called the *lower region*. The other components are the *interior components* (see Fig. 1).

Lemma 2.

$$(1) \qquad Z^{1,2}(L,M) = \sum_{\lambda} \exp\left[-\beta E(\bar{\lambda})\right] Z^1_{V_1(\lambda)} Z^2_{V_2(\lambda)} \prod_{i=1}^{k} Z^{m_i}_{W_i(\lambda)}$$

where the sum is over all interfaces, $V_1(\lambda)$ is the upper region and $V_2(\lambda)$ is the lower one; $W_i(\lambda)$, $i = 1, \ldots, k(\lambda)$, are the interior regions. They have some specified boundary conditions m_i:

$$E(\bar{\lambda}) = \sum_{p \subset \lambda} G(S_p) + \sum_{x \in \bar{\lambda}} \{F(S_x) + E(S_x)\}$$

Note that $G(S_p) = 0$ for $p \in \bar{\lambda} \backslash \lambda$.

(2) For any interface λ, the number of squares in $\lambda = |\lambda| \geqslant 2L + 1$.

Proof.

(1) Follows immediately from the definition of λ.

(2) This follows from the fact that any connected set of squares going from the 1-boundary to the 2-boundary must contain at least one irregular square. ■

Bounds of the Partition Functions. From Lemma 2, we have

$$\frac{Z_V^{1,2}}{\left(Z_V^1 Z_V^2\right)^{1/2}} = \sum_{\lambda} \exp\left\{-\beta\left[E(\lambda) - \frac{E(1)+E(2)}{2}(\bar{\lambda})\right]\right\}$$

$$\cdot \left[I_1(\lambda) I_2(\lambda) I_3(\lambda)\right]^{1/2}$$

where $(\bar{\lambda})$ = the number of sites in $\bar{\lambda}$ (the number of squares in $\bar{\lambda}$ is denoted by $|\bar{\lambda}|$. Note that $(\bar{\lambda}) \leqslant 4|\bar{\lambda}|$),

$$I_1(\lambda) = \frac{Z^1_{V_1} \cdot Z^1_{V_2} \prod_{i=1}^k Z^1_{W_i}}{Z^1_V} \exp\left[-\beta E(1)(\bar{\lambda})\right] \prod_{i=1}^k \frac{Z^{m_i}}{Z^1_{W_i}}$$

$$I_2(\lambda) = \frac{Z^2_{V_1} \cdot Z^2_{V_2} \prod_{i=1}^k Z^2_{W_i}}{Z^2_V} \exp\left[-\beta E(2)(\bar{\lambda})\right] \prod_{i=1}^k \frac{Z^{m_i}}{Z^2_{W_i}}$$

and

$$I_3(\lambda) = \frac{Z^1_{V_1} \cdot Z^2_{V_2}}{Z^1_{V_2} Z^2_{V_1}}$$

Proof of Theorem 1. Lemmas 3, 4, and 5 below yield the estimate

$$(*) \quad \frac{Z^{1,2}_V}{\left(Z^1_V Z^2_V\right)^{1/2}} \leqslant \sum_{\lambda} \exp\{\left[-\beta C_1 + C_2 + \delta(\beta)\right]|\lambda|\},$$

where $C_1 > 0$ and $C_2 > 0$ are constants, and $\delta(\beta) \to 0$, as $\beta \to \infty$.

The proof of Theorem 1 then follows from the fact that $|\lambda| \geqslant 2L + 1$ (Lemma 2(2)) and the Peierls argument. ■

Lemma 3. If the value of ϵ is sufficiently small there exists $C_1 > 0$ for each $|\mu| \leqslant \epsilon$ such that $E(\bar{\lambda}) - (1/2)[E(1) + E(2)](\bar{\lambda}) \geqslant C_1|\lambda|$

Proof. For some $c > 0$ we have

$$E(\bar{\lambda}) \geqslant c|\lambda| + \min_{1 \leqslant i \leqslant r} E(i)(\bar{\lambda} \backslash \lambda) + \min_{1 \leqslant i \leqslant n} E(i)(\lambda)$$

Since $\min E(i) = 0$ for $i \in \{1, \ldots, r\}$ we have

$$E(\bar{\lambda}) - (1/2)\left[E(1) + E(2)\right](\bar{\lambda}) \geqslant c|\lambda| - (\bar{\lambda} \backslash \lambda) \frac{E(1) + E(2)}{2} - (\lambda)\left[\frac{E(1) + E(2)}{2} - \min_{1 \leqslant i \leqslant n} E(i)\right]$$

$$\geqslant c|\lambda| - (\bar{\lambda} \backslash \lambda)\epsilon - (\lambda)c/8$$

where the last inequality follows from the assumption $|\mu| \leqslant \epsilon$ and Eq. (2.2). Now, $(\lambda) \leqslant 4|\lambda|$ and $(\bar{\lambda} \backslash \lambda) \leqslant \text{const.}|\lambda|$. So for ϵ small enough this is larger than $(c/4)|\lambda|$. ■

Lemma 4. For some $c > 0$,

$$I_1(\lambda) \leqslant \exp\left[c(\lambda)\right]$$
$$I_2(\lambda) \leqslant \exp\left[c(\lambda)\right]$$

Proof. We start by observing that, because of the Corollary of Proposition 1,

$$\prod_{i=1}^{k} \frac{Z_{W_i}^{m_i}}{Z_{W_i}^{1}} \leqslant \exp\left[c(\lambda)\right]$$

We also see that

$$Z_V^1 \geqslant Z_{V_1}^1 Z_{V_2}^1 \prod_{i=1}^{k} Z_{W_i}^1 \exp\left[-\beta E(1)(\bar{\lambda})\right]$$

because the right-hand side is simply the restriction, in the sum of the left-hand side [Eq. (2.9)] to those configurations where $S_x = 1$, $x \in \bar{\lambda}$. ■

Lemma 5.

$$I_3(\lambda) \leqslant \exp\left[\delta(\beta)(\lambda)\right]$$

where $\delta(\beta) \to 0$ exponentially as $\beta \to \infty$.

Proof. Because of Proposition 1 and since $a^1(F_1) = a^2(F_2) = 0$ one can write

$$I_3(\lambda) = \exp\left[-\beta E(1)(V_1 - V_2) - \beta E(2)(V_2 - V_1)\right] \tilde{I}_3(\lambda)$$

where

$$\tilde{I}_3(\lambda) = \frac{\Omega^0(V_1 : F_1)\Omega^0(V_2 : F_2)}{\Omega^0(V_2 : F_1)\Omega^0(V_1 : F_2)}$$

$$= \exp\left[\sum_{x \subset V_1} \phi_1^T(x) - \sum_{x \subset V_2} \phi_1^T(x) + \sum_{x \subset V_2} \phi_2^T(x) - \sum_{x \subset V_1} \phi_2^T(x)\right]$$

by Lemma 1(2).

We denote the region in λ (including the interior components of λ) by $v(\lambda)$. We denote by $R(v(\lambda))$ the region obtained by reflecting $v(\lambda)$ with

respect to the line $x_1 = 0$. Let $R(\lambda) = v(\lambda) \cup R(v(\lambda))$. Write

$$V_1 = V_1^0 \cap V_1^1, \qquad V_2 = V_2^0 \cup V_2^1$$
$$V_1^0 = V_1 \backslash R(\lambda), \qquad V_1^1 = V_1 \backslash V_1^0$$

and similarly for V_2. We have

$$V_2^0 = R(V_1^0).$$

We write

$$\sum_{x \subset V_1} \phi_1^T(x) - \sum_{x \subset V_2} \phi_1^T(x) + \sum_{x \subset V_2} \phi_2^T(x) - \sum_{x \subset V_1} \phi_2^T(x)$$

$$= \left[\sum_{x \subset V_1^0} \phi_1^T(x) + \sum_{x \subset V_1^1} \phi_1^T(x) + \sum_{\substack{x \cap V_1^0 \neq \phi \\ x \cap V_1^1 \neq \phi}} \phi_1^T(x) \right]$$

$$- \left[\sum_{x \subset V_2^0} \phi_1^T(x) + \sum_{x \subset V_2^1} \phi_1^T(x) + \sum_{\substack{x \cap V_2^0 \neq \phi \\ x \cap V_2^1 \neq \phi}} \phi_1^T(x) \right]$$

$$+ \left[\sum_{x \subset V_2^0} \phi_2^T(x) + \sum_{x \subset V_2^1} \phi_2^T(x) + \sum_{\substack{x \cap V_2^0 \neq \phi \\ x \cap V_2^1 \neq \phi}} \phi_2^T(x) \right]$$

$$- \left[\sum_{x \subset V_1^0} \phi_2^T(x) + \sum_{x \subset V_1^1} \phi_2^T(x) + \sum_{\substack{x \cap V_1^0 \neq \phi \\ x \cap V_1^1 \neq \phi}} \phi_2^T(x) \right]$$

$$= \left[\sum_{x \subset V_1^1} \phi_1^T(x) - \sum_{x \subset V_2^1} \phi_1^T(x) + \sum_{x \subset V_2^1} \phi_2^T(x) - \sum_{x \subset V_1^1} \phi_2^T(x) \right]$$

$$+ \left[\sum_{\substack{x \cap V_1^0 \neq \phi \\ x \cap V_1^1 \neq \phi}} \phi_1^T(x) - \sum_{\substack{x \cap V_2^0 \neq \phi \\ x \cap V_2^1 \neq \phi}} \phi_1^T(x) \right.$$

$$\left. + \sum_{\substack{x \cap V_2^0 \neq \phi \\ x \cap V_2^1 \neq \phi}} \phi_2^T(x) - \sum_{\substack{x \cap V_1^0 \neq \phi \\ x \cap V_1^1 \neq \phi}} \phi_2^T(x) \right] \tag{3.2}$$

From Lemma 1, part (1) we have a bound $\exp(-c\beta)(\lambda)$ on the second parenthesis in (3.2) (τ in Lemma 1 is proportional to β because of

Proposition 1). Hence we have

$$I_3(\lambda) \leqslant \exp\left[\delta(\beta)|\lambda|\right]\exp\left\{-\beta\left[E(1)\left(|V_1^1| - |V_2^1|\right) + E(2)\left(|V_2^1| - |V_1^1|\right)\right]\right\}$$
$$\times \frac{\Omega^0(V_1^1 : F_1)\Omega^0(V_2^1 : F_2)}{\Omega^0(V_2^1 : F_1)\Omega^0(V_1^1 : F_2)}$$
$$\leqslant \exp\left[\tilde{\delta}(\beta)|\lambda|\right]\exp\Big(\left\{\left[S(F_1) - \beta E(1)\right] - \left[S(F_2) - \beta E(2)\right]\right\}|V_1^1|$$
$$- \left\{\left[S(F_1) - \beta E(1)\right] - \left[S(F_2) - \beta E(2)\right]\right\}|V_2^1|\Big)$$

where $\delta(\beta)$ and $\tilde{\delta}(\beta) \leqslant \exp(-c\beta)$ as $\beta \to \infty$. The last line follows from Lemma 1, part 4. The right-hand side of the above estimate is equal to $\exp[\tilde{\delta}(\beta)|\lambda|]$, since $S(F_1) - \beta E(1) = S(F_2) - \beta E(2)$. Hence, we have the following estimate for $I_3(\lambda)$:

$$I_3(\lambda) \leqslant \exp\left[\tilde{\delta}(\beta)|\lambda|\right]$$

APPENDIX

We explain how the results of Section 2 can be extended to the more general class of models considered by Pirogov and Sinaĭ.[16] These include essentially all models with a finite set of spin values, finite-range interactions, and a finite number of ground states. We follow a formulation of these models given by Holsztynski and Slawny.[12]

Let F be a finite set. We have a copy F_x of F at each site $x \in \mathbb{Z}^d$. We also have a family of potentials $\{\phi_\Lambda\}$ where Λ runs over the finite subsets of $\mathbb{Z}^d$, and $\phi_\Lambda : F^\Lambda = \prod_{x\in\Lambda} F_x \to \mathbb{R}$; the potentials satisfy the following conditions:

(i) $\phi_\Lambda \geqslant 0$;

(ii) $\{\phi_\Lambda\}$ is periodic;

(iii) $\sup\{\operatorname{diam}\Lambda \mid \phi_\Lambda \neq 0\} = R < \infty$;

(iv) there exists a periodic configuration $\mathbf{s} \in F^{\mathbb{Z}^d}$ such that $\phi_\Lambda(\mathbf{s}) = 0\ \forall\Lambda$.

(v) $\#\{\mathbf{s} \in F^{\mathbb{Z}^d} \mid \phi_\Lambda(\mathbf{s}) = 0\ \forall\Lambda\} < \infty$.

We call *ground states* the configurations $\mathbf{s}$ such that $\phi_\Lambda(\mathbf{s}) = 0\forall\Lambda$.

Remarks.

(1) The first condition can always be satisfied by adding a constant to ϕ_Λ, and the third means that we have finite range interactions.

(2) The fourth condition is apparently restrictive; it seems that we cannot allow frustrated models. However, by a redefinition of ϕ_Λ it is often possible to satisfy (iv). For example, the antiferromagnet on a triangular

lattice does not satisfy (iv) if we take Λ = nearest-neighbor bonds and the usual interaction, but it does satisfy it if we take for Λ the elementary triangles and $\phi_\Lambda = (J/2)\sum_{\langle ij\rangle} s_i s_j$, where the sum is over the edges of the triangles.

(3) Condition (v) is the most restrictive: There are only finitely many ground states. The triangular antiferromagnet does not satisfy (v). However, this condition is essential in the Pirogov–Sinai theory.

(4) In order to make the connection with the models of Section 2 more transparent, we redefine the model. Let $d = 2$ and let us partition the lattice into translates of a box V_0.

Consider new spin variables $s_{V_0} = (s_x)_{x \in V_0} \in F^{V_0}$ that take as values the set of configurations of all the original spin variables in V_0. Then, if V_0 is large enough, we have interactions that couple at most four adjacent (new) spins, as in Section 1. For $d > 2$ we shall have 2^d–body interactions. However, it is not entirely obvious that conditions (A1) (A2) hold for this new system.

Now we explain how one can extend the results of the paper to these models. It is clear that since the Pirogov–Sinaĭ theory holds for them, we have a natural generalization of Lemma 1, of Proposition 1 and its Corollary and of Lemmas 4 and 5. What we need is a suitable extension of Lemmas 2 and 3, namely, of the following facts:

(a) One can define, in each configuration, an interface and the minimum "length" of such an interface is proportional to L (or L^{d-1} in d dimensions).

(b) Each interface has an energy, with respect to the ground state energy, that is proportional to its length.

We start with the definition of the interface in these more general models.

In Ref. 12, Holsztynski and Slawny show that the models satisfying (i)–(v) above fulfill the following Peierls condition: let, for each natural number N, $N(x) = \{y \in \mathbb{Z}^d \,|\, |x - y| < N\}$. Given a configuration $\mathbf{s}$, a square $N(x)$ is called *irregular* of the restriction of $\mathbf{s}$ to $N(x)$ does not coincide with the restriction of some ground state to $N(x)$. $B_N(\mathbf{s})$ is the union of the set of irregular squares. *Peierls' condition* states that, for each N large enough, there exists $\rho > 0$ such that, if $\mathbf{s}$ coincides with a ground state outside V,

$$\sum_{\Lambda \cap V \neq \phi} \phi_\Lambda(\mathbf{s}) > \rho |B_N(\mathbf{s})| \tag{A.1}$$

It was shown in Ref. 12 that under the assumption (i)–(v) on the potentials, Peierls' condition holds. Actually, the proof of Ref. 12 extends to the case where $V = V_{L,M}$ and $\mathbf{s}$ coincides with ground state 1 in the upper half of $V_{L,M}^c$ and with ground state 2 in the lower half.

Now, $B_N(\mathbf{s})$ can be decomposed into connected components called contours; the *interface* of a configuration with the (1, 2) boundary conditions is the contour connected to V^c. The Peierls condition (A.1) implies that every interface produces an energy proportional to its length (i.e., the number of squares contained in it). This is point (b) above. It remains to show point (a), namely, that every configuration has an interface that is long enough (at least of length L, or L^{d-1} in d dimensions). This follows from the fact that there cannot be "holes" in the interface; indeed consider any chain of squares which connects the upper half of $V^c_{L,M}$ and the lower half of $V^c_{L,M}$: $\{N(x_0), N(x_1), \ldots, N(x_K)\}$, where $N(x_0)$ is in the upper half of $V^c_{L,M}$, $N(x_K)$ is in the lower half of $V^c_{L,M}$, and $|x_i - x_{i+1}| = 1$ $i = 0, 1, \ldots, K-1$.

Let N be so large that all ground states are uniquely determined by their restriction to $N(x)$. Then there must be at least one x_j $j \in \{1, \ldots, K\}$ such that $N(x_j)$ is irregular. It is easy to see that this implies that the minimal length of an interface is proportional to L.

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