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Asymptotic phase diagrams for lattice spin systems

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Abstract. We present a method of constructing the phase diagram at low temperatures using the low temperature expansions. We consider spin lattice systems described by a Hamiltonian with a *d*-dimensional perturbation space. We prove that there is a one-to-one correspondence between subsets of the phase diagram and extremal elements of some family of convex sets. We also solve a linear programming problem of the phase diagram for a set of affine functionals.

1. Introduction

Low temperature (LT) expansions are often used as a first step in investigating the low temperature properties of a system. We will restrict our attention to lattice spin systems. Let us consider the following situation. A system is described by a finite range Hamiltonian H_0 with a finite number of periodic ground states. We assume that for any periodic ground state G, the LT expansion of a pressure is known. Next, the system is perturbed by a Hamiltonian in the form $\sum_{i=1}^{d} L_i$, where $L = (L_1, \ldots, L_d)$ is an element of a d-dimensional perturbation space. It is our goal to describe the phase diagram resulting from the LT expansion of the pressure.

If the number of ground states and dimension of the space is large, the situation is complicated, with one exception: when the number of ground states exceeds the dimension of the perturbation space by one. In this case there exist both a rigorous Pirogov-Sinai theory [1,2] and the detailed description of the phase diagram obtained from the LT expansions [3]. In [3] Slawny has also shown that this phase diagram is asymptotic (as temperature goes to zero) to the rigorous one. The phase diagram obtained from LT expansions will henceforth be called the asymptotic phase diagram. It is easy to see that as long as the number of periodic ground states of H_0 exceeds the dimension of a perturbation space (and the Hamiltonian H_0 satisfies some technical conditions necessary for the existence of the LT expansions, cf [3]), this phase diagram is asymptotic to the rigorous one. One can add new perturbations to increase the dimension of a perturbation space, so that the system satisfies the conditions of Pirogov-Sinai theory.

In this paper we present a method of constructing the asymptotic phase diagrams for a wide class of systems in the general case when the number of ground states is larger than the dimension of a perturbation space. The general idea is to locally approximate LT expansions by affine functionals. The phase diagram for a set Γ of

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affine functionals can be obtained from the properties of a convex hull of Γ . The asymptotic phase diagram is then approximated in some sense by the phase diagram for Γ .

This paper is laid out as follows. First we describe the framework and state the problem. In § 3 we consider the simpler version of the problem: the phase diagram for a set of affine functionals. Section 4 contains the main result and the description of the phase diagram in the general case. In § 5 we present examples. The proofs of theorems are contained in the appendix.

2. Framework

2.1. The description of a system

Let \mathbb{L} be a \mathbb{Z}^{ν} -invariant lattice, and $\chi = S^{t}$ the configuration space (S is finite). The system is described by a finite range Hamiltonian H_{0} , defined by an interaction Φ . If $\Lambda \subset \mathbb{L}$ is finite, then

$$(H_0)_{\Lambda} = \sum_{M \subset \Lambda} \Phi_M \qquad \Phi_M : S^M \to \mathbb{R} \qquad (M \subset \mathbb{L} \text{ finite})$$

If configurations X, Y differ in a finite number of points only, we define a relative Hamiltonian

$$H_0(X|Y) = \sum \Phi_M(X) - \Phi_M(Y)$$

(with the sum over finite subsets M of \mathbb{L}).

We say that the configuration G is *periodic* if there exists a subgroup G of \mathbb{Z}^{ν} such that G is invariant with respect to the translations from G. A periodic configuration G is a periodic ground state if, for any X differing from G in a finite number of points, $H_0(X|G) \ge 0$. X is called an excitation of G, and we define: supp $X = \{a \in \mathbb{L} : X_a \neq G_a\}$. The set of ground states is denoted by G. We assume that the set $\sigma(H_0) = \{H_0(X|G), G \in \mathcal{G}\}$ is ordered increasingly and its elements are $0 < E_1 < E_2 < \ldots$. It is not hard to see that $\sigma(H_0)$ is additive.

The equivalent definition of a periodic ground state is [1] that

$$e_G(H) \equiv \lim_{\Lambda \to \infty} \frac{1}{|\Lambda|} H_{\Lambda}(G) = \inf e_X(H)$$
(2.1)

with the infimum taken over the set of periodic configurations. We make the following assumptions about the Hamiltonian H_0 :

- (i) \mathcal{G} is finite and
- (ii) for any $G \in \mathcal{G}$, $H_0(X|G) \rightarrow \infty$ if Card(supp X) $\rightarrow \infty$.

Next, we consider the set of Hamiltonians of the form

$$H(L) = H_0 + \sum_{i=1}^{d} L_i$$
 $L = (L_1, ..., L_d)$

where L is an element of a d-dimensional perturbation space \mathcal{L} . The norm on \mathcal{L} is any norm induced by the l^1 norm in \mathbb{R}^d : $||x|| = \sum_{i=1}^d |x_i|$.

Let $G \in \mathcal{G}$. The function $L \to e_G(L)$ (cf (2.1)) defines an element of \mathcal{L}^* (the space dual to \mathcal{L}). We assume that \mathcal{L} is *transversal* to \mathcal{G} : for any fixed $G_0 \in \mathcal{G}, \{e_G - e_{G_0}: G \in \mathcal{G}\}$ spans \mathcal{L}^* .

2.2. LT expansions and cut-off pressures

As is well known, the LT expansions for general systems have to be treated as formal series in $\{\exp x(-\beta E_i)\}$. The discussion of this paragraph follows [3]. We will denote an algebra of formal series by \mathbb{D} , and \mathbb{D}^n is a direct sum of *n* copies of \mathbb{D} . Elements of \mathbb{D} (of \mathbb{D}^n) are marked by a dot.

For any $G \in \mathcal{G}$, $L \in \mathcal{L}$ and $\beta > 0$, the low temperature expansion of a pressure is a formal series given by

$$\dot{p}^{G}(\beta L) = \sum_{j=1}^{\infty} n_{j}^{G}(\beta L) \exp(-\beta E_{j}).$$
(2.2)

The dependence of n_i^G on its argument is as follows:

$$n_{i}^{G}(\beta L) = \sum_{k=1}^{r_{i}} n_{i,k}^{G} \exp(-\mu_{i,k}^{G}(\beta L))$$
(2.3)

where $\mu_{i,k}^G$ is a linear form, and some $n_{i,k}^G$ can be equal to zero. If $\dot{x} \in \mathbb{D}^d$, we define a formal series $n_j^G(\dot{x})$ by expanding $n_j^G(x)$ around zero, and replacing x by \dot{x} :

$$n_{j}^{G}(\dot{x}) = \sum_{k=1}^{r_{j}} n_{j,k}^{G} \sum_{s=0}^{\infty} \frac{1}{s!} [-\mu_{j,k}^{G}(\dot{x})]^{s}.$$

Then

$$\dot{p}^G(\dot{x}) = \sum_{j=1}^{\infty} \exp(-\beta E_j) n_j^G(\dot{x}) \equiv \sum_{j=1}^{\infty} (\dot{p}^G(\dot{x}))_j \exp(-\beta E_j).$$

Here

$$\mu_{i,k}^{G}\left(\sum_{n=0}^{\infty} x_n \exp(-\beta E_n)\right) = \sum_{n=0}^{\infty} \exp(-\beta E_n) \mu_{i,k}^{G}(x_n).$$

To describe the phase diagram, one introduces the cut-off pressures. Let $m \in \mathbb{N}$. Then the cut-off pressure in order m is

$$p_m^G(\beta L, \beta) = \sum_{i=1}^m n_j^G(\beta L) \exp(-\beta E_j).$$
(2.4)

 p_m^G is defined for all values of βL . However, we want to be able to vary L and β independently, and eventually allow β to go to infinity with L fixed. Combining (2.3) and (2.4) we obtain an equivalent expression for p_m^G as a function of L and β :

$$p_m^G(L,\beta) = \sum_{i=1}^m \sum_{k=1}^{r_i} n_{i,k}^G \exp\{-\beta [E_i + \mu_{i,k}^G(L)]\}.$$

Hence the limit $\beta \rightarrow \infty$ has meaning only if $E_i + \mu_{i,k}^G(L) > 0$. It is easy to see that there exists $c_m > 0$ such that if $||L|| < c_m$ then

$$E_i + \mu_{i,k}^G(L) > 0$$

for all G, $i \leq m$ and k. We will denote by O the ball $B(0, c_m) \subset \mathcal{L}$.

For any $G \in \mathcal{G}$, $L \in O$, and $\beta > 0$ we define

$$\pi_m^G(\beta L, \beta) = -\langle \beta L, e_G \rangle + p_m^G(\beta L, \beta)$$
(2.5)

with e_G being an element of \mathcal{L}^* introduced by (2.1), and p_m^G being defined by (2.4).

2.3. The phase diagram in order m

Suppose that $\mathscr{G} \subset \mathscr{G}$. We define a subset of $\mathscr{L} \times [0, \infty)$:

$$\Omega_{m,\beta}(\mathscr{G}') = \{ L \in \bar{\mathcal{O}}, \ \beta > 0; \ \pi_m^G(\beta L, \beta) \\ = \pi_m^{G'}(\beta L, \beta) > \pi_m^{G''}(\beta L, \beta) \text{ for all } G, \ G' \in \mathscr{G}', \ G'' \notin \mathscr{G}' \}$$
(2.6)

The phase diagram in order m is a set:

$$\Omega_m = \bigcup_{|\mathcal{G}'| \ge 2} \Omega_m(\mathcal{G}') \tag{2.7}$$

 $\Omega_m(\mathscr{G}')$ is called a *stratum* of Ω_m corresponding to \mathscr{G}' .

Let $G \in \mathcal{G}$. The domain of G is the set

$$\Omega_{m,\beta}(G) = \{ L \in \overline{O} : \pi_m^G(L,\beta) \ge \pi_m^{G'}(L,\beta) \text{ all } G' \in \mathscr{G} \}$$

$$(2.8)$$

Note that in contrast to strata, domains are closed sets.

Our goal is to describe the properties of Ω_m which are common for all *m* large enough. Therefore not all properties of an individual Ω_m are important. We are interested in stable properties: if Ω_m has the given property, then every Ω_s for $s \ge m$ also has this property. Thus, with respect to strata, we are interested in their existence rather than in the precise description of their form. We want also to have some approximation on the localisation of a stratum in the perturbation space and with respect to other strata. Finally, we will determine the conclusive order: above this order, all phase diagrams are isomorphic to one another in the sense that there is a one-to-one correspondence between their strata.

The natural set of variables for the problem is $(\beta L, \beta)$ rather than (L, β) (cf (2.4) and (2.5)). We will denote the layers of Ω_m for β fixed by $\Omega_{m,\beta}$ and layers of a stratum $\Omega_m(\mathscr{G}')$ by $\Omega_{m,\beta}(\mathscr{G}')$. The variable βL will be denoted by x.

The problem of existence of a given stratum $\Omega_m(\mathscr{G})$ is twofold. The definition (2.6) consists of the system of equations and a system of inequalities. Hence we have to determine (i) for which \mathscr{G}' the system of equations has a solution and (ii) when the system of inequalities 'cuts out' the non-empty piece from the solution set. Let us consider the first problem.

Definition 1. A family of points $x_1, x_2, ..., x_s$ in a linear vector space is said to be *linearly independent* if for any choice of i, $(1 \le i \le s)$, the set of vectors $\{x_k - x_i, k \ne i\}$ is linearly independent.

Theorem 1. Suppose that $\mathscr{G}_0 = \{G_0, G_1, \ldots, G_s\} \subset \mathscr{G}$ is such that $\{e_{G_i}, i = 1, \ldots, s\}$ is linearly independent in \mathscr{L}^* . Let $N = \bigcup_{i=1}^s \ker(e_{G_i} - e_{G_0})$ and $\mathscr{L} = N \oplus M$. Consider a system of equations:

$$\pi_m^{G_i}(x,\beta) - \pi_m^{G_0}(x,\beta) = 0.$$
(2.9)

Then there exists $\beta_m(\mathscr{G}_0)$ such that

(i) $\forall \beta > \beta_m(\mathscr{G}_0)$, the solution $y: \beta O \cap N \times (\beta_m(\mathscr{G}_0), \infty) \rightarrow M$ exists and is analytic in the first coordinate and

(ii) $\forall z \in \beta O \cap N$

$$y(z, \beta) = \sum_{j=1}^{\infty} y_j(z) \exp(-\beta E_j).$$
 (2.10)

The proof of theorem 1 may be found in appendix 1.

(Note that conditions imposed on \mathscr{G}_0 may be relaxed in the presence of symmetries (cf § 4.3).)

In general, if \mathscr{G}_0 does not satisfy the conditions of the above theorem, the solution of (2.9), and hence $\Omega_m(\mathscr{G}_0)$, does not exist. In order to avoid this problem, we will be forced to adopt an additional assumption (cf assumption 1).

The solution of the second problem of the existence of $\Omega_m(\mathscr{G})$, connected with the system of inequalities, is presented in the following sections.

Example. Blume-Capel model ([4,5]). We will use the following example to illustrate our method.

Let

$$\mathbb{L} = \mathbb{Z}^2 \qquad S = \{-\frac{5}{2}, -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}\} \qquad H_0 = \sum_{(a,b)} (s_a - s_b)^2 \qquad s_a(X) = X_a$$

where $\langle a, b \rangle$ denotes a pair of nearest neighbours.

The set of ground states of H_0 is

$$\mathscr{G} = \{(-5), (-3), (-1), (1), (3), (5)\}$$

with (k) denoting the configuration: $\forall a \in \mathbb{Z}^2$, $(k)_a = k/2$. The LT expansion coefficients in the first few orders are

- (a) $E_1 = 4$ $n_1^{(5)}(0) = n_1^{(-5)}(0) = 1$ $n_1^{(k)}(0) = 2$ if $k \neq -5, 5$
- (b) $E_2 = 6$ $n_2^{(5)}(0) = n_2^{(-5)}(0) = 2$

$$n_2^{(k)}(0) = 4$$
 if $k \neq -5,5$

(c)
$$\forall i < 7$$
 $n_i^{(k)}(0) = n_i^{(1)}(0)$ $k = -3, 3, -1.$

The order seven is the lowest order in which there exists for any (k) an excitation X such that for some $a \in \mathbb{Z}^2$, $|X_a - k| > 1$. In this order

$$n_7^{(-1)}(0) = n_7^{(1)}(0) \qquad n_7^{(3)}(0) = n_7^{(-3)}(0)$$

$$n_7^{(1)}(0) - n_7^{(3)}(0) \equiv a(3) > 0.$$

We will consider the perturbation space generated by Hamiltonians:

$$L_1 = \sum_{a \in \mathbf{L}} s_a \qquad \qquad L_2 = \sum_{a \in \mathbf{L}} s_a^3.$$

In the base generated in \mathscr{L}^* by L_1 , L_2 , the linear functional for (k) is

$$e_{(k)} = \frac{1}{8}(4k, k^3).$$

3. The phase diagrams for a set of affine functionals

As the first case in the investigation of phase diagrams for various systems, let us consider the phase diagram for a set of affine functionals. This is also a new type of problem in linear programming.

Suppose that $\Gamma = \{\rho_i, i = 1, 2, ..., N\}$ is a set of affine functionals:

$$\rho_i: \mathbb{R}^a \to \mathbb{R}: \rho_i(x) = \langle x, h_i \rangle + a_i \qquad a_i \in \mathbb{R} \qquad (d+1 \le N).$$

Assume that $\{h_i: \rho_i \in \Gamma\}$ spans \mathbb{R}^d . We will also write

$$\rho_i = (h_i, a_i) \in \mathbb{R}^{d+1}.$$

If $\Gamma' \subset \Gamma$, we define

$$\Pi(\Gamma') = \{x: \rho_i(x) = \rho_i(x) > \rho_k(x) \text{ if } \rho_i, \rho_i \in \Gamma', \rho_k \notin \Gamma'\}$$
(3.1a)

$$\Pi(\rho_i) = \{x: \rho_i(x) \ge \rho_j(x) \text{ all } j \neq i\}$$
 (closed). (3.1b)

(Different notation is used for the phase diagram in this case since later on we will introduce simultaneously phase diagrams for cut-off pressures and for some set of affine functionals.)

The set $\Pi = \bigcup \Pi(\Gamma')$, where the union is over all $\Gamma' \subset \Gamma$ such that $|\Gamma'| \ge 2$, will be called the phase diagram for Γ , and its subsets $\Pi(\Gamma')$ the strata.

Let

$$W = \operatorname{conv} \Gamma \subset \mathbb{R}^{d+1}.$$
(3.2)

We define max W as the set of maxima of W. We will say that $E \subset \max W$ is a face (extremal edge) of max W if E is a face (extremal edge) of W. $\varepsilon(\max W)$ denotes a set of extremal points of max W.

Theorem 2.

(1) There exists a one-to-one correspondence between extremal elements of max W and strata of Π . Namely, let $E \subset \max W$ be a face (extremal edge) of dimension d - r. Then $\Pi(E) \neq \emptyset$, dim $\Pi(E) = r$ and

$$\Pi(E) = \left\{ x: \rho(x) = \rho'(x) > \tilde{\rho}(x) \qquad \forall \rho, \rho' \in E, \, \tilde{\rho} \in \bigcup_{F \supset E} \varepsilon(F) \setminus E \right\}$$
(3.3)

In particular, if $\rho \in \varepsilon(\max W)$ then $\operatorname{Int} \Pi(\rho) \neq \emptyset$.

(2) If $\rho = \sum_{i=1}^{s} \lambda_i \rho_i$ (2 $\leq s \leq d+1$) with $\rho_i \in \varepsilon$ (max W) $\lambda_i \in (0,1)$ and $\sum_{i=1}^{s} \lambda_i = 1$ then $\Pi(\{\rho_1, \dots, \rho_s\})$.

(3) $\rho \notin \max W \Rightarrow \Pi(\rho) = \emptyset$.

The proof of theorem 2 is located in appendix 2.

The phase diagram Π for Γ is now constructed as follows: to any *d*-dimensional face *F* of max *W* there corresponds a point v(F) which is the unique element of $\Pi(F)$. Furthermore, for any face *E* of *F* (of dimension d-1) there exists a one-dimensional line on which elements belonging to *E* coexist. This line either goes to infinity (if some elements of $\varepsilon(E)$ are such that their linear parts belong to $\operatorname{conv}\{h, \rho \in \Gamma\}$), or it terminates at another point of coexistence v(F'), for some face *F'* sharing *E* with *F*. The process then continues for faces of Π with lower dimensions.

Remark 1. If Γ is a set of affine functionals $\{(e_G, 0), G \in \mathcal{G}(H_0)\}$, then the application of theorem 2 results in a zero temperature phase diagram.

Example. Let us apply theorem 2 to the set $\{(e_{(k)}, 0), (k) \in \mathcal{G}\}$. The set W is presented in figure 1(a). In this case, max W = W has four extremal points, four edges and one face. Hence the zero-order (zero temperature) phase diagram, figure 2(a), has one point where all six functionals coexist and four lines of two-functional coexistence. Domains of (-1) and (1) are restricted to the point.



Figure 2. The phase diagram for sets of affine functionals: (a) $\Gamma = \{(-e_{(k)}, 0), (k) \in \mathscr{G}\};$ (b) $\Gamma = \{(-e_G, n_1^{(k)}(0)), (k) \in \mathscr{G}\}.$

Next, let us consider the set $\{(e_{(k)}, n_1^{(k)}(0)), (k) \in \mathcal{G}\}$. max W_1 has five faces, as in figure 1(b). They are listed below, every face P together with elements of $\mathcal{G}_1(P)$, and $v_1(P)$:

$$F: (-1), (1), (-3), (3) \qquad v_1(F) = 0$$

$$G: (5), (3), (-1) \qquad v_1(G) = \langle \frac{1}{6}, -\frac{2}{21} \rangle$$

$$H: (5), (-1), (-3) \qquad v_1(H) = (\frac{13}{24}, -\frac{1}{6})$$

$$G': (-5), (-3), (1) \qquad v_1(G') = (-\frac{1}{6}, \frac{2}{21})$$

$$H': (-5), (1), (3) \qquad v_1(H') = (-\frac{13}{24}, \frac{1}{6})$$

The phase diagram for this case is shown in figure 2(b). It is easy to see the correspondence between extremal elements of max W and strata of the phase diagram.

4. The phase diagram in order m

We will now consider the general situation. We will show that the properties of the phase diagram $\Omega_{m,\beta}$ can be described with the help of some family of convex sets (a convex structure) in $\mathscr{L}^* \times \mathbb{R}$. This family is a generalisation of the set max W defined in § 3 (cf (3.1)).

4.1. The convex structure in order m

Recall that \mathbb{D} denotes an algebra of formal series, and elements of \mathbb{D} (of \mathbb{D}^n) are marked by a dot.

For any $G \in \mathcal{G}$, let $A_1^G = \dot{p}^G(0)_1 \equiv n_1^G(0)$. Define

$$W_1 \subset \mathscr{L} \times \mathbb{R}$$
: $W_1 = \operatorname{conv}(-e_G, A_1^G), G \in \mathscr{G}$.

In W_1 we consider the set of maxima of W_1 : max W_1 . The set $E \subset \max W_1$ is an *s*-dimensional face (edge) of $\max W_1$ if it is an *s*-dimensional face (edge) of W_1 .

Let \mathbb{F}_1 denote the set of all faces of max W_1 . If $F \in \mathbb{F}_1$, we define

$$\mathscr{G}_{1}(F) = \{ G: (-e_{G}, n_{1}^{G}(0)) \in F \}.$$

There exists a unique vector $v_1(F)$ in \mathscr{L} such that $\forall G, G_0 \in \mathscr{G}_1(F)$:

$$-\langle v_1(F), e_G - e_{G_0} \rangle + A_1^G - A_1^{G_0} = 0.$$

If G_0, G_1, \ldots, G_d are any phases corresponding to elements of $\varepsilon(F)$, then $v_1(F)$ is defined as the solution of the system of equations

$$-\langle v_1(F), e_{G_1} - e_{G_0} \rangle + A_1^{G_1} - A_1^{G_0} = 0.$$
(4.1)

For any $F \in \mathbb{F}_1$, we define the following quantities:

$$\tilde{v}_1(F,\beta) = \exp(-\beta E_1)v_1(F)$$

 $\dot{v}_1 \in \mathbb{D}^d: (\dot{v}_1)_1 = n_1 \qquad (\dot{v}_1)_k = 0 \qquad \text{if } k \ge 2.$

Let $A_2^G(F) = \dot{p}^G(\dot{v}_1(F))_2$ (for the definition of $\dot{p}^G(\dot{x})$ see § 2.2) and

$$W_2(F) = \operatorname{conv}\{(-\mathbf{e}_G, A_2^G(F)) \qquad G \in \mathscr{G}_1(F)\}.$$

We denote the set of faces of max $W_2(F)$ by $\mathbb{F}_2(F)$. The set

$$\mathbb{F}_2 = \bigcup_{F \in \mathbb{F}_1} \mathbb{F}_2(F)$$

is called the convex structure in order 2.

The convex structure in order m is defined by induction.

If $F' \in \mathbb{F}_{m-2}$ is given, then for any $F \in \mathbb{F}_{m-1}(F')$ one defines $v_{m-1}(F)$ by means of formula (4.1), and

$$\begin{split} \vec{v}_{m-1}(F,\beta) &= \vec{v}_{m-2}(F',\beta) + \exp(-\beta E_{m-1})v_{m-1}(F) \\ \vec{v}_{m-1}(F) &\in \mathbb{D}^d : (\vec{v}_{m-1}(F))_k = (\vec{v}_{m-2}(F'))_k & \text{if } k \neq m-1 \\ (\vec{v}_{m-1}(F))_{m-1} &= v_{m-1}(F) \\ \mathscr{G}_{m-1}(F) &= \{G \in \mathscr{G}_{m-2}(F') : (-e_G, A_{m-1}^G(F')) \in F\}. \end{split}$$

Let $A_m^G(F) = \dot{p}^G(\dot{v}_{m-1}(F))_m$. We define $W_m(F)$, max $W_m(F)$ and $\mathbb{F}_m(F)$ as in order 2. The convex structure in order m is the set

$$\mathbb{F}_m = \bigcup_{F \in \mathbb{F}_{m-1}} \mathbb{F}_m(F).$$

Finally, $F_0 = W_0 = \operatorname{conv}\{-e_G, G \in \mathscr{G}\}.$

Here we make the following remarks.

(i) For any F in \mathbb{F}_m , there exists a unique set of faces $\{F_0, F_1, \ldots, F_m\}$ such that $F_i \in \mathbb{F}_i(F_{i-1})$, and $F_m = F$.

(ii) For any face $F \in \mathbb{F}_k$, we can replace $A_{k+1}^G(F)$ by $A_{k+1}^G(F) - A_{k+1}^{\tilde{G}}(F)$ for any $\tilde{G} \in \mathscr{G}_k(F)$. The convex properties of max $W_{k+1}(F)$ are not changed by this replacement.

(iii) Suppose that $|\mathscr{G}(F)| = d + 1$ for some $F \in \mathbb{F}_m$. Then $\mathbb{F}_{m+1}(F) = \{F_{m+1}\}, \ldots, \mathbb{F}_{m+s}(F_{m+s-1}) = \{F_{m+s}\}$ for all s, and F, F_{m+1}, \ldots, F_{m+s} are isomorphic (as convex sets in $\mathscr{L}^* \times \mathbb{R}$, i.e. that there is a one-to-one correspondence between extremal elements of both sets).

Definition 2. The order m is conclusive if $\forall F \in \mathbb{F}_m$, $|\mathscr{G}_m(F)| = d + 1$.

Example. In § 3, we have already discussed the convex structures in zero and first orders. In order 2 $(E_2 = 6)$, one has

$$\dot{p}^{(k)}(\dot{v}_1(P))_2 = \dot{p}^{(k)}(0)_2$$

for any face P. Hence

$$A_2^{(k)}(P) = n_2^{(k)}(0) = 4 \qquad k \neq -5, 5$$

2
$$k = -5, 5.$$

Thus max $W_2(P)$ has only one element which is isomorphic (as a convex set) to P. We will denote it also as P. Moreover, it is easy to see that $v_2(P) = 2v_1(P)$. Obviously \mathbb{F}_2 is isomorphic to \mathbb{F}_1 (as collections of convex sets, see (iii) above).

Let P be any element of \mathbb{F}_2 . In order 3 ($E_3 = 8$) (see definition, § 2.2)

$$\dot{p}^{(k)}(\dot{v}_2(P))_3 = \dot{p}^{(k)}(\dot{v}_1(P))_3 = n_3^{(k)}(0) + \langle v_1(P), dn_1^{(k)} dx(0) \rangle.$$

Since the exact form of these expressions is cumbersome and of little importance, we will not reproduce it here. We note that $W_3(P)$ is again isomorphic to $W_2(P)$. If P is not F, then this holds because $\mathscr{G}_3(P)$ has three elements, and for F one has $v_2(F) = 0$, so $W_3(F)$ is a translate of $W_2(F)$. Since in any order s, higher than 2, $\mathbb{F}_s(P)$ is isomorphic to $\mathbb{F}_2(P)$ (P not equal to F), we will not investigate $\mathbb{F}_s(P)$.

Let us study $W_i(F)$ for i > 3. As we have already observed

$$\dot{p}^{(k)}(\dot{v}_2)_3 = n_3^{(k)}(0) = \text{constant}$$
 if $k = -3, -1, 1, 3$.

Hence $v_3(F) = 0$. By the inductive argument, $v_i(F) = 0$ if i < 7. In order 7

$$n_7^{(1)}(0) - n_7^{(3)}(0) \equiv a(3) > 0.$$

max $W_7(F)$ has two faces (figure 3). These are listed below together with corresponding vectors in \mathcal{L} :

$$F_1: \mathcal{G}_7(F_1) = \{(3), (1), (-1)\} \qquad v_7(F_1) = (\frac{1}{12}a(3), -\frac{1}{3}a(3))$$

$$F_2: \mathcal{G}_7(F_2) = \{(-3), (-1), (1)\} \qquad v_7(F_2) = (-\frac{1}{12}a(3), \frac{1}{3}a(3)).$$

One does not have to investigate convex structures in higher orders $(s \ge 7)$ since \mathbb{F}_s is isomorphic to \mathbb{F}_7 (in the sense of (iii) above).



Figure 3. The projection of max $W_3(F)$ on \mathcal{L}^* .

Definition 3. Let $F \in \mathbb{F}_m$, and $\{F_0, F_1, \ldots, F\}$ be as in (i) above. For any G in G, we define an affine functional:

$$\rho_{m,\beta}^{G}(F): \mathcal{L} \to \mathbb{R}$$

$$\rho_{m,\beta}^{G}(F, x) = -\langle x, e_{G} \rangle + \sum_{j=1}^{m} A_{j}^{G}(F_{j-1}) \exp(-\beta E_{j}).$$
(4.2)

Remark 2. $\forall G \in \mathscr{G}_m(F), \forall j < m$,

$$A_{j}^{G}(F_{j-1}) - \langle v_{j}(F_{j}), e_{G} \rangle = A_{j}^{G_{0}}(F_{j-1}) - \langle v_{j}(F_{j}), e_{G_{0}} \rangle$$

with $G_0 \in \mathscr{G}_m(F)$ being any fixed element.

4.2. The phase diagram in order m

Now we will show how the convex structure describes the phase diagram in order m. Let us introduce the following notation: if $F_k \in \mathbb{F}_k$, then $\Pi(F_k)$ is a phase diagram for the set of affine functionals:

$$\{\rho_{k+1,\beta}^G(F_k), G \in \mathscr{G}_k(F_k)\}$$

and $\Pi(F_k, \mathscr{G}')$ is a stratum corresponding to $\mathscr{G}' \subset \mathscr{G}$. We will also denote

$$\mathscr{G}_{k+1}(E) = \{ G \in \mathscr{G}_k(F) \colon \rho^G_{k+1,\beta}(F) \in E \}.$$

Let us first describe the restrictions of the method. Suppose that E is an *n*-dimensional face of max $W_{k+1}(F_k)$. Then $\Pi(F_k, \mathcal{G}_{k+1}(E))$ exists. However, if $\mathcal{G}_{k+1}(E)$ does not satisfy conditions imposed by theorem 1, then the solution for the system of equations

(2.9), and hence $\Omega_{m,\beta}(\mathcal{G}_{k+1}(E))$, does not generally exist. Therefore we have to make an additional assumption about the convex structure.

Assumption 1. Let $k \le m$. If E is a face (extremal edge) of max $W_k(F)(F \in \mathbb{F}_{k-1})$ with dim E < d, E contains only dim E + 1 functionals $\rho_{k,\beta}^G(F)$.

(Assumption 1 can be relaxed in the presence of symmetries, cf 4.3.)

The following theorem is the main result of this paper.

Theorem 3. Let order m be conclusive, and suppose that the system satisfies assumption 1 for all orders up to the order m. The $\exists \beta_m : \forall \beta > \beta_m$ the following holds.

(1) Suppose that $F \in \mathbb{F}_k (k \leq m)$. Then \exists open sets $U_k(F)$, $U'_k(F) : \forall \beta > \beta_m$, the following statements hold in $Z = U'_k(F) \setminus \bigcup U_{k+1}(F')$ (with the union over faces in $\mathbb{F}_{k+1}(F)$).

(a) There is a one-to-one correspondence between strata of $\Pi(F) \cap Z$ and strata of $\Omega_{m,\beta} \cap Z : \Pi(F, \mathscr{G}_0) \to \Omega_{m,\beta}(\mathscr{G}_0)$. This correspondence preserves the closure, i.e. the elements of the closure of $\Pi(F_k, \mathscr{G}_0)$ correspond to the elements of the closure of $\Omega_{m,\beta}(\mathscr{G}_0)$.

(b) $\exists a(F) > 0$: dist $(\Pi(\mathscr{G}_0) \cap Z, \Omega_{m,\beta}(\mathscr{G}_0) \cap Z) \le a(F) \exp(-\beta E_{k+1})$.

(2) If $E \subseteq \max W_m(F')$ $(F' \in \mathbb{F}_{m-1})$ is a face (edge, extremal point) of dimension d-r, then $\Omega_{m,\beta}(\mathscr{G}_m(E)) \neq \emptyset$ and has dimension r. In particular, $\Omega_{m,\beta}(G) \neq \emptyset$ if and only if $\rho_{m,\beta}^G(F') \in \varepsilon(\max W_m(F'))$. Moreover, $\forall s \ge m \exists \beta_s : \forall \beta > \beta_s$, the above holds for corresponding strata of $\Omega_{s,\beta}$.

The proof of theorem 3 is contained in appendix 3.

Remark 3. The phase diagram Ω_s , s < m, can be obtained from Ω_m (*m* conclusive) in the following way. Let $F \in \mathbb{F}_s$. If \mathscr{G}' is such that $\Omega_{s,\beta}(\mathscr{G}') \subset U_s(F)$, then we identify $\Omega_{s,\beta}(\mathscr{G}')$ with $\tilde{v}_s(F)$. There is an obvious correspondence between strata of $\Omega_{s,\beta}$ (after the identification) and extremal elements of the convex structure in order s.

Let us now show how the theorem is used to describe the phase diagram. For every $F \in \mathbb{F}_m$, there exists a unique point v(F) of coexistence of phases from $\mathscr{G}_m(F)$. Next, for any (d-1)-dimensional face E_1 of F, there is a one-dimensional surface of coexistence of phases in $\mathscr{G}_m(E_1)$ which either terminates at the boundary of $\beta \bar{O}$ (if some phases in $\mathscr{G}_m(E)$ correspond to elements of $\varepsilon(\operatorname{conv}\{-e_G, G \in \mathscr{G}\})$), or terminates at another point of coexistence v(F') (with $F' \supset E_1$). Furthermore, for any (d-2)-dimensional edge E_2 , there exists a two-dimensional surface of coexistence of phases from $\mathscr{G}_m(E_2)$. This surface is bounded by the set of lines which are the surfaces of coexistence of phases from $\mathscr{G}_m(E')$ for any $E' \supset E_2$. In addition, if some element of $\mathscr{G}_m(E_2)$ corresponds to the element of $\varepsilon(\operatorname{conv}\{-e_G, G \in \mathscr{G}\})$, then one of the boundaries is the boundary of $\beta \bar{O}$. One can make similar statements about strata of higher dimensions.

The most convenient way of representing the phase diagram is to show it separately in the blow-ups of sets $U_k(F)$, $F \in \mathbb{F}_k$. In each of these sets we can apply part (2) of the theorem to obtain the topology and localisation of strata.

Example 4. The phase diagram for our example is shown in figures 4, 5 and 6. Since $\Omega_{m,\beta}$ is constructed order by order, we represent it in the successive blow-ups of sets $U_k(F_k)$.



Figure 4. The phase diagram $\Omega_{m\beta}$ in $\beta O \setminus U_0(F_0)$. Dotted regions represent the restrictions imposed by theorem 3, part (1b).

As has been discussed before (§ 3), W_0 has four extremal points: (-5), (5), (-3), (3) and four edges: {(-5), (-3)}, {(-5), (3)}, {(5), (-3)}, {(5), (3)} (figure 1(a)). Hence, on $\beta O \setminus U_0(F_0)$, $\Omega_{m,\beta}$ has four lines of two-phase coexistence: $\Omega_{m,\beta}((-5), (-3))$, $\Omega_{m,\beta}((5), (-3))$, $\Omega_{m,\beta}((5), (3))$ and $\Omega_{m,\beta}((5), (3))$ (figure 4). Next, $\Omega_{m,\beta} \cap U_0(F_0)$ is shown in figure 5. It is easy to see the correspondence between strata of $\Omega_{m,\beta}$, strata of $\Pi(F_0)$ (figure 2(b)) and extremal features of max W_1 (cf figure 1(b)). Finally, the blow-up of $U_7(F)$ is shown in figure 6. Since \mathbb{F}_i is isomorphic to \mathbb{F}_7 if $i \ge 7$, the phase diagram of figures 4, 5 and 6 is representative for all orders higher than seven.

4.3. Phase diagrams in the presence of symmetries

Assumption 1 can be relaxed in the presence of symmetries of an original Hamiltonian H_0 .

Let R be the transformation group acting on the lattice and Q be the group of transformation acting on χ pointwise: if Q_0 is a group of transformations of S, then $Q = Q_0^{L}$.

The subgroup $\Theta \subset R * Q$ is a symmetry group of the Hamiltonian H_0 if $\forall \theta \in \Theta$, $\forall Y, X$ differing in a finite number of points:

$$H_0(\theta X | \theta Y) = H_0(X | Y).$$

 Θ induces the group of transformations T acting on \mathcal{L} : if $\theta \in \Theta$ and $L \in \mathcal{L}$, then $T_{\theta}L(X|Y) = L(\theta X|\theta Y)$.

It is easy to see that $\forall G \in \mathcal{G}, \forall m \in \mathbb{N}$,

$$\pi_m^{\theta G}(\mathbf{x},\boldsymbol{\beta}) = \pi_m^G(T_{\theta}\mathbf{x},\boldsymbol{\beta}).$$

It follows that $\Omega_{m,\beta}$ is invariant with respect to T.

Suppose now that $F \in \mathbb{F}_m(F_{m-1})$ and let $\Theta(F)$ be a symmetry group of $\mathscr{G}_m(F)$. Then $\forall \theta \in \Theta(F), T_{\theta}^*F = F$. Define

$$\mathscr{L}(F) = \{ L \colon \forall \theta \in \Theta(F) \, T_{\theta}L = L \} \qquad \qquad \mathscr{L} = \mathscr{L}(F) \oplus \mathscr{L}'(F).$$



Figure 5. The phase diagram $\Omega_{m,\beta}$ in the set $U'_0(F_0) \setminus U_7(F)$. Dotted regions represent the restrictions imposed by theorem 3, part (1*b*).

Suppose now that $\mathscr{G}_m(F)$ has $p = \dim \mathscr{L}(F) + 1$ orbits with respect to $\Theta(F)$. Let G_i , i = 0, ..., p be representatives of the orbits.

Claim. $\exists \beta(F): \forall \beta > \beta(F), \Omega_{m,\beta}(\mathscr{G}_m(F))$ exists and is contained in $\mathscr{L}(F)$.

Proof. First note that $\mathscr{L}(F) = \bigcap_{G,\theta} \ker(e_G - e_{\theta G})$. Consider the system of equations

$$\pi_m^G(x,\beta) - \pi_m^{G'}(x,\beta) = 0 \qquad G, G' \in \mathscr{G}_m(F).$$

This system can be separated into two sets of equations:

$$\langle x, e_G - e_{G_i} \rangle \qquad i = 0, \dots, p \qquad G \text{ in ith orbit}$$

$$\pi_m^{G_i}(x, \beta) - \pi_m^{G_0}(x, \beta) = 0 \qquad i = 1, \dots, p.$$

$$(4.3)$$

The solution set of the first system of equations is $\mathscr{L}(F)$, hence one can choose $d = \dim \mathscr{L}(F)$ linearly independent equations of type (4.3). The second set is linearly independent. Hence by the dimension argument one can apply the implicit function theorem.



Figure 6. The phase diagram $\Omega_{m,\beta}$ inside the set U'_{γ} . Dotted regions represent the restrictions imposed by theorem 3, part (1b).

Note that $\mathbb{F}_{m+1}(F) = \{F_{m+1}\}$, and F_{m+1} is isomorphic to F, so the proposition holds by induction for all $s \ge m$. Hence we can generalise assumption 1 to the following.

Assumption 2. Let $k \le m$ and $F \in \mathbb{F}_k$. If E is an r-dimensional face (extremal edge) of F, $\Theta(E) \subset \Theta(F)$ is the symmetry group for E and $\mathscr{L}(E)$ a subspace invariant with respect to $\Theta(E)$, then $\mathscr{G}_m(E)$ has only $s = r+1 - \dim \mathscr{L}(E)$ orbits.

If assumption 2 is satisfied, theorem 3 also holds. An example of a system with additional symmetry is given in § 5.1.

5. Examples

5.1. The Blume-Capel model with additional symmetry

This example shows how the phase diagram is constructed when there is an additional symmetry of the Hamiltonian H_0 .

The Hamiltonian H_0 is the same as in the example of § 2: $S = \{-2, -1, 0, 1, 2\}$. \mathcal{L} is generated by Hamiltonians:

$$L_1 = \sum_{a \in L} s_a \qquad \qquad L_2 = \sum_{a \in L} s_a^2.$$

In the base induced in \mathscr{L} by L_1 , L_2 , one has $e_{(k)} = (k, k^2)$.

It is easy to see that $\forall k, e_{(k)} \in \varepsilon(W_0)$; max W_1 has two faces (figure 7(a)):

H containing points corresponding to (2), (-2), (1), (-1) $v_1(H) = (0, -\frac{1}{3})$

$$F:(1), (-1), (0)$$
 $v_1(F) = 0.$



Figure 7. The phase diagram construction for the Blume-Capel model with the perturbation space generated by s_a and s_a^2 . (a) The projection of max W_1 on \mathcal{L}^* . (b) The phase diagram $\Omega_{m,\beta}$ for m > i(1).

The symmetry group for $\mathscr{G}_1(H)$ is $\{e, f\}$, where *e* is an identity transformation, and $fs_a \equiv -s_a$. This group has two orbits: $\{(-2), (2)\}$ and $\{(-1), (1)\}$. Hence one can apply theorem 3. Obviously order 1 is conclusive as to the existence of the strata. Let order i(1) be the lowest order for which $n_{i(1)}^{(1)}(0) \neq n_{i(1)}^{(0)}(0)$. If order i(1) is examined, one can see that $v_{i(1)}(F) = (0, -1)$.

The phase diagram $\Omega_{s,\beta}$ for $s \ge i(1)$ is presented in figure 7(b).

5.2. The antiferromagnet with stabilisation on the FCC lattice

As the next example let us consider the antiferromagnet on the FCC lattice in \mathbb{R}^3 . L contains four sublattices: \mathbb{Z}^3 , $\frac{1}{2}(e_1 + e_2) + \mathbb{Z}^3$, $\frac{1}{2}(e_1 + e_3) + \mathbb{Z}^3$, $\frac{1}{2}(e_2 + e_3) + \mathbb{Z}^3$. The configuration set S is $\{-1, 1\}$. The Hamiltonian H_0 is given by (cf figure 8(a))

$$H_0 = \sum_{\langle a, b \rangle} s_a s_b$$

where $\langle a, b \rangle$ denotes a pair of nearest neighbours (figure $\delta(a)$).

The reader will find an extensive description of this model in [3]. Here we cite results only, without proofs.



Figure 8. (a) The bonds for the antiferromagnet on the FCC lattice. An arrow shows the nearest-neighbour bond, the broken line, the next-nearest-neighbour bond (perturbation). (b) α pair and β pair of planes.

The ground states of H_0 are as follows. There is a class of completely symmetric ground states. We choose any two sublattices and assign +1 to every point. To every point of the remaining two sublattices we assign -1. This class has six members. Every other ground state is obtained from the completely symmetric ones in the following way. We choose one of the base vectors, say e_1 . Starting from any of the completely symmetric ground states, we flip spins in arbitrary finite numbers of lattice planes perpendicular to the e_1 axis. Then we repeat this flipping in a periodic fashion. It is evident that all ground states differing by the choice of the axis are related by a symmetry of the full Hamiltonian H_0 . We identify these states with G. Henceforth we assume that the axis of changes is the e_1 axis (x axis). Thus every ground state can be viewed as a sequence of antiferromagnetically ordered planes, with no a priori relation between spin orientations in different planes (other than that induced by periodicity).

The system described by the Hamiltonian H_0 obviously has an infinite number of ground states. In order to obtain the system with finite \mathcal{G} , we introduce a stabilisation:

$$H_1(m_1, m_2, m_3) = \sum_{i=1}^{3} \varepsilon_i \sum_{a \in \mathbb{L}} s_a s_{a+m_i e_i}$$

where $\{e_i\}$ is a canonical basis in \mathbb{R}^3 . Then the ground states of $H_0 + H_1$ are those elements of \mathscr{G} which are invariant with respect to translations from $m_1\mathbb{Z} \oplus m_2\mathbb{Z} \oplus m_3\mathbb{Z}$.

Let $G \in \mathcal{G}(H_0)$. Consider a pair of planes perpendicular to the x axis: $\{P, gP\}$, where $g \in \mathbb{Z}^3$ is the translation by vector e_1 . We say that this pair is a β pair if $\forall a \in P$, $G_a = G_{a+e_1}$.

If $G_a = -G_{a+e_1}$, then the pair is an α pair (cf figure 8(b)).

Let L be the period of G in the direction of x. We define

 $p_{\alpha}(G) = (1/L)$ Card{ α pairs with the first plane intersecting { $0, e_1, 2e_1, \ldots, (L-1)e_1$ }}.

 p_{α} is a concentration of α pairs in the ground state G. We define $p_{\beta}(G)$ in a similar fashion. By $\alpha \alpha$ we will denote three planes P, gP, g^2P such that $\{P, gP\}$ and $\{gP, g^2P\}$ are α pairs. Then $p_{\alpha\alpha}(G)$ is a concentration of $\alpha\alpha$ triples.

Let us first study the system without stabilisation. The first four terms of low temperature expansions for any ground state can be expressed in terms of concentrations p in the following way:

$E_1 = 8$	$n_1(0) = 1$
$E_2 = 12$	$n_2(0) = 4$
$E_3 = 16$	$n_3(0) = \frac{29}{2} + p_\beta(G)$
$E_4 = 20$	$n_4^G(0) = 60 + 12p_\beta(G) + 2p_{\beta\beta}(G).$

The expression for the last coefficient differs from the expression obtained by Mackenzie and Young [6]. Our result is in agreement with calculations by Styer [7]. Next we add a one-dimensional perturbation:

$$L(J) = J \sum s_a s_b$$

with the sum over pairs of next-nearest neighbours (cf figure 8(a)). It is easy to see that $e_G = 1 + 2p_\beta(G)$. Hence, for J < 0, the only ground states are those for which



Figure 9. The phase diagram for the antiferromagnet on the FCC lattice with any stabilisation.

 $p_{\beta} = 1$, i.e. the completely symmetric ground states described before. Their class will be denoted by (β).

For J > 0, the concentrations for the ground states satisfy the condition $p_{\beta} = 0$. These ground states are described as follows. Starting from any ground state (β), we flip spins in every other plane. This class has twelve elements and will be denoted as (α).

5.2.1. The convex structure in low orders

Order 1: $\rho_{1,\beta}^G = (-e_G, 1)$. There is one face F parallel to max W_0 . $v_1(F) = 0$. Order 2: $\rho_{2,\beta}^G = (-e_G, 4)$. Again max W_2 has one face F parallel to max W_0 . $v_2(F) = 0$.

Order 3: $\rho_{3,\beta}^G = (-1, \frac{29}{2}) + p_\beta(G)(-2, 1)$. Hence all functionals lie on the same line. There is one face F', $v_3(F') = \frac{1}{2}$, $\tilde{v}_3(F') = \frac{1}{2} \exp(-16\beta)$.

Order 4: $\rho_{4,\beta}^{G} = (-e_{G}, 60 + 12p_{\beta} + 20_{\beta\beta}).$

Let $G \neq (\alpha)$, (β) . Then $p_{\alpha}(G)\rho_{4,\beta}^{(\alpha)} + p_{\beta}(G)\rho_{4,\beta}^{(\beta)} > \rho_{4,\beta}^{G}$. The inequality follows from the fact that $p_{\beta}(G) > p_{\beta\beta}(G)$ if $G \neq (\alpha)$, (β) . Hence max W_4 has only one face \tilde{F} , and no phases other than (α) and (β) belong to $\mathscr{G}_4(\tilde{F})$.

Suppose now that we add to H_0 the stabilisation $H_1(m)$. Then the forms of convex structures described above do not change. We conclude that for β large enough and J small enough, there are only two phases: (α) for larger J and (β) for smaller J. The phase diagram in any order higher than three consists only of the curve separating these two phases (figure 9).

6. Conclusions

An important test for the method presented in this paper is the Pirogov-Sinai case: the number of ground states is d+1. Here the conclusive order is the zero order: by hypothesis, $\{e_G, G \in \mathcal{G}\}$ spans \mathcal{L}^* , and therefore $W = \max W$. Moreover, W has d+1extremal points, so it is a simplex. Hence the phase diagram has one point of (d+1)-phase coexistence, d+1 lines of d-phase coexistence, $\binom{d+1}{2}$ two-dimensional surfaces of d-1-phase coexistence, $\ldots, \binom{d+1}{d}$ regions where the unique phase exists. The rigorous result of [1, 2] is reproduced, as one should expect: the asymptotic phase diagram is asymptotic to the rigorous one and thus has the same topology [3]. The application of the method is restricted by assumption 1 (or 2) and by the requirement that the number of ground states be finite. The first restruction has been discussed in 4.2: we do not know how to avoid it. In the case of an infinite number of ground states some further development seems to be possible, though one loses most of the mathematical machinery used in the proof of theorem 3 (appendix 3). Hence a new approach is needed, different from the one used here.

An algorithm of the method consists of order-by-order construction, using convex polygons. Therefore it makes possible numerical analysis of the phase diagram. Work on this aspect of the problem is in progress.

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Appendix 1. Proof of theorem 1

Let $r = \sum_{j=1}^{m} r_j$, where r_j is the upper limit of the second summation in (2.3). Define a function

$$F: M \times \mathbb{R}^{r} \to M: F_{i}(y, u) = -\langle y, e_{G_{i}} - e_{G_{0}} \rangle + \sum_{j=1}^{m} \sum_{l=1}^{r_{j}} (n_{n_{j,l}}^{G_{i}} - n_{j,l}^{G_{0}}) \exp(-\beta \mu_{j,l}(y)) u_{jl}$$

with $u = (u_{11}, u_{12}, \ldots, u_{1r_1}, \ldots, u_{mr_m}) \in \mathbb{R}^r$.

It is easy to see that F satisfies conditions of the implicit function theorem. Hence there exists an open ball $B(0, q) \subset \mathbb{R}^r$ in which the solution $y: B(0, q) \to M$ of the equation F(y, u) = 0 exists. Moreover, since F is analytic, y is analytic in u. Let α be a multiplicity function, $\alpha: \{(j, l): 1 \le j \le m, 1 \le l \le r_j\} \to \mathbb{N}$, and γ a set of all multiplicity functions. There exists $q_1 > 0$ such that $\forall u \in B(0, q_1)$ we can write y(u) in the following way:

$$y(u) = \sum_{\alpha \in \gamma} y_{\alpha} u^{\alpha}$$
(A1.1)

where $u^{\alpha} = \prod_{j=1}^{m} \prod_{l=1}^{r} u_{jl}^{\alpha(j,l)}$.

Consider now the subset of $B(0, q_1)$:

$$B(0, q_1) \cap \{u \in \mathbb{R}^r : u_{j_1} = \exp[-\beta(E_j + \mu_{j_1}(L))], L \in \mathcal{O}, \beta \in \mathbb{R}_+\}.$$

Let $\beta_m(\mathscr{G}_0)$ be such that $c_m\beta_m(\mathscr{G}_0) > -\ln q_1$, with c_m defining O. For $\beta > \beta(\mathscr{G}_0)$, we define

$$y(z,\beta) = y\{\exp[-\beta E_j + \mu_{j,1}(z)]jl\} \qquad z \in \beta O \cap N.$$

Then $y(z, \beta)$ exists and is the solution of (2.9).

The substitution $u_{jl} = \exp(-\beta E_j + \mu_{j,l}(z))$ in (A1.1) yields

$$y(z, \beta) = \sum_{j=1}^{\infty} y_j(z) \exp(-\beta E_j)$$

where

$$y_j(z) = \sum_{\alpha} y_{\alpha} \exp\left(-\sum_{(n,k)} \alpha(n,k) \mu_{n,k}(z)\right)$$

and the first sum is taken over all multiplicity functions α such that $\sum_{(n,k)} \alpha(n, k) E_n = E_j$.

Appendix 2. Proof of theorem 2

(a) We will first prove statement 1 for the case where $E = \{p\}$.

Let $\Gamma' = \Gamma \setminus \{\rho\}$ and $W' = \operatorname{conv} \Gamma'$. Suppose that $\rho \in \varepsilon(\max W)$. Since W' is convex and closed, then there exists a hyperplane $P \subset \mathbb{R}^{d+1}$ strictly separating ρ from W'. Hence there exist $x_0 \in \mathbb{R}^d$, y_0 , $\alpha \in \mathbb{R}$ such that $P = \{(\eta, t) \in \mathbb{R}^{d+1} : \langle x_0, \eta \rangle + y_0 t = \alpha\}$. Note that $\rho(x_0) > \alpha$ while $\rho'(x_0) < \alpha$ for all $\rho' \in \Gamma'$. Hence $\exists \varepsilon > 0$: $||x - x_0|| < \varepsilon \Longrightarrow x \in \Pi(\rho)$. Thus dim $\Pi(\rho) = d$.

Next, let

$$\Gamma_0 = \bigcup_{\rho \in F} F \qquad \Pi_0(\rho) = \{x: \rho(x) > \rho'(x), \rho' \in \Gamma_0, \rho' \neq \rho\}.$$

Claim. $\forall \tilde{\rho} \notin \Gamma_0, \forall x \in \Pi_0(\rho), \rho(x) > \tilde{\rho}(x).$

Proof. Let $\tilde{\rho} = (\tilde{h}, \tilde{a})$. Consider $\rho_{\lambda} = (\lambda \tilde{h} + (1 - \lambda)h, a_{\lambda}), \lambda \in (0, 1)$, where a_{λ} is such that $(\tilde{h}, a_{\lambda}) \in \max W$. Then there exists F and $\lambda' \in (0, 1)$ such that $\rho, \rho_{\lambda'} \in F$. Obviously $a_{\lambda'} > \lambda' \tilde{a} + (1 - \lambda')a$, since $\tilde{\rho} \notin F$. But then $\forall x \in \Pi_0(\rho)$

$$\rho(x) > \rho_{\lambda'}(x) = \lambda' \langle x, \tilde{h} \rangle + (1 - \lambda') \langle x, h \rangle + a_{\lambda'} > \lambda' \tilde{\rho}(x) + (1 - \lambda') \rho(x) \text{ i.e. } \rho(x) > \tilde{\rho}(x).$$

Finally, note that if $\tilde{\rho} \notin \bigcup_{\rho \in F} \varepsilon(F)$ and $\tilde{\rho} = \sum_{i=1}^{s} \lambda_i \rho_i$, then the condition $\rho(x) > \rho_i(x)$ for all i = 1, ..., s induces the condition $\rho(x) > \tilde{\rho}(x)$ (see the proof of part (b)). This proves (3.3).

Now consider the general case: E has dimension d - r, r < d. Let

 $\rho_0, \rho_1, \ldots, \rho_{d-r} \in \varepsilon(E)$ and $N = \bigcap_{i=1}^{d-r} \ker(h_i - h_0).$

Then $\Pi(E) \subseteq N + x_0$, where x_0 is any solution of the system of equations

$$\langle x, h_i - h_0 \rangle = a_0 - a_i$$
 $i = 1, \ldots, d - r$

We can choose x_0 uniquely by demanding that it is orthogonal to N. Consider the map

$$pr_E: \mathbb{R}^{d+1} \to \mathbb{R}^{d-r+1}: pr_E(\rho) \equiv \tilde{\rho} = (\tilde{h}, a+h(x_0))$$

where \tilde{h} is the restriction of h to N. Obviously, for any ρ in E, $\tilde{\rho} = \tilde{\rho}_0$.

Let $\tilde{W} = pr_E W$. We will denote a phase diagram for a set $\tilde{\Gamma} = pr_E \Gamma$ by $\tilde{\Pi}$, and its strata by $\tilde{\Pi}(\tilde{\Gamma})$. It is not hard to see that $\tilde{\rho}_0 \in \varepsilon(\max W)$. Now we apply the case $E = \{\rho\}$ to \tilde{W} . Since $\Pi(E) \subset N + x_0$, the bounds (3.3) on $\tilde{\Pi}(\tilde{\rho}_0)$ give the bounds on $\Pi(E)$.

(b) Let $\rho = \sum_{i=1}^{s} \lambda_i \rho_i$. Define

$$N = \{x: \rho_i(x) = \rho_i(x), i = 1, ..., s\}.$$

Then

$$\forall x \in N, \rho(x) = \rho_i(x)$$
 for all *i*

$$\forall x \notin N \exists i: \rho(x) < \rho_i(x).$$

Hence, $\Pi(\rho) = \Pi(\{\rho_1, ..., \rho_s\}).$

(c)
$$\rho \notin \max W \Longrightarrow \exists (h, t) \in \max W : (h, t) > \rho$$
. Hence $\forall x \in \mathbb{R}^{d+1}$,

$$\langle x, h \rangle + t > \rho(x).$$

Let $(h, t) = \sum_{i=1}^{s} \lambda_i \rho_i$. It is easy to see that $\forall x \exists \rho_i: \rho(x) < \rho_i(x)$. Thus $\Pi(\rho) = \emptyset$.

Appendix 3. Proof of theorem 3

Now we present the proof of theorem 3. Proofs of lemmas cited in this section can be found in [8].

The general strategy of the proof is based on the following observation. Suppose that \mathscr{G} is a subset of \mathscr{G} and let U be an open set contained in $\bigcup_{G \in \mathscr{G}} \Omega_{m,\beta}(G)$. Define $\tilde{\Omega}_{m,\beta}$ as a phase diagram for phases in \mathscr{G}' (i.e. with other phases neglected). Then

$$\Omega_{m,\beta} \cap U = \tilde{\Omega}_{m,\beta} \cap U.$$

We will first find the covering of βO with the family of sets such that in each of these sets $\Omega_{m,\beta}$ is described by the phase diagram $\tilde{\Omega}_{m,\beta}$ defined for some subset \mathscr{G}' of \mathscr{G} .

Let $\{F_0, \ldots, F_m\}$ be a sequence of faces as in (iii) of § 4.1. With every element of this sequence we associate a set

$$U_k(F_k) = B[\tilde{v}_k(F_k,\beta), c_k(F_k) \exp(-\beta E_{k+1})] \quad (\text{open ball}).$$

Constants $c_k(F_k)$ will be specified later in this section. Slightly abusing this notation, we set $U_0(F_0) \equiv \beta O$. We will define $U_k(F_k)$ in four steps, using an induction in the order k.

Suppose that $U_{k-1}(F_{k-1})$ is defined. Then we show that:

(i) in $U_{k-1}(F_{k-1})$, the function π_m^G is approximated by $\rho_{k,\beta}^G(F_{k-1})$, so that their difference is of order $\exp(-\beta E_k)$;

(ii) in $U_{k-1}(F_{k-1})$, the phase diagram is given by phases in $\mathcal{G}_{k-1}(F_{k-1})$ (i.e. neglecting other phases);

(iii) if $\rho_{k,\beta}^G(F_{k-1}) \in \text{int } F_k$ for some $F_k \in \mathbb{F}_k(F_{k-1})$, then $\Omega_{m,\beta}(G)$ is contained in a ball with radius $r = O(\exp(-\beta E_{k+1}))$;

(iv) in step (iv) we define $U_k(F_k)$, $F_k \in \mathbb{F}_k(F_{k-1})$.

(i) Lemma A3.1. Let $F \in \mathbb{F}_m$ and $\{F_0, F_1, \ldots, F\}$ be the family of faces corresponding to F (cf (iii) of § 4.1). For $0 \le k \le m$ and c > 0, we define

$$B(F_k, c) = \{x \colon ||x - \tilde{v}_k(F_k, \beta)|| \le c \exp(-\beta E_k)\}.$$

Then $\exists \alpha_m > 0$: $\forall G \in \mathscr{G}_m(F) \exists d_k(G) > 0$: $\forall \beta > 0, \forall x \in B(F_k, c)$:

$$\left|\rho_{m,\beta}^{G}(F,x) - \pi_{m}^{G}(x,\beta)\right| \leq d_{k}(G) \exp[-\beta(E_{k} + \alpha_{m})].$$
(A3.1)

In zero order the estimate is not as good, since we demand that (A3.1) holds on $\beta \overline{O}$. Hence

$$||x|| \leq \beta c.$$

Then

$$\left|\rho_{m,\beta}^{G}(F,x)-\pi_{m}^{G}(x,\beta)\right| \leq \beta d_{0}(G) \exp(-\beta \alpha_{0}).$$

The next lemma is an immediate consequence of lemma A3.1.

Lemma A3.2. Let $\mathscr{G}_0 \equiv \{G_0, G_1, \ldots, G_s\} \subset \mathscr{G}_m(F)$ be such that $\{e_{G_i}, i = 1, \ldots, s\}$ is linearly independent. Consider the solutions $y(z, \beta)(\beta > \beta_m(\mathscr{G}_0))$ of the system of equations (2.9) (cf theorem 1) and $y_0(z, \beta)$ of the system

$$\rho_{m,\beta}^{G_i}(F, y, z) = \rho_{m,\beta}^{G_0}(F, y, z) \qquad i = 1, \dots, s.$$
(A3.2)

Here $z \in \bigcap_{i=1}^{s} \ker(e_{G_i} - e_{G_0})$.

Let $B(F_k, c)$ be in lemma A3.1. Then $\forall k \leq m, \forall c > 0, \exists a_k(c)$ such that if $\beta > \beta_m(\mathscr{G}_0)$ and $(y_0, z) \in B(F_k, c)$, then

$$||y(z, \beta) - y_0(z, \beta)|| < a_k(c) \exp(-\beta E_{k+1}).$$
 (A3.3)

Lemma A3.2 states that inside $B(F_k, c)$, the solutions of (2.9) and (A3.2) are close to one another; their distance is of order $\exp(-\beta E_{k+1})$.

(ii) Lemma A3.3. Let $F \in \mathbb{F}_k$. Then $\exists c > 0$, $\exists \gamma(c) > 0$, $\exists \beta_k(F): \forall \beta > \beta_k(F)$, $\forall \tilde{G} \notin \mathscr{G}_k(F), \forall x \in B[\tilde{v}_k(F_k, \beta), c \exp(-\beta E_k)]$:

$$\rho_{k,\beta}^{G}(F,x) - \rho_{k,\beta}^{G}(F,x) > \gamma(c) \exp(-\beta E_{k})$$
(A3.4)

for some $G \in \mathscr{G}_k(F_k)$. Hence $U_k(F_k) \subset \bigcup \Omega_{m,\beta}(G)$ with the union over elements of $\mathscr{G}_k(F_k)$.

(iii) Lemma A3.4. Let $F \in \mathbb{F}_m(F')$ and G be such that $\rho_{m,\beta}^G(F') \in \text{int } F$. Then $\forall s \ge m \exists \beta_s(G): \forall \beta > \beta_s(G), \exists r_s > 0$:

$$\Omega_{s,\beta}(G) \subset B[\tilde{v}_m(F,\beta), r_s \exp(-\beta E_{m+1})].$$
(A3.5)

(iv) The definition of sets $U_k(F_k)$. Suppose that $F_k \in \mathbb{F}_k$. Define $r_k(F_k)$ to be the smallest number such that $U'_k(F_k) \equiv B[\tilde{v}_k, (F_k, \beta), r_k(F_k) \exp(-\beta E_{k+1})]$ contains sets described below.

(1) $\Omega_{m,\beta}(G)$ if $\rho_{k,\beta}^G(F_{k-1}) \in \text{int } F_k$.

(2) If F has more than d+1 extremal points, let us consider any d-element collection of pairs $\{(G_{1,i}, G_{2,i}), i=1, \ldots, d\}$, where any phase corresponds to an extremal point of F, and some elements in different pairs may be the same. For any pair $(G_{1,i}, G_{2,i})$, let N_i be the solution set for the equation

$$\rho_{k,\beta}^{G_{1},i}(F_{k-1},x) = \rho_{k,\beta}^{G_{2},i}(F_{k-1},x).$$

Define

$$S_i = \{x: \operatorname{dist}(x, N_i) \leq a_i \exp(-\beta E_{k+1})\}$$

where a_i is given by lemma A3.2 applied to the set $\{G_{1,i}, G_{2,i}\}$. It is easy to see that for any such *d*-element collection of pairs, $\bigcap_{i=1}^{d} S_i$ is contained in a ball with radius $r = O(\exp(-\beta E_{k+1}))$. We require $r_k(F_k)$ to be such that for any collection of pairs as described above $\bigcap_{i=1}^{d} S_i \subset U'_k(F_k)$. If F_k contains exactly d+1 functionals $\rho_{k+1}^G(F_{k-1})$, then we set $U_k = \emptyset$.

Example. The construction of the set $U_0(F_0)$ for our example is shown in figure 10. We choose the collection of pairs $\{(-5), (3)\}$, $\{(-3), (3)\}$. The thin full lines represent sets N((-5), (-3)) and N((3), (-3)). The dotted lines show regions restricted by lemma A3.2. The dotted region is $S((-5), (-3)) \cap S((3), (-3))$.

Now let $\gamma > 0$ be any fixed number. We define $c_k(F_k) = r_k(F_k) + \gamma$. In the applications γ will be chosen in such a way that its value comprises a small fraction of any $r_k(F_k)$, $k \le m$.

Let $\beta_U(\gamma)$ be such that if $\beta > \beta_U(\gamma)$, then the following conditions hold for all $k \leq m$:

- (i) $U_k(F_k) \subset U'_{k-1}(F_{k-1})$
- (ii) $U_k(F_k) \subset B(F_k, c)$ (with c defined by lemma A3.3) (A3.6)
- (iii) $\forall F, F' \in \mathbb{F}_k(F_{k-1}), U_k(F) \cap U_k(F') = \emptyset.$



Figure 10. The construction of the set $U_0(F_0)$ (broken circle). The thin full lines are N((-3), (-5)) and N((-3), (3)). The dotted lines represent sets S((-3), (-5)) and S((-3), (3)).

If $\beta > \beta_U(\gamma)$, we can define a covering of βO by a family of sets:

 $\{U_k(F_k), F_k \in \mathbb{F}_k, k = 0, \ldots, m\}.$

Next, let us consider a covering of $U_k(F_k)$ by the family of sets defined in the following way. Let $\mathscr{G} \subset \mathscr{G}_k(F_k)$. We say that \mathscr{G}' is normal if

(i) $|\mathcal{G}'| = d + 1;$

(ii) all elements of \mathscr{G}' correspond to extremal points of F_k ;

(iii) $O'(F_k, \mathscr{G}') \equiv \inf[U_{k-1}(F_{k-1}) \cap \bigcup_{G \in \mathscr{G}'} \Pi(F, G)]$ is connected.

For any normal subfamily of $\mathscr{G}_k(F_k)$, we define

$$O(F_k, \mathscr{G}') = \cap \{x \in O': \operatorname{dist}(x, \Pi(F_k, G')) \leq a_k(G') \exp(-\beta E_{k+1})\} \setminus U'_k(F_k).$$

The intersection here is over all $G' \notin \mathscr{G}'$ which have common boundaries with some $G \in \mathscr{G}'$, and $a_k(G')$ is given by lemma A3.2 for the family $\mathscr{G}_0 \equiv \{G, G'\}$.

Obviously the family of sets

 $\{O(F, \mathcal{G}'), F \in \mathbb{F}_k, \mathcal{G}' \text{ normal subset of } \mathcal{G}_k(F), k = 0, \dots, m\}$

covers $\beta \overline{O}$ (since *m* is the conclusive order).

Example. In our example the covering is as follows. Only $U_0(F_0)$ and $U_7(F)$ are non-empty. The normal subfamilies of \mathscr{G} are: {(5), (3), (-3)}, {(3), (-5), (-3)}, {(-5), (-3)}, {(-5), (3), (5)}. The set $O(F_0, \{(5), (3), (-3)\})$ is dotted in figure 11(*a*). Note that $\mathscr{G}_1(H)$, $\mathscr{G}_1(G)$, $\mathscr{G}_1(H')$ and $\mathscr{G}_1(G')$ are normal.

The normal subfamilies of $\mathscr{G}_1(F)$ are $\{(-1), (3), (1)\}, \{(3), (1), (-3)\}, \{(1), (-3), (-1)\}$ and $\{(-3), (-1), (1)\}$.

The set $O(F; \{(-1), (3), (1)\})$ is dotted in figure 11(b).

Finally both $\mathscr{G}_7(F_1)$ and $\mathscr{G}_7(F_2)$ are normal.

In the presence of symmetries we modify the definition of sets $O(F\mathscr{G}')$ as follows:

$$O(F, \mathscr{G}') = O'(F, \mathscr{G}') \setminus \Delta'$$



Figure 11. The elements of covering of βO : (a) $O(F_0, \{(5), (3), (-3)\})$; (b) $O(F, \{(-1), (3), (1)\})$. The broken lines separate domains for different phases. The dotted lines show restrictions imposed by theorem 3, part (1b).

where

$$\Delta' = \{x \in \mathcal{O}'(F, \mathscr{G}') : \operatorname{dist}(x, \Pi(F_k, G') < a_k(G, G') \\ \times \exp(-\beta E_{k+1}) \text{ unless } G' = \theta G, \ \theta \in \Theta(F)\}$$

Here $a_k(G, G')$ is given by lemma A3.2.

A3.1. The proof of theorem 3

(1) Suppose that $F \in \mathbb{F}_k (k \leq m)$. Let $Z = U'_k(F) \setminus \bigcup U_{k+1}(F')$, with the union over faces in $\mathbb{F}_{k+1}(F)$. The family of sets $\{O(F_k, \mathscr{G}'), \mathscr{G}' \text{ normal in } \mathscr{G}_k(F_k)\}$ covers Z.

Claim. $\Omega_{m,\beta} \cap O(F, \mathscr{G}')$ is diffeomorphic to $\Pi(F) \cap O(F, \mathscr{G}')$.

Proof. Suppose that the elements of \mathcal{G}' are ordered:

$$\mathscr{G}' = \{G_0, G_1, \ldots, G_d\}.$$

We define the map

$$\pi_F(\beta): \mathscr{L} \to \mathbb{R}^{d+1}/\Delta: \pi_F(\beta, x)_i = [\pi_m^{G_i}(x, \beta)] \qquad i = 1, \ldots, d.$$

Here Δ is a diagonal: $\Delta = \{y \in \mathbb{R}^{d+1} : y_1 = y_2 = \ldots = y_d\}$. There exists $\beta_{\mathscr{G}}$ such that if $\beta > \beta_{\mathscr{G}}$, then $\pi_F(\beta)$ is a local diffeomorphism on β O. In addition, we have a map

$$\rho_F(\boldsymbol{\beta}): \mathcal{L} \to \mathbb{R}^{d+1} / \Delta: \rho_F(\boldsymbol{\beta}, x)_i = [\rho_{k,\boldsymbol{\beta}}^G(F_{k-1}, x)].$$

This map is also a diffeomorphism. By the definition of $O(F, \mathscr{G})$, the claim follows.

Hence, inside $O(F, \mathscr{G})$ there is an obvious correspondence between strata of $\Pi(F)$ and strata of $\Omega_{m,\beta}$. This correspondence obviously extends to the whole set Z.

The bound on the distance of corresponding strata can be easily established by applying lemma A3.2 to any \mathscr{G}_0 for which $\Omega_{m,\beta}(\mathscr{G}_0)$ is non-empty. Here $a(F_k)$ is a maximum over $a_k(\mathscr{G}_0)$ for all such $\mathscr{G}_0(a_k(\mathscr{G}_0))$ is provided by lemma (A3.2).

(2) First note that due to assumption 1, if E is an *r*-dimensional face of max $W_{k+1}(F_k)(r < d)$, then for any $s \ge k+1$, E is an *r*-dimensional face of max $W_{s+1}(F_s)$. The same holds for a *d*-dimensional face F if F contains only d+1 functionals ρ_k^G . Let k be the lowest order in which E is an extremal element of max $W_k(F_{k-1})$. By theorem 3, there exists a stratum $\Pi(F_{k-1}, \mathscr{G}_k(E))$ of $\Pi(F_{k-1})$ which corresponds to E. By part (1) of the proof, there is a stratum $\Omega_{m,\beta}(\mathscr{G}_k(E))$ which corresponds to $\Pi(F_{k-1}, \mathscr{G}_k(E))$.

If E contains more than d+1 affine functionals, then in general there is no correspondence. However, in higher orders E is replaced by max $W_{k+1}(E)$, and we apply part 1 of the theorem to the set $U'_k(E)$.

With the change of order m we have to redefine sets $U_k(F_k)$ and sets $O(F_k, \mathscr{G}')$ since there will be a change in estimation (A3.3). By lowering temperature we can compensate for these changes, so the above considerations hold for a construction of $\Omega_{s,\beta}$ with $s \ge m$.

The value of β_m is determined as the maximum of the following:

(i) β_U(γ) given as the condition that the sets U_k(F_k) do not intersect (cf (A3.6));
(ii) β_G for all F∈ F_k, k = 0,..., m (the existence of local diffeomorphism as given in the claim in part (1) of the proof);

(iii) $\beta_m(\{G, G'\})$ (as in theorem 1) for all pairs of phases, corresponding to extremal points which share a one-dimensional extremal edge. The condition $\beta > \beta_m < \{G, G'\}$) assures the existence of the stratum $\Omega_{m,\beta}(G, G')$.

Obviously β_m is finite.

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