*Journal of Statistical Physics, Vol. 52, No. 1/2, 1988*

# Phase Diagrams of Lattice Systems with Residual Entropy

**Christian Gruber**[1] **and András Sütő**[2,3]

*Received July 6, 1987; revision received March 16, 1988*

We introduce an equivalence relation on the family of ground states and generalize the Peierls and Pirogov–Sinai theory of phase transitions to systems with residual entropy. The idea consists in the replacement of the periodic ground states by equivalence classes together with an entropy factor. We apply these results to discuss the phase diagrams of diluted spin-1/2 systems.

**KEY WORDS:** Phase diagrams; first-order phase transitions; frustration; residual entropy; Pirogov–Sinai theory; spin-1 Ising models.

## 1. INTRODUCTION

The standard methods to prove the existence of phase transitions and to analyze the low-temperature phase diagrams are restricted either to ferromagnetic systems (Peierls' argument),[1,2] to systems with a finite number of periodic ground states (Pirogov–Sinai theory,[3] Slawny's asymptotic method[4]), or to systems with special properties (reflection positivity).

In the case of systems with an infinite number of periodic ground states no general results are known, although several models have been investigated. It appears that those systems, in particular the so-called frustrated models,[5] present a large variety of phase diagrams. There are many systems (such as the ANNNI model,[6]) with an infinite number of periodic ground states but vanishing residual entropy (entropy per site). They display very complicated phase diagrams, but most of the results

[1] Institut de Physique Théorique, Ecole Polytechnique Fédérale de Lausanne, PHB-Ecublens, CH-1015 Lausanne, Switzerland.

[2] Institut de Physique Théorique, Université de Lausanne, BSP, CH-1015 Lausanne, Switzerland.

[3] On leave of absence from the Central Research Institute for Physics, Budapest, Hungary.



0022-4715/88/0700-0113$06.00/0 

have been obtained by means of numerical analysis and are not always very convincing. In another class of models with interesting physical applications the number of ground states is so large that the system has finite residual entropy. These are sometimes called "superdegenerate" models[7–9]; again, most of the results are obtained from numerical analysis and it seems that even their authors are not entirely convinced.

A new approach has been recently developed[8,9] to study models with finite residual entropy. The basic idea is to introduce a concept of "restricted ensemble" and to replace the ground states in Pirogov–Sinai (PS) theory by measures over restricted ensembles. The applications, however, have been limited mainly to systems of the Widom–Rowlinson type, the interest of the authors being to prove the coexistence of the disordered phase with the ordered one, and furthermore a diluteness hypothesis was necessary. This hypothesis is not easy to check and no general condition on the interactions is known that would ensure the validity of this hypothesis.

In this paper, we extend the usual Peierls and PS theories to models with finite residual entropy in the following manner. We first introduce an equivalence relation among the ground-state configurations (more precisely, among defect-free configurations) and we decompose the family of ground states into equivalence classes. We then expect, and prove, that at low temperatures each of the equivalence classes describes a possible equilibrium phase of the system. The idea of the proof is to replace the ground states in Peierls or PS theory by equivalence classes, together with an entropy factor that takes into account the degeneracy of the class.

The equivalence relation that we introduce appears natural if one looks at standard models such as Ising models with nn magnetic and nnn nonmagnetic interactions. Indeed, for certain values of the chemical potential the ground states are determined by the nonmagnetic interaction and at each occupied site the spin is arbitrarily $+1$ or $-1$. Therefore, in this case, it is natural to define the equivalence classes in such a way that two ground states that differ locally only by the spin orientation will belong to the same class; one then expects that the same picture will occur at low temperatures (as is the case for the Griffiths model[10]).

This discussion leads us to define the equivalence relation in Section 3 in such a manner that two ground states that coincide on some (sufficiently large) cube will belong to the same class.

Although it seems to us that the existence of more than one equivalence class should be sufficient to establish the existence of a phase transition, and to conclude that there exist at low temperatures at least as many phases as the number of classes, we are forced to introduce further conditions. We first need a completeness condition (analogous to the idea of "reduced" models introduced in ref. 4 for ferromagnetic systems).

Furthermore, the systems to which our discussion applies at present are either symmetric (Section 4), i.e., all equivalence classes are related by symmetries of the interactions, or factorizable (Section 5). In the factorizable case, the phase transitions are not necessarily associated with spontaneously broken symmetry. In Section 6, we apply our results to discuss the phase diagrams of different spin-1 models.

## 2. BASIC DEFINITIONS AND PROPERTIES

Let $\mathbb{L} = \mathbb{Z}^\nu$ be a $\nu$-dimensional simple cubic lattice. With each site $i \in \mathbb{L}$ is associated a finite set $\Omega_i \cong \Omega_0$, $x(i) \in \Omega_i$ being the "value of the spin" at $i$. The configuration space is $\Omega = \Omega_0^{\mathbb{L}}$. For any $x = \{x(i)\}_{i \in \mathbb{L}} \in \Omega$ and any $A \subset \mathbb{L}$, $x_A = \{x(i) \mid i \in A\} \in \Omega_0^A = \Omega_A$. The system is defined by the formal Hamiltonian

$$H(x) = \sum_B \phi_B(x) \tag{1}$$

where the *interaction* $\phi_B$, with $B$ a finite subset of $\mathbb{L}$, is a real-valued function on $\Omega$ such that

$$\phi_B(x) = \phi_B(x_B)$$

We assume that the interaction has a *finite range* $R$, i.e., $\phi_B(x) = 0$ if

$$\operatorname{diam} B = \max_{i,j \in B} \|i - j\| > R$$

where $\|i\| = \max_{1 \leqslant k \leqslant \nu} |i_k|$. Therefore, the *relative Hamiltonian*

$$H(x \mid y) = \sum_B [\phi_B(x) - \phi_B(y)] \tag{2}$$

is well defined for any $x$, $y \in \Omega$ such that $x = y$ a.e. The interaction is assumed to be *periodic*, i.e., there is a subgroup $\hat{\mathbb{L}}$ of finite index of $\mathbb{L}$ such that $\phi_B(x) = \phi_{B+t}(T_t x)$ with $(T_t x)(i) = x(i - t)$, for any $B$, $x$ and any $t \in \hat{\mathbb{L}}$.

The main assumptions concerning the interaction are the following:

C1. $\Phi = \{\phi_B\}$ is an *m-potential*,[4] i.e., the following set $G$ is nonempty:

$$G = \{s \in \Omega \mid \phi_B(s) = \min_{y \in \Omega} \phi_B(y), \forall B \subset \mathbb{L}\} \tag{3}$$

C2. Take any cube $q$ with vertices on $\mathbb{L}$ and edges parallel to the coordinate axes, i.e.,

$$q = \{i \in \mathbb{L} \mid \|i - j\| \leqslant N/2\} \tag{4}$$

where $j \in \mathbb{L}$ if $N$ is even, and $j \in \mathbb{L}^*$, the dual of $\mathbb{L}$, if $N$ is odd. Then, for any $x \in \Omega$ such that $\phi_B(x) = \min_{y \in \Omega} \phi_B(y)$ whenever $B \cap q \neq \varnothing$, there exists some $s \in G$ such that $s_q = x_q$.

*Remark* 1. Any $s \in G$ is a *ground state* in the usual sense, that is, $H(x \mid s) \geqslant 0$ if $x = s$ a.e. Furthermore, $s$ minimizes each $\phi_B$ separately, which means that there is no competition among the $\phi_B$'s. This does not imply that models with competing interactions or frustration are excluded from the discussion: In general, $\{\phi_B\}$ is different from the set of interactions $\{J_b\}$ usually introduced for spin systems. This latter involves external fields, nearest and next-nearest neighbor interactions,..., and may exhibit frustration. It is only by suitably regrouping the bonds, i.e.,

$$\phi_B = \sum_{b: \operatorname{supp} b \subset B} J_b / \# \{B' \mid B' \supset \operatorname{supp} b\}$$

that an $m$-potential arises. An example is shown in Section 6. In "natural" models with finite-range interactions such a regrouping is usually possible. Note that the original and regrouped interactions are *equivalent* in the sense that they give rise to the same relative Hamiltonian,

$$H_\Phi(x \mid y) = H_J(x \mid y)$$

and therefore the ground states and Gibbs states are the same.

*Remark* 2. Another way to characterize the set $G$ [Eq. (3)] is to introduce the notion of a *defect-free configuration* (DFC). Let us consider any potential $\Phi$; the configuration $x \in \Omega$ is defect-free if for any finite $\Lambda \subset \mathbb{L}$ there exists a finite $\Lambda' \supset \Lambda$ and some $x' \in \Omega$ such that $x'_\Lambda = x_\Lambda$ and

$$\sum_{B \subset \Lambda'} \phi_B(x') = \min_{y \in \Omega} \sum_{B \subset \Lambda'} \phi_B(y)$$

If $\Omega_0$ is finite, the family of DFC is nonempty and for finite-range potentials any DFC is a ground state. Intuitively, a DFC is a ground state that does not contain an infinite defect surface stabilized by some boundary condition at infinity. It is conjectured that periodic ground states, if they exist, are DFC. It is clear that *if $\Phi$ is an m-potential, then $G$ coincides with the set of DFC.*

*Remark* 3. Since DFC are not defined by means of the relative Hamiltonian, it is not obvious whether equivalent interactions lead to the same family of DFC. Therefore, if $\Phi$ and $\Phi'$ are equivalent $m$-potentials, it is not clear whether $G[\Phi] = G[\Phi']$. In any case, both $G[\Phi]$ and $G[\Phi']$ contain all the periodic ground states and their pointwise limits.[4]

Moreover, if $\Phi$ is an $m$-potential and $\Phi'$ is obtained by regrouping the interactions $\phi_B$, then $\phi'_{B'}(x)$ and $\phi_B(x)$ are minimal at the same time, and $G[\Phi]=G[\Phi']$.

*Remark* 4. Condition C2 excludes potentials like Pecherski's counterexample[4]: $\mathbb{L}=\mathbb{Z}^2$, $\Omega_0=\{0,1\}$, $G$ defined by the condition that on each unit square $q$, $s_q$ is one the following configurations:

$$\begin{pmatrix}0&0\\0&0\end{pmatrix}\ \begin{pmatrix}1&1\\1&1\end{pmatrix}\ \begin{pmatrix}1&1\\0&1\end{pmatrix}\ \begin{pmatrix}0&0\\1&1\end{pmatrix}\ \begin{pmatrix}1&0\\1&0\end{pmatrix}\ \begin{pmatrix}0&1\\0&0\end{pmatrix}$$

*Remark* 5. The set $G$ is invariant under the symmetry group $\mathcal{G}$ of the Hamiltonian.

*Remark* 6. The relative Hamiltonian is unchanged if $\phi_B(x)$ is replaced by $\phi_B(x)-\min_y \phi_B(y)$. In the forthcoming discussion we will therefore suppose that

$$\phi_B(x)\geqslant 0 \qquad \text{and} \qquad \phi_B(s)=0 \quad \text{if} \quad s\in G$$

It follows from our assumptions, $|\Omega_0|<\infty$ and finite-range interactions, that

$$\inf_B \inf_{x:\,\phi_B(x)>0} \phi_B(x)=\Delta>0 \tag{5}$$

In the following, we call an $N$-cube any cube of diameter ($=$side) $N$, as given by Eq. (4). Let $Q$ denote the family of all $N$-cubes with fixed $N\geqslant R$. With any $x\in\Omega$ we associate

$$Q_x=\{q\in Q \mid x_q\neq s_q, \forall s\in G\} \tag{6}$$

and $|Q_x|$ denotes the number of cubes in $Q_x$.

We then have the following result:

**Proposition 1.** For any $s\in G$ and $x\in\Omega$ such that $x=s$ a.e.,

$$H(x\mid s)\geqslant C\,|Q_x| \tag{7}$$

with $C=\Delta/(N+1)^\nu$.

*Proof.* Let us regroup the interactions in $N$-cubes:

$$\phi_q(x)=\sum_{B\subset q}\phi_B(x)/n_B$$

where $n_B$ is the number of $N$-cubes containing $B$. Since $\phi_B \geqslant 0$ and $|q| = (N+1)^\nu$, one gets

$$\phi_q(x) \geqslant (N+1)^{-\nu} \max_{B \subset q} \phi_B(x)$$

Using the independence of $H(x \mid s)$ from the regroupment and $\phi_B(s) = 0$,

$$H(x \mid s) = \sum_{q:\, \phi_q(x) > 0} \phi_q(x) \geqslant |Q_x| \, \Delta/(N+1)^\nu$$

*Remark.* Inequality (7) looks like Peierls' condition. It would, however, be misleading to give it this name, since in all the cases we are going to discuss $G$ is an infinite set, and the inequality (7) does not guarantee that $H(x \mid s)$ increases if the domain where $x$ differs from $s$ increases. In the next section we introduce further restrictions, necessary to prove the existence of a phase transition.

## 3. EQUIVALENCE RELATION

If $G$ is finite, the phase diagram at low temperatures is described by the theory of Pirogov and Sinai (PS)[3] together with the low-temperature expansion of Slawny.[4] To extend the PS theory to the case of infinite $G$, we introduce an equivalence relation on $G$ in such a way that the equivalence classes play the role of the ground states in the PS theory.

We say that $s$, $s' \in G$ are $N$-equivalent if there exists a finite sequence $q_1, \ldots, q_n$ of $N$-cubes and $s^1, \ldots, s^{n-1} \in G$ such that $s_{q_1} = s^1_{q_1}$, $s^1_{q_2} = s^2_{q_2}, \ldots, s^{n-1}_{q_n} = s'_{q_n}$; for $n = 1$ this means $s_q = s'_q$ for some $N$-cube $q$.

Consider $P_N = \{G_p^{(N)}\}_{p=1}^{d(N)}$, the partition of $G$ into $N$-equivalence classes. If $N' > N$, then $s \sim^{N'} s'$ implies $s \sim^{N} s'$, so that the partition $P_{N'}$ is finer than $P_N$, i.e., for any $p'$ there is a unique $p$ such that $G_{p'}^{(N')} \subseteq G_p^{(N)}$. It follows that $d(N') \geqslant d(N)$, where equality holds if and only if $P_{N'} = P_N$. Let

$$N_0 = \begin{cases} \min\{N \mid d(N') = d(N) \text{ for all } N' > N\} & \text{if this set is nonempty} \\ +\infty & \text{otherwise} \end{cases} \tag{8}$$

We say that $s$ and $s'$ in $G$ are *equivalent*, $s \sim s'$, if $s \sim^N s'$ for any $N$. The number of classes $d = d(N_0)$ is called the *degeneracy of* $G$, and $P = P(N) = \{G_p\}_{p=1}^{d}$ for $N \geqslant N_0$. Note that $N_0$ is finite if and only if $d$ is finite. In fact, $\log d \leqslant (N_0+1)^\nu \log |\Omega_0|$. In the following, we consider only systems such that $N_0$ is finite.

**Definition.** Let $q$ be an $N$-cube, with $N \geqslant N_0$, and $x \in \Omega$. We call $x_q$ (and also $q$) *p-correct* if $x_q = s_q$ for some $s \in G_p$. We call $x_q$ (and $q$) *correct*

if it is $p$-correct for some $p$. The family of cubes $Q_x$ [Eq. (6)] is thus the family of noncorrect cubes.

*Properties*

*Property 1.* Any $s \in G$ can be classified by looking at $s_q$ where $q$ is any $N_0$-cube.

*Property 2.* We have the following characterisation of the equivalence: We say that $q \subset \mathbb{L}$ is an octant if for some $j = (j_1, ..., j_v) \in \mathbb{L}$,

$$q = \{i \in \mathbb{L} \mid i_1 R_1 j_1, ..., i_v R_v j_v\}$$

where $R_k$ is one of the relations $\leqslant$ and $\geqslant$. Then, $s \sim s'$ if and only if there exist octants $q_1, q_2, ..., q_n$ and DFC $s^0 = s$, $s^1$, $s^2, ..., s^{n-1}$, $s^n = s'$ such that $s^{i-1}_{q_i} = s^i_{q_i}$, $i = 1, ..., n$. This comes from the fact that the limit of increasing sequences of $N$-cubes contains an octant.

*Property 3.* $G$ is finite if and only if every $s$ in $G$ is periodic, and in this case each class consists of a single configuration: this is the situation of the PS theory. Indeed, if $G$ is finite, the periodicity of the interaction implies that every $s \in G$ is periodic. Now let $G$ be infinite and suppose that all the configurations in $G$ are periodic. Then $G$ contains an infinite sequence of periodic ground states $\{s^\alpha\}$ with increasing period which converges pointwise, i.e., there exists a configuration $s$ such that for any $i \in \mathbb{L}$, $s^\alpha(i) = s(i)$ if $\alpha$ is large enough. Now, $s \in G$, since for any $B$, $\phi_B(s) = \phi_B(s^\alpha) = 0$ for suitably large $\alpha$. According to the assumption, $s$ is periodic: there is a subgroup $\mathbb{L}(s)$ of $\mathbb{L}$ such that $s(i+t) = s(i)$, $t \in \mathbb{L}(s)$. Given $\alpha$, consider the point $i(\alpha)$ in the positive octant such that $\|i(\alpha)\| = \min_i \{\|i\| \mid s^\alpha(i) \neq s(i)\}$. Due to the convergence, $\|i(\alpha)\| \to \infty$ as $\alpha \to \infty$. Let us define a new sequence of periodic ground states $\{\tilde{s}^\alpha = T_{t(\alpha)} s^\alpha\}$, where $t(\alpha) \in \mathbb{L}(s) \cap \hat{\mathbb{L}}$, $(i(\alpha) - t(\alpha))_k \geqslant 0$, and

$$\|i(\alpha) - t(\alpha)\| = \min\{\|i(\alpha) - t\| \mid t \in \mathbb{L}(s) \cap \hat{\mathbb{L}},\ t_k \leqslant i(\alpha)_k\}$$

There exists a subsequence of $\{\tilde{s}^\alpha\}$ that converges to a limit $s'$ such that $s'$ coincides with the (periodic) $s$ on one octant and $s'_i \neq s_i$ for some $i$ at a finite distance of the origin. Therefore $s'$ cannot be periodic.

*Property 4.* Let $g \in \mathcal{G}$ be any symmetry of the Hamiltonian; then $gG_p = G_{p'}$. If the number of classes is finite, then each class is invariant under a subgroup of $\hat{\mathbb{L}}$ with finite index. For systems with a finite number of classes we thus have a scheme analogous to PS, with classes instead of ground states.

*Property 5.* Let $N > N_0$ and $x \in \Omega$ such that the $N$-cubes $q$ and $q'$ are respectively $p$- and $p'$-correct with $p \neq p'$. Take any chain of $N$-cubes

$\{q_i\}_{i=1}^n$ such that $q_1 = q$, $q_n = q'$, and $q_{i+1} = q_i + t_i$, $\|t_i\| = 1$. Then there exists some $B \subset \mathbb{L}$ with the properties $B \cap (\cup q_i) \neq \varnothing$ and $\phi_B(x) > 0$. Indeed, otherwise condition C2 would imply the existence of $s^1$, $s^2$,..., $s^n \in G$ such that $s^i_{q_i} = x_{q_i}$, $i = 1, 2, ..., n$. Since $q_i \cap q_{i+1}$ contains an $N_0$-cube, we would get $s^1 \sim s^2 \sim \cdots \sim s^n$ and hence $p = p'$.

*Remark.* Property 5 implies that there is an interface energy between nonequivalent DFCs. Observe that this is the only property that depends on C2.

Condition C2 does not rule out the possibility of an interface energy between equivalent DFCs. In order to make this remark precise, let us introduce $\bar{\Omega}^{(f)}$ as the set of configurations with a finite number of defects, i.e.,

$$\bar{\Omega}^{(f)} = \left\{ x \in \Omega \mid H(x) = \sum_B \phi_B(x) < \infty \right\}$$

Furthermore, let

$$\Omega^{(f)} = \{ x \in \Omega \mid x = s \text{ a.e. for some } s \in G \}$$

It is clear that $\Omega^{(f)} \subset \bar{\Omega}^{(f)}$, but the relation

$$\Omega^{(f)} = \bar{\Omega}^{(f)} \tag{9}$$

is not necessarily true. For instance, consider the two-dimensional spin-1 model of Section 6, defined by $J \geqslant 0$, $J + K_1 < 0$, $K_2 < 0$, and $h = 0$ in the domain of the parameters where $|G| = \infty$ and $d = 4$ (Fig. 5). Condition C2 is satisfied. The class $G_1$ is defined by configurations $s$ such that $s(i)$ is constant in each row, taking alternatively the value 0 and $+$ or $-$. The class $G_2$ is obtained by translation of $G_1$; the classes $G_3$ and $G_4$ are obtained by rotation by $\pi/2$ of $G_1$, $G_2$. Now $\bar{\Omega}^{(f)} \backslash \Omega^{(f)}$ is nonempty, since, e.g., the configuration

$$\begin{array}{ccccccc}
+ & + & + & + & + & + & + \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
+ & + & + & - & - & - & - \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
+ & + & + & + & + & + & +
\end{array}$$

is in $\bar{\Omega}^{(f)}$ but not in $\Omega^{(f)}$. In such cases there exist $s$ and $s'$, equivalent DFC, and nonoverlapping $N$-cubes $q$ and $q'$ such that the configuration $s_q \oplus s'_{q'}$ cannot be extended to a defect-free configuration in $G$. In this sense, the class containing $s$ and $s'$ is not complete: we thus consider only

$C$-potentials, i.e., potentials that satisfy condition C2 and the following "completeness" condition:

C. $\Phi$ is an $m$-potential, with $N_0$ finite; there is a partition $\mathscr{A}$ of $\mathbb{L}$ into rectangular cells $A_\alpha$ with $A_\alpha = A_0 + t_\alpha$, $t_\alpha \in \hat{\mathbb{L}}$, such that if $\Lambda$ is any (finite or infinite) union of cells and $x \in \Omega$ satisfies

(i) $\Phi_B(x) = 0$ for all $B \cap \Lambda \neq \varnothing$

(ii) $x_q$ is $p$-correct for any $N_0$-cube $q$ in $\Lambda$

then there exists $s \in G_p$ such that $s_\Lambda = x_\Lambda$.

It is clear that the $C$-potentials satisfy (9). Also note that the condition (9) is similar to the condition introduced to prove the existence of a phase transition for ferromagnetic systems.[4,11]

**Proposition 2.** Let $\Phi$ be a C-potential; then, for any class $G_p$ either $|G_p| = 1$ or $G_p$ has a nonvanishing entropy per site (residual entropy) $\sigma_p$, where

$$\sigma_p = \lim_{\Lambda \to \mathbb{L}} \frac{1}{|\Lambda|} \log |G_p(\Lambda)| \tag{10}$$

with

$$G_p(\Lambda) = \{x \in \Omega_\Lambda \mid \exists s \in G_p \text{ s.t. } s_\Lambda = x\}$$

*Proof.* Let us consider a periodic array of $N_0$-cubes separated by distances larger than $2R$. For each cube $q$ we can choose any $s \in G_p$ and define $x_q = s_q$. Condition C implies that $x$ can be extended into a DFC. If $|G_p| > 1$, then due to the periodicity of $\phi$ the limit (10) exists and is positive.

*Remark.* If $A_0$ contains more than one site, it is possible to consider the model defined by the lattice $\mathbb{L}' = \{\alpha\}$ with $\alpha$ the center of the cell $A_\alpha$, and $\Omega'_0 = \Omega_{A_0}$. In other words, we can always assume that the cells are the sites.

## 4. PHASE TRANSITIONS WITH SPONTANEOUS SYMMETRY BREAKDOWN

### 4.1. Contours

Let $\Phi$ be a $C$-potential such that the cells $A_\alpha$ are the sites of $\mathbb{L}$. For any $x \in \Omega^{(f)}$ we define the boundary $M_x$ of $x$ as the union of noncorrect $N$-cubes

$$M_x = \bigcup \{q \mid q \in Q_x\} \tag{11}$$

with

$$N > N_1 = \max\{N_0, R\} \tag{12}$$

to be specified later.

We then decompose $M_x$ into maximal 1-connected (connected) subsets $\{M_\alpha\}$, where $M_1$, $M_2$ are $r$-connected if

$$d(M_1, M_2) = \min_{\substack{i \in M_1 \\ j \in M_2}} \|i - j\| \leqslant r$$

A component $M_\alpha$ of $M_x$ is called a *contour* of $x$. Any connected, finite set $M \subset \mathbb{L}$ is a contour if it is a contour of some $x \in \Omega$. Let $M$ be a finite contour; we define Ext $M$ and $\mathrm{Int}_j M$ as maximal $N$-connected parts of $M^c = \mathbb{L} \setminus M$, Ext $M$ being the unique infinite component, and

$$\mathrm{Int}\, M = \bigcup_j \mathrm{Int}_j M, \qquad V(M) = M \cup \mathrm{Int}\, M = (\mathrm{Ext}\, M)^c \tag{13}$$

Let $\mathscr{M}_x = \{M_\alpha\}$ be the family of contours of $x \in \Omega$. The contour $M_\beta$ is an *external contour* of $\mathscr{M}_x$ if $M_\beta \subset \mathrm{Ext}\, M_\alpha$ for all $\alpha \neq \beta$. We denote by $\mathscr{M}_x^{\mathrm{ext}}$ the family of external contours. For $V \subset \mathbb{L}$, let

$$\partial_r(V) = \{i \in V \mid d(i, V^c) \leqslant r\}$$

We write $\partial(V)$ instead of $\partial_1(V)$.

**Proposition 3.** Let $x \in \Omega^{(f)}$ be such that $x = s$ a.e. for some $s$ in $G_p$.

(i) Let $M$ be a contour of $x$. Then every $N$-cube $q$ intersecting $\partial(\mathrm{Ext}\, M)$ is $p'$-correct with a common $p'$ ($p' = p$ if $M \in \mathscr{M}_x^{\mathrm{ext}}$), and every $N$-cube intersecting $\partial(\mathrm{Int}_j M)$ is $p_j$-correct with a common $p_j$.

(ii) For every $N$-cube $q$ that is not $p$-correct there exists an external contour $M$ of $x$ such that $q \subset V(M)$.

*Proof.* (i) By definition, any $N$-cube $q$ intersecting $\partial(\mathrm{Int}_j M)$ is correct. Now take some $i \in \partial(\mathrm{Int}_j M)$; then $q$ is $p(i)$-correct [with $p(i)$ independent of $q$] for any $N$-cube $q \ni i$. Indeed, since $N > N_0$, any translate of $q$ by a unit vector that contains $i$ is correct and of the same class as $q$. By repeated translation we can exhaust the set of $N$-cubes containing $i$. By definition, $\partial(\mathrm{Int}_j M)$ is $N$-connected, and this assures that $p(i)$ is the same for all $i \in \partial(\mathrm{Int}_j M)$. The same argument works for $\partial(\mathrm{Ext}\, M)$.

(ii) Any $N$-cube intersecting

$$\mathrm{Ext}(x) = \bigcap_{M \in \mathscr{M}_x^{\mathrm{ext}}} \mathrm{Ext}\, M$$

is $p$-correct. If $q$ is not $p$-correct, then $q \cap \mathrm{Ext}(x) = \varnothing$, i.e.,

$$q \subset \bigcup_{M \in \mathscr{M}_x^{\mathrm{ext}}} V(M)$$

and necessarily $q \subset V(M)$ for some $M \in \mathscr{M}_x^{\mathrm{ext}}$.

With the above definition of contour, we obtain a decomposition of the relative Hamiltonian.

**Proposition 4.** Let $x \in \Omega$ such that $x = s$ a.e. for some $s \in G$. Then,

$$H(x \mid s) = \sum_{M \in \mathscr{M}_x} H_M(x)$$

where

$$H_M(x) = H_M(x_M) = \sum_{B \subset M} \phi_B(x)$$

*Proof.* The condition $N > R$ implies that any $B$ such that $\phi_B(x) > 0$ is inside at least one noncorrect cube. Therefore

$$H(x \mid s) = \sum_B \phi_B(x) = \sum_{B \subset M_x} \phi_B(x) = \sum_{M \in \mathscr{M}_x} \sum_{B \subset M} \phi_B(x)$$

## 4.2. Peierls Argument

The Gibbs state for a finite volume $\Lambda \subset \mathbb{L}$ and boundary condition $s \in G_p$ is defined as the probability measure on

$$\Omega(s_{\Lambda^c}) = \{x \in \Omega \mid x_{\Lambda^c} = s_{\Lambda^c}\} \tag{14}$$

given by

$$\mu_\Lambda(x \mid s) = Z_\Lambda(s)^{-1} \exp[-\beta \sum_{B \cap \Lambda \neq \varnothing} \phi_B(x)]$$

Here

$$Z_\Lambda(s) = \sum_{x \in \Omega(s_{\Lambda^c})} \exp\left[-\beta \sum_{B \cap \Lambda \neq \varnothing} \phi_B(x)\right]$$

is the partition function, with boundary condition $s$, and we recall that $\phi_B(s) = 0$.

We want to estimate the probability that a given $N$-cube $q \subset \Lambda$ is not $p$-correct, which we write $\mu_\Lambda(x_q \notin G_p \mid s)$. Taking $N > N_1$ [Eq. (12)], it follows from (ii) of Proposition 3 that

$$\mu_\Lambda(x_q \notin G_p \mid s) \leqslant \sum_{M:\, q \subset V(M) \subset \Lambda \cup \partial_N(\Lambda^c)} \mu_\Lambda(M \mid s) \tag{15}$$

where

$$\mu_\Lambda(M \mid s) = \sum_{\substack{x \in \Omega(s_{\Lambda^c}) \\ M \in \mathscr{M}_x^{\mathrm{ext}}}} \mu_\Lambda(x \mid s)$$

Given a contour $M$ and $\Lambda' \supset M$, the configuration $y \in \Omega_{\Lambda'}$ is said to be *compatible* with $M$ and $s_{\Lambda^c}$, which we write $y \sim (M, s_{\Lambda^c})$, if there exists an $x \in \Omega(s_{\Lambda^c})$ such that $M \in \mathscr{M}_x^{\mathrm{ext}}$ and $x_{\Lambda'} = y$. Notice that the couple $\langle M, y \rangle$ with $y \in \Omega_M$ and $y \sim (M, s_{\Lambda^c})$ is a contour in the PS theory.

We then have

$$\mu_\Lambda(M \mid s) \leqslant \sum_{\substack{x \in \Omega_M \\ x \sim (M, s_{\Lambda^c})}} e^{-\beta H_M(x)} Z_\Lambda(s)^{-1} Z_{\Lambda \setminus V(M)}(x \oplus s_{\Lambda^c}) \prod_j Z^{\mathrm{dil}}_{\mathrm{Int}_j M}(x) \tag{16}$$

where, for $x \in \Omega_M$,

$$Z^{\mathrm{dil}}_{\mathrm{Int}_j M}(x) = \sum_{\substack{y \in \Omega_{\mathrm{Int}_j M} \\ y \oplus x \sim (M, s_{\Lambda^c})}} \exp\left[ -\beta \sum_{B \subset \mathrm{Int}_j M} \phi_B(y) \right]$$

Indeed, on the rhs of the above inequality, we have taken into account every configuration compatible with $M$ and $s_{\Lambda^c}$ and used the decomposition property (Proposition 4). An upper bound is obtained because in $\Lambda / V(M)$ we allowed also for configurations that are not compatible with $M$ and $s_{\Lambda^c}$. Furthermore, since $N > R$, for every $x \in \Omega(s_{\Lambda^c})$ such that $M \in \mathscr{M}_x^{\mathrm{ext}}$ and for any $B$ such that $B \cap M \neq \varnothing$ and $B \cap M^c \neq \varnothing$ we have $\phi_B(x) = 0$.

The following proposition implies that the boundary conditions for $Z_{\Lambda \setminus V(M)}$ and $Z^{\mathrm{dil}}_{\mathrm{Int}_j} M$ correspond to defect-free configurations, provided that $N$ is sufficiently large:

**Proposition 5.** Let $\Phi$ be a $C$-potential, $N \geqslant R + \tilde{N}$ with $\tilde{N} \geqslant N_1$, and $M$ be a contour. For any $x_M \sim (M, s_{\Lambda^c})$ with $s \in G_p$, there exist $s^0 \in G_p$ and $s^j \in G_{p_j}$ such that

$$x_M(i) = s^0(i) \qquad \text{if} \quad i \in M \text{ and } d(i, \mathrm{Ext}\, M) \leqslant \tilde{N}$$

$$x_M(i) = s^j(i) \qquad \text{if} \quad i \in M \text{ and } d(i, \mathrm{Int}_j\, M) \leqslant \tilde{N}$$

$$s^0_{\Lambda^c} = s_{\Lambda^c}$$

*Proof.* Let $x \in \Omega(s_{\Lambda^c})$ be any extension of $x_M$ such that $M \in \mathscr{M}_x^{\text{ext}}$. Consider the environment of radius $\tilde{N}$ of $\partial(\text{Int}_j M)$, i.e., the set

$$\Lambda_j = \{i \in \mathbb{L} \mid d(i, \partial(\text{Int}_j M)) \leqslant \tilde{N}\}$$

By Proposition 3, every $\tilde{N}$-cube in $\Lambda_j$ is $p_j$-correct since it is inside a $p_j$-correct $N$-cube. Moreover, $N \geqslant R + \tilde{N}$ implies that any $B$ such that $B \cap \Lambda_j \neq \varnothing$ is inside a $p_j$-correct $N$-cube, and hence $\phi_B(x) = 0$. Since $\Phi$ is a $C$-potential, there exists $s^j \in G_{p_j}$ such that $s^j_{\Lambda_j} = x_{\Lambda_j}$. Take any $i \in M$ with $d(i, \text{Int}_j M) \leqslant \tilde{N}$. Then $d(i, \partial(\text{Int}_j M)) \leqslant \tilde{N}$, so that $i \in \Lambda_j$ and $x(i) = s^j(i)$. The proof for $i \in M$, $d(i, \text{Ext } M) \leqslant \tilde{N}$, is similar.

*Remark.* Denote

$$E_r(V) = \{i \in \mathbb{L} \mid d(i, V) \leqslant r\}$$

the environment of radius $r$ of $V$. If $N > 2\tilde{N}$, then

$$E_{\tilde{N}}(\partial(M^c)) = \bigcup_j E_{\tilde{N}}(\partial(\text{Int}_j M)) \cup E_{\tilde{N}}(\partial(\text{Ext } M))$$

is a pairwise disjoint decomposition, because $d(\text{Int}_j M, \text{Int}_k M) > N$ $(j \neq k)$, $d(\text{Int}_j M, \text{Ext } M) > N$. Consider the special case of Proposition 5, when $N > 2\tilde{N}$, $\tilde{N} = R + N_1$, and $x_M \sim (M, s_{\Lambda^c})$ is such that $s^0 \in G_p$ and $s^j \in G_p$, all $j$. Then every $N$-cube in $E_{\tilde{N}}(\partial(M^c))$ is $p$-correct and thus $\phi(B) = 0$ for every $B$ intersecting with $E_{N_1}(\partial(M^c))$. Since $\Phi$ is a $C$-potential, we conclude that there exists $s' \in G_p$ such that $s' = s$ in $\Lambda^c$ and $s' = x_M$ in

$$E_{N_1}(\partial(M^c)) \cap M = \partial_{N_1}(M) \supset \partial_R(M)$$

This remark is the key to the Peierls argument.

**Definition.** We say that the potential $\Phi$ satisfies the *symmetry condition* if all the classes are related by internal and/or translational symmetry, i.e., $G_p = g_p T_{t(p)} G_1$, where $g_p$ is a pointwise transformation and $t(p) \in \hat{\mathbb{L}}$. The translational component $T_{t(p)}$ is not unique; $t(p)$ denotes a vector of minimal length. Let

$$N_2 = \max_p \|t(p)\|$$

The Peierls argument applies to a $C$-potential $\Phi$ satisfying the symmetry condition. Fix

$$N > 2(R + N_1 + N_2) = 2(\tilde{N} + N_2)$$

Let $M \subset \Lambda \cup \partial_N(\Lambda^c)$ be a contour, $s \in G_1$, $x_M \sim (M, s_{\Lambda^c})$, and $s^0 \in G_1$ and $s^j \in G_{p_j}$ the DFCs assigned to $x$, according to Proposition 5. Now, by this proposition and setting $\gamma_{p_j} = g_{p_j} T_{t(p_j)}$,

$$\gamma_{p_j}^{-1} s^j = T_{-t(p_j)} g_{p_j}^{-1} s^j \in G_1$$

coincides with $\gamma_{p_j}^{-1} x$ on $E_{\tilde{N}}(\partial(\mathrm{Int}_j M - t(p_j)))$. Due to the choice of $N$, these sets are disjoint for different $j$'s, and also disjoint from $E_{\tilde{N}}(\partial(\mathrm{Ext}\, M))$. Hence, the preceding remark is relevant: There exists $s' \in G_1$ such that $s' = s$ in $\Lambda^c$, $s' = x$ in $\partial_R(V(M))$, and $s' = \gamma_{p_j}^{-1} x$ in $\partial_R((\mathrm{Int}_j M - t(p_j))^c)$.

Since the $\gamma_{p_j}$ are symmetries of the Hamiltonian, we have

$$\phi_B(s^j) = \phi_{B - t(p_j)}(\gamma_{p_j}^{-1} s^j), \qquad \text{all } B$$

and in Eq. (16)

$$Z_{\Lambda \setminus V(M)}(x \oplus s_{\Lambda^c}) = Z_{\Lambda \setminus V(M)}(s')$$
$$Z^{\mathrm{dil}}_{\mathrm{Int}_j M}(x) = Z^{\mathrm{dil}}_{\mathrm{Int}_j M - t(p_j)}(s')$$

Then

$$Z_\Lambda(s) = Z_\Lambda(s') \geqslant Z_{\Lambda \setminus V(M)}(s') \prod_j Z_{\mathrm{Int}_j M - t(p_j)}(s')$$

and the upper bound in (16) reduces to

$$\begin{aligned} \mu_\Lambda(M \mid s) &\leqslant \sum_{\substack{x \in \Omega_M \\ x \sim (M, s_{\Lambda^c})}} \exp[-\beta H_M(x)] \\ &\leqslant \max_{x \in \Omega_M} \exp[-\beta H_M(x)]\, |\Omega_0|^M \\ &\leqslant \exp[|M|\, (\log |\Omega_0| - \beta C_1)] \end{aligned}$$

In the last inequality we used Proposition 1. Finally, for any $s \in G_p$ the estimate (15) reads

$$\begin{aligned} \mu_\Lambda(x_q \notin G_p \mid s) &\leqslant \sum_{M : q \subset V(M)} \exp[|M|\, (\log |\Omega_0| - \beta C_1)] \\ &\leqslant \sum_{l \geqslant (N+1)^\nu} \exp[-l(\beta C_1 - C_2)] \end{aligned}$$

with a suitably chosen constant $C_2$. Here, the usual exponential bound for the number of connected sets with given length is applied. The bound on the rhs is independent of $s$; by symmetry, it applies to any $p$ and goes to zero with $\beta$ going to infinity. This implies the following result:

**Theorem 1.** If the interaction is defined by a $C$-potential that satisfies the symmetry condition, then there exist at low temperatures at least as many phases as the number of classes.

## 5. EXTENSION OF THE PIROGOV–SINAI THEORY

### 5.1. Perturbed Hamiltonian

Let us consider a system with unperturbed Hamiltonian $H_0$ defined by a periodic $C$-potential $\Phi^{(0)}$, and let

$$G[H_0] = \bigcup_{p=1}^{d} G_p$$

We then introduce a perturbed Hamiltonian

$$H = H_0 + \sum_{p=1}^{d-1} \lambda_p H_p = H_0 + H'$$

where $H'$ completely splits the degeneracy between the classes, but preserves the degeneracy within each class. It is assumed that $\lambda_p$ are sufficiently small compared to

$$\Delta^{(0)} = \min_{B} \min_{x:\, \phi_B^{(0)}(x) > 0} \phi_B^{(0)}(x)$$

so that new DFCs will not appear, and

$$G[H] = \bigcup_{p \in I} G_p, \qquad I \subset \{1, \ldots, d\}$$

The perturbations $H_p$ are defined by means of periodic $C$-potentials $\Phi^{(p)}$ whose range and period do not exceed $N_1 = \max\{R^{(0)}, N_0\}$, and which satisfy

$$\phi_B^{(p)}(s) = \phi_B^{(p)}(s')$$

whenever $s$, $s' \in G[H_0]$ with $s \sim s'$.

It is easy to construct such potentials: for example, take for $\{B\}$ the family of $N_0$-cubes, and define

$$\phi_B^{(p)}(x) = \begin{cases} 1 & \text{if } x_B = s_B \text{ for some } s \in G_p \\ 0 & \text{otherwise} \end{cases}$$

The total interaction is $\phi_B = \phi_B^{(0)} + \sum_p \lambda_p \phi_B^{(p)} = \phi_B^{(0)} + \phi'_B$.

In the examples of Section 6, the approach is different: the Hamiltonian is given, and is decomposed afterward into an unperturbed part and perturbations.

## 5.2. Factorization Condition

The PS theory will be extended to periodic $m$-potentials $\Phi^{(0)}$, which satisfy the following factorization condition: There is a partition of $\mathbb{L}$ into rectangular cells $A_\alpha$, $\mathbb{L} = \bigcup_\alpha A_\alpha$, with $A_\alpha = A_0 + t_\alpha$, $t_\alpha \in \hat{\mathbb{L}}$, and a partition of $\Omega_{A_0}$

$$\Omega_{A_0} = \bigcup_{p=1}^{d+1} \Omega_{A_0}^{(p)}$$

such that

$$G = \bigcup_{p=1}^{d} G_p, \qquad \text{where} \quad G_p = \oplus \Omega_{A_\alpha}^{(p)} \tag{17}$$

and $\Omega_{A_\alpha}^{(p)}$ is related to $\Omega_{A_0}^{(p)}$ by the translation $t_\alpha$.

It is clear that $s, s' \in G_p$ implies $s \sim s'$; indeed, if $s, s' \in G_p$, there is some $s'' \in G_p$ coinciding with $s$ and $s'$ on different half-spaces. On the other hand, if $s \in G_p$, $s' \in G_{p'}$, with $p \neq p'$, then for any $\alpha$, $s_{A_\alpha} \neq s'_{A_\alpha}$, and thus an element of $G_p$ cannot be equivalent with an element of $G_{p'}$. Therefore, the decomposition (17) is the decomposition of $G$ into equivalence classes. If $N \geqslant 2 \operatorname{diam} A_0$, then any $N$-cube $q$ contains some cell $A_\alpha$, so that any $s \in G$ can be classified by inspecting $s_q$. This implies that $N_0 \leqslant 2 \operatorname{diam} A_0$. Clearly, $\Phi^{(0)}$ is a $C$-potential. The residual entropy, introduced in Eq. (10), is

$$\sigma_p = \frac{1}{|A_0|} \log |\Omega_{A_0}^{(p)}| \tag{18}$$

If $\Lambda$ is a finite union of cells $A_\alpha$ and $s$ is any element of $G_p$, then

$$\lim_{\beta \to \infty} Z_\Lambda(s) = \exp\{|\Lambda| \, \sigma_p\}$$

In this section, we assume that the unperturbed potential satisfies the factorization condition.

## 5.3. Contours

In the PS theory "contour" means a couple whose first term is a set of lattice sites and the second is a configuration on this set. We adopt this

definition and we note that the concepts introduced in this section are defined in terms of $H_0$. The *boundary* of $x \in \Omega^{(f)}$ is now defined as the couple $\langle A, x_A \rangle$, where

$$A \equiv M_x = \bigcup_{\alpha} \{A_\alpha \mid A_\alpha \cap q \neq \varnothing \text{ for some noncorrect } N\text{-cube } q\}$$

and $N \geqslant R + \max\{R, 2 \operatorname{diam} A_0\}$.

A component $M$ of $M_x$ is one of its maximal connected subsets (clearly union of cells), and

$$\Gamma = \langle M, x_M \rangle$$

is a contour of $x$, $M = \operatorname{supp} \Gamma$. Any couple $\Gamma = \langle M, x_M \rangle$ is a contour if it is the contour of some $x$ in $\Omega$. The boundary as a set of contours is $\partial_x$ (or $\partial$); $\operatorname{Ext} \Gamma$, $\operatorname{Int}_j \Gamma$, $V(\Gamma)$ are identical to $\operatorname{Ext} M$, $\operatorname{Int}_j M$, $V(M)$ introduced in Eq. (13). External contours are defined as in Section 4, and $\partial_x^{\text{ext}}$ (or $\partial^{\text{ext}}$) denotes the set of external contours of $\partial_x$ (or $\partial$).

Proposition 3 remains valid, so that there is a unique equivalence class associated with $\operatorname{Ext} \Gamma$ and each of $\operatorname{Int}_j \Gamma$. We call $\Gamma^p$ a *type p contour* if $\operatorname{Ext} \Gamma$ is associated with $G_p$. $\Gamma_p$ denotes a type $p$ contour. The decomposition property (Proposition 4) equally holds. From Eq. (7), we have

$$H_0(x \mid s) \geqslant C' |M_x|$$

## 5.4. Partition Functions

In what follows, $\Lambda$ always denotes a finite union of cells $A_\alpha$. For an $s \in G[H_0]$, let

$$\Omega(\Lambda \mid s) = \{x \in \Omega \mid x_{\Lambda^c} = s_{\Lambda^c}, d(M_x, \Lambda^c) > 1\}$$

*The dilute partition function* is defined by

$$Z(\Lambda \mid \beta H, s) = \sum_{x \in \Omega(\Lambda \mid s)} e^{-\beta H(x \mid s)}$$

where $H$ is the perturbed Hamiltonian.

The factorization condition implies that the restriction of $\Omega(\Lambda \mid s)$ to $\Lambda$ depends only on the class $G_p$ to which $s$ belongs; also $\phi_B(s) = \phi_B(s')$ if $s \sim s'$. Therefore

$$Z(\Lambda \mid \beta H, s) = Z(\Lambda \mid \beta H, s') \qquad \text{if} \quad s' \sim s$$

Indeed, for any $x \in \Omega(\Lambda \mid s)$ and $s' \sim s$, let

$$x' = \begin{cases} x \text{ on } \Lambda \\ s' \text{ on } \Lambda^c \end{cases}$$

Then $x' \in \Omega(\Lambda \mid s')$ and $H(x' \mid s') = H(x \mid s)$. To see this, take any $B$ ($\phi_B \neq 0$) such that $B \cap \Lambda \neq \phi$, $B \cap \Lambda^c \neq \phi$. There exist $\bar{s}$ and $\bar{s}'$, both equivalent to $s$ and $s'$, such that $x_B = \bar{s}_B$ and $x'_B = \bar{s}'_B$, thus $\phi_B(x) = \phi_B(\bar{s}) = \phi_B(\bar{s}') = \phi_B(x')$. This holds because of: (i) $\Lambda$ being a finite union of cells; (ii) the factorization property; (iii) the definition of diluteness; (iv) the fact that the perturbation does not split the degeneracy within a class.

Thus, the map is one-one from $\Omega(\Lambda \mid s)$ onto $\Omega(\Lambda \mid s')$ and keeps the energy unchanged. Therefore $Z(\Lambda \mid \beta H, s) = Z(\Lambda \mid \beta H, s') = Z(\Lambda \mid \beta H, p)$, if $s \in G_p$.

Furthermore, for a contour $\Gamma$, let $s(\Gamma)$ be any fixed DFC in the equivalence class associated with Ext $\Gamma$, and

$$\Omega(\Gamma) = \{x \in \Omega \mid \partial_x^{\text{ext}} = \Gamma,\ x = s(\Gamma) \text{ on Ext } \Gamma\}$$

The *crystal partition function* is

$$Z(\Gamma \mid \beta H) = \sum_{x \in \Omega(\Gamma)} e^{-\beta H(x \mid s(\Gamma))}$$

Observe that this sum does not depend on the particular choice of $s(\Gamma)$, although $\Omega(\Gamma)$ does. This is due to the fact that the summation goes over configurations in $\Omega_{\text{Int}\,\Gamma}$ and $\phi_B(s)$ is the same for all $s \in G_p$.

The two kinds of partition functions are related through the equation

$$Z(\Lambda \mid \beta H, p) = \sum_{\partial^p \subset \Lambda} e^{S_\Lambda(\partial^p)} \prod_{\Gamma \in \partial^p} Z(\Gamma \mid \beta H)$$

Here $\partial^p = \{\Gamma_i\}$ denotes a family of type $p$ external contours, i.e., $d(V(\Gamma_i), V(\Gamma_j)) > 1$ if $i \neq j$ and $s(\Gamma_i) \in G_p$ for all $i$. Furthermore, $\partial^p \subset \Lambda$ means that $d(V(\Gamma_i), \Lambda^c) > 1$ for all $i$, and $\exp\{S_\Lambda(\partial^p)\}$ is the number of DFCs coinciding with a fixed $s \in G_p$ in $\bigcup_i V(\Gamma_i) \cup \Lambda^c$. The argument of the sum represents a partial summation over all $x \in \Omega(\Lambda \mid s)$ such that $\partial_x^{\text{ext}} = \partial^p$.

On the other hand, with $x(\Gamma)$ any configuration whose unique contour is $\Gamma$, we have

$$Z(\Gamma \mid \beta H) = e^{-\beta H(\Gamma)} \sum_{x \in \Omega(\Gamma)} e^{-\beta H(x \mid x(\Gamma))}$$

where

$$H(\Gamma) = H(x(\Gamma) \mid s(\Gamma)) = \sum_{B \subset V(\Gamma)} [\phi_B(x(\Gamma)) - \phi_B(s(\Gamma))] \tag{19}$$

does not depend on the particular choice of $x(\Gamma)$. Thus,

$$Z(\Gamma \mid \beta H) = e^{-\beta H(\Gamma)} \prod_j Z(\mathrm{Int}_j \Gamma \mid \beta H, s_j)$$

where $s_j$ is an arbitrary DFC chosen from the equivalence class associated with $\mathrm{Int}_j \Gamma$.

Denoting by $\mathrm{Int}^{(p)} \Gamma$ the union of those $\mathrm{Int}_j \Gamma$ that are associated with $G_p$, we have

$$Z(\Gamma \mid \beta H) = e^{-\beta H(\Gamma)} \prod_{p=1}^{d} Z(\mathrm{Int}^{(p)} \Gamma \mid \beta H, p)$$

If $\mathrm{Int}^{(p)} \Gamma = \varnothing$, the corresponding term is 1.

Now observe that, using the factorization condition, we have

$$S_\Lambda(\partial^p) = \left( |\Lambda| - \sum_{\Gamma \in \partial^p} |V(\Gamma)| \right) \sigma_p$$

Then, introducing the *normalized partition functions*

$$\hat{Z}(\Lambda \mid \beta H, p) = [\exp(-|\Lambda| \sigma_p)] Z(\Lambda \mid \beta H, p)$$
$$\hat{Z}(\Gamma^p \mid \beta H) = \{\exp[-|V(\Gamma^p)| \sigma_p]\} Z(\Gamma^p \mid \beta H)$$

we obtain the recurrence relations

$$\hat{Z}(\Lambda \mid \beta H, p) = \sum_{\partial^p \subset \Lambda} \prod_{\Gamma \in \partial^p} \hat{Z}(\Gamma \mid \beta H) \tag{20}$$

$$\hat{Z}(\Gamma^p \mid \beta H) = \exp[-\beta \hat{H}(\Gamma^p)] \prod_q \hat{Z}(\mathrm{Int}^{(q)} \Gamma^p \mid \beta H, q) \tag{21}$$

where

$$\hat{H}(\Gamma^p) = H(\Gamma^p) + \beta^{-1} \left[ |\mathrm{supp}\, \Gamma^p| \sigma_p + \sum_q |\mathrm{Int}^{(q)} \Gamma^p| (\sigma_p - \sigma_q) \right] \tag{22}$$

## 5.5. Contour Model

Let $\mathscr{C}_p$ denote the family of type $p$ contours. With $F$ a $\tau$-functional in the sense of PS, we introduce the crystal and dilute partition functions, respectively, as

$$Z(\Gamma \mid F) = e^{-F(\Gamma)} \sum_{\partial \subset \mathrm{Int}\, \Gamma} e^{-F(\partial)} \tag{23}$$

and

$$Z(\Lambda \mid F) = \sum_{\partial \subset \Lambda} e^{-F(\partial)} \tag{24}$$

Here, $\partial \subset \mathscr{C}_p$ is a set of pairwise compatible contours (not necessarily external), i.e., $d(\text{supp } \Gamma, \text{supp } \Gamma') > 1$ if $\Gamma, \Gamma' \in \partial$ and $\Gamma \neq \Gamma'$; $\partial \subset \Lambda$ with $\Lambda \subset \mathbb{L}$ means that $d(V(\Gamma), \Lambda^c) > 1$ for all $\Gamma \in \partial$, and

$$F(\partial) = \sum_{\Gamma \in \partial} F(\Gamma)$$

The partition functions obey the recurrence relations

$$\begin{aligned} Z(\Gamma \mid F) &= e^{-F(\Gamma)} \prod_{q=1}^{d} Z(\text{Int}^{(q)} \Gamma \mid F) \\ Z(\Lambda \mid F) &= \sum_{\partial^p \subset \Lambda} \prod_{\Gamma \in \partial^p} Z(\Gamma \mid F) \end{aligned} \tag{25}$$

where $\partial^p$ denotes a set of type $p$ external contours, as earlier.

The contour model defined above through the partition functions does not differ from the one used in the original PS theory. Therefore, the results obtained therein for the existence and properties of the pressure and correlation functions will not change. When establishing the connection between the spin and the contour models a minor change will be necessary: an extra term $-\sigma_p/\beta$ has to be introduced in the expression of the energy density.

## 5.6. Phase Diagram at Low Temperatures

We define a contour functional on $\mathscr{C}_p$ by

$$\begin{aligned} \psi(\Gamma) &= H(\Gamma) + \beta^{-1} |\text{supp } \Gamma| \, \sigma_p - \sum_{q=1}^{d} (h_q - h_p) \, |\text{Int}^{(q)} \Gamma| \\ &= \hat{H}(\Gamma) - \sum_q |\text{Int}^{(q)} \Gamma| \, [(h_q - \beta^{-1}\sigma_q) - (h_p - \beta^{-1}\sigma_p)] \end{aligned}$$

Here $H(\Gamma)$ is given by (19), and $h_q$ is the specific energy of any $s \in G_q$ with respect to the perturbed Hamiltonian. In fact, since $\phi_B^{(0)}(s) = 0$,

$$h_q = \lim_{\Lambda \to \infty} \frac{1}{|\Lambda|} H'_\Lambda(s)$$

For $H' = 0$, we find

$$\psi(\Gamma) = H_0(\Gamma) + \beta^{-1} |\text{supp } \Gamma| \, \sigma_p$$

and

$$\psi(\Gamma) \geqslant \rho \, |\text{supp } \Gamma|$$

with $\rho = c' + \beta^{-1}\sigma_p$. If $H' \neq 0$, we still have

$$\left| H'(\Gamma) - \sum_{q=1}^{d} (h_q - h_p) \mid \mathrm{Int}^{(q)} \Gamma \mid \right| \leqslant \varepsilon(\lambda) \mid \mathrm{supp}\, \Gamma \mid$$

where $\varepsilon(\lambda) \to 0$ as $\lambda = (\lambda_1, \ldots, \lambda_{d-1}) \to 0$.

Hence, for sufficiently small $\lambda$

$$\psi(\Gamma) \geqslant 1/2\rho \mid \mathrm{supp}\, \Gamma \mid$$

i.e., $\psi$ is a $\tau$-functional.[3]

Consider now the contour models defined on $\mathscr{C}_1, \ldots, \mathscr{C}_d$ by using the (so far unknown) $\tau$-functionals $F_1, \ldots, F_d$, respectively. The pressures

$$\pi(F_p) = \lim_{\Lambda \to \infty} \frac{1}{|\Lambda|} \log Z(\Lambda \mid F_p) \tag{27}$$

exist for sufficiently large $\tau$. We are looking for $\{F_p\}$ that solve the equations

$$\hat{Z}(\Gamma \mid \beta H) = e^{b_p |\mathrm{Int}\, \Gamma|} Z(\Gamma \mid F_p) \tag{28}$$

for all $\Gamma \in \mathscr{C}_p$, $p = 1, \ldots, d$. Here

$$b_p = \beta h_p - \sigma_p - \pi(F_p) + \alpha \tag{29}$$

where $\alpha$ is fixed by the condition

$$\min_{1 \leqslant p \leqslant d} b_p = 0$$

At this point we can follow the proof given in ref. 3 to conclude the following result.

**Theorem 2.** If the interaction is defined by a $C$-potential with the factorization property, the low-temperature phase diagram is given by the Pirogov–Sinai theorem[3] with ground states replaced by classes.

## 6. MAGNETIC LATTICE GAS MODEL

To illustrate the definitions and to present some applications of our results, we consider a magnetic lattice gas model on the two-dimensional

square lattice $\mathbb{Z}^2$: Each lattice site $i$ can either be empty ($x_i = 0$) or occupied by a particle with spin up or spin down ($x_i = \pm 1$). In the language of binary alloys, a site is empty or occupied with an atom of type A or B. This corresponds to the so-called annealed dilution. We assume that there is a *magnetic pair interaction* $J$ between nearest neighbors (nn) and *nonmagnetic* pair *interactions* $K_1$ between nearest neighbors and $K_2$ between next nearest neighbors (nnn). The density of particles is characterized by the *chemical potential* $\mu$ and the system is subjected to a *magnetic field h.*

Written in the usual way,

$$H = -\sum_{\text{nn}} (Jx_i x_j + K_1 x_i^2 x_j^2) - \sum_{\text{nnn}} K_2 x_i^2 x_j^2 - \sum_i (hx_i + \mu x_i^2) \tag{30}$$

For general values of the five parameters the interactions do not form an $m$-potential (they do so if, e.g., all the five are positive). We may, however, rewrite $H$ in the form

$$H(x) = \sum_B \phi_B(x)$$

where $B$ are unit squares, and

$$\phi_B(x) = -1/2 \sum_{\text{nn} \subset B} (Jx_i x_j + K_1 x_i^2 x_j^2) - \sum_{\text{nnn} \subset B} K_2 x_i^2 x_j^2 - 1/4 \sum_{i \in B} (hx_i + \mu x_i^2) \tag{31}$$

This $\Phi$ already satisfies condition C1 for *any* choice of the parameters. A periodic $s \in G$ can be obtained, for example, by minimizing $\phi_B(x)$ on a square $B$ and by repeating periodically (with period 2) the resulting configuration: Due to the reflection symmetry of $H$, this yields a configuration that minimizes all the $\phi_B$ simultaneously.

This model with $K_2 = 0$ has been extensively studied in the literature by means of series expansions, mean field approximations, renormalization group techniques, and Monte Carlo methods. However, there are very few rigorous results, except at low temperatures for those values of the parameters where Pirogov–Sinai theory applies (finite number of ground states).

This model has many physical interpretations and has been used to discuss $He^3$–$He^4$ mixtures, ternary mixtures, amorphous ferromagnets, and diluted magnetic alloys that undergo crystallization as well as an order–disorder phase transition. The extended Hubbard model in the

Table I

| | $J$ | $K_1$ | $h$ |
|---|---|---|---|
| Griffiths[10] | 0 | $>0$ | 0 |
| Bernasconi and Rys[12] | 0 | $>0$ | $\neq 0$ |
| Capel[13] | $>0$ | 0 | $\neq 0$ |
| Blume, Emery, and Griffiths[14] | $>0$ | $>0$ | 0 |
| Mukamel and Blume[15] | $>0$ | $>0$ | $\neq 0$ |
| Racz and Vicsek[16] | $<0$ | $3J$ | $\mu+8J$ |
| Antiferromagnetic Potts model[17] | $<0$ | $3J$ | 0 |
| Saito[18] | $<0$ | $>0$ | $\neq 0$ |
| Hubbard[19] | $<0$ | $\lvert K_1\rvert < \lvert J\rvert$ | $\neq 0$ |

atomic limit (no hopping term) can be reduced to the Hamiltonian (30) with interactions that are temperature dependent.

We summarize some of these investigations in Table I ($K_2 = 0$).

In Fig. 1–5 we show typical phase diagrams for different domains of the parameters. We use the following convention: $n$ denotes the number of DFC, $d$ the number of equivalence classes (if $n = \infty$), $\sigma_p$ the residual entropy of the class $G_p$; $\mathscr{C}$, $\mathscr{S}$, and $\mathscr{F}$ denote that the interaction $\Phi$ satisfies, respectively, the completeness, the symmetry, or the factorization condition; on the solid lines the set of DFC is the union of the DFC on the two sides of the line; on the dashed lines $n = \infty$, $d = 1$, $\sigma > 0$, and on the two sides of these lines numbers of classes are different; on the dotted lines $n = \infty$, $\sigma > 0$, and $d$ is the same on both sides as well as on the line.

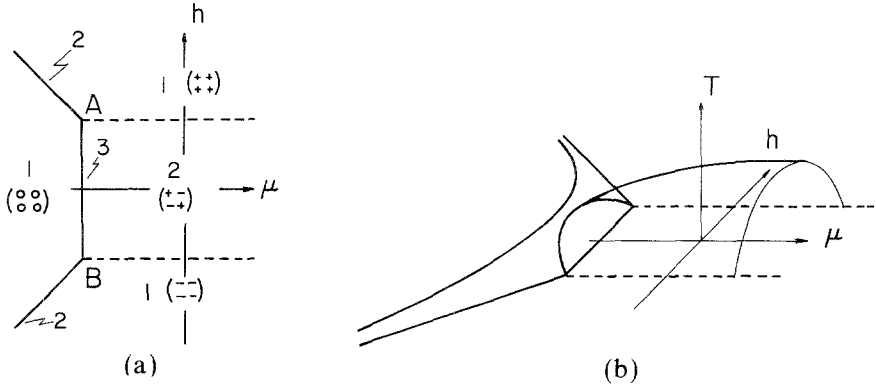



Fig. 1. Plots for $J < 0$, $K_1 > -3J$, $K_2 = 0$. The numbers of DFC are indicated. At points $A$ and $B$, $d = 2$, $\sigma_1 = 0$, $\sigma_2 > 0$, and the interaction is $\mathscr{C}$, but neither $\mathscr{S}$ nor $\mathscr{F}$.

Although our results do not give information for those values of the parameters corresponding to the dashed lines, we expect that they correspond to the boundary ($T=0$) of a surface of second-order phase transition (as is the case for the antiferromagnetic Ising model). On the other hand, we expect that the dotted lines have no special significance at nonzero temperature. This last conjecture is supported by the solvable Griffiths model,[10] where the same situation occurs, and by numerical analysis of the model described in Fig. 3.[20]

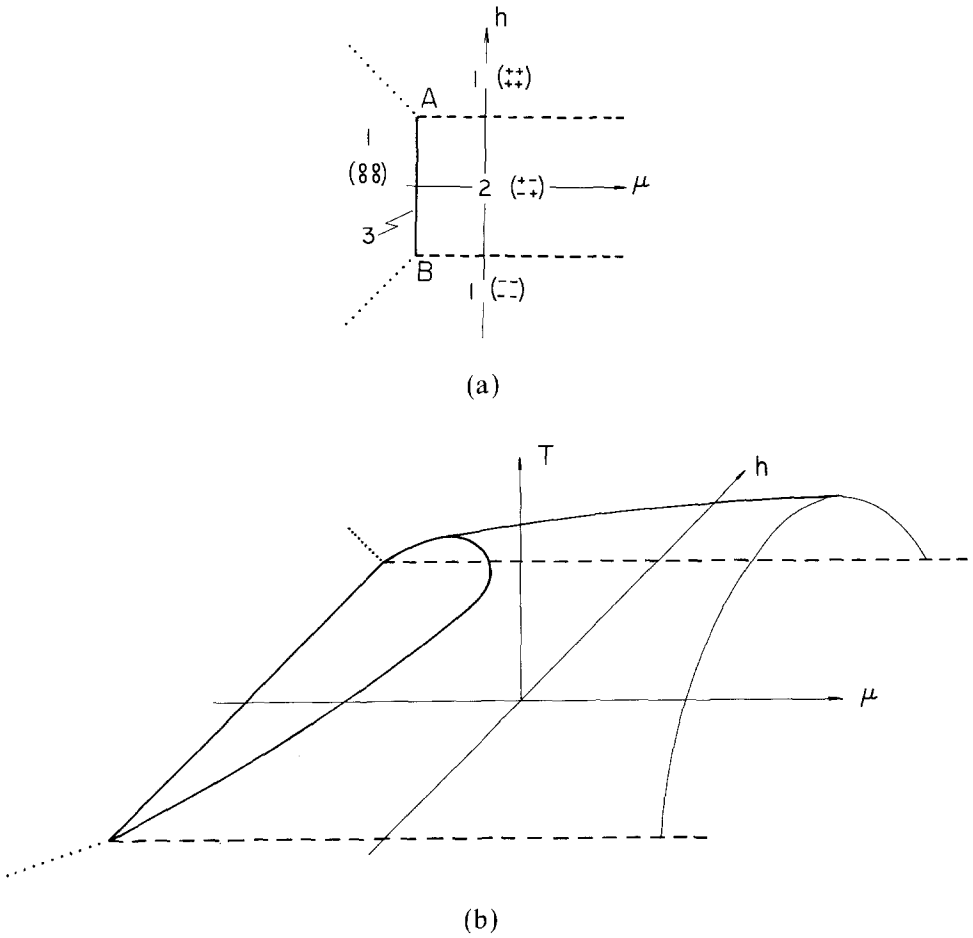
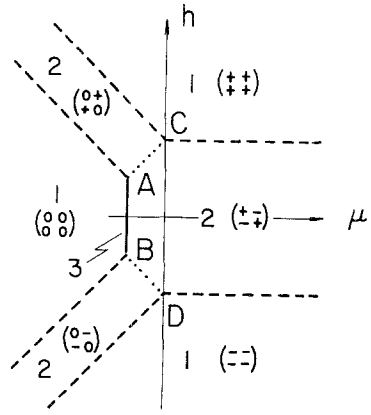
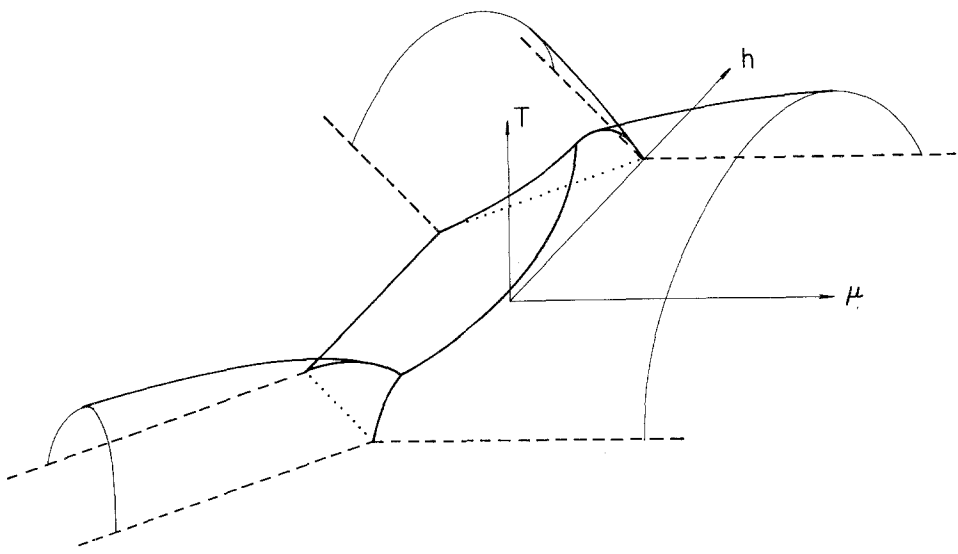



Fig. 2. Plots for $J<0$, $K_1=-J$, $K_2=0$. The numbers of DCF are indicated. At points $A$ and $B$, $d=1$, $\sigma>0$.

Figures 1–4 are $h$ versus $\mu$ plots for fixed $J<0$, $K_2=0$; the parameter $K_1$ changes from one figure to the other. The phase diagrams are symmetric with respect to the transformation $h \to -h$. In Figs. 1–4, in the $n=2$ areas there are two DFC related by translational symmetry. A Peierls–Dobrushin



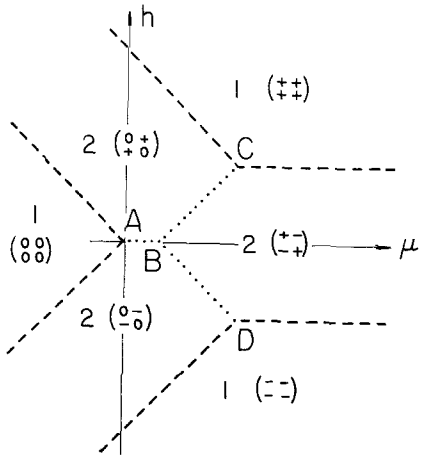

(a)



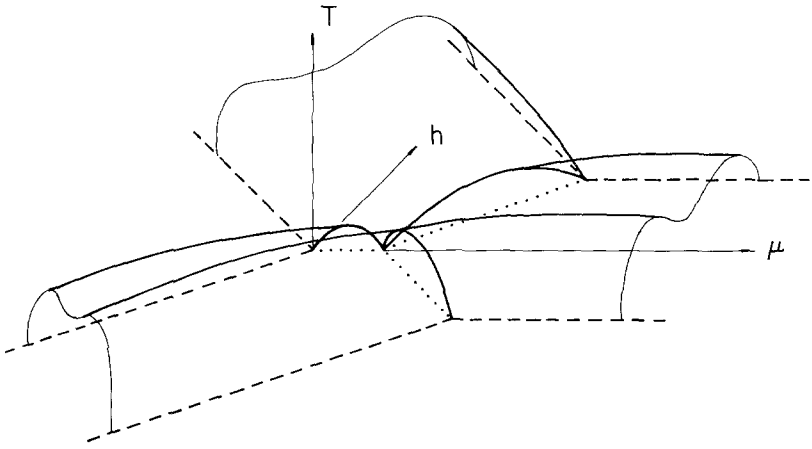

(b)

Fig. 3. Plots for $J<0$, $J<K_1<-J$, $K_2=0$. The numbers of DFC are indicated. Along the dotted lines, $d=2$, $\sigma_1=\sigma_2>0$, and the interaction is $\mathscr{C}$, $\mathscr{S}$, and $\mathscr{F}$. The $h$ axis is drawn at the value $\mu=-4K_1$.

argument, or the PS theory, shows the existence of at least two phases at $T>0$. The volume of phase coexistence is enclosed by a surface; on the largest part of this surface one expects a second-order phase transition and the existence of a unique phase. In Figs. 1–3, on the solid lines the number of DFC is finite. The interaction $\mu x_i^2$ splits the accidental degeneracy

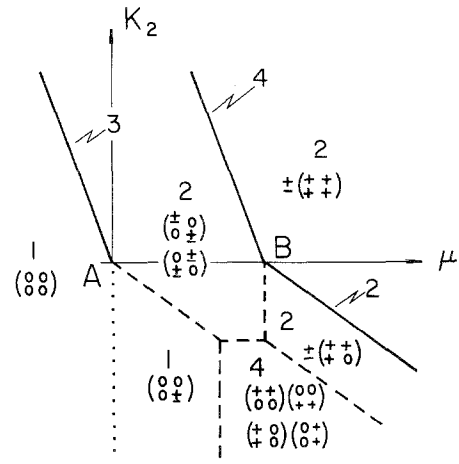


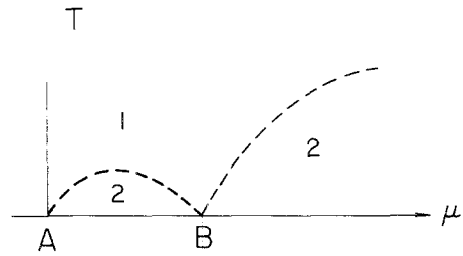

(a)




(b)

Fig. 4. Plots for $J<0$, $K_1<J$, $K_2=0$ with the numbers of DFC are indicated. The $h$ axis is drawn at the value $\mu=0$.



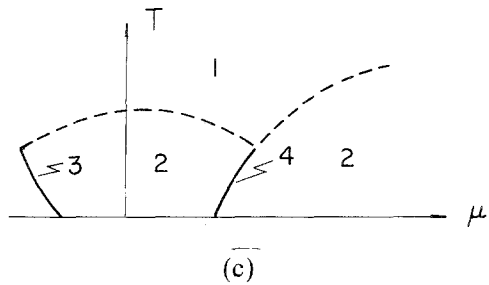




Fig. 5. Plots for $J \geqslant 0$, $J+K_1<0$, $h=0$ the numbers of (a) classes and (b, c) phases. (b) $K_2=0$, (c) $K_2>0$. The symbol $\left(\begin{smallmatrix} + & + \\ 0 & 0 \end{smallmatrix}\right)$ denotes the class of ground states such that on each unit square, the configuration is given by $\left(\begin{smallmatrix} \varepsilon & \varepsilon \\ 0 & 0 \end{smallmatrix}\right)$, $\varepsilon = +1$ or $-1$.

between the DFCs $s_i \equiv 0$ and $|s_i| \equiv 1$. Hence the PS theory predicts that there are surfaces of coexistence of two or three phases, which intersect the $T=0$ plane in the solid lines. The slope of these coexistence surfaces with respect to the $h$–$\mu$ plane varies with $K_1$ and can be calculated by Slawny's theory.[4] We expect that the intersection between the coexistence surface and the surface of second-order phase transition corresponds to a multicritical line that ends at points $A$ and $B$ (as is the case for the BEG model[14]).

At the points $A$ and $B$ of Fig. 1, there are two classes: one class consists of the single DFC $s_i \equiv 0$, the other class contains all the DFC that exist on the incident dashed line. At these points, the interaction belongs to $\mathscr{C}$, but does not belong either to $\mathscr{S}$ or $\mathscr{F}$ and we can make no conclusions.

At the points $A$ and $B$ of Fig. 2, there is just one class with $\sigma > 0$. It contains all configurations except those having $(-, -)$ nearest neighbors (at $A$), or $(+, +)$ nearest neighbors (at $B$); on the dotted line $d=1$ and the DFC are defined by $s_i \in \{0, 1\}$ for all $i$ $(h > 0)$.

At the points $A$, $B$, $C$, $D$ of Figs. 3 and 4 there is just one class with $\sigma > 0$. Along the dotted lines $d=2$, $\sigma_1 = \sigma_2 > 0$ and the two classes are symmetry-related. For instance, for $h > 0$, $s_i = 1$ on one sublattice and $s_i \in \{0, -1\}$ on the other, and the other class is obtained by translation. The interaction is $\mathscr{C}$, $\mathscr{S}$, and $\mathscr{F}$. Using our extension of the Peierls argument, one sees that along the dotted lines the two-phase coexistence persists at $T > 0$.

The use of our extension of the PS theory is best illustrated by Fig. 5. This presents a $K_2$ versus $\mu$ plot with fixed $J \geqslant 0$, $J + K_1 < 0$, and $h = 0$. For large, positive $\mu$ or $K_2$, $n=2$ and the two ferromagnetic DFC are related by spin-reversal symmetry. The Peierls argument or PS theory proves a two-phase coexistence at $T > 0$. Another domain of two-phase coexistence appears in the $d=2$ area bordered by the parallel solid lines. Here there are two symmetry-related *classes*, and the discussion of Section 4 shows the phase coexistence at $T > 0$. At low temperatures and for $K_2 > 0$ this domain is bordered by surfaces of first-order phase transition. Indeed, along the solid lines $d=3$ and 4 the interaction is a factorizable $C$-potential, and $\mu x_i^2$ splits the degeneracy between low- and high-density classes. The extension of the PS theory (Section 5) shows that we have a three-phase and a four-phase coexistence surface at the low-$\mu$ and the high-$\mu$ sides, respectively. (Slawny's method to establish the slope of these surfaces to the $T=0$ plane can be adopted and will be discussed elsewhere.) We expect that there is a piece of second-order phase transition surface between them, so that the intersections yield two multicritical lines. These lines presumably end up at $A$ and $B$ in the $T=0$ ($K_2$–$\mu$) plane (cf. Fig. 5b). A tentative $T$–$\mu$ plot for $K_2 > 0$ is shown in Fig. 5c. On the $d=2$ solid line of Fig. 5a the interaction

satisfies the symmetry condition (through spin flip), although it does not belong to $\mathscr{F}$. (In one class, $s_i \in \{0, 1\}$ without nn and nnn zeros.) The extended Peierls argument shows that the two-phase coexistence persists for $T > 0$ all along the line. There may or may not be a phase boundary here. On the low-$\mu$ side of this line $n = \infty$, $d = 2$, but $\sigma_1 = \sigma_2 = 0$, and our method is not conclusive. The same remark holds for the $d = 4$ domain and the dashed lines: since $n = \infty$ and $\sigma = 0$, the interaction is not a $C$-potential.

## ACKNOWLEDGMENTS

We are grateful to J. Jedrzejewski for several interesting and useful discussions, especially on the superdegenerate models and the Hubbard model.

This work was supported in part by the Swiss National Foundation for Scientific Research under grants FN 2.683-0.85 (A. S.) and 2.042-0.86 (C. G.).

## REFERENCES

1. R. Peierls, *Proc. Camb. Philos. Soc.* **32**:427 (1936).
2. R. B. Griffiths, in *Phase Transition and Critical Phenomena*, Vol. 1, C. Domb and M. S. Green, eds. (Academic Press, New York, 1972).
3. Ya. G. Sinai, *Theory of Phase Transition, Rigorous Results* (Pergamon, New York, 1982).
4. J. Slawny, in *Phase Transition and Critical Phenomena*, Vol. 10, C. Domb and J. C. Lebowitz, eds. (Academic Press, New York, 1987).
5. A. Sütő, *J. Stat. Phys.* **23**:203 (1980); *Helv. Phys. Acta* **54**:191, 201 (1981); *J. Phys. A* **14**:2733 (1981); for a review see R. Liebmann, *Statistical Mechanics of Periodic Frustrated Ising Systems* (Springer, 1986).
6. E. I. Dinaburg and Ya. G. Sinai, *Commun. Math. Phys.* **98**:119 (1985); E. I. Dinaburg and A. E. Mazel, in *8th International Congress on Mathematical Physics*, M. Mebkhout and R. Sénéor, eds. (World Scientific, Singapore, 1987).
7. J. L. Lebowitz, M. K. Phani, and D. F. Styer, *J. Stat. Phys.* **38**:413 (1985).
8. J. Bricmont, K. Kuroda, and J. L. Lebowitz, *Commun. Math. Phys.* **101**:501 (1985).
9. J. Bricmont and J. Slawny, in *Statistical Mechanics and Field Theory: Mathematical Aspects* (Springer, 1986).
10. R. B. Griffiths, *Physica* **33**:689 (1967).
11. C. Gruber, A. Hintermann, and D. Merlini, *Group Analysis of Classical Lattice Systems* (Springer, 1977).
12. J. Bernasconi and F. Rys, *Phys. Rev. B* **4**:3045 (1977).
13. M. W. Capel, *Physica* **32** 966 (1966).
14. M. Blume, V. J. Emery, and R. B. Griffiths, *Phys. Rev. A* **4**:1071 (1971).
15. D. Mukamel and M. Blume, *Phys. Rev. A* **10**:610 (1974).

16. Z. Racz and T. Vicsek, *Phys. Rev. B* **27**:2992 (1983).
17. J. R. Banavard and F. Y. Wu, *Phys. Rev. B* **29**:1511 (1984).
18. Y. Saito, *J. Chem. Phys.* **74**:713 (1981).
19. J. Jedrzejewski, *Z. Phys. B* **59**:325 (1985).
20. V. Schmid, Etude Numérique du diagramme de phase du modèle de Hubbard, Diploma Thesis EPF-L (1986), unpublished.