*Journal of Statistical Physics, Vol. 47, Nos. 5/6, 1987*

# An Order-by-Order Construction of Low-Temperature Phase Diagrams for Classical Lattice Systems*

**Maciek Tarnawski**[1]

*Received October 31, 1986; revision received March 17, 1987*

An inductive algorithm is presented for the construction of phase diagrams by means of the low-temperature expansion technique. First the phase diagram is studied in the set of formal series. In each step, properties of this phase diagram are related to extremal elements of some family of convex sets. Approximations of the phase diagram in order $N$ are obtained by truncating all formal series at the $N$th term.

**KEY WORDS**: Low-temperature expansions; formal phase diagram; many ground states.

We consider a classical spin lattice system described by a finite-range Hamiltonian $H_0$. We assume that $H_0$ satisfies standard assumptions which secure the existence of the low-temperature expansion (LTE) of the pressure in boundary conditions given by any periodic ground state.[1] The system is perturbed by a one-parameter perturbation $L(x) = xL$, where $L$ is a classical finite-range Hamiltonian (the many-parameter case has been discussed in Ref. 2 for systems with a finite number of ground states). In the LTE technique, each phase is connected to a periodic ground state $G$ and it is characterized by a formal series:

$$\dot{\pi}^G(x) = -x \cdot e_G + \sum_{i=1}^{\infty} n_i^G(x) \cdot e^{-\beta E_i} \tag{1}$$

Here $e_G \equiv e_G(L)$ is the average energy of the perturbation per lattice site, evaluated at the ground state $G$, and the sum is the LTE of the pressure in

* This paper was presented at the Trebon, Czechoslovakia, Symposium September 1–6, 1986.

[1] Institute of Physics, Technical University, 50-370 Wroclaw, Poland.



0022-4715/87/0600-0757$05.00/0 

$G$ boundary conditions.[3] We assume that $e_{G_1} \neq e_{G_2}$ at least for one pair $G_1, G_2$ of periodic ground states ($L$ lifts partially the ground-state degeneracy).

We propose the following two-step construction of the phase diagram. In the first step one considers the problem in the formal series algebra $\mathbb{D}$. The ground state $G$ dominates at $\dot{x} \in \mathbb{D}$ if $\dot{\pi}^G(\dot{x}) \geqslant \dot{\pi}^{G'}(\dot{x})$ for all $G'$ different from $G$. The separation of $\mathbb{D}$ into regions of a single ground-state dominance defines the formal phase diagram (FPD). In the second step, the $N$th-order approximation of the FPD in $\mathbb{R}$ is obtained by truncating all formal series at the $N$th term. This procedure is equivalent to considering from the beginning the series (1) truncated at the $N$th term. In this report we restrict our attention to the problem of constructing the formal phase diagram. The construction is inductive in order of the LTE. The $N$th-order approximation is obtained by terminating induction at order $N$.

In order zero, we consider only the linear term of (1). Suppose that $\{-e_G\}$ attains its infimum at $G_0$ and its supremum at $\bar{G}_0$. Then $G_0$ dominates at $\dot{x}$ with $x_0 < 0$, and $\bar{G}_0$ at $\dot{x}$ with $x_0 > 0$. The subset $\mathbb{D}_0 = \{\dot{x}: x_0 = 0\}$ is left for the higher order analysis. In the zeroth-order approximation (equivalent to the zero-temperature phase diagram), this subset corresponds to the point $x = 0$ at which all ground states coexist.

In order $N$, we consider a subset $\mathbb{D}_N$ of $\mathbb{D}$ in which the lower order analysis has not determined regions of dominance. In the $(N-1)$th-order approximation, $\mathbb{D}_N$ corresponds to a point of coexistence with the associated subset of ground states coexisting there. In order to study the separation of $\mathbb{D}_N$ into regions of a single ground-state dominance, we truncate series (1) at order $N$ and evaluate it in $\mathbb{D}_N$. Then the nonlinear part is constant (correction terms are of higher order), and (1) reduces to an affine functional $(-e_G, A_N^G)$. Hence, the FPD inside $\mathbb{D}_N$ is determined by the phase diagram for a set of affine functionals. This problem has been studied in Ref. 2. The idea is to construct the set $W_N = \max \operatorname{conv}\{(-e_G, A_N^G)\}$, and then extremal properties of this set provide information about the phase diagram. In particular, each extremal edge defines a subset $\mathbb{D}_{N+1}$ and a corresponding subset of ground states, which are considered in the next order.

With the help of the algorithm presented in this paper we obtained the following results. For systems with a finite number of ground states, the construction describes asymptotic phase diagrams.[2] We have also considered a class of layered systems containing the ANNNI[4] and the three-state chiral Potts model,[5] and found a technical criterion for the LTE that governs the emergence of an infinite set of phases in the phase diagram.[6]

## REFERENCES

1. J. Slawny, in *Phase Transitions and Critical Phenomena,* Vol. 10, C. Domb and J. L. Lebowitz, eds. (Academic Press, New York).
2. M. Tarnawski, *J. Phys. A* **19**:3107 (1986).
3. C. Domb, *Adv. Phys.* **9**:149 (1960).
4. M. E. Fisher and W. Selke, *Phil. Trans. R. Soc.* **302**:1 (1981).
5. J. M. Yeomans and M. E. Fisher, *Physica* **127A**:1 (1984).
6. M. Tarnawski, *J. Phys. A*, submitted.