Journal of Statistical Physics, Vol. 64, Nos. 3/4, 1991

Metastability in the Potts Model on the Cayley Tree

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Received August 16, 1990; final February 20, 1991

Metastability in the ferromagnetic p-state Potts model defined on the Cayley tree is discussed. It is shown that the sign of the boundary field H_S determines the order of the transition as well as the stability of the low-temperature phase. Lowering the temperature with $H_S > 0$, a system with $p < 2$ ($p > 2$) will display a second (first)-order transition to a metastable (stable) phase. For $H_S < 0$ a second (first)-order transition to a metastable (stable) phase occurs if $p > 2$ ($p < 2$). In this case the system also has a residual entropy which is negative for $p < 2$.

KEY WORDS: Bethe–Peierls and Bragg–Williams maps; boundary condition; metastability; residual entropy.

1. INTRODUCTION

The nature of the phase transition occurring in the p-state ferromagnetic Potts model was first discussed by Kihara *et al.*[1] in the Bragg–Williams approximation. For $p > 2$ there is a first-order transition at the critical temperature $T_c(p)$, while for $p \leqslant 2$ there is a second-order transition at $T_c(2)$. Recently another classification scheme, where the transition is first order for all $p \neq 2$ and second order for $p = 2$, has emerged from the Bethe–Peierls approximation of the Potts model.[2] This result is obtained by studying the behavior of the system deep inside the Cayley tree (Fig. 1) and by using the criterion of selecting the solution of the self-consistency condition which gives the absolute minimum of the free energy in each phase. Recalling the fact that distinct cluster approximations[3] bear the same

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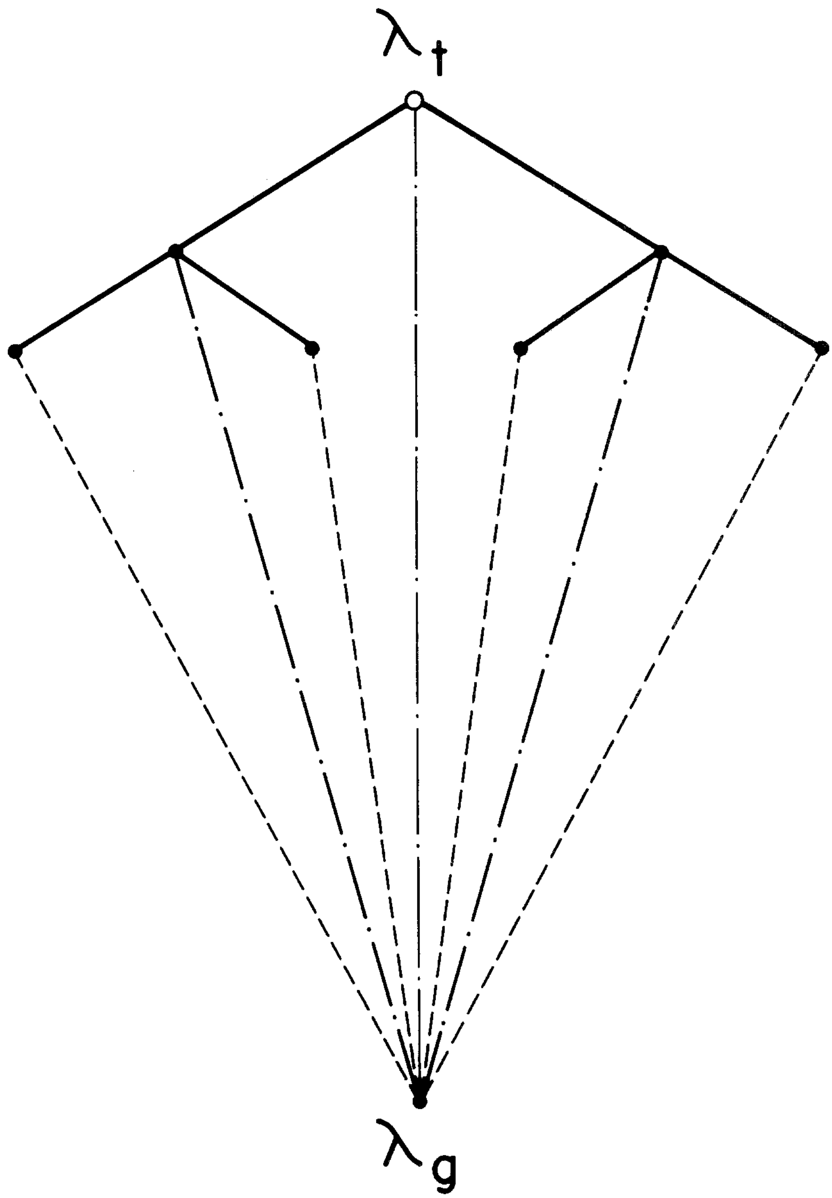


Fig. 1. A closed asymmetric Cayley branch with branching ratio $r = 2$ and with two generations. The branch with one more generation is obtained by replacing each dashed edge by the elementary cluster (cut diamond) which is formed by two solid edges representing the coupling J, two dashed edges representing the renormalized magnetic field H_N, and by the dot-dashed edge (bare magnetic field) connecting the ghost spin with the top spin in the diamond. The BP map given by Eq. (5) is obtained by calculating the effective interaction between the top and ghost spins in the cut diamond. The c.a.t is formed by connecting the top sites of three branches to an extra (central) site.

qualitative picture of a phase transition, we are led to conclude that the discrepancy between the classification schemes must not be attributed to the differences between the Bragg–Williams and the Bethe–Peierls approximations and that the explanation must be sought elsewhere.

In this paper the whole scenario where the above results can be accommodated is presented. This is accomplished by studying the effects of the sign of the boundary magnetic field H_S on the thermodynamic behavior of the system deep inside the Cayley tree. By exploring the hierarchical nature of the branches which compose the tree, a simple real-space renormalization group precedure is implemented. In this way we obtain a definite prescription to calculate the free energy, the renormalization group transformation which yields the self-consistency condition, and a criterion to select its solution. With this prescription we show that the initial condition of the renormalization group transformation is given by the boundary field H_S so that a different choice of the sign of H_S will give a different solution for the order parameter. As a consequence, phase transitions of different orders can be obtained. The classification scheme of Kihara *et al.* is recovered if the system is cooled in the presence of a positive H_S. To obtain the scheme of di Liberto *et al.*, one has to use the mixed boundary field H_S, which is positive for $p > 2$ and negative for $p < 2$. If, on the other hand, H_S is chosen to be negative, one obtains the reverse situation analyzed by Kihara *et al.*, i.e., the system with $p > 2$ will undergo a second-order transition at $T_c(2)$, while for $p < 2$ there is a first-order transition at $T_c(p)$. We have also observed that there is a region of nonphysical behavior with negative entropy in the stable phase of the system with $p < 2$. It is also shown that the low-temperature phase in the case of the first-order transitions is always the stable phase and that the coexisting metastable phase is reached if the system undergoes a second-order transition. These results are consolidated in Fig. 2.

2. THE FREE ENERGY AND THE BETHE–PEIERLS MAP

It is known that a classical spin model defined on the (loopless) Cayley tree is trivially solved having its partition function equal to that of the system defined on the open chain.[4] However, the problem of calculating the partition function becomes complex if a magnetic field is turned on. In the presence of a magnetic field the system on a Cayley tree can display two distinct kinds of behavior. As first shown for the Ising model,[5] the free energy possesses a characteristic field-dependent power term whose exponent varies with the temperature, leading to a peculiar transition of continuous order.[6] However, if the contribution to the free energy from the spins on the shells near the surface is suppressed, one recovers the Bethe–Peierls approximation, which describes the system behavior inside the tree. In order to obtain the Bethe–Peierls free energy we first calculate the free energy of the system put on the closed asymmetric tree (c.a.t) and then introduce a procedure to take into account the contribution from the surface spins.

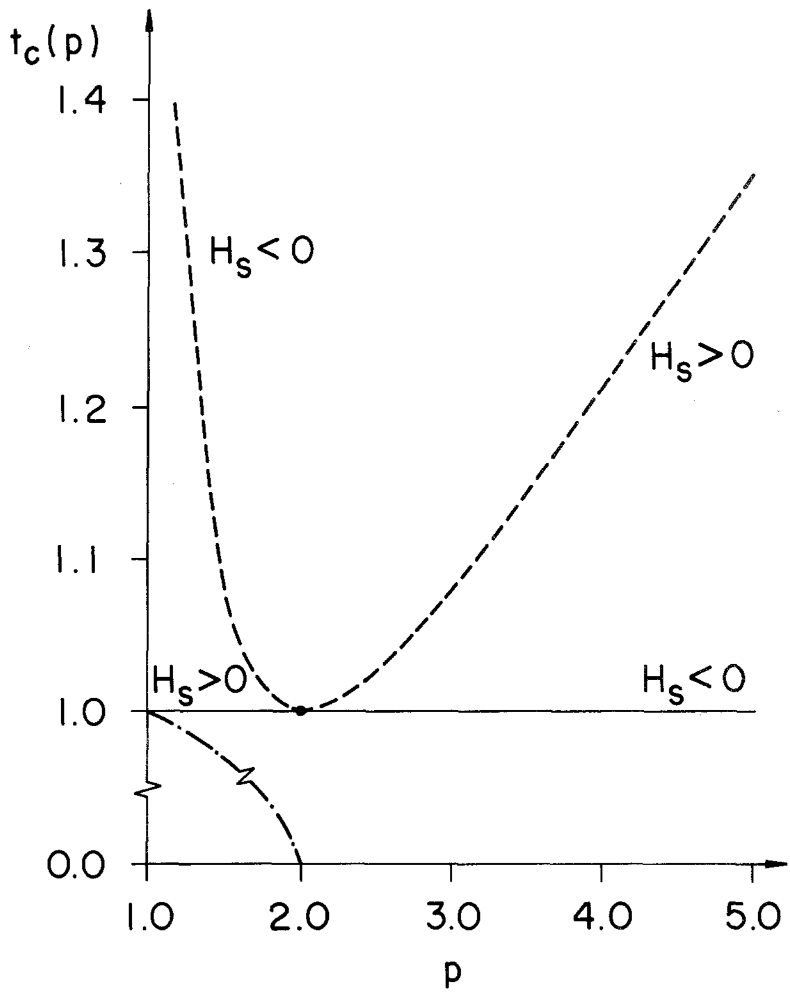


Fig. 2. The reduced transition temperature $t_c(p) = K_B T_C(p)/J$ (broken line) and $t_c(2) = K_B T_C(2)/J$ (solid line) as function of p. The transition at $t_c(p)$ [$t_c(2)$] is of first (second) order and the low-temperature free energy is an absolute (local) minimum. The sign of the boundary field to access these phases is indicated. Below the dashed-dotted curve $t_v(p)$ the (absolute minimum) free energy yields a negative entropy.

The system is defined by the Hamiltonian

$$\mathscr{H} = -pJ \sum_{\langle ij \rangle} \delta_{\lambda_i \lambda_j} - pH \sum_{i} \delta_{\lambda_i \lambda_g} - pH_S \sum_{s} \delta_{\lambda_s \lambda_g} \tag{1}$$

where $\lambda_i = 0, 1,..., p-1$ and δ is the Kronecker delta. The first summation is carried out over all n.n. pairs inside the tree, the second (third) summation is over all spins in the interior (surface) of the tree, and λ_g is the ghost spin. The advantages of introducing the c.a.t with the ghost spin are the following: (i) First, the bonds representing the interaction of the ghost spin with the other spins introduce loops in the lattice, making the system nontrivial. (ii) The closed asymmetric branches of the tree are hierarchical lattices. (iii) By freezing the ghost spins in one of its p states, in Eq. (1) one recovers the usual Hamiltonian of the model put on an open tree in the presence of a magnetic field. Finally, we observe that the partition function obtained from Eq. (1) is just p times larger than the partition function obtained when the ghost spin is frozen.

The derivation of the Bethe–Peierls free energy is carried out as follows. As the first step we calculate the partition function $Z_N(T, H, H_S; p, \sigma)$ of the system in a c.a.t with N generations (see Fig. 1) and coordination number σ. This is accomplished by freezing the central spin and those in the first generation and carrying out the summation over all other spins in the tree.[7] This is done for all possible configurations of the central spin and its neighbors λ_t. Adding all these contributions, we obtain

$$\begin{aligned} &Z_N(T, H, H_S; p, \sigma) \\ &\quad = h^{-1}[\omega^{-1} Z_N^b(\lambda_t = 0) + (p-1)\, Z_N^b(\lambda_t \neq 0)]^\sigma \\ &\qquad + (p-1)\{Z_N^b(\lambda_t = 0) + [\omega^{-1} + (p-2)]\, Z_N^b(\lambda_t \neq 0)\}^\sigma \end{aligned} \tag{2}$$

where

$$h = \exp -p\beta H, \qquad \omega = \exp -p\beta J \tag{3}$$

$Z_N^b(\lambda_t)$ is the partition function of the branch of the tree with N generations and having its top spin λ_t frozen in one of p possible states. Now a recursion relationship for $Z_N^b(\lambda_t)$ can be determined by exploring the fact that the branches are hierarchical lattices. By summing the spins on the surface of a branch with N generations the following recursive relationship between Z_N^b and Z_{N-1}^b is established:

$$\begin{aligned} &Z_N^b(T, H, H_S: p, \sigma, \lambda_t = \lambda) \\ &\quad = [h_S^1 + \omega^{-1} + (p-2)]^{(\sigma-1)^{(N-1)}}\, Z_{N-1}^b(T, H, H_1; p, \sigma, \lambda_t = \lambda) \end{aligned} \tag{4}$$

where h_s is obtained from Eq. (3) by substituting H by H_S. The renormalized field H_1, which acts on the surface spins of the branch with $N-1$ generations, is determined by the renormalization group transformation (Bethe–Peierls map)[8] given by

$$h_{i+1} = h\left(\frac{Ah_i + \omega}{Bh_i + 1}\right)^{\sigma - 1}, \qquad i = 0, 1, ..., N-1 \tag{5}$$

where

$$h_1 = \exp -p\beta H_1 \tag{6}$$

$$A = 1 + (p-2)\omega, \qquad B = (p-1)\omega \tag{7}$$

$$H_0 \equiv H_S \tag{8}$$

Having calculated the partition function for the whole tree, we now proceed to obtain the free energy deep inside the tree, therefore eliminating the contribution of the spins near and on the surface. This is accomplished by subtracting from the free energy $-K_B T \ln Z_{N+n}(T, H, H_S; p, \sigma)$ of a tree with $N+n$ generations the free energy $-(\sigma-1)^n K_B T \ln Z_N(T, H, H_S; p, \sigma)$ of $(\sigma-1)^n$ trees with N generations.[9] In the thermodynamic limit ($N \to \infty$) the dependence of the BP free energy density on n disappears and one obtains that

$$\begin{aligned} \beta f &= -[\ln Z_{N+n} - (\sigma-1)^n \ln Z_N] \\ &= -(\sigma-1)\ln(1 - tx^*) + \ln(1 - x^*) \\ &\quad + \left(\frac{\sigma-2}{2}\right)\ln[1 + (p-1)\, tx^{*2}] + \frac{\sigma}{2}\ln(1-t) - \ln p \end{aligned} \tag{9}$$

where

$$t = \frac{1-\omega}{1 + (p-1)\omega} \tag{10}$$

$$x^* = \frac{1 - h^*}{1 + (p-1)\, h^*} \tag{11}$$

and h^* is the attracting fixed point of the Bethe–Peierls map, which is obtained from Eq. (5) by letting $i \to \infty$. We notice that in this limit the BP map recovers the self-consistency condition. We want to stress that Eq. (9) refers only to the interior of the tree, since it involves the fixed point of the map. This is clear since starting from the surface each iteration take one step (generation) toward the interior of the tree such that in the limit

$i \to \infty$ the recursive relationship gives us the effective field deep inside the tree, i.e., infinitely far from the surface. Even though the contribution of the surface spins is suppressed from Eq. (9) the sign of the surface field is still relevant since it will determine the fixed point. This can be demonstrated observing first that the BP map is a rational map parametrized by the temperature, by the external field H, and by the number of states p of the Potts variable, and has its degree equal to $\sigma - 1$. The above statement concerning the effects of the initial condition H_S is supported by the following results from the theory of rational maps[10]:

(a) The number of attracting periodic orbits of a rational map $R(x)$ of degree $d \geqslant 2$ is at most $2d-2$. Since each attracting fixed point specifies a phase, the BP map with ferromagnetic interaction $J > 0$ has at most two attracting fixed points.

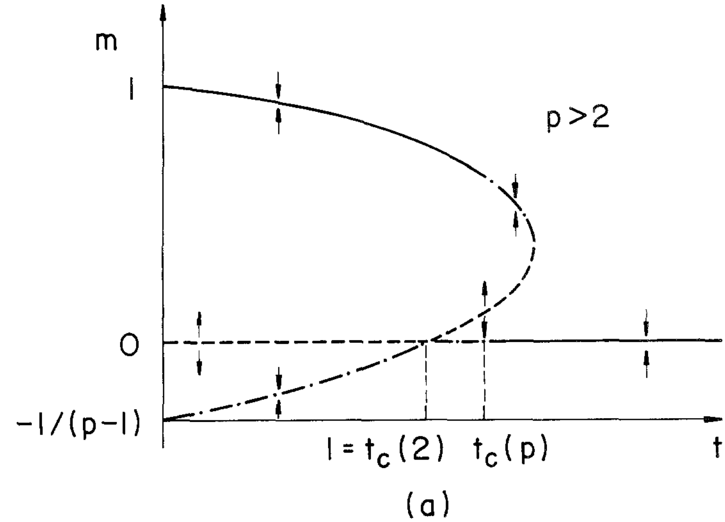
(b) The attracting orbits of a rational map $R(x)$ of degree $d \geqslant 2$ are contained in the Fatou set $F(R)$, while the repelling orbits are contained in the Julia set $J(R)$ which is the complement of $F(R)$.

(c) Let p be an attractive fixed point of $R(x)$. Then the attractive basin of p is the set $W^S(p) = \{x \mid R^n(x) \to p\}$ as $n \to \infty$ whose frontier is $J(R)$. The Julia set is also the closure of the set of repelling periodic points.

(d) The Fatou set, as well as the Julia set, is a completely invariant set, i.e., if $x \in F(R)$, then $R(x) \in F(R)$ and $R^{-1}(x) \subset F(R)$, where $R^{-1}(x)$ are the preimages of x. This means that once inside of an attracting basin (or on its border), a point will not leave it by an application of $R(x)$.

At high temperature the BP map has only one attracting basin, so that no matter what the sign is of the boundary (initial) field $H_0 = H_S$, the fixed point is the trivial paramagnetic $x^* = 0$ fixed point. For a certain range of H and T the self-consistent equation for x^* admits two other fixed points, one attracting and the other a repelling one which appear from a tangent bifurcation (Fig. 3). The sign and the strength of the surface field will determine the attracting basin in which we are starting in the recursive relationship. In other words, by determining in which attracting basin we are starting with, the boundary field also will determine the attracting fixed point of the BP map. Observing that these results are independent of the degree of the BP map we shall consider, for the sake of simplicity in carrying out numerical calculation, the limit of infinite coordination number $\sigma \to \infty$, $\lim_{\sigma \to \infty} J\sigma \to cte$ in Eqs. (5)–(11). In this limit the Bragg–Williams approximation of the free energy obtained by Kihara *et al.* is recovered,

$$\beta f = \beta J m^* + \ln(1 - m^*) + \frac{\beta J (p-1)(m^*)^2}{2} - \ln p - \frac{\beta J}{2} \tag{12}$$



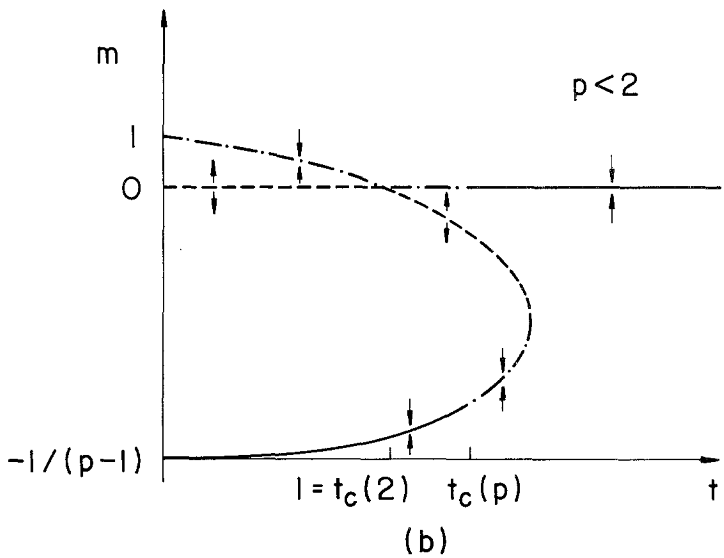


Fig. 3. Schematic plot of the zero-field, $H=0$ fixed points of the Bragg–Williams map [Eq. (13)] as a function of the reduced temperature $t=K_B T/J$. The solid, dashed-dotted, and dotted lines denotes the stable (absolute minimum free energy), metastable (local minimum free energy), and unstable (maximum free energy) phases. The arrows indicate the intervals where the fixed points are attractors or repellers.

where m^* is the fixed point of the Bragg–Williams map, which is a particular case of the Bethe–Peierls obtained in the infinite coordination limit,

$$m_{i+1} = W(T, H, p) = \frac{1 - e^{-\beta p(H + Jm_i)}}{1 + (p-1)\, e^{-\beta p(H + Jm_i)}} \tag{13}$$

$$Jm_1 = H_S; \qquad i = 1, 2,... \tag{14}$$

At $H = 0$ the fixed-point solutions of the Bragg–Williams map are shown in Figs. 3a and 3b. As shown by Kihara *et al.* the critical temperature $T_c(p)$ is obtained from the condition $f'(m) = 0$ and $f(m) = f(0)$, while the temperature $T_c(2)$ is obtained from the condition that the trivial paramagnetic fixed point $m^* = 0$ becomes indifferent. Using these condition and selecting first $H_S > 0$ and then $H_S < 0$, we have obtained the result plotted in Fig. 2.

Fixing the temperature and comparing the free energies obtained by using the different attracting fixing points of the BW, map we have verified that low-temperature phases of the first-order transition at $T_c(p)$ are the ones which give the absolute minima, while the low-temperature phases of the second-order transition are always the relative minima.

3. SUMMARY AND CONCLUSIONS

By combining Eq. (12), which gives the self-consistent free energy functional, with the Bragg–Williams map and its initial condition [Eqs. (13)–(14)], we obtain a clear prescription to obtain the thermodynamic behavior of the system. As a consequence of remark (d), an attrracting fixed point (phase) will be reached if and only if we start with a initial condition inside its basin, i.e., if we have picked up correctly the sign and strength of the surface field. Because of this property, the criterion of selecting the solution which gives the absolute minimum of the free energy can be relaxed. Any stable nonzero solution of the fixed-point equation is acceptable if it yields a thermodynamically sound behavior, i.e., if the free energy is a concave and a monotonically decreasing function of the temperature. For convenience we shall call convexity violation[11] the non-obedience of one or both of these properties of the free energy. Having the distinct free energies as functions of T, generated from the combination of Eq. (12) with the stable fixed points of Eq. (13), we obtain the following results:

(i) The transition at $T_c(p)$ is of first order. For $p > 2$ the low-temperature phase is an absolute minimum of the free energy. The system is well-behaved with a nonnegative specific heat and entropy which vanishes as $T \to 0$. For $p < 2$, although the free energy is an absolute minimum, the entropy becomes negative below $T_v(p)$ as indicated in Fig. 2.

(ii) The transition at $T_c(2)$ is of second order. There is no convexity violation for all p and the low-temperature phase is a local minimum of the free energy. For $p > 2$ there is a residual entropy $S/K_B = \ln(p-1)$.

(iii) The classification scheme of Kihara *et al.* is obtained using only the nonnegative stable fixed points $(H_S > 0)$.

(iv) The classification scheme of di Liberto *et al.* where the transitions are always of first order is obtained using $H_S > 0$ $(H_S < 0)$ for $p > 2$ $(p < 2)$. In the low-temperature phase, which is an absolute minimum of the free energy, one observes convexity violation (negative entropy) in a system with $p < 2$. In the Bethe–Peierls approximation (finite coordination number), besides the negative entropy at low temperature in the system with $p > 2$, the violation of convexity is also manifested in the low-temperature specific heat, which becomes negative for systems with $p < 2$.

In conclusion, we have discussed the nature of the phase transition as well as the physical behavior of the low-temperature phases of the ferromagnetic p-state Potts model in the Bethe–Peierls and in the Bragg–Williams approximations. It is shown that the sign of the boundary field is of vital importance, since the negative solution of the self-consistency equation may yield a free energy which violates convexity. In order to avoid nonphysical behavior it is argued that the criterion of nonviolation of convexity is hierarchically superior to the criterion of selecting the solution which yields the absolute minimum of the free energy.

ACKNOWLEDGMENTS

We would like to thank Dr. Roberto N. Onody for useful discussions during the course of this work.

REFERENCES

1. T. Kihara, Y. Midzuno, and T. Shizume, *J. Phys. Soc. Japan* **9**:681 (1954).
2. F. di Liberto, G. Monroy, and F. Peruggi, *Z. Phys. B* **66**:379 (1987).
3. J. S. Smart, *Effective Field Theories of Magnetism* (Saunders, Philadelphia, 1966).
4. T. P. Eggarter, *Phys. Rev. B* **9**:2989 (1974).
5. E. Müller-Hartmann and J. Zittartz, *Phys. Rev. Lett.* **33**:893 (1974).
6. Y. K. Wang and F. Y. Wu, *J. Phys. A* **9**:593 (1976).
7. C. J. Thompson, *J. Stat. Phys.* **27**:441 (1982).
8. P. L. Christiano and S. Goulart Rosa, Jr., *J. Phys. C* **18**:L407 (1985); A. S. Martinez and S. Goulart Rosa, Jr., *Phys. Rev. A* **38**:4304 (1988); F. S. de Aguiar, F. A. Bosco, A. S. Martinez, and S. Goulart Rosa, Jr., *J. Stat. Phys.* **58**:1231 (1990); F. S. de Aguiar and S. Goulart Rosa, Jr., *Phys. Lett. A* **143**:186 (1990).
9. H. G. Baumgärtel and E. Müller-Hartmann, *Z. Phys. B* **46**:227 (1982).
10. P. Blanchard, *Bull. Am. Math. Soc.* **11**:85 (1984).
11. R. B. Griffiths and P. D. Gujrati, *J. Stat. Phys.* **30**:563 (1983).