

A Rigorous Theory of Finite-Size Scaling at First-Order Phase Transitions

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A large class of classical lattice models describing the coexistence of a finite number of stable states at low temperatures is considered. The dependence of the finite-volume magnetization $M_{\text{per}}(h, L)$ in cubes of size L^d under periodic boundary conditions on the external field h is analyzed. For the case where two phases coexist at the infinite-volume transition point h_t , we prove that, independent of the details of the model, the finite-volume magnetization per lattice site behaves like

$$M_{\text{per}}(h_t) + M \tanh[ML^d(h - h_t)]$$

with $M_{\text{per}}(h)$ denoting the infinite-volume magnetization and $M = \frac{1}{2}[M_{\text{per}}(h_t + 0) - M_{\text{per}}(h_t - 0)]$. Introducing the finite-size transition point $h_m(L)$ as the point where the finite-volume susceptibility attains the maximum, we show that, in the case of asymmetric field-driven transitions, its shift is $h_t - h_m(L) = O(L^{-2d})$, in contrast to claims in the literature. Starting from the obvious observation that the number of stable phases has a local maximum at the transition point, we propose a new way of determining the point h_t from finite-size data with a shift that is exponentially small in L . Finally, the finite-size effects are discussed also in the case where more than two phases coexist.

KEY WORDS: First-order phase transitions; finite-size effects; universality of finite-size scaling; asymmetric first-order transitions; coexistence of several phases.

1. INTRODUCTION

The behavior of lattice systems at first-order transitions for finite lattices has been recently intensively studied.⁽¹⁻⁵⁾ The discontinuity that appears in

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the thermodynamic limit is smoothed for finite volumes. The widely accepted view is that the nature of this smoothing does not depend on the details of the model. For symmetrical models, like the Ising model, with the symmetry $h \leftrightarrow -h$ with respect to the ordering field h , the finite-size effects respect this symmetry. In fact, one expects that the magnetization M_{per} under periodic boundary conditions in a cube of size L behaves like

$$M_{\text{per}}(h, L) \sim M \tanh(M \cdot hL^d) \quad (1.1)$$

where M is the (infinte-volume) spontaneous magnetization and d is the dimension of the lattice (the inverse temperature β is included in h). This dependence follows already from the rough low-temperature approximation of the partition function

$$Z_{\text{per}}(h, L) \sim e^{hML^d} + e^{-hML^d} \quad (1.2)$$

There is a certain controversy in the literature once the models without such a symmetry are considered. It concerns both asymmetric field-driven transitions as well as temperature-driven transitions for the Potts model. Different versions of the formula (1.1) were obtained assuming different ansätze^(4,5) on equilibrium probability distribution $P_L(\psi)$ of the corresponding order parameter.

Our aim in this paper is not only to resolve this controversy, but, in general, to put the theory of finite-size effects on a rigorous footing. The theory presented here starts from the observation due to Borgs and Imbrie⁽⁶⁾ that the partition function (under periodic boundary conditions) of a model that describes the coexistence of N phases, $q = 1, \dots, N$, is well approximated⁴ by

$$Z_{\text{per}}(L, h) \cong \sum_{q=1}^N \exp(-f'_q L^d) \quad (1.3)$$

Here f'_q is some sort of “metastable free energy” of the phase q . It equals the equilibrium free energy f of the considered model whenever q is a stable phase; otherwise $f'_q > f$ and the phase q is exponentially damped in (1.3). As an implication, one can show that

$$\lim_{L \rightarrow \infty} \frac{Z_{\text{per}}(h, L)}{\exp(-\beta f L^d)} = N(h) \quad (1.4)$$

where $N(h)$ denotes the number of stable phases at the particular temperature and for the particular value of the (generalized) magnetic field h .

⁴ This result as well as the results of the present paper are valid for a large class of lattice models at low temperatures that can be rewritten in terms of contours with small activity.

The main idea of the present work is to substantiate the finite-size behavior [like than in (1.1)] by showing that the functions f'_q can be replaced by sufficiently smooth functions (for our purposes it is convenient to consider four-times differentiable functions) and by carefully estimating the involved errors. Considering the generalized magnetization

$$M_{\text{per}}(h, L) = \frac{1}{L^d} \frac{d \log Z_{\text{per}}(h, L)}{dh} \quad (1.5)$$

we can approximate it from (1.3) by

$$M_{\text{per}}(h, L) = \sum_{q=1}^N P_q(h) \cdot M_q(h) \quad (1.6)$$

with

$$M_q = -\frac{df'_q}{dh} \quad \text{and} \quad P_q = \frac{\exp(-f'_q L^d)}{\sum_{m=1}^N \exp(-f'_m L^d)}$$

Expanding now P_q and M_q around the point $h^{(0)}$ of coexistence of all phases, we get the finite-size effects in the case of the multiple phase coexistence. To our knowledge, the closed formula for the finite-size behavior around the point of coexistence of more than two phases has not been considered before in the literature (with a possible exception of the Potts models, where, however, all the ordered phases are linked by a symmetry).

In the particular case of coexistence of two phases, we get for $M_{\text{per}}(h, L)$, also in a nonsymmetric case, a formula that resembles (1.1). The (infinite-volume) coexistence point h_t may be shifted due to finite-size effects. One can imagine different ways to locate the point h_t from (say, Monte Carlo) data for a finite cube. An obvious possibility is to consider the point $h_m(L)$ where the finite-volume susceptibility $\chi_{\text{per}}(h, L)$ is maximal. We prove that this point is shifted by a term proportional to L^{-2d} with respect to h_t (the shift predicted in ref. 5 is proportional to L^{-d}). It turns out that a more natural and also more accurate estimate can be gained by considering a finite-size approximation $N(h, L)$ of the number of phases $N(h)$ as given by (1.4). Observing that the number of phases has a local maximum at the coexistence point h_t [actually, it abruptly jumps from $N(h) = 1$ for $h \neq h_t$ to $N(h_t) = 2$], we define $h_t(L)$ as the point where the function $N(h, L)$ attains the maximum. It can be shown that it is, in fact, the point where

$$M_{\text{per}}(h, L) = M_{\text{per}}(h, 2L) \quad (1.7)$$

and that its shift with respect to the infinite-volume value h_t is exponentially small in dependence on L .

Before summarizing the content of the paper, we stress two points. First, in the case of asymmetric first-order transitions it is not essential whether they are field driven or temperature driven. Thus, the parameter h actually may be replaced by β and the methods of the present work can be used also for, e.g., the Potts model.⁽⁷⁾ Second, the class of models that can be treated contains not only standard lattice models with finite numbers of spin states, but covers also first-order transitions for some models with “continuous spin” such as $P(\varphi)_2$ models (both on a lattice and a continuous space-time)⁽⁸⁾ or lattice Higgs $U(n)$ models with large n .⁽⁹⁾

We start in Section 2 by introducing the class of models to be studied. Then we show how to introduce the smooth functions f'_q . Some proofs are delegated to the Appendix. Section 3 is devoted to a detailed discussion of finite-size effects in the case of coexistence of two phases and to the evaluation of shifts of several finite-volume transition points. The proofs are collected in Section 4. The general case of multiphase coexistence is studied in Section 5.

2. CONTOUR MODELS, TRUNCATED PARTITION FUNCTIONS, STABLE AND UNSTABLE PHASES

In this section we introduce a class of models describing the systems we want to analyze. Following refs. 6, 10, and 11, we then introduce certain truncated contour models that on one hand can be analyzed by convergent cluster expansions and on the other hand agree with the original model for stable boundary conditions. The truncated partition functions and their free energies will play an important role in the analysis of this paper.

2.1. Definition of the Model

We start with the definition of the partition function $Z_q(V)$ in a region V with boundary condition $q \in Q = \{1, 2, \dots, N\}$. The index q labels the possible “ground states” of the system, and V is a finite union of unit cubes in \mathbb{R}^d , with $d \geq 2$. We use the notation V^q to indicate boundary conditions q on V , and to each ground state $q \in Q$ we associate a “ground-state energy” $e_q \in \mathbb{R}$. We define $Z_q(V)$ as a sum over contours Y in V , so we begin by defining these objects.

A contour is a pair $(Y, q(\cdot))$ where Y is a connected union of closed unit cubes and $q(\cdot)$ is an assignment of labels $q(F) \in Q$ to the boundaries F of the components C of $Y^c = \mathbb{R}^d \setminus Y$. If $q(\cdot) = q$ on the external boundary component of Y , we call Y a q -contour and we sometimes emphasize this

by a superscript q on Y . To simplify formulas, we use the symbols Y or Y^q to denote the pair $(Y, q(\cdot))$ as well as the region Y . We use $\text{Int}_m Y$ to denote the union of all finite components C of Y^c for which $q(\partial C) = m$, and write $\text{Int } Y = \bigcup_{m=1}^N \text{Int}_m Y$, $V(Y) = \text{Int } Y \cup Y$. Finally, each contour Y has a translation-invariant activity $\rho(Y) \in \mathbb{R}$ satisfying the following bound for some large τ :

$$|\rho(Y^q)| \leq \exp[-(\tau + e_0) |Y^q|] \quad (2.1)$$

Here $|Y^q|$ denotes the volume of Y^q and e_0 is defined as the energy of the lowest ground state,

$$e_0 = \min_q e_q \quad (2.2)$$

An allowed configuration of our system is a collection $\{Y_\alpha\}$ of non-overlapping⁵ contours with compatible boundary labels. The compatibility is determined by the requirement that any connected component of $V \setminus \bigcup_\alpha Y_\alpha$ has constant boundary conditions. In addition, we require that the distance of Y_α and ∂V^q is greater than or equal to one for all contours Y_α . If the complement V^c of V is not connected, we do not allow contours whose interior intersects V^c . Given a collection of contours, we finally attach energy densities to the regions occupied by each phase of the model. A connected component of $V \setminus \bigcup_\alpha Y_\alpha$ that has boundary condition m is considered to be part of R_m , the region “in the m th phase.” Thus, we have partitioned $V \setminus \bigcup_\alpha Y_\alpha$ as $\bigcup_m R_m$. Associating the energy density e_m with the region R_m , we get the expression for the partition function:

$$Z_q(V) = \sum_{\{Y_\alpha\}} \prod_\alpha \rho(Y_\alpha) \prod_{m=1}^N \exp(-e_m |R_m|) \quad (2.3)$$

The connection between this partition function and the Peierls contour picture of spin systems is clear—we have just replaced sites with cubes and thickened contours to include neighboring cubes.

The magnetic fields are introduced as real parameters $\{h_i\}$ on which the activities ρ and the energies e_q may depend. There should be at least $N-1$ such parameters, and we need a degeneracy-breaking condition. Namely, we suppose that the matrix

$$E = \left(\frac{d}{dh_i} (e_q - e_N) \right)_{q,i=1,\dots,N-1} \quad (2.4)$$

⁵ Since contours were defined as union of *closed* unit cubes, this condition is equivalent to the condition that $\text{dist}(Y_\alpha, Y_\beta) \geq 1$ for all $\alpha \neq \beta$.

is nonsingular. We further assume that ρ and e_q are C^4 functions of $h = (h_1, \dots, h_{N-1})$ satisfying the bounds

$$\left| \frac{d^k e_q}{dh^k} \right| \leq C_k \quad (2.5)$$

$$\left| \frac{d^k \rho(Y)}{dh^k} \right| \leq C_k e^{-(\tau + \epsilon_0)|Y|} \quad (2.6)$$

$$\|E^{-1}\|_\infty \equiv \max_i \sum_q |(E^{-1})_{iq}| \leq \text{const} < \infty \quad (2.7)$$

where the constants are independent of τ and $k: \{1, \dots, N-1\} \rightarrow \{0, 1, \dots\}$ is a multi-index of order $|k| \equiv \sum k_i$ between⁶ 1 and 4. We also assume that

$$e_q(h=0) = e_{\tilde{q}}(h=0) \quad \text{for all } q, \tilde{q} \in Q \quad (2.8)$$

For many purposes we need a second expression for $Z_q(V)$ which eliminates the compatibility of boundary conditions on contours. To this end, we first sum in (2.3) over all sets $\{Y_\alpha\}$ with a fixed collection of external contours (those that are not contained in $\text{Int } Y_\alpha$ for any α). For each external contour Y^q (external contours in V^q must of course have boundary condition q) this resummation produces a factor $Z_m(\text{Int}_m Y^q)$. This yields the expression

$$Z_q(V) = \sum_{\{Y_\alpha^q\}_{\text{ext}}} \prod_\alpha \left[\rho(Y_\alpha^q) \prod_m Z_m(\text{Int}_m Y_\alpha^q) \exp(-e_q |\text{Ext}|) \right] \quad (2.9)$$

where the sum runs over sets $\{Y_\alpha^q\}_{\text{ext}}$ of mutually external contours, i.e., $Y_\alpha \cup \text{Int } Y_\alpha$ and $Y_{\alpha'} \cup \text{Int } Y_{\alpha'}$ do not overlap for $\alpha' \neq \alpha$. Also, we have denoted $\text{Ext} = V \setminus \bigcup_\alpha \text{Int}_m Y_\alpha^q$. Assuming that $Z_q(\text{Int}_m Y_\alpha^q) \neq 0$, we divide each Z_m by the corresponding Z_q and multiply it back again in the formula (2.9). Iterating the same procedure on the terms $Z_q(\text{Int}_m Y_\alpha^q)$, we eventually get

$$\begin{aligned} Z_q(V) &= [\exp(-e_q |V|)] \sum_{\{Y_\alpha^q\}} \prod_\alpha \left\{ \rho(Y_\alpha^q) [\exp(e_q |Y_\alpha^q|)] \prod_m \frac{Z_m(\text{Int}_m Y_\alpha^q)}{Z_q(\text{Int}_m Y_\alpha^q)} \right\} \\ &\equiv [\exp(-e_q |V|)] \sum_{\{Y_\alpha^q\}} \prod_\alpha K(Y_\alpha^q) \end{aligned} \quad (2.10)$$

The only conditions on the collections $\{Y_\alpha^q\}$ are that the contours do not overlap and all have outer boundary q . The expression (2.10) is useful for

⁶ The reason why we take the derivatives up to namely fourth order here is that eventually we will use such a condition to evaluate the location of the maximum of the susceptibility; see Section 4.

stable q (defined below), while (2.9) is better for unstable q in view of possible zeros of $Z_q(\text{Int}_m Y_\alpha^q)$.

Remark (i). For the Ising models defined in Section 1, $N=2$. The parameter τ can be chosen as $O(\beta)$, and the magnetic field H of these models is related to the magnetic field defined in this section by $h = \beta H$.

2.2. Truncated Partition Functions, Stable and Unstable Phases

We are going to define truncated contour activities $K'(Y^q)$ and the corresponding partition functions

$$Z'_q(V) = [\exp(-e_q |V|)] \sum_{\{Y_\alpha^q\}} \prod_{\alpha} K'(Y_\alpha^q) \quad (2.11)$$

in such a way that

(i) $\log Z'_q(V)$ and the corresponding (infinite-volume) free energy f'_q can be analyzed by a convergent cluster expansion, and

(ii) $Z'_q(V) = Z_q(V)$ if $f'_q = f \equiv \min_{m \in Q} f'_m$, so that the truncated model is identical to the original model if $f'_q = f$ (following ref. 10, we call these q “stable”).

A possible choice, essentially identical to that of ref. 6, would be the definition $K'(Y) = K(Y)$ if $|K(Y)| \leq e^{-(r-8d)|Y|}$ and $K'(Y) = 0$ otherwise. This definition leads to truncated partition functions obeying the above conditions (i) and (ii), but the corresponding free energies f'_q will not be smooth functions of the magnetic fields h . While this was of no importance in the context of ref. 6, it would be inconvenient for us. We therefore prefer a different definition, motivated by ref. 11.

We proceed by induction. Assuming that $K'(Y)$ has already been defined for all contours Y with $\text{diam } Y < n$, $n \in \mathbb{N}$, and that it obeys a bound

$$|K'(Y)| \leq \varepsilon^{|Y|} \quad (2.12)$$

for some small ε , the truncated partition functions $Z'_m(V)$ are defined for all q and all volumes V with $\text{diam } V \leq n$. Their logarithm can be controlled by a convergent cluster expansion and $Z'_m(V) \neq 0$ for all $m \in Q$. We then define $K'(Y^q)$ for q -contours of diameter n by

$$K'(Y^q) = \chi'(X_q) \rho(Y^q) [\exp(e_q |Y^q|)] \prod_m \frac{Z'_m(\text{Int}_m Y^q)}{Z'_q(\text{Int}_m Y^q)} \quad (2.13a)$$

$$\chi'(Y^q) = \prod_m \chi(\log |Z'_q(V(Y^q))| - \log |Z'_m(V(Y^q))| + \alpha |Y^q|) \quad (2.13b)$$

where α will be chosen later and χ is a smoothed characteristic function. We assume that χ has been defined in such a way that χ is a C^4 function that obeys the conditions

$$0 \leq \chi(x) \leq 1 \quad (2.14a)$$

$$\chi(x) = 0 \quad \text{if } x \leq -1, \quad \chi(x) = 1 \quad \text{if } x \geq 1 \quad (2.14b)$$

$$0 \leq \frac{d}{dx} \chi(x) \leq 1 \quad (2.14c)$$

$$\left| \frac{d^k}{dx^k} \chi(x) \right| \leq \tilde{C}_k \quad \text{for } 0 \leq k \leq 4 \quad (2.14d)$$

where the constants \tilde{C}_k depend only on k .

As the final element of the construction of K' , we have to establish the bound (2.12) for $\text{diam } Y = n$. We defer the proof, together with the proof of the following Lemma 2.1, to the Appendix. We use f'_q to denote the free energy corresponding to the partition function Z'_q ,

$$f'_q = - \lim_{V \rightarrow \mathbb{Z}^d} \frac{1}{|V|} \log Z'_q(V) \quad (2.15)$$

and f, a_q are defined by

$$f = \min_m f'_m \quad (2.16)$$

$$a_q = f'_q - f \quad (2.17)$$

Lemma 2.1. Assume that $|\rho(Y^q)| \leq \exp[-(\tau + e_0)|Y^q|]$ for all possible q -contours Y^q . Then there exists a constant τ_0 (depending only on d and N) such that, for $\tau \geq \tau_0$ and $0 \leq \alpha - 3 \leq \tau - \tau_0$, the contour activities $K'(Y)$ are well defined for all Y and obey (2.12) with $\varepsilon = \exp[-(\tau - 2d - 2 - \alpha)]$. In addition, the following statements hold for $\tau \geq \tau_0$ and $0 \leq \alpha - 3 \leq \tau - \tau_0$:

- (i) $|Z_q(V)| \leq \exp(-f|V| + |\partial V|)$.
- (ii) If $a_q \text{diam } Y^q \leq \alpha - 2$, then $K(Y^q) = K'(Y^q)$.
- (iii) If $a_q \text{diam } V \leq \alpha - 2$, then $Z_q(V) = Z'_q(V)$.

Remark (ii). Due to the bound (2.12), the partition function $Z'_q(V)$ can be analyzed by a convergent cluster expansion, and

$$|\log Z'_q(V) + f'_q |V|| \leq O(\varepsilon) |\partial V| \quad (2.18)$$

$$|f'_q - e_q| \leq O(\varepsilon) \quad (2.19)$$

Remark (iii). Due to Lemma 2.1(iii), $Z_q(V)$ and $Z'_q(V)$ are equal if $a_q = 0$. One therefore says that q is stable if $a_q = 0$.

We finally turn to the continuity properties of Z_q and Z'_q . As a finite sum of C^4 functions, $Z_q(V)$ is a C^4 function of h . The following lemma gives a bound on the derivative of $Z_q(V)$.

Lemma 2.2. Assume that $\tau > \tau_0$. Then

$$\left| \frac{d^k}{dh^k} [Z_q(V) \exp(e_q |V|)] \right| \leq O(\exp(-\tau)) |V|^{|k|} \exp[(e_q - f) |V| + |\partial V|]$$

for all multi-indices k of order $1 \leq |k| \leq 4$.

Lemma 2.3. There are constants τ_0 and $K < \infty$ such that, for $\tau > \tau_0$ and $0 \leq \alpha - 3 \leq \tau - \tau_0$, $K'(Y^q)$ and $\log Z'_q(V)$ are C^4 functions of h , and

$$\left| \frac{d^k}{dh^k} K'(Y^q) \right| \leq (K\varepsilon)^{|Y^q|}$$

for all multi-indices k of order $|k| \leq 4$.

Proof. The proofs of these lemmas are given in the Appendix.

Remark (iv). By Lemma 2.3, $s_q = f'_q - e_q$ is a C^4 function of h and

$$\left| \frac{d}{dh_i} (f'_q - e_q) \right| \leq O(\varepsilon) \tag{2.20}$$

Using the *a priori* assumption (2.7), we conclude that

$$F = \left(\frac{d}{dh_i} (f'_q - f'_N) \right)_{q,i=1,\dots,N-1} \tag{2.21}$$

obeys a bound of the form (2.7) as well, with a slightly larger constant on the right-hand side; when one combines this with the inverse function theorem, one immediately obtains the existence of a point h_t for which all a_q are zero, i.e., all b.c. are stable; more generally, one may construct differentiable curves $h_q(t)$ going out of h_t , on which only q is unstable, surfaces $h_{q\bar{q}}(t, s)$ on which q, \bar{q} are unstable, etc. A possible parametrization of these curves, surfaces, etc., is given by $a_m(h_q(t)) = \delta_{mq} t$, $a_m(h_{q\bar{q}}(t, s)) = \delta_{mq} t + \delta_{m\bar{q}} s, \dots$

Remark (v). In the literature, one often assumes a bound of the form (2.1) with e_0 replaced by e_q . As one may see from (2.5), (2.7), and (2.8), such a bound will usually hold only in a neighborhood of diameter $O(\tau)$ of $h = 0$. Outside this neighborhood, one then has to distinguish between

states q for which $e_q - e_0 \leq O(\tau)$ and those for which $e_q - e_0 > O(\tau)$; the notion of a contour is then redefined in such a way that regions corresponding to a ground state q with $e_q - e_0 > O(\tau)$ are part of a contour. Our procedure avoids this procedure of redefining contours.

Remark (vi). For the rest of this paper we choose $\alpha = \tau/2$. As a consequence,

$$\left| \frac{d^k}{dh^k} K'(Y^q) \right| \leq e^{-(\tau/4)|Y^q|}$$

for all multi-indices k of order $|k| \leq 4$; and $K'(Y^q) = K(Y^q)$ if $a_q \text{ diam } Y^q \leq \tau/4$.

3. COEXISTENCE OF TWO PHASES

In this section we state our results for the finite-volume magnetization with periodic boundary conditions. We consider models defined on a d -dimensional torus T with sides of length L in each direction, whose partition function can be written as

$$Z_{\text{per}}(T) = \sum_{\{Y_\alpha\}} \prod_m [\exp(-e_m |R_m|)] \prod_\alpha \rho(Y_\alpha) \quad (3.1)$$

Contours are again $(Y, q(\cdot))$, where Y is a connected union of closed unit cubes in T and $q(\cdot)$ is an assignment of $q(F) \in Q$ to the boundaries F of the components C of $Y^c = T \setminus Y$. And R_m is again the union of all components of $T \setminus \bigcup_\alpha Y_\alpha$ which have the boundary condition m . For contours Y with

$$\text{diam } Y \leq L/3 \quad (3.2)$$

we call them *small* in this section, it is clear which component of $T \setminus Y$ is the exterior, $\text{Ext } Y$, of Y ; and $\text{Int } Y = T \setminus (Y \cup \text{Ext } Y)$ may be decomposed in the same way as before: $\text{Int } Y = \bigcup_m \text{Int}_m Y$.

We will assume that the activities $\rho(Y)$ of the small contours are the same as those introduced in Section 2 (in particular, $\rho(Y)$ is translation invariant, and does not depend on L as long as $L \geq 3 \text{ diam } Y$). We do not need any special properties of the activity ρ for large contours, apart from the condition that

$$|\rho(Y)| \leq \exp[-(\tau + e_0)|Y|] \quad (3.3a)$$

and

$$\left| \frac{d^k}{dh^k} \rho(Y) \right| \leq C_k \exp[-(\tau + e_0)|Y|] \quad (3.3b)$$

Now, we restrict ourselves to the case of two ground states, $Q = \{-1, +1\}$. We assume the bounds (2.1) and (2.5)–(2.7) for some large τ , and denote by h_t the magnetic field corresponding to the coexistence point; see Remark (iv) of Section 2. We suppose also that signs have been chosen in such a way that

$$\frac{d}{dh}(e_+ - e_-) < 0 \quad (3.4)$$

so that $+$ is stable for $h \geq h_t$ and $-$ is stable for $h \leq h_t$. We introduce further the infinite-volume magnetizations,

$$M_{\pm}(h) = \lim_{V \rightarrow \mathbb{Z}^d} \frac{1}{|V|} \frac{d}{dh} \log Z_{\pm}(V) \quad (3.5)$$

where $Z_{\pm}(V)$ are the partition functions introduced in the last section, and the finite-volume magnetization with periodic boundary conditions,

$$M_{\text{per}}(h, L) = \frac{1}{L^d} \frac{d}{dh} \log Z_{\text{per}}(T) \quad (3.6)$$

Note that $M_+(h)$ can be analyzed by a convergent cluster expansion if $h \geq h_t$, while for $M_-(h)$ we have a convergent cluster expansion if $h \leq h_t$.

Remark (i). As a finite sum of C^4 functions, $Z_{\text{per}}(T)$ is a C^4 function. Therefore $M_{\text{per}}(h, L)$ is well defined as long as $Z_{\text{per}}(T) \neq 0$.

The following lemma, together with Theorem 3.2 below, is proven in Section 4.

Lemma 3.1. For $\tau > \tau_0$, where $\tau_0 < \infty$ is a constant that depends only on d , the following statements are true:

- (i) $M_{\text{per}}(h, L)$ is well defined for all $L \in \mathbb{N}$.
- (ii) The limit $M_{\text{per}}(h) = \lim_{L \rightarrow \infty} M_{\text{per}}(h, L)$ exists and

$$M_{\text{per}}(h) = \begin{cases} M_-(h) & \text{for } h < h_t, \\ \frac{1}{2}[M_-(h) + M_+(h)] & \text{for } h = h_t, \\ M_+(h) & \text{for } h > h_t, \end{cases} \quad (3.7)$$

Remark (ii). Lemma 3.1 is an immediate generalization of a theorem proven in ref. 6, which states that the quantity

$$Z_{\text{per}}(h, L) e^{f(h)L^d}$$

goes to the number $N(h)$ of stable phases⁷ as $L \rightarrow \infty$ [we use $f(h)$ to denote the free energy].

We now turn to the finite-volume behavior of $M_{\text{per}}(h, L)$. We introduce the susceptibilities

$$\chi_{\pm} = \left. \frac{dM_{\pm}(h)}{dh} \right|_{h=h_t \pm 0} \quad (3.8)$$

and the constants

$$M_0 = \frac{M_+(h_t) + M_-(h_t)}{2} \quad (3.9a)$$

$$M = \frac{M_+(h_t) - M_-(h_t)}{2} \quad (3.9b)$$

Note that $M_0 = 0$ and $\chi_+ = \chi_-$ for a system with $+/-$ symmetry.

Theorem 3.2. There exist constants $\tau_0 < \infty$, $K_0, K_1 < \infty$, and $b_0 > 0$ such that the following statements are true for $\tau > \tau_0$.

$$(i) \quad |M_{\text{per}}(h, L) - M_{\text{per}}(h)| \leq e^{-b_0\tau L} + K_0 e^{-b_0|h-h_t|L^d} \quad (3.10)$$

$$(ii) \quad M_{\text{per}}(h, L) = M_0 + \frac{\chi_+ + \chi_-}{2} (h - h_t) + \left[M + \frac{\chi_+ - \chi_-}{2} (h - h_t) \right] \\ \times \tanh \left\{ L^d \left[M(h - h_t) + \frac{\chi_+ - \chi_-}{4} (h - h_t)^2 \right] \right\} \\ + R(h, L) \quad (3.11a)$$

with an error $R(h, L)$ bounded by

$$|R(h, L)| \leq e^{-b_0\tau L} + K_1 |h - h_t|^2 \quad (3.11b)$$

Remark (iii). Both bounds (3.10) and (3.11) of Theorem 3.2 are true for all h . The bound (3.10), however, is better if $|h - h_t|$ is large, whereas (3.11) is better if $|h - h_t|$ is small. The overlap, where both of them are nontrivial, is the region $L^{-d} \ll |h - h_t| \ll 1$.

Remark (iv). For a system with $+/-$ symmetry, $h_t = 0$, $M_0 = 0$, and $\chi_+ = \chi_- = \chi$; therefore Theorem 3.2 implies that

$$M_{\text{per}}(h, L) = \chi h + M \tanh(MhL^d) + O(h^2) + O(e^{-b_0\tau L}) \quad (3.12)$$

⁷ For the models with two ground states considered in this section, $N(h)$ is one for $h \neq h_t$ and two for $h = h_t$.

We finally discuss the shift of the coexistence point h_t due to finite-size effects. Since the order parameters have no discontinuities in finite volumes, there are several possible definitions of the coexistence point for finite L . We consider the point $h_m(L)$ where the finite-volume susceptibility

$$\chi_{\text{per}}(h, L) = \frac{dM_{\text{per}}(h, L)}{dh} \quad (3.13)$$

is maximal, the point $h_0(L)$ where $M_{\text{per}}(h, L) = M_0$, and the point $h_t(L)$ where the finite-volume approximation

$$N(h, L) = \left[\frac{Z_{\text{per}}(h, L)^{2^d}}{Z_{\text{per}}(h, 2L)} \right]^{1/(2^d - 1)} \quad (3.14)$$

to the number $N(h)$ of stable phases [see Remark (ii) after Lemma 3.1] is maximal. Since the function $M_{\text{per}}(h) - M_0$ may have additional zeros as $h \rightarrow \pm\infty$ in the abstract context considered here, one must restrict h to a certain neighborhood of h_t to ensure that $h_0(L)$ is well defined.

Theorem 3.3. There are constants $\delta > 0$ and $L_0 < \infty$ such that the following statements are true for $L > L_0$ and $\tau > \tau_0$.

(i) There is exactly one point $h_m(L)$ such that

$$\chi_{\text{per}}(h_m(L), L) > \chi_{\text{per}}(h, L) \quad \text{for all } h \neq h_m(L)$$

and

$$h_m(L) = h_t + \frac{3(\chi_+ - \chi_-)}{4M^3L^{2d}} + O(L^{-3d}) \quad (3.15)$$

(ii) There is exactly one point $h_0(L)$ in the interval $[h_t - \delta, h_t + \delta]$ such that $M_{\text{per}}(h_0(L), L) = M_0$; and

$$|h_0(L) - h_t| \leq O(e^{-b\tau L}) \quad (3.16)$$

(iii) There is exactly one point $h_t(L)$ such that

$$N(h_t(L), L) > N(h, L) \quad \text{for all } h \neq h_t(L)$$

and, for this point,

$$|h_t(L) - h_t| \leq O(e^{-b\tau L}) \quad (3.17)$$

Remark (v). The fact that $h_m(L)$ contains no corrections of $O(L^{-d})$ is a peculiarity of the coexistence of two states. If h_0 is a point where more

than two phases coexist, $h_m(L)$ may be shifted by an amount $O(L^{-d})$; see Section 5.

Remark (vi). The theorem shows that $h_0(L)$ and $h_i(L)$ are much better approximations for h_t than $h_m(L)$. Since M_0 is not known *a priori*, and since the definition of $h_0(L)$ is less obvious for systems with more than two ground states, we propose to use $h_i(L)$ for a numerical determination of the coexistence point. Note that it is not necessary to calculate the partition function itself to determine $h_i(L)$, because the local maxima of $N(h, L)$ correspond to the points h for which $M_{\text{per}}(h, L) = M_{\text{per}}(h, 2L)$.

Remark (vii). Some time ago, Binder and Landau developed a heuristic theory of finite-size scaling at first-order phase transitions, assuming that the probability distribution $p_L(\cdot)$ of the finite-volume magnetization is well approximated by a sum of two Gaussians. The relative height of these Gaussians was chosen in such a way that the *area* under both peaks of p_L is equal for $h = h_t$.⁽¹⁴⁾ Binder and Landau derived a formula for $M_{\text{per}}(h, L)$ [formula (25) of ref. 4] which is exactly our formula (3.11a), except for the error term, which cannot be systematically estimated in their theory. Later, Binder *et al.* “corrected” this theory, assuming now that for $h = h_t$ both peaks of $p_L(\cdot)$ have equal *height*, and predicting a shift $h_m(L) - h_t = O(L^{-d})$ if $\chi_+ \neq \chi_-$.⁽⁵⁾ As we know from ref. 6 (see also Theorem 4.1, Section 4), this assumption is unreasonable, because at $h = h_t$ both phases contribute to $Z_{\text{per}}(h, L)$ with equal weight $\exp[-f(h)L^d]$, except for exponentially small errors. And this corresponds to equal “*areas*,” not equal heights. This explains the discrepancy between their formulas and ours.

4. PROOF OF LEMMA 3.1, THEOREM 3.2, AND THEOREM 3.3

All results of Section 3 are based on the following theorem. Since the proof of the theorem does not depend on the fact that there are only two ground states, we formulate it for the general system with N ground states, $Q = \{1, \dots, N\}$. We define $M_{\text{per}}^i(h, L)$ by

$$M_{\text{per}}^i(h, L) = \frac{\partial}{\partial h_i} \log Z_{\text{per}}(T) \quad (4.1)$$

Theorem 4.1. There are constants $\tau_0 < \infty$ and $b_0 > 0$ depending only on N and d , such that the following statements are true for $\tau > \tau_0$:

$$(i) \quad \left| Z_{\text{per}}(T) - \sum_{q \in Q} \exp(-f'_q L^d) \right| \leq \exp(-fL^d - b_0 \tau L) \quad (4.2)$$

(ii) Let

$$P_q = \left[\sum_{m \in Q} \exp(-f'_m L^d) \right]^{-1} \exp(-f'_q L^d) \quad (4.3a)$$

Then

$$\left| \frac{d^k}{dh^k} \left[M_{\text{per}}^i(h, L) - \sum_{q \in Q} \left(-\frac{\partial f'_q}{\partial h_i} \right) P_q \right] \right| \leq \exp(-b_0 \tau L) \quad (4.3b)$$

for all multi-indices $k: \{1, \dots, N-1\} \rightarrow \{0, 1, 2, \dots\}$ of order $|k| \leq 3$.

Remark (i). Theorem 4.1 is a generalization of Theorem 5.1 of ref. 6; see also ref. 12, Theorem 5.1 and Theorem 5.5. Note that the sum over q in (4.2) and (4.3) goes over *all* $q \in Q$, whereas the theorems of refs. 6 and 12 are stated for the corresponding sums over stable q 's.

Remark (ii). It follows from Theorem 4.1(i) and the fact that $f = \min_q f'_q$ that

$$Z_{\text{per}}(T) \geq e^{-fL^d} (1 - e^{-b_0 \tau L})$$

so that $Z_{\text{per}}(T) \neq 0$ and $M_{\text{per}}^i(h, L)$ is well defined for $\tau > \tau_0$. On the other hand,

$$\lim_{L \rightarrow \infty} M_{\text{per}}^i(h, L) = \frac{1}{N(h)} \sum_{q: f'_q = f} \left(-\frac{\partial f'_q}{\partial h_i} \right)$$

by Theorem 4.1(ii); $N(h)$ is the number of stable states. For $Q = \{+, -\}$, there is only one magnetic field h , and

$$-\frac{df'_+(h)}{dh} = M_+(h) \quad \text{provided } h \leq h_t$$

while

$$-\frac{df'_-(h)}{dh} = M_-(h) \quad \text{provided } h \leq h_t$$

Therefore Lemma 3.1 follows immediately from Theorem 4.1(i) and (ii).

Proof of Theorem 4.1. The first step in the proof is a decomposition of $Z_{\text{per}}(T)$,

$$Z_{\text{per}}(T) = Z^{\text{Big}}(T) + Z^{\text{res}}(T) \quad (4.4)$$

where $Z^{\text{res}}(T)$ is obtained from $Z_{\text{per}}(T)$ by restricting the sum in (3.1) to a sum over sets $\{Y_\alpha\}$ such that $\text{diam } Y \leq L/3$ for all contours $Y \in \{Y_\alpha\}$. We further decompose $Z^{\text{res}}(T)$ as

$$Z^{\text{res}}(T) = \sum_{q \in Q} Z_q^{\text{res}}(T) \quad (4.5)$$

where a set $\{Y_\alpha\}$ contributes to $Z_q^{\text{res}}(T)$ if its external contours are q contours [if $\{Y_\alpha\}$ contains no external contours, $|R_m| = \delta_{qm} L^d$ for some $q \in Q$; the corresponding term $\exp(-e_q L^d)$ then contributes to $Z_q^{\text{res}}(T)$].

Since each configuration contribution to $Z^{\text{Big}}(T)$ contains at least one contour of size bigger than $L/3$,

$$|Z^{\text{Big}}(T)| \leq e^{-fL^d} e^{-b_1 \tau L} \quad (4.6a)$$

for some $b_1 > 0$ depending on N and d ; see Section 5 of ref. 6 for the details of the proof. In a similar way,

$$\left| \frac{d^k}{dh^k} Z^{\text{Big}}(T) \right| \leq e^{-fL^d} e^{-b_1 \tau L} \quad (4.6b)$$

for all multi-indices k of order $|k| \leq 4$.

We now turn to the properties of $Z_q^{\text{res}}(T)$. Recalling that the constant α of Section 2 was chosen as $\alpha = \tau/2$ [see remark (vi) of Section 2], let us assume for the moment that

$$a_q(h)L \leq \tau/4 \quad (4.7)$$

Then all q -contours in T (which has diameter L) have small activities by Lemma 2.1(ii) and (2.12) [see also remark (vi) of Section 2]. Therefore $Z_q^{\text{res}}(T)$ can be analyzed by a convergent cluster expansion. Comparing the expansion for $\log Z_q^{\text{res}}(T)$ with the expansion for f'_q , one obtains the bounds

$$|\log Z_q^{\text{res}}(T) + f'_q L^d| \leq e^{-b_2 \tau L} \quad (4.8a)$$

$$\left| \frac{d^k}{dh^k} [\log Z_q^{\text{res}}(T) + f'_q L^d] \right| \leq e^{-b_2 \tau L} \quad (4.8b)$$

where $b_2 > 0$ depends on d and N , and k is again a multi-index of order $|k| \leq 4$.

On the other hand, for $a_q \neq 0$,

$$\begin{aligned} & |Z_q^{\text{res}}(T)| \exp(fL^d) \\ & \leq \exp\{\exp(-b_2 \tau L)\} \max\{\exp(-a_q L^d/2), \exp(-\tau b_3 L^{d-1})\} \end{aligned} \quad (4.9a)$$

where $b_3 > 0$ again depends only on d and L . The physical origin of the bound (4.9) is clear: If q is unstable, one either pays for the higher energy of the unstable phase or for the formation of a large contour which brings the system into a stable phase. The detailed proof is given in ref. 6, Section 5; see also Appendix A, Remark (i). In a similar way,

$$\begin{aligned} \left| \frac{d^k}{dh^k} Z_q^{\text{res}}(T) \right| \exp(fL^d) \\ \leq C(|k|)(2L^d)^{|k|} \exp\{\exp(-b_2\tau L)\} \\ \times \max\{\exp(-\alpha_q L^d/2), \exp(-\tau b_3 L^{d-1})\} \end{aligned} \quad (4.9b)$$

where $C(|k|)$ is the constant defined in (A.14) and $|k| \leq 4$.

We therefore bound

$$\begin{aligned} |Z_q^{\text{res}}(T) \exp(fL^d)| &\leq \exp(-b_2\tau L) \exp(-\tau L^{d-1} \min\{1/8, b_3\}) \\ &\leq \exp(-b_4\tau L^{d-1}) \end{aligned}$$

and

$$\left| \frac{d^k}{dh^k} Z_q^{\text{res}}(T) \right| \exp(fL^d) \leq \exp(-b_4\tau L^{d-1})$$

provided τ is large enough, $|k| \leq 4$, and $a_q(h)L > \tau/4$. On the other hand,

$$\begin{aligned} |\exp(-f'_q L^d)| &\leq \exp(-fL^d) \exp(-b_4\tau L^{d-1}) \\ \left| \frac{d^k}{dh^k} \exp(-f'_q L^d) \right| &\leq \exp(-fL^d) \exp(-b_4\tau L^{d-1}) \end{aligned}$$

if $a_q(h)L > \tau/4$. Therefore,

$$|Z_q^{\text{res}}(T) - \exp(-f'_q L^d)| \leq \exp(-fL^d) \exp(-b_5\tau L^{d-1}) \quad (4.10a)$$

$$\left| \frac{d^k}{dh^k} [Z_q^{\text{res}}(T) - \exp(-f'_q L^d)] \right| \leq \exp(-fL^d) \exp(-b_5\tau L^{d-1}) \quad (4.10b)$$

if $a_q L > \tau/4$ and $|k| \leq 4$. Combining the bounds (4.6), (4.8), and (4.10), we obtain the theorem for some constant $b_0 > 0$ depending on d and N . ■

We now turn to the proof of Theorem 3.2. If $N = 2$, the bound (4.3b) can be rewritten as follows. We rewrite

$$\begin{aligned} f'_+ &= \frac{1}{2}(f'_+ + f'_-) + \frac{1}{2}(f'_+ - f'_-) \\ f'_- &= \frac{1}{2}(f'_+ + f'_-) - \frac{1}{2}(f'_+ - f'_-) \end{aligned}$$

and use the definition of the hyperbolic tangent to get

$$\left| \frac{d^k}{dh^k} \left[M_{\text{per}}(h, L) + \frac{1}{2} \frac{d(f'_+(h) + f'_-(h))}{dh} - \frac{1}{2} \frac{d(f'_+(h) - f'_-(h))}{dh} \tanh\left\{\frac{1}{2}[f'_+(h) - f'_-(h)]L^d\right\} \right] \right| \leq e^{-b_0\tau L} \quad (4.11)$$

provided $|k| \leq 3$.

On the other hand,

$$\frac{1}{2} \frac{df'_-(h) - df'_+(h)}{dh} \geq b \quad (4.12a)$$

for some constant $b > 0$; see Remark (iv), Section 2. Since $f_-(h) = f_+(h)$ for $h = h_0$, it follows that

$$\frac{1}{2} |f'_+(h) - f'_-(h)| \geq b |h - h_0| \quad (4.12b)$$

Combined with (4.11), the fact that $|\tanh x - \text{sign } x| \leq e^{-|x|}$, and the bound

$$\left| \frac{df'_q(h)}{dh} \right| \leq C_1 + O(e^{-\tau/4}) \leq 2C_1$$

where C_1 is the constant from (2.5), we conclude that

$$|M_{\text{per}}(h, L) - \lim_{L \rightarrow \infty} M_{\text{per}}(h, L)| \leq 2e^{-b_0\tau L} + 2C_1 e^{-b|h-h_0|L^d}$$

This proves Theorem 3.2(i).

Theorem 3.2(ii) follows from (4.11) by a Taylor expansion around h_0 . Using the fact that $f'_+(h_0) = f'_-(h_0)$ and

$$\begin{aligned} -\left. \frac{df'_q(h)}{dh} \right|_{h=h_0} &= M_q(h_0) = M_0 + qM \\ -\left. \frac{d^2 f'_q(h)}{dh^2} \right|_{h=h_0} &= \chi_q = \frac{\chi_+ + \chi_-}{2} + q \frac{\chi_+ - \chi_-}{2} \end{aligned}$$

where $q = \pm 1$, we expand

$$\begin{aligned} -\frac{1}{2} [f'_+(h) - f'_-(h)] &= (h - h_0)M + (h - h_0)^2 \frac{\chi_+ - \chi_-}{4} \\ &\quad + O[(h - h_0)^3] \end{aligned} \quad (4.13a)$$

$$-\frac{1}{2} \frac{d(f'_+(h) - f'_-(h))}{dh} = M + (h - h_0) \frac{\chi_+ - \chi_-}{2} + O[(h - h_0)^2] \quad (4.13b)$$

$$-\frac{1}{2} \frac{d(f'_+(h) + f'_-(h))}{dh} = M_0 + (h - h_0) \frac{\chi_+ + \chi_-}{2} + O[(h - h_0)^2] \quad (4.13c)$$

Theorem 3.2(ii) follows from (4.13) and the bound

$$\begin{aligned} & \left| \tanh \left\{ \frac{L^d}{2} [f'_+(h) - f'_-(h)] \right\} \right. \\ & \quad \left. + \tanh \left\{ L^d \left[M(h - h_0) + \frac{\chi_+ - \chi_-}{4} (h - h_0)^2 \right] \right\} \right| \\ & \leq K_2 |h - h_0|^2 \end{aligned} \quad (4.14)$$

where $K_2 < \infty$ is a constant that does not depend on L . Thus, Theorem 3.2 is proven once the bound (4.14) is established.

We use (4.13a) together with the mean value theorem of differential calculus to bound the left-hand side of (4.14) by

$$\begin{aligned} & CL^d |h - h_0|^3 \\ & \times \left(\cosh^2 \left\{ \gamma L^d [M(h - h_0)] + \frac{\chi_+ - \chi_-}{4} (h - h_0)^2 \right. \right. \\ & \quad \left. \left. + (\gamma - 1) \frac{L^d}{2} [f'_+(h) - f'_-(h)] \right\} \right)^{-1} \end{aligned}$$

where $C < \infty$ does not depend on h on L , and γ is a number between 0 and 1 (which does depend on h and L). We now use (4.12) and (4.13a) to bound the absolute value of the argument of the hyperbolic cosine from below by

$$L^d (b|h - h_0| - K|h - h_0|^3)$$

where $K < \infty$ does not depend on h or L . For $K|h - h_0|^2 < b/2$, the inequality (4.14) then follows from the observation that

$$\frac{CL^d(h - h_0)}{\cosh^2(\frac{1}{2}L^d b|h - h_0|)} \leq \frac{2C}{b}$$

For $K|h - h_0|^2 > b/2$, the bound (4.14) is trivial (choose $K_2 = 4K/b$). ■

We are left with the proof of Theorem 3.3. In a first step we assume that $|h - h_t| \geq BL^d$, where B is a constant to be fixed later, and show that

$$N(h, L) < N(h_t, L) \quad (4.15)$$

$$\chi_{\text{per}}(h, L) < \chi_{\text{per}}(h_t, L) \quad (4.16)$$

and

$$|M_{\text{per}}(h, L) - M_0| > 0 \quad (4.17)$$

provided $|h - h_t| \geq BL^{-d}$ and $L \geq L_0(B)$. In the second step we show that $M_{\text{per}}(\cdot, L) - M_0$ and the derivatives of N and χ_{per} have one and only one zero in the interval $[h_t - BL^{-d}, h_t + BL^{-d}]$, and that these zeros obey the bounds (3.15)–(3.17).

We start from Theorem 4.2(i), which will be used in the form

$$|Z_{\text{per}}(T) \exp[f(h)L^d] - 1 - \exp[-L^d |f'_+(h) - f'_-(h)|]| \leq \exp(-b_0 \tau L)$$

As a consequence,

$$\left| N(h, L) - \left[\frac{(1 + e^{-F})^n}{1 + e^{-nF}} \right]^{1/(n-1)} \right| \leq O(e^{-b_0 \tau L})$$

where we used F to denote the quantity $L^d |f'_+(h) - f'_-(h)|$ and n to denote the number 2^d . Since $(1 + e^{-x})^n / (1 + e^{-nx})$ is a monotonic function of x and

$$F = L^d |f'_+(h) - f'_-(h)| \geq 2Bb$$

provided $|h - h_t| \geq BL^{-d}$ [we used (4.12) in the last inequality], we have

$$\begin{aligned} N(h_t, L) - N(h, L) &\geq 2 - O(e^{-\tau b_0 L}) - N(h, L) \\ &\geq 2 - O(e^{-\tau b_0 L}) - \left(\frac{(1 + e^{-2Bbn})^n}{1 + e^{-2Bbn}} \right)^{1/(n-1)} \end{aligned}$$

We conclude that $N(h_t, L) > N(h, L)$ provided $|h - h_t| \geq BL^{-d}$ and $L \geq L_1(B)$.

On the other hand,

$$\begin{aligned} &\left| \chi_{\text{per}}(h, L) - \frac{L^d}{4} \left(\frac{df'_+(h)}{dh} - \frac{df'_-(h)}{dh} \right)^2 \right. \\ &\quad \left. \times \cosh^{-2} \left\{ \frac{L^d}{2} [f'_+(h) - f'_-(h)] \right\} \right| \\ &\leq 4C_2 + e^{-b_0 \tau L} \leq 1 + 4C_2 \end{aligned}$$

by the bound (4.11) and the fact that

$$\left| \frac{d^k f'_q(h)}{dh^k} \right| \leq C_k + O(e^{-\tau/4}) \leq 2C_k \quad (4.18)$$

[C_k is the constant from (2.5)]. Now, we distinguish two cases: Either $|h - h_t| \geq \tilde{B}L^{-d}$ for some large constant \tilde{B} ; then

$$\begin{aligned} \chi_{\text{per}}(h_t, L) - \chi_{\text{per}}(h, L) &\geq M^2 L^d - 4C_1^2 L^d \cosh^{-2}\{b\tilde{B}\} - 8C_2 - 2 \\ &\geq \frac{M^2 L^d}{2} - 8C_2 - 2 \end{aligned}$$

where we used the bound (4.18) to estimate $df'_q(h)/dh$. Or $BL^{-d} \leq |h - h_t| \leq \tilde{B}L^{-d}$; then

$$\frac{1}{2} \left| \frac{df'_+(h)}{dh} - \frac{df'_-(h)}{dh} \right| = |M| + O(h) \geq |M| - O(L^{-d})$$

which implies that

$$\begin{aligned} \chi_{\text{per}}(h_t, L) - \chi_{\text{per}}(h, L) &\geq M^2 L^d [1 - \cosh^{-2}(bB)] - 4C_2 - 1 - O(1) \end{aligned}$$

In both cases $\chi_{\text{per}}(h_t, L) - \chi_{\text{per}}(h, L) > 0$ provided L is chosen large enough.

Finally, by the bounds (4.11) and (4.12), and by the fact that

$$\left| \frac{df'_q(h)}{dh} + M_q \right| \leq K|h - h_t|$$

for some constant $K < \infty$,

$$\begin{aligned} |M_{\text{per}}(h, L) - M_0| &\geq M \tanh \left\{ \frac{L^d}{2} |f'_+(h) - f'_-(h)| \right\} - e^{-b_0 \tau L} - K|h - h_t| \\ &\geq M \tanh(bB) - e^{-b_0 \tau L} - K|h - h_t| \end{aligned}$$

provided $|h - h_t| \geq BL^{-d}$. We conclude that there is a constant $\delta > 0$ such that $M_{\text{per}}(h, L) - M_0 \neq 0$ for all h in the range

$$BL^{-d} \leq |h - h_t| \leq \delta$$

provided L is chosen large enough. This concludes the proof of (4.15)–(4.17).

At this point the proof of Theorem 3.3 is an easy exercise. We start with the proof of (i). We will show that $\chi_{\text{per}}(\cdot, L)$ has only one local maximum in the interval $[h_t - BL^{-d}, h_t + BL^{-d}]$, and that this maximum obeys the bound (3.15).

We start from (4.11). Calculating the derivatives with respect to h (for $k = 2$), and using the fact that

$$-\left. \frac{d^2(f'_+(h) - f'_-(h))}{dh^2} \right|_{h=h_t} = \chi_+ - \chi_-$$

we obtain that

$$\begin{aligned} & \left| \frac{d\chi_{\text{per}}(h, L)}{dh} \right|_{h=h_t} - 3L^d M \frac{\chi_+ - \chi_-}{2} \Big| \\ & \leq \frac{1}{2} \left| \frac{d^3(f'_+(h) + f'_-(h))}{dh^3} \right|_{h=h_t} + e^{-\tau b_0 L} \leq 2C_3 + 1 \end{aligned} \quad (4.19)$$

[we used (4.18) in the last step]. On the other hand, by the bound (4.11) and the fact that

$$\frac{1}{2} \frac{d(f'_+(h) - f'_-(h))}{dh} = -M + O(L^{-d})$$

provided $|h - h_t| \leq BL^{-d}$, we have

$$\begin{aligned} \frac{d^2\chi_{\text{per}}(h, L)}{dh^2} &= -2 \left(\frac{1}{2} \frac{d(f'_+(h) - f'_-(h))}{dh} \right)^4 L^{3d} \frac{1 - 3 \tanh^2 F}{\cosh^2 F} + O(L^{2d}) \\ &= -2M^4 L^{3d} \frac{1 - 3 \tanh^2 F}{\cosh^2 F} + O(L^{2d}) \end{aligned} \quad (4.20)$$

where we use F to denote the quantity $\frac{1}{2}[f'_+(h) - f'_-(h)]L^d$. We recall that $|F| \leq C_1|h - h_t| \leq BC_1$ provided $|h - h_t| \leq BL^{-d}$. Choosing B small enough and L large, we obtain that

$$\frac{d^2\chi_{\text{per}}(h, L)}{dh^2} \leq -M^4 L^{3d}$$

in the interval $[h_t - BL^{-d}, h_t + BL^{-d}]$. Together with the bound (4.19), this proves that $d\chi_{\text{per}}(h, L)/dh$ has only one zero $h_m(L)$ in the interval

$[h_t - BL^{-d}, h_t + BL_d]$, and that $h_m(L) - h_t = O(L^{-2d})$. For $|h - h_t| \leq O(L^{-2d})$, however, the bound (4.20) implies that

$$\frac{d^2 \chi_{\text{per}}(h, L)}{d^2 h^2} = -2M^4 L^{3d} + O(L^{2d})$$

Combining this bound with the bound (4.19), we obtain the bound (3.15).

The proof of (ii) proceeds in a similar way. We note that

$$|M_{\text{per}}(h_t, L) - M_0| \leq e^{-b_0 \tau L} \tag{4.21}$$

and that

$$\left| \frac{dM_{\text{per}}(h, L)}{dh} - L^d M^2 \cosh^{-2} F \right| \leq \text{const} \tag{4.22}$$

provided $|h - h_t| \leq BL^{-d}$ [the proof of (4.21) and (4.22) is completely analogous to the proof of (4.19) and (4.20)]. Since $|F| \leq BC_1$, we obtain that

$$\frac{dM_{\text{per}}(h, L)}{dh} \geq \frac{L^d M^d}{2} \cosh^{-2}(BC_1) > 0$$

provided L is large and $|h - h_t| \leq BL^{-d}$. We conclude that $M_{\text{per}}(h, L) - M_0$ has a unique zero $h_0(L)$ in the interval $[h_t - BL^{-d}, h_t + BL^{-d}]$, and that $h_0(L)$ obeys the bound (3.16).

To prove the last statement of Theorem 3.3, we note that the local maxima of $N(h, L)$ are the points for which

$$M_{\text{per}}(h, 2L) - M_{\text{per}}(h, L) = 0$$

On the other hand,

$$|M_{\text{per}}(h_t, 2L) - M_{\text{per}}(h_t, L)| \leq 2e^{-b_0 \tau L} \tag{4.23}$$

and

$$\left| \frac{d}{dh} [M_{\text{per}}(h, 2L) - M_{\text{per}}(h, L)] - L^d M^2 [2^d \cosh^{-2}(2^d F) - \cosh^{-2} F] \right| \leq \text{const} \tag{4.24}$$

provided $|h - h_t| \leq BL^{-d}$. Choosing B small enough (which implies that F is small) and L large, we obtain that

$$\frac{d}{dh} [M_{\text{per}}(h, 2L) - M_{\text{per}}(h, L)] \geq L^d L^2 L^{d-1} \cosh^{-2}(2^d BC_1) > 0$$

in the interval $[h_t - BL^{-d}, h_t + BL^{-d}]$. Together with the bound (4.23), this implies statement (iii).

5. GENERAL CASE OF MULTIPLE PHASE COEXISTENCE

Let us recall that choosing a value of the field parameters $h = \{h_i\} \in \mathbb{R}^{N-1}$, the stable phases q are characterized by vanishing of the parameter $a_q = f'_q - f$. We use $Q(h)$ to denote the set of labels of stable phases, $Q(h) = \{q \in Q; a_q(h) = 0\}$, and $N(h)$ to denote their number, $N(h) = |Q(h)|$. Recall also that in (4.1) we defined

$$M_{\text{per}}^i(h, L) = \frac{1}{L^d} \frac{\partial}{\partial h_i} \log Z_{\text{per}}(T)$$

and let us denote

$$M_q^i(h) = -\frac{\partial f'_q}{\partial h_i}$$

for every⁸ $q \in Q$.

In the Remark (ii) after Theorem 4.1 we actually proved a generalization of Lemma 3.1:

Lemma 5.1. There exist a constant τ_0 depending only on d such that, whenever $\tau \geq \tau_0$, the magnetization $M_{\text{per}}^i(h, L)$ is well defined for all $L \in \mathbb{N}$ and

$$M_{\text{per}}^i(h) = \lim_{L \rightarrow \infty} M_{\text{per}}^i(h, L) = \frac{1}{N(h)} \sum_{q \in Q(h)} M_q^i(h) \quad (5.1)$$

To evaluate the speed of convergence in (5.1), we have to bound from below the parameter $a_q(h)$ for all unstable phases q . To this end, we introduce the distance $d_q(h)$ from h to the region where q is stable,

$$d_q(h) = \text{dist}(h, \{\bar{h} \mid a_q(\bar{h}) = 0\}) \quad (5.2)$$

Lemma 5.2. There exists constants $\tau_0 < \infty$ and $M > 0$ such that, for $\tau > \tau_0$ and any q unstable for a given value of h , one has

$$a_q(h) \geq M d_q(h) \quad (5.3)$$

Proof. Let us consider, for every \bar{h} in the ball $B(h)$ of the radius $d_q(h)$ around the point h , the vector

$$v(\bar{h}) = F^{-1}u$$

⁸ If q is stable, $M_q(h)$ is just the “magnetization” of the phase q ; however, it is defined for unstable q as well and it is, in fact, a C^3 -continuation of the magnetization into the unstable regions.

where $F = F(\bar{h})$ is the matrix (2.21) and u is the vector with components $u_m = \delta_{mq}$. Recalling that the norm $\|F^{-1}\|$ satisfies a bound of the form (2.7) [cf. Remark (iv) after Lemma 2.3] and taking $0 < M < 1/\|F^{-1}\|$, we get

$$\left. \frac{d}{d\lambda} (f'_q - f'_s)[\bar{h} + \lambda v(\bar{h})] \right|_{\lambda=0} = (Fv(\bar{h}))_q - (Fv(\bar{h}))_s = 1 \geq M \cdot \|v(\bar{h})\| \quad (5.4)$$

for every $s \neq q$. Hence, there exists a smooth path C of length at least $d_q(h)$, starting at h and ending at a point $\tilde{h} \in B(h)$, such that everywhere along the path the derivative of $f'_q - f'_s$ satisfies the bound (5.4). Choosing now s stable at \tilde{h} and observing that $a_q(\tilde{h}) = f'_q(\tilde{h}) - f'_s(\tilde{h}) \geq 0$, we have

$$\begin{aligned} a_q(h) &\geq f'_q(h) - f'_s(h) \\ &= \int_C \frac{\partial(f'_q - f'_s)}{\partial h} ds + f'_q(\tilde{h}) - f'_s(\tilde{h}) \\ &\geq M \int_C ds + a_q(\tilde{h}) \\ &\geq d_q(h) \cdot M \quad \blacksquare \end{aligned}$$

Denoting now by $d(h)$ the minimum of distances $d_q(h)$ over unstable phases q ,

$$d(h) = \min_{q \in Q \setminus Q(h)} d_q(h)$$

we prove the following result.

Theorem 5.3. There exist constants τ_0 , $K_0 < \infty$ and $b_0 > 0$ such that for $\tau > \tau_0$ one has

$$|M^i_{\text{per}}(h, L) - M^i_{\text{per}}(h)| \leq e^{-b_0\tau L} + K_0 e^{-Md(h)L^d/2} \quad (5.5)$$

Proof. Taking into account the bound (4.3b) and the equality (5.1), we estimate

$$\begin{aligned} &|M^i_{\text{per}}(h, L) - M^i_{\text{per}}(h)| \\ &\leq \left| \sum_{q \in Q} P_q M^i_q(h) - \frac{1}{N(h)} \sum_{q \in Q(h)} M^i_q(h) \right| + \exp(-b_0\tau L) \\ &\leq \sum_{q \in Q(h)} |M^i_q(h)| \left[\frac{1}{N(h)} - \frac{1}{N(h) + \sum_{m \in Q \setminus Q(h)} \exp[-(f'_m - f)L^d]} \right] \\ &\quad + \sum_{q \in Q \setminus Q(h)} |M^i_q(h)| \frac{\exp[-(f'_q - f)L^d]}{N(h) + \sum_{m \in Q \setminus Q(h)} \exp[-(f'_m - f)L^d]} + \exp(-b_0\tau L) \end{aligned}$$

The needed bound follows upon taking into account that $N(h) \geq 1$ and $\exp[-(f'_q - f)L^d] \leq \exp[-Md(h)L^d]$ due to Lemma 5.2. ■

The bound (5.5) is, in analogy with Theorem 3.2(i), useful whenever the parameter h takes on values with large $d(h)$: this means far away from the curves (or surfaces) where some of the phases that are unstable at h become stable, in particular, far from the value $h^{(0)}$, where all N phases coexist [$a_q(h^{(0)}) = 0$ for all $q \in Q$].

Next, we describe the behavior of $M_{\text{per}}^i(h, L)$ in a close neighborhood of $h^{(0)}$. To this end, we start from the formulas (4.3) that express $M_{\text{per}}^i(h, L)$ in terms of $M_q^i(h)$ and $f_q^i(h)$ and expand them in $(h - h^{(0)})$. To simplify the notation, we introduce universal functions $P_q(\eta)$ that replace the hyperbolic tangent from Theorem 3.2(ii). For $\eta \in \mathbb{R}^N$, we define

$$P_q(\eta) = \frac{\exp(-\eta_q)}{\sum_{m=1}^N \exp(-\eta_m)}$$

Using also χ_q^{ij} to denote the susceptibilities, $\chi_q^{ij}(h) = -\partial^2 f_q / \partial h_i \partial h_j$, we evaluate $M_{\text{per}}^i(h, L)$ in (essentially) the first and second orders in the distance $\|h - h^{(0)}\|$ of h from the point $h^{(0)}$ of full coexistence. The crux of the statement lies in the bounds on the errors.

Theorem 5.4. There exist constants $\tau_0, K_1, K_2 < \infty$ and $b_0 > 0$ such that

$$(i) \quad M_{\text{per}}^i(h, L) = \sum_q M_q^i(h^{(0)}) P_q(\bar{\eta}) + R_1(h, L)$$

where $\bar{\eta}$ is the vector with components

$$\bar{\eta}_m = -L^d \sum_j M_m^j(h^{(0)})(h_j - h_j^{(0)})$$

and

$$(ii) \quad M_{\text{per}}^i(h, L) = \sum_q \left[M_q^i(h^{(0)}) + \sum_j \chi_q^{ij}(h^{(0)})(h_j - h_j^{(0)}) \right] P_q(\eta) + R_2(h, L)$$

where η is the vector with components

$$\eta_m = -L^d \left[\sum_j M_m^j(h^{(0)})(h - h_j^{(0)}) + \frac{1}{2} \sum_{i,j} \chi_m^{ij}(h^{(0)})(h_i - h_i^{(0)})(h_j - h_j^{(0)}) \right]$$

The errors R_1, R_2 satisfy, for $\tau > \tau_0$, the bounds

$$|R_1(h, L)| \leq e^{-b_0 \tau L} + K_1 \|h - h^{(0)}\| \min \left\{ \frac{\|h - h^{(0)}\|}{\tilde{d}(h)}, 1 + \|h - h^{(0)}\| L^d \right\} \quad (5.6i)$$

and

$$|R_2(h, L)| \leq e^{-b_0\tau L} + K_2 \|h - h^{(0)}\|^2 \min \left\{ \frac{\|h - h^{(0)}\|}{\tilde{d}(h)}, 1 + \|h - h^{(0)}\| L^d \right\} \tag{5.6ii}$$

where

$$\tilde{d}(h) = \text{dist}(h, \{\tilde{h} \in \mathbb{R}^N \mid N(h) \geq 2\})$$

We note that $\tilde{d}(h) = d(h)$ if $N(h) = 1$, whereas it vanishes on the curves (and surfaces) of phase coexistence. The bounds (5.6) are weaker than the corresponding bounds in Theorem 3.2; in the region $\|h - h^{(0)}\| \gg L^{-d}$ they become useless if h approaches the phase coexistence regions. However, changing the definition of P_q in these regions, one can evaluate the finite-volume behavior of $M_{\text{per}}(h, L)$ on the surfaces and lines of coexistence as well.

Proposition 5.5. Theorem 5.4 remains valid if the functions $P_q(\eta)$, and similarly $P_q(\bar{\eta})$, are replaced by the functions $P_q^{Q(h)}(\eta)$ which are obtained from $P_q(\eta)$ by substituting

$$\eta_0 = \frac{1}{N(h)} \sum_{m \in Q(h)} \eta_m$$

for η_q whenever q is stable. After these replacements, the bounds (5.6i) and (5.6ii) can be strengthened to

$$|R_1(h, L)| \leq e^{-b_0\tau L} + K_1 \|h - h^{(0)}\| \min \left\{ \frac{\|h - h^{(0)}\|}{d(h)}, 1 + \|h - h^0\| L^d \right\}$$

and

$$|R_2(h, L)| \leq e^{-b_0\tau L} + K_1 \|h - h^{(0)}\|^2 \min \left\{ \frac{\|h - h^{(0)}\|}{d(h)}, 1 + \|h - h^{(0)}\| L^d \right\}$$

Before proceeding to the proof of the above statements, we illustrate them by applying them to a model that is simple, yet captures main features of a general case. Namely, we consider the Blume–Capel model⁽¹³⁾ with the Hamiltonian

$$H = \frac{1}{2} \sum_{\langle a,b \rangle} (S_a - S_b)^2 - h_1 \sum_a S_a^2 - h_2 \sum_a S_a$$

where the spin takes on three values, $S_a = \pm 1, 0$. There are three translation-invariant ground states with specific energies

$$e_0 = 0, \quad e_+ = -h_1 - h_2, \quad e_- = -h_1 + h_2$$

With the help of Pirogov–Sinai theory, it can be shown^(14,15) that the phase diagram at low temperatures (Fig. 1b) is a small perturbation of the phase diagram at zero temperature (Fig. 1a). Notice that the $+$, $-$ symmetry is conserved at nonvanishing temperatures. In Fig. 2 we indicate several straight lines, along which we shall analyze, say, the formula (i) of Theorem 5.4 with the error bound (5.6i).

Considering first the dependence on a parameter h along the line l_1 , we get

$$M_{\text{per}}^i(h, L) = \sum_{q=0, \pm 1} M_q^i(h^{(0)}) \frac{\exp[-\sum_{j=1}^2 M_q^j(h^{(0)})(h_j - h_j^{(0)})L^d]}{\sum_{m=0, \pm 1} \exp[-\sum_{j=1}^2 M_m^j(h^{(0)})(h_j - h_j^{(0)})L^d]} + O(\|h - h^{(0)}\|)$$

The error is of the order $\|h - h^{(0)}\|$, since for h on l_1 one has $\tilde{d}(h) \geq \alpha \|h - h^{(0)}\|$ with a fixed $\alpha > 0$.

Along the straight line l_2 (the tangent at $h^{(0)}$ with respect to the curve of $0, -$ phase coexistence) the bound (5.6i) fails. The reason is that $\tilde{d}(h)$ vanishes quicker than $\|h - h^{(0)}\|^2$ as $h \rightarrow h^{(0)}$.

Also along the line l_3 the bound (5.6i) fails, since $\tilde{d}(h)$ goes to zero when crossing the coexistence curve, while $\|h - h^{(0)}\|$ stays bounded from below. But here we actually have the coexistence of only two phases, $+$

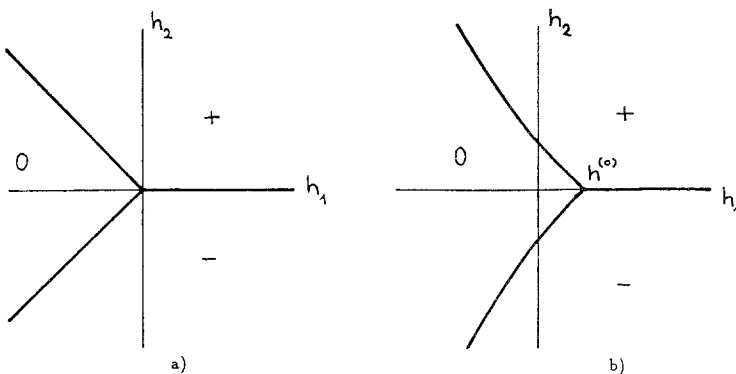


Fig. 1. The phase diagram of the Blume-Capel model at low (b) and zero (a) temperature.

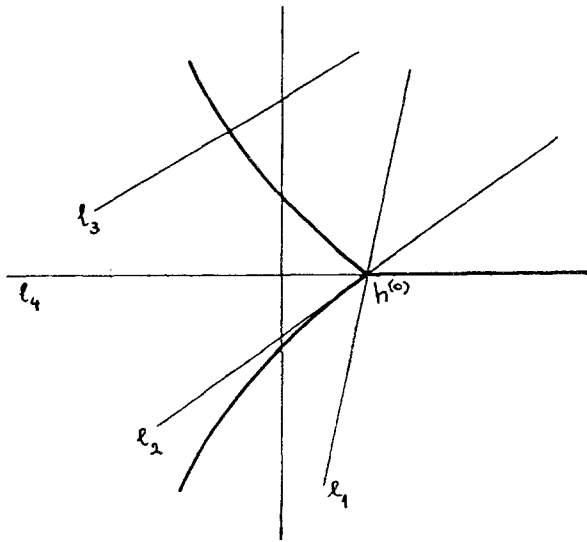


Fig. 2

and 0, and one should rather apply Theorem 3.2 replacing $h^{(0)}$ by the intersection of l_3 with the coexistence curve of + and 0 phases.

An interesting case is that of the line l_4 (the axis $h_2 = 0$). Here, one phase (the phase 0) is stable for $h_1 < h_1^{(0)}$, two phases (+ and -) are stable for $h_1 > h_1^{(0)}$, and all three of them coexist at $h_1 = h_1^{(0)}$. Observing that then $d(h) = \|h - h^{(0)}\| \equiv |h_1 - h_1^{(0)}|$ and setting

$$\bar{M}^i = \frac{1}{2} \left\{ \frac{1}{2} [M_+^i(h^{(0)}) + M_-^i(h^{(0)})] + M_0^i(h^{(0)}) \right\}$$

and $\Delta^i = -M_0^i(h^{(0)}) + \bar{M}^i$, we get

$$M_{\text{per}}^i(h, L) = \bar{M}^i + \Delta^i \tanh[\Delta^1 \cdot (h_1 - h_1^{(0)}) L^d + \log \sqrt{2}] + O(|h_1 - h_1^{(0)}|) \tag{5.7}$$

Notice that this formula has the same structure as (3.11a), except for the additional term $\log \sqrt{2}$ in the argument of the hyperbolic tangent. A direct extension to a situation with n phases coexisting along a line (say l_4) yields the formula

$$M_{\text{per}}^i(h, L) = \bar{M}^i + \Delta^i \tanh[\Delta^1 \cdot (h_1 - h_1^{(0)}) \cdot L^d + \log \sqrt{n}] + O(|h_1 - h_1^{(0)}|) \tag{5.8}$$

The term $\log \sqrt{n}$ can be traced to the fact that $n + 1$ phases coexist at $h^{(0)}$, n of them being stable for $h_1 > h_1^{(0)}$ and the remaining one for $h_1 < h_1^{(0)}$. One

would thus expect a similar behavior also for the n -state Potts model that is reminiscent of this extension. Indeed, an analog of (5.8) can be proven for $E_{\text{per}}(\beta, L)$, the mean energy of the Potts model under periodic boundary conditions.⁽⁷⁾

Proof of Theorem 5.4 and Proposition 5.5. We start with the proof of Theorem 5.4. According to (4.3b), it is sufficient to evaluate the expression

$$\sum_{q \in Q} M_q^i(h) P_q(\zeta) \quad (5.9)$$

with $\zeta = \{f'_m(h)L^d\}_{m \in Q}$. Expanding $M_m^i(h)$ and $f'_m(h)$ around $h^{(0)}$, we have

$$\left| M_m^i(h) - M_m^i(h^{(0)}) - \sum_j \chi_m^{ij}(h^{(0)})(h_j - h_j^{(0)}) \right| \leq M_1 \|h - h^{(0)}\|^2 \quad (5.10)$$

and

$$\begin{aligned} & \left| f'_m(h) - f'_m(h^{(0)}) + \sum_i M_m^i(h^{(0)})(h_i - h_i^{(0)}) \right. \\ & \quad \left. + \sum_{i,j} \chi_m^{i,j}(h^{(0)})(h_i - h_i^{(0)})(h_j - h_j^{(0)}) \right| \\ & \leq M_2 \|h - h^{(0)}\|^3 \end{aligned} \quad (5.11)$$

where the constants M_1, M_2 do not depend on h , according to (2.5) and (2.20). Taking into account (5.10) and once more (2.5) and (2.20), we see that to prove (5.6i) and (5.6ii), it is enough to show that

$$|P_q(\xi) - P_q(\bar{\eta})| \leq O(\|h - h^{(0)}\|^2) \min\{L^d, \tilde{d}(h)^{-1}\} \quad (5.12i)$$

and

$$|P_q(\zeta) - P_q(\eta)| \leq O(\|h - h^{(0)}\|^3) \min\{L^d, d(h)^{-1}\} \quad (5.12ii)$$

(Recall that $\bar{\eta}$ arises from η by omitting the quadratic terms in $h - h^{(0)}$.) Rewriting $P_q(\zeta)$ as

$$P_q(\zeta) = \exp[-(\zeta_q - \zeta_{q_0})] \left/ \sum_m \exp[-(\zeta_m - \zeta_{q_0})] \right.$$

where q_0 is chosen in such a way that q_0 is stable at h , we see that it is enough to estimate

$$\exp[-(\zeta_q - \zeta_{q_0})] - \exp[-(\eta_q - \eta_{q_0})]$$

for all $q \neq q_0$ in order to prove (5.12ii). Bounding

$$\begin{aligned} & |\exp(\zeta_q - \zeta_{q_0}) - \exp(\eta_q - \eta_{q_0})| \\ & \leq (|\zeta_q - \eta_q| + |\zeta_{q_0} - \eta_{q_0}|) \max\{\exp(\zeta_q - \zeta_{q_0}), \exp[-(\eta_q - \eta_{q_0})]\} \\ & \leq 2M_2 \|h - h^{(0)}\|^3 L^d \max\{\exp[-(\zeta_q - \zeta_{q_0})], \exp[-(\eta_q - \eta_{q_0})]\} \end{aligned}$$

we conclude that

$$\begin{aligned} & |P_q(\zeta) - P_q(\eta)| \\ & \leq O(\|h - h^{(0)}\|^3) L^d \max_{m \neq q_0} \max\{\exp[-(\zeta_q - \zeta_{q_0})], \exp[-(\eta_q - \eta_{q_0})]\} \end{aligned} \tag{5.13}$$

We now distinguish two cases. Either

$$\|h - h^{(0)}\|^3 \geq C\tilde{d}(h)$$

for some constant C to be chosen in a moment; then we use (5.13) and the trivial bound $|P_q| \leq 1$ to estimate

$$\begin{aligned} & |P_q(\zeta) - P_q(\eta)| \\ & \leq \min\{2, L^d O(\|h - h^{(0)}\|^3)\} \\ & \leq \min\left\{\frac{2\|h - h^{(0)}\|^3}{C\tilde{d}(h)}, L^d O(\|h - h^{(0)}\|^3)\right\} \end{aligned}$$

Or $\|h - h^{(0)}\|^3 < Cd(h)$ and we bound

$$\begin{aligned} & \zeta_q - \zeta_{q_0} = d_q \geq M\tilde{d}(h) \\ & \eta_q - \eta_{q_0} \geq \zeta_q - \zeta_{q_0} - M_2 \|h - h^{(0)}\|^3 L^d \\ & \geq (M_2 - C) \tilde{d}(h) L^d \end{aligned} \tag{5.14}$$

choosing $0 < C < M_2$, and using the fact that $e^{-x} \leq \min\{1, 1/x\}$, we then may use the bound (5.13) to obtain (5.12ii). The bound (5.12i) is obtained in a similar way. In order to prove Proposition 5.5, we observe that

$$\zeta_q = \zeta_0 \equiv \min_m \zeta_m$$

if q is stable. It is therefore enough to prove the bounds (5.12i) and (5.12ii) (with P_q replaced by $P_q^{Q(h)}$) for all $q \in \{0\} \cup Q \setminus Q(h)$. Rewriting

$$P_q^{Q(h)}(\zeta) = \frac{\exp[-(\zeta_q - \zeta_0)]}{|Q(h)| + \sum_{m \in Q \setminus Q(h)} \exp[-(\zeta_m - \zeta_0)]}$$

and replacing the lower bound (5.14) by the bound

$$\zeta_q - \zeta_0 \geq Md(h)$$

we then may proceed exactly as in the proof of Theorem 5.4. ■

APPENDIX. PROOF OF LEMMAS 2.1, 2.2, AND 2.3

In this Appendix we prove Lemmas 2.1–2.3. Since our results do not depend on the fact that e_q and $\rho(Y)$ are real, we allow for complex ground-state energies and activities in this Appendix. We require the bounds (2.1), (2.5), and (2.6) with (2.2) and (2.4) replaced by

$$e_0 = \min_q \operatorname{Re} e_q \tag{2.2'}$$

$$E = \left[\frac{\partial}{\partial h_i} \operatorname{Re}(e_q - e_N) \right]_{q,i=1,\dots,N-1} \tag{2.4'}$$

and generalize the definitions (2.16) and (2.17) to the complex situation by putting

$$f = \min_m \operatorname{Re} f_m \tag{2.16'}$$

$$a_q = \operatorname{Re} f_q - f \tag{2.17'}$$

The definitions of Z_q , $K'(Y)$, and Z'_q are the same as before.

We start with the proof of (2.12), assuming that it has already been proven for all contours of diameter less than n . We introduce an auxiliary contour model with activities

$$K^{(n)}(Y^q) = \begin{cases} K'(Y^q) & \text{if } \operatorname{diam} Y^q < n \\ 0 & \text{otherwise} \end{cases}$$

Denoting the corresponding free energy by $f_q^{(n)}$, we define

$$f_0^{(n)} = \min_m \operatorname{Re} f_m^{(n)} \tag{A.1}$$

$$a_q^{(n)} = \operatorname{Re} f_q^{(n)} - f_0^{(n)} \tag{A.2}$$

Since $f_q^{(n)}$ and $\log Z'_q(V)$ can be controlled by convergent cluster expansions due to the inductive assumption,

$$|\log Z'_q(V) + f_q^{(n)}|V| \leq O(\varepsilon)|\partial V| \tag{A.3a}$$

for all volumes V with $\text{diam } V \leq n$, and

$$|f_q^{(n)} - e_q| \leq O(\varepsilon) \tag{A.3b}$$

Here ε is the constant

$$\varepsilon = e^{-(\tau - \alpha - 2d - 2)} \tag{A.4}$$

We now assume inductively that

$$|K'(Y)| \leq e^{|Y|} \tag{A.5}$$

for all contours Y with $\text{diam } Y < n$, and

$$|Z_q(V)| \leq e^{|\partial V| - f_0^{(n)}|V|} \tag{A.6}$$

for all q and all volumes V with $\text{diam } V \leq n$.

Using the inductive assumption (A.6) and the bound (A.3), we bound, for $\text{diam } Y^q = n$,

$$\begin{aligned} |K'(Y^q)| &\leq \chi'(Y^q) \exp[(\text{Re } e_q - e_0 - \tau) |Y^q|] \exp(a_q^{(n)} |\text{Int } Y_q|) \\ &\quad \times \prod_m \exp\{[1 + O(\varepsilon)] |\partial \text{Int}_m Y^q|\} \\ &\leq \chi'(Y^q) \exp(a_q^{(n)} |\text{Int } Y^{qq}|) \exp\{[\text{Re } e_q - e_0 + 2d + O(\varepsilon) - \tau] |Y^q|\} \end{aligned}$$

where we used the bound

$$\sum_m |\partial \text{Int}_m Y^q| \leq |\partial Y| \leq 2d |Y| \tag{A.7}$$

Since $\chi'(Y^q) = 0$ unless

$$\text{Re}[\log Z'_q(V(Y^q)) - \log Z'_m(V(Y^q))] \geq -\alpha |Y^q| - 1$$

which, by the bounds (A.3) and the fact that $|V(Y^q)| = |\text{Int } Y^q| + |Y^q|$, implies that

$$(\text{Re } e_q - e_0) |Y^q| + a_q^{(n)} |\text{Int } Y^q| \leq [\alpha + 1 + O(\varepsilon)] |Y^q|$$

we finally obtained the desired bound

$$K'(Y^q) \leq e^{-[\tau - \alpha - 2d - 1 - O(\varepsilon)] |Y^q|} \leq e^{|Y^q|}$$

Lemma A.1. Assume that $\text{diam } Y^q \leq n$ and that $a_q^{(n)} \text{diam } Y^q \leq \alpha - 2$. Then

$$\chi'(Y^q) = 1$$

Proof. Using (A.3) and the definition of $a_q^{(n)}$, we bound

$$\begin{aligned} & \log |Z'_q(V(Y^q))| - \log |Z'_m(V(Y^q))| + \alpha |Y_q| \\ & \geq [\alpha - O(\varepsilon)] |Y^q| - a_q^{(n)} |V(Y^q)| \end{aligned}$$

Combined with the bound

$$a_q^{(n)} |V(Y^q)| \leq a_q^{(n)} \text{diam } Y^q |Y^q| \leq (\alpha - 2) |Y^q|$$

and the property (2.14b) of χ , we obtain the lemma. ■

Lemma A.2. Assume that $\text{diam } V \leq n$ and that $a_q^{(n)} \text{diam } Y^q \leq \alpha - 2$. Then

$$Z_q(V) = Z'_q(V) \tag{A.8}$$

Proof. For $\text{diam } V \leq 2$, the statement is obvious. Assume that (A.8) has been proven for all V with $\text{diam } V \leq m - 1$, $m \leq n$. Taking into account Lemma A.1, we infer that $K'(Y^q) = K(Y^q)$ for all q -contours Y^q with $\text{diam } Y^q \leq m$. Using (2.9) and the definition of $K(Y^q)$, we conclude that for all volumes with $\text{diam } V \leq m$,

$$\begin{aligned} Z_q(V) &= \sum_{\{Y_\alpha^q\}_{\text{ext}}} Z_q(\text{Int}) e^{-e_q |V \setminus \text{Int}|} \prod_{\alpha} K(Y_\alpha^q) \\ &= \sum_{\{Y_\alpha^q\}_{\text{ext}}} Z'_q(\text{Int}) e^{-e_q |V \setminus \text{Int}|} \prod_{\alpha} K'(Y_\alpha^q) \\ &= Z'_q(V) \end{aligned}$$

where Int denotes the set $\bigcup_{\alpha} \text{Int } Y_\alpha^q$. Thus, the lemma is proven by induction. ■

Lemma A.3. Assume that $\text{diam } V \leq n + 1$. Then

$$|Z_q(V)| \leq \exp(-f_0^{(n)} |V| + |\partial V|) \quad \text{for all } q \in \mathcal{Q}$$

Proof. We define a contour Y^q to be *small* if $a_q^{(n)} \text{diam } Y^q \leq \alpha - 2$ and use the relation (2.9) to rewrite $Z_q(V)$ in the following way: write a set $\{Y_\alpha^q\}$ of external q -contours in V as $\{X_\alpha^q\} \cup \{Z_\alpha^q\}$, where $\{Z_\alpha^q\}$ denotes the small contours in $\{Y_\alpha^q\}$ and $\{X_\alpha^q\}$ the large contours in $\{Y_\alpha^q\}$. Note that for fixed X_α^q , the sum over $\{Z_\alpha^q\}$ goes over all sets of mutually external small

contours in $\text{Ext} = V \setminus \bigcup_{\alpha} (X_{\alpha} \cup \text{Int } X_{\alpha})$. Thus, resumming the small contours and using the relation (2.9) for a second time, we obtain

$$Z_q(V) = \sum_{\{X_{\alpha}^q\}_{\text{ext}}} Z_q^{\text{small}}(\text{Ext}) \prod_{\alpha} \left[\rho(X_{\alpha}^q) \prod_m Z_m(\text{Int}_m X_{\alpha}^q) \right] \quad (\text{A.9})$$

where the sum goes over sets of mutually external large contours in V and $Z_q^{\text{small}}(\text{Ext})$ is obtained from $Z_q(\text{Ext})$ by dropping all large external q -contours.

By Lemmas A.1 and A.2, $K(Y^q) = K'(Y^q)$ if Y^q is small. Therefore the partition function $Z_q^{\text{small}}(\text{Ext})$ is equal to the corresponding truncated partition function, which can be controlled by convergent cluster expansions. It follows that

$$|Z_q^{\text{small}}(\text{Ext})| \leq \exp[-\text{Re } f_q^{\text{small}} |\text{Ext}| + O(\varepsilon) |\partial \text{Ext}|] \quad (\text{A.10})$$

where f_q^{small} is the free energy of the contour model with activities

$$K^{\text{small}}(Y^q) = \begin{cases} K'(Y^q) & \text{if } \text{diam } Y^q \leq n \text{ and } Y^q \text{ is small} \\ 0 & \text{otherwise} \end{cases}$$

On the other hand,

$$|Z_m(\text{Int}_m X_{\alpha}^q)| \leq \exp(-f_0^{(n)} |\text{Int}_m X_{\alpha}^q| + |\partial \text{Int}_m X_{\alpha}^q|) \quad (\text{A.11})$$

due to the inductive assumption (A.6). Combining (A.10) and (A.11) with the *a priori* bound on ρ and the bound $|f_0^{(n)} - e_0| \leq O(\varepsilon)$, we find that

$$\begin{aligned} |Z_q(V)| &\geq \sum_{\{X_{\alpha}^q\}_{\text{ext}}} \exp(-\text{Re } f_q^{\text{small}} |\text{Ext}| - f_0^{(n)} |V \setminus \text{Ext}|) \\ &\quad \times \exp[|\partial \text{Int}| + O(\varepsilon)] \cdot \prod_{\alpha} \exp[-(\tau - O(\varepsilon)) |X_{\alpha}^q|] \end{aligned}$$

Using (A.7) to bound

$$O(\varepsilon) |\partial \text{Ext}| + |\partial \text{Int}| \leq O(\varepsilon) \left(|\partial V| + \sum_{\alpha} |\partial X_{\alpha}^q| \right) + |\partial \text{Int}|$$

by $O(\varepsilon) |\partial V| + 4d \sum_{\alpha} |X_{\alpha}^q|$, we get

$$\begin{aligned} |Z_q(V)| &\leq \exp[-f_0^{(n)} |V| + O(\varepsilon) |\partial V|] \\ &\quad \times \sum_{\{X_{\alpha}^q\}_{\text{ext}}} \exp[-\text{Re}(f_q^{\text{small}} - f_0^{(n)}) |\text{Ext}|] \prod_{\alpha} \exp[-(\tau - 4d - 1) |X_{\alpha}^q|] \end{aligned}$$

At this point we extract a factor

$$\begin{aligned} & \max_{\{x_\alpha^2\}_{\text{ext}}} \exp \left\{ -\frac{a_q^{(n)}}{2} |\text{Ext}| - \frac{\tau}{2} \sum_\alpha |X_\alpha| \right\} \\ & \leq \max_{W \subset V} \exp \left\{ -\frac{a_q^{(n)}}{2} |V \setminus W| - \frac{\tau}{4d} |\partial W| \right\} \end{aligned}$$

and bound the remaining sum as in ref. 6, Section 2 (see also ref. 10, Section 2). We get the estimate

$$|Z_q(V)| \leq \exp(-f_0^{(n)}|V| + |\partial V|) \max_{W \subset V} \exp \left\{ -\frac{a_q^{(n)}}{2} |V \setminus W| - \frac{\tau}{4d} |\partial W| \right\} \tag{A.12}$$

Bounding the last factor by one, we obtain the lemma. ■

This completes the inductive proof of (2.12). On the other hand, $f = \lim_{n \rightarrow \infty} f_0^{(n)}$ and $a_q = \lim_{n \rightarrow \infty} a_q^{(n)}$. Therefore Lemma 2.1 follows from Lemmas A.1–A.3 by taking the limit $n \rightarrow \infty$.

We now turn to the proof of Lemma 2.2, which we will prove in the form

$$\begin{aligned} & \left| \left(\prod_{i=1}^k \frac{d}{dh_{p(i)}} \right) [Z_q(V) e^{e_q} |V|] \right| \\ & \leq \text{const} \cdot e^{-\tau} C(k) (4e^{2d} |V|)^k e^{(e_q - f)|V| + |\partial V|} \end{aligned} \tag{A.13}$$

where $k = 1, \dots, 4$, $p: \{1, \dots, k\} \rightarrow \{1, \dots, N-1\}$, and

$$C(k) = \max_{\substack{k_1, \dots, k_k \geq 0 \\ \sum k_i = k}} \prod_{i=1}^k C_{k_i} \tag{A.14}$$

C_{k_i} are the constants from (2.5) and (2.6), $C_0 = 1$, and the constant const in (A.13) does not depend on k and V .

By the definition (2.3) of $Z_q(V)$

$$[Z_q(V) e^{e_q |V|}] = \sum_{\{Y_\alpha\}} \prod_\alpha \rho(Y_\alpha) e^{e_q |Y_\alpha|} \prod_{x \in V \setminus \cup Y_\alpha} e^{e_q - e(x)} \tag{A.15}$$

where $e(x) = e_m$ if $x \in R_m$. A derivative $d/dh_{p(i)}$ now either acts on a factor $e^{e_q - e(x)}$ or on a factor $\rho(Y_\alpha) e^{e_q |Y_\alpha|}$. We fix all contours Y which are differentiated or which contain a point x in their interior such that $e^{e_q - e(x)}$ is differentiated, as well as all contours Y' such that there is a contour $Y \subset \text{Int } Y'$ which is differentiated, and resum all other contours. We then

use Lemma 2.1(i) to bound the resulting partition functions, and the bounds (2.5) and (2.6) to bound the derivatives of ρ and e_q . As a result, we obtain the estimate

$$\begin{aligned} & \left| \left(\prod_{i=1}^k \frac{d}{dh_{p(i)}} \right) [Z_q(V) \exp(e_q |V|)] \right| \\ & \leq C(k) 2^k \exp(e_q |V|) \sum_{x_1, \dots, x_k \in V} \sum'_{\{Y_\alpha\}} \\ & \quad \times \exp \left(-f |V \setminus \cup Y_\alpha \setminus \{x_1, \dots, x_k\}| + |\partial V| + \sum_{i=1}^k 2d + \sum_{\alpha} |\partial Y_\alpha| \right) \\ & \quad \times \prod_{i=1}^k \exp[-e(x_i)] \prod_{\alpha} \exp[-(\tau + e_0) |Y_\alpha|] \end{aligned} \tag{A.16}$$

where the sum \sum' goes over all sets $\{Y_\alpha\}$ for which each Y_α either contains or surrounds a point x_i . Note that a term for which $x_i \in Y_\alpha$ comes from a term where $\rho(Y_\alpha) \exp(e_q |Y_\alpha|)$ was differentiated with respect to $h_{p(i)}$, while the terms for which x_i lies in $V \setminus \cup Y_\alpha$ come from those terms where $\exp[e_q - e(x_i)]$ was differentiated with respect to $h_{p(i)}$. We now extract a factor

$$C(k) (2e^{2d})^k e^{(e_q - f)|V| + |\partial V|}$$

from the right-hand side of the above inequality and bound the remaining sum as follows:

$$\begin{aligned} & \sum'_{\{Y_\alpha\}} \prod_{i=1}^k e^{f - e(x_i)} \prod_{\alpha} e^{-(\tau + e_0 - f) |Y_\alpha| + |\partial Y_\alpha|} \\ & \leq \sum'_{\{Y_\alpha\}} e^{kO(e)} \prod_{\alpha} e^{-[\tau - O(e) - 2d] |Y_\alpha|} \\ & \leq \prod_{i=1}^k e^{O(e)} \sum^{(i)}_{\{Y_\alpha\}} \prod_{\alpha} e^{-[\tau - O(e) - 2d] |Y_\alpha|} \\ & \leq e^{kO(e)} [1 + O(e^{-\tau})]^k \leq 2^k \end{aligned}$$

where the sum $\sum^{(i)}$ goes over sets $\{Y_\alpha\}$ of contours Y such that $x_i \in Y \cup \text{Int } Y$ for all $Y \in \{Y_\alpha\}$. Finally, we note that the expansion of the left-hand side of (A.13) contains at least one contour because the term without any contour in (A.15) becomes zero when differentiated. Thus, a factor $\text{const} \cdot e^{-\tau}$ can be extracted from the sum over contours without destroying the remaining estimates. This concludes the proof of (A.13). ■

We are left with the proof of Lemma 2.3. Proceeding by induction, we assume that the lemma has already been proven for $\text{diam } Y^q \leq n - 1$ and $\text{diam } V \leq n$. For $\text{diam } Y^q = n$, we rewrite

$$K'(Y^q) = \rho(Y^q) \exp(e_q |Y^q|) \times \prod_m Z_m(\text{Int}_m Y^q) \{ \exp[-\log Z'_q(\text{Int}_m Y^q)] \} \chi_m(Y^q) \quad (\text{A.17})$$

with

$$\chi_m(Y^q) = \chi(\text{Re } \log Z'_q(V(Y^q)) - \text{Re } \log Z'_m(V(Y^q)) + \alpha |Y^q|) \quad (\text{A.18})$$

By the inductive assumption, Lemma 2.2, and the fact that χ is a C^4 function, $K'(Y^q)$ is a C^4 function for $\text{diam } Y^q = n$.

One may now use the inductive assumptions and the fact that $\log Z'_m(V) - e_m |V|$ can be analyzed by a convergent cluster expansion to bound [see Remark (iii) below]

$$\left| \frac{d^k}{dh^k} \log Z'_m(V) \right| \leq [C_k + O(\varepsilon)] |V| \leq 2C_k |V| \quad (\text{A.19})$$

provided $\text{diam } V \leq n$. Using the properties of the function χ , one obtains the bound

$$\left| \frac{d^k}{dh^k} \chi_m(Y^q) \right| \leq \text{const} \cdot |V(Y^q)|^{|k|} \quad (\text{A.20})$$

with a constant that depends on N and on k . On the other hand,

$$\left| \frac{d^k}{dh^k} [\rho(Y^q) \exp(e_q |Y^q|)] \right| \leq \text{const} \cdot (1 + |Y^q|)^{|k|} \exp[(\text{Re } e_q - e_0 - \tau) |Y^q|] \quad (\text{A.21})$$

and

$$\left| \frac{d^k}{dh^k} \exp[-\log Z_q(\text{Int } Y^q)] \right| \leq \text{const} \cdot |\text{Int } Y^q|^k \exp[\text{Re } f_q |\text{Int } Y^q| + O(\varepsilon) |Y^q|] \quad (\text{A.22})$$

We then use (A.17) to rewrite the derivatives of $K'(Y^q)$, and (A.20)–(A.22) together with Lemmas 2.1 and 2.2 to bound the resulting terms. We obtain the bound

$$\begin{aligned}
 \left| \frac{d^k}{dh^k} K'(Y^q) \right| &\leq \text{const} \cdot [1 + |Y^q| + |\text{Int } Y^q|]^{|\kappa|} \\
 &\quad \times \exp\{a_q |\text{Int } Y^q| + [\text{Re } e_q - e_0 + 2d + O(\varepsilon) - \tau] |Y^q|\} \\
 &\leq \text{const} \cdot [1 + |Y^q| + 2d |Y^q|^2]^4 \\
 &\quad \times \exp\{a_q |\text{Int } Y^q| + [\text{Re } e_q - e_0 + 2d + O(\varepsilon) - \tau] |Y^q|\} \\
 &\leq \exp[a_q |\text{Int } Y^q| + (\text{Re } e_q - e_0 + \text{const} - \tau) |Y^q|] \\
 &\leq (K\varepsilon)^{|Y^q|} \tag{A.23}
 \end{aligned}$$

where we used the fact that $\chi'(Y^q) = \prod \chi_m(Y^q)$ and all its derivatives are zero if

$$a_q |\text{Int } Y^q| + (\text{Re } e_q - e_0) |Y^q| > [\alpha + 1 + O(\varepsilon)] |Y^q|$$

We finally have to show that $\log Z'_q(V)$ is a C^4 function of h for $\text{diam } V = n + 1$. Since $\log Z'_q(V)$ can be analyzed by a convergent cluster expansion involving only contours Y^q of diameter less than or equal to n , this property of $\log Z'_q(V)$ follows immediately from the fact that $K'(Y^q)$ is C^4 for $\text{diam } Y^q \leq n$ and the fact that the cluster expansion for $d^k \log Z_q(V)/dh^k$ converges uniformly in h by the bound (A.23).⁹ ■

Remark (i). For $a_q \neq 0$, the bound (i) of Lemma 2.1 can be sharpened as follows: Taking the limit $n \rightarrow \infty$ of (A.12), and bounding $|\partial W|$ from below with the help of the isoperimetric inequality, we estimate

$$|Z_q(V)| \leq \exp(-f|V| + |\partial V|) \max_{W \subset V} \exp\left\{-\frac{a_q}{2}|V \setminus W| - \tau K|W|^{(d-1)/d}\right\}$$

where $K > 0$ is a constant which depends only on the dimension d . The maximum is obtained for either $W = V$ or $W = \emptyset$; therefore,

$$|Z_q(V)| \leq \exp(-f|V| + |\partial V|) \max\left\{\exp\left(-\frac{a_q}{2}|V|\right), \exp(-\tau K|V|^{(d-1)/d})\right\} \tag{A.24}$$

This is the announced improvement of Lemma 2.1(i).

Remark (ii). In a similar way, one may improve the bounds on the derivatives of $Z_q(V)$, using Eq. (A.9) and the fact that the derivatives of

⁹ The argument is the same as that leading to (A.9); see Remark (iii) below.

Z_q^{small} can be controlled by a convergent cluster expansion. One obtains the bound

$$\left| \frac{d^k Z_q(V)}{dh^k} \right| \leq C(|k|)(2|V|)^{|k|} \exp(-f|V| + |\partial V|) \\ \times \max \left\{ \exp\left(-\frac{a_q}{2}|V|\right), \exp(-\tau K|V|^{d/(d-1)}) \right\} \quad (\text{A.25})$$

Remark (iii). In standard polymer expansions (see, e.g., ref. 15), the partition function $\log Z'_m(V) - e_m |V|$ is expressed as a sum over term of the form

$$\phi_c(Y_1^m, \dots, Y_n^m) \prod_{i=1}^n K'(Y_i^m)$$

with coefficients ϕ_c (not depending on h) satisfying suitable bounds. These bounds are sufficient to ensure not only (A.19) for $k=0$, but, differentiating explicitly this sum and taking into account the inductive bounds on derivatives for K' , also for $k>0$.

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