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FINITE-SIZE SCALING FOR POTTS MODELS

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Abstract — Recently, two of the authors (C.B. and R.K.) developed a rigorous theory of finite-size effects near first-order phase transitions. Here we apply this theory to the ferromagnetic q state Potts model, which (for q large and $d \geq 2$) undergoes a first-order phase transition as the inverse temperature β is varied. We prove a formula for the internal energy in a periodic cube of side length L which describes the rounding of the infinite volume jump ΔE in terms of a hyperbolic tangent, and show that the position of the maximum of the specific heat is shifted by $\Delta\beta_m(L) = (\ln q/\Delta E)L^{-d} + O(L^{-2d})$ with respect to the infinite volume transition point β_t. We also propose an alternative definition of the finite volume transition temperature $\beta_t(L)$ which might be useful for numerical calculations because it differs only by exponentially small corrections from β_t.

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1. Introduction

First-order phase transitions are characterized by discontinuities in the first derivative of the free energy, i.e., discontinuities of an order parameter like the internal energy or the magnetization. As a consequence, the specific heat and the susceptibility show δ-function singularities at the transition. In finite systems, however, these singularities do not occur. Instead, the jump in the order parameter is smoothed out and one observes finite peaks in the susceptibility and the specific heat.

Recently the precise form of the order parameter in a finite volume has been studied by several authors [1–3,12]. For cubic volumes, it has been predicted that it can be described by a universal function, and that the jump is smoothed out in a region of width L^{-d} in the driving field or temperature, where d is the dimension and L is the side length of the cube.

In [4], two of the authors developed a rigorous theory of these finite-size effects that can be applied whenever it is possible to rewrite the partition function in terms of contour models with small activities that allow to control the behavior around the transition point. Note that it is not important for the methods of [4], whether the transition is "field-driven" or "temperature-driven", as long as it is first-order.[1]

In this note we will apply these methods to the q state Potts models. For q large enough (and $d \geq 2$) this model undergoes a first-order phase transition as the inverse temperature, $\beta = 1/(kT)$, is varied. At the transition point, β_t, the number of stable phases goes from 1 below β_t to q above β_t. Actually, for $\beta = \beta_t$, the q ordered low temperature phases and the disordered high temperature phase coexist, and the inner energy $E(\beta)$ jumps from $E_d = E(\beta_t - 0)$ to $E_o = E(\beta_t + 0)$ [5].

Here we prove that the internal energy, $E_{\text{per}}(\beta, L)$, and the specific heat, $C_{\text{per}}(\beta, L)$,

[1] Actually, for an asymmetric, field driven transition, the distinction between field driven and temperature driven transitions is somewhat artificial.

in a periodic box of side length L behave like

$$E_{\text{per}}(\beta, L) \sim \frac{E_d + E_o}{2} - \frac{E_d - E_o}{2} \,\text{th} \left\{ \frac{E_d - E_o}{2} \,(\beta - \beta_t) L^d + \frac{\log q}{2} \right\} \tag{1}$$

and

$$C_{\text{per}}(\beta, L) \sim L^d k \beta^2 \left(\frac{E_d - E_o}{2} \right)^2 \,\text{ch}^{-2} \left\{ \frac{E_d - E_o}{2} \,(\beta - \beta_t) L^d + \frac{\log q}{2} \right\} \tag{2}$$

if $L \to \infty$ and $\beta \to \beta_t$ in such a way that $(\beta - \beta_t)L^d$ is fixed. As a consequence, we locate the maximum of the specific heat at a point $\beta_m(L)$, which is shifted by

$$\Delta\beta_m(L) = \frac{\log q}{E_o - E_d} L^{-d} + O(L^{-2d}) \tag{3}$$

with respect to the infinite volume value β_t. We will also analyze the parameter $V_L(\beta) = 1 - \frac{1}{3}\langle H^4 \rangle_L \langle H^2 \rangle_L^{-2}$ introduced in [2], where $\langle \cdot \rangle_L$ denotes expectation values in L^d with periodic boundary conditions and H is the Hamiltonian in L^d. We find that the minimum of V_L is located at a point $\beta_V(L)$ which is shifted by

$$\Delta\beta_V(L) = \frac{L^{-d}}{E_o - E_d} \log(q \, E_o^2 / E_d^2) + O(L^{-2d}) \tag{4}$$

with respect to β_t. Note that the coefficients of L^{-d} in (3) and (4) differ from those derived in [2] using a phenomenological thermodynamic fluctuation theory. It is interesting to compare (3) and (4), as well as the predictions of [2] with the numerical data shown in Fig. 9 of [2]: both (3) and the corresponding prediction in [2] are in good agreement with the numerical data, while the prediction of [2] that $\Delta\beta_V(L) = \Delta\beta_m(L)$ in the leading order in L^{-d} is not consistent with them; on the other side the above prediction (4) is again in excellent agreement with the numerical data presented in [2] (see Section 4, Remark (i)).

We would like to stress that our results are derived directly from first principles, controlling all approximations made provided q is large enough. Actually, our method allows to calculate the higher order corrections to the first-order approximations (1) and (2). For simplicity, however, we only calculate the second-order corrections (see Theorem 3, Sect. 3).

In the course of proving (1) and (2), we also show that the number $N(\beta)$ of stable phases at temperature $1/\beta$ is given by

$$N(\beta) = \lim_{L\to\infty} \frac{Z_{\text{per}}(\beta, L)}{e^{-\beta f(\beta) L^d}}, \tag{5}$$

where Z_{per} is the partition function with periodic boundary conditions and $f(\beta)$ the free energy; namely,

$$N(\beta) = \begin{cases} 1 & \text{for} \quad \beta < \beta_t \\ q+1 & \text{for} \quad \beta = \beta_t \\ q & \text{for} \quad \beta > \beta_t. \end{cases}$$

This extends the results of [4], Section 5, to Potts models with large q.

In view of (5), it is natural to take the location of the maximum of $N(\beta, L)$, the finite volume approximation to (5), as an alternative definition of the finite-size transition point, $\beta_t(L)$. In fact we prove in Section 4 that this value differs from β_t only by an exponential error of the order $q^{-b\,L}$, where $b > 0$ is a constant. We also propose an equivalent definition that might be more useful for numerical applications as the point where $E_{\text{per}}(\beta, 2L) - E_{\text{per}}(\beta, L)$ passes through zero.

The paper is organized as follows. In Section 2 we use the Fortuin-Kasteleyn expansion along the lines of [7] to rewrite the model in terms of contours; this allows us to use the methods of [6] in the form of [4] to derive a formula for the finite volume internal energy involving only exponential errors in L. In Section 3 we further expand these formulae in order to compare them to the formulae in the literature, namely those proposed in [2]. Section 4 is devoted to the analysis of the finite-size shift of the transition temperature for the following three candidates of the finite-size transition point β_t(L): the location of the maximum of the specific heat, the minimum of V_L and the maximum of $N(\beta, L)$ mentioned above.

We note that some of the results presented in this paper (in particular the scaling form (2) for the specific heat and the corrected minimum value of the Binder parameter V_L given in Section 4) were independently obtained by Jooyoung Lee and J.M. Kosterlitz in their recent work [11]. We consider their results as comlementary to ours, since Lee and Kosterlitz present several numerical calculations (we don't do any), while we are more concerned with the rigorous aspects of the theory in order to definitely settle some of the controversies in the literature.

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2. Contour Analysis of the Model

In the Potts model, spin variables σ_i which take values in a discrete set $\{1, 2, \ldots, q\}$ are associated with each site i of a d-dimensional cubic lattice $\mathbf{Z}^d$. Two nearest-neighbor spins σ_i and σ_j interact with interaction energy $-J\delta(\sigma_i, \sigma_j)$ where $J > 0$ for ferromagnetic systems and δ is the Kronecker delta.

We start by considering the finite system defined in a periodic cube T of side length L. If we use Λ to denote the set of all dL^d nearest-neighbor bonds in T, the Hamiltonian of the system is

$$H = -J \sum_{\langle i,j \rangle \in \Lambda} \delta(\sigma_i, \sigma_j). \tag{6}$$

According to the Fortuin-Kasteleyn representation of the Potts model [8], the partition function $Z_{\text{per}}(\beta, L)$ on the torus T can be written as

$$Z_{\text{per}}(\beta, L) = \sum_{X \subset \Lambda} (e^{\beta} - 1)^{|X|} q^{C_\Lambda(X)} \,, \tag{7}$$

where the summation runs over all sets of bonds $X \subset \Lambda$ and we use $|X|$ and $C_\Lambda(X)$ to denote the number of bonds and connected components (regarding each isolated site as a component), respectively, and $\beta = 1/kT$ (without loss of generality we are choosing the coupling constant J=1). The subsets of Λ could therefore be regarded as the configurations of the system.

In [7], equation (7) was used as the starting point for a contour analysis of large q Potts models, which allowed a new and intuitive proof of the fact that the model undergoes a first-order phase transition at β_t. Here we follow this strategy to rewrite $Z_{\text{per}}(\beta, L)$ in a form which makes it possible to apply the methods of [4] and [6]. As a consequence we will be able to define smooth functions $f_o(\beta)$ and $f_d(\beta)$ such that $f_o(\beta)$ is identical with the free energy $f(\beta)$ for $\beta \geq \beta_t$, $f_d(\beta) = f(\beta)$ for $\beta \leq \beta_t$, $f(\beta) = \min\{f_o(\beta), f_d(\beta)\}$, and

$$\boxed{Z_{\text{per}}(\beta, L) = e^{-\beta L^d f_d(\beta)} + q e^{-\beta L^d f_o(\beta)} + O(q^{-bL}) e^{-\beta L^d f(\beta)}} \tag{8}$$

for some constant $b > 0$, provided q is large enough (and $d \geq 2$). Similar expressions will hold for the derivatives of $Z_{\text{per}}(\beta, L)$, see Theorem 1 below.

In order to prove (8) by the methods of [4] and [6], we first rewrite $Z_{\text{per}}(\beta, L)$ in terms of contours starting from the expansion (7). For any set of bonds $X \subset \Lambda$, we use $C(X)$ to denote the number of connected subsets of X, $S(X)$ to denote the set of sites which belong to some bond of X and δX to denote the set of bonds which belong to $\Lambda \backslash X$ and are connected to X. We notice that

$$\delta X = \delta_1 X \cup \delta_2 X,$$

where

$$\delta_k X = \{b \in \Lambda \backslash X; |S(b) \cap S(X)| = k\} \qquad k = 1, 2$$

and also that

$$|S(X)| - (1/d)|X| = (1/2d)(|\delta_1 X| + 2|\delta_2 X|)$$

which follows from the fact that 2d bonds meet at every site of the lattice. Hereafter $|E|$ denotes the cardinality of the set E. Taking into account this formula and the fact that $C_\Lambda(X) = C(X) + |S(\Lambda) \backslash S(X)|$ we get

$$Z_{\text{per}}(\beta, L) = \sum_{X \subset \Lambda} (e^\beta - 1)^{|X|} q^{\frac{1}{d}|\Lambda \backslash X|} q^{-\frac{1}{2d}\|\delta X\| + C(X)}\,, \tag{9}$$

where $\|\delta X\| = |\delta_1 X| + 2|\delta_2 X|$. The formula (9) already expresses the fact that (for $(e^\beta - 1) \approx q^{1/d}$) the partition function $Z_{\text{per}}(\beta, L)$ describes the coexistence of an ordered phase (small empty islands in a sea of bonds X) and a disordered phase (small oases of X in an empty desert), with excitations suppressed as $q^{-\ell/2d}$ where ℓ is the length of their boundary.

Now, our aim is to express the partition function in terms of contours describing these excitations. To this end we immerse the graph Λ inside the continuum torus $\mathbf{T}$ of linear size L (i.e., the real manifold $(\mathbf{R}/L\mathbf{Z})^d$). Considering the bonds, plaquettes, ... in Λ as subsets of $\mathbf{T}$, we define $P(X)$ as the union of all bonds in X and all plaquettes in Λ which contain 4 bonds of X if $d = 2$. For $d = 3$ the set $P(X)$ contains in addition the cubes whose all 12 bonds are in X, etc. We then consider the neighborhood of $P(X)$ which contains all points of distance less than 1/3 from $P(X)$. The boundary of this set (which is non empty except for $X = \Lambda$ or $X = \phi$) splits into connected components (with respect to the usual topology of $\mathbf{T}$), say, $\gamma_1, \ldots, \gamma_n$, which we call the contours corresponding to the configuration $X \subset \Lambda$. Moreover, we define the length, $\|\gamma\|$, of a contour as the number of intersections of the contour γ with the bounds of Λ, and we observe that

$$\sum_{k=1}^{n} \|\gamma_k\| = \|\delta X\|.$$

Notice that the contours $\gamma_1, \ldots, \gamma_n$ separate the ordered region X from the disordered region $\Lambda \backslash X$. Now, we divide the set of configurations $X \subset \Lambda$ into two classes: those configurations which contain at least one contour of diameter larger than $L/3$, and those where no such contour is present. The contribution of the former to the partition function (9) is denoted $Z^{\text{big}}(\beta, L)$. The contributions of the latter can be uniquely decomposed into perturbations of $X = \Lambda$ or $X = \phi$, and will be written as

$$qZ_o^{\text{res}}(\beta, L) + Z_d^{\text{res}}(\beta, L)\,, \tag{10}$$

with

$$Z_m^{\text{res}}(\beta, L) = \sum_X{}^{(m)} (e^\beta - 1)^{|X|} q^{\frac{1}{d}|\Lambda \backslash X|} \prod_\gamma \rho(\gamma)\,, \tag{11}$$

where the sum $\sum^{(m)}$ goes over the perturbations of Λ for $m = o$ and of ϕ if $m = d$; the product runs over all contours corresponding to X, and $\rho(\gamma)$ is defined locally as

$$\rho(\gamma) = q^{-\frac{1}{2d}\|\gamma\|} \tag{12}$$

if γ describes the transition from an ordered exterior to a disordered interior, and as

$$\rho(\gamma) = q \cdot q^{-\frac{1}{2d}\|\gamma\|} \tag{13}$$

for a contour with ordered interior (see appendix for the precise definitions). Note that $C(X)$ is equal to the number of contours with ordered interior if X can be described as a perturbation of ϕ, and equal to the number of contours with ordered interior plus 1 if X is a perturbation of Λ. This explains the factor q in (10).

Given the representation (11) for $Z_m^{\text{res}}(\beta, L)$ and the fact that

$$Z_{\text{per}}(\beta, L) = Z_d^{\text{res}}(\beta, L) + qZ_o^{\text{res}}(\beta, L) + Z^{\text{big}}(\beta, L) \tag{14}$$

the bound (8) can now be easily proven using the methods of [4] and [6]. We first note that the logarithm of $Z_o^{\text{res}}(\beta, L)$ can be controlled by a convergent cluster expansion if $\beta \geq \beta_t$, while $\log Z_d^{\text{res}}(\beta, L)$ can be controlled if $\beta \leq \beta_t$. Comparing the corresponding expansions with that for $\beta L^d f(\beta)$, one finds that

$$\left| - \log Z_m^{\text{res}}(\beta, L) - \beta L^d f(\beta) \right| \leq O(q^{-bL}) \tag{15}$$

for some constant $b > 0$, and hence

$$\left| Z_m^{\text{res}}(\beta, L) - e^{-\beta L^d f(\beta)} \right| \leq O(q^{-bL}) e^{-\beta L^d f(\beta)} ,$$

provided $m = o$ and $\beta \geq \beta_t$ or $m = d$ and $\beta \leq \beta_t$. Note that there are no surface corrections to the leading behavior of $\log Z_m^{\text{res}}$ because Z_m^{res} is defined on a torus.

Even though the validity of the bound (15) for $m = o$ and $m = d$ overlaps only at $\beta = \beta_t$, it is possible to define smooth functions $f_o(\beta)$ and $f_d(\beta)$, such that $f_o(\beta) = f(\beta)$ if $\beta \geq \beta_t$, $f_d(\beta) = f(\beta)$ if $\beta \leq \beta_t$, $f(\beta) = \min\{f_o(\beta), f_d(\beta)\}$ and

$$\left| Z_m^{\text{res}}(\beta, L) - e^{-\beta L^d f_m(\beta)} \right| \leq O(q^{-bL}) e^{-\beta L^d f(\beta)} \tag{16}$$

becomes true for all β, see Section 4 of [4] (and the appendix of this paper) for details.

On the other hand, one may use the fact that all configurations X contributing to $Z^{\rm big}$ contain at least one contour of size larger than $L/3$ to prove that

$$|Z^{\rm big}(\beta, L)| \leq O(q^{-bL}) e^{-\beta L^d f(\beta)} \tag{17}$$

(c.f. [6], Lemma 5.5). Combining (14), (16), and (17), we get (8). Generalizing the bounds (16) and (17) to derivatives in the same way as in [4] and using the notation

$$E_{\rm per}(\beta, L) = -L^{-d} \frac{d}{d\beta} \log Z_{\rm per}(\beta, L),$$

we get the following theorem.

Theorem 1. *There exist two six times differentiable functions $f_o(\beta)$ and $f_d(\beta)$ and constants $b, b_1 > 0$ such that the following statements are true whenever q is large enough (and $d \geq 2$).*

(i) $$f(\beta) = \begin{cases} f_o(\beta) & \text{if} \quad \beta \geq \beta_t \\ f_d(\beta) & \text{if} \quad \beta \leq \beta_t\,, \end{cases}$$

(ii) $$f(\beta) = \min\,\{f_o(\beta), f_d(\beta)\},\;\; E_d(\beta) - E_o(\beta) \geq b_1,\;\; \text{and}\;\; |f_o(\beta) - f_d(\beta)| \geq b_1\, \frac{|\beta - \beta_t|}{\beta},$$

(iii) $$\Big| Z_{\rm per}(\beta, L) - \Big[q e^{-\beta L^d f_o(\beta)} + e^{-\beta L^d f_d(\beta)} \Big] \Big| \leq e^{-\beta L^d f(\beta)} O(q^{-bL}),\;\; \text{and}$$

(iv) $$\left| \frac{d^k}{d\beta^k} \Big[E_{\rm per}(\beta, L) - (P_d(\beta) E_d(\beta) + P_o(\beta) E_o(\beta)) \Big] \right| \leq O(q^{-bL}),$$

where $0 \leq k \leq 5$,

$$P_d(\beta) = \frac{e^{-\beta L^d f_d(\beta)}}{qe^{-\beta L^d f_o(\beta)} + e^{-\beta L^d f_d(\beta)}}\,,$$

$$P_o(\beta) = \frac{qe^{-\beta L^d f_o(\beta)}}{qe^{-\beta L^d f_o(\beta)} + e^{-\beta L^d f_d(\beta)}}\,,$$

and

$$E_m(\beta) = \frac{d}{d\beta}\left(\beta f_m(\beta)\right), \quad m = o, d.$$

Remark. Notice that the relation (5) mentioned in the introduction follows immediately from (i)–(iii) above.

3. Finite-Size Scaling for the Mean Energy and the Specific Heat

In this section we derive the finite-size behavior of the mean energy $E_{\rm per}(\beta, L)$ and the specific heat,

$$C_{\rm per}(\beta, L) = -k\beta^2 \frac{d}{d\beta} E_{\rm per}(\beta, L) . \tag{18}$$

Letting $C_m(\beta) = \frac{d}{dT} E_m(\beta) = -k\beta^2 \frac{d}{d\beta} E_m(\beta)$, where E_m is defined in Theorem 1, $m = o, d$, and observing that

$$P_d(\beta) - P_o(\beta) = \text{th} \left\{ \frac{\beta L^d}{2} \left(f_o(\beta) - f_d(\beta)\right) - \frac{\ln q}{2} \right\}$$

while $P_d(\beta) + P_o(\beta) = 1$, we rewrite the statement (iv) of Theorem 1 (for $k = 0, 1$) as

$$E_{\rm per}(\beta, L) = \frac{E_d(\beta) + E_o(\beta)}{2} + \frac{E_d(\beta) - E_o(\beta)}{2} \, \text{th}\, Y + O(q^{-bL}) \tag{19a}$$

$$C_{\rm per}(\beta, L) = \frac{(E_d(\beta) - E_o(\beta))^2}{4} \, \frac{k\beta^2 L^d}{\text{ch}^2 Y} + \frac{C_d(\beta) + C_o(\beta)}{2}$$

$$+ \frac{C_d(\beta) - C_o(\beta)}{2} \, \text{th}\, Y + O(\beta^2 q^{-bL}) \tag{19b}$$

where we used the abbreviation

$$Y = \frac{\beta L^d}{2} \left(f_o(\beta) - f_d(\beta)\right) - \frac{\ln q}{2} . \tag{19c}$$

As a corollary, we immediately get the following

Corollary 2. *For $d \geq 2$ and q large enough, the following statements hold*

(i) *The limit $E_{\rm per}(\beta) = \lim_{L\to\infty} E_{\rm per}(\beta, L)$ exists for all $\beta \in \mathbf{R}^+$ and*

$$E_{\rm per}(\beta) = \begin{cases} E_o(\beta) & \text{for} \quad \beta > \beta_t \\ \frac{1}{q+1}\, E_d(\beta) + \frac{q}{q+1}\, E_o(\beta) & \text{for} \quad \beta = \beta_t \\ E_d(\beta) & \text{for} \quad \beta < \beta_t\,. \end{cases}$$

(ii) *For $\beta \neq \beta_t$, the limit $C_{\rm per}(\beta) = \lim_{L\to\infty} C_{\rm per}(\beta, L)$ exists, and*

$$C_{\rm per}(\beta) = \begin{cases} C_o(\beta) & \text{for} \quad \beta > \beta_t \\ C_d(\beta) & \text{for} \quad \beta < \beta_t\,, \end{cases}$$

while $$\lim_{L\to\infty} L^{-d} C_{\rm per}(\beta_t, L) = \frac{k\beta^2}{q^2+1+q^{-2}}\, (E_d - E_o)^2\,.$$

(iii) $|E_{\rm per}(\beta, L) - E_{\rm per}(\beta)| \leq O(q^{-bL}) + O(e^{-b_1|\beta-\beta_t|L^d})$.

(iv) $|C_{\rm per}(\beta, L) - C_{\rm per}(\beta)| \leq O(\beta^2 q^{-bL}) + O(\beta^2 L^d e^{-b_1|\beta-\beta_t|L^d})$ *provided $\beta \neq \beta_t$.*

Here E_o and E_d are defined as $E_o(\beta_t) = E_{\rm per}(\beta+0)$ and $E_d(\beta_t) = E_{\rm per}(\beta-0)$, respectively.

Note that the bounds (iii) and (iv) of Corollary 2, while valid for all $\beta \neq \beta_t$, are only useful if $|\beta - \beta_t| >> L^{-d}$. We now turn to the analysis of the region $(\beta - \beta_t) \leq O(L^{-d})$, which is the region where the finite-size rounding takes place. We introduce the constants $C_o = C_o(\beta_t) = C_{\rm per}(\beta + 0)$, and $C_d = C_d(\beta_t) = C_{\rm per}(\beta - 0)$, and expand $f_m(\beta)$, $E_m(\beta)$ and $C_m(\beta)$ around β_t. Using the fact that $f_o(\beta_t) = f_d(\beta_t)$, one gets the following

Theorem 3. *For $d \geq 2$ and q large enough,*

$$(i) \quad E_{\rm per}(\beta, L) = \left(\frac{E_d + E_o}{2} - \frac{(C_d + C_o)}{2k\beta^2}(\beta - \beta_t)\right) + \left(\frac{\Delta E}{2} - \frac{\Delta C}{2k\beta^2}(\beta - \beta_t)\right) \operatorname{th} Y_2 + O(q^{-bL}) + O((\beta - \beta_t)^2)\,;$$

$$(ii) \quad C_{\rm per}(\beta, L) = \frac{C_d + C_o}{2} + \frac{\Delta C}{2} \operatorname{th} Y_2 + k\beta^2 \left(\frac{\Delta E}{2} - \frac{\Delta C}{2k\beta^2}(\beta - \beta_t)\right)^2 L^d \operatorname{ch}^{-2} Y_2 + O(\beta^2 q^{-bL}) + O(\beta^2 \max\{|\beta - \beta_t|, |\beta - \beta_t|^2 L^d\})\,,$$

where $\Delta E = E_d - E_o$, $\Delta C = C_d - C_0$ *and*

$$Y_2 = L^d \left\{ (\beta - \beta_t)\frac{\Delta E}{2} - (\beta - \beta_t)^2 \frac{\Delta C}{2k\beta^2} \right\} - \frac{\ln q}{2}\,.$$

Proof. The proof is obvious, except for the error bounds [2]

$$|\mathrm{th}\, Y_2 - \mathrm{th}\, Y| \leq O(|\beta - \beta_t|^2)\,, \tag{20a}$$

$$|\mathrm{ch}^{-2} Y - \mathrm{ch}^{-2} Y_2| \leq O(|\beta - \beta_t|^2)\,, \tag{20b}$$

which are needed in the course of the proof. As an example, we prove the bound (20b) and leave the proof of (20a) to the reader.

By the fundamental theorem of calculus

$$|\mathrm{ch}^{-2} Y - \mathrm{ch}^{-2} Y_2| = \left| \int_{Y_2}^{Y} ds\, \frac{\partial}{\partial s}\, \mathrm{ch}^{-2} s \right| = \left| \int_{Y_2}^{Y} ds\, \frac{2\mathrm{th}\, s}{\mathrm{ch}^2 s} \right|$$

$$\leq 2|Y - Y_2| \sup_{t\in[0,1]} \frac{1}{\mathrm{ch}(tY + (1-t)Y_2)^2}$$

$$\leq \sup_{t\in[0,1]} \frac{2|Y - Y_2|}{\exp(2|tY + (1-t)Y_2|)} \leq \sup_{t\in[0,1]} \frac{2|Y - Y_2|}{1 + 2|tY + (1-t)Y_2|}\,.$$

We now use Theorem 1(ii) to bound

$$\inf_{t\in[0,1]} 2|tY + (1-t)Y_2| \geq L^d b_1(\beta - \beta_t) - O((L^d(\beta - \beta_t)^2) - \log q\,.$$

[2] The bounds (20) are in fact not uniform in q, as may be seen from the proof below. A more precise statement would involve errors $O(|\beta - \beta_t|^2 \log q)$ that explicitely expresses the dependence of the constants on q.

If the second term on the r.h.s. dominates the first, $|\beta - \beta_t| \geq K$ for some constant K not depending on β and L and the bound (20b) is a trivial statement. So we may assume without loss of generality that

$$\inf_{t\in(0,1)} 2|tY + (1-t)Y_2| \geq \frac{b_1}{2} L^d |\beta - \beta_t| - \log q$$

which implies that

$$\sup_{t\in(0,1)} \frac{2(Y-Y_2)}{1+2|tY+(1-t)Y_2|} \leq \frac{2|Y-Y_2|}{\max\left\{1, \frac{b_1}{2} L^d|\beta-\beta_t| - \log q\right\}} .$$

Inserting the bound $|Y - Y_2| \leq \text{const } L^d |\beta - \beta_t|^3$ the inequality (20) follows. □

Remark: (i) If one expresses β in terms of $T = 1/k\beta$, the bounds of Theorem 3 become ($\Delta T = T_t - T$)

$$E_{\text{per}}(T,L) = \left(\frac{E_d + E_o}{2} + \frac{C_d + C_o}{2}\Delta T\right) + \left(\frac{\Delta E}{2} + \frac{\Delta C}{2}\,\Delta T\right) \text{th}\, Y_2 \tag{21}$$
$$+ O(q^{-bL}) + O\Big(\Big(\frac{\Delta T}{kTT_t}\Big)^2\Big)$$

and

$$C_{\text{per}}(T,L) = \frac{C_d + C_o}{2} + \frac{\Delta C}{2}\,\text{th}\, Y_2 + \left(\frac{\Delta E}{2} + \frac{\Delta C}{2}\,\Delta T\right)^2 \frac{L^d \text{ch}^{-2} Y_2}{kT^2} \tag{22}$$
$$+ O\Big(\frac{1}{(kT)^2}\, q^{-bL}\Big) + O\Big(\frac{1}{(kT)^2} \max\Big\{\frac{|\Delta T|}{kTT_t}\,,\, \frac{|\Delta T|^2}{k^2T^2T_t^2}\, L^d\Big\}\Big),$$

with

$$Y_2 = -L^d \left\{\frac{\Delta E}{2kT}\,\frac{\Delta T}{T_t} + \frac{\Delta C}{2k}\left(\frac{\Delta T}{T_t}\right)^2\right\} - \frac{\ln q}{2}\,. \tag{23}$$

The formulae (7) and (9) of [2] are exactly of the same form, with the only difference that they involve the argument

$$\widetilde{Y} = Y - \frac{1}{4}\,\ln(C_0/C_d)$$

where we have the argument Y_2. In order to discuss this discrepancy, we briefly describe the theory of [2]. It starts from the assumption that the probability distribution, $P_L(E)$ of the energy in a finite volume L, can be well approximated by the sum of two Gaussians centered at $E_m + C_m \Delta T$, $m = o, d$ (in the notation of [2] o is denoted $-$ and d is denoted $+$), with width $(kT^2 C_m L^{-d})^{1/2}$. The normalization of these Gaussians is then chosen in such a way that $P_L(E_o) = q P_L(E_d)$ for $T = T_t$.

In fact, this normalization is incorrect because at $T = T_t$, all phases contribute to the periodic Gibbs state with the same weight. This has already been observed in [6] and also follows from Corollary 2 above (recall that there are q ordered phases and 1 disordered phase at $T = T_t$). And the weight of a given phase includes the fluctuations around the corresponding maximum of P_L. Therefore the correct normalization is obtained if one requires that the *area* under the peak at E_d is q times the area under the peak of E_o, which corresponds to $P_L(E_o) = q(C_d/C_o)^{1/2} P_L(E_d)$ for $T = T_t$. This explains the discrepancy between the formulae given in [2] and our formulae.

(ii) It is obvious that one could calculate the higher order corrections for E_{per} and C_{per} as well, starting from (19) again and expanding further in $(\beta - \beta_t)$.

We close this section with the discussion of the quantity

$$V_L(\beta) = 1 - \frac{\langle E^4 \rangle_L}{3 \langle E^2 \rangle_L^2} \tag{24}$$

introduced in [2]. (The expectation value $\langle E^k \rangle_L$ is defined as

$$(-1)^k \, \frac{L^{-kd}}{Z_{\text{per}}(\beta, L)} \, \frac{d^k}{d\beta^k} \, Z_{\text{per}}(\beta, L) \, ,$$

$k = 2, 4$). Obviously $V_L(\beta) \to V_\infty(\beta) = 2/3$ as $L \to \infty$ if we fix $\beta \neq \beta_t$. For a second-order transition it is expected that $V_L(\beta) \to 2/3$ at $\beta = \beta_t$ as well, while $V_\infty(\beta_t)$ is expected to be smaller than $2/3$ for a first-order phase transition. Here

$$V_L(\beta_t) \underset{L \to \infty}{\longrightarrow} 1 - \frac{(q E_o^4 + E_d^4)(q + 1)}{3(q E_o^2 + E_d^2)^2} \, ,$$

which is indeed strictly smaller than 2/3. Definig $\beta_V(L)$ as the point where the finite volume quantity $V_L(\beta)$ is minimal, one may now discuss the shift of $\beta_V(L)$ with respect to β_t. We defer this discussion to the next section.

4. The Shift of the Transition Point

In this section we discuss the shift of the finite-volume transition point with respect to the infinite-volume value β_t. Defining $V_L(\beta)$ as in the last section and the finite volume approximation to the number $N(\beta)$ of stable phases at β as

$$N(\beta, L) := \left[\frac{Z_{\text{per}}(h, L)^{2^d}}{Z_{\text{per}}(h, 2L)} \right]^{\frac{1}{2^d-1}} \tag{25}$$

we consider the following three points

— the point $\beta_m(L)$ where the specific heat is maximal,

— the point $\beta_V(L)$ where $V_L(\beta)$ is minimal,

— and the point $\beta_N(L)$ where $N(\beta, L)$ is maximal.

Theorem 4. *For $d \geq 2$ and q large enough, the following statements are true provided L is large:* (i) *There is exactly one point $\beta_m(L)$, such that $C_{\text{per}}(\beta_m(L), L) > C_{\text{per}}(\beta, L)$ for all $\beta \neq \beta_m(L)$. In addition*

$$\beta_m(L) - \beta_t = \frac{L^{-d}}{E_o - E_d} \ln q \, + \, O(L^{-2d}) \, . \tag{26}$$

(ii) *There is exactly one point $\beta_V(L)$, such that $V_L(\beta_V(L)) < V_L(\beta)$ for all $\beta \neq \beta_V(L)$. In addition*

$$\beta_V(L) - \beta_t = \frac{L^{-d}}{E_o - E_d} \ln(qE_o^2/E_d^2) + O(L^{-2d}) \, . \tag{27}$$

(iii) *There is exactly one point $\beta_N(L)$, such that $N(\beta_N(L), L) > N(\beta, L)$ for all $\beta \neq \beta_N(L)$. In addition*

$$|\beta_N(L) - \beta_t| = O(q^{-bL}) \, . \tag{28}$$

Remarks:

(i) For $d = 2$, the exact values of β_t, E_o and E_d are known [9,10]. For the $q = 10$ Potts Model, $\beta_t^{-1} = 0.701232$, $E_d = -0.9682$ and $E_o = -1.6643$. Reexpressing (26) and (27) in terms of $kT = \beta^{-1}$, we get

$$kT_m(L) = kT_t + \frac{(kT_t)^2 L^{-d}}{E_d - E_o} \ln q + O(L^{-2d}) \tag{26'}$$

$$kT_V(L) = kT_t + \frac{(kT_t)^2 L^{-d}}{E_d - E_o} \ln(qE_o^2/E_d^2) + O(L^{-2d}) \,. \tag{27'}$$

In particular, for $q = 10$ and $d = 2$, we get

$$kT_m(L) = 0.7012 + 1.63L^{-2} + O(L^{-4})$$
$$kT_V(L) = 0.7012 + 2.39L^{-2} + O(L^{-4})$$

which is in very good agreement with the numerical data of Challa *et al.* as shown in Fig. 9 of [2].

(ii) Inserting the value of $\beta_V(L)$ into $V_L(\beta)$, one finds that

$$V_L^{\min} = \min_\beta \; V_L(\beta) = \frac{2}{3} - \frac{1}{3}\left(\frac{E_d^2 - E_o^2}{2E_dE_o}\right)^2 + O(L^{-d}) \,, \tag{29}$$

which, for $d = 2$ and $q = 10$, gives

$$V_L^{\min} = 0.559 + O(L^{-2})$$

which is in better agreement with the data of Challa *et al.* as shown in Fig. 8 of [2] than their theoretical value 0.58.

(iii) Theorem 4 shows that the point $\beta_N(L)$ where $N(\beta, L)$ is maximal is a much better approximation for β_t than $\beta_m(L)$, which might seem the most natural definition of the finite volume transition point at first sight. Remark that $N(\beta, L)$ may either be obtained directly using the available numerical methods to calculate partition functions, or indirectly using the observation that

$$E_{\text{per}}(\beta_N(L), L) = E_{\text{per}}(\beta_N(L), 2L)\,. \tag{30}$$

We therefore propose $\beta_N(L)$ as a new way to determine β_t from the finite size data.

(iv) Before actually proving Theorem 4, we indicate the heuristic ideas behind the proof. Starting with the shift of $\beta_m(L)$ we recall that

$$C_{\text{per}}(\beta, L) \sim L^d k \beta^2 \left(\frac{\Delta E}{2}\right)^2 \text{ch}^{-2} \left\{\frac{\Delta E}{2}\,(\beta - \beta_t) L^d + \frac{\log q}{2}\right\}$$

if $L \to \infty$ and $\beta \to \beta_t$ in such a way that $(\beta - \beta_t)L^d$ is fixed. This leads to the shift

$$\Delta\beta_m(L) \sim -\frac{\log q}{\Delta E}\, L^{-d}\,.$$

On the other hand

$$E_{\text{per}}(\beta_t, L) - E_{\text{per}}(\beta_t, 2L) = O(q^{-bL})$$

and

$$\frac{d}{d\beta}\left(E_{\text{per}}(\beta_t, L) - E_{\text{per}}(\beta_t, 2L)\right) = -\frac{1}{k\beta^2}\left(C_{\text{per}}(\beta_t, L) - C_{\text{per}}(\beta_t, 2L)\right) = O(L^d)$$

by the bounds (19a) and (19b). Using the fact that $\beta_N(L)$ may be characterized by (30) one expects only an exponentially small shift

$$\Delta\beta_N(L) = O(q^{-bL})\,.$$

In order to determine $\beta_V(L)$ we first note that it is the point where

$$U(L, \beta) = \frac{\langle E^2\rangle_L^2}{\langle E^4\rangle_L} \tag{31}$$

is minimal. By Theorem 1

$$U(L,\beta) = \left[\sum_m P_m(\beta) A_m(\beta) \right]^2 \left[\sum_m P_m(\beta) B_m(\beta) \right]^{-1} + O(q^{-bL}) \tag{32}$$

where

$$A_m(\beta) = L^{-2d} e^{L^d \beta f_m(\beta)} \frac{d^2}{d\beta^2} e^{-L^d \beta f_m(\beta)} = E_m^2(\beta) + O(L^{-d}) \tag{33a}$$

and

$$B_m(\beta) = L^{-4d} e^{L^d \beta f_m(\beta)} \frac{d^4}{d\beta^4} e^{-L^d \beta f_m(\beta)} = E_m^4(\beta) + O(L^{-d}) \ . \tag{33b}$$

Neglecting the dependence of A_m, B_m on β and taking only the leading term in L^{-d} into account we obtain

$$U(L,\beta) \approx \left(\sum_m E_m^2 P_m(\beta) \right)^2 \left(\sum_m E_m^4 P_m(\beta) \right)^{-1} . \tag{34}$$

Since $P_o(\beta) + P_d(\beta) = 1$, this depends on β only through the variable

$$x = P_d(\beta) - P_o(\beta) = \text{th}\, Y(\beta)\,. \tag{35}$$

We rewrite the right-hand side of (34) as

$$\frac{(E_o^2 P_o + E_d^2 P_d)^2}{E_o^4 P_o + E_d^4 P_d} = \frac{\left(\frac{1}{2}(E_o^2 + E_d^2) + \frac{x}{2}(E_d^2 - E_o^2)\right)^2}{\frac{1}{2}(E_o^4 + E_d^4) + \frac{x}{2}(E_d^4 - E_o^4)} = \frac{(F + Gx)^2}{F^2 + 2FGx + G^2} = g(x)\,, \tag{36}$$

where $F = (E_o^2 + E_d^2)/2$ and $G = (E_d^2 - E_o^2)/2$. Calculating the derivative of g one immediately finds the minimum of g at the location

$$x_0 = -\frac{G}{F} = \frac{E_o^2 - E_d^2}{E_o^2 + E_d^2}\,,$$

corresponding to

$$Y(\beta) = \operatorname{arth} \frac{E_o^2 - E_d^2}{E_o^2 + E_d^2} = \frac{1}{2} \log(E_o^2/E_d^2) \, .$$

Up to technical details, which we present below, this proves (27).

Proof of Theorem 4. (i) Choose $\tilde{\beta} = \tilde{\beta}(L)$ in such a way that

$$\beta L^d \left(f_o(\beta) - f_d(\beta) \right) = \ln q \, .$$

Then $Y(\tilde{\beta}) = 0$ and $|Y(\beta)| \geq \frac{b_1}{2} \, |\beta - \tilde{\beta}| L^d$, where b_1 is the constant from Theorem 1(ii) (recall that $E_m(\beta) = d(\beta f_m(\beta))/d\beta$). As a consequence of this bound and the bound (19b),

$$C_{\mathrm{per}}(\beta, L) < C_{\mathrm{per}}(\tilde{\beta}, L)$$

for all β with $|\beta - \tilde{\beta}| \geq K L^{-d}$, provided $K > 0$ and L is chosen large enough (depending on K). It is therefore enough to analyze $C_{\mathrm{per}}(\cdot, L)$ in an interval $I = [\tilde{\beta} - K L^{-d}, \tilde{\beta} + K L^{-d}]$. Taking derivatives in (19b), which is justified by Theorem 1(iv), one easily shows that $C_{\mathrm{per}}(\cdot, L)$ has one and only one local maximum $\beta_m(L)$ in I, that

$$- \frac{d^2 C_{\mathrm{per}}(\beta, L)}{d\beta^2} \geq k \beta^2 L^{3d} \left(\frac{\Delta E}{2} \right)^4 \qquad \text{for all} \qquad \beta \in I \, ,$$

and that

$$\left| \frac{d C_{\mathrm{per}}(\beta, L)}{d\beta} \right|_{\beta = \tilde{\beta}} \leq O(\beta^2 L^d) \, ,$$

provided K is chosen small enough. As a consequence of the last two bounds

$$|\beta_m(L) - \tilde{\beta}| \leq O(L^{-2d}) \, ,$$

which, together with the fact that

$$\tilde{\beta} = \beta_t - L^{-d}\, \frac{\ln q}{E_d - E_o} + O(L^{-2d})$$

completes the proof of (i).

(iii) The structure of the proof of (iii) is identical to that of (i), with the only difference that β_t takes the role of $\tilde{\beta}(L)$. The fact that $|\beta_t - \beta_N(L)| \leq O(q^{-bL})$ follows from the bound

$$\left| \frac{d}{d\beta}\, \log N(\beta, L) \right|_{\beta=\beta_t} = \frac{(2L)^d}{2^d - 1}\, |E_{\mathrm{per}}(\beta_t, 2L) - E_{\mathrm{per}}(\beta_t, L)| = L^d O(q^{-bL})$$

and the fact that

$$-\frac{d^2}{d\beta^2}\, \log N(\beta, L) = \frac{(2L)^d}{(2^d - 1)k\beta^2}\, (C_{\mathrm{per}}(\beta, 2L) - C_{\mathrm{per}}(\beta, L)) = O(L^{2d})$$

provided $|\beta - \beta_t| \leq KL^{-d}$. (We used the bound (19); and again K has to be chosen small enough.)

(ii) Motivated by the heuristic analysis above we define $\tilde{\beta}$ as the value of β for which

$$\mathrm{th}\, Y(\tilde{\beta}) = x_o \equiv (E_o^2 - E_d^2)/(E_o^2 + E_d^2)\,.$$

Let $g(x)$ be the function defined in (36). Then

$$g'(x_o) = 0, \quad g''(x_o) > 0\,, \tag{37}$$

$$g'(x) < 0 \qquad \text{for} \qquad x \in (-1, x_o) \qquad \text{and} \qquad g'(x) > 0 \qquad \text{for} \qquad x \in (x_o, 1)\,. \tag{38}$$

Using (37) and the definition of $x(\beta) = \text{th}\, Y(\beta)$ with Y given in (19c) one easily shows that

$$\frac{d^2 g(x(\beta))}{d\beta^2} \geq \frac{1}{2} \left.\frac{d^2 g(x(\beta))}{d\beta^2}\right|_{\beta=\tilde{\beta}} = \frac{g''(x_o)}{2} \left(\frac{E_o(\tilde{\beta}) - E_d(\tilde{\beta})}{2\text{ch}^2 Y(\tilde{\beta})} \, L^d \right)^2 =: \epsilon L^{2d} \qquad (39)$$

provided $|\beta - \tilde{\beta}| \leq \alpha L^{-d}$ and $\alpha > 0$ is chosen small enough. On the other hand,

$$\frac{d^2 U(L,\beta)}{d\beta^2} = \frac{d^2 g(x(\beta))}{d\beta^2} + O(L^d) + O(L^{2d}|\beta - \beta_t|) = \frac{d^2 g(x(\beta))}{d\beta^2} + O(L^d)$$

in the interval $I = [\tilde{\beta} - \alpha L^{-d},\ \tilde{\beta} + \alpha L^{-d}]$ (recall that $|\tilde{\beta} - \beta_t| = O(L^{-d})$). We therefore conclude that

$$\frac{d^2 U(L,\beta)}{d\beta^2} \geq \frac{\epsilon L^{2d}}{2} \qquad \text{for} \qquad \beta \in I\,,$$

provided L is chosen large enough. In a similar way one obtains

$$\left| \frac{dU(L,\beta)}{d\beta} \right|_{\beta=\tilde{\beta}} \leq \text{const}(1 + L^d|\tilde{\beta} - \beta_t|) \leq O(1)\,.$$

We conclude that $U(L,\beta)$ has exactly one local minimum $\beta_V(L)$ in I, and that

$$|\beta_V(L) - \tilde{\beta}| \leq O(L^{-2d})\,.$$

Since

$$\tilde{\beta} = \beta_t - \frac{L^{-d}}{\Delta E} \log(qE_o^2/E_d^2) + O(L^{-2d})\,,$$

this proves the bound (27).

We are left with the proof that

$$U(L,\beta) > U(L,\beta_V(L)) \qquad \text{provided} \qquad |\beta - \tilde{\beta}| \geq \alpha L^{-d}\,.$$

Let $x_{1,2} = x(\tilde{\beta} \pm \alpha L^{-d})$. Then

$$g(x) \geq \min\{g(x_1), g(x_2)\} =: g(x_0) + \tilde{\epsilon} \qquad \text{for all} \qquad x \notin (x_1, x_2)$$

by the bounds (38). Since $U(L, \beta) - g(x(\beta)) = O(L^{-d}) + O(\beta - \beta_t)$ we conclude that

$$U(L, \beta) > U(L, \tilde{\beta})$$

provided $|\beta - \beta_t| \leq K$, $K > 0$ is chosen small enough and L is large. But for $|\beta - \beta_t| \geq K$ either $P_+(\beta) \leq O(e^{-b_1 K L^d})$ or $P_-(\beta) \leq O(e^{-b_1 K L^d})$, where b_1 is the constant from Theorem 1. Combined with the bounds (32) and (33) we obtain that

$$U(L, \beta) = 1 + O(L^{-d})$$

if $|\beta - \beta_t| \leq K$; this completes the proof because $U(L, \beta_V(L)) < 1$. $\square$

Appendix: The Definition of f_m and $Z_m^{\rm res}$

We divide the set of contours into two classes: those of diameter less than $L/3$ to be called short in the sequel, and the remaining ones to be called long. It is a consequence of our definition of contours that the set $\mathbf{T}\backslash\gamma$ splits into two connected components for all short contours γ. We write Ext γ for the larger one and Int γ for the smaller one. Given a short contour, γ, there is a unique configuration, $X(\gamma)$, such that γ is the only contour corresponding to $X(\gamma)$. If $X(\gamma) \subset$ Ext γ, γ will be called an ordered contour, if $X(\gamma) \subset$ Int γ it is called disordered.

A set ∂ of contours is called admissible if there exists a configuration X such that ∂ is the set of contours corresponding to X. If ∂ is an admissible set of short contours, a contour $\gamma \in \partial$ is called external, if it touches the set $\bigcap_{\gamma\in\partial} \text{Ext}\,\gamma$. A set ∂ of contours is called a set of mutually external contours if, for all γ, $\gamma' \in \partial$, $\text{dist}(\text{Int}\gamma, \text{Int}\gamma') \geq 1/3$.

The partition functions $Z_m^{\rm res}(\beta, L)$ introduced in (11) are defined by restricting the sum in (9) to the sum over all admissible sets of short contours with ordered external contours if $m = o$ and disordered ones if $m = d$. The activity, $\rho(\gamma)$, of a short contour γ is defined by (10) if γ is an ordered contour, and by (11) if γ is a disordered contour; that is

$$\rho(\gamma) = q^{-\|\gamma\|/2d}$$

if γ is ordered and

$$\rho(\gamma) = q \cdot q^{-\|\gamma\|/2d}$$

if γ is disordered. Note that the minimal length of an ordered contour is $\|\gamma\| = 2$ while the length of the smallest disordered contour is $4d - 2$.

Given a volume $V \subset \mathbf{R}^d$ such that $V =$ Int γ_o for some contour γ_o, we introduce $B(V)$ as the set of all bonds whose center lies in V and define

$$Z_m(V) = \sum_{\partial} (e^\beta - 1)^{|B(V)\cap X(\partial)|}\, q^{\frac{1}{d}|B(V)\backslash X(\partial)|} \prod_{\gamma\in\partial} \rho(\gamma)\,, \tag{A.1}$$

where the sum goes over all admissible families ∂ of contours such that the external contours in ∂ are m contours with $\mathrm{dist}(\gamma, V^c) \geq 1/3$. We use $X(\partial)$ to denotes the uniquely determined configuration X corresponding to ∂. With this definition we may rewrite

$$Z_o^{\mathrm{res}}(\beta, L) = \sum_{\partial} (e^{\beta} - 1)^{|B(\mathrm{Ext}\partial)|} \prod_{\gamma \in \partial} \rho(\gamma) Z_d(\mathrm{Int}\ \gamma), \tag{A.2}$$

and

$$Z_d^{\mathrm{rest}}(\beta, L) = \sum_{\partial} q^{|B(\mathrm{Ext}\partial)|} \prod_{\gamma \in \partial} \rho(\gamma) Z_o(\mathrm{Int}\ \gamma), \tag{A.3}$$

where the summations are over sets of families ∂ of mutually external short m contours ($m = o,\ d,$ resp.) and $\mathrm{Ext}\partial = \cap_{\gamma \in \partial} \mathrm{Ext}\gamma$.

Multiplying every term $Z_d(\mathrm{Int}\gamma)$ by $1 = Z_o(\mathrm{Int}\gamma)/Z_o(\mathrm{Int}\gamma)$, we may iterate (A.2) to get

$$Z_o^{\mathrm{res}}(\beta, L) = (e^{\beta} - 1)^{dL^d} \sum_{\partial}^{(o)} \prod_{\gamma \in \partial} K(\gamma), \tag{A.4}$$

where the contour weight $K(\gamma)$ is defined by

$$K(\gamma) = \rho(\gamma)\ \frac{Z_d(\mathrm{Int}\ \gamma)}{Z_o(\mathrm{Int}\ \gamma)}. \tag{A.5}$$

and the sum goes over all collections ∂ of short *ordered* contours such that dist $(\gamma, \gamma') \geq \frac{1}{3}$ for all $\gamma, \gamma' \in \partial$, $\gamma \neq \gamma'$. Similarly, introducing for *disordered* contours γ the weight

$$K(\gamma) = \rho(\gamma)\ \frac{Z_o(\mathrm{Int}\ \gamma)}{Z_d(\mathrm{Int}\ \gamma)}, \tag{A.6}$$

we get

$$Z_d^{\mathrm{res}}(\beta, L) = q^{L^d} \sum_{\partial}^{(d)} \prod_{\gamma \in \partial} K(\gamma), \tag{A.7}$$

where the sum goes over all collections ∂ of of short disordered contours such that dist$(\gamma,\gamma')\geq \frac{1}{3}$ for all $\gamma,\gamma'\in\partial$, $\gamma\neq\gamma'$.

Using the methods of [4,6] one now shows that there exist a constant $b>0$ and a uniquely defined inverse temperature β_t such that the following statements are true provided q is large enough:

i) $|Z_m(V)|\leq e^{-\beta f(\beta)|B(V)|/d+O(|\partial V|)}$ for all inverse temperatures β.

ii) $|K(\gamma)|\leq q^{-b\|\gamma\|}$ if γ is disordered and $(\bar\beta-\bar\beta_t)\mathrm{diam}\,\gamma\leq b\log q$.

iii) $|K(\gamma)|\leq q^{-b\|\gamma\|}$ if γ is ordered and $(\bar\beta_t-\bar\beta)\mathrm{diam}\,\gamma\leq b\log q$.

Here

$$\begin{aligned}\bar\beta&=d\log(e^{\beta}-1)\\ \bar\beta_t&=d\log(e^{\beta_t}-1).\end{aligned}\tag{A.8}$$

Note that the bound (15) mentioned in section 2 is an immedeate consequence of ii), iii), (A.4), (A.7) and the standard techniques of Mayer expansions for dilute polymer systems.

We now define the extensions $f_m(\beta)$ of the free energy $f(\beta)$. We introduce

$$K'(\gamma):=K(\gamma)\,\chi\left(b\log q+(\bar\beta-\bar\beta_t)\mathrm{diam}\,\gamma\right)\tag{A.9}$$

if γ is an ordered contour, and

$$K'(\gamma):=K(\gamma)\,\chi\left(b\log q+(\bar\beta_t-\bar\beta)\mathrm{diam}\,\gamma\right)\tag{A.10}$$

if γ is a disordered contour. Here χ is a smoothed version of the characteristic function ($\chi\in C^6$, $0\leq\chi\leq 1$, $\chi(x)=0$ if $x\leq 0$ and $\chi(x)=1$ if $x\geq 1$). Note that

$$|K'(\gamma)|\leq q^{-b\|\gamma\|}\tag{A.11}$$

for all γ and all $\beta\geq 0$ by the definition of K' and the bounds ii) and iii) above. We conclude that the free energy, $f_m(\beta)$, corresponding to the partition function

$$Z'_m(\beta,L)=e^{-e_mL^d}\sum_{\partial}{}^{(m)}\prod_{\gamma\in\partial}K'(\gamma),\tag{A.12}$$

with

$$
\begin{aligned}
e_o &= -d\log(e^\beta - 1) = -\bar\beta, \\
e_d &= -\log q,
\end{aligned}
\tag{A.13}
$$

is well defined and may be analysed by a convergent cluster expansion. Theorem 1 then follows using the methods of [4], Section 4. Note that statement i) of Theorem 1 is obvious at this point since $K'(\gamma) = K(\gamma)$ for all ordered contours if $\beta \geq \beta_t$, while $K'(\gamma) = K(\gamma)$ for all disordered contours if $\beta \leq \beta_t$.

Remark. In order to apply the methods of [4], on needs bounds of the form

$$
\left| \left(\frac{de_m(\beta)}{d\beta} \right)^k \right| \leq C_k \tag{A.14}
$$

for some constants $C_k < \infty$ which do not depend on β. The bounds (A.14) are obviously fulfilled if we restrict β to, say, $[1, \infty)$. On the other hand, $|d^k e_m / d(\bar\beta)^k| \leq 1$ for all β. As a consequence

$$
|\beta(f_o(\beta) - f_d(\beta))| \geq b_1 |\bar\beta - \bar\beta_t| \,,
$$

which, together with the fact that

$$
\bar\beta_t = \log q + O(q^{-b})
$$

implies that

$$
|P_o(\beta)| \leq q^{-bL^d} (e^\beta - 1)^{L^d}.
$$

(Similar bounds hold for the derivatives). We conclude that

$$
\left| \frac{d^k}{d\beta^k} \left[E_{\text{per}}(\beta, L) - (P_d(\beta) E_d(\beta) + P_o(\beta) E_o(\beta)) \right] \right| \leq \left| \frac{d^k}{d\beta^k} \left[E_{\text{per}}(\beta, L) - E_d(\beta) \right] \right| + O(q^{-bL}) \,, \tag{A.15}
$$

if $\beta \leq 1$. For $\beta \leq 1$, however, $E_{\text{per}}(\beta, L)$ may be analysed by a standard high temperature expansion which immediately gives a bound of the form $O(q^{-bL})$ for the right hand side of (A.15).

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