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Finite-Size Effects for the Potts Model with Weak Boundary Conditions

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Using the Pirogov–Sinai theory, we study finite-size effects for the ferromagnetic q-state Potts model in a cube with boundary conditions that interpolate between free and constant boundary conditions. If the surface coupling is about half of the bulk coupling and q is sufficiently large, we show that only small perturbations of the ordered and disordered ground states are dominant contributions to the partition function in a finite but large volume. This allows a rigorous control of the finite-size effects for these "weak boundary conditions." In particular, we give explicit formulæ for the rounding of the infinite-volume jumps of the internal energy and magnetization, as well as the position of the maximum of the finite-volume specific heat. While the width of the rounding window is of order L^{-d}, the same as for periodic boundary conditions, the shift is much larger, of order L^{-1}. For "strong boundary conditions"—the surface coupling is either close to zero or close to the bulk coupling—the finite size effects at the transition point are shown to be dominated by either the disordered or the ordered phase, respectively. In particular, it means that sufficiently small boundary fields lead to the disordered, and not to the ordered Gibbs state. This gives an explicit proof of A. van Enter's result that the phase transition in the Potts model is not robust.

KEY WORDS: Lattice systems; finite-size scaling; Potts model; surface coupling.

1. INTRODUCTION

First-order phase transitions are characterized by discontinuities in the mean values of order parameters in the thermodynamic limit. However, in

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a finite volume the transition is rounded and, possibly, shifted with respect to the infinite-volume transition point.

The details of the finite-size effects depend crucially on the choice of boundary conditions that, in turn, depend on the physical situation under consideration. The simplest and best studied case is that of classical lattice systems with periodic boundary conditions. This investigation goes back to the work of Imry,[(1)] Fisher and Berker,[(2)] Blöte and Nightingale,[(3)] Binder and co-workers,[(4, 5)] and others. Rigorous results concerning finite-size effects with periodic boundary conditions[(6–11)] show a universal behaviour of the rounded transition and yield details of the asymptotics of the finite-size shift of the transition. One of the results of these papers is that for cubic volumes of linear size L, the inflection point $h_t(L)$ of the mean value of the order parameter is shifted by a correction which is typically of order L^{-d}, where $d \geqslant 2$ is the dimension of the lattice under consideration. For the special case of two phase coexistence, this shift is much smaller, namely, of order $O(L^{-2d})$. (More precisely, the required property is that both phases have the same finite degeneracy.)

While periodic boundary conditions are studied most often (and are also the easiest to implement in computer simulations), free boundary conditions, constant boundary conditions, and, more generally, boundary conditions with boundary fields are more natural from the point of view of realistic systems. The case of fixed constant boundary conditions, where one has to investigate the balancing effect of boundary conditions and an opposite driving force (say, the external magnetic field) is rather difficult to control rigorously, and only results for two-dimensional Ising model are available.[(12)] On the other hand, when boundary conditions are sufficiently weak ("close" to the free boundary conditions), a rather general class of models was rigorously studied in ref. 13. The asymptotics of the rounding and the shift of the transition point were precisely evaluated. In contrast to periodic boundary conditions, the shift is typically of order L^{-1}, due to the contribution of the surface free energies.

Even though the results of ref. 13 cover a rather general class of systems, the case of the temperature-driven transition for the Potts model is included only in principle. The details of the contour analysis depend on a slightly different type of contours and, in addition, the discussion of the Fortuin–Kasteleyn representation with the corresponding boundary condition has to be included. Given also the fact that the Potts model is often used as a typical case of a weak and asymmetric first-order transition for computer simulations, we find it useful to analyze it separately in the present paper. Finally, it is interesting to discuss the very meaning of "weak" boundary conditions for the Potts model. Fixing the bulk coupling constant J to 1, we consider a variable strength λ with which the spins on the inner boundary of the volume are enforced to align with a fixed spin value, say, 1. The particular value $\lambda = 1$ corresponds to standard fixed boundary conditions yielding, at the phase coexistence temperature, the ordered 1-phase. On the other hand, the value $\lambda = 0$ (i.e., the free boundary conditions) does not correspond to a "uniform mixture" of pure phases—it actually strongly enforces the disordered phase. The role of "weak" boundary conditions, where the contributions of the ordered and disordered phases are of comparable importance, turns out to be played by the values $\lambda \sim \frac{1}{2}$. To see this in the leading approximation, let us take, for the main contributions to the partition function in a hypercube L^d, the terms $e^{-\beta(dL^d - dL^{d-1} + \lambda 2dL^{d-1})}$ corresponding to the ground state for the ordered 1-phase and q^{L^d} corresponding to the disordered state. Their equality at the approximate coexistence inverse temperature $\beta_0 = \frac{\log q}{d}$ yields $\lambda = \frac{1}{2}$. Of course, the important task of the rigorous analysis will be to show that this reasoning remains approximately true even when allowing arbitrary excitations.

In the following section we introduce the model and present our results. In accordance with the discussion of the preceding paragraph, it is useful to consider three separate regions for the strength λ of the boundary condition: the interval $[\frac{1-\mu}{2}, \frac{1+\mu}{2}]$ containing the value $\lambda = \frac{1}{2}$, with an arbitrary fixed parameter $\mu \in (0, 1)$, and the complementary intervals $[0, \frac{1-\mu}{2}]$ and $[\frac{1+\mu}{2}, \infty)$. For λ in the latter two intervals, the Gibbs state is close to the corresponding pure (disordered and ordered, respectively) phase, as described in Theorem 2.1, while the former yields a transition region where the interpolation between the two phases occurs. The corresponding results are presented in Theorem 2.3, including the claim that the maximum of the specific heat occurs at the inverse temperature

$$\beta^{(\lambda)}_{\max}(L) = \beta_t \left[1 + \frac{d}{\Delta e} \left(\frac{1}{2} - \lambda + O\left(\frac{q^{-\nu}}{\log q} \right) \right) \frac{1}{L} + O(L^{-2}) \right]$$

with Δe denoting the latent heat at β_t and ν being of the order $(1-\mu)/4d$. Theorems 2.1 and 2.3 extend the results of the Master thesis of one of the authors,[14] who proved similar statements for $|\lambda - \frac{1}{2}| \leqslant \delta$ and $|\frac{\beta}{\beta_t} - 1| \leqslant \delta$, where $\delta = \delta(d) < 1/52d$.

Note that our results in the window $[0, \frac{1-\mu}{2}]$ imply that the phase transition in the Potts model is not robust. Here robustness is defined in the sense introduced by Pemantle and Steif in ref. 15: A phase transition is said to be robust if the different extremal states are obtained as limits of Gibbs states with arbitrarily weak boundary fields. More precisely, robustness is defined in terms of (limiting) marginal single site measures at the origin instead of Gibbs states. Theorem 2.1 immediately implies that the temperature driven first-order phase transition of the Potts model is not robust, since sufficiently small boundary fields lead to the disordered, and not the ordered Gibbs state.[4] A proof of this statement was already sketched in ref. 16.

After stating our results in Section 2, we use, in Section 3, the Fortuin–Kasteleyn representation to derive a suitable contour representation of the model, paying particular attention to the specific boundary conditions. Section 4 is devoted to the cluster expansion analysis of the finite-volume partition functions. In particular, the needed results from the Pirogov–Sinai theory are discussed with a special view on boundary contours and smoothness of truncated contour weights. The proofs of Theorems 2.1 and 2.3 are then presented in Sections 5 and 6, respectively. Proofs of several technical lemmas are deferred to the appendix.

2. RESULTS

In this paper, we consider the q-state Potts model in the d-dimensional cube

$$\Lambda=\Lambda(L)=\left\{x\in\mathbb{Z}^d \,\middle|\, -\frac{L}{2}<x_i\leqslant\frac{L}{2} \text{ for all } i=1,\dots,d\right\},\qquad L=1,2,\dots, \tag{2.1}$$

with boundary conditions interpolating between free and constant 1-boundary conditions.[5] As usual, the spin configurations of this model are maps σ_Λ from Λ into $Q=\{1,\dots,q\}$. We use $\mathbb{B}=\mathbb{B}(\Lambda)$ to denote the set of all bonds $\langle x,y\rangle$ of nearest-neighbour sites $x, y\in\mathbb{Z}^d$ with both end-points in Λ and $\partial\mathbb{B}=\partial\mathbb{B}(\Lambda)$ to denote the set $\{\langle x,y\rangle \mid x\in\Lambda,\, y\in\mathbb{Z}^d\setminus\Lambda\}$. We consider the Hamiltonian

$$H^{(\lambda)}(\sigma_\Lambda)=-\sum_{\langle x,y\rangle\in\mathbb{B}}\delta_{\sigma_x,\sigma_y}-\lambda\sum_{\substack{\langle x,y\rangle\in\partial\mathbb{B}:\\ x\in\Lambda}}\delta_{\sigma_x,1}, \tag{2.2}$$

[4] This statement already follows from the results of ref. 14, which imply that for $\beta=\beta_t$ and $\lambda=\frac{1}{2}(1-\delta)$ the limiting Gibbs state is the disordered state. Using FKG-monotonicity, we conclude that any $\lambda\in(0,\frac{1}{2}(1-\delta))$ leads to a limiting Gibbs state that is identical to the one obtained from free boundary conditions.

[5] Without loss of generality, we use 1-boundary conditions, $\sigma_x=1$ for all $x\in\mathbb{Z}^d\setminus\Lambda$, instead of general fixed boundary conditions.

where $\lambda \geqslant 0$ is the surface coupling. The value $\lambda = 0$ represents *free boundary conditions*, while $\lambda = 1$ represents *standard* 1-*boundary conditions*. The Gibbs state corresponding to the Hamiltonian (2.2) is given by

$$\langle \cdot \rangle_L^{(\beta, \lambda)} = \frac{1}{Z_L(\beta, \lambda)} \sum_{\sigma_\Lambda \in Q^\Lambda} \cdot e^{-\beta H^{(\lambda)}(\sigma_\Lambda)}, \tag{2.3}$$

where $Z_L(\beta, \lambda)$ is the partition function,

$$Z_L(\beta, \lambda) = \sum_{\sigma_\Lambda \in Q^\Lambda} e^{-\beta H^{(\lambda)}(\sigma_\Lambda)}. \tag{2.4}$$

It is well known by now that for all $d \geqslant 2$ and all $q \geqslant 2$ the infinite-volume system exhibits a phase transition at some value β_t characterized by the appearance of a spontaneous magnetization for $\beta > \beta_t$. For q sufficiently large, this transition is known to be first-order[17] with a discontinuity in both the magnetization[6]

$$m(\beta) = \lim_{L \to \infty} \frac{1}{L^d} \frac{1}{q-1} \left\langle \sum_{x \in \Lambda(L)} (q\, \delta_{\sigma_x, 1} - 1) \right\rangle_L^{(\beta, \lambda = 1)} \tag{2.5}$$

and the mean energy

$$e(\beta) = \lim_{L \to \infty} \frac{1}{L^d} \langle H^{(\lambda = 1)}(\sigma_{\Lambda(L)}) \rangle_L^{(\beta, \lambda = 1)}. \tag{2.6}$$

The magnetization $m(\beta)$ is zero for $\beta < \beta_t$, it jumps from

$$m_{\text{dis}}(\beta_t) = 0$$

to

$$m_{\text{ord}}(\beta_t) = \lim_{\beta \downarrow \beta_t} m(\beta) = m(\beta_t) > 0$$

at β_t, and it is strictly increasing for $\beta > \beta_t$, while the mean energy $e(\beta)$ is strictly decreasing for all β, with a jump from

$$e_{\text{dis}}(\beta_t) = \lim_{\beta \uparrow \beta_t} e(\beta)$$

[6] The existence of the limits (2.5) and (2.6) with the constant 1-boundary conditions follows from either GKS-inequalities[18] or FK-monotonicity, see, e.g., ref. 19. By the same methods, one can also show that the functions m and e are right continuous, $m(\beta) = m(\beta + 0)$, $e(\beta) = e(\beta + 0)$.

to

$$e_{\rm ord}(\beta_t) = \lim_{\beta \downarrow \beta_t} e(\beta) = e(\beta_t)$$

at β_t.

Here we study the finite-volume magnetization and the mean energy defined by

$$M_L(\beta, \lambda) = \frac{1}{q-1} \left\langle \sum_{x \in \Lambda(L)} (q\delta_{\sigma_x, 1} - 1) \right\rangle_L^{(\beta, \lambda)} \tag{2.7}$$

and

$$E_L(\beta, \lambda) = \langle H^{(\lambda)}(\sigma_\Lambda) \rangle_L^{(\beta, \lambda)} = -\frac{\partial}{\partial \beta} \log Z_L(\beta, \lambda), \tag{2.8}$$

respectively. The case of the free boundary conditions ($\lambda = 0$) can, for q sufficiently large, be analyzed by the standard Pirogov–Sinai theory as long as $\beta \leqslant \beta_t$, while the case of the standard 1-boundary conditions ($\lambda = 1$) can be analyzed as long as $\beta \geqslant \beta_t$. This, in particular, gives

$$\lim_{L \to \infty} \frac{1}{L^d} M_L(\beta_t, 0) = 0, \qquad \lim_{L \to \infty} \frac{1}{L^d} E_L(\beta_t, 0) = e_{\rm dis}(\beta_t) \tag{2.9}$$

and

$$\lim_{L \to \infty} \frac{1}{L^d} M_L(\beta_t, 1) = m_{\rm ord}(\beta_t), \qquad \lim_{L \to \infty} \frac{1}{L^d} E_L(\beta_t, 1) = e_{\rm ord}(\beta_t). \tag{2.10}$$

The main contribution of this paper is the analysis of the asymptotic behaviour (as $L \to \infty$) of $M_L(\beta, \lambda)$ and $E_L(\beta, \lambda)$ for any $\lambda \geqslant 0$ and q large. It turns out that the behaviour for $\lambda \in (0, \frac{1}{2})$ and $\beta \leqslant \beta_t$ is qualitatively the same as that for the free boundary conditions: the specific magnetization $\frac{1}{|\Lambda(L)|} M_L(\beta, \lambda)$ and the specific mean energy $\frac{1}{|\Lambda(L)|} E_L(\beta, \lambda)$ still converge to the bulk quantities in the disordered phase with corrections of the order L^{-1}. Similarly, for $\lambda \in (\frac{1}{2}, \infty)$ and $\beta \geqslant \beta_t$, we are still in the ordered phase. These two cases are jointly referred to as the *strong boundary conditions*. Finite-size behaviour for intermediate values of λ—"around" $\lambda = \frac{1}{2}$, the *weak boundary conditions*—and any $\beta > 0$ is governed by the competition between contributions coming from the configurations which are either in the ordered or in the disordered phase for the whole of Λ. Surface effects, in dependence on the particular value of λ, then determine the resulting finite-size rounding of the phase transition.

Our results are summarized in the following theorems. In order to state them, we first introduce the specific heat

$$C_L(\beta, \lambda) = \beta^2 \left(\langle (H^{(\lambda)}(\sigma_\Lambda))^2\rangle_L^{(\beta,\lambda)} - (\langle H^{(\lambda)}(\sigma_\Lambda)\rangle_L^{(\beta,\lambda)})^2\right) = -\beta^2 \frac{\partial E_L(\beta, \lambda)}{\partial \beta} \tag{2.11}$$

and the shorthands $m^* = m(\beta_t)$, the derivative $c(\beta) = -\beta^2 \frac{de(\beta)}{d\beta}$ (known to exist as a smooth function as long as $\beta \neq \beta_t$),

$$e_0 = \frac{e_{\mathrm{dis}}(\beta_t) + e_{\mathrm{ord}}(\beta_t)}{2}, \qquad \text{and} \qquad \Delta e = \frac{e_{\mathrm{dis}}(\beta_t) - e_{\mathrm{ord}}(\beta_t)}{2}. \tag{2.12}$$

Theorem 2.1. Let $d \geqslant 2$ and $\mu \in (0, 1]$. For q and L sufficiently large, we have:

(a) If $0 \leqslant \lambda \leqslant \frac{1}{2}(1-\mu)$ and $\beta \leqslant \beta_t$, then

$$M_L(\beta, \lambda) = O(L^{d-1}) \tag{2.13}$$

and

$$E_L(\beta, \lambda) = e(\beta - 0)\, L^d + O(L^{d-1}). \tag{2.14}$$

(b) If $\lambda \geqslant \frac{1}{2}(1+\mu)$ and $\beta \geqslant \beta_t$, then

$$M_L(\beta, \lambda) = m(\beta)\, L^d + O(L^{d-1}) \tag{2.15}$$

and

$$E_L(\beta, \lambda) = e(\beta + 0)\, L^d + (1+\lambda)\, O(L^{d-1}). \tag{2.16}$$

Remark 2.2. In the above theorem, as well as in the rest of this paper, all constants implicit in the O-symbols depend only on d and μ. In particular, the corresponding bounds are uniform in β, L, and q.

Our second theorem concerns weak boundary conditions, i.e., values of λ in the interval $[\frac{1-\mu}{2}, \frac{1+\mu}{2}]$, where μ is an arbitrary fixed parameter $\mu \in (0, 1)$. For these boundary conditions we control the finite-size behaviour of $M_L(\beta, \lambda)$, $E_L(\beta, \lambda)$, and $C_L(\beta, \lambda)$ for all $\beta \in (0, \infty)$.

Theorem 2.3. Let $d \geqslant 2$ and $0 < \mu < 1$ and let $\nu = \min\{1/12d, (1-\mu)/4d\}$. Then, for q and L sufficiently large, and $|\lambda - \frac{1}{2}| \leqslant \frac{\mu}{2}$, we have:

(a) There exists a unique point $\beta_{\max}^{(\lambda)}(L)$ at which the specific heat $C_L(\beta, \lambda)$ attains its maximum. Furthermore, there exists a function $b(\lambda, q)$ such that

$$\beta_{\max}^{(\lambda)}(L) = \beta_t \left[1 + \frac{b(\lambda, q)}{L} + O(L^{-2}) \right] \tag{2.17}$$

and

$$b(\lambda, q) = \frac{d}{\Delta e} \left(\frac{1}{2} - \lambda + O\left(\frac{q^{-\nu}}{\log q} \right) \right). \tag{2.18}$$

(b) For all $\beta \geqslant 1$, we have

$$\begin{aligned} M_L(\beta, \lambda) &= \frac{m^*}{2} L^d + \frac{m^*}{2} L^d \tanh(\Delta e(\beta - \beta_{\max}^{(\lambda)}(L))\, L^d) \\ &\quad + O\left(\frac{\beta - \beta_t}{\beta_t} L^d \right) + O(L^{d-1}), \end{aligned} \tag{2.19}$$

$$\begin{aligned} E_L(\beta, \lambda) &= e_0 L^d - \Delta e\, L^d \tanh(\Delta e(\beta - \beta_{\max}^{(\lambda)}(L))\, L^d) \\ &\quad + O\left(\frac{\beta - \beta_t}{\beta_t} L^d \right) + O(L^{d-1}), \end{aligned} \tag{2.20}$$

and

$$\begin{aligned} C_L(\beta, \lambda) &= \beta^2 (\Delta e)^2 L^{2d} \cosh^{-2}(\Delta e(\beta - \beta_{\max}^{(\lambda)}(L))\, L^d) \\ &\quad + \beta_t^2 O\left(\frac{\beta - \beta_t}{\beta_t} L^{2d} \right) + \beta_t^2\, O(L^{2d-1}). \end{aligned} \tag{2.21}$$

(c) Let

$$\frac{|\beta - \beta_t|}{\beta_t} \geqslant \frac{\mu d}{\Delta e} \frac{1}{L}. \tag{2.22}$$

Then

$$M_L(\beta, \lambda) = m(\beta)\, L^d + O(L^{d-1}), \tag{2.23}$$

$$E_L(\beta, \lambda) = e(\beta)\, L^d + O(L^{d-1}), \qquad \text{and} \tag{2.24}$$

$$C_L(\beta, \lambda) = c(\beta)\, L^d + \beta_t^2 O(L^{d-1}). \tag{2.25}$$

Remark 2.4. (i) As can be seen from the proof of the theorem, the function $b(\lambda, q)$ can actually be written as

$$\beta_t b(\lambda, q) = 2d\,\frac{s_{\mathrm{dis}}(\beta_t) - s_{\mathrm{ord}}(\beta_t)}{e_{\mathrm{dis}}(\beta_t) - e_{\mathrm{ord}}(\beta_t)}, \tag{2.26}$$

where s_{dis} and s_{ord} are the surface free energies of the disordered and ordered phase, respectively. See Section 4 for the definition of the surface free energies. The explicit terms in (2.18) come from the ground state energy contributions to the surface free energies. Notice that the shift can actually be made to be of order L^{-2} by tuning λ in such a way that $s_{\mathrm{dis}}(\beta_t) = s_{\mathrm{ord}}(\beta_t)$, and thus $b(\lambda, q) = 0$. As can be seen from (2.18), this happens for $\lambda = \frac{1}{2} + O(\frac{q^{-\nu}}{\log q})$.

(ii) Notice that the results of Theorem 2.1 and Theorem 2.3 are, in the regions of overlapping parameters, in agreement. Indeed, let $\lambda \in (0, \frac{1}{2})$ and $\beta \leqslant \beta_t$ first. If $\beta < \beta_t$, then Theorem 2.3(c) yields (2.13) and (2.14), respectively, whenever one takes L such that $\frac{|\beta - \beta_t|}{\beta_t} \gg \frac{\mu d}{\Delta e} \frac{1}{L}$. If $\beta = \beta_t$, the Eqs. (2.13) and (2.14) follow from Theorem 2.3(a) and (b): one just uses that $\tanh x = 1 + O(e^{-2x})$ for $x \gg 1$ and observes that $\beta_t - \beta_{\max}^{(\lambda)}(L)$ is negative and of the order L^{-1} by virtue of (2.17). The case $\lambda \in (\frac{1}{2}, 1)$ and $\beta \geqslant \beta_t$ is similar.

(iii) In order to prove the above theorems, one in fact needs to exclude the values of β close to 0 (cf. Lemma A.1), and we take $\beta \geqslant 1$ where necessary. Nevertheless, the restriction of β to the interval $[1, \infty)$ is not serious: if $\beta \leqslant 1$, we may use, for q large, a standard high-temperature expansion to obtain the results of Theorem 2.1(a) and Theorem 2.3(a) and (c).

(iv) The techniques used in this paper do not allow to study the finite-size scaling of $M_L(\beta, \lambda)$ and $E_L(\beta, \lambda)$ for boundary conditions which *strongly* favour the ordered or the disordered phase near the boundary of Λ. In this case, the leading contributions to $Z_L(\beta, \lambda)$ feature a flip along a large contour from one of the two phases near the boundary to the other phase within the bulk. To analyze the finite-size scaling, a control over the behaviour of this large contour would be necessary, involving, in particular, the analysis of the so-called Wulff shape of a contour filling essentially the whole volume. This is out of the scope of this paper. As will be shown in Section 4, such a detailed analysis of large contours is not necessary in the case of the weak boundary conditions.

(v) In the general setting of the Pirogov–Sinai theory, surface-induced finite-size effects for first-order phase transitions were studied in ref. 13, and one could try to apply this approach to our model. To this end, the model must be first rewritten in terms of contours and then the assumptions under which ref. 13 can be used have to be checked; this was done in ref. 14. Whereas the assumptions (3.7) to (3.9) of ref. 13 are fulfilled in our situation (if we suppose that, say, $\beta \geqslant 1$), the assumption (3.11) of ref. 13 imposes drastic constrains on the values of λ and β. Namely, one must assume that $|\lambda - \frac{1}{2}| \leqslant \delta$ and $|\frac{\beta}{\beta_t} - 1| \leqslant \delta$, where $\delta = \delta(d) < \frac{1}{52d}$, see (4.47b) in ref. 13. With such restrictions, the general setting of ref. 13 enables us to establish the results of Theorem 2.3. Here we weakened these constrains (both for λ and β), using the methods of ref. 13 with a more careful evaluation of boundary terms.

3. CONTOUR REPRESENTATIONS

In order to analyze the finite-volume quantities $M_L(\beta, \lambda)$ and $E_L(\beta, \lambda)$, we use the machinery of the Pirogov–Sinai theory in the form developed in ref. 13. To this end, we first rewrite the partition function (2.4) in terms of contours.

Throughout this section, we assume that $d \geqslant 2$, $\lambda \geqslant 0$ and $\beta > 0$. Moreover, the cube Λ (and, thus, the sets $\mathbb{B} = \mathbb{B}(\Lambda)$ and $\partial\mathbb{B}$) is fixed, and we write $\overline{\mathbb{B}}$ for $\mathbb{B} \cup \partial\mathbb{B}$.

First, we express $Z_L(\beta, \lambda)$ with the help of the Fortuin–Kasteleyn random-cluster representation.[20] Modifying the approach of ref. 8 to take into account the effect of the boundary, one obtains

$$Z_L(\beta, \lambda) = \sum_{X \subset \overline{\mathbb{B}}} e^{-G(X)} q^{-\frac{1}{2d}\|\delta X\| + C_{\text{in}}(X)}, \tag{3.1}$$

see ref. 14 for details. Here $C_{\text{in}}(X)$ is the number of the connected components of X which do not include any bond of $\partial\mathbb{B}$, $\|\delta X\| = |\delta_1 X| + 2\,|\delta_2 X|$, where

$$\delta_i X = \{\langle x, y\rangle \in \overline{\mathbb{B}} \setminus X : |\{x, y\} \cap S(X)| = i\}, \qquad i = 1, 2,$$

with

$$S(X) = \{x \in \Lambda : \langle x, y\rangle \in X \text{ for some } y \in \mathbb{Z}^d\},$$

and $G(X) = \sum_{b \in \overline{\mathbb{B}}} g_X(b)$, with

$$g_X(b) = \begin{cases} -\log(e^{\beta} - 1) & \text{if} \quad b \in \mathbb{B} \cap X, \\ -\log(e^{\lambda\beta} - 1) & \text{if} \quad b \in \partial\mathbb{B} \cap X, \end{cases}$$
$$g_X(b) = \begin{cases} -\frac{1}{d}\log q & \text{if} \quad b \in \mathbb{B} \setminus X, \\ -\frac{1}{2d}\log q & \text{if} \quad b \in \partial\mathbb{B} \setminus X. \end{cases} \tag{3.2}$$

Remark 3.1. Note that for the free boundary conditions, $\lambda = 0$, the contribution of any random-cluster configuration $X \subset \overline{\mathbb{B}}$ to $Z_L(\beta, \lambda)$ vanishes unless $X \cap \partial\mathbb{B} = \varnothing$.

Next, let us introduce $V = V(L)$ as the closed d-dimensional cube in $\mathbb{R}^d$, of side length[7] $L+1$, centred at the same point as Λ. As usual, the boundary ∂W of any set $W \subset \mathbb{R}^d$ is the set of points x with $\operatorname{dist}(x, W) = \operatorname{dist}(x, \mathbb{R}^d \setminus W) = 0$, where $\operatorname{dist}(x, W) = \inf_{y \in W} \operatorname{dist}(x, y)$, with $\operatorname{dist}(x, y)$ standing for the ℓ_∞-distance $\operatorname{dist}(x, y) = \max_{i=1,\dots,d} |x_i - y_i|$. If $W \subset V$, we will also consider the *inner* boundary of W, defined as $\partial_V W = \{x \in V : \operatorname{dist}(x, W) = \operatorname{dist}(x, V \setminus W) = 0\}$.

Our aim is to rewrite every random-cluster configuration $X \subset \overline{\mathbb{B}}$ in terms of collections of contours. It turns out that it is convenient to introduce two different types of contours, depending on the boundary conditions: for weak boundary conditions it is natural to consider open contours "ending on the boundary ∂V," while for strong boundary conditions the natural setting is to consider closed contours only. Accordingly, the following definition distinguishes these cases. Nevertheless, the differences concern only contours "touching" the boundary ∂V—for those in the interior, all the definitions are independent of the boundary conditions.

Let $X \subset \overline{\mathbb{B}}$ be a random-cluster configuration. In order to define contours, we first identify the bonds $\langle x, y \rangle \in X$ with the corresponding line segments in $\mathbb{R}^d$, and then define a closed k-dimensional unit hypercube $c \subset \mathbb{R}^d$ with vertices in $\mathbb{Z}^d$ to be occupied if all bonds $b \subset c$ are bonds in X. We use $\mathscr{P}(X)$ to denote the union of all occupied hypercubes. In a similar way, we define $\overline{\mathscr{P}}(X) \supset \mathscr{P}(X)$ as the union of all closed unit hypercubes c with vertices in $\mathbb{Z}^d$ for which all bonds $b \subset c$ lie in $X \cup \partial V$. Next, we introduce the sets $\mathscr{P}_w$, $\mathscr{P}_\mathrm{o}$, and $\mathscr{P}_\mathrm{d}$ as

(a) the intersection of the $\frac{1}{4}$-neighbourhood of $\overline{\mathscr{P}}(X) \setminus \partial V$ with V,

(b) the intersection of the $\frac{1}{4}$-neighbourhood of $\overline{\mathscr{P}}(X)$ with V,

(c) the $\frac{1}{4}$-neighbourhood of $\mathscr{P}(X) \cap \{x \in V : \operatorname{dist}(x, \partial V) \geqslant \frac{1}{2}\}$.

Here the neighbourhood is defined with respect to the ℓ_∞ distance.

Given these sets, we define the set of contours $Y_\mathrm{o}(X)$ and $Y_\mathrm{d}(X)$ as the sets of connected components of the boundaries of $\mathscr{P}_\mathrm{o}$ and $\mathscr{P}_\mathrm{d}$, respectively, and the set of contours $Y(X)$ as the set of connected components of the inner boundary $\partial_V \mathscr{P}_w$ of $\mathscr{P}_w$, see Fig. 1. Elements of $Y(X)$ are called *w-contours*, while elements of $Y_\mathrm{o}(X)$ or $Y_\mathrm{d}(X)$ are called *s-contours*, and we

[7] Note that $V(L)$ is thus defined to be the smallest closed cube containing all bonds from $\overline{\mathbb{B}}$.

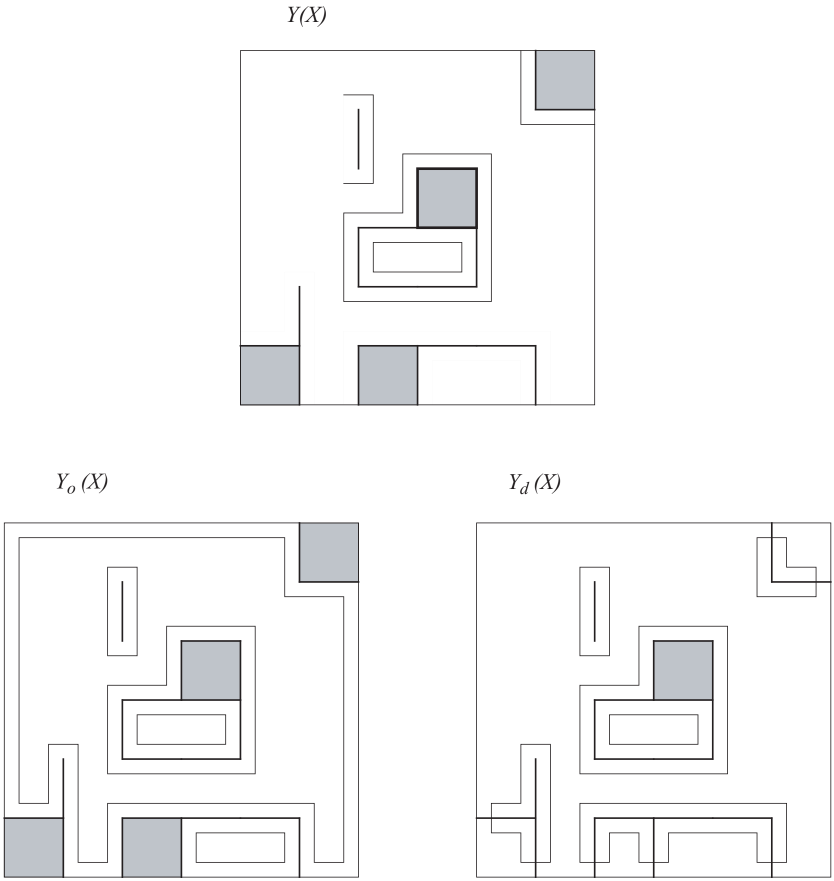

Fig. 1. Contours under different boundary conditions.

shall use γ to denote any of them. Furthermore, we say that a set ∂ of w-contours (s-contours) is *admissible* if there exists a configuration $X \subset \overline{\mathbb{B}}$ such that $\partial = Y(X)$ ($\partial = Y_{\mathrm{o}}(X)$ or $\partial = Y_{\mathrm{d}}(X)$). This configuration is necessarily unique whenever ∂ is not empty, while

$$Y(\overline{\mathbb{B}}) = Y(\varnothing) = Y_{\mathrm{o}}(\overline{\mathbb{B}}) = Y_{\mathrm{d}}(\varnothing) = \varnothing.$$

If $\partial \neq \varnothing$, we use $X(\partial)$ to denote the unique configuration corresponding to ∂.

Define the "octant" $\mathcal{O}(k)$ of each corner $k = [k_1,..., k_d]$ of the box V by

$$\mathcal{O}(k) = \{x \in \mathbb{R}^d : x_i \geqslant k_i \text{ if } i \in I_-, x_i \leqslant k_i \text{ if } i \in I_+\}, \tag{3.3}$$

where $i \in I_-$ as long as $y_i \geqslant k_i$ for all $y \in V$, while $i \in I_+$ as long as $y_i \leqslant k_i$ for all $y \in V$. If, for a given γ, there is a corner k of V such that $\gamma \cap \partial V \subset \partial \mathcal{O}(k)$, then $\operatorname{Int} \gamma$, the *interior* of γ, is defined as the finite component of $\mathcal{O}(k) \setminus \gamma$.[8] However, if there is no such a corner, then $\operatorname{Int} \gamma$ is defined as the smaller of the two components of $V \setminus \gamma$.[9] In addition, we set $V(\gamma) = \gamma \cup \operatorname{Int} \gamma$ and $\operatorname{Ext} \gamma = V \setminus V(\gamma)$. Any γ from an admissible set of w- or s-contours ∂ is *external* if there is no $\tilde{\gamma} \in \partial$ such that $\gamma \subset \operatorname{Int} \tilde{\gamma}$.

The set $\{\gamma\}$ with γ arbitrary is admissible and non-empty, and thus there exists a unique configuration $X_\gamma \subset \overline{\mathbb{B}}$ for which $Y(X_\gamma) = \{\gamma\}$ if γ is a w-contour, while $Y_{\mathrm{o}}(X_\gamma) = \{\gamma\}$ or $Y_{\mathrm{d}}(X_\gamma) = \{\gamma\}$ if γ is an s-contour. We call γ *ordered* (or *o-labeled*) if $X_\gamma \subset \operatorname{Ext} \gamma$ and *disordered* (or *d-labeled*) if $X_\gamma \subset \operatorname{Int} \gamma$. If $X_\gamma = \varnothing$, one necessarily has $\{\gamma\} = Y_{\mathrm{o}}(X_\gamma)$, and we say that γ is o-labeled. Note that all the external contours of an admissible set of w- or s-contours are either ordered or disordered; for instance, the external contours of $Y_{\mathrm{m}}(X)$ with $\mathrm{m} = \mathrm{o}, \mathrm{d}$ and any $X \subset \overline{\mathbb{B}}$ are m-labeled.

Let the *length* $\|\gamma\|$ of a contour γ be the number of its intersections with the bonds of $\overline{\mathbb{B}}$. Observing that, for any set of admissible contours ∂, the number of disordered contours in ∂ with $\operatorname{dist}(\gamma, \partial V) \geqslant \frac{3}{4}$ is $C_{\mathrm{in}}(X(\partial))$, we introduce the *weight* of γ by

$$\varrho(\gamma) = \begin{cases} q^{-\frac{1}{2d}\|\gamma\|} & \text{if } \gamma \text{ is ordered or if } \gamma \text{ is disordered with } \operatorname{dist}(\gamma, \partial V) \leqslant \frac{1}{4}, \\ q^{-\frac{1}{2d}\|\gamma\| + 1} & \text{if } \gamma \text{ is disordered with } \operatorname{dist}(\gamma, \partial V) \geqslant \frac{3}{4}. \end{cases} \tag{3.4}$$

If ∂ is a non-empty admissible set of w-contours, then one easily sees that

$$\sum_{\gamma \in \partial} \|\gamma\| = \|\delta X(\partial)\|, \tag{3.5}$$

whereas if ∂ is a non-empty admissible set of s-contours, then

$$\sum_{\gamma \in \partial} \|\gamma\| = \begin{cases} \|\delta X(\partial)\| + |\partial \mathbb{B} \setminus X(\partial)| & \text{if external } s\text{-contours in } \partial \text{ are ordered,} \\ \|\delta X(\partial)\| + |\partial \mathbb{B} \cap X(\partial)| & \text{if external } s\text{-contours in } \partial \text{ are disordered.} \end{cases} \tag{3.6}$$

Here $X(\partial)$ is the unique configuration corresponding to ∂.

A set $\{\gamma_1, \ldots, \gamma_n\}$ of w-contours (s-contours) is called a *set of non-overlapping w-contours (s-contours)* if $\operatorname{dist}(\gamma_i, \gamma_j) \geqslant \frac{1}{2}$ for all $1 \leqslant i < j \leqslant n$. Any admissible set of w-contours (s-contours) may serve as an example.

[8] This definition clearly does not depend on the choice of k if more corners are possible.

[9] If both the components of $V \setminus \gamma$ are of the same size, take the one which contains the corner k of V for which $k_i \leqslant x_i$, $i = 1, \ldots, d$, for all $x \in V$.

Let $W \subset V$ be of the form

$$V \setminus \bigcup_{\gamma \in \partial^*} V(\gamma) \qquad \text{or} \qquad \operatorname{Int} \gamma_0 \setminus \bigcup_{\gamma \in \tilde{\partial}^*} V(\gamma), \tag{3.7}$$

where γ_0 is a w-contour (s-contour) and ∂^* and $\tilde{\partial}^*$ are, possibly empty, sets of non-overlapping w-contours (s-contours) with $V(\gamma) \subset \operatorname{Int} \gamma_0$ for all $\gamma \in \tilde{\partial}^*$. Then $\mathbb{B}(W)$ and $\partial\mathbb{B}(W)$ stand for the sets of all bonds of $\mathbb{B}$ and $\partial\mathbb{B}$, respectively, whose centres lie in W and $\overline{\mathbb{B}}(W) = \mathbb{B}(W) \cup \partial\mathbb{B}(W)$. Further, let $\|\partial_i W\|$, $\|\partial_e W\|$, and $\|\partial W\| = \|\partial_i W\| + \|\partial_e W\|$ be the number of intersections of bonds from $\overline{\mathbb{B}}$ with $\partial W \setminus \partial V$, $\partial W \cap \partial V$, and ∂W, respectively. Notice that for any contour γ, the closure of $\partial \operatorname{Int} \gamma \setminus \partial V$ actually equals γ, implying that $\|\gamma\| = \|\partial_i \operatorname{Int} \gamma\|$. Note further that $|\partial\mathbb{B}(W)| = \|\partial_e W\|$ if γ_0 and all contours from ∂^* and $\tilde{\partial}^*$ in (3.7) are w-contours.

In order to express the weight of a configuration X in terms of its contours, we also introduce the ordered and disordered "regions,"

$$\Omega_{\mathrm{m}}(W, \partial) = \begin{cases} \overline{\mathbb{B}}(W) \cap X(\partial) & \text{if} \quad \mathrm{m} = \mathrm{o}, \\ \overline{\mathbb{B}}(W) \setminus X(\partial) & \text{if} \quad \mathrm{m} = \mathrm{d}, \end{cases} \tag{3.8}$$

for any admissible set of w- or s-contours ∂, where we set $X(\emptyset)$ to be equal to $\overline{\mathbb{B}}$ if $\mathrm{m} = \mathrm{o}$ and to $\emptyset$ if $\mathrm{m} = \mathrm{d}$.

When expressing the partition function in terms of contour weights, we distinguish the case of weak and strong boundary conditions.

Weak b.c. For every $B \subset \overline{\mathbb{B}}$ and $\mathrm{m} = \mathrm{o}, \mathrm{d}$, we set

$$G_{\mathrm{m}}(B) = \frac{g_{\mathrm{m}}}{d} |\mathbb{B} \cap B| + h_{\mathrm{m}} |\partial\mathbb{B} \cap B| \tag{3.9}$$

with

$$g_{\mathrm{o}} = -d \log(e^{\beta} - 1), \quad g_{\mathrm{d}} = -\log q, \quad h_{\mathrm{o}} = -\log(e^{\lambda\beta} - 1), \quad h_{\mathrm{d}} = -\frac{1}{2d} \log q. \tag{3.10}$$

Let us call γ *short* if[10] $\operatorname{diam} \gamma < \omega(L)$ and *long* otherwise; the parameter $\omega(L)$, to be specified later, is supposed to be fixed so that $1 < \omega(L) \leqslant L + 1$. For W of the form (3.7), we define

$$Z_{\mathrm{m}, W}(\beta, \lambda) = \sum_{\partial \sqsubset W}^{(\mathrm{m})} e^{-G_{\mathrm{o}}(\Omega_{\mathrm{o}}(W, \partial)) - G_{\mathrm{d}}(\Omega_{\mathrm{d}}(W, \partial))} \prod_{\gamma \in \partial} \varrho(\gamma), \qquad \mathrm{m} = \mathrm{o}, \mathrm{d}, \tag{3.11}$$

[10] The *diameter* of any subset $\mathscr{W}$ of $\mathbb{R}^d$, $\operatorname{diam} \mathscr{W}$, is defined here as the length of the side of the smallest square box in $\mathbb{R}^d$ into which $\mathscr{W}$ can fit.

where the sum is taken over all admissible sets ∂ of short w-contours such that the external contours in ∂ are m-labeled and $V(\gamma) \subset W$ for all $\gamma \in \partial$.

As it is standard in the Pirogov–Sinai theory, one may derive another, more suitable expression for the partition function (3.11) (in a context similar to the present one, see, e.g., Section 4.2 of ref. 13), namely,

$$Z_{\mathrm{m}, W}(\beta, \lambda) = e^{-G_{\mathrm{m}}(\overline{\mathbb{B}}(W))} \sum_{\partial^* \sqsubset W}^{(\mathrm{m})} \prod_{\gamma \in \partial^*} K_{\mathrm{m}}(\gamma), \qquad \mathrm{m} = \mathrm{o}, \mathrm{d}. \tag{3.12}$$

Here the summation is over all sets ∂^* of non-overlapping short m-labeled w-contours with $V(\gamma) \subset W$ for every $\gamma \in \partial^*$ and

$$K_{\mathrm{o}}(\gamma) = \varrho(\gamma) \frac{Z_{\mathrm{d}, \mathrm{Int}\, \gamma}(\beta, \lambda)}{Z_{\mathrm{o}, \mathrm{Int}\, \gamma}(\beta, \lambda)}, \qquad K_{\mathrm{d}}(\gamma) = \varrho(\gamma) \frac{Z_{\mathrm{o}, \mathrm{Int}\, \gamma}(\beta, \lambda)}{Z_{\mathrm{d}, \mathrm{Int}\, \gamma}(\beta, \lambda)}, \tag{3.13}$$

where we skipped the dependence of $K_{\mathrm{m}}(\gamma)$ on β and λ.

In addition, we introduce

$$Z_{\mathrm{big}, V}(\beta, \lambda) = \sum_{\partial}^{(\mathrm{long})} e^{-G_{\mathrm{o}}(\Omega_{\mathrm{o}}(V, \partial)) - G_{\mathrm{d}}(\Omega_{\mathrm{d}}(V, \partial))} \prod_{\gamma \in \partial} \varrho(\gamma) \tag{3.14}$$

with the sum going over all the admissible sets ∂ of w-contours which contain at least one long $\gamma \in \partial$. Given such a set ∂, let ∂_l be the set of its long w-contours; it is obviously admissible. Then $V \setminus \partial_l$ splits into connected components $\mathscr{C}_1, \ldots, \mathscr{C}_N$ and, for each $i = 1, \ldots, N$, either $\overline{\mathbb{B}}(\mathscr{C}_i) \subset \Omega_{\mathrm{o}}(V, \partial_l)$ or $\overline{\mathbb{B}}(\mathscr{C}_i) \subset \Omega_{\mathrm{d}}(V, \partial_l)$. We use $W_{\mathrm{o}}(\partial_l)$ to denote the union of the former components and $W_{\mathrm{d}}(\partial_l)$ to denote the union of the latter ones. Now, let us decompose ∂ into the disjoint union $\partial_l \cup \partial^{\mathrm{o}} \cup \partial^{\mathrm{d}}$, where ∂^{m}, $\mathrm{m} = \mathrm{o}, \mathrm{d}$, is the set of all the short w-contours of ∂ with $V(\gamma) \subset W_{\mathrm{m}}(\partial_l)$ for every $\gamma \in \partial^{\mathrm{m}}$. Clearly, the external w-contours of ∂^{m} are m-labeled and

$$\Omega_{\mathrm{m}}(V, \partial) = \Omega_{\mathrm{m}}(W_{\mathrm{m}}(\partial_l), \partial^{\mathrm{m}}) \cup \Omega_{\mathrm{m}}(W_{\mathrm{m}^c}(\partial_l), \partial^{\mathrm{m}^c}) \tag{3.15}$$

is also a disjoint union (here $\mathrm{m}^c = \mathrm{o}$ if $\mathrm{m} = \mathrm{d}$ and vice versa). Re-summing all the short w-contours contributing to $Z_{\mathrm{big}, V}(\beta, \lambda)$, we therefore obtain

$$Z_{\mathrm{big}, V}(\beta, \lambda) = \sum_{\partial_l} Z_{\mathrm{o}, W_{\mathrm{o}}(\partial_l)}(\beta, \lambda)\, Z_{\mathrm{d}, W_{\mathrm{d}}(\partial_l)}(\beta, \lambda) \prod_{\gamma \in \partial_l} \varrho(\gamma). \tag{3.16}$$

Let ∂ be an admissible set of w-contours. Then the number of disordered w-contours in ∂ with $\mathrm{dist}(\gamma, \partial V) \geqslant \frac{3}{4}$ is $C_{\mathrm{in}}(X(\partial))$. Hence,

$$\prod_{\gamma \in \partial} \varrho(\gamma) = q^{-\frac{1}{2d} \|\delta X(\partial)\| + C_{\mathrm{in}}(X(\partial))} \tag{3.17}$$

by (3.5) and the definition (3.4) of $\varrho(\gamma)$. Combining this with (3.1), we get the contour representation

$$Z_L(\beta, \lambda) = \sum_{\partial} e^{-G_{\mathrm{o}}(\Omega_{\mathrm{o}}(V,\partial)) - G_{\mathrm{d}}(\Omega_{\mathrm{d}}(V,\partial))} \prod_{\gamma \in \partial} \varrho(\gamma) \tag{3.18}$$

with the sum going over all the admissible sets ∂ of w-contours. Here we use the convention that the empty set of contours counts twice: once with $X(\partial) = \emptyset$, and once with $X(\partial) = \overline{\mathbb{B}}$, corresponding to the weights $e^{-G_{\mathrm{d}}(\overline{\mathbb{B}})}$ and $e^{-G_{\mathrm{o}}(\overline{\mathbb{B}})}$, respectively. This is made more explicit in the following representation, which follows immediately from (3.11) and (3.14),

$$Z_L(\beta, \lambda) = Z_{\mathrm{o}, V(L)}(\beta, \lambda) + Z_{\mathrm{d}, V(L)}(\beta, \lambda) + Z_{\mathrm{big}, V(L)}(\beta, \lambda). \tag{3.19}$$

To analyze the magnetization, we will also introduce "modified" partition functions. Namely, for W of the form (3.7) and $x \in \Lambda$, we define

$$Z^{(x)}_{\mathrm{m}, W}(\beta, \lambda) = \sum_{\partial \sqsubset W}^{(\mathrm{m})} \mathbb{I}[x \in \mathscr{M}(W, \partial)]\, e^{-G_{\mathrm{o}}(\Omega_{\mathrm{o}}(W,\partial)) - G_{\mathrm{d}}(\Omega_{\mathrm{d}}(W,\partial))} \prod_{\gamma \in \partial} \varrho(\gamma),$$

$$\mathrm{m} = \mathrm{o}, \mathrm{d}, \tag{3.20}$$

where the sum is as in (3.11), $\mathscr{M}(W, \partial)$ is the set of points $x \in \Lambda$ that are endpoints of a bond in a component of $\Omega_{\mathrm{o}}(W, \partial)$ that contains bonds from $\partial\mathbb{B}$, and $\mathbb{I}[x \in \mathscr{M}(W, \partial)]$ is the indicator function of the event $x \in \mathscr{M}(W, \partial)$. For $\partial = \emptyset$, we set $\mathscr{M}(W, \partial) = \emptyset$ if m in (3.20) is d, and $\mathscr{M}(W, \partial) = \Lambda$ if $\mathrm{m} = \mathrm{o}$.

The partition function $Z^{(x)}_{\mathrm{big}, V}(\beta, \lambda)$ is defined analogously. With these definitions,

$$M_L(\beta, \lambda) = \sum_{x \in \Lambda} \frac{Z^{(x)}_{\mathrm{o}, V}(\beta, \lambda) + Z^{(x)}_{\mathrm{d}, V}(\beta, \lambda) + Z^{(x)}_{\mathrm{big}, V}(\beta, \lambda)}{Z_L(\beta, \lambda)}. \tag{3.21}$$

Again, one may rewrite the partition functions $Z^{(x)}_{\mathrm{m}, W}(\beta, \lambda)$ in a form similar to (3.12). To this end, we introduce the notion of a weak x-contour γ_x. Such a contour is either a standard contour with $x \in \mathrm{Int}\, \gamma_x \cap \Lambda$, or the empty set. We then define

$$K^{(x)}_{\mathrm{m}}(\gamma_x) = \frac{Z^{(x)}_{\mathrm{m}^c, \mathrm{Int}\, \gamma_x}(\beta, \lambda)}{Z_{\mathrm{m}^c, \mathrm{Int}\, \gamma_x}(\beta, \lambda)} K_{\mathrm{m}}(\gamma_x), \tag{3.22}$$

where $\frac{Z^{(x)}_{\mathrm{m}^c, \mathrm{Int}\, \gamma_x}(\beta, \lambda)}{Z_{\mathrm{m}^c, \mathrm{Int}\, \gamma_x}(\beta, \lambda)}$ stands for the Kronecker delta $\delta_{\mathrm{m}, \mathrm{o}}$ if $\gamma_x = \emptyset$. Finally, we say that a standard contour γ' is compatible with γ_x if $(\{x\} \cup \gamma_x) \cap V(\gamma') = \emptyset$. With these definitions, we rewrite $Z^{(x)}_{\mathrm{m}, V}(\beta, \lambda)$ as

$$Z^{(x)}_{\mathrm{m}, V}(\beta, \lambda) = e^{-G_{\mathrm{m}}(\overline{\mathbb{B}}(V))} \sum_{\gamma_x}^{(\mathrm{m})} K^{(x)}_{\mathrm{m}}(\gamma_x) \sum_{\partial^* \sim \gamma_x}^{(\mathrm{m})} \prod_{\gamma \in \partial^*} K_{\mathrm{m}}(\gamma), \qquad \mathrm{m} = \mathrm{o}, \mathrm{d}. \tag{3.23}$$

Here the first sum goes over all weak x-contours in V, while the second goes over all sets ∂^* of non-overlapping short m-labeled w-contours in V such that each of them is compatible with γ_x.

Strong b.c. For these boundary conditions, our definitions are slightly more involved. This stems in part from our definition of contours, in particular from the extra terms in (3.6), and in part from our desire to rewrite $Z_L(\beta, \lambda)$ as a partition function with disordered or ordered boundary conditions, depending on whether we are in the situation of Theorem 2.1(a) or (b).

For every $B \subset \overline{\mathbb{B}}$, let

$$G^{\mathrm{m}}_{\mathrm{m}'}(B) = \frac{g_{\mathrm{m}'}}{d} |\mathbb{B} \cap B| + h^{\mathrm{m}}_{\mathrm{m}'} |\partial\mathbb{B} \cap B|, \qquad \mathrm{m}, \mathrm{m}' = \mathrm{o}, \mathrm{d}, \tag{3.24}$$

where g_{o} and g_{d} were defined in (3.10) and

$$\begin{aligned} h^{\mathrm{m}}_{\mathrm{o}} &= \begin{cases} -\log(e^{\lambda\beta} - 1) & \text{if} \quad \mathrm{m} = \mathrm{o}, \\ -\log(e^{\lambda\beta} - 1) - \frac{1}{2d} \log q & \text{if} \quad \mathrm{m} = \mathrm{d}, \end{cases} \\ h^{\mathrm{m}}_{\mathrm{d}} &= \begin{cases} -\frac{1}{d} \log q & \text{if} \quad \mathrm{m} = \mathrm{o}, \\ -\frac{1}{2d} \log q & \text{if} \quad \mathrm{m} = \mathrm{d}. \end{cases} \end{aligned} \tag{3.25}$$

Moreover, for any W of the form (3.7), we define

$$\tilde{Z}_{\mathrm{m}, W}(\beta, \lambda) = \sum_{\partial \sqsubset W}^{(\mathrm{m})} e^{-G^{\mathrm{m}}_{\mathrm{o}}(\Omega_{\mathrm{o}}(W, \partial)) - G^{\mathrm{m}}_{\mathrm{d}}(\Omega_{\mathrm{d}}(W, \partial))} \prod_{\gamma \in \partial} \varrho(\gamma), \qquad \mathrm{m} = \mathrm{o}, \mathrm{d}, \tag{3.26}$$

where the sum goes over all admissible sets ∂ of s-contours such that the external s-contours in ∂ are m-labeled and $V(\gamma) \subset W$ for every $\gamma \in \partial$. With this definition, we get

$$Z_L(\beta, \lambda) = \tilde{Z}_{\mathrm{o}, V(L)}(\beta, \lambda) = \tilde{Z}_{\mathrm{d}, V(L)}(\beta, \lambda). \tag{3.27}$$

Indeed, consider $\tilde{Z}_{\mathrm{o}, V}(\beta, \lambda)$ defined by (3.26). Then every ∂ contributing to it contains exactly $C_{\mathrm{in}}(X(\partial))$ disordered s-contours, all with $\mathrm{dist}(\gamma, \partial V) \geqslant \frac{3}{4}$. Analogously, any ∂ contributing to $\tilde{Z}_{\mathrm{d}, V}(\beta, \lambda)$ contains $C_{\mathrm{in}}(X(\partial))$ disordered s-contours for which $\mathrm{dist}(\gamma, \partial V) \geqslant \frac{3}{4}$. Combining this with (3.1), (3.4), (3.6), and (3.24)–(3.26), we obtain (3.27), and hence two more contour representations for our model. They will be used to prove Theorem 2.1.

Again, it will be useful to rewrite $\tilde{Z}_{\mathrm{m}, W}(\beta, \lambda)$ as

$$\tilde{Z}_{\mathrm{m}, W}(\beta, \lambda) = e^{-G^{\mathrm{m}}_{\mathrm{m}}(\overline{\mathbb{B}}(W))} \sum_{\partial^* \sqsubset W}^{(\mathrm{m})} \prod_{\gamma \in \partial^*} \tilde{K}_{\mathrm{m}}(\gamma), \qquad \mathrm{m} = \mathrm{o}, \mathrm{d}, \tag{3.28}$$

where the sum goes over all collections ∂^* of non-overlapping m-labeled s-contours such that $V(\gamma) \subset W$ for every $\gamma \in \partial^*$ and

$$\tilde{K}_{\mathrm{o}}(\gamma) = \varrho(\gamma)\, q^{\frac{1}{2d}|\partial\mathbb{B}(\mathrm{Int}\,\gamma)|} \frac{\tilde{Z}_{\mathrm{d},\,\mathrm{Int}\,\gamma}(\beta, \lambda)}{\tilde{Z}_{\mathrm{o},\,\mathrm{Int}\,\gamma}(\beta, \lambda)}, \quad \tilde{K}_{\mathrm{d}}(\gamma) = \varrho(\gamma)\, q^{\frac{1}{2d}|\partial\mathbb{B}(\mathrm{Int}\,\gamma)|} \frac{\tilde{Z}_{\mathrm{o},\,\mathrm{Int}\,\gamma}(\beta, \lambda)}{\tilde{Z}_{\mathrm{d},\,\mathrm{Int}\,\gamma}(\beta, \lambda)}. \tag{3.29}$$

Defining $\tilde{Z}^{(x)}_{\mathrm{m},W}(\beta, \lambda)$ as in (3.20), we now get

$$M_L(\beta, \lambda) = \sum_{x \in \Lambda} \frac{\tilde{Z}^{(x)}_{\mathrm{o},V}(\beta, \lambda)}{\tilde{Z}_{\mathrm{o},V}(\beta, \lambda)} = \sum_{x \in \Lambda} \frac{\tilde{Z}^{(x)}_{\mathrm{d},V}(\beta, \lambda)}{\tilde{Z}_{\mathrm{d},V}(\beta, \lambda)}. \tag{3.30}$$

Defining $\tilde{K}^{(x)}_{\mathrm{m}}(\gamma_x)$ as in (3.22), the modified partition function $\tilde{Z}^{(x)}_{\mathrm{m},W}(\beta, \lambda)$ again has a contour representation of the form (3.23):

$$\tilde{Z}^{(x)}_{\mathrm{m},V}(\beta, \lambda) = e^{-G^{\mathrm{m}}_{\mathrm{m}}(\bar{\mathbb{B}}(V))} \sum_{\gamma_x}^{(\mathrm{m})} \tilde{K}^{(x)}_{\mathrm{m}}(\gamma_x) \sum_{\partial^* \sim \gamma_x}^{(\mathrm{m})} \prod_{\gamma \in \partial^*} \tilde{K}_{\mathrm{m}}(\gamma), \qquad \mathrm{m} = \mathrm{o}, \mathrm{d}. \tag{3.31}$$

Remark 3.2. Since the partition functions defined by (3.11) and (3.26) depend on λ only through $G_{\mathrm{o}}((\Omega_{\mathrm{o}}(W, \partial))$ and $G^{\mathrm{m}}_{\mathrm{o}}((\Omega_{\mathrm{o}}(W, \partial))$, respectively, they are independent of λ once $\partial\mathbb{B}(W) = \emptyset$, i.e., once $\mathrm{dist}(W, \partial V) \geqslant \frac{3}{4}$. As a result, the activities $K_{\mathrm{m}}(\gamma)$ and $\tilde{K}_{\mathrm{m}}(\gamma)$, $\mathrm{m} = \mathrm{o}, \mathrm{d}$, are independent of λ if $\mathrm{dist}(\gamma, \partial V) \geqslant \frac{3}{4}$.[11] Notice also that the partition functions $Z_{\mathrm{m},W}(\beta, \lambda)$ and $\tilde{Z}_{\mathrm{m},W}(\beta, \lambda)$ coincide whenever W is "not too large and not touching the boundary." Namely, we have $Z_{\mathrm{m},W}(\beta, \lambda) = \tilde{Z}_{\mathrm{m},W}(\beta, \lambda)$ and $K_{\mathrm{m}}(\gamma) = \tilde{K}_{\mathrm{m}}(\gamma)$ as soon as $\mathrm{diam}\, W < \omega(L)$, $\mathrm{dist}(W, \partial V) \geqslant \frac{3}{4}$ and $\mathrm{diam}\, \gamma < \omega(L)$, $\mathrm{dist}(\gamma, \partial V) \geqslant \frac{3}{4}$, respectively. The same holds for $K^{(x)}_{\mathrm{m}}(\gamma_x)$ and $\tilde{K}^{(x)}_{\mathrm{m}}(\gamma_x)$ as well as for $Z^{(x)}_{\mathrm{m},W}(\beta, \lambda)$ and $\tilde{Z}^{(x)}_{\mathrm{m},W}(\beta, \lambda)$.

We close this section with the following straightforward lemma.

Lemma 3.3. There exist constants $D_k < \infty$ such that for any $k = 1, 2, \ldots$, $\mathrm{m} = \mathrm{o}, \mathrm{d}$, $\lambda \in [0, \infty)$, and β in the interval $[1, \infty)$, we have

$$\left| \frac{\partial^k}{\partial \beta^k} Z_{\mathrm{m},W}(\beta, \lambda) \right| \leqslant D_k (|\partial\mathbb{B}(W)|\, (1+\lambda) + |\mathbb{B}(W)|)^k\, Z_{\mathrm{m},W}(\beta, \lambda), \tag{3.32}$$

provided $W \subset V$ is a volume of the form (3.7), and

$$\left| \frac{\partial^k}{\partial \beta^k} K_{\mathrm{m}}(\gamma) \right| \leqslant D_k (|\partial\mathbb{B}(\mathrm{Int}\,\gamma)|\, (1+\lambda) + |\mathbb{B}(\mathrm{Int}\,\gamma)|)^k\, K_{\mathrm{m}}(\gamma), \tag{3.33}$$

[11] Note that in this case the multiplicative factor $q^{\frac{1}{2d}|\partial\mathbb{B}(\mathrm{Int}\,\gamma)|}$ in (3.29) vanishes.

provided γ is a short m-labeled w-contour. The same bounds hold for the partition functions $Z_{\mathrm{big},V}(\beta,\lambda)$, $\tilde{Z}_{\mathrm{m},W}(\beta,\lambda)$, and the contour weights $\tilde{K}_{\mathrm{m}}(\gamma)$, as well as for the modified partition functions $Z^{(x)}_{\mathrm{m},W}(\beta,\lambda)$, $Z^{(x)}_{\mathrm{big},V}(\beta,\lambda)$, and $\tilde{Z}^{(x)}_{\mathrm{m},W}(\beta,\lambda)$, and the modified contour weights $K^{(x)}_{\mathrm{m}}(\gamma)$ and $\tilde{K}^{(x)}_{\mathrm{m}}(\gamma)$.

Proof. The bound (3.32) follows directly from definition (3.11), the fact that $\varrho(\gamma)$ does not depend on β, and Lemmas A.1 and A.9, which, in turn, immediately implies (3.33). ∎

4. CLUSTER EXPANSION AND PIROGOV–SINAI THEORY FOR WEAK BOUNDARY CONDITIONS

The decomposition (3.19) of the partition function $Z_L(\beta,\lambda)$ suggests that the finite-size scaling for the energy $E_L(\beta,\lambda)$ and the heat capacity $C_L(\beta,\lambda)$ may be evaluated with the help of a cluster-expansion analysis of the partition functions $Z_{\mathrm{m},V}(\beta,\lambda)$, $\mathrm{m}=\mathrm{o},\mathrm{d}$. To this end, a bound $K_{\mathrm{m}}(\gamma)\leqslant\epsilon^{\|\gamma\|}$, where $\epsilon>0$ is small, would be needed for every short w-contour γ.

Before proving such a bound, let us summarize the implications of the cluster expansions for the finite-size asymptotics. We will formulate these results in a generic situation, which will allow us to apply them to weak boundary conditions (done later in this section) as well as to strong boundary conditions (see Section 5).

Let us consider contours of a single type (ordered s-contours, disordered s-contours, ordered w-contours, or disordered w-contours), and use $\mathscr{L}_V$ to denote the set of all contours in V of given type. Further, let $\tilde{\mathscr{L}}_V$ be the set of those contours $\gamma\in\mathscr{L}_V$ with $\operatorname{dist}(\gamma,\partial V)\geqslant 3/4$, and let $\mathscr{L}_\infty=\bigcup_L\tilde{\mathscr{L}}_{V(L)}$.

We also introduce a set of contours $\mathscr{L}_<$ attached to the hyperplane $x_1=0$. To this end, let $P(L)=\{x\in\partial V(L)\mid x_1=\lceil\frac{L+1}{2}\rceil\}$, and let $T_L\colon\mathbb{R}^d\to\mathbb{R}^d$ be the translation that maps $(x_1,x_2,\dots,x_d)$ into $(x_1-\lceil\frac{L+1}{2}\rceil,x_2,\dots,x_d)$. We say that a contour $\gamma\in\mathscr{L}_V$ touches only the face $P(L)$ if $\operatorname{dist}(\gamma,P(L))\leqslant 1/4$ and $\operatorname{dist}(\gamma,\partial V\setminus P(L))\geqslant 3/4$, and similarly for the remaining $2d-1$ faces of V. We then define $\mathscr{L}^{(L)}_<$ as the set of all contours $\tilde{\gamma}$ that are translations by T_L of contours γ touching only the face $P(L)$ and introduce $\mathscr{L}_<=\bigcup_L\mathscr{L}^{(L)}_<$.

Lemma 4.1. Let $\mathscr{K}_V\colon\mathscr{L}_V\to\mathbb{R}$ be a contour weight such that

(i) there exists a translation-invariant weight $\mathscr{K}\colon\mathscr{L}_\infty\to\mathbb{R}$ such that $\mathscr{K}_V(\gamma)=\mathscr{K}(\gamma)$ whenever $\operatorname{dist}(\gamma,\partial V)\geqslant 3/4$;

(ii) there exists a weight $\mathscr{K}_<\colon\mathscr{L}_<\to\mathbb{R}$, invariant under translations parallel to the hyperplane $x_1=0$, such that $\mathscr{K}_V(\gamma)=\mathscr{K}_<(T_L(\gamma))$ whenever $\gamma\in\mathscr{L}_V$ is a contour that touches only the face $P(L)$;

(iii) the weight $\mathscr{K}_V$ is invariant under lattice rotations around the center of V; and

(iv) $|\mathscr{K}_V(\gamma)| \leqslant \epsilon^{\|\gamma\|}$ with $\epsilon > 0$ sufficiently small.

Let ω: $\mathbb{N} \to (0, \infty]$ with $\omega(L)/\log L \to \infty$ as $L \to \infty$; for any W of the form (3.7), let

$$\mathscr{Z}(W) = \sum_{\partial^* \sqsubset W} \prod_{\gamma \in \partial^*} \mathscr{K}_V(\gamma),$$

where the sum is over all families ∂^* of non-intersecting contours such that $V(\gamma) \subset W$ and $\operatorname{diam} \gamma < \omega(L)$ for every $\gamma \in \partial^*$. Then $\mathscr{Z}(W) \neq 0$ for all volumes W of the form (3.7), the limits

$$\phi = -\lim_{L \to \infty} \frac{1}{L^d} \log \mathscr{Z}(V(L)) \qquad \text{and}$$

$$\sigma = -\lim_{L \to \infty} \frac{1}{2\, dL^{d-1}} (\log \mathscr{Z}(V(L)) + \phi |\mathbb{B}|/d) \tag{4.1}$$

exist, and

$$\log \mathscr{Z}(W) = -\Phi(W) + O(\epsilon)\, \|\partial_i W\| + O(\epsilon)\, \|\partial^{(d-2)} W\| \tag{4.2}$$

where $\Phi(W) = \phi\, |\mathbb{B}(W)|/d + \sigma\, \|\partial_e W\|$, while $\|\partial^{(d-2)} W\|$ is the $(d-2)$-dimensional area of the intersection of ∂W with the union of all $(d-2)$-dimensional edges of V. Here, the error terms $O(\epsilon)$ are uniform in L and $W \subset V(L)$, provided that L is sufficiently large (how large depends on the function ω).

Remark 4.2. The formula (4.2) is a suitable generalization of the standard expression $\log \mathscr{Z}(W) = -\phi\, |\mathbb{B}(W)|/d + O(\epsilon\, \|\partial W\|)$. An important fact to notice is that if W is touching the boundary $\partial V(L)$, $\|\partial_e W\| \neq 0$, the term proportional to $\|\partial_e W\|$ is explicitly considered and not included into the error term.

Proof. Let us first prove the lemma without the restriction $\operatorname{diam} \gamma < \omega(L)$, i.e., putting formally $\omega(L) = \infty$. By the usual Mayer expansion for polymer systems, the logarithm of $\mathscr{Z}(W)$ can be expanded in the form

$$\log \mathscr{Z}(W) = \sum_{Y:\, V(Y) \subset W} a(Y)\, \mathscr{K}_V^Y. \tag{4.3}$$

Here the sum goes over all multi-indices Y: $\mathscr{L}_V \to \mathbb{N}_0$ with $|Y| = \sum_{\gamma \in \mathscr{L}_V} Y(\gamma) < \infty$, $V(Y) = \bigcup_{\gamma:\, Y(\gamma) > 0} V(\gamma)$, $\mathscr{K}_V^Y = \prod_{\gamma \in \mathscr{L}_V} \mathscr{K}_V(\gamma)^{Y(\gamma)}$, and $a(Y) \in \mathbb{Z}$ is a combinatorial coefficient that does not depend on V, see, any standard exposition on cluster expansions like ref. 21, or more recently, refs. 22 and 23).

First, let us split the sum on the right hand side of (4.3) into two terms,

$$\log \mathscr{Z}(W) = \sum_{\substack{Y:\, V(Y) \subset W,\\ \overline{\mathbb{B}}(Y) \subset \mathbb{B}(W)}} a(Y)\, \mathscr{K}_V^Y + \sum_{\substack{Y:\, V(Y) \subset W,\\ \partial\mathbb{B}(Y) \neq \emptyset}} a(Y)\, \mathscr{K}_V^Y, \tag{4.4}$$

where $\overline{\mathbb{B}}(Y) = \bigcup_{\gamma:\, Y(\gamma) > 0} \overline{\mathbb{B}}(\gamma)$ and $\partial\mathbb{B}(Y) = \bigcup_{\gamma:\, Y(\gamma) > 0} \partial\mathbb{B}(\gamma)$. For the first sum, observing that $\mathscr{K}_V = \mathscr{K}$ for all contributing terms and introducing the explicit expression

$$\phi = -\sum_{Y:\, \overline{\mathbb{B}}(Y) \ni b} \frac{a(Y)}{|\overline{\mathbb{B}}(Y)|} \mathscr{K}^Y, \tag{4.5}$$

where the sum is over multi-indices $Y: \mathscr{L}_\infty \to \mathbb{N}_0$ and b is any fixed bond, we get

$$\begin{aligned} \sum_{\substack{Y:\, V(Y) \subset W,\\ \overline{\mathbb{B}}(Y) \subset \mathbb{B}(W)}} a(Y)\, \mathscr{K}^Y = -\phi\, |\mathbb{B}(W)| - \sum_{Y:\, \overline{\mathbb{B}}(Y) \not\subset \mathbb{B}(W)} a(Y)\, \mathscr{K}^Y \frac{|\mathbb{B}(W) \cap \overline{\mathbb{B}}(Y)|}{|\overline{\mathbb{B}}(Y)|} \\ - \sum_{\substack{Y:\, V(Y) \not\subset W,\\ \overline{\mathbb{B}}(Y) \subset \mathbb{B}(W)}} a(Y)\, \mathscr{K}^Y. \end{aligned} \tag{4.6}$$

Using (4.4) for $W = V(L)$ and noticing that the second sum in (4.4) as well as both sums on the right hand side in (4.6) are of he order of $|\partial V(L)|$, the existence of the first limit in (4.1) and the fact that it equals (4.5) follows.

Let now $\partial\mathbb{B}_<$ be the set of bonds of the form $b = \langle(-1, x_2,..., x_d), (0, x_2,..., x_d)\rangle$, $\mathbb{B}_<$ be the set of bonds $b = \langle(x_1, x_2,..., x_d), (y_1, y_2,..., y_d)\rangle\}$ with $x_1, y_1 \leqslant -1$, $P_<$ be the halfspace $P_< = \{x \in \mathbb{R}^d;\, x_1 \leqslant 0\}$, and, for any multiindex Y on $\mathscr{L}_<$, let $\partial\mathbb{B}_<(Y) = \overline{\mathbb{B}}(Y) \cap \partial\mathbb{B}_<$. Further, let us introduce

$$\sigma_1 = -\sum_{Y:\, \partial\mathbb{B}_<(Y) \ni b} \frac{a(Y)}{|\partial\mathbb{B}_<(Y)|} \mathscr{K}_<^Y \tag{4.7}$$

with the sum over multiindices on $\mathscr{L}_<$ and b any bond from $\partial\mathbb{B}_<$, as well as

$$\sigma_2 = \sum_{\substack{Y:\, \partial_+\mathbb{B}(Y) \ni b,\\ \overline{\mathbb{B}}(Y) \not\subset \mathbb{B}_<}} \frac{a(Y)}{|\partial_+\mathbb{B}(Y)|} \frac{|\mathbb{B}_< \cap \overline{\mathbb{B}}(Y)|}{|\overline{\mathbb{B}}(Y)|} \mathscr{K}^Y \tag{4.8}$$

and

$$\sigma_3 = \sum_{\substack{Y:\,\partial_+\mathbb{B}(Y)\ni b,\\ V(Y)\not\subset P_<,\\ \overline{\mathbb{B}}(Y)\subset\mathbb{B}_<}} \frac{a(Y)}{|\partial_+\mathbb{B}(Y)|}\mathscr{K}^Y. \tag{4.9}$$

Here, again $b\in\partial\mathbb{B}_<$, the sums are over multiindices on $\mathscr{L}_\infty$, and

$$\partial_+\mathbb{B}(Y)=\{b\in\partial\mathbb{B}_< : \mathrm{dist}(b, V(Y))\leqslant\tfrac{1}{2}\}. \tag{4.10}$$

Let us observe that all terms in the second sum in (4.4) touching only one face of V can be attributed to the expression $\sigma_1\|\partial_e W\|$. The terms not accounted for are necessarily such that, either bonds from $\overline{\mathbb{B}}(Y)$ intersect $\partial W\setminus\partial V$ or $\partial\mathbb{B}(Y)$ is intersecting at least two faces of V. Their sum is yielding an error of the order $O(\epsilon)(\|\partial_i W\|+\|\partial^{(d-2)}W\|)$. Similarly, we can evaluate the two sums on the right hand side of (4.6) by $(\sigma_2+\sigma_2)\,\|\partial_e W\|$, again with error $O(\epsilon)(\|\partial_i W\|+\|\partial^{(d-2)}W\|)$. Taking $\sigma=\sigma_1+\sigma_2+\sigma_3$, we get the claim (4.2) and thus, applying it to $W=V(L)$, also the existence of the second limit in (4.1).

Returning now to the case of a general function ω: $\mathbb{N}\to(0,\infty)$ obeying the condition $\omega(L)/\log L\to\infty$, we observe that the restriction to contours of diameter $\mathrm{diam}\,\gamma<\omega(L)$ introduces an extra error term of the form $O(L^d(C\epsilon)^{\omega(L)})$, where C is a dimension dependent constant. The condition $\omega(L)/\log L\to\infty$ ensures that the error term can be bounded by $O(\epsilon)$, which in turn can be absorbed into the error terms already present in (4.2). ∎

In order to apply the lemma to the partition functions $Z_{\mathrm{m},V}(\beta,\lambda)$, $\mathrm{m}=\mathrm{o},\mathrm{d}$, a bound[12] $K_{\mathrm{m}}(\gamma)\leqslant\epsilon^{\|\gamma\|}$, where $\epsilon>0$ is small, would be needed for every short w-contour γ. It turns out, though, that a bound of this form does not hold for both $\mathrm{m}=\mathrm{o},\mathrm{d}$ and for all $\beta>0$. Therefore, one first constructs[(6, 13)] truncated contour activities $\bar{K}_{\mathrm{m}}(\gamma)$ and the corresponding partition functions[13]

$$\bar{Z}_{\mathrm{m},W}(\beta,\lambda)=e^{-G_{\mathrm{m}}(\overline{\mathbb{B}}(W))}\sum_{\partial^*\sqsubset W}^{(\mathrm{m})}\prod_{\gamma\in\partial^*}\bar{K}_{\mathrm{m}}(\gamma), \qquad \mathrm{m}=\mathrm{o},\mathrm{d}, \tag{4.11}$$

[12] Actually, as will be explained below, we will consider such a bound in two different forms in dependence on whether the considered contour is (or is not) touching the boundary ∂V.

[13] The sum in (4.11) runs over the same collections of w-contours as in (3.12).

defined for every W of the form (3.7). This will be done in such a way that $\bar{K}_{\mathrm{m}}(\gamma)$ is a smooth function of β and $\bar{K}_{\mathrm{m}}(\gamma) \leqslant \epsilon^{\|\gamma\|}$ for some small $\epsilon > 0$ and all short w-contours γ. In addition, whenever

$$f_{\mathrm{m}}(\beta) = -\lim_{L \to \infty} \frac{1}{L^d} \log \bar{Z}_{\mathrm{m}, V(L)}(\beta, \lambda) \tag{4.12}$$

equals

$$f(\beta) = \min\{f_{\mathrm{o}}(\beta), f_{\mathrm{d}}(\beta)\}, \tag{4.13}$$

then, necessarily, $\bar{K}_{\mathrm{m}}(\gamma) = K_{\mathrm{m}}(\gamma)$ so that $\bar{Z}_{\mathrm{m}, W}(\beta, \lambda) = Z_{\mathrm{m}, W}(\beta, \lambda)$.

Different approaches for a construction of the truncated model were proposed (see, for example, ref. 13 or ref. 24). Even though the contours with weights depending on their position with respect to the boundary ∂V were discussed already in ref. 24, we need a more careful evaluation of the boundary terms to get weaker constrains on the surface coupling λ. On the other hand, the truncation procedure in the spirit of ref. 24 is simpler in our case since we effectively have only two coexisting phases.

First, let $\chi_\eta(u_1, u_2)$ be a smoothed version of $\min(u_1, u_2)$ satisfying the following conditions:

(i) $\chi_\eta(u) \leqslant \min(u)$,

(ii) $\chi_\eta(u) = u_i$ whenever $u_i \leqslant \min\{u_j; j \neq i\} - \eta$,

(iii) χ_η is C^∞, $0 \leqslant \frac{\partial \chi_\eta(u)}{\partial u_i} \leqslant 1$, and $\|\frac{\partial^k \chi_\eta(u)}{\partial u_1^k}\| \leqslant \eta^{-k+1} c_k$ for $k \geqslant 2$ and some $c_k < \infty$.

As shown in ref. 24, one can define such function by a convolution of min with a suitable function. Here, we take any fixed nonnegative symmetric function $f \in C^\infty(\mathbb{R}^2)$ such that $\int_{\mathbb{R}^2} f(u)\, du = 1$ and $f(u) = 0$ whenever $\|u\| \geqslant \frac{1}{2}$, and define

$$\chi_\eta(u) = \eta \int f\left(\frac{u}{\eta} - v\right) \min(v)\, dv. \tag{4.14}$$

Further, let

$$\nu_0 = \frac{1}{12d} \qquad \text{and} \qquad \nu = \min\left\{\nu_0, \frac{1-\mu}{4d}\right\} \tag{4.15}$$

and, for any contour γ, let

$$\tau(\gamma) = \begin{cases} \nu_0 \|\gamma\| & \text{if } \operatorname{dist}(\gamma, \partial V) \geqslant 3/4 \\ \nu \|\gamma\| & \text{otherwise.} \end{cases} \tag{4.16}$$

We introduce the *truncated activities* $\bar{K}_{\mathrm{m}}(\gamma)$, $\mathrm{m}=\mathrm{o},\mathrm{d}$, for any short w-contour γ, in the following manner:

$$\bar{K}_{\mathrm{m}}(\gamma)=\exp\{\chi_{\|\gamma\|}(\log K_{\mathrm{m}}(\gamma),-\tau(\gamma)\log q)\}, \tag{4.17}$$

where we took the function χ_η with $\eta=\|\gamma\|$. Notice that $\bar{K}_{\mathrm{m}}(\gamma)$ is well defined since $K_{\mathrm{m}}(\gamma)>0$ by definition. We also introduce the truncated equivalent of the modified weights $K_{\mathrm{m}}^{(x)}(\gamma)$ as

$$\bar{K}_{\mathrm{m}}^{(x)}(\gamma_x)=\frac{Z^{(x)}_{\mathrm{m}^c,\,\mathrm{Int}\,\gamma_x}(\beta,\lambda)}{Z_{\mathrm{m}^c,\,\mathrm{Int}\,\gamma_x}(\beta,\lambda)}\,\bar{K}_{\mathrm{m}}(\gamma_x), \tag{4.18}$$

with $\bar{K}_{\mathrm{m}}(\emptyset)=1$, so that, in particular, $\bar{K}_{\mathrm{m}}^{(x)}(\emptyset)=K_{\mathrm{m}}^{(x)}(\emptyset)=\delta_{\mathrm{m},\mathrm{o}}$. We also define a truncated version of the modified partition functions $Z^{(x)}_{\mathrm{m},V}(\beta,\lambda)$ as

$$\bar{Z}^{(x)}_{\mathrm{m},V}(\beta,\lambda)=e^{-G_{\mathrm{m}}(\bar{\mathbb{B}}(V))}\sum_{\gamma_x}^{(\mathrm{m})}\bar{K}_{\mathrm{m}}^{(x)}(\gamma_x)\sum_{\partial^*\sim\gamma_x}^{(\mathrm{m})}\prod_{\gamma\in\partial^*}\bar{K}_{\mathrm{m}}(\gamma),\qquad \mathrm{m}=\mathrm{o},\mathrm{d}. \tag{4.19}$$

Lemma 4.3. Let $d\geqslant 2$, $0\leqslant\mu<1$, and $k_0\in\mathbb{Z}$, $k_0\geqslant 0$. Then there exists a finite positive constant D_0 such that the following statements are true for $\mathrm{m}=\mathrm{o},\mathrm{d}$ and all m-labelled w-contours γ.

(a) For $\beta>0$ and $\lambda\in[\frac{1-\mu}{2},\frac{1+\mu}{2}]$, one has

$$\bar{K}_{\mathrm{m}}(\gamma)\leqslant q^{-\tau(\gamma)}. \tag{4.20}$$

(b) For any $\lambda\in[\frac{1-\mu}{2},\frac{1+\mu}{2}]$, the activity $\bar{K}_{\mathrm{m}}(\gamma)$ is a C^{k_0} function of β in the interval $[1,\infty)$, and

$$\left|\frac{\partial^k}{\partial\beta^k}\bar{K}_{\mathrm{m}}(\gamma)\right|\leqslant(D_0\,|\bar{\mathbb{B}}(\mathrm{Int}(\gamma))|)^k\,q^{-\tau(\gamma)}\qquad\text{for all}\quad k\leqslant k_0. \tag{4.21}$$

(c) With the conventions $\tau(\emptyset)=0$ and $|\bar{\mathbb{B}}(\mathrm{Int}(\emptyset))|=0$, the same bounds hold for the modified activities $\bar{K}_{\mathrm{m}}^{(x)}(\gamma_x)$.

Proof. The claim (a) is a direct consequence of the definition (4.17) and the property (i) of χ_η. For the bound on derivatives, we use Lemma A.9 to combine the property (iii) of χ_η with (3.33). The bounds for $\bar{K}_{\mathrm{m}}^{(x)}(\gamma_x)$ are obtained in an identical way. ▮

Lemma 4.3 allows us to apply convergent cluster expansions to analyze the functions $\log\bar{Z}_{\mathrm{m},V(L)}(\beta,\lambda)$, $\mathrm{m}=\mathrm{o},\mathrm{d}$. In particular, the limits (4.12) and

$$s_{\mathrm{m}}(\beta)=-\lim_{L\to\infty}\frac{1}{2\,dL^{d-1}}\left(\log\bar{Z}_{\mathrm{m},V(L)}(\beta,\lambda)+\frac{1}{d}f_{\mathrm{m}}(\beta)\,|\mathbb{B}|\right), \tag{4.22}$$

exist for q large enough and all $\beta > 0$, the functions f_{m} and s_{m} are C^{k_0} functions of β on the interval $[1, \infty)$, and

$$\frac{d^k f_{\mathrm{m}}}{d\beta^k} = \frac{d^k g_{\mathrm{m}}}{d\beta^k} + O(q^{-\nu_0}) \qquad \text{and} \qquad \frac{d^k s_{\mathrm{m}}}{d\beta^k} = \frac{d^k h_{\mathrm{m}}}{d\beta^k} + O(q^{-\nu}) \tag{4.23}$$

for any $k = 0,..., k_0$. For $k = 0$, the bounds (4.23) are valid for all $\beta \in (0, \infty)$.

Lemma 4.3 also allows us to analyze the functions $\log \bar{Z}_{\mathrm{m},W}(\beta, \lambda)$, $\mathrm{m} = \mathrm{o}, \mathrm{d}$ for more general volumes W. Assuming that q and L are sufficiently large, taking $W \subset V$ to be a volume of the form (3.7), with γ_0 and all contours from ∂^* and $\tilde{\partial}^*$ being w-contours, so that, in particular, $|\partial \mathbb{B}(W)| = \|\partial_e W\|$, and introducing

$$F_{\mathrm{m}}(W) = \frac{1}{d} f_{\mathrm{m}} \, |\mathbb{B}(W)| + s_{\mathrm{m}} \, \|\partial_e W\|, \tag{4.24}$$

we get

$$\frac{\partial^k}{\partial \beta^k} \log \bar{Z}_{\mathrm{m},W}(\beta, \lambda) = -\frac{\partial^k F_{\mathrm{m}}(W)}{\partial \beta^k} + O(q^{-\nu} \, \|\partial_i W\|) + O(q^{-\nu} \, \|\partial^{(d-2)} W\|), \tag{4.25}$$

provided $\lambda \in [\frac{1-\mu}{2}, \frac{1+\mu}{2}]$, $\beta \in [1, \infty)$, and $k \leqslant k_0$. For $k = 0$, this bound again holds for all $\beta > 0$. While (4.25) can be used to analyze the ratio $\bar{Z}_{\mathrm{m},W}(\beta, \lambda)/\bar{Z}_{\mathrm{m},V}(\beta, \lambda)$, it is sometimes useful to have a better bound. Expressing $\log \bar{Z}_{\mathrm{m},V}(\beta, \lambda) - \log \bar{Z}_{\mathrm{m},W}(\beta, \lambda)$ with the help of the cluster expansion of the form (4.3), we notice that only terms with clusters in $W^c = V \setminus W$ or those intersecting its boundary will not be cancelled. As a result, we get

$$\frac{\partial^k}{\partial \beta^k} \left(\log \frac{\bar{Z}_{\mathrm{m},W}(\beta, \lambda)}{\bar{Z}_{\mathrm{m},V}(\beta, \lambda)} \right) = \frac{\partial^k F_{\mathrm{m}}(W^c)}{\partial \beta^k} + O(q^{-\nu} \, \|\partial_i W^c\|) + O(q^{-\nu} \, \|\partial^{(d-2)} W^c\|) \tag{4.26}$$

or, less precisely,

$$\frac{\partial^k}{\partial \beta^k} \left(\log \frac{\bar{Z}_{\mathrm{m},W}(\beta, \lambda)}{\bar{Z}_{\mathrm{m},V}(\beta, \lambda)} \right) = \frac{\partial^k F_{\mathrm{m}}(W^c)}{\partial \beta^k} + O(q^{-\nu} \, \|\partial W^c\|). \tag{4.27}$$

Finally, Lemma 4.3(c) allows us to use convergent cluster expansions to analyze the ratios $\frac{\bar{Z}^{(x)}_{\mathrm{m},V}(\beta,\lambda)}{\bar{Z}_{\mathrm{m},V}(\beta,\lambda)}$, and thus the "meta-stable" magnetizations $M_{\mathrm{m},L}(\beta,\lambda)$ defined as

$$M_{\mathrm{m},L}(\beta,\lambda)=\sum_{x\in\Lambda}\frac{\bar{Z}^{(x)}_{\mathrm{m},V(L)}(\beta,\lambda)}{\bar{Z}_{\mathrm{m},V(L)}(\beta,\lambda)}. \tag{4.28}$$

In particular, the limits

$$m_{\mathrm{m}}(\beta)=\lim_{L\to\infty}\frac{1}{L^d}M_{\mathrm{m},L}(\beta,\lambda) \tag{4.29}$$

exist, they are independent of λ and obey the bounds

$$m_{\mathrm{m}}(\beta)=\delta_{\mathrm{m},\mathrm{o}}+O(q^{-\nu_0}) \tag{4.30}$$

and

$$\frac{d^k m_{\mathrm{m}}(\beta)}{d\beta^k}=O(q^{-\nu_0}),\qquad 1\leqslant k\leqslant k_0. \tag{4.31}$$

In addition, we get the following bounds on finite-size corrections,

$$\frac{\partial^k M_{\mathrm{m},L}(\beta,\lambda)}{\partial\beta^k}=\frac{d^k m_{\mathrm{m}}(\beta)}{d\beta^k}L^d+O(q^{-\nu})\,L^{d-1},\qquad 0\leqslant k\leqslant k_0. \tag{4.32}$$

Lemma 4.4. Let $d\geqslant 2$, $0\leqslant\mu<1$, and let $\omega\colon\mathbb{N}\to[0,\infty]$ be a function with $\omega(L)\leqslant L+1$ and $\omega(L)/\log L\to\infty$ as $L\to\infty$. Define

$$\alpha=\frac{\nu\log q-2}{4}\qquad\text{and}\qquad\alpha_0=\frac{\nu_0\log q-2}{4}, \tag{4.33}$$

and assume that q, L are sufficiently large. For any m-labeled short w-contour γ, $\mathrm{m}=\mathrm{o},\mathrm{d}$, and any volume W of the form (3.7), the truncated activity $\bar{K}_{\mathrm{m}}(\gamma)$ and the corresponding partition function $\bar{Z}_{\mathrm{m},W}(\beta,\lambda)$ satisfy the following claims (a)–(f), provided $|\lambda-\frac{1}{2}|\leqslant\frac{\mu}{2}$ and $\beta>0$:

(a) Let $a_{\mathrm{m}}(\beta)=f_{\mathrm{m}}(\beta)-f(\beta)$. If $a_{\mathrm{m}}(\beta)\operatorname{diam}\gamma\leqslant 2d\alpha$, then $\bar{K}_{\mathrm{m}}(\gamma)=K_{\mathrm{m}}(\gamma)$.

(b) If $a_{\mathrm{m}}(\beta)\operatorname{diam}\gamma\leqslant 2d\alpha_0$ and $\operatorname{dist}(\gamma,\partial V)\geqslant\frac{3}{4}$, then $\bar{K}_{\mathrm{m}}(\gamma)=K_{\mathrm{m}}(\gamma)$.

(c) If $a_{\mathrm{m}}(\beta)\min\{\operatorname{diam}W,\omega(L)\}\leqslant 2d\alpha$, then $\bar{Z}_{\mathrm{m},W}(\beta,\lambda)=Z_{\mathrm{m},W}(\beta,\lambda)$.

(d) If $a_{\mathrm{m}}(\beta)\min\{\operatorname{diam} W, \omega(L)\} \leqslant 2\, d\alpha_0$ and $\operatorname{dist}(W, \partial V) \geqslant \frac{3}{4}$, then $\bar{Z}_{\mathrm{m}, W}(\beta, \lambda) = Z_{\mathrm{m}, W}(\beta, \lambda)$.

(e) If $a_{\mathrm{m}}(\beta) > 0$, then

$$Z_{\mathrm{m}, W}(\beta, \lambda) \leqslant e^{-F_{\mathrm{m}^c}(W) + \frac{\mu}{2d} \log q \, \|\partial_e W\| + O(q^{-\nu}) \, \|\partial W\|}, \tag{4.34}$$

with m^c defined as in (3.15).

Proof. The claims of the lemma will be proven by induction in $|\overline{\mathbb{B}}(\operatorname{Int} \gamma)|$ and $v(W)$, where

$$v(W) = \max_{\substack{\gamma:\, V(\gamma) \subset W, \\ \gamma \text{ short } w\text{-contour}}} |\overline{\mathbb{B}}(\operatorname{Int} \gamma)|. \tag{4.35}$$

• *Proof of (a)–(e) for $|\overline{\mathbb{B}}(\operatorname{Int} \gamma)|=0$ and $v(W)=0$.* Since there is no w-contour γ with $|\overline{\mathbb{B}}(\operatorname{Int} \gamma)| = 0$, there is nothing to prove in the claims (a) and (b).

Next, let $v(W) = 0$. Then (3.12) directly yields

$$Z_{\mathrm{m}, W}(\beta, \lambda) = e^{-G_{\mathrm{m}}(\overline{\mathbb{B}}(W))} = \bar{Z}_{\mathrm{m}, W}(\beta, \lambda), \tag{4.36}$$

proving thus (c) and (d). Further, in view of (4.2), and the fact that $f_{\mathrm{m}} \geqslant f_{\mathrm{m}^c}$ if $a_{\mathrm{m}}(\beta) \geqslant 0$, we get

$$\begin{aligned} Z_{\mathrm{m}, W}(\beta, \lambda) = \bar{Z}_{\mathrm{m}, W}(\beta, \lambda) &= e^{-F_{\mathrm{m}}(W) + O(q^{-\nu}) \, \|\partial W\|} \\ &\leqslant e^{-F_{\mathrm{m}^c}(W) + (s_{\mathrm{m}^c} - s_{\mathrm{m}}) \, |\partial \mathbb{B}(W)| + O(q^{-\nu}) \, \|\partial W\|} \end{aligned} \tag{4.37}$$

whenever $a_{\mathrm{m}}(\beta) \geqslant 0$. Referring to (4.23), and using first Lemma A.6(b) with $\xi = 0$, and then the bound (A.9) of Lemma A.6(a), we get

$$\sup_{\beta:\, a_{\mathrm{m}}(\beta) > 0} (s_{\mathrm{m}^c} - s_{\mathrm{m}})(\beta) \leqslant \frac{\mu}{2d} \log q + O(q^{-\nu}) \tag{4.38}$$

and hence the claim (e).

Next, assume that $n \geqslant 1$ and that the lemma has already been proven for all γ such that $|\overline{\mathbb{B}}(\operatorname{Int} \gamma)| < n$ and all W such that $v(W) < n$.

• *Proof of (a) and (b) for γ with $|\overline{\mathbb{B}}(\operatorname{Int} \gamma)|=n$.* Using, by the inductive assumption, the claim (c) for $Z_{\mathrm{m}, \operatorname{Int} \gamma}(\beta, \lambda)$, the bound $\|\partial \operatorname{Int} \gamma\| = \|\gamma\| + |\partial \mathbb{B}(\operatorname{Int} \gamma)| \leqslant 2 \, \|\gamma\|$, and, in dependence on the value of β, either the claim (c) or (e) for $Z_{\mathrm{m}^c, \operatorname{Int} \gamma}(\beta, \lambda)$, we get

$$\frac{Z_{\mathrm{m}^c, \operatorname{Int} \gamma}(\beta, \lambda)}{Z_{\mathrm{m}, \operatorname{Int} \gamma}(\beta, \lambda)} = e^{a_{\mathrm{m}} |\mathbb{B}(\operatorname{Int} \gamma)|/d + (s_{\mathrm{m}} - s_{\mathrm{m}^c}) \, |\partial \mathbb{B}(\operatorname{Int} \gamma)| + O(q^{-\nu}) \, \|\gamma\|} \tag{4.39}$$

for all $\beta > 0$ such that a_{m^c} diam $\gamma \leqslant 2\, d\alpha$ (the former case) and

$$\frac{Z_{\mathrm{m}^c,\,\mathrm{Int}\,\gamma}(\beta,\lambda)}{Z_{\mathrm{m},\,\mathrm{Int}\,\gamma}(\beta,\lambda)} \leqslant e^{(\frac{\mu}{2d}\log q + O(q^{-\nu}))\,|\partial\mathbb{B}(\mathrm{Int}\,\gamma)| + O(q^{-\nu})\,\|\gamma\|} \tag{4.40}$$

otherwise (the latter case).

Observing that $a_{\mathrm{m}} \geqslant f_{\mathrm{m}} - f_{\mathrm{m}^c}$ and using Lemma A.4, we get

$$(f_{\mathrm{m}} - f_{\mathrm{m}^c})\,|\overline{\mathbb{B}}(\mathrm{Int}\,\gamma)|/d \leqslant a_{\mathrm{m}}|\overline{\mathbb{B}}(\mathrm{Int}\,\gamma)|/d \leqslant \frac{2}{d}\, a_{\mathrm{m}} \text{ diam } \gamma\, \|\gamma\|. \tag{4.41}$$

As a result,

$$\begin{aligned}\frac{Z_{\mathrm{m}^c,\,\mathrm{Int}\,\gamma}(\beta,\lambda)}{Z_{\mathrm{m},\,\mathrm{Int}\,\gamma}(\beta,\lambda)} &\leqslant \max\Big\{\sup_{\beta>0} e^{\frac{2}{d}a_{\mathrm{m}}\mathrm{diam}\,\gamma\,\|\gamma\| + (s_{\mathrm{m}} - s_{\mathrm{m}^c} - a_{\mathrm{m}}/d)\,|\partial\mathbb{B}(\mathrm{Int}\,\gamma)|},\\ &\qquad e^{(\frac{\mu}{2d}\log q + O(q^{-\nu}))\,|\partial\mathbb{B}(\mathrm{Int}\,\gamma)|}\Big\}\, e^{O(q^{-\nu})\,\|\gamma\|}.\end{aligned} \tag{4.42}$$

Using first Lemma A.6(c) and Lemma A.6(a) to bound $(s_{\mathrm{m}} - s_{\mathrm{m}^c} - a_{\mathrm{m}}/d)$, and then Lemma A.2 to bound $|\partial\mathbb{B}(\mathrm{Int}\,\gamma)|$, we get

$$\frac{Z_{\mathrm{m}^c,\,\mathrm{Int}\,\gamma}(\beta,\lambda)}{Z_{\mathrm{m},\,\mathrm{Int}\,\gamma}(\beta,\lambda)} \leqslant e^{(\frac{2}{d}a_{\mathrm{m}}\mathrm{diam}\,\gamma + O(q^{-\nu}))\,\|\gamma\| + \frac{\mu}{2d}\log q\,|\partial\mathbb{B}(\mathrm{Int}\,\gamma)|}. \tag{4.43}$$

If $|\partial\mathbb{B}(\mathrm{Int}\,\gamma)| = 0$, we have $\mathrm{dist}(\gamma, \partial V) \geqslant \frac{3}{4}$ and $\varrho(\gamma) \leqslant q^{-\frac{1}{6d}\|\gamma\|}$.[14] Then (3.13), (4.33), and (4.43) combined with the assumption a_{m} diam $\gamma \leqslant 2\, d\alpha_0$ yield

$$K_{\mathrm{m}}(\gamma) \leqslant q^{(-\frac{1}{6d}+\nu_0)\,\|\gamma\|} e^{-\|\gamma\|} \leqslant q^{-\tau(\gamma)} e^{-\|\gamma\|}, \tag{4.44}$$

provided that q is large enough to guarantee that the error term $O(q^{-\nu})\,\|\gamma\|$ in (4.43) is smaller than $\|\gamma\|$. Referring to the definition (4.17) and to the property (ii) of the function χ_η, we get $\bar{K}_{\mathrm{m}}(\gamma) = K_{\mathrm{m}}(\gamma)$, proving thus (b).

On the other hand, if $|\partial\mathbb{B}(\mathrm{Int}\,\gamma)| \geqslant 1$, then $\mathrm{dist}(\gamma, \partial V) = 0$ and $\varrho(\gamma) = q^{-\frac{1}{2d}\|\gamma\|}$. The bound (4.43) combined with the assumption a_{m} diam $\gamma \leqslant 2\, d\alpha$ now yields

$$K_{\mathrm{m}}(\gamma) \leqslant q^{(-\frac{1-\mu}{2d}+\nu)\,\|\gamma\|} e^{-\|\gamma\|} \leqslant q^{-\tau(\gamma)} e^{-\|\gamma\|}, \tag{4.45}$$

implying again $\bar{K}_{\mathrm{m}}(\gamma) = K_{\mathrm{m}}(\gamma)$ and thus verifying (a).

- *Proof of (c) and (d) for $v(W)=n$.* This part is an immediate consequence of the just proved claims (a) and (b).

[14] To see the latter bound, we use (3.4) and realize that the shortest disordered contour γ with $\mathrm{dist}(\gamma, \partial V) \geqslant \frac{3}{4}$ has the length $4d - 2$.

• *Proof of (e) for v(W)=n.* We call a contour γ *stable* if $a_{\mathrm{m}}(\beta)\,\mathrm{diam}\,\gamma \leqslant 2\,d\alpha$ and *unstable* if $a_{\mathrm{m}}(\beta)\,\mathrm{diam}\,\gamma > 2\,d\alpha$. Splitting the external w-contours of every set ∂ contributing to $Z_{\mathrm{m},W}(\beta,\lambda)$ in (3.11) into stable and unstable and summing over non-external and stable external w-contours of ∂, we get

$$Z_{\mathrm{m},W}(\beta,\lambda) = \sum_{\partial_{\mathrm{ext}} \sqsubset W}^{(\mathrm{m})} Z^{\mathrm{stable}}_{\mathrm{m,\,Ext}}(\beta,\lambda) \prod_{\gamma \in \partial_{\mathrm{ext}}} [\varrho(\gamma)\; Z_{\mathrm{m}^c,\,\mathrm{Int}\,\gamma}(\beta,\lambda)]. \tag{4.46}$$

Here the sum is over sets of m-labelled unstable short w-contours such that every $\gamma \in \partial_{\mathrm{ext}}$ is external and $V(\gamma) \subset W$. Moreover, we use Ext to denote $W \setminus \bigcup_{\gamma \in \partial_{\mathrm{ext}}} V(\gamma)$ and $Z^{\mathrm{stable}}_{\mathrm{m,\,Ext}}(\beta,\lambda)$ is obtained from $Z_{\mathrm{m,\,Ext}}(\beta,\lambda)$ by dropping all the unstable external short w-contours.

Since all external w-contours contributing to $Z^{\mathrm{stable}}_{\mathrm{m,\,Ext}}(\beta,\lambda)$ are stable, so is any other m-labeled w-contour contributing to its representation in the form (3.12). Thus, using Lemma 4.3 and the inductive assumption (c), we can control this partition function by a convergent cluster expansion, obtaining

$$Z^{\mathrm{stable}}_{\mathrm{m,\,Ext}}(\beta,\lambda) = e^{-F^{\mathrm{stable}}_{\mathrm{m}}(\mathrm{Ext}) + O(q^{-\nu})\,\|\partial_i\,\mathrm{Ext}\| + O(q^{-\nu})\,\|\partial^{(d-2)}\,\mathrm{Ext}\|}, \tag{4.47}$$

where $F^{\mathrm{stable}}_{\mathrm{m}}(\mathrm{Ext}) = f^{\mathrm{stable}}_{\mathrm{m}}\,|\mathbb{B}(\mathrm{Ext})|/d + s^{\mathrm{stable}}_{\mathrm{m}}\,|\partial\mathbb{B}(\mathrm{Ext})|$ with $f^{\mathrm{stable}}_{\mathrm{m}}$ and $s^{\mathrm{stable}}_{\mathrm{m}}$ corresponding to the contour model with the activities

$$K^{\mathrm{stable}}_{\mathrm{m}}(\gamma) = \begin{cases} \bar{K}_{\mathrm{m}}(\gamma) & \text{if } \gamma \text{ is a stable short } w\text{-contour,} \\ 0 & \text{otherwise.} \end{cases} \tag{4.48}$$

Since $2\,\|\gamma\| \geqslant \mathrm{diam}\,\gamma$ for any w-contour γ, we have a lower bound on the length of every unstable w-contour, namely, $\|\gamma\| > \zeta \equiv \frac{d\alpha}{a_{\mathrm{m}}(\beta)}$. Hence,

$$|f_{\mathrm{m}} - f^{\mathrm{stable}}_{\mathrm{m}}| \leqslant (\tilde{D}_1 q^{-\nu})^{\zeta} \leqslant q^{-\frac{\nu\zeta}{2}} \leqslant \frac{2}{d\alpha\,\nu\,\log q}\,a_{\mathrm{m}}(\beta) \leqslant \frac{\varepsilon}{2}\,a_{\mathrm{m}}(\beta) \tag{4.49}$$

and, similarly,

$$|s_{\mathrm{m}} - s^{\mathrm{stable}}_{\mathrm{m}}| \leqslant q^{-\frac{\nu\zeta}{2}} \leqslant \frac{\varepsilon}{2}\,a_{\mathrm{m}}(\beta) \tag{4.50}$$

for any $\varepsilon > 0$ once q is sufficiently large. Consequently,

$$Z^{\mathrm{stable}}_{\mathrm{m,\,Ext}}(\beta,\lambda) \leqslant e^{-F_{\mathrm{m}}(\mathrm{Ext}) + \frac{\varepsilon}{2} a_{\mathrm{m}}(|\mathbb{B}(\mathrm{Ext})|/d + |\partial\mathbb{B}(\mathrm{Ext})|) + O(q^{-\nu})\,\|\partial_i\,\mathrm{Ext}\| + O(q^{-\nu})\,\|\partial^{(d-2)}\,\mathrm{Ext}\|}. \tag{4.51}$$

Consider now a contour $\gamma \in \partial_{\text{ext}}$. Since $v(\text{Int}\,\gamma) < v(W) \leqslant n$ and $a_{\text{m}^c}(\beta) = 0$ by assumption, we can apply the proven claims (a) through (d) of the lemma to $Z_{\text{m}^c,\,\text{Int}\,\gamma}(\beta, \lambda)$. In view of (4.2) this allows us to get

$$Z_{\text{m}^c,\,\text{Int}\,\gamma}(\beta, \lambda) = \bar{Z}_{\text{m}^c,\,\text{Int}\,\gamma}(\beta, \lambda) = e^{-F_{\text{m}^c}(\text{Int}\,\gamma) + O(q^{-\nu})\,\|\gamma\|} \tag{4.52}$$

for all $\beta > 0$ such that $a_{\text{m}^c}(\beta) = 0$.

Combining (4.46), (4.51), and (4.52) with

$$|\mathbb{B}(W)| = |\mathbb{B}(\text{Ext})| + \sum_{\gamma \in \partial_{\text{ext}}} |\mathbb{B}(\text{Int}\,\gamma)|, \quad |\partial\mathbb{B}(W)| = |\partial\mathbb{B}(\text{Ext})| + \sum_{\gamma \in \partial_{\text{ext}}} |\partial\mathbb{B}(\text{Int}\,\gamma)|, \tag{4.53}$$

and $\|\partial_i\,\text{Ext}\,\| = \|\partial_i W\| + \sum_{\gamma \in \partial_{\text{ext}}} \|\gamma\|$, while $\|\partial^{(d-2)}\,\text{Ext}\,\| \leqslant \|\partial^{(d-2)} W\|$, it follows that

$$\begin{aligned} Z_{\text{m},W}(\beta, \lambda) &\leqslant e^{-F_{\text{m}^c}(W) + O(q^{-\nu})\,\|\partial_i W\| + O(q^{-\nu})\,\|\partial^{(d-2)} W\|} \sum_{\partial_{\text{ext}} \sqsubset W}^{(\text{m})} e^{-(1-\frac{\varepsilon}{2})\,a_{\text{m}}\,|\mathbb{B}(\text{Ext})|/d} \\ &\quad \times e^{(s_{\text{m}^c} - s_{\text{m}} + \frac{\varepsilon}{2} a_{\text{m}})\,|\partial\mathbb{B}(\text{Ext})|} \prod_{\gamma \in \partial_{\text{ext}}} [\varrho(\gamma)\; e^{O(q^{-\nu})\,\|\gamma\|}] \end{aligned} \tag{4.54}$$

$$\begin{aligned} &\leqslant e^{-F_{\text{m}^c}(W) + O(q^{-\nu})\,\|\partial_i W\| + O(q^{-\nu})\,\|\partial^{(d-2)} W\| + \max\{s_{\text{m}^c} - s_{\text{m}} + \varepsilon a_{\text{m}},\, 0\}\,|\partial\mathbb{B}(W)|} \\ &\quad \times \sum_{\partial_{\text{ext}} \sqsubset W}^{(\text{m})} e^{-\frac{\varepsilon}{2} a_{\text{m}}(|\mathbb{B}(\text{Ext})|/d + |\partial\mathbb{B}(\text{Ext})|)} \prod_{\gamma \in \partial_{\text{ext}}} [\varrho(\gamma)\; e^{\|\gamma\|}]. \end{aligned} \tag{4.55}$$

Next, we apply Lemma A.5, taking $\mathscr{K}_V(\gamma) = \varrho(\gamma)\, e^{\|\gamma\|}$ if γ is a w-contour contributing to the sum in (4.55), whereas $\mathscr{K}_V(\gamma) = 0$ otherwise. Since $\varrho(\gamma) \leqslant q^{-\frac{1}{6d}\|\gamma\|}$ (cf. the footnote on p. 94), we have $\mathscr{K}_V(\gamma) \leqslant (eq^{-2\nu})^{\|\gamma\|}$. Since $\|\gamma\| > \zeta$, where $\zeta > 0$ is the constant from (4.49) and (4.50), the quantities ϕ^* and σ^* introduced in Lemma A.5 satisfy the bounds $0 \leqslant -\phi^* \leqslant q^{-\frac{\nu\zeta}{2}}$ and $0 \leqslant -\sigma^* \leqslant q^{-\frac{\nu\zeta}{2}}$. As $q^{-\frac{\nu\zeta}{2}} \leqslant \frac{\varepsilon}{2} a_{\text{m}}$, Lemma A.5 allows us to bound the sum in (4.55), yielding

$$Z_{\text{m},W}(\beta, \lambda) \leqslant e^{-F_{\text{m}^c}(W) + O(q^{-\nu})\,\|\partial_i W\| + O(q^{-\nu})\,\|\partial^{(d-2)} W\| + \max\{s_{\text{m}^c} - s_{\text{m}} + \varepsilon a_{\text{m}},\, 0\}\,|\partial\mathbb{B}(W)|}. \tag{4.56}$$

Moreover, Lemma A.6(b) and (a) with $\kappa_2 = \nu$ yield

$$\sup_{\beta:\, a_{\text{m}}(\beta) > 0} (s_{\text{m}^c} - s_{\text{m}} + \varepsilon a_{\text{m}})(\beta) = \frac{\mu}{2d} \log q + O(q^{-\nu}) \tag{4.57}$$

for all $|\lambda - \frac{1}{2}| \leqslant \frac{\mu}{2}$ and $\varepsilon \leqslant \frac{\lambda^2}{d}$. Since $\varepsilon > 0$ can be chosen arbitrarily small (for q large enough) and, by assumption, we consider β such that $a_{\text{m}}(\beta) > 0$, we get (4.34). ∎

The next lemma states that the quantity $f(\beta)$ defined by (4.13) is actually the free energy of our model, and that the transition point β_t is identical to the unique point where f_o and f_d coincide. Here, the the transition point β_t is defined by the onset of a spontaneous magnetization, $\beta_t = \inf\{\beta: m(\beta) > 0\}$.

Lemma 4.5. Under the conditions of Lemma 4.4, the quantity $f(\beta)$ defined by (4.13) is the free energy of our model,

$$-\lim_{L\to\infty} \frac{1}{L^d} \log Z_L(\beta, \lambda) = \min\{f_\mathrm{o}(\beta), f_\mathrm{d}(\beta)\}. \tag{4.58}$$

The transition point β_t is the unique point where f_o and f_d coincide, and

$$f(\beta) = \begin{cases} f_\mathrm{o}(\beta) & \text{if} \quad \beta \geqslant \beta_t, \\ f_\mathrm{d}(\beta) & \text{if} \quad \beta \leqslant \beta_t. \end{cases} \tag{4.59}$$

Furthermore

$$\beta_t = \frac{\log q}{d} + O(q^{-\nu_0}), \tag{4.60}$$

and

$$\Delta e = \frac{1}{2} \frac{d(f_\mathrm{d} - f_\mathrm{o})}{d\beta}\bigg|_{\beta_t} = \frac{d}{2} + O(q^{-\nu_0}). \tag{4.61}$$

Remark 4.6. By (4.23) and (3.10),

$$\frac{d(f_\mathrm{d} - f_\mathrm{o})}{d\beta}\bigg|_{\beta} \geqslant d + O(q^{-\nu_0}) > 0 \qquad \text{if} \quad \beta \geqslant 1. \tag{4.62}$$

In view of this bound and (4.59), the functions $a_\mathrm{o}(\beta)$ and $a_\mathrm{d}(\beta)$ vanish for $\beta \geqslant \beta_t$ and $\beta \leqslant \beta_t$, respectively. Moreover, for $1 \leqslant \beta < \beta_t$, the function $a_\mathrm{o}(\beta) = (f_\mathrm{o} - f_\mathrm{d})(\beta) > 0$ is decreasing, whereas for $\beta > \beta_t$ the function $a_\mathrm{d}(\beta) = -(f_\mathrm{o} - f_\mathrm{d})(\beta) > 0$ is increasing.

Proof of Lemma 4.5. Given $\beta > 0$, let m be such that $a_\mathrm{m} = 0$. By Lemma 4.4 and the definition (4.12) of f_m we then have

$$-\lim_{L\to\infty} \frac{1}{L^d} \log Z_{\mathrm{m}, V(L)}(\beta, \lambda) = -\lim_{L\to\infty} \frac{1}{L^d} \log \bar{Z}_{\mathrm{m}, V(L)}(\beta, \lambda) = f_\mathrm{m} = f. \tag{4.63}$$

Next we use (4.25) in combination with Lemma 4.4(c) to estimate $Z_{\mathrm{m}, V(L)}(\beta, \lambda)$ and the bound (4.34) of Lemma 4.4 to estimate $Z_{\mathrm{m}^c, V(L)}(\beta, \lambda)$. We conclude that

$$\frac{Z_{\mathrm{m}^c, V(L)}(\beta, \lambda)}{Z_{\mathrm{m}, V(L)}(\beta, \lambda)} \leqslant e^{\frac{\mu}{2d} \log q \, \|\partial_e V\| + O(q^{-\nu}) \, \|\partial V\|} = e^{(\mu \log q + O(q^{-\nu})) \, L^{d-1}}, \tag{4.64}$$

where we have used that $\|\partial V\| = \|\partial_e V\| = |\partial \mathbb{B}| = 2\, dL^{d-1}$.

In order to bound the ratio

$$\delta_{\mathrm{m}}(\beta) = \frac{Z_{\mathrm{big}, V}(\beta, \lambda)}{Z_{\mathrm{m}, V(L)}(\beta, \lambda)}, \tag{4.65}$$

let us consider a set of contours ∂_l contributing to (3.16). Using the shorthand $W_{\mathrm{o}} = W_{\mathrm{o}}(\partial_l)$ and $W_{\mathrm{d}} = W_{\mathrm{d}}(\partial_l)$, and applying the bounds (4.27) and (4.34), we get

$$\frac{Z_{\mathrm{o}, W_{\mathrm{o}}}(\beta, \lambda) \, Z_{\mathrm{d}, W_{\mathrm{d}}}(\beta, \lambda)}{Z_{\mathrm{m}, V(L)}(\beta, \lambda)} \leqslant e^{\frac{\mu}{2d} \log q \, \|\partial_e W_{\mathrm{m}^c}\| + O(q^{-\nu}) \, \|\partial W_{\mathrm{m}^c}\| + O(q^{-\nu}) \, \|\partial_i W_{\mathrm{m}}\|}. \tag{4.66}$$

Observing that $\|\partial_i W_{\mathrm{m}}\| = \|\partial_i W_{\mathrm{m}^c}\| = \sum_{\gamma \in \partial_l} \|\gamma\|$, while $\|\partial_e W_{\mathrm{m}^c}\| \leqslant \|\partial_e V\| = 2\, dL^{d-1}$, we obtain the bound

$$\frac{Z_{\mathrm{o}, W_{\mathrm{o}}}(\beta, \lambda) \, Z_{\mathrm{d}, W_{\mathrm{d}}}(\beta, \lambda)}{Z_{\mathrm{m}, V(L)}(\beta, \lambda)} \leqslant e^{(\mu \log q + O(q^{-\nu})) \, L^{d-1}} \prod_{\gamma \in \partial_l} e^{O(q^{-\nu}) \, \|\gamma\|}. \tag{4.67}$$

Observing that $2\,\|\gamma\| \geqslant \operatorname{diam} \gamma$ holds for every contour γ, any long w-contour γ satisfies $\|\gamma\| \geqslant \ell_0 \equiv \frac{1}{2}\,\omega(L)$. Then (3.4) gives $\varrho(\gamma) \leqslant q^{-c\,\|\gamma\|}$ with $c = \frac{1}{2d} - \frac{2}{\omega(L)}$. Combined with (3.16) and (4.67), we get that the ratio (4.65) can be bounded by

$$\delta_{\mathrm{m}}(\beta) \leqslant e^{(\mu \log q + O(q^{-\nu})) \, L^{d-1}} \sum_{\partial_l} \prod_{\gamma \in \partial_l} q^{-\frac{1}{4d} \|\gamma\|} \tag{4.68}$$

for all q and L large enough. Now,

$$\sum_{\partial_l} \prod_{\gamma \in \partial_l} q^{-\frac{1}{4d} \|\gamma\|} \leqslant \sum_{n=1}^{\infty} \sum_{\partial_l :\, |\partial_l| = n} \prod_{\gamma \in \partial_l} q^{-\frac{1}{4d} \|\gamma\|} \leqslant \sum_{n=1}^{\infty} \frac{1}{n!} \Big(\sum_{\gamma} q^{-\frac{1}{4d} \|\gamma\|} \Big)^n, \tag{4.69}$$

where the last sum is over all long w-contours γ in $V(L)$. Bounding the number of w-contours in $V(L)$ whose length is ℓ by $C^{\ell} L^d$, where $C > 0$ is a constant depending on d, it follows that

$$\begin{aligned}\sum_\gamma q^{-\frac{1}{4d}\|\gamma\|} &\leqslant \sum_{\ell=\ell_0}^{\infty} \sum_{\gamma:\,\|\gamma\|=\ell} q^{-\frac{1}{4d}\ell} \leqslant \sum_{\ell=\ell_0}^{\infty} C^\ell L^d q^{-\frac{1}{4d}\ell} \leqslant L^d \sum_{\ell=\ell_0}^{\infty} q^{-\frac{1}{5d}\ell}\\ &\leqslant q^{-\frac{1}{6d}\ell_0} = q^{-\frac{1}{12d}\omega(L)}\end{aligned} \tag{4.70}$$

whenever q and L are taken large enough. As a result,

$$\delta_m(\beta) \leqslant e^{(\mu \log q + O(q^{-\nu}))\, L^{d-1}} (e^{q^{-\frac{1}{12d}\omega(L)}} - 1) \leqslant e^{(\mu \log q + O(q^{-\nu}))\, L^{d-1}} q^{-\frac{1}{14d}\omega(L)} \tag{4.71}$$

as soon as q and L are sufficiently large. Combining (4.63) and (4.64) with (4.65) and (4.71), we get (4.58).

In order to prove the remaining statements, we first use the well know fact that for large q, the transition point β_t can be equivalently defined as the unique point where the derivative of the free energy jumps, see refs. 17 and 25. By (4.23) and Lemma A.6, there is a unique point $\hat{\beta}$ where f_{o} and f_{d} coincide. Combined with (4.62), we conclude that $f(\beta) = f_{\mathrm{d}}(\beta)$ if $\beta \leqslant \hat{\beta}$, and $f(\beta) = f_{\mathrm{o}}(\beta)$ if $\beta \geqslant \hat{\beta}$, implying in particular that at $\hat{\beta}$ the derivative of the free energy is discontinuous. This identifies β_t, and proves at the same time (4.59) and (4.60), see Lemma A.6(a).

To prove (4.61), we invoke (3.10) and (4.23), together with the observation that

$$\Delta e := \frac{1}{2}\left(\frac{df}{d\beta}\bigg|_{\beta_t - 0} - \frac{df}{d\beta}\bigg|_{\beta_t + 0}\right) = \frac{1}{2}\frac{d(f_{\mathrm{d}} - f_{\mathrm{o}})}{d\beta}\bigg|_{\beta_t}. \quad \blacksquare \tag{4.72}$$

5. PROOF OF THEOREM 2.1

We now prove Theorem 2.1, restricting our attention to $\beta \geqslant 1$, see Remark 2.4(iii). We consider strong boundary conditions, recall the definition (3.26) of the corresponding partition functions $\tilde{Z}_{\mathrm{m},W}(\beta, \lambda)$ in terms of s-contours, and their reformulation (3.28) in terms of the weights $\tilde{K}_{\mathrm{m}}(\gamma)$. Throughout this section, f_{o} and f_{d} are the meta-stable free energies defined in (4.12), ν_0 is the constant defined in (4.15), $\tau(\gamma)$ is as in (4.16), $D_0 < \infty$ is the constant from Lemma 4.3, and a_{m}, $\mathrm{m} = \mathrm{o}, \mathrm{d}$, is defined in Lemma 4.4(a).

Lemma 5.1. Let $d \geqslant 2$, $k_0 = 0, 1, \ldots$. If q and L are sufficiently large, $\beta \geqslant 1$, $\lambda \geqslant 0$, $0 \leqslant k \leqslant k_0$, and $\mathrm{m} = \mathrm{o}, \mathrm{d}$, we have:

(a) For any m-labeled s-contour γ with $\operatorname{dist}(\gamma, \partial V) \geqslant \frac{3}{4}$, the activity $\tilde{K}_{\mathrm{m}}(\gamma)$ does not depend on λ. Moreover, if $a_{\mathrm{m}}(\beta) \operatorname{diam} \gamma \leqslant 2\, d\alpha_0$, then $\tilde{K}_{\mathrm{m}}(\gamma)$ is a C^{k_0} function of β, and $|\frac{\partial^k}{\partial \beta^k} \tilde{K}_{\mathrm{m}}(\gamma)| \leqslant (D_0\, |\mathbb{B}(\operatorname{Int}(\gamma))|)^k\, q^{-\tau(\gamma)}$.

(b) For any volume W of the form (3.7) with $\operatorname{dist}(W, \partial V) \geqslant \frac{3}{4}$, the partition function $\tilde{Z}_{\mathrm{m},W}(\beta, \lambda)$ is independent of λ. In addition, if $a_{\mathrm{m}}(\beta) \operatorname{diam} W \leqslant 2\, d\alpha_0$, then

$$\frac{\partial^k}{\partial \beta^k} \log \tilde{Z}_{\mathrm{m},W}(\beta, \lambda) = -\frac{1}{d} \frac{\partial^k f_{\mathrm{m}}}{\partial \beta^k} |\mathbb{B}(W)| + O(q^{-\nu_0})\, \|\partial W\|. \tag{5.1}$$

(c) The same bounds as in (a) hold also for activities $\tilde{K}^{(x)}_{\mathrm{m}}(\gamma_x)$.

Proof. Let γ and γ_x be m-labeled s-contours with $\operatorname{dist}(\gamma, \partial V) \geqslant \frac{3}{4}$ and $\operatorname{dist}(\gamma_x, \partial V) \geqslant \frac{3}{4}$, and let W be the volume of the form (3.7) with $\operatorname{dist}(W, \partial V) \geqslant \frac{3}{4}$. Then, in view of Remark 3.2, the activities $\tilde{K}_{\mathrm{m}}(\gamma)$ and $\tilde{K}^{(x)}_{\mathrm{m}}(\gamma_x)$, and the partition function $\tilde{Z}_{\mathrm{m},W}(\beta, \lambda)$ are independent of λ. Choosing $\omega(L) = L+1$, we have $\tilde{K}_{\mathrm{m}}(\gamma) = K_{\mathrm{m}}(\gamma)$, $\tilde{K}^{(x)}_{\mathrm{m}}(\gamma_x) = K^{(x)}_{\mathrm{m}}(\gamma_x)$, and $\tilde{Z}_{\mathrm{m},W}(\beta, \lambda) = Z_{\mathrm{m},W}(\beta, \lambda)$. Taking now into account Lemmas 4.3 and 4.4 combined with (4.25), the remaining claims readily follow. ∎

Lemma 5.2. Let $d \geqslant 2$, assume that q and L are sufficiently large, $\beta \geqslant 1$, and $\lambda \geqslant \frac{1}{2\beta_t}$. Let γ_0 be a s-contour, $W = \operatorname{Int} \gamma_0$, and let

$$\tilde{\delta}_{\mathrm{o},W}(\beta) = \frac{\tilde{Z}_{\mathrm{d},W}(\beta, \lambda)}{\tilde{Z}_{\mathrm{o},W}(\beta, \lambda)} \qquad \text{and} \qquad \tilde{\delta}_{\mathrm{d},W}(\beta) = \frac{\tilde{Z}_{\mathrm{o},W}(\beta, \lambda)}{\tilde{Z}_{\mathrm{d},W}(\beta, \lambda)}. \tag{5.2}$$

Then the function $\tilde{\delta}_{\mathrm{o},W}(\cdot)$ is decreasing on the interval $[\beta_t, \infty)$, while the function $\tilde{\delta}_{\mathrm{d},W}(\cdot)$ is increasing on the interval $[1, \beta_t]$.

Proof. We will explicitly only prove the monotonicity of $\tilde{\delta}_{\mathrm{o},W}(\cdot)$. The monotonicity of $\tilde{\delta}_{\mathrm{d},W}(\cdot)$ is proven analogously and will be left to the reader.

We first rewrite the partition function $\tilde{Z}_{\mathrm{d},W}(\beta, \lambda)$. Namely, in its expression in the form (3.26), we resum over all sets ∂ whose external contours are fixed, to get

$$\tilde{Z}_{\mathrm{d},W}(\beta, \lambda) = \sum_{\partial_{\mathrm{ext}} \sqsubset W}^{(\mathrm{d})} e^{-G^{\mathrm{d}}_{\mathrm{d}}(\mathbb{B}(\mathrm{Ext}))} \tilde{Z}_{\mathrm{o},\mathrm{Int}}(\beta, \lambda) \prod_{\gamma \in \partial_{\mathrm{ext}}} q^{\frac{1}{2d}|\partial \mathbb{B}(\operatorname{Int} \gamma)|} \varrho(\gamma). \tag{5.3}$$

Here, the summation is over sets ∂_{ext} of mutually external, short, d-labelled s-contours with $V(\gamma) \subset W$, $\mathrm{Int} = \bigcup_{\gamma \in \partial_{\mathrm{ext}}} \operatorname{Int} \gamma$, and $\mathrm{Ext} = W \setminus \bigcup_{\gamma \in \partial_{\mathrm{ext}}} V(\gamma)$. In this way we get

$$\frac{\tilde{Z}_{\mathrm{d},W}(\beta, \lambda)}{\tilde{Z}_{\mathrm{o},W}(\beta, \lambda)} = \sum_{\partial_{\mathrm{ext}} \sqsubset W}^{(\mathrm{d})} e^{\xi(\beta)} \prod_{\gamma \in \partial_{\mathrm{ext}}} \varrho(\gamma), \tag{5.4}$$

where

$$\xi(\beta) = -G_{\mathrm{d}}^{\mathrm{d}}(\overline{\mathbb{B}}(\mathrm{Ext})) + \log \frac{\tilde{Z}_{\mathrm{o,\,Int}}(\beta, \lambda)}{\tilde{Z}_{\mathrm{o},W}(\beta, \lambda)}. \tag{5.5}$$

Notice that ξ is the only term in (5.4) depending on β. Notice also that, since the distance of any pair of non-overlapping (s- or w-) contours must be at least $\frac{1}{2}$, any contour γ contributing to $\tilde{Z}_{\mathrm{o,\,Int}}(\beta, \lambda)$ or $\tilde{Z}_{\mathrm{o},W}(\beta, \lambda)$ has $\mathrm{dist}(\gamma, \partial V) \geqslant \frac{3}{4}$. By Lemma 5.1(a), we may use the cluster expansion of the form (4.3) to analyze $\log \tilde{Z}_{\mathrm{o,\,Int}}(\beta, \lambda) - \log \tilde{Z}_{\mathrm{o},W}(\beta, \lambda)$. Defining

$$\tilde{F}_{\mathrm{m}}(\overline{\mathbb{B}}(W)) = \frac{1}{d} f_{\mathrm{m}}\, |\mathbb{B}(W)| + h_{\mathrm{m}}\, |\partial \mathbb{B}(W)|, \tag{5.6}$$

we get

$$\frac{d\xi}{d\beta} = \frac{d}{d\beta}\, [\tilde{F}_{\mathrm{o}}(\overline{\mathbb{B}}(\mathrm{Ext})) - G_{\mathrm{d}}^{\mathrm{d}}(\overline{\mathbb{B}}(\mathrm{Ext}))] + \|\partial(\mathrm{Ext})\|\, O(q^{-\nu}). \tag{5.7}$$

The first term can be explicitly estimated,

$$\frac{d}{d\beta}\, (\tilde{F}_{\mathrm{o}}(\overline{\mathbb{B}}(\mathrm{Ext})) - G_{\mathrm{d}}^{\mathrm{d}}(\overline{\mathbb{B}}(\mathrm{Ext}))) < (-\lambda + O(q^{-\nu}))\, |\overline{\mathbb{B}}(\mathrm{Ext})| \tag{5.8}$$

due to (4.23) and (3.24). Hence,

$$\frac{d\xi}{d\beta} < (-\lambda + O(q^{-\nu}))\, |\overline{\mathbb{B}}(\mathrm{Ext})| + \|\partial(\mathrm{Ext})\|\, O(q^{-\nu}). \tag{5.9}$$

Since, obviously, $\|\partial(\mathrm{Ext})\| \leqslant O(|\overline{\mathbb{B}}(\mathrm{Ext})|)$ with $|\overline{\mathbb{B}}(\mathrm{Ext})| \geqslant 1$, while $\frac{1}{2\beta_t} \geqslant \frac{d}{4 \log q}$, we get $\frac{d\xi}{d\beta} \leqslant -\frac{\lambda}{2} < 0$ for all q large and $\lambda \geqslant \frac{1}{2\beta_t}$. ∎

Lemma 5.3. Let $d \geqslant 2$, $0 < \mu \leqslant 1$, $k_0 = 0, 1, \ldots$, and $\tilde{\nu} = \min(\nu_0, \frac{\mu}{4d})$. There exist a finite constant $\tilde{D}_0 < \infty$ such that, for all q and L sufficiently large and $0 \leqslant k \leqslant k_0$, we have:

(a) If $1 \leqslant \beta \leqslant \beta_t$ and $0 \leqslant \lambda \leqslant \frac{1}{2}(1 - \mu)$, then $\tilde{K}_{\mathrm{d}}(\gamma)$ is a C^{k_0} function of β for any disordered s-contour γ, and $|\frac{\partial^k}{\partial \beta^k} \tilde{K}_{\mathrm{d}}(\gamma)| \leqslant \tilde{D}_0 q^{-\tilde{\nu}\, \|\gamma\|}$.

(b) If $\beta \geqslant \beta_t$ and $\lambda \geqslant \frac{1}{2}\,(1 + \mu)$, then $\tilde{K}_{\mathrm{d}}(\gamma)$ is a C^{k_0} function of β for any ordered s-contour γ, and $|\frac{\partial^k}{\partial \beta^k} \tilde{K}_{\mathrm{o}}(\gamma)| \leqslant \tilde{D}_0 q^{-\tilde{\nu}\, \|\gamma\|}$.

(c) The same bounds hold for the activities $\tilde{K}_{\mathrm{d}}^{(x)}(\gamma_x)$ and $\tilde{K}_{\mathrm{o}}^{(x)}(\gamma_x)$.

Proof. According to Lemma 5.1(b) and (c), the claims hold for any s-contour γ (respectively γ_x) for which $\operatorname{dist}(\gamma, \partial V) \geqslant \frac{3}{4}$. Hence, let us consider only the remaining contours, i.e., those with distance $\frac{1}{4}$ from the boundary.

To bound the derivatives, we evoke Lemmas 3.3 and A.3 to get

$$\left|\frac{\partial^k}{\partial \beta^k} \tilde{K}_{\mathrm{m}}(\gamma)\right| \leqslant \tilde{D}_0((1+\lambda)\, |\partial \mathbb{B}(\operatorname{Int}\gamma)| + |\mathbb{B}(\operatorname{Int}\gamma)|)^{k_0}\, \tilde{K}_{\mathrm{m}}(\gamma)$$
$$\leqslant \tilde{D}_0 e^{\lambda\, |\partial \mathbb{B}(\operatorname{Int}\gamma)|} e^{dk_0\, \|\gamma\|}\, \tilde{K}_{\mathrm{m}}(\gamma) \tag{5.10}$$

for some constant $\tilde{D}_0 = \tilde{D}_0(k_0) < \infty$.

Consider now the case $k = 0$ and observe that, since the distance of any pair of non-overlapping (s- or w-) contours must be at least $\frac{1}{2}$, any contour γ contributing to $\tilde{Z}_{\mathrm{m},\operatorname{Int}\gamma}(\beta, \lambda)$ has $\operatorname{dist}(\gamma, \partial V) \geqslant \frac{3}{4}$. According to Lemma 5.1(a), the corresponding activity $\tilde{K}_{\mathrm{m}}(\gamma)$ is independent of λ. Taking now into account the explicit expression (3.28), we observe that neither $\tilde{Z}_{\mathrm{d},\operatorname{Int}\gamma}(\beta, \lambda)$ nor the ratio $\frac{\tilde{Z}_{\mathrm{o},\operatorname{Int}\gamma}(\beta, \lambda)}{(e^{\lambda\beta}-1)^{\|\partial \mathbb{B}(\operatorname{Int}\gamma)\|}}$ is depending on λ. Using temporarily $\tilde{K}_{\mathrm{m}}^{(\beta,\lambda)}(\gamma)$ to denote explicitly the dependence of the weights $\tilde{K}_{\mathrm{m}}(\gamma)$ on β and λ, the above observation yields

$$e^{\lambda\, |\partial \mathbb{B}(\operatorname{Int}\gamma)|} \tilde{K}_{\mathrm{m}}^{(\beta,\lambda)}(\gamma) \leqslant \tilde{K}_{\mathrm{m}}^{(\beta,\lambda_{\mathrm{m}})}(\gamma), \tag{5.11}$$

where $\lambda_{\mathrm{d}} = \frac{1}{2}(1-\mu) + \frac{1}{2\beta_t}$ and $\lambda_{\mathrm{o}} = \frac{1}{2}(1+\mu) - \frac{1}{2\beta_t}$. Here we used the fact that for the case $\mathrm{m} = \mathrm{d}$ we assume that $\beta \leqslant \beta_t$ and $\lambda \leqslant \frac{1}{2}(1-\mu)$, while for $\mathrm{m} = \mathrm{o}$ we assume that $\beta \geqslant \beta_t$ and $\lambda \geqslant \frac{1}{2}(1+\mu)$. Further, let us notice that the monotonicity in β according to Lemma 6.3 is true, with the same proof, also for the ratio $\frac{\tilde{Z}_{\mathrm{m}^c, W}(\beta, \lambda_{\mathrm{m}})}{\tilde{Z}_{\mathrm{m}, W}(\beta, \lambda_{\mathrm{m}})}$. Hence,

$$\frac{\tilde{Z}_{\mathrm{m}^c,\operatorname{Int}\gamma}(\beta, \lambda_{\mathrm{m}})}{\tilde{Z}_{\mathrm{m},\operatorname{Int}\gamma}(\beta, \lambda_{\mathrm{m}})} \leqslant \frac{\tilde{Z}_{\mathrm{m}^c,\operatorname{Int}\gamma}(\beta_t, \lambda_{\mathrm{m}})}{\tilde{Z}_{\mathrm{m},\operatorname{Int}\gamma}(\beta_t, \lambda_{\mathrm{m}})} \tag{5.12}$$

and, combining it with (5.11), we get

$$e^{\lambda\, |\partial \mathbb{B}(\operatorname{Int}\gamma)|} \tilde{K}_{\mathrm{m}}^{(\beta,\lambda)}(\gamma) \leqslant \varrho(\gamma)\, q^{\frac{1}{2d}|\partial \mathbb{B}(\operatorname{Int}\gamma)|} \frac{\tilde{Z}_{\mathrm{m}^c,\operatorname{Int}\gamma}(\beta_t, \lambda_{\mathrm{m}})}{\tilde{Z}_{\mathrm{m},\operatorname{Int}\gamma}(\beta_t, \lambda_{\mathrm{m}})}. \tag{5.13}$$

Applying now, for both phases, λ-independent cluster expansions according to Lemma 5.1(b) and taking explicitly into account the boundary terms $h_{\mathrm{m}}^{\mathrm{m}}$ and $h_{\mathrm{m}^c}^{\mathrm{m}^c}$ from (3.28), we get

$$\tilde{K}_{\mathrm{m}}(\gamma) \leqslant e^{-\lambda\, |\partial \mathbb{B}(\operatorname{Int}\gamma)|} \varrho(\gamma)\, q^{\frac{1}{2d}\|\gamma\|} e^{(h_{\mathrm{m}}^{\mathrm{m}} - h_{\mathrm{m}^c}^{\mathrm{m}^c})(\beta_t, \lambda_{\mathrm{m}})\, \|\partial \mathbb{B}(\operatorname{Int}\gamma)\| + O(q^{-\nu_0})\, \|\partial \operatorname{Int}\gamma\|}. \tag{5.14}$$

Using the fact that $\varrho(\gamma)=q^{-\frac{1}{2d}\|\gamma\|}$ if $\operatorname{dist}(\gamma, \partial V)=1/4$, see (3.4), and applying Lemma A.4, we get

$$\tilde{K}_{\mathrm{d}}(\gamma) \leqslant e^{-\lambda\,|\partial\mathbb{B}(\operatorname{Int}\gamma)|}\left(\frac{e^{\beta_t\lambda_{\mathrm{d}}}-1}{q^{\frac{1}{2d}}}\right)^{\|\gamma\|} e^{O(q^{-\nu_0})\,\|\gamma\|} \tag{5.15}$$

and

$$\tilde{K}_{\mathrm{o}}(\gamma) \leqslant e^{-\lambda\,|\partial\mathbb{B}(\operatorname{Int}\gamma)|}\left(\frac{q^{\frac{1}{2d}}}{e^{\beta_t\lambda_{\mathrm{o}}}-1}\right)^{\|\gamma\|} e^{O(q^{-\nu_0})\,\|\gamma\|}. \tag{5.16}$$

Using further the explicit bound on β_t from (4.60), we obtain in both cases

$$\tilde{K}_{\mathrm{m}}(\gamma) \leqslant e^{-\lambda\,|\partial\mathbb{B}(\operatorname{Int}\gamma)|} q^{-(\frac{\mu}{2d}+O(q^{-\nu_0})+O(\frac{1}{\log q}))\,\|\gamma\|} \leqslant e^{-\lambda\,|\partial\mathbb{B}(\operatorname{Int}\gamma)|} q^{-\frac{\mu}{3d}\|\gamma\|}. \tag{5.17}$$

Thus, we got the claims (a) and (b) for $k=0$ and, applying (5.10), also for $k=1,\ldots,k_0$.

To prove (c), we note that as before,

$$\left|\frac{\partial^k}{\partial\beta^k}\tilde{K}_{\mathrm{m}}^{(x)}(\gamma_x)\right| \leqslant \tilde{D}_0 e^{\lambda\,|\partial\mathbb{B}(\operatorname{Int}\gamma_x)|} e^{dk_0\,\|\gamma_x\|}\,\tilde{K}_{\mathrm{m}}^{(x)}(\gamma_x). \tag{5.18}$$

Combined with the fact that $\tilde{K}_{\mathrm{m}}^{(x)}(\gamma_x) \leqslant \tilde{K}_{\mathrm{m}}(\gamma_x)$, this completes the proof. ∎

Proof of Theorem 2.1. First, let us prove the claim (a). By virtue of (3.28) and Lemma 5.3(a), the function $\log\tilde{Z}_{\mathrm{d},V}(\beta,\lambda)$ and its derivatives can be analyzed by convergent cluster expansions for q, L large and any $0\leqslant\lambda<\frac{1}{2}(1-\mu)$ whenever $1\leqslant\beta\leqslant\beta_t$. Taking an arbitrary $k\leqslant k_0$, we have

$$\frac{\partial^k}{\partial\beta^k}\log\tilde{Z}_{\mathrm{d},V}(\beta,\lambda) = -\frac{d^k\tilde{F}_{\mathrm{d}}(\overline{\mathbb{B}})}{d\beta^k}+O(q^{-\tilde{\nu}}L^{d-1}), \tag{5.19}$$

where $\tilde{F}_{\mathrm{d}}$ is defined in (5.6). Combining this with (3.27), (2.8), and (3.10), we get

$$\frac{\partial^{k-1}}{\partial\beta^{k-1}}E_L(\beta,\lambda)=\frac{\partial f_{\mathrm{d}}}{\partial\beta}L^d+L^{d-1}O(q^{-\tilde{\nu}}),$$

which, together with (4.59), proves (2.14).

To prove (2.13), we use the representation (3.30) of $M_L(\beta,\lambda)$ in terms of the ratios $\tilde{Z}_{V,\mathrm{d}}^{(x)}(\beta,\lambda)/\tilde{Z}_{V,\mathrm{d}}(\beta,\lambda)$. Next, we use the contour representations (3.28) and (3.31), together with the fact that for $\beta\leqslant\beta_t$, the phase d is stable and thus $|\frac{\partial^k}{\partial\beta^k}\tilde{K}_{\rm d}(\gamma)| \leqslant \tilde{D}_0 q^{-\tilde{\nu}\|\gamma\|}$ and $|\frac{\partial^k}{\partial\beta^k}\tilde{K}_{\rm d}^{(x)}(\gamma_x)| \leqslant \tilde{D}_0 q^{-\tilde{\nu}\|\gamma_x\|}$, see Lemma 5.3. This allows us to analyze the terms in (3.30) by a convergent cluster expansion, yielding, in particular, the existence and λ-independence of the limit

$$\tilde{m}_{\rm d}(\beta) = \lim_{L\to\infty} \frac{1}{L^d} M_L(\beta, \lambda), \tag{5.20}$$

as well as the following bounds on finite-size corrections:

$$M_L(\beta, \lambda) = \tilde{m}_{\rm d}(\beta)\, L^d + O(q^{-\nu})\, L^{d-1}. \tag{5.21}$$

Combining the observation that $M_L(\beta, \lambda) = 0$ if $\lambda = 0$ with the λ-independence of $\tilde{m}_{\rm d}(\beta)$, we conclude that $\tilde{m}_{\rm d}(\beta) = 0$ whenever $\beta \leqslant \beta_t$. The bound (5.21) is then identical with the claim (2.13).

The proof of the claim (b) is similar, noticing that for the derivatives of $h_{\rm o}$ one can use the bounds from Lemma A.1. In particular, $\frac{\partial h_{\rm o}}{\partial\beta} \leqslant 1+\lambda$. We also note that for $\beta \geqslant \beta_t$, the limit

$$\tilde{m}_{\rm o}(\beta) = \lim_{L\to\infty} \frac{1}{L^d} M_L(\beta, \lambda) \tag{5.22}$$

is again independent of λ, and can be identified with the value at $\lambda = 1$, which equals $m(\beta)$ as defined in (2.5). ∎

Remark 5.4. Notice that, for $\beta \leqslant \beta_t$, the convergent cluster expansions for $m_{\rm d}(\beta)$ (cf. (4.29)) and for $\tilde{m}_{\rm d}(\beta)$ (cf. (5.20)) are identical. Indeed, taking into account Remark 3.2 and Lemma 4.4(b), the corresponding cluster expansion terms have contributions only from contours from $\mathscr{L}_\infty$ for which the corresponding weights do not depend on λ and one has $\tilde{K}_{\rm d}(\gamma) = K_{\rm d}(\gamma) = \bar{K}_{\rm d}(\gamma)$ and $\tilde{K}_{\rm d}^{(x)}(\gamma_x) = K_{\rm d}^{(x)}(\gamma_x) = \bar{K}_{\rm d}^{(x)}(\gamma_x)$. Hence, $m_{\rm d}(\beta) = \tilde{m}_{\rm d}(\beta) = 0$.

Similarly, for $\beta \geqslant \beta_t$, one can identify $m_{\rm o}(\beta) = \tilde{m}_{\rm o}(\beta) = m(\beta)$.

6. FINITE SIZE EFFECTS FOR WEAK BOUNDARY CONDITIONS

In this section we prove Theorem 2.3. We start with a more accurate bound on the derivatives of $f_{\rm m}$ and $s_{\rm m}$ near $\beta = \beta_t$.

Lemma 6.1. Let $k_0 \in \mathbb{N}$, and let $0 \leqslant \mu < 1$. If q is sufficiently large, then

$$\frac{d^k f_{\rm m}}{d\beta^k} = O(q^{-\nu_0}) \qquad \text{and} \qquad \frac{d^k s_{\rm m}}{d\beta^k} = O(q^{-\nu}) \tag{6.1}$$

provided $\beta \geqslant \beta_t/2$, $|\lambda - \frac{1}{2}| \leqslant \frac{\mu}{2}$ and $2 \leqslant k \leqslant k_0$. For $m = \mathrm{d}$, these bounds remain true for all $\beta \geqslant 1$.

Proof. This follows immediately from (4.23), Lemma A.1, (4.60), and the definitions (4.15) of ν and ν_0. ∎

The next lemma is the first step in the proof of (2.17).

Lemma 6.2. Let $d \geqslant 2$, $0 \leqslant \mu < 1$ and let ν and α be defined by (4.15) and (4.33), respectively. Let $\omega\colon \mathbb{N} \to [0, \infty)$ be a function satisfying the conditions

$$\limsup_{L \to \infty} \frac{\omega(L)}{L} \leqslant \frac{\nu}{6} \qquad \text{and} \qquad \liminf_{L \to \infty} \frac{\omega(L)}{\log L} = \infty. \tag{6.2}$$

For q and L sufficiently large and $|\lambda - \frac{1}{2}| \leqslant \frac{\mu}{2}$, we have:

(a) The equation $a_{\mathrm{m}}(\beta) = \frac{\alpha}{\omega(L)}$, $\mathrm{m} = \mathrm{o}, \mathrm{d}$, has a single solution $\beta_{\mathrm{m}}(L)$, and $a_{\mathrm{o}}(\beta) \leqslant \frac{\alpha}{\omega(L)}$ iff $\beta \geqslant \beta_{\mathrm{o}}(L)$, while $a_{\mathrm{d}}(\beta) \leqslant \frac{\alpha}{\omega(L)}$ iff $\beta \leqslant \beta_{\mathrm{d}}(L)$. Furthermore, we have $\beta_{\mathrm{m}}(L) = \beta_t(1 + O((\omega(L))^{-1}))$, and, more precisely,

$$\begin{aligned} \beta_{\mathrm{o}}(L) &= \beta_t - \frac{\alpha}{2\,\Delta e}\,\frac{1}{\omega(L)} + \left(\frac{\alpha}{\omega(L)}\right)^2 O(q^{-\nu}), \\ \beta_{\mathrm{d}}(L) &= \beta_t + \frac{\alpha}{2\,\Delta e}\,\frac{1}{\omega(L)} + \left(\frac{\alpha}{\omega(L)}\right)^2 O(q^{-\nu}). \end{aligned} \tag{6.3}$$

(b) There is a unique point $\beta_{=}^{(\lambda)}(L) \in (\beta_{\mathrm{o}}(L), \beta_{\mathrm{d}}(L))$ at which $Z_{\mathrm{o},V}(\beta, \lambda)$ and $Z_{\mathrm{d},V}(\beta, \lambda)$ coincide, and $\beta_{=}^{(\lambda)}(L) = \beta_t(1 + O(L^{-1}))$. More precisely,

$$\beta_{=}^{(\lambda)}(L) = \beta_t + \frac{\vartheta(\lambda, q, L)}{L} + \left(\frac{\vartheta(\lambda, q, L)}{L}\right)^2 O(q^{-\nu}), \tag{6.4}$$

where $\vartheta(\lambda, q, L)$ is a function that obeys the bounds

$$\vartheta(\lambda, q, L) = \frac{d\beta_t}{\Delta e}\left(\frac{1}{2} - \lambda + O\left(\frac{q^{-\nu}}{\log q}\right)\right)(1 + O(L^{-1})) \tag{6.5}$$

and

$$\vartheta(\lambda, q, L) = \frac{d(s_{\mathrm{d}} - s_{\mathrm{o}})(\beta_t)}{\Delta e} + O(\beta_t L^{-1}). \tag{6.6}$$

Proof. (a) Let us consider $\mathrm{m}=\mathrm{o}$, for instance. For $0<\beta\leqslant 1$, we have

$$a_{\mathrm{o}}(\beta)-\frac{\alpha}{\omega(L)}\geqslant \log q-d\log(e-1)+O(q^{-\nu})-\frac{\alpha}{\omega(L)}>0$$

whenever q and L are large enough; we used (4.23) with $k=0$ and the fact that $\omega(L)\to\infty$ by the second condition in (6.2). Since $a_{\mathrm{o}}(\beta)$ is continuous and decreasing on $[1,\beta_t)$ once q is large, while $a_{\mathrm{o}}(\beta)=0$ for $\beta\geqslant\beta_t$, there is a single solution $\beta_{\mathrm{o}}(L)\in(1,\beta_t)$. The Lagrange mean-value theorem then yields

$$\frac{\alpha}{\omega(L)}=a_{\mathrm{o}}(\beta_{\mathrm{o}}(L))=(f_{\mathrm{o}}-f_{\mathrm{d}})(\beta_{\mathrm{o}}(L))=(\beta_{\mathrm{o}}(L)-\beta_t)\left.\frac{d(f_{\mathrm{o}}-f_{\mathrm{d}})}{d\beta}\right|_{\tilde\beta} \tag{6.7}$$

for some $\tilde\beta$ between $\beta_{\mathrm{o}}(L)$ and β_t. Since the derivative of $f_{\mathrm{o}}-f_{\mathrm{d}}$ is bounded away from zero by (4.62), it follows that $\beta_{\mathrm{o}}(L)-\beta_t=\alpha O((\omega(L))^{-1})=\beta_t O((\omega(L))^{-1})$. Using this and Lemma 6.1, the Taylor expansion around β_t gives

$$\begin{aligned}\frac{\alpha}{\omega(L)}&=(f_{\mathrm{o}}-f_{\mathrm{d}})(\beta_{\mathrm{o}}(L))\\&=(\beta_{\mathrm{o}}(L)-\beta_t)\left.\frac{d(f_{\mathrm{o}}-f_{\mathrm{d}})}{d\beta}\right|_{\beta_t}+(\omega(L))^{-2}\,O(q^{-\nu}\log^2 q),\end{aligned} \tag{6.8}$$

which along with (4.61) directly implies the first equality of (6.3). One proceeds similarly for $\mathrm{m}=\mathrm{d}$.

(b) Let us introduce

$$\xi_L(\beta)=\log\frac{Z_{\mathrm{o},V(L)}(\beta,\lambda)}{Z_{\mathrm{d},V(L)}(\beta,\lambda)}. \tag{6.9}$$

If $\beta\in[\beta_{\mathrm{o}}(L),\beta_{\mathrm{d}}(L)]$, we may use the proved part (a) of this lemma, Lemma 4.4(c), the relation (4.25) with $k=0$, Eq. (4.23), and Lemma A.1 to get

$$\begin{aligned}\xi_L(\beta_{\mathrm{m}}(L))=&-\frac{1}{d}(f_{\mathrm{o}}-f_{\mathrm{d}})(\beta_{\mathrm{m}}(L))\,|\mathbb{B}|\\&-\left[(s_{\mathrm{o}}-s_{\mathrm{d}})(\beta_t)+\alpha O\left(\frac{1}{\omega(L)}\right)\right]|\partial\mathbb{B}|+L^{d-2}O(q^{-\nu})\end{aligned}$$

for m = o, d. By Lemma A.6(a) with $\kappa_2 = \nu$, we have

$$(s_{\mathrm{o}} - s_{\mathrm{d}})(\beta_t) = -\frac{1}{d}\left(\lambda - \frac{1}{2}\right)\log q + O(q^{-\nu}). \tag{6.10}$$

Observing that

$$|\mathbb{B}| = |\mathbb{B}(\Lambda(L))| = dL^{d-1}(L-1), \qquad |\partial\mathbb{B}| = |\partial\mathbb{B}(\Lambda(L))| = 2\,dL^{d-1}, \tag{6.11}$$

and taking into account (6.7), (4.33), and (6.2), we eventually obtain

$$\begin{aligned}\xi_L(\beta_{\mathrm{o}}(L)) &= \left[-\frac{\alpha}{\log q}\frac{L-1}{\omega(L)} + 2\left(\lambda - \frac{1}{2}\right) + O\left(\frac{q^{-\nu}}{\log q}\right)\right] L^{d-1}\log q + \alpha O\left(\frac{L^{d-1}}{\omega(L)}\right)\\ &\leqslant \left[-\left(\frac{\nu}{4} - \frac{1}{2\log q}\right)\frac{5}{\nu} + \mu + O\left(\frac{q^{-\nu}}{\log q}\right)\right] L^{d-1}\log q + \alpha O\left(\frac{L^{d-1}}{\omega(L)}\right)\\ &\leqslant -\frac{1}{5}L^{d-1}\log q\left[1 + O\left(\frac{1}{\omega(L)}\right)\right] \leqslant -\frac{1}{6}L^{d-1}\log q < 0\end{aligned} \tag{6.12}$$

for q, L large. Similarly,

$$\xi_L(\beta_{\mathrm{d}}(L)) \geqslant \tfrac{1}{6}L^{d-1}\log q > 0 \tag{6.13}$$

once q, L are large enough.

Next, for large q and L and any $\beta \in [\beta_{\mathrm{o}}(L), \beta_{\mathrm{d}}(L)]$, we have

$$\xi'_L(\beta) = \frac{\partial \xi_L}{\partial \beta} = \frac{\partial G_{\mathrm{o}}(\overline{\mathbb{B}})}{\partial \beta} + L^d O(q^{-\nu}) \geqslant (d + O(q^{-\nu}))\,L^{d-1}(L-1) \geqslant \frac{d}{2}L^d. \tag{6.14}$$

Taking into account that $\xi_L(\beta)$ is continuous, a result of (6.12), (6.13), and (6.14) is that the equation $Z_{\mathrm{o},V}(\beta,\lambda) = Z_{\mathrm{d},V}(\beta,\lambda)$ has necessarily a unique solution $\beta_{=}^{(\lambda)}(L)$ on the interval $(\beta_{\mathrm{o}}(L), \beta_{\mathrm{d}}(L))$. To find its position, we first use the Lagrange mean-value theorem to write

$$0 = \xi_L(\beta_{=}^{(\lambda)}(L)) = \xi_L(\beta_t) + (\beta_{=}^{(\lambda)}(L) - \beta_t)\,\xi'_L(\hat{\beta}) \tag{6.15}$$

where $\hat{\beta}$ is a point between $\beta_{=}^{(\lambda)}(L)$ and β_t. In view of (6.14), we get

$$\beta_{=}^{(\lambda)}(L) - \beta_t = \xi_L(\beta_t)\,O(L^{-d}) \tag{6.16}$$

and due to (4.25), (4.23), and Lemma A.1, we have

$$\xi'_L(\beta_t) = 2\,\Delta e\,L^d[1 + O(L^{-1})] \tag{6.17}$$

and, using also Lemma 6.1,

$$\frac{\partial^2 \xi_L}{\partial \beta^2} = L^d O(q^{-\nu}) \tag{6.18}$$

for any $\beta \in [\beta_{\mathrm{o}}(L), \beta_{\mathrm{d}}(L)]$. The Taylor expansion of $\xi_L(\beta_{=}^{(\lambda)}(L))$ around β_t then implies

$$0 = \xi_L(\beta_t) + (\beta_{=}^{(\lambda)}(L) - \beta_t)\, \xi_L'(\beta_t) + [\xi_L(\beta_t)]^2\, L^{-d} O(q^{-\nu}). \tag{6.19}$$

Defining

$$\vartheta(\lambda, q, L) = \frac{\xi_L(\beta_t)}{\xi_L'(\beta_t)}\, L, \tag{6.20}$$

and referring to (6.17), we immediately get (6.4).

Due to (4.25), (6.10), and (6.11), we have

$$\begin{aligned} \xi_L(\beta_t) &= (s_{\mathrm{d}} - s_{\mathrm{o}})(\beta_t)\, |\partial \mathbb{B}| + L^{d-2} O(q^{-\nu}) \\ &= 2\left[\left(\lambda - \frac{1}{2}\right) \log q + O(q^{-\nu})\right] L^{d-1}. \end{aligned} \tag{6.21}$$

Combining (6.21) and (4.60) with (6.16) gives the bound $\beta_{=}^{(\lambda)}(L) = \beta_t(1 + O(L^{-1}))$, while (6.21), (4.60), and (6.17) yields the more precise bound (6.5). ▮

For a more detailed bounds on $Z_{\mathrm{big},\, V(L)}(\beta, \lambda)$ then those in the proof of Lemma 4.5, we use the following claims to restrict its evaluation to β from a suitably chosen small range.

Lemma 6.3. Let W be a volume of the form (3.7). Under the conditions of Lemma 6.2 we have:

(a) The functions

$$\delta_{\mathrm{o}}(\beta) = \frac{Z_{\mathrm{big},\, V(L)}(\beta, \lambda)}{Z_{\mathrm{o},\, V(L)}(\beta, \lambda)} \quad \text{and} \quad \delta_{\mathrm{o},\, W}(\beta) = \frac{Z_{\mathrm{d},\, W}(\beta, \lambda)}{Z_{\mathrm{o},\, W}(\beta, \lambda)} \tag{6.22}$$

are decreasing on the interval $[\beta_{\mathrm{o}}(L), \infty)$.

(b) The functions

$$\delta_{\mathrm{d}}(\beta) = \frac{Z_{\mathrm{big},\, V(L)}(\beta, \lambda)}{Z_{\mathrm{d},\, V(L)}(\beta, \lambda)} \quad \text{and} \quad \delta_{\mathrm{d},\, W}(\beta) = \frac{Z_{\mathrm{o},\, W}(\beta, \lambda)}{Z_{\mathrm{d},\, W}(\beta, \lambda)} \tag{6.23}$$

are increasing on the interval $[1, \beta_{\mathrm{d}}(L)]$.

Proof. We will explicitly only prove the monotonicity of $\delta_{\mathrm{o}}(\beta)$. The remaining cases are proven analogously and will be left to the reader.

We proceed similarly as in the proof of Lemma 5.2. To evaluate $Z_{\mathrm{big},\, V(L)}(\beta, \lambda)$, we rewrite the factor $Z_{\mathrm{d},\, W_{\mathrm{d}}(\partial_l)}(\beta, \lambda)$ in (3.16) in analogy with (5.3),

$$Z_{\mathrm{d},\, W_{\mathrm{d}}(\partial_l)}(\beta, \lambda) = \sum_{\partial_{\mathrm{ext}} \sqsubset W_{\mathrm{d}}(\partial_l)}^{(\mathrm{d})} e^{-G_{\mathrm{d}}(\overline{\mathbb{B}}(\mathrm{Ext}))} Z_{\mathrm{o},\, \mathrm{Int}}(\beta, \lambda) \prod_{\gamma \in \partial_{\mathrm{ext}}} \varrho(\gamma). \tag{6.24}$$

Here, the summation is over sets ∂_{ext} of mutually external, short, d-labelled w-contours with $V(\gamma) \subset W_{\mathrm{d}}(\partial_l)$, $\mathrm{Int} = \bigcup_{\gamma \in \partial_{\mathrm{ext}}} \mathrm{Int}\, \gamma$, and $\mathrm{Ext} = W_{\mathrm{d}}(\partial_l) \setminus \bigcup_{\gamma \in \partial_{\mathrm{ext}}} V(\gamma)$. In this way we get

$$\frac{Z_{\mathrm{big},\, V}(\beta, \lambda)}{Z_{\mathrm{o},\, V}(\beta, \lambda)} = \sum_{\partial_l} \prod_{\gamma \in \partial_l} \varrho(\gamma) \sum_{\partial_{\mathrm{ext}} \sqsubset W_{\mathrm{d}}(\partial_l)}^{(\mathrm{d})} e^{\xi(\beta)} \prod_{\tilde{\gamma} \in \partial_{\mathrm{ext}}} \varrho(\tilde{\gamma}), \tag{6.25}$$

where

$$\xi(\beta) = -G_{\mathrm{d}}(\overline{\mathbb{B}}(\mathrm{Ext})) + \log \frac{Z_{\mathrm{o},\, W_{\mathrm{o}}(\partial_l)}(\beta, \lambda)\, Z_{\mathrm{o},\, \mathrm{Int}}(\beta, \lambda)}{Z_{\mathrm{o},\, V}(\beta, \lambda)}. \tag{6.26}$$

Using now the cluster expansion of the form (4.3) to analyze $\log Z_{\mathrm{o},\, W_{\mathrm{o}}(\partial_l)}(\beta, \lambda) + \log Z_{\mathrm{o},\, \mathrm{Int}}(\beta, \lambda) - \log Z_{\mathrm{o},\, V}(\beta, \lambda)$, we get

$$\frac{d\xi}{d\beta} = \frac{d}{d\beta}(F_{\mathrm{o}}(\mathrm{Ext}) - G_{\mathrm{d}}(\overline{\mathbb{B}}(\mathrm{Ext}))) + \|\partial(\mathrm{Ext})\|\, O(q^{-\nu}). \tag{6.27}$$

Hence, in view (4.23) and (3.10),

$$\frac{d\xi}{d\beta} < (-\lambda + O(q^{-\nu}))\, |\overline{\mathbb{B}}(\mathrm{Ext})| + \|\partial(\mathrm{Ext})\|\, O(q^{-\nu}) \leqslant -\frac{\lambda}{2} < 0 \tag{6.28}$$

for all q large, in the same way as for (5.9). ▮

Remark 6.4. The above proof shows that in the interval $[\beta_{\mathrm{o}}(L), \infty)$, the derivatives of $\log \delta_{\mathrm{o}}(\beta)$ and $\log \delta_{\mathrm{o},\, W}(\beta)$ are at most $-\frac{\lambda}{2}$, while on the interval $[1, \beta_{\mathrm{d}}(L)]$, the derivatives of $\log \delta_{\mathrm{d}}(\beta)$ and $\log \delta_{\mathrm{d},\, W}(\beta)$ are at least $\frac{\lambda}{2}$.

Lemma 6.5. Let $d \geqslant 2$ and $0 \leqslant \mu < 1$. Let $\omega\colon \mathbb{N} \to [0, \infty)$ be a function satisfying the conditions (6.2) from Lemma 6.2, and let $k_0 \in \mathbb{Z}$, $k_0 \geqslant 0$. For all q and L sufficiently large, $|\lambda - \frac{1}{2}| \leqslant \frac{\mu}{2}$, and $0 \leqslant k \leqslant k_0$, we have:

(a) If $\beta \in [1, \infty)$, then

$$\left| \frac{\partial^k}{\partial \beta^k} \frac{Z_{\text{big}, V(L)}(\beta, \lambda)}{Z_{\text{o}, V(L)}(\beta, \lambda) + Z_{\text{d}, V(L)}(\beta, \lambda)} \right| < q^{-\frac{1-\mu}{16d} \omega(L)}. \tag{6.29}$$

(b) If $\beta \geqslant \beta_{\text{d}}(L)$, then

$$\left| \frac{\partial^k}{\partial \beta^k} \frac{Z_{\text{d}, V(L)}(\beta, \lambda) + Z_{\text{big}, V(L)}(\beta, \lambda)}{Z_{\text{o}, V(L)}(\beta, \lambda)} \right| < q^{-\frac{1-\mu}{16d} \omega(L)}. \tag{6.30}$$

(c) If $1 \leqslant \beta \leqslant \beta_{\text{o}}(L)$, then

$$\left| \frac{\partial^k}{\partial \beta^k} \frac{Z_{\text{o}, V(L)}(\beta, \lambda) + Z_{\text{big}, V(L)}(\beta, \lambda)}{Z_{\text{d}, V(L)}(\beta, \lambda)} \right| < q^{-\frac{1-\mu}{16d} \omega(L)}. \tag{6.31}$$

Proof. For $k = 0$ we will actually prove a stronger claim with the right hand sides above replaced by $q^{-\frac{1-\mu}{14d} \omega(L)}$. Taking into account the first condition in (6.2), the claim for $k > 0$ then follows by Lemma 3.3.

(a) Let

$$\delta_{=} = \frac{Z_{\text{big}, V(L)}(\beta_{=}^{(\lambda)}(L), \lambda)}{Z_{\text{o}, V(L)}(\beta_{=}^{(\lambda)}(L), \lambda)} = \frac{Z_{\text{big}, V(L)}(\beta_{=}^{(\lambda)}(L), \lambda)}{Z_{\text{d}, V(L)}(\beta_{=}^{(\lambda)}(L), \lambda)} \tag{6.32}$$

where $\beta_{=}^{(\lambda)}(L)$ is the point where $Z_{\text{o}, V}(\beta, \lambda) = Z_{\text{d}, V}(\beta, \lambda)$, see Lemma 6.2. Applying Lemma 6.3, we get

$$\sup_{\beta \in [1, \infty)} \frac{Z_{\text{big}, V}(\beta, \lambda)}{Z_{\text{o}, V}(\beta, \lambda) + Z_{\text{d}, V}(\beta, \lambda)} \leqslant \sup_{\beta \in [1, \infty)} \min\{\delta_{\text{o}}(\beta), \delta_{\text{d}}(b)\} \leqslant \delta_{=}, \tag{6.33}$$

where δ_{o} and δ_{d} are the quantities defined in Lemma 6.3. Referring to (3.16), we now have to bound the factor

$$\frac{Z_{\text{o}, W_{\text{o}}}(\beta_{=}^{(\lambda)}(L), \lambda)\, Z_{\text{d}, W_{\text{d}}}(\beta_{=}^{(\lambda)}(L), \lambda)}{Z_{\text{o}, V}(\beta_{=}^{(\lambda)}(L), \lambda)} = \frac{Z_{\text{o}, W_{\text{o}}}(\beta_{=}^{(\lambda)}(L), \lambda)\, Z_{\text{d}, W_{\text{d}}}(\beta_{=}^{(\lambda)}(L), \lambda)}{Z_{\text{d}, V}(\beta_{=}^{(\lambda)}(L), \lambda)}, \tag{6.34}$$

where we used the shorthand $W_{\text{o}} = W_{\text{o}}(\partial_l)$ and $W_{\text{d}} = W_{\text{d}}(\partial_l)$. Notice that, due to Lemma 6.2, both phases at $\beta = \beta_{=}^{(\lambda)}(L)$ can be analyzed by convergent cluster expansions. For each particular configuration ∂_l, let $\text{m} = \text{m}(\partial_l)$ be the label for which

$$\|\partial_e W_{\text{m}}\| = \min\{\|\partial_e W_{\text{o}}\|, \|\partial_e W_{\text{d}}\|\}. \tag{6.35}$$

Choosing the form of (6.34) with denominator $Z_{\mathrm{m}^c,V}(\beta_{=}^{(\lambda)}(L),\lambda)$, and using the bounds (4.25) and (4.27), together with the observation that $\|\partial_i W_{\mathrm{m}}\| = \|\partial_i W_{\mathrm{m}^c}\|$, we get the estimate

$$\frac{Z_{\mathrm{o},W_{\mathrm{o}}}(\beta_{=}^{(\lambda)}(L),\lambda)\,Z_{\mathrm{d},W_{\mathrm{d}}}(\beta_{=}^{(\lambda)}(L),\lambda)}{Z_{\mathrm{m}^c,V}(\beta_{=}^{(\lambda)}(L),\lambda)} \leqslant e^{F_{\mathrm{m}^c}(W_{\mathrm{m}})-F_{\mathrm{m}}(W_{\mathrm{m}})+\|\partial W_{\mathrm{m}}\|\,O(q^{-\nu})}, \tag{6.36}$$

and hence

$$\delta_{=} \leqslant \sum_{\partial_l} e^{F_{\mathrm{m}^c}(W_{\mathrm{m}})-F_{\mathrm{m}}(W_{\mathrm{m}})+\|\partial_e W_{\mathrm{m}}\|\,O(q^{-\nu})} \prod_{\gamma\in\partial_l} \varrho(\gamma)\, e^{O(q^{-\nu})\,\|\gamma\|}. \tag{6.37}$$

Here we used that $\|\partial W_{\mathrm{m}}\| = \|\partial_i W_{\mathrm{m}}\| + \|\partial_e W_{\mathrm{m}}\|$ and $\|\partial_i W_{\mathrm{m}}\| = \sum_{\gamma\in\partial_l}\|\gamma\|$.

As $F_{\mathrm{o}}(V) = F_{\mathrm{d}}(V) + L^{d-2}\,O(q^{-\nu})$ at $\beta_{=}^{(\lambda)}(L)$ by virtue of Lemma 6.2(b) and the bound (4.25), we have

$$(f_{\mathrm{o}}-f_{\mathrm{d}})(\beta_{=}^{(\lambda)}(L))\,|\mathbb{B}|/d = -(s_{\mathrm{o}}-s_{\mathrm{d}})(\beta_{=}^{(\lambda)}(L))\,|\partial\mathbb{B}| + L^{d-2}O(q^{-\nu}). \tag{6.38}$$

In conjunction with (6.11), we get

$$\begin{aligned}
&|F_{\mathrm{m}^c}(W_{\mathrm{m}}) - F_{\mathrm{m}}(W_{\mathrm{m}})| \\
&\quad\leqslant |(s_{\mathrm{o}}-s_{\mathrm{d}})(\beta_{=}^{(\lambda)}(L))| \left|\frac{2\,|\mathbb{B}(W_{\mathrm{m}})|}{L-1} - |\partial\mathbb{B}(W_{\mathrm{m}})|\right| + \frac{|\mathbb{B}(W_{\mathrm{m}})|}{L^2}\,O(q^{-\nu}).
\end{aligned} \tag{6.39}$$

Further, by Lemma 6.2(b), $\beta_{=}^{(\lambda)}(L) = \beta_t(1+o(1))$, implying that the derivative of $(s_{\mathrm{o}}-s_{\mathrm{d}})(\beta)$ is bounded between $\beta_{=}^{(\lambda)}(L)$ and β_t. Since $\beta_{=}^{(\lambda)}(L) - \beta_t = \log q\,O(L^{-1})$ by the same lemma and Eq. (4.60), we can conclude that

$$\begin{aligned}
|(s_{\mathrm{o}}-s_{\mathrm{d}})(\beta_{=}^{(\lambda)}(L))| &= |(s_{\mathrm{o}}-s_{\mathrm{d}})(\beta_t)| + \log q\,O(L^{-1}) \\
&\leqslant \frac{\mu}{2d} + \log q\,O(L^{-1}) + O(q^{-\nu}),
\end{aligned} \tag{6.40}$$

where we have used (6.10) in the last step. Combining (6.37) with (6.39), (6.40), and Lemma A.7, we arrive at

$$\delta_{=} \leqslant \sum_{\partial_l} e^{\|\partial_e W_{\mathrm{m}}\|\,O(q^{-\nu})} \prod_{\gamma\in\partial_l} \varrho(\gamma)\, e^{(\frac{\mu}{2d}+O(q^{-\nu})+\log q\,O(L^{-1}))\,\|\gamma\|}. \tag{6.41}$$

Using now Lemma A.8 to bound $\|\partial_e W_{\mathrm{m}}\|$ and then continuing as in the proof of (4.71), we get

$$\delta_{=} \leqslant q^{-\frac{1-\mu}{14d}\,\omega(L)} \tag{6.42}$$

as soon as q and L are sufficiently large.

(b) Using the proven claim (a), it is sufficient to bound $\delta_{\mathrm{o},V}(\beta)=\frac{Z_{\mathrm{d},V}(\beta,\lambda)}{Z_{\mathrm{o},V}(\beta,\lambda)}$. In view of monotonicity of $\delta_{\mathrm{o},V}(\beta)$ according Lemma 6.3, we can bound it by $\delta_{\mathrm{o},V}(\beta_{\mathrm{d}}(L))$, at which point we can control both $\log Z_{\mathrm{o},V}(\beta,\lambda)$ and $\log Z_{\mathrm{d},V}(\beta,\lambda)$ by convergent cluster expansions,

$$\delta_{\mathrm{o},V}(\beta_{\mathrm{d}}(L))\leqslant e^{-F_{\mathrm{d}}(V)+F_{\mathrm{o}}(V)+L^{d-2}\,O(q^{-\nu})}\leqslant e^{-\frac{\alpha}{\omega(L)}|\mathbb{B}|+(\frac{\mu}{2d}\log q+O(q^{-\nu}))\,|\partial\mathbb{B}|+L^{d-2}\,O(q^{-\nu})} \tag{6.43}$$

since $a_{\mathrm{d}}(\beta_{\mathrm{d}}(L))=\frac{\alpha}{\omega(L)}$ and $(s_{\mathrm{o}}-s_{\mathrm{d}})(\beta_{\mathrm{d}}(L))\leqslant\frac{\mu}{2d}\log q+O(q^{-\nu})$ due to (4.57) with $\varepsilon=0$. Using now (6.11) and the first condition in (6.2), we get

$$\begin{aligned}&\frac{\alpha}{\omega(L)}|\mathbb{B}|-\left(\frac{\mu}{2d}\log q+O(q^{-\nu})\right)|\partial\mathbb{B}|\\&\quad\geqslant\left(\left(\frac{3(L-1)}{4L}-\frac{\mu}{2d}\right)\log q+O(q^{-\nu})-\frac{3(L-1)}{2L\nu}\right)|\partial\mathbb{B}|\geqslant\frac{1}{2L}|\partial\mathbb{B}|\log q.\end{aligned} \tag{6.44}$$

As a result, we get

$$\delta_{\mathrm{o},V}(\beta_{\mathrm{d}}(L))\leqslant q^{-dL^{d-1}} \tag{6.45}$$

for q and L large.

(c) The proof of the claim (c) is analogous to the proof of (b). ∎

Let us now use Lemmas 4.4, 6.2, and 6.5, to study the behaviour of the finite-volume mean energy $E_L(\beta,\lambda)$ and its derivatives (with respect to β) for large values of q and L.

Lemma 6.6. Let $d\geqslant 2$, $0\leqslant\mu<1$, and $k_0=1,2\ldots$ For q and L large enough, $|\lambda-\frac{1}{2}|\leqslant\frac{\mu}{2}$, $\beta\geqslant 1$, and $2\leqslant k\leqslant k_0$, we have

$$\begin{aligned}M_L(\beta,\lambda)=&\frac{m^*}{2}L^d+\frac{m^*}{2}L^d\tanh(\Delta e(\beta-\beta_{=}^{(\lambda)}(L))\,L^d)\\&+O(|\beta-\beta_t|\,L^dq^{-\nu_0})+O(L^{d-1}),\end{aligned} \tag{6.46}$$

$$\begin{aligned}E_L(\beta,\lambda)=&e_0\,L^d-\Delta e\,L^d\tanh(\Delta e(\beta-\beta_{=}^{(\lambda)}(L))\,L^d)\\&+O(|\beta-\beta_t|\,L^dq^{-\nu_0})+O(L^{d-1}),\end{aligned} \tag{6.47}$$

and

$$\begin{aligned}\frac{\partial^{k-1}}{\partial\beta^{k-1}}E_L(\beta,\lambda)=&-(\Delta e\,L^d)^k\,\frac{d^{k-1}}{dx^{k-1}}\tanh x\Big|_{x=\Delta e(\beta-\beta_{=}^{(\lambda)}(L))\,L^d}\\&+O(|\beta-\beta_t|\,L^{kd}q^{-\nu_0})+O(L^{kd-1}).\end{aligned} \tag{6.48}$$

Here $\beta_{=}^{(\lambda)}(L)$ is the temperature introduced in Lemma 6.2(b).

Proof. We first prove the statements for the mean energy $E_L(\beta, \lambda)$ and its derivatives. Using (3.19), we have

$$\begin{aligned} E_L(\beta, \lambda) &= -\frac{\partial}{\partial \beta}\Bigg[\log(Z_{\mathrm{o},V}(\beta, \lambda) + Z_{\mathrm{d},V}(\beta, \lambda)) \\ &\quad + \log\left(1 + \frac{Z_{\mathrm{big},V(L)}(\beta, \lambda)}{Z_{\mathrm{o},V}(\beta, \lambda) + Z_{\mathrm{d},V}(\beta, \lambda)}\right)\Bigg] \\ &= -\frac{1}{2}\frac{\partial}{\partial \beta}\log(Z_{\mathrm{o},V}(\beta, \lambda)\, Z_{\mathrm{d},V}(\beta, \lambda)) \\ &\quad -\frac{1}{2}\left(\frac{\partial}{\partial \beta}\log\frac{Z_{\mathrm{o},V}(\beta, \lambda)}{Z_{\mathrm{d},V}(\beta, \lambda)}\right)\tanh\left(\frac{1}{2}\log\frac{Z_{\mathrm{o},V}(\beta, \lambda)}{Z_{\mathrm{d},V}(\beta, \lambda)}\right) \\ &\quad -\frac{\partial}{\partial \beta}\log\left(1 + \frac{Z_{\mathrm{big},V(L)}(\beta, \lambda)}{Z_{\mathrm{o},V}(\beta, \lambda) + Z_{\mathrm{d},V}(\beta, \lambda)}\right). \end{aligned} \tag{6.49}$$

Applying Lemma A.9 to $\psi_1(x) = \log x$ and $\psi_2(\beta) = 1 + \frac{Z_{\mathrm{big},V}(\beta, \lambda)}{Z_{\mathrm{o},V}(\beta, \lambda) + Z_{\mathrm{d},V}(\beta, \lambda)}$ and using Lemma 6.5(a), we get

$$\begin{aligned} &\frac{\partial^k}{\partial \beta^k}\log\left(1 + \frac{Z_{\mathrm{big},V(L)}(\beta, \lambda)}{Z_{\mathrm{o},V}(\beta, \lambda) + Z_{\mathrm{d},V}(\beta, \lambda)}\right) = \\ &= \sum_{j=1}^{k} (1 + O(q^{-\frac{1-\mu}{16d}\omega(L)}))^{-j}\, O(q^{-j\frac{1-\mu}{16d}\omega(L)}) = O(q^{-\frac{1-\mu}{16d}\omega(L)}) \end{aligned} \tag{6.50}$$

for any $k \leqslant k_0$.

Suppose now that $\beta \in [\beta_{\mathrm{o}}(L), \beta_{\mathrm{d}}(L)]$. Taking into account (4.25), (4.23), Lemmas A.1, 6.1, and using the shorthand (6.9), we get

$$\begin{aligned} E_L(\beta, \lambda) &= e_0\, L^d - \Delta e\, L^d \tanh(\tfrac{1}{2}\,\xi_L(\beta)) + |\beta - \beta_t|\, L^d O(q^{-\nu_0}) \\ &\quad + O(L^{d-1}) + O(q^{-\frac{1-\mu}{16d}\omega(L)}). \end{aligned} \tag{6.51}$$

Here e_0 introduced in (2.12) is, taking into account Lemma 4.5 and the fact that $\frac{df_{\mathrm{d}}}{d\beta} = O(q^{-\nu_0})$ according to (4.23) and (3.10),

$$e_0 = \frac{1}{2}\frac{d(f_{\mathrm{o}} + f_{\mathrm{d}})}{d\beta}\bigg|_{\beta_t} = -\frac{d}{2} + O(q^{-\nu_0}). \tag{6.52}$$

Next, let us find expressions for the derivatives of $E_L(\beta, \lambda)$. Since the derivatives of $\tanh x$ are bounded due to (A.21), we may use Lemma A.9, (4.25), (4.23), Lemma A.1 and Lemma 6.1 to get

$$\begin{aligned}
&\frac{\partial^{k-1}}{\partial\beta^{k-1}}\left[\frac{1}{2}\left(\frac{\partial}{\partial\beta}\log\frac{Z_{\mathrm{o},V}(\beta,\lambda)}{Z_{\mathrm{d},V}(\beta,\lambda)}\right)\tanh\left(\frac{1}{2}\log\frac{Z_{\mathrm{o},V}(\beta,\lambda)}{Z_{\mathrm{d},V}(\beta,\lambda)}\right)\right]\\
&\quad=\left(\frac{1}{2}\frac{\partial}{\partial\beta}\log\frac{Z_{\mathrm{o},V}(\beta,\lambda)}{Z_{\mathrm{d},V}(\beta,\lambda)}\right)^k\frac{d^{k-1}}{dx^{k-1}}\tanh x\Big|_{x=\frac{1}{2}\xi_L(\beta)}+\sum_{j=1}^{k-1}L^{jd}O(q^{-\nu})\\
&\quad=(\Delta e\,L^d)^k\,(1+|\beta-\beta_t|\,O(q^{-\nu_0})+O(L^{-1}))\\
&\qquad\times\frac{d^{k-1}}{dx^{k-1}}\tanh x\Big|_{x=\frac{1}{2}\xi_L(\beta)}+L^{(k-1)\,d}O(q^{-\nu}).
\end{aligned}$$

Along with (6.49), (4.25), (6.50), and the observation that the derivatives of the first term on the right hand side of (6.49) can be bounded by $L^dO(q^{-\nu})\leqslant L^{(k-1)\,d}O(q^{-\nu})$, this implies

$$\begin{aligned}
\frac{\partial^{k-1}}{\partial\beta^{k-1}}E_L(\beta,\lambda)&=(\Delta e\,L^d)^k\,(1+|\beta-\beta_t|\,O(q^{-\nu_0})+O(L^{-1}))\\
&\quad\times\frac{d^{k-1}}{dx^{k-1}}\tanh x\Big|_{x=\frac{1}{2}\xi_L(\beta)}+L^{(k-1)\,d}O(q^{-\nu}).
\end{aligned}\tag{6.53}$$

Finally, we Taylor expand $\xi_L(\beta)=\log\frac{Z_{\mathrm{o},V}(\beta,\lambda)}{Z_{\mathrm{d},V}(\beta,\lambda)}$ around the point $\beta_{=}^{(\lambda)}(L)$ of Lemma 6.2(b). Using (4.25), (4.61), Lemma A.1, Lemma 4.5, we obtain

$$\begin{aligned}
\log\frac{Z_{\mathrm{o},V}(\beta,\lambda)}{Z_{\mathrm{d},V}(\beta,\lambda)}&=(\beta-\beta_{=}^{(\lambda)}(L))\bigg(\frac{d(f_{\mathrm{d}}-f_{\mathrm{o}})}{d\beta}\Big|_{\beta_t}L^d+O(L^{d-1})\\
&\quad+(|\beta-\beta_{=}^{(\lambda)}(L)|+|\beta_t-\beta_{=}^{(\lambda)}(L)|)\,L^dO(q^{-\nu_0})\bigg)\\
&=2\,\Delta e\,(\beta-\beta_{=}^{(\lambda)}(L))\,L^d(1+O(L^{-1})+|\beta-\beta_t|\,O(q^{-\nu_0})),
\end{aligned}\tag{6.54}$$

where we observed that $|\beta-\beta_{=}^{(\lambda)}(L)|\leqslant|\beta-\beta_t|+|\beta_t-\beta_{=}^{(\lambda)}(L)|$ and $|\beta_t-\beta_{=}^{(\lambda)}(L)|=\log q\,O(L^{-1})$. Using now Lemma A.10, we get

$$\begin{aligned}
&\frac{d^{k-1}}{dx^{k-1}}\tanh x\Big|_{x=\frac{1}{2}\xi_L(\beta)}\\
&\quad=\frac{d^{k-1}}{dx^{k-1}}\tanh x\Big|_{x=\Delta e(\beta-\beta_{=}^{(\lambda)}(L))\,L^d}+O(L^{-1})+|\beta-\beta_t|\,O(q^{-\nu_0})
\end{aligned}\tag{6.55}$$

for any $k=1,\ldots$. The relations (6.51), (6.53), and (6.55) complete the proof of (6.47) and (6.48) for β in the interval $[\beta_{\mathrm{o}}(L),\beta_{\mathrm{d}}(L)]$.

Using (3.21) and (3.19), and referring to the bounds $Z^{(x)}_{\mathrm{o},V}(\beta,\lambda) \leqslant Z_{\mathrm{o},V}(\beta,\lambda)$, $Z^{(x)}_{\mathrm{d},V}(\beta,\lambda) \leqslant Z_{\mathrm{d},V}(\beta,\lambda)$, and $Z^{(x)}_{\mathrm{big},V}(\beta,\lambda) \leqslant Z_{\mathrm{big},V}(\beta,\lambda)$, Lemma 6.5 implies that

$$M_L(\beta,\lambda) = \sum_{x\in\Lambda} \frac{Z^{(x)}_{\mathrm{o},V}(\beta,\lambda) + Z^{(x)}_{\mathrm{d},V}(\beta,\lambda)}{Z_{\mathrm{o},V}(\beta,\lambda) + Z_{\mathrm{d},V}(\beta,\lambda)} + L^d O(q^{-\frac{1-\mu}{16d}\omega(L)}). \tag{6.56}$$

Let us now assume that $\beta \in [\beta_{\mathrm{o}}(L), \beta_{\mathrm{d}}(L)]$, so that $Z_{\mathrm{m},V}(\beta,\lambda) = \bar{Z}_{\mathrm{m},V}(\beta,\lambda)$ and $Z^{(x)}_{\mathrm{m},V}(\beta,\lambda) = \bar{Z}^{(x)}_{\mathrm{m},V}(\beta,\lambda)$ for both $\mathrm{m}=\mathrm{d}$ and $\mathrm{m}=\mathrm{o}$. Taking into account the definition (4.28), we then get

$$\begin{aligned} M_{\mathrm{m},L}(\beta,\lambda) = {} & \frac{M_{\mathrm{o},L}(\beta,\lambda) + M_{\mathrm{d},L}(\beta,\lambda)}{2} + \frac{M_{\mathrm{o},L}(\beta,\lambda) - M_{\mathrm{d},L}(\beta,\lambda)}{2} \\ & \times \tanh\left(\frac{1}{2}\log\frac{Z_{\mathrm{o},V}(\beta,\lambda)}{Z_{\mathrm{d},V}(\beta,\lambda)}\right) + L^d O(q^{-\frac{1-\mu}{16d}\omega(L)}). \end{aligned} \tag{6.57}$$

Combined with the finite-size scaling bound (4.32), this gives

$$\begin{aligned} M_{\mathrm{m},L}(\beta,\lambda) = {} & \frac{m_{\mathrm{o}}(\beta) + m_{\mathrm{d}}(\beta)}{2} L^d + \frac{m_{\mathrm{o}}(\beta) - m_{\mathrm{d}}(\beta)}{2} L^d \\ & \times \tanh\left(\frac{1}{2}\log\frac{Z_{\mathrm{o},V}(\beta,\lambda)}{Z_{\mathrm{d},V}(\beta,\lambda)}\right) + L^{d-1} O(q^{-\nu}). \end{aligned} \tag{6.58}$$

Finally, using first the bound (4.31) for $k=1$ to bound the difference between $m_{\mathrm{m}}(\beta)$ and $m_{\mathrm{m}}(\beta_t)$ by $|\beta-\beta_t|\, O(q^{-\nu_0})$ and then Remark 5.4 to conclude that $m_{\mathrm{d}}(\beta_t) = 0$ and $m_{\mathrm{o}}(\beta_t) = m^*$, we get

$$\begin{aligned} M_{\mathrm{m},L}(\beta,\lambda) = {} & \frac{m^*}{2} L^d + \frac{m^*}{2} L^d \tanh\left(\frac{1}{2}\log\frac{Z_{\mathrm{o},V}(\beta,\lambda)}{Z_{\mathrm{d},V}(\beta,\lambda)}\right) + \\ & + L^{d-1} O(q^{-\nu}) + |\beta-\beta_t|\, L^d O(q^{-\nu_0}). \end{aligned} \tag{6.59}$$

Combined with (6.55), this gives the bound (6.46) for $\beta \in [\beta_{\mathrm{o}}(L), \beta_{\mathrm{d}}(L)]$.

For β outside this interval, the claims of the lemma follow from the more precise estimates of the next lemma. ∎

Lemma 6.7. Let $d \geqslant 2$, $0 \leqslant \mu < 1$, and $k_0 = 1, 2 \ldots$. Assume that q and L are sufficiently large, $|\lambda - \frac{1}{2}| \leqslant \frac{\mu}{2}$, $1 \leqslant k \leqslant k_0$ and $\beta \geqslant 1$. If

$$|\beta - \beta_t| \geqslant \frac{\mu d \beta_t}{\Delta e} \frac{1}{L}, \tag{6.60}$$

one has

$$M_L(\beta, \lambda) = m(\beta)\, L^d + O(L^{d-1}) \tag{6.61}$$

and

$$\frac{\partial^{k-1}}{\partial \beta^{k-1}} E_L(\beta, \lambda) = \frac{d^k f(\beta)}{d\beta^k} L^d + O(L^{d-1}). \tag{6.62}$$

Here f is the free energy introduced by (4.13), and

$$\frac{d^k f(\beta)}{d\beta^k} = \begin{cases} \dfrac{d^k f_{\mathrm{d}}(\beta)}{d\beta^k} & \text{if} \quad \beta < \beta_t, \\ \dfrac{d^k f_{\mathrm{o}}(\beta)}{d\beta^k} & \text{if} \quad \beta > \beta_t. \end{cases} \tag{6.63}$$

Proof. Let $\beta_\pm = \beta_t \pm \frac{\mu d \beta_t}{\Delta e} \frac{1}{L}$. By Lemma 6.2(b), the condition (6.60) and the fact that we assumed $|\lambda - \frac{1}{2}| \leqslant \frac{\mu}{2}$, we have

$$\beta_- \leqslant \beta_{=}^{(\lambda)}(L) - \frac{\mu d \beta_t}{3 \Delta e} \frac{1}{L} \qquad \text{and} \qquad \beta_+ \geqslant \beta_{=}^{(\lambda)}(L) + \frac{\mu d \beta_t}{3 \Delta e} \frac{1}{L}, \tag{6.64}$$

provided L and q are large enough. Assume that $\beta \geqslant \beta_+$. Using first the monotonicity according to Lemma 6.3(a), then the bound (6.14) to control the difference of $\log[Z_{\mathrm{o},V}(\beta_{=}^{(\lambda)}(L), \lambda)/Z_{\mathrm{d},V}(\beta_{=}^{(\lambda)}(L), \lambda)] = 0$ and $\log[Z_{\mathrm{o},V}(\beta_+, \lambda)/Z_{\mathrm{d},V}(\beta_+, \lambda)]$ and finally the bound (6.64) to control the difference between β_+ and $\beta_{=}^{(\lambda)}(L)$, we get

$$\frac{1}{2} \log \frac{Z_{\mathrm{o},V}(\beta, \lambda)}{Z_{\mathrm{d},V}(\beta, \lambda)} \geqslant \frac{1}{2} \log \frac{Z_{\mathrm{o},V}(\beta_+, \lambda)}{Z_{\mathrm{d},V}(\beta_+, \lambda)} \geqslant \frac{d}{4} L^d (\beta_+ - \beta_{=}^{(\lambda)}(L)) \geqslant \eta\, L^{d-1}, \tag{6.65}$$

where $\eta = \frac{\mu d^2 \beta_t}{12 \Delta e}$. Combining this bound with the fact that $\tanh x = \operatorname{sign} x + O(e^{-2|x|})$, we now use (6.58) and Remark 5.4 to get the claim (6.61) for $\beta \geqslant \beta_+$.

For the mean energy, we combine (6.65) with (6.49) and Lemmas 3.3 and 6.5(a) to get

$$E_L(\beta, \lambda) = -\frac{\partial}{\partial \beta} \log Z_{\mathrm{o},V}(\beta, \lambda) + O(L^d e^{-2\eta L^{d-1}}) + O(q^{-\frac{1-\mu}{16d} \omega(L)}). \tag{6.66}$$

On the other hand, (6.49) combined with Lemmas 3.3 and 6.5(a) and the fact that the leading term in the derivatives of the second term on the right hand side of (6.49) does not contain derivatives of $\tanh x$ since $\frac{d^k}{dx^k}\tanh x = O(e^{-2x})$ whenever $k \geqslant 1$, leads to

$$\frac{\partial^{k-1}}{\partial \beta^{k-1}} E_L(\beta, \lambda) = -\frac{\partial^k}{\partial \beta^k} \log Z_{\mathrm{o}, V}(\beta, \lambda) + O(L^{dk} e^{-2\eta L^{d-1}}) + O(q^{-\frac{1-\mu}{16d}\omega(L)}). \tag{6.67}$$

Finally, the relation (4.25) and Lemma A.1 imply that

$$\frac{\partial^k}{\partial \beta^k} \log Z_{\mathrm{o}, V}(\beta, \lambda) = -\frac{d^k f_{\mathrm{o}}}{d\beta^k} L^d + O(L^{d-1}). \tag{6.68}$$

Inserted into (6.66) and (6.67) this completes the proof of the lemma for $\beta \geqslant \beta_+$. The proof for $\beta \leqslant \beta_-$ is almost identical. ∎

Finally, we prove the following

Lemma 6.8. Let $d \geqslant 2$ and $0 \leqslant \mu < 1$. For q and L sufficiently large and $|\lambda - \frac{1}{2}| \leqslant \frac{\mu}{2}$, the specific heat $C_L(\beta, \lambda)$ attains its maximal value at a unique temperature $\beta_{\max}^{(\lambda)}(L)$. Moreover,

$$\beta_{\max}^{(\lambda)}(L) = \beta_{=}^{(\lambda)}(L) + \beta_t^{-1} O(L^{-2d}), \tag{6.69}$$

where $\beta_{=}^{(\lambda)}(L)$ was introduced in Lemma 6.2(b).

Proof. Let $\beta_\pm$ be as in the proof of Lemma 6.7. We first prove that

$$C_L(\beta, \lambda) = \beta_t^2 O(L^d) \tag{6.70}$$

uniformly in $\beta \in (0, \beta_-] \cup [\beta_+, \infty)$. In the interval $[0, 1]$, this claim follows from the standard high temperature expansion, while in the interval $[1, \beta_-]$ it follows from Lemma 6.7. For $\beta \geqslant \beta_+$, however, Lemma 6.7 yields only a bound $C_L(\beta, \lambda) = \beta^2 O(L^d)$, which is not uniform in β. To improve this bound, we first use Remark 6.4 to sharpen the bound of Lemma 6.5(a). For $\beta \geqslant \beta_{=}^{(\lambda)}(L)$, this gives

$$\left| \frac{\partial^k}{\partial \beta^k} \frac{Z_{\mathrm{big}, V(L)}(\beta, \lambda)}{Z_{\mathrm{o}, V(L)}(\beta, \lambda) + Z_{\mathrm{d}, V(L)}(\beta, \lambda)} \right| < e^{-\frac{\lambda}{2}(\beta - \beta_{=}^{(\lambda)}(L))} q^{-\frac{1-\mu}{16d}\omega(L)}. \tag{6.71}$$

In a similar way, the bound (6.65) can be sharpened to

$$\frac{1}{2} \log \frac{Z_{\mathrm{o}, V}(\beta, \lambda)}{Z_{\mathrm{d}, V}(\beta, \lambda)} \geqslant \eta L^{d-1} + \frac{\lambda}{2}(\beta - \beta_+). \tag{6.72}$$

This leads to the following improvement of (6.67):

$$\frac{\partial^{k-1}}{\partial\beta^{k-1}} E_L(\beta,\lambda) = -\frac{\partial^k}{\partial\beta^k}\log Z_{\mathrm{o},V}(\beta,\lambda) + e^{-\frac{\lambda}{2}(\beta-\beta_+)}(O(L^{dk}e^{-2\eta L^{d-1}}) + O(q^{-\frac{1-\mu}{16d}\omega(L)})). \tag{6.73}$$

As a final application of Remark 6.4, we obtain that for any w-contour γ, the ratio of partition functions $\frac{Z_{\mathrm{d},\,\mathrm{Int}\,\gamma}(\beta,\lambda)}{Z_{\mathrm{o},\,\mathrm{Int}\,\gamma}(\beta,\lambda)}$ can be bounded by its value at β_t multiplied by $e^{-\frac{\lambda}{2}(\beta-\beta_t)}$. This leads to the bound

$$K_{\mathrm{o}}(\gamma) \leqslant q^{-\tau(\gamma)} e^{-\frac{\lambda}{2}(\beta-\beta_t)} \tag{6.74}$$

and similar improvements for the derivatives. As a consequence,

$$\frac{\partial^k}{\partial\beta^k}\log Z_{\mathrm{o},V}(\beta,\lambda) = -\frac{\partial^k}{\partial\beta^k} G_{\mathrm{o}}(\overline{\mathbb{B}}(V)) + L^d e^{-\frac{\lambda}{2}(\beta-\beta_t)} O(q^{-\nu}) \tag{6.75}$$

and

$$\frac{\partial^k}{\partial\beta^k}[\log Z_{\mathrm{o},V}(\beta,\lambda) + f_{\mathrm{o}} L^{d-1}(L-1)] = -\frac{\partial^k h_{\mathrm{o}}}{\partial\beta^k}|\partial\overline{\mathbb{B}}(V)| + L^{d-1} e^{-\frac{\lambda}{2}(\beta-\beta_t)} O(q^{-\nu}). \tag{6.76}$$

Combining the bounds (6.73) and (6.75) with Lemma A.1(b), we obtain that $C_L(\beta,\lambda) = \beta^2 e^{-(\beta-\beta_+)} O(L^d) \leqslant \beta_t^2 O(L^d)$ whenever $\beta \geqslant \beta_+$.

On the other hand, the bound (6.48) of Lemma 6.6 and the fact that $\beta_=^{(\lambda)}(L) = \beta_t(1+O(L^{-1}))$ (see Lemma 6.2(b)) yield that

$$C_L(\beta_=^{(\lambda)}(L),\lambda) = \beta_t^2(\Delta e\, L^d)^2\,(1+O(L^{-1})). \tag{6.77}$$

We conclude that

$$C_L(\beta,\lambda) < C_L(\beta_=^{(\lambda)}(L),\lambda)$$

for all $\beta \notin [\beta_-, \beta_+]$ and q, L large enough. In other words, if the temperature $\beta_{\max}^{(\lambda)}(L)$ exists, then $\beta_{\max}^{(\lambda)}(L) \in [\beta_-, \beta_+]$.

Let us, therefore, take $\beta \in [\beta_-, \beta_+]$ in the following. Then Lemma 6.6 gives

$$\frac{\partial^2 C_L(\beta,\lambda)}{\partial\beta^2} = \beta^2(\Delta e\, L^d)^4 \frac{d^3}{dx^3}\tanh x\bigg|_{x=\Delta e(\beta-\beta_=^{(\lambda)}(L))\,L^d} + \beta^2 O(L^{4d-1}). \tag{6.78}$$

Observing that there exist constants $A, B > 0$ such that $\frac{d^3 \tanh x}{dx^3} < -B < 0$ once $|x| \leqslant A$, we conclude that

$$\frac{\partial^2 C_L(\beta, \lambda)}{\partial \beta^2} \leqslant -\beta^2 (\Delta e\, L^d)^4 B + \beta^2 O(L^{4d-1}) \leqslant -\frac{B}{2}\, \beta^2 (\Delta e\, L^d)^4 \tag{6.79}$$

whenever $|\beta - \beta_{=}^{(\lambda)}(L)| \leqslant \frac{A}{\Delta e} \frac{1}{L^d}$ and q, L are large. On the other hand, (2.11), (6.53), Lemma 6.2, and the fact that $\frac{d^2 \tanh x}{dx^2} = 0$ at $x = 0$ imply that

$$\left.\frac{\partial C_L(\beta, \lambda)}{\partial \beta}\right|_{\beta_{=}^{(\lambda)}(L)} = -2\beta \left.\frac{\partial E_L(\beta, \lambda)}{\partial \beta}\right|_{\beta = \beta_{=}^{(\lambda)}(L)} + O(L^{2d} \beta_t^2 q^{-\nu}) = O(\beta_t L^{2d}). \tag{6.80}$$

Combining (6.80) with the bound (6.79), we conclude that, for q and L large, there exists a unique temperature $\beta_0(L)$ such that $|\beta_0(L) - \beta_{=}^{(\lambda)}(L)| = O(\beta_t^{-1} L^{-2d})$ and

$$C_L(\beta_0(L), \lambda) > C_L(\beta, \lambda)$$

for all $\beta \neq \beta_0(L)$ and $|\beta - \beta_{=}^{(\lambda)}(L)| \leqslant \frac{A}{\Delta e} \frac{1}{L^d}$. However, if $|\beta - \beta_{=}^{(\lambda)}(L)| > \frac{A}{\Delta e} \frac{1}{L^d}$, then, in view of (2.11) and Lemma 6.6,

$$\begin{aligned} C_L(\beta, \lambda) &= \beta^2 (\Delta e\, L^d)^2 \cosh^{-2}(\Delta e(\beta - \beta_{=}^{(\lambda)}(L))\, L^d) + O(L^{2d-1}) \\ &< \beta^2 (\Delta e\, L^d)^2\, [\cosh^{-2} A + O(L^{-1})] \end{aligned} \tag{6.81}$$

so that

$$C_L(\beta_{=}^{(\lambda)}(L), \lambda) - C_L(\beta, \lambda) \geqslant \beta^2 (\Delta e\, L^d)^2\, [1 - \cosh^{-2} A + O(L^{-1})] > 0 \tag{6.82}$$

once q and L are large. Hence, $\beta_0(L) = \beta_{\max}^{(\lambda)}(L)$, which proves Lemma 6.8. ∎

Proof of Theorem 2.3. The claim (a) of the theorem, with

$$b(\lambda, q) = \frac{d(s_{\mathrm{d}} - s_{\mathrm{o}})(\beta_t)}{\beta_t \Delta e} \tag{6.83}$$

follows from Lemmas 6.8 and 6.2(b), taking into account that

$$\beta_t^{-1}\, |(s_{\mathrm{d}} - s_{\mathrm{o}})(\beta_t)|^2\, O(q^{-\nu}) \leqslant \beta_t\, O(q^{-\nu}) = O(1).$$

To get (2.18), we use (6.10) and (4.60).

To prove the claim (b), we first note that in view of the preceding lemma and Lemma A.10, we have

$$\frac{d^k}{dx^k}\tanh x|_{x=\Delta e(\beta-\beta_{=}^{(\lambda)}(L))\,L^d}=\frac{d^k}{dx^k}\tanh x|_{x=\Delta e(\beta-\beta_{\max}^{(\lambda)}(L))\,L^d}+\beta_t^{-1}O(L^{-d}). \tag{6.84}$$

Combined with Lemma 6.6, this implies statement (b) of Theorem 2.3, except for (2.21), which is stronger than the resulting bound if, say, $\beta\geqslant 2\beta_t$. But in this region, $\beta\geqslant\beta_+$, and we can use (6.70) to get $C_L(\beta,\lambda)=\beta_t^2O(L^d)$, which is, in fact, a much stronger bound than (2.21) if $\beta\geqslant 2\beta_t$ since $x^2\cosh^{-2}x\to 0$ as $x\to\infty$.

For $|\beta-\beta_t|\geqslant\frac{\mu\,d\beta_t}{\Delta e}\frac{1}{L}$, the first two claims of Theorem 2.3(c) are contained in Lemma 6.7. The same is true for the last claim in the region $\beta\leqslant\beta_-$, where $\beta\leqslant\beta_t$. For $\beta\geqslant\beta_+$, we insert (6.76) into (6.73). This improves the bound (6.62) to

$$\frac{\partial^{k-1}}{\partial\beta^{k-1}}E_L(\beta,\lambda)=\frac{d^k}{d\beta^k}\left[f_\circ(\beta)\,L^{d-1}(L-1)+2\,dh_\circ L^{d-1}\right]+L^{d-1}e^{-\frac{\lambda}{2}(\beta-\beta_+)}O(q^{-\nu}). \tag{6.85}$$

Observing finally that for $k\geqslant 2$, we have $\frac{d^kf_\circ}{d\beta^k}=e^{-\frac{\lambda}{2}(\beta-\beta_+)}O(q^{-\nu})$ and $\frac{\partial^kh_\circ}{\partial\beta^k}=O(e^{-\frac{\lambda}{2}(\beta-\beta_+)})$ by (6.75) and Lemma A.1, we conclude that

$$\frac{\partial}{\partial\beta}E_L(\beta,\lambda)=\frac{d^2f_\circ(\beta)}{d\beta^2}L^d+L^{d-1}\,O(e^{-\frac{\lambda}{2}(\beta-\beta_+)}), \tag{6.86}$$

which implies the final claim of the theorem. ∎

APPENDIX: AUXILIARY LEMMAS

Lemma A.1. For any $k\in\mathbb{N}$, there exists a finite constant $\mathcal{D}_k$ such that, for all $\beta\geqslant 1$, the kth derivative (with respect to β) of any of the functions $g_\circ$, $h_\circ$, and $h_\circ^{\mathrm{m}}$, $\mathrm{m}=\mathrm{o},\mathrm{d}$, defined by (3.10) and (3.25), respectively, can be bounded by

(a) $\frac{a}{1-e^{-a}}$ if $k=1$,

(b) $\mathcal{D}_k(1+a)^k\,e^{-a\beta}$ if $k\geqslant 2$.

Here $a=1$ for the function $g_\circ$, and $a=\lambda$ otherwise.

Proof. Let us consider the function $f(x)=-\log(e^{ax}-1)$. Obviously, the absolute value of

$$\frac{df}{dx}=-\frac{a}{1-e^{-ax}}$$

is bounded by $\frac{a}{1-e^{-a}}\leqslant 1+a$ on $[1,\infty)$. Using the identity

$$\frac{d^2f}{dx^2}=e^{-ax}\left(\frac{df}{dx}\right)^2,$$

one shows by induction that, for any $k=2,3,\ldots$, there exist constants $C_{k1},\ldots,C_{k(k-1)}$ such that

$$\frac{d^kf}{dx^k}=\sum_{\ell=1}^{k-1}C_{k\ell}\,a^{k-1-\ell}\,e^{-a\ell x}\left(\frac{df}{dx}\right)^{\ell+1}.$$

Using the bound $|df/dx|\leqslant 1+a$, we thus get the bound

$$\left|\frac{d^kf}{dx^k}\right|\leqslant \mathscr{D}_k(1+a)^k\,e^{-ax},\qquad k\geqslant 2, \tag{A.1}$$

where $\mathscr{D}_k=\sum_\ell |C_{k\ell}|$. Taking into account the definitions (3.10) and (3.25), the lemma is proved. ▮

Lemma A.2. Let γ be a contour with $\operatorname{diam}\gamma<\operatorname{diam}V$. Then $|\partial\mathbb{B}(\operatorname{Int}\gamma)|\leqslant\|\gamma\|$.

Proof. The lemma is trivial if γ is an s-contour, or if it is a w-contour with $\operatorname{dist}(\gamma,\partial V)\geqslant\frac{3}{4}$ (in the first case all bonds in $\partial\mathbb{B}(\operatorname{Int}\gamma)$ intersect γ, and in the second case $|\partial\mathbb{B}(\operatorname{Int}\gamma)|=0$). Assume therefore that γ is a w-contour with $\operatorname{dist}(\gamma,\partial V)\leqslant\frac{1}{4}$. Since $\operatorname{diam}\gamma<\operatorname{diam}V$, there is a corner k of V for which $\gamma\cap\partial V\subset\partial\mathscr{O}(k)$. Necessarily, the line $p(b)\subset\mathbb{R}^d$ that passes through the end-points of $b\in\partial\mathbb{B}(\operatorname{Int}\gamma)$, intersects the boundary of $V(\gamma)$ at least twice, and at most one of these intersections can occur on ∂V (recall that $\operatorname{diam}\gamma=\operatorname{diam}V(\gamma)<\operatorname{diam}V$). As a consequence, introducing the segment

$$\mathfrak{s}(b)=\{\langle x,y\rangle\in\overline{\mathbb{B}}:x,y\in p(b)\}, \tag{A.2}$$

at least one of its bonds intersects the contour γ. Observing that $\mathfrak{s}(b)\cap\mathfrak{s}(b')=\varnothing$ for any two different bonds b,b' of $\partial\mathbb{B}(\operatorname{Int}\gamma)$, the lemma is proved. ▮

Lemma A.3. Let γ be an arbitrary contour. Then

(i) $\operatorname{diam} \gamma \leqslant \|\gamma\|+1$,

(ii) $|\overline{\mathbb{B}}(\operatorname{Int} \gamma)| \leqslant (\|\gamma\|+|\partial\mathbb{B}(\operatorname{Int} \gamma)|) \operatorname{diam} \gamma$, and

(iii) $|\overline{\mathbb{B}}(\operatorname{Int} \gamma)| \leqslant 2d \, \|\gamma\|^d$.

Proof. The claim (i) is a direct consequence of the fact that the contour is connected and that it is touching two opposite faces of a cube of side $\operatorname{diam} \gamma$. Indeed, any of $\lfloor \operatorname{diam} \gamma \rfloor \geqslant \operatorname{diam} \gamma - 1$ parallel hyperplanes between this two faces, necessarily containes at least one bond intersecting γ. Otherwise, the contour γ would split into two disconnected pieces.

To prove (ii), consider the set $\mathfrak{S}(\gamma)=\{\mathfrak{s}(b)\}_{b \in \overline{\mathbb{B}}(\operatorname{Int} \gamma)}$ of all segments $\mathfrak{s}(b)$, as defined in (A.2), associated with the bonds of $\overline{\mathbb{B}}(\operatorname{Int} \gamma)$. Then $|\mathfrak{s} \cap \overline{\mathbb{B}}(\operatorname{Int} \gamma)| \leqslant \operatorname{diam} \gamma + \frac{1}{2}$, so that

$$|\overline{\mathbb{B}}(\operatorname{Int} \gamma)| \leqslant 2\, |\mathfrak{S}(\gamma)| \operatorname{diam} \gamma. \tag{A.3}$$

Since, for every segment from $\mathfrak{S}(\gamma)$, we have $2 \leqslant |\mathfrak{s} \cap \partial\mathbb{B}(\operatorname{Int} \gamma)| + \|\gamma\|_{\mathfrak{s}}$, where $\|\gamma\|_{\mathfrak{s}}$ is the number of intersections of bonds from $\mathfrak{s}$ with γ, we have

$$2\, |\mathfrak{S}(\gamma)| \leqslant \|\gamma\| + |\partial\mathbb{B}(\operatorname{Int} \gamma)|. \tag{A.4}$$

Finally, to prove (iii), we notice that for $\operatorname{diam} \gamma < \operatorname{diam} V$ it is a direct consequence of the claims (i), (ii), and Lemma A.2. If $\operatorname{diam} \gamma = \operatorname{diam} V = L+1$, we have $|\overline{\mathbb{B}}(\operatorname{Int} \gamma)| \leqslant |\overline{\mathbb{B}}| = dL^d + \frac{2d}{2} L^{d-1} \leqslant 2\, dL^d$ implying (iii) since $L = \operatorname{diam} \gamma - 1 \leqslant \|\gamma\|$ according to (i). ∎

Lemma A.4. Let γ be a contour with $\operatorname{diam} \gamma < \operatorname{diam} V$. Then $|\overline{\mathbb{B}}(\operatorname{Int} \gamma)| \leqslant 2\, \|\gamma\| \operatorname{diam} \gamma$.

Proof. The claim follows from Lemma A.3(ii) combined with Lemma A.2. ∎

Lemma A.5. Let $\mathscr{K}_V\colon \mathscr{L}_V \to \mathbb{R}$ be a contour weight obeying the conditions (i)–(iv) of Lemma 4.1. Let us define

$$\mathscr{Z}^*(W) = \sum_{\partial^* \subset W} \prod_{\gamma \in \partial^*} (\mathscr{K}_V(\gamma)\, e^{\|\gamma\|})$$

for any W of the form (3.7), where the sum is over all families ∂^* of non-intersecting contours with $V(\gamma) \subset W$ for every $\gamma \in \partial^*$. Further, let

$$\phi^* = -\lim_{L\to\infty} \frac{1}{L^d} \log \mathscr{Z}^*(V), \quad \text{and}$$

$$\sigma^* = -\lim_{L\to\infty} \frac{1}{2\,dL^{d-1}} (\log \mathscr{Z}^*(V) + \phi^* \, |\mathbb{B}|/d).$$

Then, for any $c_1 \geqslant -\phi^*$ and $c_2 \geqslant -\sigma^*$,

$$\sum_{\partial_{\text{ext}} \sqsubset W} e^{-c_1 |\mathbb{B}(\text{Ext})|/d - c_2 \, \|\partial_e \text{Ext}\,\|} \prod_{\gamma\in\partial_{\text{ext}}} \mathscr{K}_V(\gamma) \leqslant e^{O(\epsilon)\,\|\partial_i W\| + O(\epsilon)\,\|\partial^{(d-2)} W\|},$$

where the sum goes over sets ∂_{ext} of contours which are all external with $V(\gamma) \subset W$ for any $\gamma \in \partial_{\text{ext}}$ and $\text{Ext} = W \setminus \bigcup_{\gamma\in\partial_{\text{ext}}} V(\gamma)$.

Proof. If $\mathscr{K}_V(\gamma) \leqslant \epsilon^{\|\gamma\|}$, then $\mathscr{K}_V(\gamma)\, e^{\|\gamma\|} \leqslant \tilde{\epsilon}^{\|\gamma\|}$ with $\tilde{\epsilon} = e\epsilon$. By Lemma 4.1,

$$\log \mathscr{Z}^*(W) = -\Phi^*(W) + O(\epsilon)\,\|\partial_i W\| + O(\epsilon)\,\|\partial^{(d-2)} W\| \tag{A.5}$$

with $\Phi^*(W) = \phi^* |\mathbb{B}(W)|/d + \sigma^*\,\|\partial_e W\|$, where we used that $O(\tilde{\epsilon}) = O(\epsilon)$. Assuming now that $c_1 \geqslant -\phi^*$ and $c_2 \geqslant -\sigma^*$ and using (A.5) together with the fact that for all contours γ we have $\|\partial_i \text{ Int}\,\gamma\| = \|\gamma\|$, we get

$$\begin{aligned}
&\sum_{\partial_{\text{ext}} \sqsubset W} e^{-c_1 |\mathbb{B}(\text{Ext})|/d - c_2\, |\partial_e \text{Ext}|} \prod_{\gamma\in\partial_{\text{ext}}} \mathscr{K}_V(\gamma) \\
&\quad\leqslant e^{\Phi^*(W)} \sum_{\partial_{\text{ext}} \sqsubset W} \prod_{\gamma\in\partial_{\text{ext}}} (\mathscr{K}_V(\gamma)\, e^{-\Phi^*(\text{Int}\,\gamma)}) \\
&\quad= e^{\Phi^*(W) + O(\epsilon)\,\|\partial^{(d-2)} W\|} \sum_{\partial_{\text{ext}} \sqsubset W} \prod_{\gamma\in\partial_{\text{ext}}} (\mathscr{K}_V(\gamma)\, \mathscr{Z}^*(\text{Int}\,\gamma)\, e^{O(\epsilon)\,\|\gamma\|}) \\
&\quad\leqslant e^{\Phi^*(W) + O(\epsilon)\,\|\partial^{(d-2)} W\|} \mathscr{Z}^*(W) = e^{O(\epsilon)\,\|\partial_i W\| + O(\epsilon)\,\|\partial^{(d-2)} W\|}. \qquad \blacksquare
\end{aligned}$$

Lemma A.6. Let g_{m}, h_{m}, $\text{m} = \text{o, d}$, be the quantities defined in (3.10). Let $\kappa_0 \geqslant \kappa > 0$, and $\varphi_{\text{m}}(\beta)$ and $\varsigma_{\text{m}}(\beta)$ be arbitrary functions such that

(i) $\varphi_{\text{m}}(\beta)$ and $\varsigma_{\text{m}}(\beta)$ are continuous, and $\varphi_{\text{m}} = g_{\text{m}} + O(q^{-\kappa_0})$, $\varsigma_{\text{m}} = h_{\text{m}} + O(q^{-\kappa})$;

(ii) $\varphi_{\text{m}}(\beta)$ and $\varsigma_{\text{m}}(\beta)$ are differentiable on $[1, \infty)$, and

$$\frac{d\varphi_{\text{m}}}{d\beta} = \frac{dg_{\text{m}}}{d\beta} + O(q^{-\kappa_0}), \quad \frac{d\varsigma_{\text{m}}}{d\beta} = \frac{dh_{\text{m}}}{d\beta} + O(q^{-\kappa}). \tag{A.6}$$

For $\lambda \in (0, 1)$, and q sufficiently large, the following claims are valid:

(a) There exists a unique point $\hat{\beta}$ such that $\varphi_{\mathrm{o}}(\hat{\beta}) = \varphi_{\mathrm{d}}(\hat{\beta})$. Moreover,

$$\varphi(\beta) = \min\{\varphi_{\mathrm{o}}(\beta), \varphi_{\mathrm{d}}(\beta)\} = \begin{cases} \varphi_{\mathrm{o}}(\beta) & \text{if } \beta \geqslant \hat{\beta}, \\ \varphi_{\mathrm{d}}(\beta) & \text{if } \beta \leqslant \hat{\beta}, \end{cases} \tag{A.7}$$

$$\hat{\beta} = \frac{\log q}{d} + O(q^{-\kappa_1}), \tag{A.8}$$

and

$$(\varsigma_{\mathrm{o}} - \varsigma_{\mathrm{d}})(\hat{\beta}) = -\frac{1}{d}\left(\lambda - \frac{1}{2}\right)\log q + O(q^{-\kappa_2}), \tag{A.9}$$

where $\kappa_1 = \min\{\kappa_0, \frac{1}{d}\}$ and $\kappa_2 = \min\{\kappa, \frac{1}{d}, \frac{\lambda}{d}\} = \min\{\kappa, \frac{\lambda}{d}\}$.

(b) Let $\mathscr{F}_{\mathrm{m}} = \varsigma_{\mathrm{m}} - \varsigma_{\mathrm{m}^c} + \frac{\xi}{d}(\varphi_{\mathrm{m}^c} - \varphi)$ with $\mathrm{m}^c = \mathrm{o}$ if $\mathrm{m} = \mathrm{d}$ and vice versa. If $\xi \leqslant \lambda^2$, then

$$\sup_{\beta:\, \varphi(\beta) = \varphi_{\mathrm{m}}(\beta)} \mathscr{F}_{\mathrm{m}}(\beta) = \mathscr{F}_{\mathrm{m}}(\hat{\beta}).$$

(c) Let $\mathscr{G}_{\mathrm{m}} = \varsigma_{\mathrm{m}} - \varsigma_{\mathrm{m}^c} - \frac{1}{d}(\varphi_{\mathrm{m}} - \varphi)$. Then

$$\sup_{\beta > 0} \mathscr{G}_{\mathrm{m}}(\beta) = \mathscr{G}_{\mathrm{m}}(\hat{\beta}).$$

Proof. Throughout the proof, we assume that q is large.

(a) The function $\varphi_{\mathrm{o}} - \varphi_{\mathrm{d}}$ is decreasing on $[1, \infty)$ since

$$\frac{d}{d\beta}(\varphi_{\mathrm{o}} - \varphi_{\mathrm{d}}) = -\frac{d}{1 - e^{-\beta}} + O(q^{-\kappa_0}) \leqslant -d + O(q^{-\kappa_0}) < 0 \tag{A.10}$$

by (3.10) and (A.6). In addition,

$$(\varphi_{\mathrm{o}} - \varphi_{\mathrm{d}})(\beta) \geqslant \log q - d\log(e-1) + O(q^{-\kappa_0}) > 0$$

for all $\beta \in (0, 1]$ and $\lim_{\beta \to \infty} (\varphi_{\mathrm{o}} - \varphi_{\mathrm{d}})(\beta) = -\infty$. Referring to the assumed continuity of $\varphi_{\mathrm{o}} - \varphi_{\mathrm{d}}$, we get the existence of a unique point $\hat{\beta}$ for which $\varphi_{\mathrm{o}} - \varphi_{\mathrm{d}} \geqslant 0$ if $\beta \leqslant \hat{\beta}$ and $\varphi_{\mathrm{o}} - \varphi_{\mathrm{d}} \leqslant 0$ if $\beta \geqslant \hat{\beta}$. The equality (A.8) is now an immediate consequence of (A.10) and the fact that for $\tilde{\beta} = \frac{1}{d}\log q$ we have $(\varphi_{\mathrm{o}}-\varphi_{\mathrm{d}})(\tilde{\beta})=(g_{\mathrm{o}}-g_{\mathrm{d}})(\beta)+O(q^{-\kappa_0})=O(q^{-\min\{\kappa_0,1/d\}})$. Finally, according to (A.8), we have $e^{\lambda\hat{\beta}}-1=q^{\frac{\lambda}{d}}(1+O(q^{-\kappa_2}))$. Combined with (3.10) and assumption (i) of the lemma we thus get

$$(\varsigma_{\mathrm{o}}-\varsigma_{\mathrm{d}})(\hat{\beta})=(h_{\mathrm{o}}-h_{\mathrm{d}})(\hat{\beta})+O(q^{-\kappa})=-\frac{1}{d}\left(\lambda-\frac{1}{2}\right)\log q+O(q^{-\kappa_2}). \quad \text{(A.11)}$$

(b) Let $\xi\leqslant\lambda^2$. We start by showing that $\ell_1=h_{\mathrm{o}}-\frac{\xi}{d}g_{\mathrm{o}}$ is a decreasing function of β. Indeed,

$$\frac{d\ell_1}{d\beta}=\frac{\xi}{1-e^{-\beta}}-\frac{\lambda}{1-e^{-\lambda\beta}}$$

in view of (3.10). Using that $\pi_c(x)=\frac{e^{-cx}}{(1-e^{-cx})^2}$ is a decreasing function of $c>0$ for any $x>0$, we get

$$\frac{d^2\ell_1}{d\beta^2}=-\xi\pi_1(\beta)+\lambda^2\pi_\lambda(\beta)>(\lambda^2-\xi)\,\pi_1(\beta)\geqslant 0.$$

Thus,

$$\frac{d\ell_1}{d\beta}\leqslant\left.\frac{d\ell_1}{d\beta}\right|_{\beta=\infty}=\xi-\lambda\leqslant-\lambda(1-\lambda)<0$$

for all $\lambda\in(0,1)$ as was claimed.

Now, by virtue of the assumption (i) and the fact that h_{d} and g_{d} do not depend on β, we have

$$\mathscr{F}_{\mathrm{d}}(2)-\mathscr{F}_{\mathrm{d}}(\beta)=\ell_1(\beta)-\ell_1(2)+O(q^{-\kappa})\geqslant\ell_1(1)-\ell_1(2)+O(q^{-\kappa})>0$$

for all $\beta\in(0,1]$ since $\ell_1(1)-\ell_1(2)$ is, according to the monotonicity of ℓ_1, a positive number which, in addition, does not depend on q. Next, with the help of the assumption (ii) and (A.7), we observe that $\mathscr{F}_{\mathrm{m}}$, m = o, d, is differentiable in β on $[1,\infty)\setminus\{\hat{\beta}\}$. The Lagrange mean-value theorem thus yields

$$\begin{aligned}\mathscr{F}_{\mathrm{d}}(\hat{\beta})-\mathscr{F}_{\mathrm{d}}(\beta)&=(\hat{\beta}-\beta)\left.\frac{d\mathscr{F}_{\mathrm{d}}}{d\beta}\right|_{\beta_1}=(\hat{\beta}-\beta)\left(-\left.\frac{d\ell_1}{d\beta}\right|_{\beta_1}+O(q^{-\kappa})\right)\\&\geqslant\frac{\lambda}{2}(1-\lambda)\,(\hat{\beta}-\beta)>0\end{aligned}$$

for any $\beta \in [1, \hat{\beta})$ and some $\beta_1 \in (\beta, \hat{\beta})$. Similarly,

$$\mathscr{F}_{\mathrm{o}}(\hat{\beta}) - \mathscr{F}_{\mathrm{o}}(\beta) \geqslant (\hat{\beta} - \beta) \left(\frac{d\ell_1}{d\beta}\bigg|_{\beta_2} + O(q^{-\kappa}) \right) \geqslant -\frac{\lambda}{2}(1-\lambda)(\hat{\beta} - \beta) > 0$$

for any $\beta \in (\hat{\beta}, \infty)$ and some $\beta_2 \in (\hat{\beta}, \beta)$. The last three bounds justify the claim (b).

(c) Let us prove the statement only for $\mathrm{m} = \mathrm{o}$. First, we show that $\ell_2 = h_{\mathrm{o}} - \frac{1}{d} g_{\mathrm{o}}$ is an increasing function of β. To this end, one observes that $\eta_c(x) = \frac{c\, e^{cx}}{e^{cx}-1}$ is an increasing function of $c > 0$ for all $x > 0$, which, in view of (3.10), implies that $\frac{d\ell_2}{d\beta} = \eta_1(\beta) - \eta_\lambda(\beta) > 0$. Next, using (A.8) and the fact that $\kappa_0 \geqslant \kappa$, we have

$$e^{a\hat{\beta}} - 1 = q^{\frac{a}{d}}(1 + O(\delta)), \qquad \delta = \max\{q^{-1/d}, q^{-\kappa}, q^{-\frac{a}{d}}\} \tag{A.12}$$

for any $0 < a \leqslant 1$. Combined with the assumption (i), (A.7), and (3.10), we get

$$\begin{aligned} \mathscr{G}_{\mathrm{o}}(\hat{\beta}) - \mathscr{G}_{\mathrm{o}}(\beta) &= \ell_2(\hat{\beta}) - \ell_2(\beta) + O(q^{-\kappa}) \geqslant \ell_2(\hat{\beta}) - \ell_2\left(\frac{\hat{\beta}}{2}\right) + O(q^{-\kappa}) \\ &= \log\left(\frac{e^{\frac{\lambda\hat{\beta}}{2}} - 1}{e^{\lambda\hat{\beta}} - 1} \frac{e^{\hat{\beta}} - 1}{e^{\frac{\hat{\beta}}{2}} - 1} \right) + O(q^{-\kappa}) \\ &= \frac{1-\lambda}{2d} \log q + O(\delta) > 0 \end{aligned}$$

for all $\beta \in (0, \frac{\hat{\beta}}{2}]$. Analogously, using also the assumption (ii),

$$\frac{d\mathscr{G}_{\mathrm{o}}}{d\beta}\bigg|_{a\hat{\beta}} = \frac{d\ell_2}{d\beta}\bigg|_{a\hat{\beta}} + O(q^{-\kappa}) = \eta_1(a\hat{\beta}) - \eta_\lambda(a\hat{\beta}) + O(q^{-\kappa}) = 1 - \lambda + O(\delta) > 0$$

for all $a \in [\frac{1}{2}, 1)$, whereas

$$\frac{d\mathscr{G}_{\mathrm{o}}}{d\beta} = \frac{dh_{\mathrm{o}}}{d\beta} + O(q^{-\kappa}) = -\frac{\lambda}{1 - e^{-\lambda\beta}} + O(q^{-\kappa}) \leqslant -\lambda + O(q^{-\kappa}) < 0$$

for all $\beta > \hat{\beta}$. As a result, $\mathscr{G}_{\mathrm{o}}(\hat{\beta}) \geqslant \mathscr{G}_{\mathrm{o}}(\beta)$ for any $\beta \geqslant \frac{\hat{\beta}}{2}$ by the Lagrange mean-value theorem (see above). ▮

For any non-empty admissible set ∂ of w-contours, let us consider the connected components $\mathscr{C}_1, \ldots, \mathscr{C}_n$ of $V \setminus \partial$. Observing that $\overline{\mathbb{B}}(\mathscr{C}_i) \subset \Omega_{\mathrm{o}}(V, \partial)$ or $\overline{\mathbb{B}}(\mathscr{C}_i) \subset \Omega_{\mathrm{d}}(V, \partial)$ for every $1 \leqslant i \leqslant n$, we define $W_{\mathrm{o}}(\partial)$ as the union of all of the former components and $W_{\mathrm{d}}(\partial)$ as the union of the latter ones.

Lemma A.7. Let $\partial \neq \emptyset$ be an admissible set of w-contours and let $W_{\mathrm{o}}(\partial)$, $W_{\mathrm{d}}(\partial)$ be defined as above. Then, for any $\mathrm{m} = \mathrm{o}, \mathrm{d}$, we have the bound

$$\sum_{\gamma \in \partial} \|\gamma\| \geqslant \left| \frac{2\,|\mathbb{B}(W_{\mathrm{m}}(\partial))|}{L-1} - |\partial \mathbb{B}(W_{\mathrm{m}}(\partial))| \right|. \tag{A.13}$$

Proof. Let $\mathrm{m} = \mathrm{o}$ or $\mathrm{m} = \mathrm{d}$. Given a component $\mathscr{C}_i \subset W_{\mathrm{m}}(\partial)$, let $\partial \mathscr{C}_i$ be the boundary of $\mathscr{C}_i$ and $\partial_i = \{\gamma \in \partial : \gamma \subset \overline{\partial \mathscr{C}_i \setminus \partial V}\}$. One obviously has

$$\partial_i \cap \partial_j = \emptyset \qquad \text{for all} \quad 1 \leqslant i < j \leqslant n, \quad \partial = \bigcup_{i:\, \mathscr{C}_i \in W_{\mathrm{m}}(\partial)} \partial_i.$$

In addition, let $\tilde{\mathscr{C}}_i = \{x \in \mathscr{C}_i : \operatorname{dist}(x, \partial V) > \frac{1}{4}\}$ and let $\|\Gamma_i\|$ be the number of the intersections of the boundary of $\tilde{\mathscr{C}}_i$ with the bonds of $\overline{\mathbb{B}}$. Clearly,

$$\|\Gamma_i\| = \sum_{\gamma \in \partial_i} \|\gamma\| + |\partial \mathbb{B}(\mathscr{C}_i)|, \qquad \sum_{i:\, \mathscr{C}_i \subset W_{\mathrm{m}}(\partial)} \|\Gamma_i\| = \sum_{\gamma \in \partial} \|\gamma\| + |\partial \mathbb{B}(W_{\mathrm{m}}(\partial))|.$$

Finally, let π be the set of all the lines $p(b)$ in $\mathbb{R}^d$ each of which passes through the end-points of some $b \in \partial \mathbb{B}$ and let $\pi_i = \{p \in \pi : p \cap \tilde{\mathscr{C}}_i \neq \emptyset\}$. Then $|\mathbb{B}(\mathscr{C}_i)| \leqslant (L-1)\,|\pi_i|$, where $L-1$ is the maximal number of bonds from $\mathbb{B}$ that can lie on a single line $p \in \pi$. Moreover, any line $p \in \pi_i$ contains either at least one bond of $\mathbb{B}$ that intersect twice the boundary of $\tilde{\mathscr{C}}_i$ or at least two bonds of $\overline{\mathbb{B}}$ such that the boundary of $\tilde{\mathscr{C}}_i$ intersects each of them once. In any case, there are at least two intersections of this boundary with bonds from $\overline{\mathbb{B}}$ contained in $p \in \pi_i$, i.e., $2|\pi_i| \leqslant \|\Gamma_i\|$. Hence,

$$|\mathbb{B}(\mathscr{C}_i)| \leqslant (L-1)\,|\pi_i| \leqslant (L-1)\,\frac{\|\Gamma_i\|}{2}.$$

Consequently,

$$\begin{aligned} \sum_{\gamma \in \partial} \|\gamma\| + |\partial \mathbb{B}(W_{\mathrm{m}}(\partial))| &= \sum_{i:\, \mathscr{C}_i \subset W_{\mathrm{m}}(\partial)} \|\Gamma_i\| \\ &\geqslant \frac{2}{L-1} \sum_{i:\, \mathscr{C}_i \in W_{\mathrm{m}}(\partial)} |\mathbb{B}(\mathscr{C}_i)| = \frac{2\,|\mathbb{B}(W_{\mathrm{m}}(\partial))|}{L-1} \end{aligned}$$

and the lemma holds as soon as $\frac{2\,|\mathbb{B}(W_{\mathrm{m}}(\partial))|}{L-1} - |\partial \mathbb{B}(W_{\mathrm{m}}(\partial))| \geqslant 0$. Observing that $|\mathbb{B}| = dL^{d-1}(L-1)$ and $|\partial \mathbb{B}| = 2\,dL^{d-1}$, we get

$$\frac{2\,|\mathbb{B}(W_{\mathrm{o}}(\partial))|}{L-1} - |\partial \mathbb{B}(W_{\mathrm{o}}(\partial))| + \frac{2\,|\mathbb{B}(W_{\mathrm{d}}(\partial))|}{L-1} - |\partial \mathbb{B}(W_{\mathrm{d}}(\partial))| = \frac{2\,|\mathbb{B}|}{L-1} - |\partial \mathbb{B}| = 0.$$

Thus, the absolute value in (A.13) is the same for both $\mathrm{m} = \mathrm{o}$ and $\mathrm{m} = \mathrm{d}$ and non-negative for one of them. ▮

Lemma A.8. Let $\partial \neq \varnothing$ be an admissible set of w-contours and let $W_{\mathrm{o}}(\partial)$, $W_{\mathrm{d}}(\partial)$ be defined as above. Then

$$\min\{\|\partial_e W_{\mathrm{o}}(\partial)\|, \|\partial_e W_{\mathrm{d}}(\partial)\|\} \leqslant \frac{2^{1/d}+1}{2^{1/d}-1} \sum_{\gamma \in \partial} \|\gamma\|. \tag{A.14}$$

Proof. We will reduce the statement to that of Lemma B.3 of ref. 13. Given $x \in \mathbb{Z}^d$, let $c(x)$ be the closed unit cube in $\mathbb{R}^d$ that is centered at x. For W of the form (3.7), let $\bar{W} = \bigcup_{x \in \Lambda \cap W} c(x)$, and let $|\partial \bar{W}|$ be the $(d-1)$-dimensional area of the boundary of $\bar{W}$ in $\mathbb{R}^d$. Note that with this notation, $\|\partial_e V\| = |\partial \mathbb{B}| = |\partial \bar{\Lambda}|$. Introducing the shorthand $W_{\mathrm{o}} = W_{\mathrm{o}}(\partial)$ and $W_{\mathrm{d}} = W_{\mathrm{d}}(\partial)$, we also note that

$$\|\partial_e W_{\mathrm{o}}\| = |\partial \mathbb{B}(W_{\mathrm{o}})| = |\partial \bar{W}_{\mathrm{o}} \cap \partial \bar{\Lambda}|, \tag{A.15}$$

while

$$\|\partial_e W_{\mathrm{d}}\| = |\partial \mathbb{B}(W_{\mathrm{d}})| = |\partial \bar{W}_{\mathrm{d}} \cap \partial \bar{\Lambda}| + |\partial R(W_{\mathrm{d}})|, \tag{A.16}$$

where $\partial R(W_{\mathrm{d}})$ is the set of bonds in $\partial \mathbb{B}(W_{\mathrm{d}})$ that have no endpoint in $W_{\mathrm{d}} \cap \Lambda$. Similarly, introducing $R(W_{\mathrm{d}})$ as the set of bonds in $\mathbb{B}(W_{\mathrm{d}})$ with no endpoint in $W_{\mathrm{d}} \cap \Lambda$, we get

$$\begin{aligned} \|\partial_i W_{\mathrm{d}}\| = \|\partial_i W_{\mathrm{o}}\| &= |\partial \bar{W}_{\mathrm{d}} \setminus \partial \bar{\Lambda}| + |\partial R(W_{\mathrm{d}})| + 2\,|R(W_{\mathrm{d}})| \\ &= |\partial \bar{W}_{\mathrm{o}} \setminus \partial \bar{\Lambda}| + |\partial R(W_{\mathrm{d}})| + 2\,|R(W_{\mathrm{d}})|. \end{aligned} \tag{A.17}$$

Let now m be such that the volume of $\bar{W}_{\mathrm{m}}$ is at most $L^d/2$. By Lemma B.3 of ref. 13, we then have

$$|\partial \bar{W}_{\mathrm{m}} \cap \partial \bar{\Lambda}| \leqslant \frac{2^{1/d}+1}{2^{1/d}-1} |\partial \bar{W}_{\mathrm{m}} \setminus \partial \bar{\Lambda}|. \tag{A.18}$$

Combined with (A.15)–(A.17), we get the claim of the lemma. ▮

Lemma A.9. Let $\psi_r \colon \mathbb{R} \to \mathbb{R}$, $r = 1, 2$, be two C^∞ functions. Then, for any $k \in \mathbb{N}$,

$$\frac{d^k \psi_1(\psi_2(x))}{dx^k} = \sum_{j=1}^{k} \left.\frac{d^j \psi_1(y)}{dy^j}\right|_{y=\psi_2(x)} \sum_{\{I_1,\dots,I_j\}} \prod_{i=1}^{j} \frac{d^{|I_i|}\psi_2(x)}{dx^{|I_i|}},$$

where $\{I_1, \ldots, I_j\}$, $j = 1, \ldots, k$, is a set of non-empty sub-sequences which partition $\{1, \ldots, k\}$ and $|I_i|$, $i = 1, \ldots, j$, is the cardinality of I_i.

Proof. By induction on $k \in \mathbb{N}$. ▮

Lemma A.10. Let x_1, x_2 be two real numbers. For any $k = 0, 1, \ldots,$ there is constant $\theta_k > 0$ such that

$$\left| \left(\frac{d^k}{dx^k} \tanh x \right)_{x_1} - \left(\frac{d^k}{dx^k} \tanh x \right)_{x_2} \right| \leqslant \theta_k \min \left\{ \frac{\tanh x_1}{x_1}, \frac{\tanh x_2}{x_2} \right\} |x_1 - x_2|. \tag{A.19}$$

and

$$\left| \left(\frac{d^k}{dx^k} \tanh x \right)_{x_1} - \left(\frac{d^k}{dx^k} \tanh x \right)_{x_2} \right| \leqslant \theta_k \max \left\{ \frac{1}{\cosh^2 x_1}, \frac{1}{\cosh^2 x_2} \right\} |x_1 - x_2|. \tag{A.20}$$

Proof. Let $x_1, x_2 \in \mathbb{R}$ be given. Without loss of generality, we may suppose that $x_1 > x_2$. Then $\tanh x_1 > \tanh x_2$ and $\frac{\tanh x_1}{x_1} < \frac{\tanh x_2}{x_2}$. Thus,

$$|\tanh x_1 - \tanh x_2| \frac{x_1}{\tanh x_1} = \left(1 - \frac{\tanh x_2}{\tanh x_1} \right) |x_1| < \left| 1 - \frac{x_2}{x_1} \right| |x_1| = |x_1 - x_2|,$$

which verifies the first bound of the lemma for $k = 0$ (with $\theta_0 = 1$). To prove the second bound for $k = 0$, we just observe that

$$|\tanh x_1 - \tanh x_2| = \int_{x_2}^{x_1} dx \frac{1}{\cosh^2 x} \leqslant \max \left\{ \frac{1}{\cosh^2 x_1}, \frac{1}{\cosh^2 x_2} \right\} | x_1 - x_2|.$$

Let $k \geqslant 1$ be fixed now. It is easy to show by induction that there exist constants $\Xi_{k1}, \ldots, \Xi_{kk}$ such that

$$\frac{d^k}{dx^k} \tanh x = \left(\frac{d}{dx} \tanh x \right) \sum_{j=0}^{k} \Xi_{kj} \tanh^j x \tag{A.21}$$

for any $x \in \mathbb{R}$. Using that $|\tanh x| \leqslant 1$ for real $x \in \mathbb{R}$, we get

$$\left| \left(\frac{d^k}{dx^k} \tanh x \right)_{x_1} - \left(\frac{d^k}{dx^k} \tanh x \right)_{x_2} \right| = \left| \int_{x_1}^{x_2} \frac{d^{k+1} \tanh x}{dx^{k+1}} dx \right|$$
$$\leqslant \left| \sum_{j=0}^{k+1} \Xi_{k+1, j} \right| \left| \int_{x_1}^{x_2} \frac{d \tanh x}{dx} dx \right| = \theta_k \, |\tanh x_2 - \tanh x_1| . \quad ▮$$

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