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Partition Function Zeros at First-Order Phase Transitions: Pirogov–Sinai Theory[1]

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This paper is a continuation of our previous analysis[(2)] of partition functions zeros in models with first-order phase transitions and periodic boundary conditions. Here it is shown that the assumptions under which the results of ref. 2 were established are satisfied by a large class of lattice models. These models are characterized by two basic properties: The existence of only a finite number of ground states and the availability of an appropriate contour representation. This setting includes, for instance, the Ising, Potts, and Blume–Capel models at low temperatures. The combined results of ref. 2 and the present paper provide complete control of the zeros of the partition function with periodic boundary conditions for all models in the above class.

KEY WORDS: Partition function zeros; Lee–Yang theorem; Pirogov–Sinai theory; contour models.

This paper is dedicated to Elliott Lieb on the occasion of his 70 th birthday. Elliott was thesis advisor to one of us (J.T.C.) and an inspiration to us all.

1. INTRODUCTION

1.1. Overview

In the recent papers,[(1, 2)] we presented a general theory of partition function zeros in models with periodic boundary conditions and interaction depending on one complex parameter. The analysis was based on a set of

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assumptions, called Assumptions A and B in ref. 2, which are essentially statements concerning differentiability properties of certain free energies supplemented by appropriate non-degeneracy conditions. On the basis of these assumptions we characterized the topology of the resulting phase diagram and showed that the partition function zeros are in one-to-one correspondence with the solutions to specific (and simple) equations. In addition, the maximal degeneracy of the zeros was proved to be bounded by the number of thermodynamically stable phases, and the distance between the zeros and the corresponding solutions was shown to be generically exponentially small in the linear size of the system.

The reliance on Assumptions A and B in ref. 2 permitted us to split the analysis of partition function zeros into two parts, which are distinct in both mathematical and physical content: one concerning the zeros of a complex (in fact, analytic) function—namely the partition function with periodic boundary conditions—subject to specific requirements, and the other concerning the control of the partition function in a statistical mechanical model depending on one complex parameter. The former part of the analysis was carried out in ref. 2; the latter is the subject of this paper. Explicitly, the principal goal of this paper can be summarized as follows: We will define a large class of lattice spin models (which includes several well-known systems, e.g., the Ising and Blume–Capel models) and show that Assumptions A and B are satisfied for every model in this class. On the basis of ref. 2, for any model in this class we then have complete control of the zeros of the partition function with periodic boundary conditions.

The models we consider are characterized by two properties: the existence of only a finite number of *ground states* and the availability of a *contour* representation. In our setting, the term ground state will simply mean a constant—or, after some reinterpretations, a periodic—infinite volume spin configuration. Roughly speaking, the contour representation will be such that the contours correspond to finite, connected subsets of the lattice where the spin configuration differs from any of the possible ground states. A precise definition of these notions is a bit technical; details will be provided in Section 3. Besides these properties, there will also be a few quantitative requirements on the ground state energies and the scaling of the excess contour energy with the size of the contour—the Peierls condition—see Sections 2.1 and 3.2.

These two characteristic properties enable us to apply Pirogov–Sinai theory—a general method for determining low-temperature properties of a statistical mechanical model by perturbing about zero-temperature. The first formulation of this perturbation technique[16, 17] applied to a class of models with real, positive weights. The original "Banach space" approach of refs. 16 and 17 was later replaced by inductive methods,[9] which resulted in a complete classification of translation-invariant Gibbs states.[21] The inductive techniques also permitted a generalization of the characterization of phase stability/coexistence to models with complex weights.[5] However, most relevant for our purposes are the results of ref. 6, dealing with finite-size scaling in the vicinity of first-order phase transitions. There Pirogov–Sinai theory was used to derive detailed asymptotics of finite volume partition functions. The present paper provides, among other things, a variant of ref. 6 that ensures appropriate differentiability of the so-called metastable free energies as required for the analysis of partition function zeros.

The remainder of this paper is organized as follows. Section 1.2 outlines the class of models of interest. Section 1.3 defines the ground state and excitation energies and introduces the torus partition function—the main object of interest in this paper. Section 2.1 lists the assumptions on the models and Section 2.2 gives the statements of the main results of this paper. These immediately imply Assumptions A and B of ref. 2 for all models in the class considered. Sections 3 and 4 introduce the necessary tools from Pirogov–Sinai theory. These are applied in Section 5 to prove the main results of the paper.

1.2. Models of Interest

Here we define the class of models to be considered in this paper. Most of what is to follow in this and the forthcoming sections is inspired by classic texts on spin models, Gibbs states, and Pirogov–Sinai theory, e.g., refs. 8, 18, 20, and 21.

We will consider finite-state spin models on the d-dimensional hypercubic lattice $\mathbb{Z}^d$ for $d \geqslant 2$. At each site $x \in \mathbb{Z}^d$ the *spin*, denoted by σ_x, will take values in a finite set $\mathscr{S}$. A *spin configuration* $\sigma = (\sigma_x)_{x \in \mathbb{Z}^d}$ is an assignment of a spin to each site of the lattice. The interaction Hamiltonian will be described using a collection of potentials (Φ_Λ), where Λ runs over all finite subsets of $\mathbb{Z}^d$. The Φ_Λ are functions on configurations from $\mathscr{S}^{\mathbb{Z}^d}$ with the following properties:

(1) The value $\Phi_\Lambda(\sigma)$ depends only on σ_x with $x \in \Lambda$.

(2) The potential is translation invariant, i.e., if σ' is a translate of σ and Λ' is the corresponding translate of Λ, then $\Phi_{\Lambda'}(\sigma) = \Phi_\Lambda(\sigma')$.

(3) There exists an $R \geqslant 1$ such that $\Phi_\Lambda \equiv 0$ for all Λ with diameter exceeding $R+1$.

Here the *diameter* of a cubic box with $L \times \cdots \times L$ sites is defined to be L while for a general $A \subset \mathbb{Z}^d$ it is the diameter of the smallest cubic box containing A. The constant R is called the *range of the interaction.*

Remark 1.1. Condition (2) has been included mostly for convenience of exposition. In fact, all of the results of this paper hold under the assumption that Φ_Λ are periodic in the sense that $\Phi_{\Lambda'}(\sigma) = \Phi_\Lambda(\sigma')$ holds for Λ and σ related to Λ' and σ' by a translation from $(a\mathbb{Z})^d$ for some fixed integer a. This is seen by noting that the periodic cases can always be converted to translation-invariant ones by considering block-spin variables and integrated potentials.

As usual, the energy of a spin configuration is specified by the Hamiltonian. Formally, the Hamiltonian is represented by a collection of functions (βH_Λ) indexed by finite subsets of $\mathbb{Z}^d$, where βH_Λ is defined by the formula

$$\beta H_\Lambda(\sigma) = \sum_{\Lambda' : \Lambda' \cap \Lambda \neq \varnothing} \Phi_{\Lambda'}(\sigma). \tag{1.1}$$

(The superfluous β, playing the role of the inverse temperature, appears only to maintain formal correspondence with the fundamental formulas of statistical mechanics.) In light of our restriction to finite-range interactions, the sum is always finite.

We proceed by listing a few well known examples of models in the above class. With the exception of the second example, the range of each interaction is equal to 1:

Ising Model. Here $\mathscr{S} = \{-1, +1\}$ and $\Phi_\Lambda(\sigma) \not\equiv 0$ only for Λ containing a single site or a nearest-neighbor pair. In this case we have

$$\Phi_\Lambda(\sigma) = \begin{cases} -h\sigma_x, & \text{if } \Lambda = \{x\}, \\ -J\sigma_x\sigma_y, & \text{if } \Lambda = \{x, y\} \text{ with } |x-y| = 1. \end{cases} \tag{1.2}$$

Here J is the coupling constant, h is an external field and $|x-y|$ denotes the Euclidean distance between x and y.

Perturbed Ising Model. Again $\mathscr{S} = \{-1, +1\}$, but now we allow for arbitrary finite range perturbations. Explicitly,

$$\Phi_\Lambda(\sigma) = \begin{cases} -h\sigma_x, & \text{if } \Lambda = \{x\}, \\ -J_\Lambda \prod_{x \in \Lambda} \sigma_x & \text{if } |\Lambda| \geqslant 2 \text{ and } \operatorname{diam} \Lambda \leqslant R+1. \end{cases} \tag{1.3}$$

The coupling constants J_Λ are assumed to be translation invariant (i.e., $J_\Lambda = J_{\Lambda'}$ if Λ and Λ' are translates of each other). The constant h is again the external field.

Blume–Capel Model. In this case $\mathscr{S}=\{-1,0,+1\}$ and $\Phi_\Lambda(\sigma)\equiv 0$ unless Λ is just a single site or a nearest-neighbor pair. Explicitly, we have

$$\Phi_\Lambda(\sigma)=\begin{cases}-\lambda\sigma_x^2-h\sigma_x, & \text{if}\quad \Lambda=\{x\},\\ J(\sigma_x-\sigma_y)^2, & \text{if}\quad \Lambda=\{x,y\}\quad\text{with } |x-y|=1.\end{cases}\tag{1.4}$$

Here J is the coupling constant, λ is a parameter favoring ± 1 against 0-spins and h is an external field splitting the symmetry between $+1$ and -1.

Potts Model in an External Field. The state space has q elements, $\mathscr{S}=\{1,\dots,q\}$ and Φ_Λ is again nontrivial only if Λ is a one-element set or a pair of nearest-neighbor sites. Explicitly,

$$\Phi_\Lambda(\sigma)=\begin{cases}-h\delta_{\sigma_x,1}, & \text{if}\quad \Lambda=\{x\},\\ -J\delta_{\sigma_x,\sigma_y}, & \text{if}\quad \Lambda=\{x,y\}\quad\text{with } |x-y|=1.\end{cases}\tag{1.5}$$

Here $\delta_{\sigma,\sigma'}$ equals one if $\sigma=\sigma'$ and zero otherwise, J is the coupling constant and h is an external field favoring spin value 1. Actually, the results of this paper will hold only for the low-temperature regime (which in our parametrization corresponds to $J\gg\log q$); a more general argument covering *all* temperatures (but under the condition that q is sufficiently large) will be presented elsewhere.[3, 4]

Any of the constants appearing in the above Hamiltonian can in principle be complex. However, not all complex values of, e.g., the coupling constant will be permitted by our additional restrictions. See Section 2.3 for more discussion.

1.3. Ground States, Excitations, and Torus Partition Function

The key idea underlying our formulation is that *constant* configurations represent the potential ground states of the system. (A precise statement of this fact appears in Assumption C2 later.) This motivates us to define the dimensionless *ground state energy density* e_m associated with spin $m\in\mathscr{S}$ by the formula

$$e_m=\sum_{\Lambda:\,\Lambda\ni 0}\frac{1}{|\Lambda|}\Phi_\Lambda(\sigma^m),\tag{1.6}$$

where $|\Lambda|$ denotes the cardinality of the set Λ and where σ^m is the spin configuration that is equal to m at every site. By our restriction to finite-range interactions, the sum is effectively finite.

The constant configurations represent the states with minimal energy; all other configurations are to be regarded as excitations. Given a spin configuration σ, let $B_R(\sigma)$ denote the union of all cubic boxes $\Lambda \subset \mathbb{Z}^d$ of diameter $2R+1$ such that σ is not constant in Λ. We think of $B_R(\sigma)$ as the set on which σ is "bad" in the sense that it is not a ground state at scale R. The set $B_R(\sigma)$ will be referred to as the *R-boundary* of σ. Then the *excitation energy* $E(\sigma)$ of configuration σ is defined by

$$E(\sigma) = \sum_{x \in B_R(\sigma)} \sum_{\Lambda:\, x \in \Lambda} \frac{1}{|\Lambda|} \Phi_\Lambda(\sigma). \tag{1.7}$$

To ensure that the sum is finite (and therefore meaningful) we will only consider the configurations σ for which $B_R(\sigma)$ is a finite set.

The main quantity of interest in this paper is the partition function with periodic boundary conditions which we now define. Let $L \geqslant 2R+1$, and let $\mathbb{T}_L$ denote the torus of $L \times L \times \cdots \times L$ sites in $\mathbb{Z}^d$, which can be thought of as the factor of $\mathbb{Z}^d$ with respect to the action of the subgroup $(L\mathbb{Z})^d$. Let us consider the Hamiltonian $\beta H_L\colon \mathscr{S}^{\mathbb{T}_L} \to \mathbb{C}$ defined by

$$\beta H_L(\sigma) = \sum_{\Lambda:\, \Lambda \subset \mathbb{T}_L} \Phi_\Lambda(\sigma), \qquad \sigma \in \mathscr{S}^{\mathbb{T}_L}, \tag{1.8}$$

where Φ_Λ are retractions of the corresponding potentials from $\mathbb{Z}^d$ to $\mathbb{T}_L$. (Here we use the translation invariance of Φ_Λ.) Then the *partition function with periodic boundary conditions* in $\mathbb{T}_L$ is defined by

$$Z_L^{\text{per}} = \sum_{\sigma \in \mathscr{S}^{\mathbb{T}_L}} e^{-\beta H_L(\sigma)}. \tag{1.9}$$

In general, Z_L^{per} is a complex quantity which depends on all parameters of the Hamiltonian. We note that various other partition functions will play an important role throughout this paper. However, none of these will be needed for the statement of our main results in Section 2, so we postpone the additional definitions and discussion to Section 4.

We conclude this section with a remark concerning the interchangeability of the various spin states. There are natural examples (e.g., the Potts model) where several spin values are virtually indistinguishable from each other. To express this property mathematically, we will consider the situation where there exists a subgroup $\mathfrak{G}$ of the permutations of $\mathscr{S}$ such that if $\pi \in \mathfrak{G}$ then $e_{\pi(m)} = e_m$ and $E(\pi(\sigma)) = E(\sigma)$ for each $m \in \mathscr{S}$ and each configuration σ with finite $B_R(\sigma)$, where $\pi(\sigma)$ is the spin configuration taking value $\pi(\sigma_x)$ at each x. (Note that $B_R(\pi(\sigma)) = B_R(\sigma)$ for any such permutation π.) Then we call two spin states m and n *interchangeable* if m and n belong to the same orbit of the group $\mathfrak{G}$ on $\mathscr{S}$.

While this extra symmetry has absolutely no effect on the contour analysis of the torus partition sum, it turns out that interchangeable spin states cannot be treated separately in our analysis of partition function zeros. (The precise reason is that interchangeable spin states would violate our non-degeneracy conditions; see Assumption C3, C4 and Theorems 2.33, 2.34 later.) To avoid this difficulty, we will use the factor set $\mathscr{R}=\mathscr{S}/\mathfrak{G}$ instead of the original index set $\mathscr{S}$ when stating our assumptions and results. In accordance with the notation of ref. 2, we will also use r to denote the cardinality of the set $\mathscr{R}$, i.e., $\mathscr{R}=\{1,2,\ldots,r\}$, and q_m to denote the cardinality of the orbit corresponding to $m\in\mathscr{R}$.

2. ASSUMPTIONS AND RESULTS

In this section we list our precise assumptions on the models of interest and state the main results of this paper.

2.1. Assumptions

We will consider the setup outlined in Sections 1.2 and 1.3 with the additional assumption that the parameters of the Hamiltonian depend on one complex parameter z which varies in some open subset $\widetilde{\mathcal{O}}$ of the complex plane. Typically, we will take $z=e^h$ or $z=e^{2h}$ where h is an external field; see the examples at the end of Section 1.2. Throughout this paper we will assume that the spin space $\mathscr{S}$, the factor set $\mathscr{R}$, the integers q_m and the range of the interaction are independent of the parameter z. We will also assume that the spatial dimension d is no less than two.

The assumptions below will be expressed in terms of complex derivatives with respect to z. For brevity of exposition, let us use the standard notation

$$\partial_z=\frac{1}{2}\left(\frac{\partial}{\partial x}-i\frac{\partial}{\partial y}\right)\qquad\text{and}\qquad\partial_{\bar z}=\frac{1}{2}\left(\frac{\partial}{\partial x}+i\frac{\partial}{\partial y}\right)\tag{2.1}$$

for the derivatives with respect to z and $\bar z$, respectively. Here $x=\mathfrak{Re}\,z$ and $y=\mathfrak{Im}\,z$. Our assumptions will be formulated for the exponential weights

$$\varphi_A(\sigma,z)=e^{-\Phi_A(\sigma,z)},\qquad\rho_z(\sigma)=e^{-E(\sigma,z)},\qquad\text{and}\qquad\theta_m(z)=e^{-e_m(z)},\tag{2.2}$$

where we have now made the dependence on z notationally explicit. In terms of the θ_m's and the quantity

$$\theta(z)=\max_{m\in\mathscr{R}}|\theta_m(z)|\tag{2.3}$$

we define the set $\mathscr{L}_\alpha(m)$ by

$$\mathscr{L}_\alpha(m) = \{z \in \widetilde{\mathscr{O}} : |\theta_m(z)| \geqslant \theta(z)\, e^\alpha\}. \tag{2.4}$$

Informally, $\mathscr{L}_\alpha(m)$ is the set of z for which m is "almost" a ground state of the Hamiltonian.

Since we want to refer back to Assumptions A and B of ref. 2, we will call our new hypothesis Assumption C.

Assumption C. There exist a domain $\widetilde{\mathscr{O}} \subset \mathbb{C}$ and constants $\alpha, M, \tau \in (0, \infty)$ such that the following conditions are satisfied.

(0) For each $\sigma \in \mathscr{S}^{\mathbb{Z}^d}$ and each finite $\Lambda \subset \mathbb{Z}^d$, the function $z \mapsto \varphi_\Lambda(\sigma, z)$ is holomorphic in $\widetilde{\mathscr{O}}$.

(1) For all $m \in \mathscr{S}$, all $z \in \widetilde{\mathscr{O}}$, and all $\ell = 0, 1, 2$, the ground state weights obey the bounds

$$|\partial_z^\ell \theta_m(z)| \leqslant M^\ell \theta(z). \tag{2.5}$$

In addition, the quantity $\theta(z)$ is uniformly bounded away from zero in $\widetilde{\mathscr{O}}$.

(2) For every configuration σ with finite R-boundary $B_R(\sigma)$, the Peierls condition

$$|\partial_z^\ell \rho_z(\sigma)| \leqslant (M\, |B_R(\sigma)|)^\ell\, (e^{-\tau} \theta(z))^{|B_R(\sigma)|} \tag{2.6}$$

holds for all $z \in \widetilde{\mathscr{O}}$ and $\ell = 0, 1, 2$.

(3) For all distinct $m, n \in \mathscr{R}$ and all $z \in \mathscr{L}_\alpha(m) \cap \mathscr{L}_\alpha(n)$, we have

$$\left| \frac{\partial_z \theta_m(z)}{\theta_m(z)} - \frac{\partial_z \theta_n(z)}{\theta_n(z)} \right| \geqslant \alpha. \tag{2.7}$$

(4) If $\mathscr{Q} \subset \mathscr{R}$ is such that $|\mathscr{Q}| \geqslant 3$, then for any $z \in \bigcap_{m \in \mathscr{Q}} \mathscr{L}_\alpha(m)$ we assume that the complex quantities $v_m(z) = \theta_m(z)^{-1}\, \partial_z \theta_m(z)$, $m \in \mathscr{Q}$, regarded as vectors in $\mathbb{R}^2$, are vertices of a strictly convex polygon. Explicitly, we demand that the bound

$$\inf \left\{ \left| v_m(z) - \sum_{n \in \mathscr{Q} \setminus \{m\}} \omega_n v_n(z) \right| : \omega_n \geqslant 0,\ \sum_{n \in \mathscr{Q} \setminus \{m\}} \omega_n = 1 \right\} \geqslant \alpha \tag{2.8}$$

holds for every $m \in \mathscr{Q}$ and every $z \in \bigcap_{n \in \mathscr{Q}} \mathscr{L}_\alpha(n)$.

Assumptions C0–C2 are very natural; indeed, they are typically a consequence of the fact that the potentials $\varphi_\Lambda(\sigma, z)$—and hence also $\theta_m(z)$ and $\rho_z(\sigma)$—arise by analytic continuation from the positive real axis.

Assumptions C3 and C4 replace the "standard" multidimensional non-degeneracy conditions which are typically introduced to control the topological structure of the phase diagram, see, e.g., refs. 16, 17, and 20. (However, unlike for the "standard" non-degeneracy conditions, here this control requires a good deal of extra work, see ref. 2.) Assumption C4 is only important in the vicinity of multiple coexistence points (see Section 3.2); otherwise, it can be omitted.

Remark 2.1. For many models, including the first three of our examples, the partition function has both zeros and poles, and sometimes even involves non-integer powers of z. In this situation it is convenient to multiply the partition function by a suitable power of z to obtain a function that is analytic in a larger domain. Typically, this different normalization also leads to a larger domain $\widetilde{\mathcal{O}}$ for which Assumption C holds. Taking, e.g., the Ising model with $z = e^{2h}$, one easily verifies that for low enough temperatures, Assumption C holds everywhere in the complex plane—provided we replace the term $-h\sigma_x$ by $-h(\sigma_x + 1)$. By contrast, in the original representation (where $\varphi_{\{x\}}(\sigma, z) = (\sqrt{z})^{\sigma_x}$), one needs to take out a neighborhood of the negative real axis (or any other ray from zero to infinity) to achieve the analyticity required by Assumption C0.

Remark 2.2. If we replace the term $-h\sigma_x$ in (1.2)–(1.4) by $-h(\sigma_x + 1)$, Assumption C (with $z = e^{2h}$ for the Ising models, and $z = e^h$ for the Blume–Capel and Potts model) holds for all four examples listed in Section 1.2, provided that the nearest-neighbor couplings are ferromagnetic and the temperature is low enough. (For the perturbed Ising model, one also needs that the nearest-neighbor coupling is sufficiently dominant.)

2.2. Main Results

Now we are in a position to state our main results, which show that Assumptions A and B from ref. 2 are satisfied and hence our conclusions concerning the partition function zeros hold. The structure of these theorems parallels the structure of Assumptions A and B. We caution the reader that the precise statement of these results is quite technical. For a discussion of the implications of these theorems, see Section 2.3. The first theorem establishes the existence of metastable free energies and their relation to the quantities θ_m.

Theorem A. Let $M \in (0, \infty)$ and $\alpha \in (0, \infty)$. Then there is a constant τ_0 depending on M, α, the number of spin states $|\mathcal{S}|$ and the dimension d such that if Assumption C holds for the constants M, α, some open domain $\widetilde{\mathcal{O}} \subset \mathbb{C}$ and some $\tau \geqslant \tau_0$, then there are functions $\zeta_m: \widetilde{\mathcal{O}} \to \mathbb{C}$, $m \in \mathscr{R}$, for which the following holds:

(1) There are functions $s_m: \widetilde{\mathcal{O}} \to \mathbb{C}$, $m \in \mathscr{R}$, such that $\zeta_m(z)$ can be expressed as

$$\zeta_m(z) = \theta_m(z)\, e^{s_m(z)} \qquad \text{and} \qquad |s_m(z)| \leqslant e^{-\tau/2}. \tag{2.9}$$

In particular, the quantity $\zeta(z) = \max_{m \in \mathscr{R}} |\zeta_m(z)|$ is uniformly positive in $\widetilde{\mathcal{O}}$.

(2) Each function ζ_m, viewed as a function of two real variables $x = \mathfrak{Re}\, z$ and $y = \mathfrak{Im}\, z$, is twice continuously differentiable on $\widetilde{\mathcal{O}}$ and satisfies the Cauchy–Riemann equations $\partial_{\bar{z}} \zeta_m(z) = 0$ for all $z \in \mathscr{S}_m$, where

$$\mathscr{S}_m = \{ z \in \widetilde{\mathcal{O}} : |\zeta_m(z)| = \zeta(z) \}. \tag{2.10}$$

In particular, ζ_m is analytic in the interior of $\mathscr{S}_m$.

(3) For any pair of distinct indices $m, n \in \mathscr{R}$ and any $z \in \mathscr{S}_m \cap \mathscr{S}_n$ we have

$$\left| \frac{\partial_z \zeta_m(z)}{\zeta_m(z)} - \frac{\partial_z \zeta_n(z)}{\zeta_n(z)} \right| \geqslant \alpha - 2e^{-\tau/2}. \tag{2.11}$$

(4) If $\mathscr{Q} \subset \mathscr{R}$ is such that $|\mathscr{Q}| \geqslant 3$, then for any $z \in \bigcap_{m \in \mathscr{Q}} \mathscr{S}_m$,

$$v_m(z) = \frac{\partial_z \zeta_m(z)}{\zeta_m(z)}, \qquad m \in \mathscr{Q}, \tag{2.12}$$

are the vertices of a strictly convex polygon in $\mathbb{C} \simeq \mathbb{R}^2$.

Theorem A ensures the validity of Assumption A in ref. 2 for any model satisfying Assumption C with τ sufficiently large. Assumption A, in turn, allows us to establish several properties of the topology of the phase diagram, see Section 2.3 later for more details.

Following ref. 2, we will refer to the indices in $\mathscr{R}$ as *phases*, and call a phase $m \in \mathscr{R}$ *stable at* z if $|\zeta_m(z)| = \zeta(z)$. We will say that a point $z \in \widetilde{\mathcal{O}}$ is a point of *phase coexistence* if there are at least two phases $m \in \mathscr{R}$ which are stable at z. In ref. 2 we introduced these definitions without further motivation, anticipating, however, the present work which provides the technical justification of these concepts. Indeed, using the expansion techniques developed in Sections 3 and 4, one can show that, for each $m \in \mathscr{S}$ that corresponds to a stable phase in $\mathscr{R}$, the finite volume states with m-boundary conditions tend to a unique infinite-volume limit $\langle \cdot \rangle_m$ in the sense of weak convergence on linear functionals on local observables. (Here a local observable refers to a function depending only on a finite number of spins.) The limit state is invariant under translations of $\mathbb{Z}^d$, exhibits exponential clustering, and is a small perturbation of the ground state σ^m in the sense that $\langle \delta_{\sigma_x, k} \rangle_m = \delta_{m,k} + O(e^{-\tau/2})$ for all $x \in \mathbb{Z}^d$.

Remark 2.3. Note that two states $\langle \cdot \rangle_m$ and $\langle \cdot \rangle_{m'}$ are considered as two different versions of the same phase if m and m' are indistinguishable, in accordance with our convention that $\mathscr{R}$, and not $\mathscr{S}$, labels phases. Accordingly, the term phase coexistence refers to the coexistence of *distinguishable* phases, and not to the coexistence of two states labelled by different indices in the same orbit $\mathscr{R}$. This interpretation of a "thermodynamic phase" agrees with that used in physics, but disagrees with that sometimes used in the mathematical physics literature.

While Theorem A is valid in the whole domain $\widetilde{\mathcal{O}}$, our next theorem will require that we restrict ourselves to a subset $\mathcal{O} \subset \widetilde{\mathcal{O}}$ with the property that there exists some $\epsilon > 0$ such that for each point $z \in \mathcal{O}$, the disc $\mathbb{D}_\epsilon(z)$ of radius ϵ centered at z is contained in $\widetilde{\mathcal{O}}$. (Note that this condition requires $\mathcal{O}$ to be a strict subset of $\widetilde{\mathcal{O}}$, unless $\widetilde{\mathcal{O}}$ consists of the whole complex plane.) In order to state the next theorem, we will need to recall some notation from ref. 2. Given any $m \in \mathscr{R}$ and $\delta > 0$, let $\mathscr{S}_\delta(m)$ denote the region where the phase m is "almost stable,"

$$\mathscr{S}_\delta(m) = \{z \in \mathcal{O} : |\zeta_m(z)| > e^{-\delta}\zeta(z)\}. \tag{2.13}$$

For any $\mathscr{Q} \subset \mathscr{R}$, we also introduce the region where all phases from $\mathscr{Q}$ are "almost stable" while the remaining ones are not,

$$\mathscr{U}_\delta(\mathscr{Q}) = \bigcap_{m \in \mathscr{Q}} \mathscr{S}_\delta(m) \Big\backslash \bigcup_{n \in \mathscr{Q}^{\mathrm{c}}} \overline{\mathscr{S}_{\delta/2}(n)}, \tag{2.14}$$

with the bar denoting the set closure.

Theorem B. Let $M, \alpha, \epsilon \in (0, \infty)$, and let $\tau \geqslant \tau_0$, where τ_0 is the constant from Theorem A, and let $\kappa = \tau/4$. Let $\widetilde{\mathcal{O}} \subset \mathbb{C}$ and $\mathcal{O} \subset \widetilde{\mathcal{O}}$ be open domains such that that Assumption C holds in $\widetilde{\mathcal{O}}$ and $\mathbb{D}_\epsilon(z) \subset \widetilde{\mathcal{O}}$ for all $z \in \mathcal{O}$. Then there are constants C_0 (depending only on M), M_0 (depending on M and ϵ), and L_0 (depending on d, M, τ, and ϵ) such that for each $m \in \mathscr{R}$ and each $L \geqslant L_0$ there is a function $\zeta_m^{(L)}: \mathscr{S}_{\kappa/L}(m) \to \mathbb{C}$ such that the following holds for all $L \geqslant L_0$:

(1) The function Z_L^{per} is analytic in $\widetilde{\mathcal{O}}$.

(2) Each $\zeta_m^{(L)}$ is non-vanishing and analytic in $\mathscr{S}_{\kappa/L}(m)$. Furthermore,

$$\left|\log \frac{\zeta_m^{(L)}(z)}{\zeta_m(z)}\right| \leqslant e^{-\tau L/8} \tag{2.15}$$

and

$$\left|\partial_z \log \frac{\zeta_m^{(L)}(z)}{\zeta_m(z)}\right| + \left|\partial_{\bar{z}} \log \frac{\zeta_m^{(L)}(z)}{\zeta_m(z)}\right| \leqslant e^{-\tau L/8} \tag{2.16}$$

hold for all $m \in \mathscr{R}$ and all $z \in \mathscr{S}_{\kappa/L}(m)$.

(3) For each $m \in \mathscr{R}$, all $\ell \geqslant 1$, and all $z \in \mathscr{S}_{\kappa/L}(m)$, we have

$$\left|\frac{\partial_z^\ell \zeta_m^{(L)}(z)}{\zeta_m^{(L)}(z)}\right| \leqslant (\ell!)^2 M_0^\ell. \tag{2.17}$$

Moreover, for all distinct $m, n \in \mathscr{R}$ and all $z \in \mathscr{S}_{\kappa/L}(m) \cap \mathscr{S}_{\kappa/L}(n)$,

$$\left|\frac{\partial_z \zeta_m^{(L)}(z)}{\zeta_m^{(L)}(z)} - \frac{\partial_z \zeta_n^{(L)}(z)}{\zeta_n^{(L)}(z)}\right| \geqslant \alpha - 2e^{-\tau/2}. \tag{2.18}$$

(4) For any $\mathscr{Q} \subset \mathscr{R}$, the difference

$$\Xi_{\mathscr{Q},L}(z) = Z_L^{\text{per}}(z) - \sum_{m \in \mathscr{Q}} q_m [\zeta_m^{(L)}(z)]^{L^d} \tag{2.19}$$

satisfies the bound

$$|\partial_z^\ell \Xi_{\mathscr{Q},L}(z)| \leqslant \ell!\,(C_0 L^d)^{\ell+1}\, \zeta(z)^{L^d} \left(\sum_{m \in \mathscr{R}} q_m\right) e^{-\tau L/16} \tag{2.20}$$

for all $\ell \geqslant 0$ and all $z \in \mathscr{U}_{\kappa/L}(\mathscr{Q})$.

Theorem B proves the validity of Assumption B from ref. 2. Together with Theorem A, this in turn allows us to give a detailed description of the positions of the partition function zeros for all models in our class, see Section 2.3.

The principal result of Theorem B is stated in part (4): The torus partition function can be approximated by a finite sum of terms—one for each "almost stable" phase $m \in \mathscr{R}$—which have well controlled analyticity properties. As a consequence, the zeros of the partition function arise as a result of destructive interference between almost stable phases, and all zeros are near to the set of coexistence points $\mathscr{G} = \bigcup_{m \neq n} \mathscr{S}_m \cap \mathscr{S}_n$; see Section 2.3 for further details. Representations of the form (2.19) were crucial for the analysis of finite-size scaling near first-order phase transitions.[6] The original derivation goes back to ref. 5. In our case the situation is complicated by the requirement of analyticity; hence the restriction to $z \in \mathscr{U}_{\kappa/L}(\mathscr{Q})$ in (4).

2.3. Discussion

As mentioned previously, Theorems A and B imply the validity of Assumptions A and B of ref. 2, which in turn imply the principal conclusions of ref. 2 for any model of the kind introduced in Section 1.2 that satisfies Assumption C with τ sufficiently large. Instead of giving the full statements of the results of ref. 2, we will only describe these theorems on a qualitative level. Readers interested in more details are referred to Section 2 of ref. 2.

Our first result concerns the set of coexistence points, $\mathscr{G} = \bigcup_{m \neq n} \mathscr{S}_m \cap \mathscr{S}_n$, giving rise to the complex phase diagram. Here Theorem 2.1 of ref. 2 asserts that $\mathscr{G}$ is the union of a set of simple, smooth (open and closed) curves such that exactly two phases coexist at any interior point of the curve, while at least three phases coexist at the endpoints—these are the *multiple points*. Moreover, in each compact set, any two such curves cannot get too close without intersecting and there are only a finite number of multiple points. These properties are of course direct consequences of the non-degeneracy conditions expressed in Theorems A3 and A4.

Having discussed the phase diagram, we can now turn our attention to the zeros of Z_L^{per}. The combined results of Theorems 2.2–2.4 of ref. 2 yield the following: First, all zeros lie within $O(L^{-d})$ of the set $\mathscr{G}$. Second, along the two-phase coexistence lines with stable phases $m, n \in \mathscr{R}$, the zeros are within $O(e^{-cL})$, for some $c > 0$, of the solutions to the equations

$$q_m^{1/L^d}\,|\zeta_m(z)| = q_n^{1/L^d}\,|\zeta_n(z)|, \tag{2.21}$$

$$L^d\,\mathrm{Arg}(\zeta_m(z)/\zeta_n(z)) = \pi \bmod 2\pi. \tag{2.22}$$

Consecutive solutions to these equations are separated by distances of order L^{-d}, i.e., there are of the other L^d zeros per unit length of the coexistence line. Scaling by L^d, this allows us to define a *density of zeros* along each two-phase coexistence line, which in the limit $L \to \infty$ turns out to be a smooth function varying only over distances of order one.

Near the multiple points the zeros are still in one-to-one correspondence with the solutions of a certain equation. However, our control of the errors here is less precise than in the two-phase coexistence region. In any case, all zeros are at most $(r-1)$-times degenerate. In addition, for models with an Ising-like plus-minus symmetry, Theorem B of ref. 2 gives conditions under which zeros will lie exactly on the unit circle. This is the local Lee–Yang theorem.

Let us demonstrate these results in the context of some of our examples from Section 1.2. We will begin with the standard Ising model at low temperatures. In this case there are two possible phases, labeled + and −, with the corresponding metastable free energies given as functions of $z = e^{2h}$ by

$$\zeta_{\pm}(z) = \exp\{\pm h + e^{-2dJ \mp 2h} + O(e^{-(4d-2)J})\}. \tag{2.23}$$

Symmetry considerations now imply that $|\zeta_+(z)| = |\zeta_-(z)|$ if and only if $\mathfrak{Re}\, h = 0$, i.e., $|z| = 1$, and, as already known from the celebrated Lee–Yang Circle Theorem,[11] the same is true for the actual zeros of Z_L^{per}. However, our analysis allows us to go further and approximately calculate the solutions to the system (2.21) and (2.22), which shows that the zeros of Z_L^{per} lie near the points $z = e^{i\theta_k}$, where $k = 0, 1, \ldots, L^d - 1$ and

$$\theta_k = \frac{2k+1}{L^d}\pi + 2e^{-2dJ} \sin\left(\frac{2k+1}{L^d}\pi\right) + O(e^{-(4d-2)J}). \tag{2.24}$$

Of course, as L increases, higher and higher-order terms in e^{-J} are needed to pinpoint the location of any particular zero (given that the distance of close zeros is of the order L^{-d}). Thus, rather than providing the precise location of any given zero, the above formula should be used to calculate the quantity $\theta_{k+1} - \theta_k$, which is essentially the distance between two consecutive zeros. The resulting derivation of the *density of zeros* is new even in the case of the standard Ising model. A qualitative picture of how the zeros span the unit circle is provided in Fig. 1.

A similar discussion applies to the "perturbed" Ising model, provided the nearest-neighbor coupling is ferromagnetic and the remaining terms in the Hamiltonian are small in some appropriate norm. In the case of general multi-body couplings, the zeros will lie on a closed curve which, generically, is not a circle. (For instance, this is easily verified for the three-body interaction.) However, if only even terms in (σ_x) appear in the Hamiltonian, the models have the plus-minus symmetry required by Theorem 2.5 of ref. 2 and all of the zeros will lie exactly on the unit circle. This shows that the conclusions of the Lee–Yang theorem hold well beyond the set of models to which the classic proof applies.

Finally, in order to demonstrate the non-trivial topology of the set of zeros, let us turn our attention to the Blume–Capel model. In this case there are three possible stable phases, each corresponding to a particular

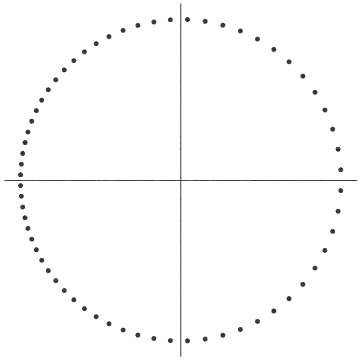

Fig. 1. A schematic figure of the solutions to (2.21) and (2.22) giving the approximate locations of partition function zeros of the Ising model in parameter z which is related to the external field h by $z = e^{2h}$. The plot corresponds to dimension $d = 2$ and torus side $L = 8$. The expansion used for calculating the quantities $\zeta_\pm$ is shown in (2.23). To make the non-uniformity of the spacing between zeros more apparent, the plot has been rendered for the choice $e^{2J} = 2.5$ even though this is beyond the region where we can prove convergence of our expansions.

spin value. In terms of the complex parameter $z = e^h$, the corresponding metastable free energies are computed from the formulas

$$\begin{aligned}
\zeta_+(z) &= z\, e^{\lambda} \exp\{z^{-1} e^{-2dJ-\lambda} + dz^{-2}\, e^{-(4d-2)\,J-2\lambda} + O(e^{-4dJ})\},\\
\zeta_-(z) &= z^{-1} e^{\lambda} \exp\{z e^{-2dJ-\lambda} + dz^{2}\, e^{-(4d-2)\,J-2\lambda} + O(e^{-4dJ})\},\\
\zeta_0(z) &= \exp\{(z+z^{-1})\, e^{-2dJ+\lambda} + d(z^2+z^{-2})\, e^{-(4d-2)\,J+2\lambda} + O(e^{-4dJ})\}.
\end{aligned} \tag{2.25}$$

Here it is essential that the energy of the plus-minus neighboring pair exceeds that of zero-plus (or zero-minus) by a factor of four.

A calculation[1] shows that the zeros lie on two curves which are symmetrical with respect to circle inversion and which may coincide along an arc of the unit circle, depending on the value of λ; see Fig. 2. As λ increases, the shared portion of these curves grows and, for positive λ exceeding a constant of order e^{-2dJ}, all zeros will lie on the unit circle. Note that by the methods of ref. 13, the last result can be established[12] for all temperatures provided λ is sufficiently large, while our results give the correct critical λ but only hold for low temperatures.

3. CONTOUR MODELS AND CLUSTER EXPANSION

Let us turn to the proofs. We begin by establishing the necessary tools for applying Pirogov–Sinai theory. Specifically, we will define contours and show that spin configurations and collections of matching contours are

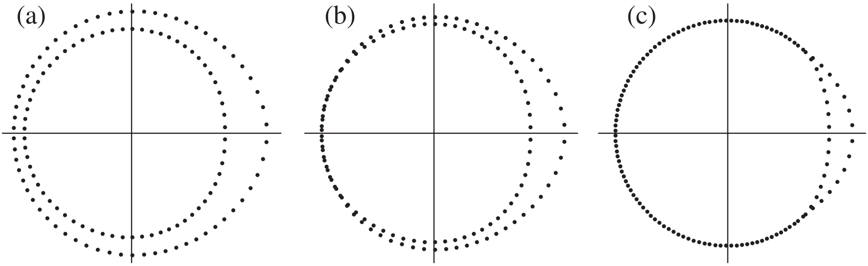

Fig. 2. A picture demonstrating the location of partition function zeros of the Blume–Capel model. Here the zeros concentrate on two curves, related by the circle inversion, which may or may not coincide along an arc of the unit circle. There are two critical values of λ, denoted by $\lambda_c^{\pm}$, both of order e^{-2dJ}, such that for $\lambda < \lambda_c^- < 0$, the two curves do not intersect; see (a). Once λ increases through λ_c^-, a common piece starts to develop which grows as λ increases through the interval $[\lambda_c^-, \lambda_c^+]$, see (b) and (c). Finally, both curves collapse on the unit circle at $\lambda = \lambda_c^+ > 0$ and stay there for all $\lambda > \lambda_c^+$. With the exception of the "bifurcation" points, the zeros lie *exactly* on the unit circle along the shared arc. The non-uniform spacing of the zeros in (b) comes from the influence of the "unstable" phase near the multiple points.

in one-to-one correspondence. This will induce a corresponding relation between the contour and spin partition functions. We will also summarize the facts we will need from the theory of cluster expansions.

3.1. Contours

The goal of this section is to represent spin configurations in terms of contours. Based on the fact—following from Assumption C—that the constant configurations are the only possible minima of (the real part of) the energy, we will define contours as the regions where the spin configuration is not constant.

Recalling our assumption $L \geqslant 2R+1$, let σ be a spin configuration on $\mathbb{T}_L$ and let $B_R(\sigma)$ be the R-boundary of σ. We equip $B_R(\sigma)$ with a graph structure by placing an edge between any two distinct sites $x, y \in B_R(\sigma)$ whenever x and y are contained in a cubic box $\Lambda \subset \mathbb{T}_L$ of diameter $2R+1$ where σ is not constant. We will denote the resulting graph by $G_R(\sigma)$. Some of our definitions will involve the connectivity induced by the graph $G_R(\sigma)$ but we will also use the usual concept of connectivity on $\mathbb{T}_L$ (or $\mathbb{Z}^d$): We say that a set of sites $\Lambda \subset \mathbb{T}_L$ is connected if every two sites from Λ can be connected by a nearest-neighbor path on Λ. Note that the connected components of $B_R(\sigma)$ and the (vertex sets corresponding to the) components of the graph $G_R(\sigma)$ are often very different sets.

Now we are ready to define contours. We start with contours on $\mathbb{Z}^d$, and then define contours on the torus in such a way that they can be easily embedded into $\mathbb{Z}^d$.

Definition 3.1. A *contour* on $\mathbb{Z}^d$ is a pair $Y = (\operatorname{supp} Y, \sigma_Y)$ where $\operatorname{supp} Y$ is a *finite* connected subset of $\mathbb{Z}^d$ and where σ_Y is a spin configuration on $\mathbb{Z}^d$ such that the graph $G_R(\sigma_Y)$ is connected and $B_R(\sigma_Y) = \operatorname{supp} Y$.

A *contour* on $\mathbb{T}_L$ is a pair $Y = (\operatorname{supp} Y, \sigma_Y)$ where $\operatorname{supp} Y$ is a non-empty, connected subset of $\mathbb{T}_L$ with diameter strictly less than $L/2$ and where σ_Y is a spin configuration on $\mathbb{T}_L$ such that the graph $G_R(\sigma_Y)$ is connected and $B_R(\sigma_Y) = \operatorname{supp} Y$.

A *contour network* on $\mathbb{T}_L$ is a pair $\mathcal{N} = (\operatorname{supp} \mathcal{N}, \sigma_{\mathcal{N}})$, where $\mathcal{N}$ is a (possibly empty or non-connected) subset of $\mathbb{T}_L$ and where $\sigma_{\mathcal{N}}$ is a spin configuration on $\mathbb{T}_L$ such that $B_R(\sigma_{\mathcal{N}}) = \operatorname{supp} \mathcal{N}$ and such that the diameter of the vertex set of each component of $G_R(\sigma_{\mathcal{N}})$ is at least $L/2$.

Note that each contour on $\mathbb{T}_L$ has an embedding into $\mathbb{Z}^d$ which is unique up to translation by multiples of L. (Informally, we just need to unwrap the torus without cutting through the contour.) As long as we restrict attention only to finite contours, the concept of a contour network has no counterpart on $\mathbb{Z}^d$, so there we will always assume that $\mathcal{N} = \emptyset$.

Having defined contours and contour networks on $\mathbb{T}_L$ abstractly, our next task is to identify the contours $Y_1, \dots, Y_n$ and the contour network $\mathcal{N}$ from a general spin configuration on $\mathbb{T}_L$. Obviously, the supports of $Y_1, \dots, Y_n$ will be defined as the vertex sets of the components of the graph $G_R(\sigma)$ with diameter less than $L/2$, while $\operatorname{supp} \mathcal{N}$ will be the remaining vertices in $B_R(\sigma)$. To define the corresponding spin configurations we need to demonstrate that the restriction of σ to $\operatorname{supp} Y_i$ (resp., $\operatorname{supp} \mathcal{N}$) can be extended to spin configurations σ_{Y_i} (resp., $\sigma_{\mathcal{N}}$) on $\mathbb{T}_L$ such that $B_R(\sigma_{Y_i}) = \operatorname{supp} Y_i$ (resp., $B_R(\sigma_{\mathcal{N}}) = \operatorname{supp} \mathcal{N}$). It will turn out to be sufficient to show that σ is constant on the *boundary* of each connected component of $\mathbb{T}_L \setminus B_R(\sigma)$.

Given a set $\Lambda \subset \mathbb{T}_L$ (or $\Lambda \subset \mathbb{Z}^d$), let $\partial\Lambda$ denote the external boundary of Λ, i.e., $\partial\Lambda = \{x \in \mathbb{T}_L : \operatorname{dist}(x, \Lambda) = 1\}$. For the purposes of this section, we also need to define the set Λ° which is just Λ reduced by the boundary of its complement, $\Lambda^\circ = \Lambda \setminus \partial(\mathbb{T}_L \setminus \Lambda)$. An immediate consequence of Definition 3.1 (and the restriction to $2R+1 \geqslant 3$) is the following fact:

Lemma 3.2. Let (Λ, σ) be either a contour or a contour network on $\mathbb{T}_L$, and let C be a connected component of $\mathbb{T}_L \setminus \Lambda^\circ$. Then σ is constant on C. If (Λ, σ) is a contour on $\mathbb{Z}^d$, then σ is constant on each connected component C of $\mathbb{Z}^d \setminus \Lambda^\circ$, with Λ° now defined as $\Lambda^\circ = \Lambda \setminus \partial(\mathbb{Z}^d \setminus \Lambda)$.

Proof. Assume that σ is not constant on C. Then there must exist a pair of nearest-neighbor sites $x, y \in C$ such that $\sigma_x \neq \sigma_y$. But then x and all of its nearest neighbors lie in $\Lambda = B_R(\sigma)$. Since $C \cap \Lambda^\circ = \emptyset$ and $x \in C$, we are forced to conclude that $x \in \Lambda \setminus \Lambda^\circ$. But that contradicts the fact that all of the neighbors of x also lie in Λ. The same proof applies to contours on $\mathbb{Z}^d$. ▮

Definition 3.3. Let (Λ, σ) be either a contour or a contour network on $\mathbb{T}_L$ and let C be a connected component of $\mathbb{T}_L \setminus \Lambda$. The common value of the spin on this component in configuration σ will be called the *label* of C. The same definition applies to contours on $\mathbb{Z}^d$, and to connected components C of $\mathbb{Z}^d \setminus \Lambda$.

Let $\Lambda \subset \mathbb{T}_L$ be a connected set with diameter less than $L/2$. Since the diameter was defined by enclosure into a "cubic" box (see Section 1.2), it follows that each such Λ has a well defined exterior and interior. Indeed, any box of side less than $L/2$ enclosing Λ contains less than $(L/2)^d \leqslant L^d/2$ sites, so we can define the *exterior* of Λ, denoted by $\mathrm{Ext}\, \Lambda$, to be the unique component of $\mathbb{T}_L \setminus \Lambda$ that contains more than $L^d/2$ sites. The *interior* $\mathrm{Int}\, \Lambda$ is defined simply by putting $\mathrm{Int}\, \Lambda = \mathbb{T}_L \setminus (\Lambda \cup \mathrm{Ext}\, \Lambda)$. On the other hand, if Λ is the union of disjoint connected sets each with diameter at least $L/2$ we define $\mathrm{Ext}\, \Lambda = \emptyset$ and $\mathrm{Int}\, \Lambda = \mathbb{T}_L \setminus \Lambda$. These definitions for connected sets imply the following definitions for contours on $\mathbb{T}_L$:

Definition 3.4. Let Y be a contour or a contour network on $\mathbb{T}_L$. We then define the *exterior* of Y, denoted by $\mathrm{Ext}\, Y$, as the set $\mathrm{Ext}\, \mathrm{supp}\, Y$, and the *interior* of Y, denoted by $\mathrm{Int}\, Y$, as the set $\mathrm{Int}\, \mathrm{supp}\, Y$. For each $m \in \mathscr{S}$, we let $\mathrm{Int}_m\, Y$ be the union of all components of $\mathrm{Int}\, Y$ with label m. If Y is a contour on T_L, we say that Y is a *m-contour* if the label of $\mathrm{Ext}\, Y$ is m.

Analogous definitions apply to contours on $\mathbb{Z}^d$, except that the exterior of a contour Y is now defined as the infinite component of $\mathbb{Z}^d \setminus \mathrm{supp}\, Y$, while the interior is defined as the union of all finite components of $\mathbb{Z}^d \setminus \mathrm{supp}\, Y$.

While most of the following statements can be easily modified to hold for $\mathbb{Z}^d$ as well as for the torus $\mathbb{T}_L$, for the sake of brevity, we henceforth restrict ourselves to the torus.

Lemma 3.5. Let $R \geqslant 1$ and fix $L > 2R+1$. Let σ be a spin configuration on $\mathbb{T}_L$ and let Λ be either the vertex set of a component of the graph $G_R(\sigma)$ with diameter less than $L/2$ or the union of the vertex sets of all components with diameter at least $L/2$. Let Λ' be of the same form with $\Lambda' \neq \Lambda$. Then exactly one of the following is true:

(1) $\Lambda \cup \mathrm{Int}\, \Lambda \subset \mathrm{Int}\, \Lambda'$ and $\Lambda' \cup \mathrm{Ext}\, \Lambda' \subset \mathrm{Ext}\, \Lambda$, or

(2) $\Lambda' \cup \mathrm{Int}\, \Lambda' \subset \mathrm{Int}\, \Lambda$ and $\Lambda \cup \mathrm{Ext}\, \Lambda \subset \mathrm{Ext}\, \Lambda'$, or

(3) $\Lambda \cup \mathrm{Int}\, \Lambda \subset \mathrm{Ext}\, \Lambda'$ and $\Lambda' \cup \mathrm{Int}\, \Lambda' \subset \mathrm{Ext}\, \Lambda$.

Proof. It is clearly enough to prove the first half of each of the statements (1)–(3), since the second half follow from the first by taking complements (for example in (3), we just use that $\Lambda \cup \operatorname{Int} \Lambda \subset \operatorname{Ext} \Lambda'$ implies $\mathbb{T}_L \setminus (\Lambda \cup \operatorname{Int} \Lambda) \supset \mathbb{T}_L \setminus \operatorname{Ext} \Lambda'$, which is nothing but the statement that $\Lambda' \cup \operatorname{Int} \Lambda' \subset \operatorname{Ext} \Lambda$ by our definition of interiors and exteriors).

In order to prove the first halves of the statements (1)–(3), we first assume that both Λ and Λ' are vertex sets of components of the graph $G_R(\sigma)$ with diameter less than $L/2$. Clearly, since Λ and Λ' correspond to different components of $G_R(\sigma)$, we have $\Lambda \cap \Lambda' = \emptyset$. Moreover, Λ and Λ' are both connected (as subsets of $\mathbb{T}_L$) so we have either $\Lambda \subset \operatorname{Int} \Lambda'$ or $\Lambda \subset \operatorname{Ext} \Lambda'$ and *vice versa*. Hence, exactly one of the following four statements is true:

(a) $\Lambda \subset \operatorname{Int} \Lambda'$ and $\Lambda' \subset \operatorname{Int} \Lambda$, or

(b) $\Lambda \subset \operatorname{Int} \Lambda'$ and $\Lambda' \subset \operatorname{Ext} \Lambda$, or

(c) $\Lambda \subset \operatorname{Ext} \Lambda'$ and $\Lambda' \subset \operatorname{Int} \Lambda$, or

(d) $\Lambda \subset \operatorname{Ext} \Lambda'$ and $\Lambda' \subset \operatorname{Ext} \Lambda$.

We claim that the case (a) cannot happen. Indeed, suppose that $\Lambda \subset \operatorname{Int} \Lambda'$ and observe that if B is a box of size less than $L^d/2$ such that $\Lambda' \subset B$, then $\operatorname{Ext} \Lambda' \supset \mathbb{T}_L \setminus B$. Hence $\operatorname{Int} \Lambda' \subset B$. But then B also encloses Λ and thus $\operatorname{Ext} \Lambda \cap \operatorname{Ext} \Lambda' \supset \mathbb{T}_L \setminus B \neq \emptyset$. Now $\Lambda' \cup \operatorname{Ext} \Lambda'$ is a connected set intersecting $\operatorname{Ext} \Lambda$ but not intersecting Λ (because we assumed that $\Lambda \subset \operatorname{Int} \Lambda'$). It follows that $\Lambda' \cup \operatorname{Ext} \Lambda' \subset \operatorname{Ext} \Lambda$, and hence $\operatorname{Int} \Lambda' \supset \Lambda \cup \operatorname{Int} \Lambda$. But then we cannot have $\Lambda' \subset \operatorname{Int} \Lambda$ as well. This excludes the case (a) above, and also shows that (b) actually gives $\Lambda \cup \operatorname{Int} \Lambda \subset \operatorname{Int} \Lambda'$, which is the first part of the claim (1), while (c) gives $\Lambda' \cup \operatorname{Int} \Lambda' \subset \operatorname{Int} \Lambda$, which is the first part of the claim (2).

Turning to the remaining case (d), let us observe that $\Lambda' \subset \operatorname{Ext} \Lambda$ implies $\operatorname{Int} \Lambda \cap \Lambda' \subset \operatorname{Int} \Lambda \cap \operatorname{Ext} \Lambda = \emptyset$. Since $\Lambda \cap \Lambda' = \emptyset$ as well, this implies $(\Lambda \cup \operatorname{Int} \Lambda) \cap \Lambda' = \emptyset$. But $\Lambda \cup \operatorname{Int} \Lambda$ is a connected subset of $\mathbb{T}_L$, so either $\Lambda \cup \operatorname{Int} \Lambda \subset \operatorname{Int} \Lambda'$ or $\Lambda \cup \operatorname{Int} \Lambda \subset \operatorname{Ext} \Lambda'$. Since $\Lambda \subset \operatorname{Ext} \Lambda'$ excludes the first possibility, we have shown that in case (d), we necessarily have $\Lambda \cup \operatorname{Int} \Lambda \subset \operatorname{Ext} \Lambda'$, which is the first part of statement (3). This concludes the proof of the lemma for the case when both Λ and Λ' are vertex sets of components of the graph $G_R(\sigma)$ with diameter less than $L/2$.

Since it is not possible that both Λ and Λ' are the union of the vertex sets of all components of diameter at least $L/2$, it remains to show the statement of the lemma for the case when Λ is the vertex set of a component of the graph $G_R(\sigma)$ with diameter less than $L/2$, while Λ' is the union of the vertex sets of all components of diameter at least $L/2$. By definition we now have $\operatorname{Ext} \Lambda' = \emptyset$, so we will have to prove that $\Lambda \cup \operatorname{Int} \Lambda \subset \operatorname{Int} \Lambda'$, or equivalently, $\Lambda' \subset \operatorname{Ext} \Lambda$. To this end, let us first observe that $\Lambda \cap \Lambda' = \emptyset$, since Λ has diameter less than $L/2$ while all components of Λ' have diameter at least $L/2$. Consider the set $\operatorname{Int} \Lambda$. Since Λ has diameter less than $L/2$, we can find a box B of side length smaller than $L/2$ that contains Λ, and hence also $\operatorname{Int} \Lambda$. But this implies that none of the components of Λ' can lie in $\operatorname{Int} \Lambda$ (their diameter is too large). Since all these components are connected subsets of $\operatorname{Int} \Lambda \cup \operatorname{Ext} \Lambda$, we conclude that they must be part of $\operatorname{Ext} \Lambda$. This gives the desired conclusion $\Lambda' \subset \operatorname{Ext} \Lambda$. ∎

The previous lemma allows us to organize the components of $G_R(\sigma)$ into a tree-like structure by regarding Λ' to be the "ancestor" of Λ (or, equivalently, Λ to be a "descendant" of Λ') if the first option in Lemma 3.5 occurs. Explicitly, let $W_R(\sigma)$ be the collection of all sets $\Lambda \subset \mathbb{T}_L$ that are either the vertex set of a connected component of $G_R(\sigma)$ with diameter less than $L/2$ or the union of the vertex sets of all connected components of diameter at least $L/2$. We use Λ_0 to denote the latter. If there is no component of diameter $L/2$ or larger, we define $\Lambda_0 = \emptyset$ and set $\operatorname{Int} \Lambda_0 = \mathbb{T}_L$.

We now define a *partial order* on $W_R(\sigma)$ by setting $\Lambda \prec \Lambda'$ whenever $\Lambda \cup \operatorname{Int} \Lambda \subset \operatorname{Int} \Lambda'$. If $\Lambda \prec \Lambda'$, but there is no $\Lambda'' \in W_R(\sigma)$ such that $\Lambda \prec \Lambda'' \prec \Lambda'$, we say that Λ is a child of Λ' and Λ' is a parent of Λ. Using Lemma 3.5, one easily shows that no child has more than one parent, implying that the parent child relationship leads to a tree structure on $W_R(\sigma)$, with root Λ_0. This opens the possibility for inductive arguments from the innermost contours (the leaves in the above tree) to the outermost contours (the children of the root). Our first use of such an argument will be to prove that unique labels can be assigned to the connected components of the complement of $B_R(\sigma)$.

Lemma 3.6. Let σ be a spin configuration on $\mathbb{T}_L$ and let Λ be either the vertex set of a component of the graph $G_R(\sigma)$ with diameter less than $L/2$ or the set of sites in $B_R(\sigma)$ that are not contained in any such component. If C is a connected component of $\mathbb{T}_L \setminus \Lambda^{\circ}$, then σ is constant on $C \cap \Lambda$.

The proof is based on the following fact which is presumably well known:

Lemma 3.7. Let $A \subset \mathbb{Z}^d$ be a finite connected set with a connected complement. Then ∂A^{c} is $*$-connected in the sense that any two sites $x, y \in \partial A^{\mathrm{c}}$ are connected by a path on ∂A^{c} whose individual steps connect only pairs of sites of $\mathbb{Z}^d$ with Euclidean distance not exceeding $\sqrt{2}$.

Proof. The proof will proceed in three steps. In the first step, we will prove that the *edge* boundary of A, henceforth denoted by δA, is a *minimal cutset*. (Here we recall that a set of edges E' in a graph $G=(V,E)$ is called a cutset if the graph $G'=(V,E\setminus E')$ has at least two components, and a cutset E' is called minimal if any proper subset of E' is not a cutset.) In the second step, we will prove that the dual of the edge boundary δA is a connected set of facets, and in the third step we will use this fact to prove that ∂A^{c} is $*$-connected.

Consider thus a set A which is connected and whose complement is connected. Let δA be the edge boundary of A and let E_d be the set of nearest-neighbor edges in $\mathbb{Z}^d$. The set δA is clearly a cutset since any nearest-neighbor path joining A to A^{c} must pass through one of the edges in δA. To show that δA is also minimal, let E' be a proper subset of δA, and let $e\in\delta A\setminus E'$. Since both A and A^{c} are connected, an arbitrary pair of sites $x,y\in\mathbb{Z}^d$ can be joined by a path that uses only edges in $\{e\}\cup(E_d\setminus\delta A)$ $\subset E_d\setminus E'$. Hence such E' is not a cutset which implies that δA is minimal as claimed.

To continue with the second part of the proof, we need to introduce some notation. As usual, we use the symbol $\mathbb{Z}^{*d}$ to denote the set of all points in $\mathbb{R}^d$ with half-integer coordinates. We say that a set $c\subset\mathbb{Z}^{*d}$ is a *k-cell* if the vertices in c are the "corners" of a k-dimensional unit cube in $\mathbb{R}^d$. A d-cell $c\subset\mathbb{Z}^{*d}$ and a vertex $x\in Z^d$ are called dual to each other if x is the center of c (considered as a subset of $\mathbb{R}^d$). Similarly, a facet f (i.e., a $(d-1)$-cell in $\mathbb{Z}^{*d}$) and a nearest-neighbor edge $e\subset\mathbb{Z}^d$ are called dual to each other if the midpoint of e (considered as a line segment in $\mathbb{R}^d$) is the center of f. The boundary ∂C of a set C of d-cells in $\mathbb{Z}^{*d}$ is defined as the set of facets that are contained in an odd number of cells in C, and the boundary ∂F of a set F of facets in $\mathbb{Z}^{*d}$ is defined as the set of $(d-2)$-cells that are contained in an odd number of facets in F. Finally, a set of facets F is called connected if any two facets $f,f'\in F$ can be joined by a path of facets $f_1=f,\ldots,f_n=f'$ in F such that for all $i=1,\ldots,n-1$, the facets f_i and f_{i+1} share a $(d-2)$-cell in $\mathbb{Z}^{*d}$.

Note that an arbitrary finite set of facets F has empty boundary if and only if there exists a finite set of cubes C such that $F=\partial C$, which follows immediately from the fact $\mathbb{R}^d$ has trivial homology. Using this fact, we now prove that the set F of facets dual to δA is connected. Let W be the set of d-cells dual to A, and let $F=\partial W$ be the boundary of W. We will now prove that F is a connected set of facets. Indeed, since $F=\partial W$, we have that F has empty boundary, $\partial F=\varnothing$. Assume that F has more than one component, and let $\tilde{F}\subset F$ be one of them. Then $\tilde{F}$ and $F\setminus\tilde{F}$ are not connected to each other, and hence share no $(d-2)$-cells. But this implies that the boundary of $\tilde{F}$ must be empty itself, so that $\tilde{F}$ is the boundary of some set $\tilde{W}$. This in turn implies that the dual of $\tilde{F}$ is a cutset, contradicting the fact that δA is a minimal cutset.

Consider now two points $x, y \in \partial A^{\mathrm{c}} \subset A$. Then there are points $\tilde{x}, \tilde{y} \in A^{\mathrm{c}}$ such that $\{x, \tilde{x}\}$ and $\{y, \tilde{y}\}$ are edges in δA. Taking into account the connectedness of the dual of δA, we can find a sequence of edges $e_1 = \{x, \tilde{x}\},..., e_n = \{y, \tilde{y}\}$ in δA such that for all $k = 1,..., n-1$, the facets dual to e_k and e_{k+1} share a $(d-2)$ cell in $\mathbb{Z}^{*d}$. As a consequence, the edges e_k and e_{k+1} are either parallel, and the four vertices in these two edges form an elementary plaquette of the form $\{x, x+\mathbf{n}_1, x+\mathbf{n}_2, x+\mathbf{n}_1+\mathbf{n}_2\}$ where $\mathbf{n}_1$ and $\mathbf{n}_2$ are unit vectors in two different lattice directions, or e_k and e_{k+1} are orthogonal and share exactly one endpoint. Since both e_k and e_{k+1} are edges in δA, each of them must contains a point in ∂A^{c}, and by the above case analysis, the two points are at most $\sqrt{2}$ apart. The sequence $e_1,..., e_n$ thus gives rise to a sequence of (not necessarily distinct) points $x_1,..., x_n \in \partial A^{\mathrm{c}}$ such that $x = x_1$, $y = x_n$ and $\mathrm{dist}(x_k, x_{k+1}) \leqslant \sqrt{2}$ for all $k = 1,..., n-1$. This proves that ∂A^{c} is $*$-connected. ▮

Proof of Lemma 3.6. Relying on Lemma 3.5, we will prove the statement by induction from innermost to outermost components of diameter less than $L/2$. Let Λ be the vertex set of a component of the graph $G_R(\sigma)$ with diameter less than $L/2$ and suppose $B_R(\sigma) \cap \mathrm{Int}\,\Lambda = \emptyset$. (In other words, Λ is an innermost component of $B_R(\sigma)$.) Then the same argument that was used in the proof of Lemma 3.2 shows that all connected components of $\mathrm{Int}\,\Lambda$ clearly have the desired property, so we only need to focus on $\mathrm{Ext}\,\Lambda$.

Let us pick two sites $x, y \in \partial\,\mathrm{Ext}\,\Lambda = \Lambda \cap \partial\,\mathrm{Ext}\,\Lambda$ and let $\Lambda' = \Lambda \cup \mathrm{Int}\,\Lambda$. Then Λ' is connected with a connected complement and since Λ has a diameter less than $L/2$, we may as well think of Λ' as a subset of $\mathbb{Z}^d$. Now Lemma 3.7 guarantees that $\partial(\Lambda')^{\mathrm{c}} = \partial\,\mathrm{Ext}\,\Lambda$ is $*$-connected and hence x and y are connected by a $*$-connected path entirely contained in $\partial\,\mathrm{Ext}\,\Lambda$. But the spin configuration must be constant on any box $(z+[-R, R]^d) \cap \mathbb{Z}^d$ with $z \in \partial\,\mathrm{Ext}\,\Lambda$ and thus the spin is constant along the path. It follows that $\sigma_x = \sigma_y$.

The outcome of the previous argument is that now we can "rewrite" the configuration on Λ' without changing the rest of $B_R(\sigma)$. The resulting configuration will have fewer connected components of diameter less than $L/2$ and, proceeding by induction, the proof is reduced to the cases when there are no such components at all. But then we are down to the case when Λ simply equals $B_R(\sigma)$. Using again the argument in the proof of Lemma 3.2, the spin must be constant on each connected component C of $\mathbb{T}_L \setminus B_R(\sigma)^{\circ}$. ▮

The previous lemma shows that each component of the graph $G_R(\sigma)$ induces a unique label on every connected component C of its complement. Consequently, if two contours share such a component—which includes the case when their supports are adjacent to each other—they must induce the same label on it. A precise statement of this "matching" condition is as follows. (Note, however, that not all collections of contours will have this matching property.)

Definition 3.8. We say that the pair $(\mathbb{Y}, \mathscr{N})$—where $\mathbb{Y}$ is a set of contours and $\mathscr{N}$ is a contour network on $\mathbb{T}_L$—is a *collection of matching contours* if the following is true:

(1) $\operatorname{supp} Y \cap \operatorname{supp} Y' = \emptyset$ for any two distinct $Y, Y' \in \mathbb{Y}$ and $\operatorname{supp} Y \cap \operatorname{supp} \mathscr{N} = \emptyset$ for any $Y \in \mathbb{Y}$.

(2) If C is a connected component of $\mathbb{T}_L \setminus [(\operatorname{supp} \mathscr{N})^\circ \cup \bigcup_{Y \in \mathbb{Y}} (\operatorname{supp} Y)^\circ]$, then the restrictions of the spin configurations σ_Y (and $\sigma_{\mathscr{N}}$) to C are the same for all contours $Y \in \mathbb{Y}$ (and contour network $\mathscr{N}$) with $\operatorname{supp} Y \cap C \neq \emptyset$ ($\operatorname{supp} \mathscr{N} \cap C \neq \emptyset$). In other words, the contours/contour network intersecting C induce the same label on C.

Here we use the convention that there are altogether $|\mathscr{S}|$ distinct pairs $(\mathbb{Y}, \mathscr{N})$ with both $\mathbb{Y} = \emptyset$ and $\mathscr{N} = \emptyset$, each of which corresponds to one $m \in \mathscr{S}$.

Definition 3.8 has an obvious analogue for sets $\mathbb{Y}$ of contours on $\mathbb{Z}^d$, where we require that (1) $\operatorname{supp} Y \cap \operatorname{supp} Y' = \emptyset$ for any two distinct $Y, Y' \in \mathbb{Y}$ and (2) all contours intersecting a connected component C of $\mathbb{Z}^d \setminus [\bigcup_{Y \in \mathbb{Y}} (\operatorname{supp} Y)^\circ]$ induce the same label on C.

It remains to check the intuitively obvious fact that spin configurations and collections of matching contours are in one-to-one correspondence:

Lemma 3.9. For each spin configuration $\sigma \in \mathscr{S}^{\mathbb{T}_L}$, there exists a unique collection $(\mathbb{Y}, \mathscr{N})$ of matching contours on $\mathbb{T}_L$ and for any collection $(\mathbb{Y}, \mathscr{N})$ of matching contours on $\mathbb{T}_L$, there exists a unique spin configuration $\sigma \in \mathscr{S}^{\mathbb{T}_L}$ such that the following is true:

(1) The supports of the contours in $\mathbb{Y}$ (of the contour network $\mathscr{N}$) are the vertex sets (the union of the vertex sets) of the connected components of the graph $G_R(\sigma)$ with diameter strictly less than (at least) $L/2$.

(2) The spin configuration corresponding to a collection $(\mathbb{Y}, \mathscr{N})$ of matching contours arise by restricting σ_Y for each $Y \in \mathbb{Y}$ as well as $\sigma_{\mathscr{N}}$ to

the support of the corresponding contour (contour network) and then extending the resulting configuration by the common label of the adjacent connected components.

Proof. Let σ be a spin configuration and let Λ be a component of the graph $G_R(\sigma)$ with diameter less than $L/2$. Then Lemma 3.6 ensures that σ is constant on the boundary ∂C of each component C of Λ^c. Restricting σ to Λ and extending the resulting configuration in such a way that the new configuration, $\tilde{\sigma}$, restricted to a component component C of Λ^c, is equal to the old configuration on ∂C, the pair $(\Lambda, \tilde{\sigma})$ thus defines a contour. Similarly, if Λ is the union of all components of the graph $G_R(\sigma)$ with diameter at least $L/2$ and C is a connected component of $\mathbb{T}_L \setminus \Lambda^\circ$, then σ is, after removal of all contours, constant on C. The contours/contour network $(\mathbb{Y}, \mathcal{N})$ then arise from σ in the way described. The supports of these objects are all disjoint, so the last property to check is that the labels induced on the adjacent connected components indeed match. But this is a direct consequence of the construction.

To prove the converse, let $(\mathbb{Y}, \mathcal{N})$ denote a set of matching contours and let σ be defined by the corresponding contour configuration on the support of the contours (or contour network) and by the common value of the spin in contour configurations for contours adjacent to a connected component of $\mathbb{T}_L \setminus [(\operatorname{supp} \mathcal{N})^\circ \cup \bigcup_{Y \in \mathbb{Y}} (\operatorname{supp} Y)^\circ]$. (If at least one of $\mathbb{Y}, \mathcal{N}$ is nonempty, then this value is uniquely specified because of the matching condition; otherwise, it follows by our convention that empty $(\mathbb{Y}, \mathcal{N})$ carries an extra label.)

It remains to show that $\mathbb{Y}$ are the contours and $\mathcal{N}$ is the contour network of σ. Let A be a component of the graph $G_R(\sigma)$. We have to show that it coincides with $\operatorname{supp} Y$ for some $Y \in \mathbb{Y}$ or with a component of $\operatorname{supp} \mathcal{N}$ (viewed as a graph). We start with the observation that $A \subset \operatorname{supp} \mathcal{N} \cup (\bigcup_{Y \in \mathbb{Y}} \operatorname{supp} Y)$. Next we note that for each $Y \in \mathbb{Y}$, the graph $G_R(\sigma_Y)$ is connected. Since the restriction of σ_Y to $\operatorname{supp} Y$ is equal to the corresponding restriction of σ, we conclude that $\operatorname{supp} Y \cap A \neq \emptyset$ implies $\operatorname{supp} Y \subset A$, and similarly for the components of $\operatorname{supp} \mathcal{N}$. To complete the proof, we therefore only have to exclude that $\operatorname{supp} Y \subset A$ for more than one contour $Y \in \mathbb{Y}$, or that $\Lambda \subset A$ for more than one component Λ of $\operatorname{supp} \mathcal{N}$, and similarly for the combination of contours in Y and components of $\operatorname{supp} \mathcal{N}$.

Let us assume that $\operatorname{supp} Y \subset A$ for more than one contour $Y \in \mathbb{Y}$. Since A is a connected component of the graph $G_R(\sigma)$, this implies that there exists a box $B_z = (z + [-R, R]^d) \cap \mathbb{Z}^d$ and two contours $Y_1, Y_2 \in Y$ such that σ is not constant on B_z, $\operatorname{supp} Y_1 \cup \operatorname{supp} Y_2 \subset A$ and B_z is intersecting both $\operatorname{supp} Y_1$ and $\operatorname{supp} Y_2$. But this is in contradiction with the fact that $\mathbb{Y}$ is a collection of matching contours (and a configuration on any such box not contained in the support of one of the contours in $\mathbb{Y}$ or in a component of supp $\mathcal{N}$ must be constant). In the same way one excludes the case combining supp Y with a component of supp $\mathcal{N}$ or combining two components of supp $\mathcal{N}$. Having excluded everything else, we thus have shown that A is either the support of one of the contours in Y, or one of the components of supp $\mathcal{N}$. ▮

3.2. Partition Functions and Peierls' Condition

A crucial part of our forthcoming derivations concerns various contour partition functions, so our next task will be to define these quantities. We need some notation: Let $(\mathbb{Y}, \mathcal{N})$ be a collection of matching contours on $\mathbb{T}_L$. A contour $Y \in \mathbb{Y}$ is called an *external contour in* $\mathbb{Y}$ if $\operatorname{supp} Y \subset \operatorname{Ext} Y'$ for all $Y' \in \mathbb{Y}$ different from Y, and we will call two contours $Y, Y' \in \mathbb{Y}$ *mutually external* if $\operatorname{supp} Y \subset \operatorname{Ext} Y'$ and $\operatorname{supp} Y' \subset \operatorname{Ext} Y$. Completely analogous definitions apply to a set of matching contours $\mathbb{Y}$ on $\mathbb{Z}^d$ (recall that on $\mathbb{Z}^d$, we always set $\mathcal{N} = \varnothing$). Note that, by Lemma 3.5, two contours of a configuration σ on $\mathbb{T}_L$ are either mutually external or one is contained in the interior of the other. Inspecting the proof of this Lemma 3.5, the reader may easily verify that this remains true for configurations on $\mathbb{Z}^d$, provided the set $B_R(\sigma)$ is finite.

Given a contour $Y = (\operatorname{supp} Y, \sigma_Y)$ or a contour network $\mathcal{N} = (\operatorname{supp} \mathcal{N}, \sigma_{\mathcal{N}})$ let $E(Y, z)$ and $E(\mathcal{N}, z)$ denote the corresponding excitation energies $E(\sigma_Y, z)$ and $E(\sigma_{\mathcal{N}}, z)$ from (1.7). We then introduce exponential weights $\rho_z(Y)$ and $\rho_z(\mathcal{N})$, which are related to the quantities $E(Y, z)$ and $E(\mathcal{N}, z)$ according to

$$\rho_z(Y) = e^{-E(Y, z)} \qquad \text{and} \qquad \rho_z(\mathcal{N}) = e^{-E(\mathcal{N}, z)}. \tag{3.1}$$

The next lemma states that the exponential weights $\theta_m(z)$, $\rho_z(Y)$ and $\rho_z(\mathcal{N})$ are analytic functions of z.

Lemma 3.10. Suppose that Assumption C0 holds, let $q \in \mathcal{S}$, let Y be a q-contour and let $\mathcal{N}$ be a contour network. Then $\theta_q(z)$, $\rho_z(Y)$, and $\rho_z(\mathcal{N})$ are analytic functions of z in $\widetilde{\mathcal{O}}$.

Proof. By Assumption C0, the functions $z \mapsto \varphi_A(\sigma, z) = \exp\{-\Phi_A(\sigma, z)\}$ are holomorphic in $\widetilde{\mathcal{O}}$. To prove the lemma, we will show that $\theta_q(z)$, $\rho_z(Y)$, and $\rho_z(\mathcal{N})$ can be written as products over the exponential potentials $\varphi_A(\sigma, z)$, with $\sigma = \sigma^q$, $\sigma = \sigma_Y$, and $\sigma = \sigma_{\mathcal{N}}$, respectively.

Let us start with $\theta_q(z)$. Showing that θ_q is the product of exponential potentials $\varphi_\Lambda(\sigma^q, z)$ is clearly equivalent to showing that e_q can be rewritten in the form

$$e_q = \sum_{\Lambda \in \mathbb{V}_e} \Phi_\Lambda(\sigma^q), \tag{3.2}$$

where $\mathbb{V}_e$ is a collection of subsets $\Lambda \subset \mathbb{T}_L$. But this is obvious from the definition (1.6) of e_q: just choose $\mathbb{V}_e$ in such a way that it contains exactly one representative from each equivalence class under translations.

Consider now a contour $Y = (\operatorname{supp} Y, \sigma_Y)$ and the corresponding excitation energy $E(Y, z)$. We will want to show that $E(Y, z)$ can be written in the form

$$E(Y, z) = \sum_{\Lambda \in \mathbb{V}_Y} \Phi_\Lambda(\sigma_Y), \tag{3.3}$$

where $\mathbb{V}_Y$ is again a collection of subsets $\Lambda \subset \mathbb{T}_L$. Let $\Lambda_q = \operatorname{Ext} Y \cup \operatorname{Int}_q Y$, and $\Lambda_m = \operatorname{Int}_m Y$ for $m \neq q$. Consider a point $x \in \Lambda_m$. Since $x \notin \operatorname{supp} Y = B_R(\sigma_Y)$, the configuration σ_Y must be constant on any subset $\Lambda \subset \mathbb{T}_L$ that has diameter $2R+1$ or less and contains the point x, implying that

$$\sum_{\Lambda:\, x \in \Lambda} \frac{1}{|\Lambda|} \Phi_\Lambda(\sigma_Y) = \sum_{\Lambda:\, x \in \Lambda} \frac{1}{|\Lambda|} \Phi_\Lambda(\sigma^m) = e_m \tag{3.4}$$

whenever $x \in \Lambda_m$. Using these facts, we now rewrite $E(Y, z)$ as

$$\begin{aligned} E(Y, z) &= \beta H_L(\sigma_Y) - \sum_{x \in \mathbb{T}_L \setminus \operatorname{supp} Y} \; \sum_{\Lambda :\, x \in \Lambda} \frac{1}{|\Lambda|} \Phi_\Lambda(\sigma_Y) \\ &= \sum_{\Lambda \subset \mathbb{T}_L} \Phi_\Lambda(\sigma_Y) - \sum_{m \in \mathscr{S}} |\Lambda_m| \, e_m \\ &= \sum_{\Lambda \subset \operatorname{supp} Y} \Phi_\Lambda(\sigma_Y) + \sum_{m \in \mathscr{S}} \Biggl\{ \Biggl(\sum_{\substack{\Lambda \subset \mathbb{T}_L \\ \Lambda \cap \Lambda_m \neq \varnothing}} \Phi_\Lambda(\sigma^m) \Biggr) - |\Lambda_m| \, e_m \Biggr\}. \end{aligned} \tag{3.5}$$

To complete the proof, we note that the sum over all Λ with $\Lambda \cap \Lambda_m \neq \varnothing$ contains at least $|\Lambda_m|$ translates of each $\Lambda \subset \mathbb{T}_L$ contributing to the right hand side of (3.2). As a consequence, the difference on the right hand side of (3.5) can be written in the form (3.3), proving that $E(Y, z)$ is of the form (3.3). The proof that $\rho_z(\mathcal{N})$ is an analytic function of z is virtually identical. ∎

Next we define partition functions in finite subsets of $\mathbb{Z}^d$. Fix an index $q \in \mathscr{S}$. Let $\Lambda \subset \mathbb{Z}^d$ be a finite set and let $\mathscr{M}(\Lambda, q)$ be the set of all collections $\mathbb{Y}$ of matching contours in $\mathbb{Z}^d$ with the following properties:

(1) For each $Y \in \mathbb{Y}$, we have $\operatorname{supp} Y \cup \operatorname{Int} Y \subset \Lambda$.

(2) The external contours in $\mathbb{Y}$ are q-contours.

Note that $\operatorname{supp} Y \cup \operatorname{Int} Y \subset \Lambda$ is implied by the simpler condition that $\operatorname{supp} Y \subset \Lambda$ if $\mathbb{Z}^d \setminus \Lambda$ is connected, while in the case where $\mathbb{Z}^d \setminus \Lambda$ is not connected, the condition $\operatorname{supp} Y \cup \operatorname{Int} Y \subset \Lambda$ is stronger, since it implies that none of the contours $Y \in \mathbb{Y}$ contain any hole of Λ in its interior. (Here a hole is defined as a finite component of $\mathbb{Z}^d \setminus \Lambda$.) In the sequel, we will say that *Y is a contour in Λ* whenever Y obeys the condition $\operatorname{supp} Y \cup \operatorname{Int} Y \subset \Lambda$.

The *contour partition function* in Λ with boundary condition q is then defined by

$$Z_q(\Lambda, z) = \sum_{\mathbb{Y} \in \mathscr{M}(\Lambda, q)} \Bigg[\prod_{m \in \mathscr{S}} \theta_m(z)^{|\Lambda_m(\mathbb{Y})|} \Bigg] \prod_{Y \in \mathbb{Y}} \rho_z(Y), \tag{3.6}$$

where $\Lambda_m(\mathbb{Y})$ denotes the union of all components of $\Lambda \setminus \bigcup_{Y \in \mathbb{Y}} \operatorname{supp} Y$ with label m, and $|\Lambda_m(\mathbb{Y})|$ stands for the cardinality of $\Lambda_m(\mathbb{Y})$.

If we add the condition that the contour network $\mathscr{N}$ is empty, the definitions of the set $\mathscr{M}(\Lambda, q)$ and the partition function $Z_q(\Lambda, z)$ clearly extends to any subset $\Lambda \subset \mathbb{T}_L$, because on $\mathbb{T}_L$ every contour has a well defined exterior and interior. However, our goal is to have a contour representation for the full torus partition function. Let $\mathscr{M}_L$ denote the set of all collections $(\mathbb{Y}, \mathscr{N})$ of matching contours in $\mathbb{T}_L$ which, according to our convention, include an extra label $m \in \mathscr{S}$ when both $\mathbb{Y}$ and $\mathscr{N}$ are empty. If $(\mathbb{Y}, \mathscr{N}) \in \mathscr{M}_L$ is such a collection, let $\Lambda_m(\mathbb{Y}, \mathscr{N})$ denote the union of the components of $\mathbb{T}_L \setminus (\operatorname{supp} \mathscr{N} \cup \bigcup_{Y \in \mathbb{Y}} \operatorname{supp} Y)$ with label m. Then we have:

Proposition 3.11 (Contour Representation). The partition function on the torus $\mathbb{T}_L$ is given by

$$Z_L^{\mathrm{per}}(z) = \sum_{(\mathbb{Y}, \mathscr{N}) \in \mathscr{M}_L} \Bigg[\prod_{m \in \mathscr{S}} \theta_m(z)^{|\Lambda_m(\mathbb{Y}, \mathscr{N})|} \Bigg] \rho_z(\mathscr{N}) \prod_{Y \in \mathbb{Y}} \rho_z(Y). \tag{3.7}$$

In particular, we have

$$Z_L^{\mathrm{per}}(z) = \sum_{(\varnothing, \mathscr{N}) \in \mathscr{M}_L} \rho_z(\mathscr{N}) \prod_{m \in \mathscr{S}} Z_m(\Lambda_m(\varnothing, \mathscr{N}), z). \tag{3.8}$$

Proof. By Lemma 3.9, the spin configurations σ are in one-to-one correspondence with the pairs $(\mathbb{Y}, \mathcal{N}) \in \mathcal{M}_L$. Let $(\mathbb{Y}, \mathcal{N})$ be the pair corresponding to σ. Rewriting (1.8) as

$$\beta H_L(\sigma) = \sum_{x \in \mathbb{T}_L} \sum_{\substack{\Lambda:\, \Lambda \subset \mathbb{T}_L \\ \Lambda \ni x}} \frac{1}{|\Lambda|} \Phi_\Lambda(\sigma), \tag{3.9}$$

we can now split the first sum into several parts: one for each $m \in \mathscr{S}$ corresponding to $x \in \Lambda_m(\mathbb{Y}, \mathcal{N})$, one for each $Y \in \mathbb{Y}$ corresponding to $x \in \operatorname{supp} Y$, and finally, one for the part of the sum corresponding to $x \in \operatorname{supp} \mathcal{N}$. Invoking the definitions of the energies $e_m(z)$, $E(Y, z)$ and $E(\mathcal{N}, z)$, this gives

$$\beta H_L(\sigma) = \sum_{m \in \mathscr{S}} e_m(z) \, |\Lambda_m(\mathbb{Y}, \mathcal{N})| + \sum_{Y \in \mathbb{Y}} E(Y, z) + E(\mathcal{N}, z). \tag{3.10}$$

Strictly speaking, the fact that the excitation energy factors (technically, sums) over contours and contour networks requires a proof. Since this is straightforward using induction as in the proof of Lemma 3.6, starting again with the innermost contours, we leave the formal proof to the reader. Using the definitions of $\theta_m(z)$, $\rho_z(Y)$, and $\rho_z(\mathcal{N})$ and noting that, by Lemma 3.9, the sum over σ can be rewritten as the sum over $(\mathbb{Y}, \mathcal{N}) \in \mathcal{M}_L$, formula (3.7) directly follows.

The second formula, (3.8), formally arises by a resummation of all contours that can contribute together with a given contour network $\mathcal{N}$. It only remains to check that if $\mathbb{Y}_m \subset \mathbb{Y}$ is the set of $Y \in \mathbb{Y}$ with $\operatorname{supp} Y \subset \Lambda_m = \Lambda_m(\emptyset, \mathcal{N})$, then $\mathbb{Y}_m$ can take any value in $\mathcal{M}(\Lambda_m, m)$. But this follows directly from Definition 3.8 and the definition of $\mathcal{M}(\Lambda_m, m)$. ▮

In order to be useful, the representations (3.7) and (3.8) require that contours and contour networks are sufficiently suppressed with respect to the maximal ground state weight θ. This is ensured by Assumption C2, which guarantees that $|\rho_z(Y)| \leqslant \theta(z)^{|Y|} \, e^{-\tau |Y|}$ and $|\rho_z(\mathcal{N})| \leqslant \theta(z)^{|\mathcal{N}|} \, e^{-\tau |\mathcal{N}|}$, where we used the symbols $|Y|$ and $|\mathcal{N}|$ to denote the cardinality of $\operatorname{supp} Y$ and $\operatorname{supp} \mathcal{N}$, respectively.

3.3. Cluster Expansion

The last ingredient that we will need is the *cluster expansion*, which will serve as our principal tool for evaluating and estimating logarithms of various partition functions. The cluster expansion is conveniently formulated in the context of so-called abstract polymer models.[7, 10, 14, 19] Let K be a countable set—the set of all *polymers*—and let $\nsim$ be the *relation of incompatibility* which is a reflexive and symmetric binary relation on K. For each $\mathsf{A} \subset \mathsf{K}$, let $\mathscr{M}(\mathsf{A})$ be the set of multi-indices $\mathsf{X}: \mathsf{K} \to \{0\} \cup \mathbb{N}$ that are finite, $\sum_{\gamma \in \mathsf{K}} \mathsf{X}(\gamma) < \infty$, and that satisfy $\mathsf{X}(\gamma) = 0$ whenever $\gamma \notin \mathsf{A}$. Further, let $\mathscr{C}(\mathsf{A})$ be the set of all multi-indices $\mathsf{X} \in \mathscr{M}(\mathsf{A})$ with values in $\{0, 1\}$ that satisfy $\mathsf{X}(\gamma)\, \mathsf{X}(\gamma') = 0$ whenever $\gamma \nsim \gamma'$ and $\gamma \neq \gamma'$.

Let $\mathfrak{z}: \mathsf{K} \to \mathbb{C}$ be a polymer functional. For each finite subset $\mathsf{A} \subset \mathsf{K}$, let us define the polymer partition function $\mathscr{Z}(\mathsf{A})$ by the formula

$$\mathscr{Z}(\mathsf{A}) = \sum_{\mathsf{X} \in \mathscr{C}(\mathsf{A})} \prod_{\gamma \in \mathsf{K}} \mathfrak{z}(\gamma)^{\mathsf{X}(\gamma)}. \tag{3.11}$$

In the most recent formulation,[7,14] the cluster expansion corresponds to a multidimensional Taylor series for the quantity $\log \mathscr{Z}(\mathsf{A})$, where the complex variables are the $\mathfrak{z}(\gamma)$. Here *clusters* are simply multi-indices $\mathsf{X} \in \mathscr{M}(\mathsf{K})$ for which any nontrivial decomposition of X leads to incompatible multi-indices. Explicitly, if X can be written as $\mathsf{X}_1 + \mathsf{X}_2$ with $\mathsf{X}_1, \mathsf{X}_2 \not\equiv 0$, then there exist two (not necessary distinct) polymers $\gamma_1, \gamma_2 \in \mathsf{K}$, $\gamma_1 \nsim \gamma_2$, such that $\mathsf{X}_1(\gamma_1)\, \mathsf{X}_2(\gamma_2) \neq 0$.

Given a finite sequence $\Gamma = (\gamma_1, \ldots, \gamma_n)$ of polymers in K, let $n(\Gamma) = n$ be the length of the sequence Γ, let $\mathscr{G}(\Gamma)$ be the set of all connected graphs on $\{1, \ldots, n\}$ that have no edge between the vertices i and j if $\gamma_i \sim \gamma_j$, and let X_Γ be the multi-index for which $\mathsf{X}_\Gamma(\gamma)$ is equal to the number of times that γ appears in Γ. For a finite multi-index X, we then define

$$a^{\mathrm{T}}(\mathsf{X}) = \sum_{\Gamma: \mathsf{X}_\Gamma = \mathsf{X}} \frac{1}{n(\Gamma)!} \sum_{\mathfrak{g} \in \mathscr{G}(\Gamma)} (-1)^{|\mathfrak{g}|}, \tag{3.12}$$

with $|\mathfrak{g}|$ denoting the number of edges in $\mathfrak{g}$, and

$$\mathfrak{z}^{\mathrm{T}}(\mathsf{X}) = a^{\mathrm{T}}(\mathsf{X}) \prod_{\gamma \in \mathsf{K}} \mathfrak{z}(\gamma)^{\mathsf{X}(\gamma)}. \tag{3.13}$$

Note that $\mathscr{G}(\Gamma) = \emptyset$ if X_Γ is not a cluster, implying, in particular, that $\mathfrak{z}^{\mathrm{T}}(\mathsf{X}) = 0$ whenever X is not a cluster. We also use the notation $\mathsf{X} \nsim \gamma$ whenever X is a cluster such that $\mathsf{X}(\gamma') > 0$ for at least one $\gamma' \nsim \gamma$.

The main result of ref. 14 (building upon ref. 7) is then as follows:

Theorem 3.12 (Cluster Expansion). Let $a: \mathsf{K} \to [0, \infty)$ be a function and let $\mathfrak{z}_0: \mathsf{K} \to [0, \infty)$ be polymer weights satisfying the bound

$$\sum_{\substack{\gamma' \in \mathsf{K} \\ \gamma' \nsim \gamma}} \mathfrak{z}_0(\gamma')\, e^{a(\gamma')} \leqslant a(\gamma), \qquad \gamma \in \mathsf{K}. \tag{3.14}$$

Then $\mathscr{Z}(\mathsf{A}) \neq 0$ for any finite set $\mathsf{A} \subset \mathsf{K}$ and any collection of polymer weights $\mathfrak{z}\colon \mathsf{K} \to \mathbb{C}$ in the multidisc $\mathbb{D}_\mathsf{A} = \{(\mathfrak{z}(\gamma))\colon |\mathfrak{z}(\gamma)| \leqslant \mathfrak{z}_0(\gamma), \gamma \in \mathsf{A}\}$. Moreover, if we define $\log \mathscr{Z}(\mathsf{A})$ as the unique continuous branch of the complex logarithm of $\mathscr{Z}(\mathsf{A})$ on $\mathbb{D}_\mathsf{A}$ normalized so that $\log \mathscr{Z}(\mathsf{A}) = 0$ when $\mathfrak{z}(\gamma) = 0$ for all $\gamma \in \mathsf{A}$, then

$$\log \mathscr{Z}(\mathsf{A}) = \sum_{\mathsf{X} \in \mathscr{M}(\mathsf{A})} \mathfrak{z}^\mathrm{T}(\mathsf{X}) \tag{3.15}$$

holds for each finite set $\mathsf{A} \subset \mathsf{K}$. Here the power series on the right hand side converges absolutely on the multidisc $\mathbb{D}_\mathsf{A}$. Furthermore, the bounds

$$\sum_{\substack{\mathsf{X} \in \mathscr{M}(\mathsf{K}) \\ \mathsf{X}(\gamma) \geqslant 1}} |\mathfrak{z}^\mathrm{T}(\mathsf{X})| \leqslant \sum_{\mathsf{X} \in \mathscr{M}(\mathsf{K})} \mathsf{X}(\gamma)\, |\mathfrak{z}^\mathrm{T}(\mathsf{X})| \leqslant |\mathfrak{z}(\gamma)|\, e^{a(\gamma)} \tag{3.16}$$

and

$$\sum_{\substack{\mathsf{X} \in \mathscr{M}(\mathsf{K}) \\ \mathsf{X} \not\sim \gamma}} |\mathfrak{z}^\mathrm{T}(\mathsf{X})| \leqslant a(\gamma) \tag{3.17}$$

hold for each $\gamma \in \mathsf{K}$.

Proof. This is essentially the main result of ref. 14 stated under the (stronger) condition (3.14), which is originally due to refs. 10 and 15. To make the correspondence with ref. 14 explicit, let

$$\mu(\gamma) = \log(1 + |\mathfrak{z}(\gamma)|\, e^{a(\gamma)}) \tag{3.18}$$

and note that $\mu(\gamma) \leqslant |\mathfrak{z}(\gamma)|\, e^{a(\gamma)} \leqslant \mathfrak{z}_0(\gamma)\, e^{a(\gamma)}$. The condition (3.14) then guarantees that we have $\sum_{\gamma' \not\sim \gamma} \mu(\gamma') \leqslant a(\gamma)$ and hence

$$|\mathfrak{z}(\gamma)| = (e^{\mu(\gamma)} - 1)\, e^{-a(\gamma)} \leqslant (e^{\mu(\gamma)} - 1) \exp\Big\{-\sum_{\gamma' \not\sim \gamma} \mu(\gamma')\Big\}. \tag{3.19}$$

This implies that any collection of weights $\mathfrak{z}\colon \mathsf{K} \to \mathbb{C}$ such that $|\mathfrak{z}(\gamma)| \leqslant \mathfrak{z}_0(\gamma)$ for all $\gamma \in \mathsf{K}$ will fulfill the principal condition of the main theorem of ref. 14. Hence, we can conclude that $\mathscr{Z}(\mathsf{A}) \neq 0$ in $\mathbb{D}_\mathsf{A}$ and that (3.15) holds. Moreover, as shown in ref. 14, both quantities on the left-hand side of (3.16) are bounded by $e^{\mu(\gamma)} - 1$ which simply equals $|\mathfrak{z}(\gamma)|\, e^{a(\gamma)}$. The bound (3.16) together with the condition (3.14) immediately give (3.17). ∎

To facilitate the future use of this result, we will extract the relevant conclusions into two lemmas. Given a spin state $q \in \mathscr{S}$, let K_q denote the set of all q-contours in $\mathbb{Z}^d$. If $Y, Y' \in \mathsf{K}_q$, let us call Y and Y' *incompatible* if

$\operatorname{supp} Y \cap \operatorname{supp} Y' \neq \emptyset$. If A is a finite set of q-contours, we will let $\mathscr{Z}(\mathsf{A})$ be the polymer sum (3.11) defined using this incompatibility relation. Then we have:

Lemma 3.13. There exists a constant $c_0 = c_0(d, |\mathscr{S}|) \in (0, \infty)$ such that, for all $q \in \mathscr{S}$ and all contour functionals $\mathfrak{z}\colon \mathsf{K}_q \to \mathbb{C}$ satisfying the condition

$$|\mathfrak{z}(Y)| \leqslant \mathfrak{z}_0(Y) = e^{-(c_0+\eta)\,|Y|} \qquad \text{for all} \quad Y \in \mathsf{K}_q, \tag{3.20}$$

for some $\eta \geqslant 0$, the following holds for all $k \geqslant 1$:

(1) $\mathscr{Z}(\mathsf{A}) \neq 0$ for all finite $\mathsf{A} \subset \mathscr{K}_q$ with $\log \mathscr{Z}(\mathsf{A})$ given by (3.15), and

$$\sum_{\substack{\mathsf{X} \in \mathscr{M}(\mathsf{K}_q) \\ V(\mathsf{X}) \ni 0,\, \|\mathsf{X}\| \geqslant k}} |\mathfrak{z}^{\mathrm{T}}(\mathsf{X})| \leqslant e^{-\eta k}. \tag{3.21}$$

Here $V(\mathsf{X}) = \bigcup_{Y:\, \mathsf{X}(Y)>0} V(Y)$ with $V(Y) = \operatorname{supp} Y \cup \operatorname{Int} Y$ and $\|\mathsf{X}\| = \sum_{Y \in \mathsf{K}_q} \mathsf{X}(Y)\,|Y|$.

(2) Furthermore, if the activities $\mathfrak{z}(Y)$ are twice continuously differentiable (but not necessarily analytic) functions of a complex parameter z such that the bounds

$$|\partial_w \mathfrak{z}(Y)| \leqslant \mathfrak{z}_0(Y) \qquad \text{and} \qquad |\partial_w \partial_{w'} \mathfrak{z}(Y)| \leqslant \mathfrak{z}_0(Y) \tag{3.22}$$

hold for any $w, w' \in \{z, \bar{z}\}$ and any $Y \in \mathsf{K}_q$, then

$$\sum_{\substack{\mathsf{X} \in \mathscr{M}(\mathsf{K}_q) \\ V(\mathsf{X}) \ni 0,\, \|\mathsf{X}\| \geqslant k}} |\partial_w \mathfrak{z}^{\mathrm{T}}(\mathsf{X})| \leqslant e^{-\eta k} \qquad \text{and} \qquad \sum_{\substack{\mathsf{X} \in \mathscr{M}(\mathsf{K}_q) \\ V(\mathsf{X}) \ni 0,\, \|\mathsf{X}\| \geqslant k}} |\partial_w \partial_{w'} \mathfrak{z}^{\mathrm{T}}(\mathsf{X})| \leqslant e^{-\eta k}, \tag{3.23}$$

for any $w, w' \in \{z, \bar{z}\}$.

Using, for any finite $\Lambda \subset \mathbb{Z}^d$, the notation $\mathsf{K}_{q,\Lambda} = \{Y \in \mathsf{K}_q : \operatorname{supp} Y \cup \operatorname{Int} Y \subset \Lambda\}$ and $\partial\Lambda$ for the set of sites in $\mathbb{Z}^d \setminus \Lambda$ that have a nearest neighbor in Λ, we get the following lemma as an easy corollary:

Lemma 3.14. Suppose that the weights $\mathfrak{z}$ satisfy the bound (3.20) and are invariant under the translations of $\mathbb{Z}^d$. Then the *polymer pressure* $s_q = \lim_{\Lambda \uparrow \mathbb{Z}^d} |\Lambda|^{-1} \log \mathscr{Z}(\mathsf{K}_{q,\Lambda})$ exists and is given by

$$s_q = \sum_{\mathsf{X} \in \mathscr{M}(\mathsf{K}_q) :\, V(\mathsf{X}) \ni 0} \frac{1}{|V(\mathsf{X})|}\, \mathfrak{z}^{\mathrm{T}}(\mathsf{X}). \tag{3.24}$$

Moreover, the bounds

$$|s_q| \leqslant e^{-\eta} \tag{3.25}$$

and

$$\big|\log \mathscr{Z}(\mathsf{K}_{q,\Lambda}) - s_q\, |\Lambda|\big| \leqslant e^{-\eta}\, |\partial\Lambda| \tag{3.26}$$

hold. Finally, if the conditions (3.22) on derivatives of the weights $\mathfrak{z}(Y)$ are also met, the polymer pressure s_q is twice continuously differentiable in z with the bounds

$$|\partial_w s_q| \leqslant e^{-\eta} \qquad \text{and} \qquad |\partial_w \partial_{w'} s_q| \leqslant e^{-\eta}, \tag{3.27}$$

valid for any $w, w' \in \{z, \bar{z}\}$.

Proof of Lemma 3.13. Let us consider a polymer model where polymers are either a single site of $\mathbb{Z}^d$ or a q-contour from K_q. (The reason for including single sites as polymers will become apparent below.) Let the compatibility between contours be defined by disjointness of their supports while that between a contour Y and a site x by disjointness of $\{x\}$ and $\operatorname{supp} Y \cup \operatorname{Int} Y$. If we let $\mathfrak{z}(\gamma) = 0$ whenever γ is just a single site, this polymer model is indistinguishable from the one considered in the statement of the lemma. Let us choose c_0 so that

$$\sum_{Y \in \mathsf{K}_q : V(Y) \ni 0} e^{(2-c_0)\,|Y|} \leqslant 1. \tag{3.28}$$

To see that this is possible with a constant c_0 depending only on the dimension and the cardinality of $\mathscr{S}$, we note that each polymer is a connected subset of $\mathbb{Z}^d$. As is well known, the number of such sets of size n containing the origin grows only exponentially with n. Since there are only finitely many spin states, this shows that it is possible to choose c_0 as claimed.

Defining $a(\gamma) = 1$ if γ is a single site and $a(Y) = |Y|$ if Y is a q-contour in K_q, the assumption (3.14) of Theorem 3.12 is then satisfied. (Note that assumption (3.14) requires slightly less than (3.28), namely the analogue of (3.28) with the exponent of $(1-c_0)\,|Y|$ instead of $(2-c_0)\,|Y|$; the reason why we chose c_0 such that (3.28) holds will become clear momentarily.) Theorem 3.12 guarantees that $\mathscr{Z}(\mathsf{A}) \neq 0$ and (3.15) holds for the corresponding cluster weights $\mathfrak{z}^{\mathsf{T}}$. Actually, assumption (3.14) is, for all $\eta \geqslant 0$, also satisfied when $\mathfrak{z}(Y)$ is replaced by $\mathfrak{z}(Y)\, e^{b(Y)}$ with $b(Y) = \eta\, |Y|$, yielding

$$\sum_{\substack{\mathsf{X} \in \mathscr{M}(\mathsf{K}) \\ \mathsf{X} \not\sim \gamma}} e^{b(\mathsf{X})}\, |\mathfrak{z}^{\mathsf{T}}(\mathsf{X})| \leqslant a(\gamma) \tag{3.29}$$

with $b(\mathsf{X}) = \eta \, \|\mathsf{X}\|$ instead of (3.17). Using (3.29) with γ chosen to be the polymer represented by the site at the origin and observing that the quantity $b(\mathsf{X})$ exceeds ηk for any cluster contributing to the sum in (3.21), we get the bound

$$e^{\eta k} \sum_{\substack{\mathsf{X} \in \mathscr{M}(\mathsf{K}_q) \\ V(\mathsf{X}) \ni 0, \, \|\mathsf{X}\| \geqslant k}} |\mathfrak{z}^{\mathrm{T}}(\mathsf{X})| \leqslant \sum_{\substack{\mathsf{X} \in \mathscr{M}(\mathsf{K}_q) \\ V(\mathsf{X}) \ni 0}} |\mathfrak{z}^{\mathrm{T}}(\mathsf{X})| \, e^{b(\mathsf{X})} \leqslant 1, \tag{3.30}$$

i.e., the bound (3.21).

In order to prove the bounds (3.23), we first notice that, in view of (3.13) and (3.22) we have

$$|\partial_w \mathfrak{z}^{\mathrm{T}}(\mathsf{X})| \leqslant \|\mathsf{X}\| \, |\mathfrak{z}_0^{\mathrm{T}}(\mathsf{X})| \leqslant e^{\|\mathsf{X}\|} \, |\mathfrak{z}_0^{\mathrm{T}}(\mathsf{X})| \tag{3.31}$$

and

$$|\partial_w \partial_{w'} \mathfrak{z}^{\mathrm{T}}(\mathsf{X})| \leqslant \|\mathsf{X}\|^2 \, |\mathfrak{z}_0^{\mathrm{T}}(\mathsf{X})| \leqslant e^{\|\mathsf{X}\|} \, |\mathfrak{z}_0^{\mathrm{T}}(\mathsf{X})|. \tag{3.32}$$

Using (3.29) with $b(Y) = (\eta + 1) \, |Y|$ (which is also possible since we choose c_0 such that (3.28) holds as stated, instead of the weaker condition where $(2 - c_0) \, |Y|$ is replaced by $(1 - c_0) \, |Y|$) we get (3.23) in the same way as (3.21). ∎

Proof of Lemma 3.14. The bound (3.21) for $k = 1$ immediately implies that the sum in (3.24) converges with $|s_q| \leqslant e^{-\eta}$. Using (3.15) and standard resummation techniques, we rewrite the left hand side of (3.26) as

$$\left| \log \mathscr{Z}(\mathsf{K}_{q,\Lambda}) - s_q \, |\Lambda| \right| = \left| \sum_{\substack{\mathsf{X} \in \mathscr{M}(\mathsf{K}_q) \\ V(\mathsf{X}) \not\subset \Lambda}} \frac{|V(\mathsf{X}) \cap \Lambda|}{|V(\mathsf{X})|} \, \mathfrak{z}^{\mathrm{T}}(\mathsf{X}) \right|. \tag{3.33}$$

Next we note that for any cluster $\mathsf{X} \in \mathscr{M}(\mathsf{K}_q)$, the set $V(\mathsf{X})$ is a connected subset of $\mathbb{Z}^d$, which follows immediately from the observations that $\operatorname{supp} Y \cup \operatorname{Int} Y$ is connected for all contours Y, and that incompatibility of two contours Y, Y' implies that $\operatorname{supp} Y \cap \operatorname{supp} Y' \neq \varnothing$. Since only clusters with $V(\mathsf{X}) \cap \Lambda \neq \varnothing$ and $V(\mathsf{X}) \cap \Lambda^{\mathrm{c}} \neq \varnothing$ contribute to the right hand side of (3.33), we conclude that the right hand side of (3.33) can be bounded by a sum over clusters $\mathsf{X} \in \mathsf{K}_q$ with $V(\mathsf{X}) \cap \partial\Lambda \neq \varnothing$. Using this fact and the bound (3.21) with $k = 1$, (3.26) is proved.

Similarly, using the bounds (3.23) in combination with explicit expression (3.24) in terms of absolutely converging cluster expansions, the claims (3.27) immediately follow. ∎

Remark 3.15. The proof of Lemma 3.13 holds without changes if we replace the set of all q-contours in $\mathbb{Z}^d$ by the set of all q-contours on the torus $\mathbb{T}_L$. This is not true, however, for the proof of the bound (3.26) from Lemma 3.14 since one also has to take into account the difference between clusters wrapped around the torus and clusters in $\mathbb{Z}^d$. The corresponding modifications will be discussed in Section 4.4.

4. PIROGOV–SINAI ANALYSIS

The main goal of this section is to develop the techniques needed to control the torus partition function. Along the way we will establish some basic properties of the metastable free energies which will be used to prove the statements concerning the quantities ζ_m. Most of this section concerns the contour model on $\mathbb{Z}^d$. We will return to the torus in Sections 4.4 and 5.

All of the derivations in this section are based on assumptions that are slightly more general than Assumption C. Specifically, we only make statements concerning a contour model satisfying the following three conditions (which depend on two parameters, τ and M):

(1) The partition functions $Z_q(\Lambda, z)$ and $Z_L^{\text{per}}(z)$ are expressed in terms of the energy variables $\theta_m(z)$ and contour weights ρ_z as stated in (3.6) and (3.7), respectively.

(2) The weights ρ_z of contours and contour networks are translation invariant and are twice continuously differentiable functions on $\widetilde{\mathscr{O}}$. They obey the bounds

$$|\partial_z^{\ell}\partial_{\bar{z}}^{\bar{\ell}}\rho_z(Y)| \leqslant (M\,|Y|)^{\ell+\bar{\ell}}\, e^{-\tau\,|Y|}\theta(z)^{|Y|} \tag{4.1}$$

and

$$|\partial_z^{\ell}\partial_{\bar{z}}^{\bar{\ell}}\rho_z(\mathcal{N})| \leqslant (M\,|\mathcal{N}|)^{\ell+\bar{\ell}}\, e^{-\tau\,|\mathcal{N}|}\theta(z)^{|\mathcal{N}|} \tag{4.2}$$

as long as $\ell, \bar{\ell} \geqslant 0$ and $\ell+\bar{\ell} \leqslant 2$.

(3) The energy variables θ_m are twice continuously differentiable functions on $\widetilde{\mathscr{O}}$ and obey the bounds

$$|\partial_z^{\ell}\partial_{\bar{z}}^{\bar{\ell}}\theta_m(z)| \leqslant (M)^{\ell+\bar{\ell}}\,\theta(z) \tag{4.3}$$

as long as $\ell, \bar{\ell} \geqslant 0$ and $\ell+\bar{\ell} \leqslant 2$. We will assume that $\theta(z)$ is bounded uniformly from below throughout $\widetilde{\mathscr{O}}$. However, we allow that some of the θ_m vanish at some $z \in \widetilde{\mathscr{O}}$.

In particular, throughout this section we will not require that any of the quantities θ_m, $\rho_z(Y)$, or $\rho_z(\mathcal{N})$ is analytic in z.

4.1. Truncated Contour Weights

The key idea of contour expansions is that, for phases that are thermodynamically stable, contours appear as heavily suppressed perturbations of the corresponding ground states. At the points of the phase diagram where all ground states lead to stable phases, cluster expansion should then allow us to calculate all important physical quantities. However, even in these special circumstances, the direct use of the cluster expansion on (3.6) is impeded by the presence of the energy terms $\theta_m(z)^{|\Lambda_m(\mathbb{Y})|}$ and, more seriously, by the requirement that the contour labels match.

To solve these problems, we will express the partition function in a form which does not involve any matching condition. First we will rewrite the sum in (3.6) as a sum over mutually external contours $\mathbb{Y}^{\text{ext}}$ times a sum over collections of contours which are contained in the interior of one of the contours in $\mathbb{Y}^{\text{ext}}$. For a fixed contour $Y \in \mathbb{Y}^{\text{ext}}$, the sum over all contours inside $\text{Int}_m Y$ then contributes the factor $Z_m(\text{Int}_m Y, z)$, while the exterior of the contours in $\mathbb{Y}^{\text{ext}}$ contributes the factor $\theta_m(z)^{|\text{Ext}|}$, where $\text{Ext} = \text{Ext}_\Lambda(\mathbb{Y}^{\text{ext}}) = \bigcap_{Y \in \mathbb{Y}^{\text{ext}}} (\text{Ext}\, Y \cap \Lambda)$. As a consequence, we can rewrite the partition function (3.6) as

$$Z_q(\Lambda, z) = \sum_{\mathbb{Y}^{\text{ext}}} \theta_q(z)^{|\text{Ext}|} \prod_{Y \in \mathbb{Y}^{\text{ext}}} \left\{ \rho_z(Y) \prod_m Z_m(\text{Int}_m Y, z) \right\}, \tag{4.4}$$

where the sum goes over all collections of compatible external q-contours in Λ.

At this point, we use an idea which originally goes back to ref. 9. Let us multiply each term in the above sum by 1 in the form

$$1 = \prod_{Y \in \mathbb{Y}^{\text{ext}}} \prod_m \frac{Z_q(\text{Int}_m Y, z)}{Z_q(\text{Int}_m Y, z)}. \tag{4.5}$$

Associating the partition functions in the denominator with the corresponding contour, we get

$$Z_q(\Lambda, z) = \sum_{\mathbb{Y}^{\text{ext}}} \theta_q(z)^{|\text{Ext}|} \prod_{Y \in \mathbb{Y}^{\text{ext}}} (\theta_q(z)^{|Y|} K_q(Y, z)\, Z_q(\text{Int}\, Y, z)), \tag{4.6}$$

where $K_q(Y, z)$ is given by

$$K_q(Y, z) = \rho_z(Y)\, \theta_q(z)^{-|Y|} \prod_{m \in \mathscr{S}} \frac{Z_m(\text{Int}_m Y, z)}{Z_q(\text{Int}_m Y, z)}. \tag{4.7}$$

Proceeding by induction, this leads to the representation

$$Z_q(\Lambda, z) = \theta_q(z)^{|\Lambda|} \sum_{\mathbb{Y} \in \mathscr{C}(\Lambda, q)} \prod_{Y \in \mathbb{Y}} K_q(Y, z), \tag{4.8}$$

where $\mathscr{C}(\Lambda, q)$ denotes the set of all collections of non-overlapping q-contours in Λ. Clearly, the sum on the right hand side is exactly of the form needed to apply cluster expansion, provided the contour weights satisfy the necessary convergence assumptions.

Notwithstanding the appeal of the previous construction, a bit of caution is necessary. Indeed, in order for the weights $K_q(Y, z)$ to be well defined, we are forced to assume—or prove by cluster expansion, provided we somehow know that the weights K_q have the required decay—that $Z_q(\mathrm{Int}_m\, Y, z) \neq 0$. In the "physical" cases when the contour weights are real and positive (and the ground-state energies are real-valued), this condition usually follows automatically. However, here we are considering contour models with general complex weights and, in fact, our ultimate goal is actually to look at situations where a partition function vanishes.

Matters get even more complicated whenever there is a ground state which fails to yield a stable state (which is what happens at a generic point of the phase diagram). Indeed, for such ground states, the occurrence of a large contour provides a mechanism for flipping from an unstable to a stable phase—which is the favored situation once the volume gain of free energy exceeds the energy penalty at the boundary. Consequently, the relative weights of (large) contours in unstable phases are generally large, which precludes the use of the cluster expansion altogether. A classic solution to this difficulty is to modify the contour functionals for unstable phases.[5, 6, 21] We will follow the strategy of ref. 6, where contour weights are truncated with the aid of a smooth mollifier.

To introduce the truncated contours weights, let us consider a $C^2(\mathbb{R})$-function $x \mapsto \chi(x)$, such that $0 \leqslant \chi(\cdot) \leqslant 1$, $\chi(x) = 0$ for $x \leqslant -2$, and $\chi(x) = 1$ for $x \geqslant -1$. Let c_0 be the constant from Lemma 3.13. Using χ as a regularized truncation factor, we shall inductively define new contour weights $\widetilde{K}'_q(\cdot, z)$ so that $|\widetilde{K}'_q(Y, z)| \leqslant e^{-(c_0+\tau/2)\,|Y|}$ for all q-contours Y. By Lemma 3.13, the associated partition functions $Z'_q(\cdot, z)$ defined by

$$Z'_q(\Lambda, z) = \theta_q(z)^{|\Lambda|} \sum_{\mathbb{Y} \in \mathscr{C}(\Lambda, q)} \prod_{Y \in \mathbb{Y}} \widetilde{K}'_q(Y, z) \tag{4.9}$$

can then be controlled by cluster expansion. (Of course, later we will show that $\widetilde{K}'_q(\cdot, z) = K_q(\cdot, z)$ and $Z'_q(\Lambda, z) = Z_q(\Lambda, z)$ whenever the ground state q gives rise to a stable phase.)

Let $\theta_q(z) \neq 0$, let Y be a q-contour in Λ, and suppose that $Z'_m(\Lambda', z)$ has been defined by (4.9) for all $m \in \mathscr{S}$ and all $\Lambda' \subsetneqq \Lambda$. Let us further assume by induction that $Z'_q(\Lambda', z) \neq 0$ for all $m \in \mathscr{S}$ and all $\Lambda' \subsetneqq \Lambda$. We then define a smoothed cutoff function $\phi_q(Y, z)$ by

$$\phi_q(Y, z) = \prod_{m \in \mathscr{S}} \chi_{q;\, m}(Y, z), \tag{4.10}$$

where

$$\chi_{q;\, m}(Y, z) = \chi\left(\frac{\tau}{4} + \frac{1}{|Y|} \log \left|\frac{Z'_q(\operatorname{Int} Y, z)\, \theta_q(z)^{|Y|}}{Z'_m(\operatorname{Int} Y, z)\, \theta_m(z)^{|Y|}}\right|\right). \tag{4.11}$$

Here $\chi_{q;\, m}(Y, z)$ is interpreted as 1 if $\theta_m(z)$ or $Z'_m(\operatorname{Int} Y, z)$ is zero.

As a consequence of the above definitions and the fact that $\operatorname{Int}_m Y \subsetneqq \Lambda$ for all $m \in \mathscr{S}$, the expressions

$$K'_q(Y, z) = \rho_z(Y)\, \theta_q(z)^{-|Y|}\, \phi_q(Y, z) \prod_{m \in \mathscr{S}} \frac{Z_m(\operatorname{Int}_m Y, z)}{Z'_q(\operatorname{Int}_m Y, z)} \tag{4.12}$$

and

$$\tilde{K}'_q(Y, z) = \begin{cases} K'_q(Y, z), & \text{if } \quad |K'_q(Y, z)| \leqslant e^{-(c_0 + \tau/2)\,|Y|}, \\ 0, & \text{otherwise,} \end{cases} \tag{4.13}$$

are meaningful for all z with $\theta_q(z) \neq 0$. By Lemma 3.13 we now know that $Z'_q(\Lambda, z) \neq 0$ and the inductive definition can proceed.

In the exceptional case $\theta_q(z) = 0$, we let $\tilde{K}'_q(\cdot\,, z) = K'_q(\cdot\,, z) \equiv 0$ and $Z'_q(\cdot\,, z) \equiv 0$. Note that this is consistent with $\phi_q(Y, z) \equiv 0$.

Remark 4.1. Theorem 4.3 stated and proved below will ensure that $|K'_q(Y, z)| < e^{-(c_0 + \tau/2)\,|Y|}$ for all q-contours Y and all $q \in \mathscr{S}$, provided $\tau \geqslant 4c_0 + 16$. Hence, as it turns out *a posteriori*, the second alternative in (4.13) never occurs and, once we are done with the proof of Theorem 4.3, we can safely replace $\tilde{K}'_q$ everywhere by K'_q. The additional truncation allows us to define and use the relevant metastable free energies before stating and proving the (rather involved) Theorem 4.3. An alternative strategy would be to define scale dependent free energies as was done, e.g., in ref. 6.

4.2. Metastable Free Energies

Let us rewrite $Z'_q(\Lambda, z)$ as

$$Z'_q(\Lambda, z) = \theta_q(z)^{|\Lambda|}\, \mathscr{Z}'_q(\Lambda, z) \tag{4.14}$$

where

$$\mathscr{Z}'_q(\Lambda, z) = \sum_{\mathbb{Y} \in \mathscr{C}(\Lambda, q)} \prod_{Y \in \mathbb{Y}} \widetilde{K}'_q(Y, z). \tag{4.15}$$

We then define

$$\zeta_q(z) = \theta_q(z)\, e^{s_q(z)}, \tag{4.16}$$

where

$$s_q(z) = \lim_{|\Lambda| \to \infty,\ \frac{|\partial\Lambda|}{|\Lambda|} \to 0} \frac{1}{|\Lambda|} \log \mathscr{Z}'_q(\Lambda, z). \tag{4.17}$$

By Lemma 3.14, the partition functions $\mathscr{Z}'_q(\Lambda, z)$ and the polymer pressure $s_q(z)$ can be analyzed by a convergent cluster expansion, leading to the following lemma.

Lemma 4.2. For each $q \in \mathscr{S}$ and each $z \in \widetilde{\mathscr{O}}$, the van Hove limit (4.17) exists and obeys the bound

$$|s_q(z)| \leqslant e^{-\tau/2}. \tag{4.18}$$

If Λ is a finite subset of $\mathbb{Z}^d$ and $\theta_q(z) \neq 0$, we further have that $Z'_q(\Lambda, z) \neq 0$ and

$$|\log(\zeta_q(z)^{-|\Lambda|}\, Z'_q(\Lambda, z))| \leqslant e^{-\tau/2}\, |\partial\Lambda|, \tag{4.19}$$

while $\zeta_q(z) = 0$ and $Z'_q(\Lambda, z) = 0$ if $\theta_q(z) = 0$.

Proof. Recalling the definition of compatibility between q-contours from the paragraph before Lemma 3.13, $\mathscr{C}(\Lambda, q)$ is exactly the set of all compatible collections of q-contours in Λ. Using the bound (4.13), the statements of the lemma are now direct consequences of Lemma 3.14, the definition (4.16), the representation (4.14) for $Z'_q(\Lambda, z)$ and the fact that we set $\widetilde{K}'_q(Y, z) = 0$ if $\theta_q(z) = 0$. ∎

The logarithm of $\zeta_q(z)$—or at least its real part—has a natural interpretation as the *metastable free energy* of the ground state q. To state our next theorem, we actually need to define these (and some other) quantities explicitly: For each $z \in \widetilde{\mathscr{O}}$ and each $q \in \mathscr{S}$ with $\theta_q(z) \neq 0$, let

$$\begin{aligned} f_q(z) &= -\log |\zeta_q(z)|, \\ f(z) &= \min_{m \in \mathscr{S}} f_m(z), \\ a_q(z) &= f_q(z) - f(z). \end{aligned} \tag{4.20}$$

If $\theta_q(z)=0$, we set $f_q(z)=\infty$ and $a_q=\infty$. (Note that $\sup_{z\in\tilde{\mathcal{O}}} f(z)<\infty$ by (4.16), the bound (4.18) and our assumption that $\theta(z)=\max_q |\theta_q(z)|$ is bounded away from zero.)

In accord with our previous definition, a phase q is stable at z if $a_q(z)=0$. We will also say that a q-contour Y is *stable at* z if $K'_q(Y,z)=K_q(Y,z)$. As we will see, stability of the phase q implies that all q-contours are stable. Now we can formulate an analogue of Theorem 3.1 of ref. 5 and Theorem 1.7 of ref. 21.

Theorem 4.3. Suppose that $\tau\geqslant 4c_0+16$ where c_0 is the constant from Lemma 3.13, and let $\tilde{\epsilon}=e^{-\tau/2}$. Then the following holds for all $z\in\widetilde{\mathcal{O}}$:

(i) For all $q\in\mathcal{S}$ and all q-contours Y, we have $|K'_q(Y,z)|<e^{-(c_0+\tau/2)\,|Y|}$ and, in particular, $\widetilde{K}'_q(Y,z)=K'_q(Y,z)$.

(ii) If Y is a q-contour with $a_q(z)\operatorname{diam} Y\leqslant\frac{\tau}{4}$, then $K'_q(Y,z)=K_q(Y,z)$.

(iii) If $a_q(z)\operatorname{diam}\Lambda\leqslant\frac{\tau}{4}$, then $Z_q(\Lambda,z)=Z'_q(\Lambda,z)\neq 0$ and

$$|Z_q(\Lambda,z)|\geqslant e^{-f_q(z)\,|\Lambda|-\tilde{\epsilon}\,|\partial\Lambda|}. \tag{4.21}$$

(iv) If $m\in\mathcal{S}$, then

$$|Z_m(\Lambda,z)|\leqslant e^{-f(z)\,|\Lambda|}e^{2\tilde{\epsilon}\,|\partial\Lambda|}. \tag{4.22}$$

Before proving Theorem 4.3, we state and prove the following simple lemma which will be used both in the proof of Theorem 4.3 and in the proof of Proposition 4.6 in the next subsection.

Lemma 4.4. Let $m,q\in\mathcal{S}$, let $z\in\widetilde{\mathcal{O}}$ and let Y be a q-contour.

(i) If $\phi_q(Y,z)>0$, then

$$a_q(|\mathrm{Int}\,Y|+|Y|)\leqslant(\tau/4+2+4e^{-\tau/2})\,|Y|. \tag{4.23}$$

(ii) If $\phi_q(Y,z)>0$ and $\chi_{q;m}(Y,z)<1$, then

$$a_m(|\mathrm{Int}\,Y|+|Y|)\leqslant(1+8e^{-\tau/2})\,|Y|. \tag{4.24}$$

Proof of Lemma 4.4. By the definitions (4.10) and (4.11), the condition $\phi_q(Y,z)>0$ implies that

$$\max_{n\in\mathcal{S}}\log\left|\frac{Z'_n(\mathrm{Int}\,Y,z)\,\theta_n(z)^{|Y|}}{Z'_q(\mathrm{Int}\,Y,z)\,\theta_q(z)^{|Y|}}\right|\leqslant(2+\tau/4)\,|Y|. \tag{4.25}$$

Next we observe that $\phi_q(Y,z)>0$ implies $\theta_q(z)\neq 0$. Since the maximum in (4.25) is clearly attained for some n with $\theta_n(z)\neq 0$, we may use the bound (4.19) to estimate the partition functions on the left hand side of (4.25). Combined with (4.16), (4.18), (4.20) and the estimate $|\partial \operatorname{Int} Y|\leqslant |Y|$, this immediately gives the bound (4.23).

Next we use that the condition $\chi_{q;m}(Y,z)<1$ implies that

$$\log\left|\frac{Z'_m(\operatorname{Int} Y,z)\,\theta_m(z)^{|Y|}}{Z'_q(\operatorname{Int} Y,z)\,\theta_q(z)^{|Y|}}\right|\geqslant (1+\tau/4)\,|Y|. \tag{4.26}$$

Since (4.26) is not consistent with $\theta_m(z)=0$, we may again use (4.19), (4.16), (4.18), and (4.20) to estimate the left hand side, leading to the bound

$$(f_q-f_m)(|\operatorname{Int} Y|+|Y|)\geqslant (\tau/4+1-4e^{-\tau/2})\,|Y|. \tag{4.27}$$

Combining (4.27) with (4.23) and expressing a_m as $a_q-(f_q-f_m)$, one easily obtains the bound (4.24). ∎

As in ref. 5, Theorem 4.3 is proved using induction on the diameter of Λ and Y. The initial step for the induction, namely, (i) and (ii) for $\operatorname{diam} Y=1$—which is trivially valid since no such contours exist—and (iii), (iv) for $\operatorname{diam}\Lambda=1$, is established by an argument along the same lines as that which drives the induction, so we just need to prove the induction step. Let $N\geqslant 1$ and suppose that the claims (i)–(iv) have been established (or hold automatically) for all Y', Λ' with $\operatorname{diam} Y'$, $\operatorname{diam}\Lambda'<N$. Throughout the proof we will omit the argument z in $f_m(z)$ and $a_m(z)$.

The proof of the induction step is given in four parts:

Proof of (i). Let Y be such that $\operatorname{diam} Y=N$. First we will show that the second alternative in (4.13) does not apply. By the bounds (4.1) and (4.18), we have that

$$|\rho_z(Y)\,\theta_q(z)^{-|Y|}|\leqslant e^{-\tau|Y|}\left(\frac{\theta(z)}{|\theta_q(z)|}\right)^{|Y|}\leqslant e^{-(\tau-2\tilde{\varepsilon})\,|Y|}e^{a_q\,|Y|}, \tag{4.28}$$

while the inductive assumption (iv), the bound (4.19) and the fact that $\sum_m |\operatorname{Int}_m Y|=|\operatorname{Int} Y|$ and $\sum_m |\partial \operatorname{Int}_m Y|=|\partial\operatorname{Int} Y|\leqslant |Y|$, imply that

$$\left|\prod_{m\in\mathscr{S}}\frac{Z_m(\operatorname{Int}_m Y,z)}{Z'_q(\operatorname{Int}_m Y,z)}\right|\leqslant e^{a_q\,|\operatorname{Int} Y|}e^{3\tilde{\varepsilon}\,|Y|}. \tag{4.29}$$

Assuming without loss of generality that $\phi_q(Y,z)>0$ (otherwise there is nothing to prove), we now combine the bounds (4.28) and (4.29) with

(4.23) and the fact that $\tilde{\epsilon} = e^{-\tau/2} \leqslant 2/\tau \leqslant 1/8$, to conclude that $|K'_q(Y, z)| \leqslant e^{-(\frac{3}{4}\tau - \frac{5}{2} - 5\tilde{\epsilon})|Y|} < e^{-(\frac{3}{4}\tau - 4)|Y|}$. By the assumption $\tau \geqslant 4c_0 + 16$, this is bounded by $e^{-(c_0 + \tau/2)|Y|}$, as desired. ∎

Proof of (ii). Let $\operatorname{diam} Y = N$ and suppose that Y is a q-contour satisfying $a_q \operatorname{diam} Y \leqslant \tau/4$. Using the bounds (4.18) and (4.19), the definitions (4.16) and (4.20), and the fact that $|\partial \operatorname{Int} Y| \leqslant |Y|$ we can conclude that

$$\max_{m \in \mathscr{S}} \frac{1}{|Y|} \log \left| \frac{Z'_m(\operatorname{Int} Y, z)\, \theta_m(z)^{|Y|}}{Z'_q(\operatorname{Int} Y, z)\, \theta_q(z)^{|Y|}} \right| \leqslant a_q \frac{|\operatorname{supp} Y \cup \operatorname{Int} Y|}{|Y|} + 4\tilde{\epsilon} \leqslant \frac{\tau}{4} + 1. \tag{4.30}$$

In the last inequality, we used the bound $|\operatorname{supp} Y \cup \operatorname{Int} Y| \leqslant |Y| \operatorname{diam} Y$, the assumption that $a_q \operatorname{diam} Y \leqslant \tau/4$ and the fact that $4\tilde{\epsilon} \leqslant 1$. We also used that $a_q < \infty$ implies $\theta_q \neq 0$, which justifies the use of the bound (4.19). By the definitions (4.10) and (4.11), the bound (4.30) implies that $\phi_q(\operatorname{Int} Y, z) = 1$. On the other hand, $Z_q(\operatorname{Int}_m Y, z) = Z'_q(\operatorname{Int}_m Y, z)$ for all $m \in \mathscr{S}$ by the inductive assumption (iii) and the fact that $\operatorname{diam} \operatorname{Int}_m Y < \operatorname{diam} Y = N$. Combined with the inductive assumption (i), we infer that $\tilde{K}'_q(Y, z) = K'_q(Y, z) = K_q(Y, z)$. ∎

Proof of (iii). Let $\Lambda \subset \mathbb{Z}^d$ be such that $\operatorname{diam} \Lambda = N$ and $a_q \operatorname{diam} \Lambda \leqslant \tau/4$. By the fact that (ii) is known to hold for all contours Y with $\operatorname{diam} Y \leqslant N$, we have that $K'_q(Y, z) = K_q(Y, z)$ for all Y in Λ, implying that $Z_q(\Lambda, z) = Z'_q(\Lambda, z)$. Invoking (4.19) and (4.20), the bound (4.21) follows directly. ∎

Proof of (iv). Let Λ be a subset of $\mathbb{Z}^d$ with $\operatorname{diam} \Lambda = N$. Following refs. 5 and 21, we will apply the cluster expansion only to contours that are sufficiently suppressed and handle the other contours by a crude upper bound. Given a compatible collection of contours $\mathbb{Y}$, recall that *internal* contours are those contained in $\operatorname{Int} Y$ of some other $Y \in \mathbb{Y}$ while the others are *external*. Let us call an m-contour Y *small* if $a_m \operatorname{diam} Y \leqslant \tau/4$; otherwise we will call it *large*. The reason for this distinction is that if Y is small then it is automatically stable.

Bearing in mind the above definitions, let us partition any collection of contours $\mathbb{Y} \in \mathscr{M}(\Lambda, m)$ into three sets $\mathbb{Y}^{\text{int}} \cup \mathbb{Y}^{\text{ext}}_{\text{small}} \cup \mathbb{Y}^{\text{ext}}_{\text{large}}$ of internal, small-external and large-external contours, respectively. Fixing $\mathbb{Y}^{\text{ext}}_{\text{large}}$ and resumming the remaining two families of contours, the partition function $Z_m(\Lambda, z)$ can be recast in the form

$$Z_m(\Lambda, z) = \sum_{\tilde{\mathbb{Y}}} Z^{\text{small}}_m(\text{Ext}, z) \prod_{Y \in \tilde{\mathbb{Y}}} \left\{ \rho_z(Y) \prod_{n \in \mathscr{S}} Z_n(\operatorname{Int}_n Y) \right\}. \tag{4.31}$$

Here the sum runs over all sets $\widetilde{\mathbb{Y}}$ of mutually external large m-contours in Λ, the symbol $\mathrm{Ext} = \mathrm{Ext}_\Lambda(\widetilde{\mathbb{Y}})$ denotes the set $\bigcap_{Y \in \widetilde{\mathbb{Y}}} (\mathrm{Ext}\, Y \cap \Lambda)$ and $Z_m^{\mathrm{small}}(\mathrm{Ext}, z)$ is the partition sum in Ext induced by $\widetilde{\mathbb{Y}}$. Explicitly, $Z_m^{\mathrm{small}}(\Lambda, z)$ is the quantity from (3.6) with the sum restricted to the collections $\mathbb{Y} \in \mathscr{M}(\Lambda, m)$ for which all external contours are small according to the above definition.

In the special case where $\theta_m(z) = 0$, all contours are large by definition (recall that $a_m = \infty$ if θ_m vanishes) and the partition function $Z_m^{\mathrm{small}}(\Lambda, z)$ is defined to be zero unless $\Lambda = \varnothing$, in which case we set it to one. We will not pay special attention to the case $\theta_m = 0$ in the sequel of this proof, but as the reader may easily verify, all our estimates remain true in this case, and can be formally derived by considering the limit $a_m \to \infty$.

Using the inductive assumption (iv) to estimate the partition functions $Z_n(\mathrm{Int}_n\, Y)$, the Peierls condition (4.1) to bound the activities $\rho_z(Y)$, and the bound (4.18) to estimate $\theta(z)$ by $e^{-f} e^{\tilde{\epsilon}}$, we get

$$\prod_{Y \in \widetilde{\mathbb{Y}}} \Big\{ \rho_z(Y) \prod_{n \in \mathscr{S}} Z_n(\mathrm{Int}_n\, Y) \Big\} \leqslant \prod_{Y \in \widetilde{\mathbb{Y}}} \{ e^{-\tau |Y|} e^{-f(|\mathrm{Int}\, Y| + |Y|) + 3\tilde{\epsilon}\, |Y|} \}$$
$$= e^{-f\, |\Lambda \setminus \mathrm{Ext}|} \prod_{Y \in \widetilde{\mathbb{Y}}} e^{-(\tau - 3\tilde{\epsilon})\, |Y|}. \tag{4.32}$$

Next we will estimate the partition function $Z_m^{\mathrm{small}}(\mathrm{Ext}, z)$. Since all small m-contours are stable by the inductive hypothesis, this partition function can be analyzed by a convergent cluster expansion. Let us consider the ratio of $Z_m^{\mathrm{small}}(\mathrm{Ext}, z)$ and $Z'_m(\mathrm{Ext}, z)$. Expressing the logarithm of this ratio as a sum over clusters we obtain a sum over clusters that contain at least one contour of size $|Y| \geqslant \mathrm{diam}\, Y > \tau / a_m \geqslant 2 / a_m$. Using the bound (3.21) with $\eta = \tau/2$ we conclude that

$$\left| \frac{Z_m^{\mathrm{small}}(\mathrm{Ext}, z)}{Z'_m(\mathrm{Ext}, z)} \right| \leqslant e^{|\mathrm{Ext}|\, e^{-\tau/a_m}}. \tag{4.33}$$

Combined with Lemma 4.2 and the definitions (4.20), this gives

$$|Z_m^{\mathrm{small}}(\mathrm{Ext}, z)| \leqslant e^{-(f_m - e^{-\tau/a_m})\, |\mathrm{Ext}|}\, e^{\tilde{\epsilon}\, |\partial \Lambda|} \prod_{Y \in \widetilde{\mathbb{Y}}} e^{\tilde{\epsilon}\, |Y|}. \tag{4.34}$$

We thus conclude that the left hand side of (4.31) is bounded by

$$|Z_m(\Lambda, z)| \leqslant \max_{\widetilde{\mathbb{Y}}} \Big(e^{-(a_m/2)\, |\mathrm{Ext}|} \prod_{Y \in \widetilde{\mathbb{Y}}} e^{-(\tau/4)\, |Y|} \Big)$$
$$\times e^{-f\, |\Lambda|} e^{\tilde{\epsilon}\, |\partial \Lambda|} \sum_{\widetilde{\mathbb{Y}}} e^{-b\, |\mathrm{Ext}|} \prod_{Y \in \widetilde{\mathbb{Y}}} e^{-(3\tau/4 - 4\tilde{\epsilon})\, |Y|}, \tag{4.35}$$

where $b = a_m/2 - e^{-\tau/a_m}$. Note that $b \geqslant e^{-\tau/a_m}$ which is implied by the fact that $4e^{-\tau/a_m} \leqslant 4a_m/\tau \leqslant a_m$.

For the purposes of this proof, it suffices to bound the first factor in (4.35) by 1. In a later proof, however, we will use a more subtle bound. To bound the second factor, we will invoke Zahradník's method (see ref. 21, Main Lemma or ref. 5, Lemma 3.2): Consider the contour model with weights $\hat{K}(Y) = e^{-(3\tau/4-4)\,|Y|}$ if Y is a large m-contour and $\hat{K}(Y) = 0$ otherwise. Let $\hat{Z}(\Lambda)$ be the corresponding polymer partition function in Λ—see (3.11)—and let φ be the corresponding free energy. Clearly $\hat{Z}(\Lambda) \geqslant 1$ so that $-\varphi \geqslant 0$. Since $3\tau/4 - 4 \geqslant c_0 + \tau/2$, we can use Lemmas 3.13 and 3.14 to obtain further bounds. For the free energy, this gives $0 \leqslant -\varphi \leqslant \min\{\tilde{\varepsilon}, e^{-\tau/a_m}\}$ because the weights of contours smaller than $2/a_m$ identically vanish. Since $b \geqslant e^{-\tau/a_m}$, this allows us to bound the sum on the right hand side of (4.35) by

$$\sum_{\tilde{\mathbb{Y}}} e^{\varphi\,|\mathrm{Ext}|} \prod_{Y \in \tilde{\mathbb{Y}}} e^{-(3\tau/4-4\tilde{\varepsilon})\,|Y|} \leqslant \sum_{\tilde{\mathbb{Y}}} e^{\varphi\,|\mathrm{Ext}|} \prod_{Y \in \tilde{\mathbb{Y}}} \{e^{\varphi\,|Y|} e^{-(3\tau/4-5\tilde{\varepsilon})\,|Y|}\}. \tag{4.36}$$

Using Lemma 3.14 once more, we have that $\hat{Z}(\mathrm{Int}\,Y)\, e^{\varphi\,|\mathrm{Int}\,Y|} e^{\tilde{\varepsilon}\,|Y|} \geqslant 1$. Inserting into (4.36), we obtain

$$\begin{aligned} &\sum_{\tilde{\mathbb{Y}}} e^{-b\,|\mathrm{Ext}|} \prod_{Y \in \tilde{\mathbb{Y}}} e^{-(3\tau/4-4\tilde{\varepsilon})\,|Y|} \\ &\quad \leqslant \sum_{\tilde{\mathbb{Y}}} e^{\varphi(|\mathrm{Ext}| + \sum_{Y \in \tilde{\mathbb{Y}}} (|\mathrm{Int}\,Y| + |Y|))} \prod_{Y \in \tilde{\mathbb{Y}}} \{\hat{Z}(\mathrm{Int}\,Y)\, \hat{K}(Y)\} \\ &\quad = e^{\varphi\,|\Lambda|} \sum_{\tilde{\mathbb{Y}}} \prod_{Y \in \tilde{\mathbb{Y}}} \{\hat{Z}(\mathrm{Int}\,Y)\, \hat{K}(Y)\}. \end{aligned} \tag{4.37}$$

Consider, on the other hand, the polymer partition function $\hat{Z}(\Lambda)$ in the representation (3.11). Resuming all contours but the external ones, we obtain precisely the right hand side of (4.37), except for the factor $e^{\varphi\,|\Lambda|}$. This shows that the right hands side of (4.37) is equal to $\hat{Z}(\Lambda)\, e^{\varphi\,|\Lambda|}$ which—again by Lemma 3.14—is bounded by $e^{\tilde{\varepsilon}\,|\partial\Lambda|}$. Putting this and (4.35) together we obtain the proof of the claim (iv). ∎

4.3. Differentiability of Free Energies

Our next item of concern will be the existence of two continuous and bounded derivatives of the metastable free energies. To this end, we first prove the following proposition, which establishes a bound of the form (4.22) for the derivatives of the partition functions $Z_m(\Lambda, z)$.

Proposition 4.5. Let τ and M be the constants from (4.1) and (4.3), let $\tilde{\varepsilon}=e^{-\tau/2}$, and suppose that $\tau \geqslant 4c_0+16$ where c_0 is the constant from Lemma 3.13. Then

$$|\partial_z^{\ell}\partial_{\bar{z}}^{\bar{\ell}} Z_m(\Lambda, z)| \leqslant e^{-f(z)\,|\Lambda|}(2M\,|\Lambda|)^{\ell+\bar{\ell}}\, e^{2\tilde{\varepsilon}\,|\partial\Lambda|}, \tag{4.38}$$

holds for all $z \in \widetilde{\mathcal{O}}$, all $m \in \mathscr{S}$, and all $\ell, \bar{\ell} \geqslant 0$ with $\ell+\bar{\ell} \leqslant 2$.

Proof. Again, we proceed by induction on the diameter of Λ. We start from the representation (4.4) which we rewrite as

$$Z_m(\Lambda, z)=\sum_{\mathbb{Y}^{\text{ext}}} \prod_{x \in \text{Ext}} \theta_m(z) \prod_{Y \in \mathbb{Y}^{\text{ext}}} Z(Y, z), \tag{4.39}$$

where we abbreviated $Z(Y,z)=\rho_z(Y)\prod_n Z_n(\text{Int}_n\, Y, z)$. Let $1 \leqslant \ell < \infty$ be fixed (later, we will use that actually, $\ell \leqslant 2$) and let us consider the impact of applying ∂_z^{ℓ} on $Z_m(\Lambda, z)$. Clearly, each of the derivatives acts either on some of θ_m's, or on some of the $Z(Y,z)$'s. Let k_x be the number of times the term $\theta_m(z)$ is differentiated "at x," and let i_Y be the number of times the factor $Z(Y,z)$ is differentiated. Let $\mathbf{k}=(k_x)$ and $\mathbf{i}=(i_Y)$ be the corresponding multiindices. The resummation of all contours Y for which $i_Y=0$ and $k_x=0$ for all $x \in \operatorname{supp} Y \cup \operatorname{Int} Y$ then contributes a factor $Z_m(\text{Ext}_\Lambda(\overline{\mathbb{Y}}^{\text{ext}}) \setminus \Lambda', z)$, where we used $\overline{\mathbb{Y}}^{\text{ext}}$ to denote the set of all those $Y \in \mathbb{Y}^{\text{ext}}$ for which $i_Y>0$, $\text{Ext}_\Lambda(\overline{\mathbb{Y}}^{\text{ext}})=\Lambda \setminus \bigcup_{Y \in \overline{\mathbb{Y}}^{\text{ext}}} (\operatorname{supp} Y \cup \operatorname{Int} Y)$, and $\Lambda'=\{x\colon k_x>0\}$. (Remember the requirement that no contour in $\text{Ext}_\Lambda(\overline{\mathbb{Y}}^{\text{ext}}) \setminus \Lambda'$ surrounds any of the "holes.") Using this notation, the result of differentiating can be concisely written as

$$\begin{aligned}\partial_z^{\ell} Z_m(\Lambda, z) = &\sum_{\overline{\mathbb{Y}}^{\text{ext}}} \sum_{\Lambda' \subset \text{Ext}_\Lambda(\overline{\mathbb{Y}}^{\text{ext}})} Z_m(\text{Ext}_\Lambda(\overline{\mathbb{Y}}^{\text{ext}}) \setminus \Lambda', z)\\ &\times \sum_{\substack{\mathbf{k},\,\mathbf{i}\\ \mathbf{k}+\mathbf{i}=\ell}} \frac{\ell!}{\mathbf{k}!\,\mathbf{i}!} \prod_{x \in \Lambda'} \partial_z^{k_x}\theta_m(z) \prod_{Y \in \overline{\mathbb{Y}}^{\text{ext}}} \partial_z^{i_Y} Z(Y, z).\end{aligned} \tag{4.40}$$

Here the first sum goes over all collections (including the empty one) $\overline{\mathbb{Y}}^{\text{ext}}$ of mutually external contours in Λ and the third sum goes over all pairs of multiindices $(\mathbf{k}, \mathbf{i})$, $k_x=1,2,\dots$, $x \in \Lambda'$, $i_Y=1,2,\dots$, $Y \in \overline{\mathbb{Y}}^{\text{ext}}$. (The terms with $|\Lambda'|+|\overline{\mathbb{Y}}^{\text{ext}}|>\ell$ vanish.) We write $\mathbf{k}+\mathbf{i}=\ell$ to abbreviate $\sum_x k_x + \sum_Y i_Y=\ell$ and use the symbols $\mathbf{k}!$ and $\mathbf{i}!$ to denote the multi-index factorials $\prod_x k_x!$ and $\prod_Y i_Y!$, respectively.

We now use (4.3) and (4.18) to bound $|\partial_z^{k_x}\theta_m(z)|$ by $(M)^{k_x} e^{\tilde{\varepsilon}} e^{-f(z)}$. Employing (4.1) and (4.18) to bound the derivatives of $\rho_z(Y)$, and the inductive hypothesis to bound the derivatives of $Z_m(\text{Int}_m\, Y, z)$, we estimate $|\partial_z^{i_Y} Z(Y,z)|$ by $[2M\,|V(Y)|]^{i_Y} e^{-(\tau-3\tilde{\varepsilon})\,|Y|} e^{-f(z)\,|V(Y)|}$ (recall that $V(Y)$ was defined as $\operatorname{supp} Y \cup \operatorname{Int} Y$). Finally, we may use the bound (4.22) to estimate

$$|Z_m(\operatorname{Ext}_\Lambda(\overline{\mathbb{Y}}^{\mathrm{ext}}) \setminus \Lambda', z)| \leqslant e^{2\tilde{\varepsilon}\, |\partial(\operatorname{Ext}_\Lambda(\overline{\mathbb{Y}}^{\mathrm{ext}}) \setminus \Lambda')} e^{-f(z)\, |\operatorname{Ext}_\Lambda(\overline{\mathbb{Y}}^{\mathrm{ext}}) \setminus \Lambda'|}. \tag{4.41}$$

Combining these estimates and invoking the inequality

$$|\partial(\operatorname{Ext}_\Lambda(\overline{\mathbb{Y}}^{\mathrm{ext}}) \setminus \Lambda')| \leqslant |\partial\Lambda| + |\Lambda'| + \sum_{Y \in \overline{\mathbb{Y}}^{\mathrm{ext}}} |Y|, \tag{4.42}$$

we get

$$|\partial_z^\ell Z_m(\Lambda, z)| \leqslant e^{2\tilde{\varepsilon}\, |\partial\Lambda|} e^{-f(z)\, |\Lambda|} \sum_{\overline{\mathbb{Y}}^{\mathrm{ext}}} \sum_{\Lambda' \subset \operatorname{Ext}_\Lambda(\overline{\mathbb{Y}}^{\mathrm{ext}})} \sum_{\substack{\mathbf{k}, \mathbf{i} \\ \mathbf{k}+\mathbf{i}=\ell}} \frac{\ell!}{\mathbf{k}!\, \mathbf{i}!}$$

$$\times \prod_{x \in \Lambda'} (M e^{3\tilde{\varepsilon}})^{k_x} \prod_{Y \in \overline{\mathbb{Y}}^{\mathrm{ext}}} (2M\, |V(Y)|)^{i_Y}\, e^{-(\tau - 5\tilde{\varepsilon})\, |Y|}. \tag{4.43}$$

Let us now consider the case $\ell = 1$ and $\ell = 2$. For $\ell = 1$, the sum on the right hand side of (4.43) can be rewritten as

$$\sum_{x \in \Lambda} \left(M e^{3\tilde{\varepsilon}} + \sum_{Y:\, x \in V(Y) \subset \Lambda} 2M e^{-(\tau - 5\tilde{\varepsilon})\, |Y|} \right), \tag{4.44}$$

while for $\ell = 2$, it becomes

$$\sum_{x,\, y \in \Lambda} \left\{ (M e^{3\tilde{\varepsilon}})^2 + 2M e^{3\tilde{\varepsilon}} 2M \sum_{\substack{Y:\, x \in \Lambda \setminus V(Y) \\ y \in V(Y) \subset \Lambda}} e^{-(\tau - 5\tilde{\varepsilon})\, |Y|} + (2M)^2 \sum_{\overline{\mathbb{Y}}^{\mathrm{ext}}} \prod_{Y \in \overline{\mathbb{Y}}^{\mathrm{ext}}} e^{-(\tau - 5\tilde{\varepsilon})\, |Y|} \right\}, \tag{4.45}$$

where the last sum goes over sets of mutually external contours $\overline{\mathbb{Y}}^{\mathrm{ext}}$ in Λ such that $\{x, y\} \subset \bigcup_{Y \in \overline{\mathbb{Y}}^{\mathrm{ext}}} V(Y)$ and $\{x, y\} \cap V(Y) \neq \emptyset$ for each $Y \in \overline{\mathbb{Y}}^{\mathrm{ext}}$. Note that the last condition can only be satisfied if $\overline{\mathbb{Y}}^{\mathrm{ext}}$ contains either one or two contours. Introducing the shorthand

$$S = \sum_{Y:\, 0 \in V(Y) \subset \mathbb{Z}^d} e^{-(\tau - 5\tilde{\varepsilon})\, |Y|} \tag{4.46}$$

we bound the expression (4.44) by $(e^{3\tilde{\varepsilon}} + 2S)\, M\, |\Lambda|$, and the expression (4.45) by $(e^{6\tilde{\varepsilon}} + 4e^{3\tilde{\varepsilon}} S + 4(S + S^2))\, M^2\, |\Lambda|^2$. Recalling that c_0 was defined in such a way that the bound (3.28) holds, we may now use the fact that $\tau - 5\tilde{\varepsilon} - c_0 \geqslant \frac{1}{2}\tau$ to bound S by $e^{-2}\tilde{\varepsilon}$. Since $\tilde{\varepsilon} \leqslant 1/8$, this implies that the above two terms can be estimated by $(e^{3/8} + \frac{1}{4} e^{-2})\, M\, |\Lambda| \leqslant 2M\, |\Lambda|$ and $(e^{6/8} + \frac{1}{2} e^{3/8-2} + \frac{1}{2}(e^{-2} + \frac{1}{8} e^{-4}))\, M^2\, |\Lambda|^2 \leqslant 4M^2\, |\Lambda|^2$, as desired.

This completes the proof for the derivatives with respect to z. The proof for the derivatives with respect to $\bar{z}$ and the mixed derivatives is completely analogous and is left to the reader. ▌

Next we will establish a bound on the first two derivatives of the contour weights K'_q. Before formulating the next proposition, we recall the definitions of the polymer partition function $\mathscr{Z}'_q(\Lambda, z)$ and the polymer pressure s_q in (4.17) and (4.15) .

Proposition 4.6. Let τ and M be the constants from (4.1) and (4.3), let c_0 be the constant from Lemma 3.13, and let $\tilde{\epsilon} = e^{-\tau/2}$. Then there exists a finite constant $\tau_1 \geqslant 4c_0 + 16$ depending only on M, d, and $|\mathscr{S}|$ such that if $\tau \geqslant \tau_1$, the contour weights $K'_q(Y, \cdot)$ are twice continuously differentiable in $\widetilde{\mathscr{O}}$. Furthermore, the bounds

$$|\partial_z^{\ell} \partial_{\bar{z}}^{\bar{\ell}} K'_q(Y, z)| \leqslant e^{-(c_0+\tau/2)\,|Y|} \tag{4.47}$$

and

$$|\partial_z^{\ell} \partial_{\bar{z}}^{\bar{\ell}} \mathscr{Z}'_q(\Lambda, z)| \leqslant |\Lambda|^{\ell+\bar{\ell}}\, e^{s_q(z)\,|\Lambda| + \tilde{\epsilon}\,|\partial\Lambda|} \tag{4.48}$$

hold for all $q \in \mathscr{S}$, all $z \in \widetilde{\mathscr{O}}$, all q-contours Y, all finite $\Lambda \subset \mathbb{Z}^d$ and all $\ell, \bar{\ell} \geqslant 0$ with $\ell + \bar{\ell} \leqslant 2$.

Proposition 4.6 immediately implies that the polymer pressures s_q are twice continuously differentiable and obey the bounds of Lemma 3.14. For future reference, we state this in the following corollary.

Corollary 4.7. Let τ_1 be as in Proposition 4.6. If $\tau \geqslant \tau_1$ and $q \in \mathscr{S}$, then s_q is a twice continuously differentiable function in $\widetilde{\mathscr{O}}$ and obeys the bounds

$$|\partial_w s_q| \leqslant e^{-\tau/2} \qquad \text{and} \qquad |\partial_w \partial_{w'} s_q| \leqslant e^{-\tau/2}, \tag{4.49}$$

valid for any $w, w' \in \{z, \bar{z}\}$ and any $z \in \widetilde{\mathscr{O}}$.

Proof of Proposition 4.6. Let $\tau \geqslant \tau_1 \geqslant 4c_0 + 16$. Then Theorem 4.3 is at our disposal. It will be convenient to cover the set $\widetilde{\mathscr{O}}$ by the open sets

$$\widetilde{\mathscr{O}}_1^{(q)} = \{z \in \widetilde{\mathscr{O}} : |\theta_q(z)| < e^{-(\tau/4+2+6\tilde{\epsilon})}\theta(z)\} \tag{4.50}$$

and

$$\widetilde{\mathscr{O}}_2^{(q)} = \{z \in \widetilde{\mathscr{O}} : |\theta_q(z)| > e^{-(\tau/4+2+8\tilde{\epsilon})}\theta(z)\}. \tag{4.51}$$

We first note that $K'_q(Y,z)=0$ if $z\in\widetilde{\mathscr{O}}_1^{(q)}$. Indeed, assuming $K'_q(Y,z)\neq 0$ we necessarily have $\phi_q(Y,z)>0$, which, by (4.23), implies that $a_q\leqslant\tau/4+2+4\tilde{\epsilon}$ and thus $\log\theta(z)-\log|\theta_q(z)|\leqslant\tau/4+2+6\tilde{\epsilon}$, which is incompatible with $z\in\widetilde{\mathscr{O}}_1^{(q)}$. Hence, the claims trivially hold in $\widetilde{\mathscr{O}}_1^{(q)}$ and it remains to prove that $K'_q(Y,\cdot)$ is twice continuously differentiable in $\mathscr{O}_2^{(q)}$, and that (4.47) and (4.48) hold for all $z\in\widetilde{\mathscr{O}}_2^{(q)}$. As in the proof of Theorem 4.3 we will proceed by induction on the diameter of Y and Λ. Let $N\geqslant 1$ and suppose that $K'_q(Y,\cdot)\in C^2(\widetilde{\mathscr{O}}_2^{(q)})$ and obeys the bounds (4.47) for all $q\in\mathscr{S}$ and all q-contours Y with diam $Y<N$, and that (4.48) holds for all $q\in\mathscr{S}$ and all $\Lambda\subset\mathbb{Z}^d$ with diam $\Lambda<N-1$.

We start by proving that $K'_q(Y,\cdot)\in C^2(\widetilde{\mathscr{O}}_2^{(q)})$ whenever Y is a q-contour Y of diameter N. To this end, we first observe that in $\widetilde{\mathscr{O}}_2^{(q)}$, we have that $\theta_q(z)\neq 0$ and hence also $Z'_q(\operatorname{Int}Y,z)\neq 0$. Using the inductive assumption, this implies that the quotient

$$Q_{m,Y}(z)=\frac{Z'_m(\operatorname{Int}Y,z)\,\theta_m(z)^{|Y|}}{Z'_q(\operatorname{Int}Y,z)\,\theta_q(z)^{|Y|}} \tag{4.52}$$

is twice continuously differentiable in $\widetilde{\mathscr{O}}_2^{(q)}$, which in turn implies that $\chi_{q;m}(Y,z)$ is twice continuously differentiable. Combined with the corresponding continuous differentiability of $\rho_z(Y)$, $\theta_q(z)$, $Z_m(\operatorname{Int}_m Y,z)$, and $Z'_q(\operatorname{Int}_m Y,z)$, this proves the existence of two continuous derivatives of $z\mapsto K'_q(Y,z)$ with respect to both z and $\bar{z}$.

Next we prove the bound (4.48) for diam $\Lambda=N-1$. As we will see, these bounds follow immediately from the inductive assumptions (4.47) and Lemma 3.14. Indeed, let $\mathfrak{z}_q(Y)=K'_q(Y,z)$ if diam $Y\leqslant N-1$, and $\mathfrak{z}_q(Y)=0$ if diam $Y>N-1$. The inductive assumptions (4.47) then guarantee the conditions (3.22) of Lemma 3.14. Combining the representation (3.15) for $\log\mathscr{Z}'_q(\Lambda,z)$ with the estimate (3.23) from Lemma 3.14 we thus conclude that

$$|\partial_z^{\ell}\partial_{\bar{z}}^{\bar{\ell}}\log\mathscr{Z}'_q(\Lambda,z)|\leqslant|\Lambda|\,\tilde{\epsilon}, \tag{4.53}$$

while (3.26) gives the bound

$$|\mathscr{Z}'_q(\Lambda,z)|\leqslant e^{s_q|\Lambda|+\tilde{\epsilon}\,|\partial\Lambda|}. \tag{4.54}$$

Combining these bounds with the estimates $\tilde{\epsilon}\,|\Lambda|\leqslant|\Lambda|$ and $\tilde{\epsilon}^2\,|\Lambda|^2+\tilde{\epsilon}\,|\Lambda|\leqslant|\Lambda|^2$, we obtain the desired bounds (4.48).

Before turning to the proof of (4.47) we will show that for $z\in\widetilde{\mathscr{O}}_2^{(q)}$, the bound (4.48) implies

$$|\partial_z^{\ell}\partial_{\bar{z}}^{\bar{\ell}}Z'_q(\Lambda,z)|\leqslant(M_1e^{\tau/4+3}\,|\Lambda|)^{\ell+\bar{\ell}}\,e^{-f_q(z)\,|\Lambda|+\tilde{\epsilon}\,|\partial\Lambda|} \tag{4.55}$$

with $M_1 = 1 + M$. Indeed, invoking the assumption (4.3), the definition of $\widetilde{\mathcal{O}}_2^{(q)}$, and the fact that $\tilde{\epsilon} \leqslant 1/8$, we may estimate the first and second derivative of $\theta_q(z)^{|\Lambda|}$ by

$$|\partial_z^\ell \partial_{\bar{z}}^{\bar{\ell}} \theta_q(z)^{|\Lambda|}| \leqslant \left(M\,|\Lambda|\,\frac{\theta(z)}{|\theta_q(z)|} \right)^{\ell+\bar{\ell}} |\theta_q(z)|^{|\Lambda|}$$
$$\leqslant (M\,|\Lambda|\,e^{\tau/4+3})^{\ell+\bar{\ell}}\,|\theta_q(z)|^{|\Lambda|}. \tag{4.56}$$

Combined with (4.14) and (4.48) this gives (4.55).

Let Y be a q-contour with diam $Y = N$, and let us consider the derivatives with respect to z; the other derivatives are handled analogously. By the assumption (4.1) and the bound (4.18), we have

$$|\partial_z^\ell \rho_z(Y)| \leqslant |Y|^\ell\, M^\ell e^{-(\tau - 2\tilde{\epsilon})\,|Y|} e^{a_q\,|Y|}\, |\theta_q(z)|^{|Y|}, \tag{4.57}$$

while (4.3) and the assumption that $z \in \widetilde{\mathcal{O}}_2^{(q)}$ (cf. (4.56)) yields

$$|\partial_z^\ell \theta_q(z)^{-|Y|}| \leqslant (|Y|+1)^\ell\,(M e^{\tau/4+3})^\ell\,|\theta_q(z)|^{-|Y|}. \tag{4.58}$$

Further, combining the bound (4.55) with Theorem 4.3 and Proposition 4.5 we have

$$\left| \partial_z^\ell \prod_{m \in \mathscr{S}} \frac{Z_m(\operatorname{Int}_m Y, z)}{Z_q'(\operatorname{Int}_m Y, z)} \right| \leqslant |\operatorname{Int} Y|^\ell\,(2M + 2M_1 e^{2\tilde{\epsilon}\,|Y|} e^{3+\tau/4})^\ell\, e^{3\tilde{\epsilon}\,|Y|} e^{a_q\,|\operatorname{Int} Y|}. \tag{4.59}$$

Finally, let us consider one of the factors $\chi_{q;m}(Y, z)$. To bound its derivative, we may assume that z is an accumulation point of z' with $\chi_{q;m}(Y, z') < 1$ (otherwise its derivative is zero), so by Lemma 4.4(ii) we have that $a_m \leqslant 1 + 8\tilde{\epsilon}$ and thus $\log \theta(z) - \log |\theta_m(z)| \leqslant 1 + 10\tilde{\epsilon} < \tau/4 + 2 + 8\tilde{\epsilon}$, implying that $z \in \widetilde{\mathcal{O}}_2^{(m)}$. We may therefore use the bounds (4.56) and (4.55) to estimate the derivatives of $\chi_{q;m}(Y, z)$, yielding the bound

$$|\partial_z^\ell \chi_{q;m}(Y, z)| \leqslant C(|\operatorname{Int} Y| + |Y|)^\ell\,(4M_1 e^{3+\tau/4} e^{2\tilde{\epsilon}\,|Y|})^\ell \tag{4.60}$$

where C is a constant bounding both the first and the second derivative of the mollifier function χ. Combining all these estimates, we obtain a bound of the form

$$|\partial_z^\ell K_q'(Y, z)| \leqslant \tilde{C}(|\operatorname{Int} Y| + |Y|)^\ell\, e^{\ell\tau/4} e^{-(\tau - \tilde{c}\tilde{\epsilon})\,|Y|} e^{a_q(|\operatorname{Int} Y| + |Y|)} \tag{4.61}$$

with a constant $\tilde{C}$ that depends on M and the number of spin states $|\mathscr{S}|$, and a constant $\tilde{c}$ that depends only on $|\mathscr{S}|$. Using the bound (4.23) and the fact that $e^{\ell\tau/4} \leqslant e^{(\tau/8)|Y|}$ (note that $|Y| \geqslant (2R+1)^d > 4$ by our definition of contours), we conclude that

$$|\partial_z^\ell K'_q(Y,z)| \leqslant \tilde{C}(|\text{Int}\,Y| + |Y|)^\ell\, e^{-(5\tau/8-3-\tilde{c}\tilde{\epsilon})\,|Y|}. \tag{4.62}$$

Increasing τ_1 if necessary to absorb all of the prefactors, the bound (4.47) follows. ▮

We close the subsection with a lemma concerning the Lipschitz continuity of real-valued functions $z \mapsto f(z)$ and $z \mapsto e^{-a_q(z)}$ on $\widetilde{\mathcal{O}}$:

Lemma 4.8. Let τ_1 be as in Proposition 4.6 and let $\widetilde{M}_1 = 4M+1$. If $\tau \geqslant \tau_1$, $q \in \mathscr{S}$, and if $z, z_0 \in \widetilde{\mathcal{O}}$ are such that $[z_0, z] = \{sz + (1-s)\, z_0 : 0 \leqslant s \leqslant 1\} \subset \widetilde{\mathcal{O}}$, then

$$|f(z_0) - f(z)| \leqslant \widetilde{M}_1\, |z - z_0| \tag{4.63}$$

and

$$|e^{-a_q(z)} - e^{-a_q(z_0)}| \leqslant 2\widetilde{M}_1\, |z - z_0|\, e^{\widetilde{M}_1\,|z-z_0|}. \tag{4.64}$$

Proof. Let $\zeta_q(z)$ be the quantity defined in (4.16), and let $\tilde{\epsilon} = e^{-\tau/2}$. Combining the assumption (4.3) with the bounds (4.49) and (4.18), we get the estimate

$$|\partial_w \zeta_q(z)| \leqslant (Me^{2\tilde{\epsilon}} + \tilde{\epsilon})\, e^{-f(z)}, \qquad w, w' \in \{z, \bar{z}\}. \tag{4.65}$$

With the help of the bound $Me^{2\tilde{\epsilon}} + \tilde{\epsilon} \leqslant 2M + 1/2 = \widetilde{M}_1/2$, we conclude that

$$|e^{-f_q(z_1)} - e^{-f_q(z_2)}| \leqslant \widetilde{M}_1 \int_{[z_1,z_2]} e^{-f(z')}\, |\mathrm{d}z'|, \qquad z_1, z_2 \in [z_0, z], \tag{4.66}$$

where $|\mathrm{d}z'|$ denotes the Lebesgue measure on the interval $[z_0, z]$. Using that $f = \max_q f_q$, this implies

$$|e^{-f(z_1)} - e^{-f(z_2)}| \leqslant \widetilde{M}_1 \int_{[z_1,z_2]} e^{-f(z')}\, |\mathrm{d}z'|, \qquad z_1, z_2 \in [z_0, z]. \tag{4.67}$$

Now if (4.63) is violated, i.e., when $|f(z) - f(z_0)| \geqslant (\widetilde{M}_1 + \epsilon)\, |z - z_0|$, then the same is true either about the first or the second half of the segment $[z_0, z]$. This shows that there is a sequence of intervals $[z_{1,n}, z_{2,n}]$ of length

$2^{-n}|z_0-z|$ where $|f(z_{1,n})-f(z_{2,n})| \geqslant (\widetilde{M}_1+\epsilon)\,|z_{1,n}-z_{2,n}|$. But that would be in contradiction with (4.67) which implies that

$$\lim_{n\to\infty}\frac{|f(z_{1,n})-f(z_{2,n})|}{|z_{1,n}-z_{2,n}|}=\lim_{n\to\infty}\frac{|e^{-f(z_{1,n})}-e^{-f(z_{2,n})}|}{\int_{[z_{1,n},z_{2,n}]}e^{-f(z')}\,|\mathrm{d}z'|}\leqslant \widetilde{M}_1, \tag{4.68}$$

where we use the mean-value Theorem and a compactness argument to infer the first equality. Hence, (4.63) must be true after all.

To prove (4.64), we combine the triangle inequality and the bound $f_q(z_0)\geqslant f(z_0)$ with (4.66) and (4.67) to conclude that

$$\begin{aligned}|e^{-a_q(z)}-e^{-a_q(z_0)}| &= |e^{f(z)}e^{-f_q(z)}-e^{f(z_0)}e^{-f_q(z_0)}|\\ &\leqslant e^{f(z)}\,|e^{-f_q(z)}-e^{-f_q(z_0)}|+\frac{e^{-f_q(z_0)}}{e^{-f(z)}e^{-f(z_0)}}\,|e^{-f(z_0)}-e^{-f(z)}|\\ &\leqslant 2\widetilde{M}_1\int_{z_0}^{z}e^{f(z)-f(z')}\,|\mathrm{d}z'|.\end{aligned} \tag{4.69}$$

Bounding $f(z)-f(z')$ by $\widetilde{M}_1\,|z-z_0|$, we obtain the bound (4.64). ∎

4.4. Torus Partition Functions

In this subsection we consider the partition functions $Z_q(\Lambda,z)$, defined for $\Lambda\subset\mathbb{T}_L$ in (3.6). Since all contours contributing to $Z_q(\Lambda,z)$ have diameter strictly less than $L/2$, the partition function $Z_q(\Lambda,z)$ can be represented in the form (4.8), with $K_q(Y,z)$ defined by embedding the contour Y into $\mathbb{Z}^d$. Let $Z'_q(\Lambda,z)$ be the corresponding truncated partition function, defined with weights $K'_q(Y,z)$ given by (4.12). Notice, however, that even though every contour $Y\subset\Lambda$ can be individually embedded into $\mathbb{Z}^d$, the relation of incompatibility is formulated on torus. The polymer partition function $\mathscr{Z}'_q(\Lambda,z)$ and $Z'_q(\Lambda,z)$ can then again be analyzed by a convergent cluster expansion, bearing in mind, however, the torus incompatibility relation. The torus analogue of Lemma 4.2 is then as follows:

Lemma 4.9. Assume that $\tau\geqslant\tau_1$, where τ_1 is the constant from Proposition 4.6 and let $q\in\mathscr{S}$ and $z\in\widetilde{\mathscr{O}}$ be such that $\theta_q(z)\neq 0$. Then

$$|\partial_w^\ell\log(\zeta_q(z)^{-|\Lambda|}Z'_q(\Lambda,z))|\leqslant e^{-\tau/2}\,|\partial\Lambda|+2\,|\Lambda|\,e^{-\tau L/4} \tag{4.70}$$

for any $\Lambda\subset\mathbb{T}_L$, any $z\in\widetilde{\mathscr{O}}$, $\ell=0,1$, and $w\in\{z,\bar z\}$.

Proof. Let us write $Z'_q(\Lambda,z)$ in the form (4.14). Taking into account the torus compatibility relation when comparing the cluster expansion for

$\log \mathcal{Z}'_q(\Lambda, z)$ with the corresponding terms contributing to $s_q\,|\Lambda|$, we see that the difference stems not only from clusters passing through the boundary $\partial\Lambda$, but also from the clusters that are wrapped around the torus in the former as well as the clusters that cannot be placed on the torus in the latter. For such clusters, however, we necessarily have $\sum_Y \mathsf{X}(Y)\,|Y| \geqslant L/2$. Since the functional $\mathfrak{z}(Y) = K'_q(Y, z)$ satisfies the bound (3.20) with $\eta = \tau/2$, we may use the bound (3.21) to estimate the contribution of these clusters. This yields

$$\left|\log \mathcal{Z}'_q(\Lambda, z) - s_q\,|\Lambda|\right| \leqslant e^{-\tau/2}\,|\partial\Lambda| + 2\,|\Lambda|\,e^{-\tau L/4}, \tag{4.71}$$

which is (4.70) for $\ell = 0$. To handle the case $\ell = 1$, we just need to recall that, by Proposition 4.6, the functional $\mathfrak{z}(Y) = K'_q(Y, z)$ satisfies the bounds (3.22) with $\eta = \tau/2$. Then the desired estimate for $\ell = 1$ follows with help of (3.23) by a straightforward generalization of the above proof of (4.71). ▮

Next we provide the corresponding extension of Theorem 4.3 to the torus:

Theorem 4.10. Let $\tau \geqslant 4c_0 + 16$ where c_0 is the constant from Lemma 3.13, and let us abbreviate $\tilde{\epsilon} = e^{-\tau/2}$. For all $z \in \widetilde{\mathcal{O}}$, the following holds for all subsets Λ of the torus $\mathbb{T}_L$:

(i) If $a_q(z)\,\mathrm{diam}\,\Lambda \leqslant \frac{\tau}{4}$, then $Z_q(\Lambda, z) = Z'_q(\Lambda, z) \neq 0$ and

$$|Z_q(\Lambda, z)| \geqslant e^{-f_q(z)\,|\Lambda|} e^{-\tilde{\epsilon}\,|\partial\Lambda| - 2\,|\Lambda|\,e^{-\tau L/4}}. \tag{4.72}$$

(ii) If $m \in \mathcal{S}$, then

$$|Z_m(\Lambda, z)| \leqslant e^{-f(z)\,|\Lambda| + 2\tilde{\epsilon}\,|\partial\Lambda| + 4\,|\Lambda|\,e^{-\tau L/4}}. \tag{4.73}$$

(iii) If $m \in \mathcal{S}$, then

$$|Z_m(\mathbb{T}_L, z)| \leqslant e^{-f(z)\,L^d} \max\{e^{-a_m(z)\,L^d/2}, e^{-\tau L^{d-1}/4}\}\, e^{4L^d e^{-\tau L/4}}. \tag{4.74}$$

Remark 4.11. The bounds (4.72) and (4.73) are obvious generalizations of the corresponding bounds in Theorem 4.3 to the torus. But unlike in Proposition 4.6, we will not need to prove the bounds for the derivatives with respect to z. When such bounds will be needed in the next section, we will invoke analyticity in z and estimate the derivatives using Cauchy's Theorem.

Proof of (i). Since all contours can by definition be embedded into $\mathbb{Z}^d$, Theorem 4.3(ii) guarantees that $K'_q(Y, z) = K_q(Y, z)$ for all q-contours in Λ and hence $Z_q(\Lambda, z) = Z'_q(\Lambda, z)$. Then (4.72) follows by Lemma 4.9 and the definition of f_q. ∎

Proof of (ii). We will only indicate the changes relative to the proof of part (iv) of Theorem 4.3. First, since all contours can be embedded into $\mathbb{Z}^d$, we have that a corresponding bound—namely, (4.22)—holds for the interiors of all contours in Λ. This means that all of the derivation (4.31)–(4.35) carries over, with the exception of the factor $e^{\tilde{\varepsilon}\,|\partial\Lambda|}$ in (4.34) and (4.35) which by Lemma 4.9 should now be replaced by $e^{\tilde{\varepsilon}\,|\partial\Lambda|+2\,|\Lambda|\,e^{-\tau L/4}}$. In order to estimate the last sum in (4.35), we will again invoke the trick described in (4.36) and (4.37). This brings in yet another factor $e^{\tilde{\varepsilon}\,|\partial\Lambda|+2\,|\Lambda|\,e^{-\tau L/4}}$. From here (4.73) follows. ∎

Proof of (iii). The estimate is analogous to that in (ii); the only difference is that now we have to make use of the extra decay from the maximum in (4.35). (Note that for $\Lambda = \mathbb{T}_L$ we have $|\partial\Lambda| = 0$ and $|\Lambda| = L^d$.) Following ref. 5, this is done as follows: If Y is a contour, a standard isoperimetric inequality yields

$$|Y| \geqslant \frac{1}{2d}\,|\partial(\operatorname{supp} Y \cup \operatorname{Int} Y)| \geqslant |\operatorname{supp} Y \cup \operatorname{Int} Y|^{\frac{d-1}{d}}. \tag{4.75}$$

Hence, if $\tilde{\mathbb{Y}}$ is a collection of external contours in $\mathbb{T}_L$ and Ext is the corresponding exterior set, we have

$$\begin{aligned}\sum_{Y\in\tilde{\mathbb{Y}}} |Y| &\geqslant \sum_{Y\in\tilde{\mathbb{Y}}} |\operatorname{supp} Y \cup \operatorname{Int} Y|^{\frac{d-1}{d}}\\ &\geqslant \Big(\sum_{Y\in\tilde{\mathbb{Y}}} |\operatorname{supp} Y \cup \operatorname{Int} Y|\Big)^{\frac{d-1}{d}} = (L^d - |\mathrm{Ext}|)^{\frac{d-1}{d}}.\end{aligned} \tag{4.76}$$

Writing $|\mathrm{Ext}| = (1-x)\,L^d$ where $x\in[0,1]$, the maximum in (4.35) is bounded by

$$\sup_{x\in[0,1]} \exp\left\{-\frac{a_m}{2}\,L^d(1-x) - \frac{\tau}{4}\,L^{d-1}x^{\frac{d-1}{d}}\right\}. \tag{4.77}$$

The function in the exponent is convex and the supremum is thus clearly dominated by the bigger of the values at $x=0$ and $x=1$. This gives the maximum in (4.74). ∎

Apart from the partition functions $Z_m(\mathbb{T}_L, z)$, we will also need to deal with the situations where there is a non-trivial contour network. To this end, we need a suitable estimate on the difference

$$Z_L^{\text{big}}(z) = Z_L^{\text{per}}(z) - \sum_{m \in \mathscr{S}} Z_m(\mathbb{T}_L, z). \tag{4.78}$$

This is the content of the last lemma of this section.

Lemma 4.12. There exists a constant $\tilde{c}_0$ depending only on d and $|\mathscr{S}|$ such that for $\tau \geqslant 4\tilde{c}_0 + 16$ and all $z \in \widetilde{\mathcal{O}}$, we have

$$|Z_L^{\text{big}}(z)| \leqslant L^d e^{-\tau L/4} e^{5L^d e^{-\tau L/4}} \zeta(z)^{L^d}. \tag{4.79}$$

Proof. Let c_0 be the constant from Lemma 3.13, and let $\tilde{c}_0 = \tilde{c}_0(d, |\mathscr{S}|) \geqslant c_0$ be such that

$$\sum_{\Lambda \subset \mathbb{T}_L} (|\mathscr{S}|\, e^{-c_0})^{|\Lambda|} \leqslant L^d, \tag{4.80}$$

where the sum goes over all connected subsets Λ of the torus $\mathbb{T}_L$ (the existence of such a constant follows immediately from the fact that the number of connected subsets $\Lambda \subset \mathbb{Z}^d$ that contain a given point x and have size k is bounded by a d-dependent constant raised to the power k).

The proof of the lemma is now a straightforward corollary of Theorem 4.10. Indeed, invoking the representation (3.8) we have

$$Z_L^{\text{big}}(z) = \sum_{\substack{(\varnothing, \mathcal{N}) \in \mathscr{M}_L \\ \mathcal{N} \neq \varnothing}} \rho_z(\mathcal{N}) \prod_{m \in \mathscr{S}} Z_m(\Lambda_m(\varnothing, \mathcal{N}), z), \tag{4.81}$$

where $\Lambda_m(\varnothing, \mathcal{N})$ is defined before Proposition 3.11. Using (4.2) and (4.73) in conjunction with the bounds $\theta(z) \leqslant \zeta(z)\, e^{2\tilde{\varepsilon}}$ and $\sum_{m \in \mathscr{S}} |\partial \Lambda_m(\varnothing, \mathcal{N})| \leqslant |\mathcal{N}|$, we get

$$|Z_L^{\text{big}}(z)| \leqslant \zeta(z)^{L^d}\, e^{4L^d e^{-\tau L/4}} \sum_{\substack{(\varnothing, \mathcal{N}) \in \mathscr{M}_L \\ \mathcal{N} \neq \varnothing}} e^{-(\tau - 4\tilde{\varepsilon})\,|\mathcal{N}|}. \tag{4.82}$$

Taking into account that each connected component of supp $\mathcal{N}$ has size at least $L/2$, the last sum can be bounded by

$$\sum_{\substack{(\varnothing, \mathcal{N}) \in \mathscr{M}_L \\ \mathcal{N} \neq \varnothing}} e^{-(\tau - 4\tilde{\varepsilon})\,|\mathcal{N}|} \leqslant \sum_{n=1}^{\infty} \frac{1}{n!} S^n \leqslant S e^S \tag{4.83}$$

where

$$S = \sum_{\substack{\Lambda \subset \mathbb{T}_L \\ |\Lambda| \geqslant L/2}} (|\mathscr{S}| \, e^{-(\tau - 4\tilde{\epsilon})})^{|\Lambda|} \tag{4.84}$$

is a sum over connected sets $\Lambda \subset \mathbb{T}_L$ of size at least $L/2$. Extracting a factor $e^{-\tau L/4}$ from the right hand side of (4.84), observing that $\tau/2 - 4\tilde{\epsilon} \geqslant \tilde{c}_0$, and recalling that $\tilde{c}_0$ was defined in such a way that (4.80) holds, we get the estimate $S \leqslant L^d e^{-\tau L/4}$. Combined with (4.82) and (4.83) this gives the desired bound (4.79). ∎

5. PROOFS OF MAIN RESULTS

We are finally in a position to prove our main results. Unlike in Section 4, all of the derivations will assume the validity of Assumption C. Note that the assumptions (4.1)–(4.3) follow from Assumptions C0–C2, so all results from Section 4 are at our disposal. Note also that $\rho_z(Y)$, $\rho_z(\mathscr{N})$, and $\theta_m(z)$ are analytic functions of z by Lemma 3.10, implying that the partition functions $Z_m(\Lambda, \cdot)$ and Z_L^{per} are analytic functions of z.

We will prove Theorems A and B for

$$\tau_0 = \max\{\tau_1, 4\tilde{c}_0 + 16, 2\log(2/\alpha)\} \tag{5.1}$$

where τ_1 is the constant from Proposition 4.6, $\tilde{c}_0$ is the constant from Lemma 4.12 and α is the constant from Assumption C. Recall that $\tau_1 \geqslant 4c_0 + 16$, so for $\tau \geqslant \tau_0$ we can use all results of Section 4.

First, we will attend to the proof of Theorem A:

Proof of Theorem A. Most of the required properties have already been established. Indeed, let ζ_q be as defined in (4.16). Then (2.9) is exactly (4.18) which proves part (1) of the Theorem A.

In order to prove that $\partial_{\bar{z}}\zeta_q(z) = 0$ whenever $z \in \mathscr{S}_q$, we recall that $\zeta_q(z) = \theta_q(z)\, e^{s_q(z)}$ where $\theta_q(z)$ is holomorphic in $\widetilde{\mathscr{O}}$ and $s_q(z)$ is given in terms of its Taylor expansion in the contour activities $K'_q(Y, z)$. Now, if $a_q(z) = 0$—which is implied by $z \in \mathscr{S}_q$—then $K'_q(Y, z) = K_q(Y, z)$ for any q-contour Y by Theorem 4.3. But $\partial_{\bar{z}} K_q(Y, z) = 0$ by the fact that $\rho_z(Y)$, $Z_q(\text{Int}_m\, Y, z)$, and $Z_m(\text{Int}_m\, Y, z)$ are holomorphic and $Z_q(\text{Int}_m\, Y, z) \neq 0$. Since s_q is given in terms of an absolutely converging power series in the K_q's, we thus also have that $\partial_{\bar{z}} e^{s_q(z)} = 0$. Hence $\partial_{\bar{z}}\zeta_q(z) = 0$ for all $z \in \mathscr{S}_q$.

To prove part (3), let $z \in \mathscr{S}_m \cap \mathscr{S}_n$ for some distinct indices $m, n \in \mathscr{R}$. Using Lemma 4.2 we then have

$$\theta_m(z) \geqslant \theta(z)\, e^{-2e^{-\tau/2}} \tag{5.2}$$

and similarly for n. Since $\alpha \geqslant 2e^{-\tau_0/2} \geqslant 2e^{-\tau/2}$, we thus have $z \in \mathscr{L}_\alpha(m) \cap \mathscr{L}_\alpha(n)$. Using the first bound in (4.49), we further have

$$\left| \frac{\partial_z \zeta_m(z)}{\zeta_m(z)} - \frac{\partial_z \zeta_n(z)}{\zeta_n(z)} \right| \geqslant |\partial_z e_m(z) - \partial_z e_n(z)| - 2e^{-\tau/2}. \tag{5.3}$$

Applying Assumption C3, the right hand side is not less than $\alpha - 2e^{-\tau/2}$. Part (4) is proved analogously; we leave the details to the reader. ▮

Before proving Theorem B, we prove the following lemma.

Lemma 5.1. Let $\epsilon > 0$, let τ_1 be the constant from Proposition 4.6, and let

$$s_q^{(L)}(z) = \frac{1}{|\Lambda|} \log \mathscr{Z}'_q(\mathbb{T}_L, z) \tag{5.4}$$

and

$$\zeta_q^{(L)}(z) = \theta_q(z)\, e^{s_q^{(L)}(z)}. \tag{5.5}$$

Then there exists a constant M_0 depending only on ϵ and M such that

$$|\partial_z^\ell \zeta_q^{(L)}(z)| \leqslant (\ell!)^2\, (M_0)^\ell\, |\zeta_q^{(L)}(z)| \tag{5.6}$$

holds for all $q \in \mathscr{S}$, all $\ell \geqslant 1$, all $\tau \geqslant \tau_1$, all $L \geqslant \tau/2$, and all $z \in \widetilde{\mathscr{O}}$ with $a_q(z) \leqslant \tau/(4L)$ and $\operatorname{dist}(z, \widetilde{\mathscr{O}}^c) \geqslant \epsilon$.

Proof. We will prove the lemma withe the help of Cauchy's theorem. Starting with the derivatives of θ_q, let $\epsilon_0 = \min\{\epsilon, 1/(4\widetilde{M}_1)\}$ where $\widetilde{M}_1 = 1 + 4M$ is the constant from Lemma 4.8, and let z' be a point in the disc $\mathbb{D}_{\epsilon_0}(z)$ of radius ϵ_0 around z. Using the bounds (4.18) and (4.63), we now bound

$$|\theta_q(z')| \leqslant e^{\tilde{\varepsilon} - f(z')} \leqslant e^{\tilde{\varepsilon} + \widetilde{M}_1 \epsilon_0} e^{-f(z)} \leqslant e^{\tilde{\varepsilon} + \widetilde{M}_1 \epsilon_0 + a_q(z)} e^{-f_q(z)} \leqslant |\theta_q(z)|\, e^{2\tilde{\varepsilon} + \widetilde{M}_1 \epsilon_0 + a_q(z)}. \tag{5.7}$$

With the help of Cauchy's theorem and the estimates $\tilde{\varepsilon} \leqslant 1/8$, $\widetilde{M}_1 \epsilon \leqslant 1/4$, and $a_q(z) \leqslant 1/2$, this implies

$$\frac{|\partial_z^\ell \theta_q(z)|}{|\theta_q(z)|} \leqslant \ell!\, \epsilon_0^{-\ell} e^{1/4 + 1/4 + 1/2} \leqslant \ell!\, (2\epsilon_0^{-1})^\ell. \tag{5.8}$$

In order to bound the derivatives of $s_q^{(L)}$, let us consider a multiindex X contributing to the cluster expansion of $s_q^{(L)}$, and let $k=\max_{Y:\,\mathsf{X}(Y)>0}\operatorname{diam} Y$. Defining

$$\epsilon_k=\min\{\epsilon,\,(20e\widetilde{M}_1k)^{-1}\},\tag{5.9}$$

where $\widetilde{M}_1=1+4M$ is the constant from Lemma 4.8, we will show that the weight $K_q'(Y,\cdot)$ of any contour Y with $\mathsf{X}(Y)>0$ is analytic inside the disc $\mathbb{D}_{\epsilon_k}(z)$ of radius ϵ_k about z. Indeed, let $|z-z'|\leqslant\epsilon_k$. Combining the assumption $a_q(z)\leqslant\tau/(4L)\leqslant 1/2$ with Lemma 4.8, we have

$$\begin{aligned}e^{-a_q(z')}&\geqslant e^{-a_q(z)}-2e\widetilde{M}_1\epsilon_k\geqslant 1-a_q(z)-2e\widetilde{M}_1\epsilon_k\\&\geqslant 1-\tfrac{6}{5}\max\{a_q(z),\,10e\widetilde{M}_1\epsilon_k\}\geqslant e^{-2\max\{a_q(z),\,10e\widetilde{M}_1\epsilon_k\}}.\end{aligned}\tag{5.10}$$

Here we used the fact that $x+y\leqslant\frac{6}{5}\max\{x,5y\}$ whenever $x,y\geqslant 0$ in the last but one step, and the fact that $e^{-2x}\leqslant 1-(1-e^{-1})\,2x\leqslant 1-\frac{6}{5}x$ whenever $x\leqslant 1/2$ in the last step. We thus have proven that

$$a_q(z')\leqslant\max\{2a_q(z),\,20e\widetilde{M}_1\epsilon_k\}\leqslant\max\left\{\frac{\tau}{2L},\frac{1}{k}\right\}\leqslant\frac{\tau}{4k},\tag{5.11}$$

so by Theorem 4.3, $K_q'(Y,z')=K_q(Y,z')$ and $Z_q(\operatorname{Int}_m Y,z')\neq 0$ for all $m\in\mathscr{S}$ and $z'\in\mathbb{D}_{\epsilon_k}(z)$. As a consequence, $K_q'(Y,\cdot)$ is analytic inside the disc $\mathbb{D}_{\epsilon_k}(z)$, as claimed.

At this point, the proof of the lemma is an easy exercise. Indeed, combining Cauchy's theorem with the bound $|K_q'(Y,z')|\leqslant e^{-(\tau/2+c_0)\,|Y|}\leqslant e^{-c_0\,|Y|}e^{-(\tau/2)\operatorname{diam}Y}$, we get the estimate

$$\begin{aligned}\left|\partial_z^\ell\prod_Y K_q'(Y,z')^{\mathsf{X}(Y)}\right|&\leqslant\ell!\,\epsilon_k^\ell\prod_Y e^{-(c_0+\tau/2)\,|Y|\,\mathsf{X}(Y)}\\&\leqslant\ell!\,\epsilon_k^{-\ell}e^{-(\tau/2)\,k}\prod_Y e^{-c_0\,|Y|\,\mathsf{X}(Y)}.\end{aligned}\tag{5.12}$$

Bounding $\epsilon_k^{-\ell}e^{-(\tau/2)\,k}$ by $\epsilon_1^{-\ell}k^\ell e^{-k}\leqslant(\ell e^{-1}\epsilon_1^{-1})^\ell$, we conclude that

$$\left|\partial_z^\ell\prod_Y K_q'(Y,z')^{\mathsf{X}(Y)}\right|\leqslant\ell!\,(\ell e^{-1}\epsilon_1^{-1})^\ell\prod_Y e^{-c_0\,|Y|\,\mathsf{X}(Y)}.\tag{5.13}$$

Inserted into the cluster expansion for $s_q^{(L)}$, this gives the bound

$$|\partial_z^\ell s_q^{(L)}(z)|\leqslant\ell!\,(\ell e^{-1}\epsilon_1^{-1})^\ell,\tag{5.14}$$

which in turn implies that

$$|\partial_z^\ell e^{s_q^{(L)}(z)}| \leqslant \ell!\, (\ell e^{-1}\epsilon_1^{-1})^\ell\, 2^\ell\, |e^{s_q^{(L)}(z)}|. \tag{5.15}$$

Combining this bound with the bound (5.8), we obtain the bound (5.6) with a constant M_0 that depends only on ϵ and $\widetilde{M}_1$, and hence only on ϵ and M. ▮

Next we will prove Theorem B. Recall the definitions of the sets $\mathscr{S}_\epsilon(m)$ and $\mathscr{U}_\epsilon(\mathscr{Q})$ from (2.13) and (2.14) and the fact that in Theorem B, we set $\kappa = \tau/4$.

Proof of Theorem B(1)–(3). Part (1) is a trivial consequence of the fact that $\theta_m(z)$, $\rho_z(\mathscr{N})$, and $\rho_z(Y)$ are analytic functions of z throughout $\widetilde{\mathscr{O}}$.

In order to prove part (2), we note that $z \in \mathscr{S}_{\kappa/L}(q)$ implies that $a_q(z) \leqslant \kappa/L = \tau/(4L)$ and hence by Theorem 4.3(ii) we have that $K'_q(Y, z) = K_q(Y, z)$ for any q-contour contributing to $\mathscr{Z}_q(\mathbb{T}_L, z)$. This immediately implies that the functions $s_q^{(L)}$ and $\zeta_q^{(L)}(z)$ defined in (5.4) and (5.5) are analytic function in $\mathscr{S}_{\kappa/L}(q)$. Next we observe that $\tau \geqslant 4\tilde{c}_0 + 16$ implies that $\tau L/8 \geqslant \tau/8 \geqslant \log 4$ and hence $4e^{-\tau L/4} \leqslant e^{-\tau L/8}$. Since $z \in \mathscr{S}_{\kappa/L}(q)$ implies $a_q(z) < \infty$ and hence $\theta_q(z) \neq 0$, the bounds (2.15) and (2.16) are then direct consequences of Lemma 4.9 and the fact that $\partial \mathbb{T}_L = \varnothing$.

The bound (2.17) in part (3) finally is nothing but the bound (5.6) from Lemma 5.1, while he bound (2.18) is proved exactly as for Theorem A. Note that so far, we only have used that $\tau \geqslant \tau_0$, except for the proof of (2.17), which through the conditions from Lemma 5.1 requires $L \geqslant \tau/2$, and give a constant M_0 depending on ϵ and M. ▮

Proof of Theorem B(4). We will again rely on analyticity and Cauchy's Theorem. Let $\mathscr{Q} \subset \mathscr{R}$ and let $\mathscr{Q}' \subset \mathscr{S}$ be the set of corresponding interchangeable spin states. Clearly, if m and n are interchangeable, then $\zeta_m^{(L)} = \zeta_n^{(L)}$ and, recalling that q_m denotes the set of spins corresponding to $m \in \mathscr{R}$, we have

$$\Xi_{\mathscr{Q}}(z) = Z_L^{\text{per}}(z) - \sum_{n \in \mathscr{Q}'} [\zeta_n^{(L)}(z)]^{L^d} = Z_L^{\text{per}}(z) - \sum_{n \in \mathscr{Q}'} Z'_n(\mathbb{T}_L, z). \tag{5.16}$$

Pick a $z_0 \in \mathscr{U}_{\kappa/L}(\mathscr{Q})$. For $n \in \mathscr{Q}'$, we then have $a_n(z_0) \leqslant \tau/(4L)$, and by the argument leading to (5.11) we have that $a_n(z) \leqslant \tau/(2L)$ provided $\tau/(4L) \leqslant 1/2$ and $2e\widetilde{M}_1\, |z - z_0| \leqslant \frac{1}{5}\frac{\tau}{4L}$. On the other hand, if $m \in \mathscr{S} \setminus \mathscr{Q}'$, then $a_m(z_0) \geqslant \tau/(8L)$, and by a similar argument, we get that $a_m(z) \geqslant \tau/(16L)$ if

$\tau/(8L) \leqslant 1$ and $2e\widetilde{M}_1\, |z - z_0| \leqslant \frac{1}{10}\frac{\tau}{8L}$. Noting that $\tau \geqslant \tilde{\tau}_0$ implies $\tau \geqslant 4c_0 + 16 \geqslant 16$, we now set

$$\epsilon^{(L)} = \min\{\epsilon, (10e\widetilde{M}_1 L^d)^{-1}\}. \tag{5.17}$$

For $z \in \mathbb{D}_{\epsilon^{(L)}}(z_0)$ and $n \in \mathscr{Q}'$, we then have $a_n(z)\frac{L}{2} \leqslant \tau/4$ and hence $Z'_n(\mathbb{T}_L, z) = Z_n(\mathbb{T}_L, z)$, implying in particular that

$$\Xi_{\mathscr{Q}}(z) = Z_L^{\text{big}}(z) + \sum_{m \in \mathscr{S} \setminus \mathscr{Q}'} Z_m(\mathbb{T}_L, z). \tag{5.18}$$

Note that this implies, in particular, that $\Xi_{\mathscr{Q}}(\cdot)$ is analytic in $\mathbb{D}_{\epsilon^{(L)}}(z_0)$.

Our next goal is to prove a suitable bound on the right hand side of (5.18). By Lemma 4.12, the first term contributes no more than $2L^d \zeta(z)^{L^d} e^{-\tau L/4}$, provided $\tau \geqslant 4\tilde{c}_0 + 16$ and L is so large that $5L^d e^{-\tau L/4} \leqslant \log 2$. On the other hand, since $z \in \mathbb{D}_{\epsilon^{(L)}}(z_0)$ implies that $a_m(z) \geqslant \tau/(16L)$ for all $m \notin \mathscr{Q}'$, the bound (4.74) implies that each $Z_m(\mathbb{T}_L, z)$ on the right hand side of (5.18) contributes less than $2\zeta(z)^{L^d} e^{-\tau L^{d-1}/32}$ once L is so large that $4L^d e^{-\tau L/4} \leqslant \log 2$. By putting all of these bounds together and using that $\zeta(z)^{L^d} \leqslant \zeta(z_0)^{L^d} e^{\widetilde{M}_1 |z - z_0|\, L^d} \leqslant e^{1/(10e)} \zeta(z_0)^{L^d}$ by the bound (4.63) and our definition of $\epsilon^{(L)}$, we get that

$$|\Xi_{\mathscr{Q}}(z)| \leqslant 5\, |\mathscr{S}|\, L^d \zeta(z_0)^{L^d} e^{-\tau L^{d-1}/32} \tag{5.19}$$

whenever $z \in \mathbb{D}_{\epsilon^{(L)}}(z_0)$ and L is so large that $L \geqslant \tau/2$ and $5L^d e^{-\tau L/4} \leqslant \log 2$. Increasing L if necessary to guarantee that $\epsilon^{(L)} = (10e\widetilde{M}_1 L^d)^{-1}$ and applying Cauchy's theorem to bound the derivatives of $\Xi_{\mathscr{Q}}(z)$, we thus get

$$|\partial_z^\ell \Xi_{\mathscr{Q}}(z)|_{z=z_0} \leqslant \ell!\, (10e\widetilde{M}_1)^\ell\, 5\, |\mathscr{S}|\, L^{d(\ell+1)} \zeta(z_0)^{L^d} e^{-\tau L^{d-1}/32} \tag{5.20}$$

provided $L \geqslant L_0$, where $L_0 = L_0(d, M, \tau, \epsilon)$ is chosen in such a way that for $L \geqslant L_0$, we have $L \geqslant \tau/2$, $5L^d e^{-\tau L/4} \leqslant \log 2$, and $(10e\widetilde{M}_1 L^d)^{-1} \leqslant \epsilon$. Since $z_0 \in \mathscr{U}_{\kappa/L}(\mathscr{Q})$ was arbitrary and $|\mathscr{S}| = \sum_{m \in \mathscr{R}} q_m$, this proves the desired bound (2.20) with $C_0 = 10e\widetilde{M}_1 = 10e(1 + 4M)$. ▮

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