FUB-HEP 5/92,
February 1992

CROSSOVER FINITE-SIZE SCALING AT FIRST ORDER TRANSITIONS

Christian Borgs*
Institut für Theoretische Physik
Freie Universität Berlin
Arnimallee 14
D-1000 Berlin 33
Germany

John Z. Imbrie**
Department of Mathematics
University of Virginia
Charlottesville, VA 22903
USA

ABSTRACT

In a recent paper we developed a method which allows to rigorously control the finite-size behavior in long cylinders near first-order phase transitions at low temperature. Here we apply this method to asymmetric transitions with two competing phases, and to the q-state Potts model as a typical model of a temperature driven transition, where q low temperature phases compete with one high temperature phase. We obtain the finite-size scaling of the first N eigenvalues (where N is the number of competing phases) of the transfer matrix in a periodic box of volume $L \times \ldots \times L \times t$, and, as a corollary the finite-size scaling of the shape of the order parameter in a hypercubic box ($t = L$), the infinite cylinder ($t = \infty$), and the crossover regime from hypercubic to cylindrical scaling. For the two-phase case ($N = 2$) we find that the crossover length ξ_L is given by $O(L^w)e^{\beta\sigma L^\nu}$, where β is the inverse temperature, σ is the surface tension and $w = 1/2$ if $\nu + 1 = 2$ while $w = 0$ if $\nu + 1 > 2$. For the standard Ising model we also consider free boundary conditions, showing that $\xi_L = \exp(\beta\sigma L^\nu + O(L^{\nu-1}))$ for any dimension $\nu + 1 \geq 2$. For $\nu + 1 = 2$ we finally discuss a class of boundary conditions which interpolate between free (corresponding to the interpolating parameter $g = 0$) and periodic boundary conditions (corresponding to $g = 1$), finding that $\xi_L = O(L^w)e^{\beta\sigma L^\nu}$ with $w = 0$ for $g = 0$ and $w = 1/2$ for $0 < g \leq 1$.

* Research partially supported by the A. P. Sloan Foundation and by the NSF under DMS-8858073.
** Research partially supported by the NSF under DMS-8858073 and DMS-9008827.

1. Introduction

In recent years, finite-size effects at first-order transitions have been widely studied [1]. For a wide class of models the finite-size scaling in a cubic box V with periodic boundary conditions can be derived from the ansatz

$$Z_{\text{per}}(V,\mu) \cong \sum_{m=1}^{N} e^{-\beta f_m(\mu)|V|} \tag{1.1}$$

for the partition function. Here $|V|$ is the volume of the cubic box V, μ is the driving parameter of the transition, N is the number of stable phases at the transition point, β is the inverse temperature and $f_m(\mu)$ is some sort of metastable free energy of the phase m. It is equal to the free energy $f(\mu)$ if m is stable, and strictly larger than $f(\mu)$ if m is unstable.

If the model in consideration allows for a contour representation in which the configurations of the system may be described in terms of "ground state regions" separated by energetically unfavorable "contours [1]," a formula of the form (1.1) can actually be proven, together with a bound $O(|V|e^{-b\text{diam}V})$ for the error term [2,3]. Here diam$V$ is the diameter of the cube, and $b > 0$ is a constant. Actually, these results remain true in the the more general case where V is a $\nu + 1$ dimensional cylinder with $L \times \cdots \times L \times t$ points, provided

$$|V|e^{-\min(L,t)} \le 1 \ . \tag{1.2}$$

For long cylinders, however, the effects neglected in the approximation (1.1) play an important role. Using a linear scaling ansatz to scale the cylinder down to a one-dimensional interval of length t/L, Blöte and Nightingale [4] have developed a heuristic theory of finite-size scaling in long cylinders. A little bit later, Privman and Fisher [5] developed an alternative theory, starting from the observation that the periodic partition function may be written as

$$Z_{\text{per}}(V,\mu) = \sum_{i=1}^{\infty} \lambda_i(L)^t \tag{1.3}$$

[1] For the ferromagnetic Ising model, the ground states regions are the regions where the spin is constant, while the contours are just the usual Peierls contours.

if the model in consideration has a positive transfer matrix (as many models of statistical mechanics do). Here $\lambda_1(L) \geq \lambda_2(L) \geq \cdots$ are the eigenvalues of the transfer matrix. They then argue, for $N = 2$ and models with a symmetry relating μ to $-\mu$, that only λ_1 and λ_2 are important for the asymptotic behavior of $Z_{\text{per}}(V, \mu)$, and that λ_1 and λ_2 may be calculated by diagonalizing a certain 2×2 matrix. As a consequence, they were able to calculate the finite-size scaling of the magnetization from cubic boxes up to infinite cylinders, finding a crossover regime when t diverges with L like

$$\xi_L = D(L) \exp(\beta \sigma L^\nu)$$

where σ is the surface tension between the two phases and $D(L)$ is a "slowly varying function of L." Privman and Fisher predicted $D(L) \sim L^{1/2}$ for $\nu = 1$ and Brézin and Zinn-Justin [6] predicted $D(L) \sim L^{(2-\nu)/2}$ for $\nu \geq 1$, see also [7]. As we will see, this prediction is incorrect for $\nu > 2$ and low temperature. (As pointed out in [8], the exponent may be different above the roughening transition.)

Here we continue the rigorous analysis in [9] of finite-size scaling in long cylinders at low temperature. Among other results we will obtain a rigorous derivation of the results of Privman and Fisher, a formula for the slowly varying function $D(L)$, the generalization of these results to a wide class of two-phase systems without any symmetry assumptions, and — as an example of a temperature driven transition — the finite-size scaling for the q-state Potts model.

In order to describe the ideas and results of [9] let us consider a perturbed Ising model with Hamiltonian

$$\beta H = \beta \sum_{\substack{x,y \\ |x-y|=1}} |\sigma_y - \sigma_y| + \beta \sum_X J_X \prod_{x \in X} \sigma_x - \mu \sum_x \sigma_x \,, \tag{1.4}$$

where $J_X = 0$ if diam $X > r_0$ ($r_0 < \infty$ is the range of the interaction), $\sum_{X \ni x} |J_X|$ is small and β is large. Note that μ is β times the usual magnetic field. This model is a typical example of a model describing an asymmetric first order transition between two different low temperature phases and allows for a Peierls contour expansion with exponentially suppressed contours.

Neglecting for the moment contours which wind around the cylinder in the time direction, we now distinguish two different kinds of contours: interfaces which separate two different phases in the lower and upper part of an infinite cylinder, and ordinary contours which do not. Resumming the ordinary contours we get an effective weight, $\kappa(Y)$, for the interfaces, a "renormalized" ground state energy, $f_{\pm}(L)$, for the regions between interfaces, and an interaction between interfaces. Using iterative cluster expansions to control this interaction (see Section 4 of [9]) and a variant of Dobrushin's surface expansion [10] to control the deviation from flat interfaces (Section 5 of [9]), we obtain a system of non-interacting flat interfaces with weight $O(L^{-1/2})e^{-\beta\sigma L^\nu}$ for $\nu = 1$ and $(1+O(e^{-bL}))e^{-\beta\sigma L^\nu}$ for $\nu > 1$. Since a system of flat interfaces is equivalent to a one-dimensional system we obtain Theorem A (below) for the perturbed Ising model (1.4).

In fact, Theorem A is proven in a much wider context, see Section 2 and 5 of [9] for a description of the class of models to which it applies. Essentially we need a contour or cluster representation with a Peierls condition, translation invariance, and invariance under reflection in the t-direction, together with several assumptions on the structure of interfaces, essentially locality and suppression of defects relative to a flat interface. The notation is as follows: $Z_{\rm per}(V,\mu)$ is the periodic partition function in volume V, $|V| = L^\nu t$, μ is an $(N-1)$-vector of parameters driving transitions amongst N states, μ^* is the coexistence point, $f = f(\mu)$ is the free energy density, σ_{mn} is the surface tension between the phases m and n, and τ is the parameter in the Peierls condition ($\tau = O(\beta)$ for the perturbed Ising model (1.4)). It is assumed throughout that L, t are positive integers.

Theorem A. *There are C^4 functions $f_m(\mu) \geq f(\mu)$, $m = 1, \cdots, N$, agreeing with $f(\mu)$ if and only if the corresponding phase is stable, such that the following statements are true provided τ is sufficiently large and $|\mu - \mu^*|L^\nu \leq 1$.*

(i) *There exists an $N \times N$ symmetric matrix R such that for all $t \geq \nu \log L$ and for $0 \leq k \leq 4$,*

$$\left| \frac{d^k}{d\mu^k} (Z_{\rm per}(V,\mu) - \operatorname{Tr} R^t) \right| \leq e^{-\beta f |V|} e^{-(\tau - O(1))t}. \tag{1.5}$$

(ii)
$$\left| \frac{d^k}{d\mu^k} \left(L^{-\nu} \log R_{mm} + \beta f_m(\mu)\right) \right| \leq e^{-(\tau - O(1))L} \tag{1.6}$$

(iii)
$$\left| \frac{d^k}{d\mu^k} R_{mn} \right| \leq e^{-(\beta f + \tau - O(1))L^\nu} \qquad \textit{if} \qquad n \neq m \tag{1.7}$$

(iv) *Let $N = 2$. Then there are constants $0 < b_1 < 1$ and $C_{+-} > 0$ such that the off-diagonal matrix elements $R_{+-} = R_{-+}$ of R are*

$$R_{+-} = e^{-\beta f(\mu)L^\nu} \begin{cases} C_{+-}\ L^{-1/2} e^{-\beta\sigma L}(1 + O(L^{-1}))\ , & \nu = 1,\ L \gg 1 \\ e^{-\beta\sigma L^\nu}(1 + O(e^{-b_1\tau L}))\ , & \nu \geq 2\ , \end{cases} \tag{1.8}$$

provided $|\mu - \mu^*| \leq e^{-\tau L/2}$.

This theorem reduces the determination of the asymptotics of $Z_{\text{per}}(V,\mu)$ to a calculation of an $N \times N$ matrix R. If the original model has a positive transfer matrix T, it implies that the first N eigenvalues of T are just the eigenvalues of R, and that $\lambda_i(L) \leq e^{-O(\tau)}\lambda_1$ for the remaining ones.

In the present note, we use the results of [9], in particular Theorem A above, to derive the explicit scaling form for the magnetization, $M_{\text{per}}(V,\mu)$, and the internal energy, $E_{\text{per}}(V,\beta)$, respectively, of models like the perturbed Ising model (1.4) or the q-state Potts model (at low temperatures and large q, respectively). For the perturbed Ising model and more generally for any two-phase model satisfying the assumptions described before Theorem A, our main results are summarized in the following Theorem B. We need the infinite volume magnetizations of the two phases, which we write as

$$M_0 \pm \Delta M \equiv -\frac{d(\beta f)}{d\mu}(\mu^{*\pm}). \tag{1.9}$$

Theorem B. *Let $N = 2$, let τ be sufficiently large, and let $\mu^*(L) = \mu^* + e^{-(\tau - O(1))L}$ be the point for which the diagonal matrix elements R_{++} and R_{--} of the matrix R are equal. There exists a ξ_L satisfying*

$$\xi_L = \begin{cases} \frac{1}{2C_{+-}}\ L^{1/2} e^{\beta\sigma L}(1 + O(L^{-1}))\ , & \nu = 1,\ L \gg 1 \\ \frac{1}{2} e^{\beta\sigma L^\nu}(1 + O(e^{-b_1\tau L}))\ , & \nu \geq 2\ , \end{cases} \tag{1.10}$$

such that in terms of scaling variables

$$y_B = tL^\nu(\mu - \mu^*(L))\Delta M \tag{1.11}$$

$$y_C = \xi_L L^\nu(\mu - \mu^*(L))\Delta M \tag{1.12}$$

and the scaling function

$$Y(y_B, y_C) = \frac{2y_C}{\sqrt{1+4y_C^2}}\tanh\left[\frac{y_B}{2y_C}\sqrt{1+4y_C^2}\right], \tag{1.13}$$

the magnetization obeys the following bound:

$$M_{\text{per}}(V,\mu) = M_0 + \Delta M\, Y(y_B, y_C) + e^{-O(\tau)L} + e^{-O(\tau)t} + O(\mu-\mu^*), \tag{1.14}$$

for any t, L, μ which fulfills the conditions $L^\nu e^{-t} \leq 1$ and $|\mu-\mu^*| \leq O(1)$. Here C_{+-} is the constant from Theorem A.

Theorem B is the announced generalization of Privman and Fisher's results to asymmetric two-phase systems. Note that the formula (1.10) for ξ_L (which is the inverse of the smallest splitting of the eigenvalues of $\log R$ in (1.5) as μ varies near μ^*) agrees with their prediction for $\nu = 1$, and corrects the prediction of Brézin and Zinn-Justin for $\nu > 2$. We emphasize that (1.10) is a low temperature result and that ξ_L may behave differently above the roughening transition in $\nu + 1 = 3$. For $\nu + 1 > 3$, however, it is not expected that there is a roughening transition. Nevertheless, numerical simulations of the four-dimensional Ising model near T_c [11,12] seem to support the continuum calculations of [7], who predicts $\xi_L = C(\beta)L^{-1/2}e^{\beta\sigma L^\nu}$ with $C(\beta)$ given explicitely in terms of the renormalized mass and coupling constant. It is an interesting open problem to explain the transition from the apparent continuum behaviour near T_c to the low temperature behaviour proven in this paper.

While (1.14) holds for all t, L, μ within the prescribed range, it is natural to consider a limit $t, L, |\mu-\mu^*|^{-1} \to \infty$ fixing y_B, y_C. In this limit $t \sim \xi_L$, the crossover length scale, $(\mu - \mu^*(L)) \sim 1/(L^\nu \xi_L)$, all error terms in (1.14) are exponentially small, and

$$M_{\text{per}}(V,\mu) \to M_0 + \Delta M\, Y(y_B, y_C)\ ,$$

If one considers, on the other hand, a limit where y_B is kept fixed while $y_C \to \infty$,

$$M_{\text{per}}(V,\mu) \to M_0 + \Delta M\ \tanh y_B\ ,$$

which is the usual scaling form in the block limit. Considering finally the cylinder limit, where $t, L, |\mu - \mu^*|^{-1} \to \infty$ in such a way that y_C is kept fixed while $y_B \to \infty$,

$$M_{\rm per}(V,\mu) \to M_0 + \Delta M \, \frac{2y_C}{\sqrt{1+4y_C^2}} \ ,$$

which is the typical form for a one-dimensional system.

We emphasize that the width of the transition in the crossover and in the cylinder regime is of the order $\mu - \mu^* = O(1/(L^\nu \xi_L))$, which is (at least for $\nu+1 \geq 3$) much smaller than the shift $\mu^*(L) - \mu^* = e^{-O(\tau)L}$ allowed by the bound (1.6) [2]. Note, however, that $\mu^*(L) = \mu^*$ for a model like the ordinary Ising model, where the two phases are related by a symmetry $\mu - \mu^* \to \mu^* - \mu$.

We finally discuss the q-state Potts model, which is a spin model with spin variable $\sigma_x \in \mathbf{Z}_q := \{1, e^{2\pi i/q}, \ldots, e^{2\pi i(q-1)/q}\}$ and Hamiltonian

$$H = -\tfrac{1}{2} \sum_{\substack{x,y \\ |x-y|=1}} \delta(\sigma_y, \sigma_y) \ , \tag{1.15}$$

where δ is the Kronecker delta (for a review of the Potts model, see *e.g.* [13]). For q large enough (and $\nu + 1 \geq 2$) this model undergoes a first-order phase transition as the inverse temperature, $\beta = 1/(kT)$, is varied. At the transition point, β_t, the number of stable phases goes from 1 below β_t to q above β_t. Actually, for $\beta = \beta_t$, the q ordered low temperature phases and the disordered high temperature phase coexist and the internal energy $E(\beta)$ jumps from $E_d = E(\beta_t - 0)$ to $E_o = E(\beta_t + 0)$ ([14,15]).

The next theorem summarizes our main results concerning the finite-size scaling of this model. The constant σ_{od} appearing in (1.17) below is the surface tension between the disordered and an ordered phase.

Theorem C. *Let q and L be sufficiently large. Then there exists a finite volume transition point $\beta^*(L)$ and a length scale ξ_L satisfying*

$$|\beta_t - \beta^*(L)| \leq q^{-O(1)L} \ , \tag{1.16}$$

$$\xi_L = \begin{cases} C(q) L^{1/2} (1 + O(L^{-1})) e^{\beta \sigma_{od} L} \ , & \nu = 1 \ , \\ q^{-1/2} e^{\beta \sigma_{od} L^\nu} (1 + O(q^{-O(1)L})) \ , & \nu \geq 2 \ , \end{cases} \tag{1.17}$$

[2] We expect that the actual shift is $\mu^*(L) - \mu^* = O(e^{-L/\max(\xi_+, \xi_-)})$, where $\xi_\pm$ are the infinite volume correlation lengths of the two phases.

for some $C(q)$ such that in terms of scaling variables

$$y_B = tL^\nu(\beta - \beta^*(L))\frac{E_d - E_o}{2} \tag{1.18}$$

$$y_C = \xi_L L^\nu(\beta - \beta^*(L))\frac{E_d - E_o}{2} \tag{1.19}$$

and the scaling function

$$Y(y_B, y_C) = \frac{(q-1)e^{y_B} + (1+y_C^{-2})^{-1/2} 2\sinh\left(y_B\sqrt{1+y_C^{-2}}\right)}{(q-1)e^{y_B} + 2\cosh\left(y_B\sqrt{1+y_C^{-2}}\right)} \tag{1.20}$$

the internal energy obeys the following bound:

$$\begin{aligned} E_{\text{per}}(V,\beta) = {}& \frac{E_o + E_d}{2} + \frac{E_o - E_d}{2} Y(y_B, y_C) + q^{-O(1)L} + q^{-O(1)t} \\ & + O(q|\beta - \beta_t|) + O(\xi_L^{-(1-\epsilon)}) \min\{1 + |y_C|, y_B/y_C\}\ , \end{aligned} \tag{1.21}$$

for any t, L, β which fulfill the conditions $L^\nu e^{-t} \leq 1$ and $|\beta - \beta^*| \leq O(1)$. Here $\epsilon = \epsilon(q)$ is a small positive constant which goes to zero as $q \to \infty$.

Note that the asymptotics (1.21) simplifies in the block limit where t, L, and $(\beta_t - \beta)^{-1} \to \infty$ in such a way that $y_C \to \infty$ while y_B is kept fixed; in this case

$$E_{\text{per}}(V,\beta) \to \frac{E_o + E_d}{2} + \frac{E_o - E_d}{2}\ \tanh(y_B + \tfrac{1}{2}\log q)$$

(in accordance with the results of [3]). On the other hand, in the cylinder limit where t, L, and $(\beta_t - \beta)^{-1} \to \infty$ in such a way that $y_B \to \infty$ while y_C is kept fixed, we have that

$$E_{\text{per}}(V,\beta) \to \frac{E_o + E_d}{2} + \frac{E_o - E_d}{2}\ \frac{y_C}{\sqrt{1+y_C^2}}\ .$$

Outline. We derive the finite-size scaling for the two-phase system in Section 2, where we also state a more precise version of Theorem B. Among other things we eliminate the error term $\exp(-O(\tau)L)$ by using L-dependent quantities in defining the block and cylinder scaling variables y_B, y_C. In Section 3 we discuss the finite-size scaling of the internal energy and the specific heat for the Potts model, and in Section 4 we discuss free boundary conditions (and more generally a class of boundary conditions interpolating between free and periodic), restricting ourselves to a situation where two phases related by a symmetry are coexisting to avoid technical complications. Some of the more technical aspects of Section 4 are dealt with in an appendix.

2. Asymmetric First-Order Phase Transitions with Two Competing Phases

In this section we consider a large class of models describing this coexistence of two infinite volume phases, $m = \pm 1$, at the value $\mu = \mu^*$ of the driving field μ. We need a contour or cluster representation with a Peierls condition, translation invariance, and invariance under reflection in the t-direction (see Section 2 of [9] for the precise assumptions), together with several assumptions on the structure of interfaces, essentially locality and suppression of defects relative to a flat interface (see Section 5, Assumption 5.1 through 5.5, of [9]). As a typical example, the reader should keep in mind the perturbed Ising model (1.4) at low temperatures. We will prove Theorem B stated in the introduction, and its more precise version Theorem 2.1 below.

Recall that we are interested in the behavior of the partition function $Z_{\text{per}}(V, \mu)$ and the magnetization

$$M_{\text{per}}(V, \mu) = \frac{1}{tL^\nu} \frac{d}{d\mu} \log Z_{\text{per}}(V, \mu) , \tag{2.1}$$

in a cylinder $V = A \times T$, where A is the ν-dimensional torus of side length L, and T is the one dimensional torus of length $|T| = t$. Due to Theorem A,

$$\left| Z_{\text{per}}(V, \mu) - \sum_{i=1}^{2} \lambda_i(L)^t \right| \leq e^{-\beta f(\mu)|V|} e^{-(\tau - O(1))t};, \tag{2.2}$$

$$\left| \frac{d^k}{d\mu^k} \left[M_{\text{per}}(V, \mu) - \sum_i M_i(L, \mu) P_i(V, \mu) \right] \right| \leq e^{-(\tau - O(1))t} , \tag{2.3}$$

if $k \leq 3$, $t \geq \nu \log L$ and $|\mu - \mu^*| L^\nu \leq 1$. Here $\lambda_i(L)$ are the eigenvalues of the 2×2 matrix R described in Theorem A, and

$$M_i(L, \mu) \equiv \frac{1}{L^\nu} \frac{d}{d\mu} \log \lambda_i(L) , \tag{2.4}$$

$$P_i(V, \mu) \equiv \lambda_i(L)^t \left[\sum_j \lambda_j(L)^t \right]^{-1} . \tag{2.5}$$

As a consequence, the asymptotic behavior of $Z_{\text{per}}(V, \mu)$ and $M_{\text{per}}(V, \mu)$ is determined once the asymptotic behavior of the eigenvalues $\lambda_{1,2}(L)$ is given.

We start with a heuristic derivation of this behavior in the region $|\mu-\mu^*|L^\nu \leq 1$. Let us neglect the L-dependence in the diagonal elements of R, so that (in the approximation given by (1.6))

$$R = \begin{pmatrix} \exp(-L^\nu \beta f_+(\mu)) & R_{+-}(\mu) \\ R_{+-}(\mu) & \exp(-L^\nu \beta f_-(\mu)) \end{pmatrix} .$$

Now we pull out an overall factor $\exp(-L^\nu\beta(f_+(\mu)+f_-(\mu))/2)$ from this matrix, leaving

$$\widetilde{R} = \begin{pmatrix} \exp(-L^\nu \beta (f_+(\mu)-f_-(\mu))/2) & \widetilde{R}_{+-} \\ \widetilde{R}_{+-} & \exp(L^\nu \beta (f_+(\mu)-f_-(\mu))/2) \end{pmatrix} .$$

Ignoring the μ-dependence of $\widetilde{R}_{+-}$ we have $\widetilde{R}_{+-} = \widetilde{R}_{+-}(\mu^*)$. Finally, we linearize $f_\pm(\mu)$ about μ^*, so that

$$\widetilde{R} = \begin{pmatrix} e^x & \widetilde{R}_{+-} \\ \widetilde{R}_{+-} & e^{-x} \end{pmatrix}$$

with $x = \Delta M(\mu-\mu^*)L^\nu$. The eigenvalues of this matrix are $\cosh x \pm \sqrt{\sinh^2 x + \widetilde{R}_{+-}^2}$ which for small x and $\widetilde{R}_{+-}$ becomes

$$1 \pm \sqrt{x^2 + \widetilde{R}_{+-}^2} = 1 \pm \frac{1}{2}\,\xi_L^{-1}\sqrt{1+4y_C^2}\ ,$$

where $\xi_L = (2\widetilde{R}_{+-}(\mu^*))^{-1}$ and $y_C = \xi_L L^\nu(\mu-\mu^*(L))\,\Delta M$ is the scaling variable defined in (1.12). As a consequence,

$$\lambda_{1,2}(L) = \exp\left(-\frac{1}{2}\,L^\nu\beta(f_+ + f_-)\right)\left[1 \pm \frac{1}{2}\,\xi_L^{-1}\sqrt{1+4y_C^2}\right] .$$

To see the form of the magnetization, differentiate the eigenvalues with respect to μ, as required by (2.4):

$$M_{1,2}(L,\mu) = \frac{1}{L^\nu}\frac{d}{d\mu}\log\lambda_{1,2} \cong M_0 \pm \frac{1}{2}\xi_L^{-1}\frac{4y_C y_C'}{\sqrt{1+4y_C^2}} = M_0 \pm \Delta M \frac{2y_C}{\sqrt{1+4y_C^2}} .$$

(In the second equality, we have neglected second and higher order terms in the expansion of the log.) The relative weightings $P_{1,2}$ given by (2.5) are determined by

$$\lambda_{1,2}^t \sim \exp\left(\pm(t/2\xi_L)\sqrt{1+4y_C^2}\right) = \exp\left(\pm\frac{y_B}{2y_C}\sqrt{1+4y_C^2}\right) ,$$

so that

$$M_{\rm per} = M_1 P_1 + M_2 P_2 = M_0 + \Delta M \frac{2y_C}{\sqrt{1+4y_C^2}} \tanh\left[\frac{y_B}{2y_C}\sqrt{1+4y_C^2}\right] \ ,$$

as in Theorem B.

In order to obtain the optimal asymptotics for Theorem 2.1 below, we now introduce scaling variables y_B and y_C where the constant ΔM is replaced by an L-dependent constant $\widetilde{\Delta M}$. Our definitions are based on the exact matrix R of Theorem A. We write

$$R = \begin{pmatrix} \exp(-L^\nu \beta \tilde{f}_+) & R_{+-} \\ R_{+-} & \exp(-L^\nu \beta \tilde{f}_-) \end{pmatrix} \ , \tag{2.6}$$

and recall that

$$\left| \frac{d^k}{d\mu^k} \Big(\beta f_\pm(\mu) - \beta \tilde{f}_\pm(L,\mu) \Big) \right| \le e^{-(\tau - O(1))L} \ , \tag{2.7}$$

provided $k \le 4$ and $|\mu - \mu^*| L^\nu \le 1$. We define $\mu^*(L)$ by the equation $\tilde{f}_+(\mu^*(L)) = \tilde{f}_-(\mu^*(L))$, and introduce the magnetizations of the two phases in $\mathbf{R}^{\nu+1}$, and the corresponding L-dependent quantities

$$M_\pm = -\frac{d(\beta f_\pm)}{d\mu}(\mu^*) \ , \qquad \widetilde{M}_\pm = \widetilde{M}_\pm(L) = -\frac{d(\beta \tilde{f}_\pm)}{d\mu}(\mu^*(L)) \ . \tag{2.8}$$

We also define

$$\begin{aligned} M_0 &= \tfrac{1}{2}(M_+ + M_-) \ , &\qquad \Delta M &= \tfrac{1}{2}(M_+ - M_-) \ , \\ \widetilde{M}_0 &= \tfrac{1}{2}(\widetilde{M}_+ + \widetilde{M}_-) \ , &\qquad \widetilde{\Delta M} &= \tfrac{1}{2}(\widetilde{M}_+ - \widetilde{M}_-) \ . \end{aligned} \tag{2.9}$$

Note that the assumption (2.7) formulated in [9] implies that ΔM, $\widetilde{\Delta M}$ are nonzero. Furthermore, Theorem A, (ii) implies that

$$|\mu^*(L) - \mu^*| \le e^{-(\tau - O(1))L} \ , \tag{2.10}$$

$$|\widetilde{\Delta M} - \Delta M| \le e^{-(\tau - O(1))L} \ , \tag{2.11}$$

$$|\widetilde{M}_0 - M_0| \le e^{-(\tau - O(1))L} \ . \tag{2.12}$$

Next, we introduce a characteristic length scale

$$\xi_L = \tfrac{1}{2} R_{+-}(L, \mu^*(L))^{-1} \exp\left(-\tfrac{1}{2} L^\nu \beta(\tilde{f}_+(\mu^*(L)) + \tilde{f}_-(\mu^*(L)))\right) ,$$

which governs transitions between phases along the t-axis at $\mu^*(L)$. Finally, we introduce block and cylinder scaling parameters:

$$y_B = t L^\nu (\mu - \mu^*(L)) \widetilde{\Delta M} , \tag{2.13}$$

$$y_C = \xi_L L^\nu (\mu - \mu^*(L)) \widetilde{\Delta M} . \tag{2.14}$$

Remark: If the model in consideration has a positive transfer matrix T with eigenvalues $\lambda_1 > \lambda_2 \geq \cdots$, the correlation length $\xi_\parallel$ in time direction is just

$$\xi_\parallel = [\log(\lambda_1/\lambda_2)]^{-1} .$$

Due to Theorem A, λ_1 and λ_2 may be calculated from the matrix R, and

$$\xi_\parallel(\mu = \mu^*(L)) = \left[\log \left(\frac{1 + (2\xi_L)^{-1}}{1 - (2\xi_L)^{-1}} \right) \right]^{-1} = \xi_L (1 + O(\xi_L^{-2}))$$

by the above definition of ξ_L.

Theorem 2.1. *Consider a two-phase system satisfying the assumptions formulated in Section 2 and 5 of [9], and suppose τ is sufficiently large. Then $Z_{\rm per}(V, \mu)$, the partition function in periodic cylindrical volume $V = L^\nu t$, obeys the asymptotics* (2.2) *with*

$$\begin{aligned} \lambda_{1,2}(L) = & \exp\left(\frac{1}{2} \, L^\nu \beta(\tilde{f}_+ + \tilde{f}_-) \right) \\ & \times \left[1 + O(|\mu - \mu^*(L)|^2 L^{2\nu}) \pm \frac{1}{2} \, \xi_L^{-1} \sqrt{1 + 4y_C^2} \, (1 + O(|\mu - \mu^*(L)| L^\nu)) \right] , \end{aligned} \tag{2.15}$$

provided $|\mu - \mu^*| L^\nu \leq 1$ and $t \geq \nu \log L$. Under the same conditions the magnetization is described by

$$M_{\rm per}(V, \mu) = \widetilde{M}_0 + \widetilde{\Delta M} \, Y(y_B, y_C) + O(\xi_L^{-1}) + O(e^{-(\tau - O(1))t}) + O(\mu - \mu^*(L)) . \tag{2.16}$$

Here y_B and y_C are block and cylinder scaling variables defined in (2.13) *and* (2.14) *and* $Y(\cdot,\cdot)$ *is the scaling function*

$$Y(y_B, y_C) = \frac{2y_C}{\sqrt{1+4y_C^2}} \tanh\left[\frac{y_B}{2y_C}\sqrt{1+4y_C^2}\right] . \tag{2.17}$$

Finally,

$$\xi_L = \begin{cases} \frac{1}{2C_{+-}} L^{1/2} e^{\beta\sigma L}(1+O(L^{-1})) , & \nu = 1,\, L \gg 1 \\ \frac{1}{2} e^{\beta\sigma L^\nu}(1+O(e^{-b\tau L})) , & \nu \geq 2 , \end{cases} \tag{2.18}$$

where C_{+-} is the constant introduced in Theorem A and σ is the string tension at the coexistence point μ^*.

It is interesting to consider three types of scaling limits $t, L, |\mu-\mu^*|^{-1} \to \infty$: the cylinder limit where y_C is fixed while $y_B \to \infty$, so that $t/\xi_L = y_B/y_C \to \infty$, the block limit where y_B is fixed and $y_C \to \infty$, so that $t/\xi_L \to 0$, and the crossover limit where y_B and y_C are fixed in $(0,\infty)$, so that $t \sim \xi_L$. Note that in any of these cases

$$|\mu - \mu^*(L)|L^\nu = |y_B|/(t\widetilde{\Delta M}) = |y_C|/(\xi_L\widetilde{\Delta M}) \to 0 , \tag{2.19}$$

since both t and ξ_L tend to infinity.

Cylinder geometry: y_C fixed, $y_B \to \infty$. In this case we have $t >> \xi_L \sim L^w e^{\beta\sigma L^\nu}$,

$$Y(y_B, y_C) = \frac{2y_C}{\sqrt{1+4y_C^2}}(1+O(e^{-2y_B})) .$$

Since $(\mu - \mu^*(L)) = O(\xi_L^{-1})$ in this geometry, we get

$$M_{\rm per}(V,\mu) = \widetilde{M}_0 + O(\xi_L^{-1}) + \widetilde{\Delta M}\frac{2y_C}{\sqrt{1+4y_C^2}}(1+O(e^{-2y_B})) . \tag{2.20}$$

Block geometry: y_B fixed, $y_C \to \infty$. In this case $t/\xi_L \to 0$,

$$Y(y_B, y_C) = (\tanh y_B)(1+O(y_C^{-2})) ,$$

and

$$M_{\rm per}(V,\mu) = \widetilde{M}_0 + O(\xi_L^{-1}) + O(e^{-(\tau - O(1))t}) + \widetilde{\Delta M}(1 + O(y_C^{-2}))\tanh y_B + O(\mu - \mu^*(L)) \ . \tag{2.21}$$

Block geometry still allows diverging t/L. If instead we consider fixed aspect ratio, then (2.21) simplifies to

$$M_{\rm per}(V,\mu) = M_0 + e^{-O(\tau L)} + \Delta M \tanh y_B + O(\mu - \mu^*) \ . \tag{2.22}$$

In this case there is no gain in using quantities defined at $\mu^*(L)$ and we recover the asymptotics of [2].

Crossover geometry: y_B, y_C fixed. Recalling that $|\mu - \mu^*(L)|L^\nu \sim y_C\xi_L^{-1} = y_B t^{-1}$ we can write

$$M_{\rm per}(V,\mu) = \widetilde{M}_0 + O((1+y_C)\xi_L^{-1}) + \widetilde{\Delta M}\ Y(y_B, y_C) \ . \tag{2.23}$$

Before proving Theorem 2.1, we note that it is actually possible to eliminate the error term $O(\mu - \mu^*(L))$ in (2.16) if one introduces μ-dependent quantities

$$\widetilde{M}_0(L,\mu) = -\frac{d}{d\mu}\frac{\tilde f_+(L,\mu) + \tilde f(_-L,\mu)}{2} \ , \tag{2.24}$$

$$\widetilde{\Delta M}(L,\mu) = -\frac{d}{d\mu}\frac{\tilde f_+(L,\mu) - \tilde f(_-L,\mu)}{2} \ , \tag{2.25}$$

$$x = \tfrac{1}{2}(\tilde f_- - \tilde f_+)L^\nu = \widetilde{\Delta M}(\mu - \mu^*(L))L^\nu(1 + O(\mu - \mu^*(L)) \ . \tag{2.26}$$

Then

$$M_{\rm per}(V,\mu) = \widetilde{M}_0(L,\mu) + \widetilde{\Delta M}(L,\mu)\ Y\left(y_B\sqrt{\frac{1+4(x\xi_L)^2}{1+4y_C^2}}, y_C\right) + O(\xi_L^{-1}) + O(e^{-(\tau - O(1))t}) \ . \tag{2.27}$$

The bound (2.16) is obtained from (2.27) by expanding $\widetilde{M}_0(L,\mu)$, $\widetilde{\Delta M}(L,\mu)$ and $x\xi_L$ about $\mu^*(L)$ (note that $x\xi_L = y_C(1 + O(\mu - \mu^*(L)))$). If one went further to second derivatives in μ, one would obtain the more detailed shape (involving the susceptibility) predicted in [16]. We will prove the bound (2.27) together with Theorem 2.1.

Proof of Theorem 2.1. Let us write R as

$$R = \exp\left(-\tfrac{1}{2}L^\nu(\tilde{f}_+ + \tilde{f}_-)\right) \begin{pmatrix} e^x & \widetilde{R} \\ \widetilde{R} & e^{-x} \end{pmatrix} , \tag{2.28}$$

where x is defined in (2.26). We have $\widetilde{R}(\mu^*(L)) = \frac{1}{2}\xi_L^{-1}$, and we would like this equality to hold approximately for $\mu \neq \mu^*(L)$. This is the content of the following proposition.

Proposition 2.2. *If τ is large and $|\mu - \mu^*|L^\nu \leq 1$, then*

$$\widetilde{R}(\mu) = \tfrac{1}{2}\xi_L^{-1}(1 + O(|\mu - \mu^*(L)|L^\nu) + O(|\mu - \mu^*(L)|^2 L^{2\nu} e^{O(L)})) . \tag{2.29}$$

The last term in (2.29) *may be omitted if $\nu \geq 2$.*

The proof is based on the results of Section 5 of [9]. We defer it to the end of this section.

If we put $C = \cosh x$, $S = \sinh x$, then the eigenvalues of R are

$$\lambda_{1,2} = \exp\left(-\tfrac{1}{2}L^\nu(\tilde{f}_+ + \tilde{f}_-)\right) (C \pm \sqrt{S^2 + \widetilde{R}^2}) , \tag{2.30}$$

with the $+$ sign corresponding to the larger eigenvalue λ_1, the $-$ sign corresponding to λ_2. Proceeding with the proof of Theorem 2.1, we need to approximate $C \pm \sqrt{S^2 + \widetilde{R}^2}$ as $1 \pm \frac{1}{2}\xi_L^{-1}\sqrt{1 + 4y_C^2}$. We have

$$C = 1 + O(x^2) = 1 + O((\mu - \mu^*(L))^2 L^{2\nu}) ,$$

and by (2.26), (2.29) we have

$$\begin{aligned}
\sqrt{S^2 + \widetilde{R}^2} &= \sqrt{x_0^2(1 + O(\mu - \mu^*(L)) + O(x_0^2)) + \tfrac{1}{4}\xi_L^{-2}(1 + O(x_0) + O(x_0^2)e^{O(L)})} \\
&= \tfrac{1}{2}\xi_L^{-1}\sqrt{1 + 4y_C^2}\left(1 + \frac{O(\mu - \mu^*(L))y_C^2 + O(x_0^2)y_C^2 + O(x_0) + O(x_0^2)e^{O(L)}}{1 + 4y_C^2}\right) \\
&= \tfrac{1}{2}\xi_L^{-1}\sqrt{1 + 4y_C^2}\,(1 + O(|\mu - \mu^*(L)|L^\nu)) ,
\end{aligned} \tag{2.31}$$

where $x_0 = \widetilde{\Delta M}(\mu - \mu^*(L))L^\nu = y_C \xi_L^{-1}$. The last term was estimated using $x_0 e^{O(L)} = y_C \xi_L^{-1} e^{O(L)} \leq y_C \leq 1 + 4y_C^2$. Altogether we find that

$$\begin{aligned}
\tfrac{1}{2}(\lambda_1 + \lambda_2) &= \exp\left(-\tfrac{1}{2}L^\nu(\tilde{f}_+ + \tilde{f}_-)\right)(1 + O(|\mu - \mu^*(L)|L^\nu)^2) \\
\lambda_1 - \lambda_2 &= \exp\left(-\tfrac{1}{2}L^\nu(\tilde{f}_+ + \tilde{f}_-)\right)\xi_L^{-1}\sqrt{1 + 4y_C^2}(1 + O(|\mu - \mu^*(L)|L^\nu))\ .
\end{aligned}$$

This proves the first part of Theorem 2.1.

Next we evaluate and approximate

$$M_{1,2} = L^{-\nu}\ \frac{d}{d\mu}\ \log \lambda_{1,2}\ . \tag{2.32}$$

A calculation shows that

$$M_{1,2} = \widetilde{M}_0(L,\mu) \pm \left(\frac{S}{\sqrt{S^2 + \widetilde{R}^2}}\ \widetilde{\Delta M}(L,\mu) + \frac{\widetilde{R}L^{-\nu}\ \frac{d\widetilde{R}}{d\mu}}{\left(C \pm \sqrt{S^2 + \widetilde{R}^2}\right)\sqrt{S^2 + \widetilde{R}^2}}\right)\ . \tag{2.33}$$

Since we assume $|\mu - \mu^*|L^\nu \leq 1$, x is bounded. Also $\widetilde{R} << 1$, so the last term can be bounded by $O(1)L^{-\nu}\widetilde{R}\ \frac{d\widetilde{R}}{d\mu}\ (S^2 + \widetilde{R}^2)^{-1/2}$.

Lemma 2.3. *If τ is large and $|\mu - \mu^*|L^\nu \leq 1$, then*

$$\left|\mathrm{L}^{-\nu}\widetilde{R}\ \frac{d\widetilde{R}}{d\mu}\ (S^2 + \widetilde{R}^2)^{-1/2}\right| \leq O(\xi_L^{-1})\ . \tag{2.34}$$

The proof is deferred to the end of this section.

We expand $S(S^2 + \widetilde{R}^2)^{-1/2}$ as in (2.31) using $\widetilde{R}/S = [1 + O(x_0) + O(x_0^2)e^{O(L)}]/(2y_C)$:

$$\frac{S}{\sqrt{S^2 + \widetilde{R}^2}} = \frac{2y_C}{\sqrt{1 + 4y_C^2}}\ \left(1 + \frac{O(x_0) + O(x_0^2)e^{O(L)}}{1 + 4y_C^2}\right) = \frac{2y_C}{\sqrt{1 + 4y_C^2}}\ (1 + O(\xi_L^{-1}))\ .$$

This leads to the following result:

Proposition 2.4. *If τ is large and $|\mu - \mu^*|L^\nu \leq 1$, then*

$$\frac{M_1 + M_2}{2} = \widetilde{M}_0(L,\mu) + O(\xi_L^{-1})\ , \tag{2.35}$$

$$\frac{M_1 - M_2}{2} = \widetilde{\Delta M}(L,\mu)\frac{2y_C}{\sqrt{1 + 4y_C^2}} + O(\xi_L^{-1})\ . \tag{2.36}$$

We need to approximate the relative weights

$$P_{1,2} = \lambda_{1,2}^t (\lambda_1^t + \lambda_2^t)^{-1} \ , \tag{2.37}$$

which determine how $M_{1,2}$ are represented in the true magnetization M_{per}. We have

$$\begin{aligned} \lambda_{1,2}^t &= (\lambda_1 \lambda_2)^{t/2} \left(\frac{\lambda_1}{\lambda_2} \right)^{\pm t/2} \ , \\ P_1 - P_2 &= \tanh \left(\frac{t}{2} \log \frac{\lambda_1}{\lambda_2} \right) \ , \end{aligned}$$

and if we define $\hat{x}$ by the equation

$$\tanh \hat{x} = \sqrt{\tanh^2 x + (\widetilde{R}/C)^2} \ , \tag{2.38}$$

then (2.30) yields

$$\log \frac{\lambda_1}{\lambda_2} = \log \frac{1 + \tanh \hat{x}}{1 - \tanh \hat{x}} = 2\hat{x} \ .$$

If we express $\hat{x}^2$ in terms of x and $\widetilde{R}$ and perturb in $(\widetilde{R}/C)^2$, we find

$$\begin{aligned} \hat{x}^2 &= x^2 + (\widetilde{R}/C)^2 (1 + O(x^2) + O(\widetilde{R}^2)) \\ \hat{x} &= \sqrt{x^2 + \widetilde{R}^2} \left(1 + (O(x^2) + O(\widetilde{R}^2)) \frac{\widetilde{R}^2}{x^2 + \widetilde{R}^2} \right) \\ &= \sqrt{x^2 + \widetilde{R}^2} \, (1 + O(\widetilde{R}^2)) \ . \end{aligned}$$

Then Proposition 2.2 implies that

$$\begin{aligned} \hat{x} &= \sqrt{x^2 + (2\xi_L)^{-2}} \left(1 + \left[O(x) + O\left(x^2 e^{O(L)} \right) \right] \frac{(2\xi_L)^{-2}}{x^2 + (2\xi_L)^{-2}} \right) \\ &= \sqrt{x^2 + (2\xi_L)^{-2}} \, (1 + O(\xi_L^{-1})) \ . \end{aligned}$$

Since $t/\xi_L = y_B/y_C$, we obtain the following

Proposition 2.5. *If τ is large and $|\mu-\mu^*|L^\nu \le 1$, then*

$$\log(\lambda_1/\lambda_2) = 2\sqrt{x^2+(2\xi_L)^{-2}}\,(1+O(\xi_L^{-1}))\ , \tag{2.39}$$

and

$$P_1 - P_2 = \tanh\left[\frac{y_B}{2y_C}\ \sqrt{1+4(x\xi_L)^2}\,(1+O(\xi_L^{-1}))\right]\ . \tag{2.40}$$

Using (2.26), which implies that $x\xi_L = y_C(1+O(\mu-\mu^*(L)))$, we have

$$P_1 - P_2 = \tanh\left[\frac{y_B}{2y_C}\ \sqrt{1+4y_C^2}\,(1+O(\mu-\mu^*(L))+O(\xi_L^{-1}))\right]\ .$$

Of course $P_1+P_2=1$. Finally, we put these results together to compute, using the bound (2.3):

$$\begin{aligned} M_{\text{per}}(V,\mu) &= M_1P_1 + M_2P_2 + O(e^{-(\tau-O(1))t}) \\ &= \frac{M_1+M_2}{2} + \frac{M_1-M_2}{2}(P_1-P_2) + O(e^{-(\tau-O(1))t}) \\ &= \widetilde{M}_0 + O(\xi_L^{-1}) + O(e^{-(\tau-O(1))t}) + O(\mu-\mu^*(L)) \\ &\quad + \widetilde{\Delta M}\frac{2y_C}{\sqrt{1+4y_C^2}}\tanh\left[\frac{y_B}{2y_C}\ \sqrt{1+4y_C^2}\right]\ . \end{aligned} \tag{2.41}$$

Here we see the scaling function

$$Y(y_B,y_C) = \frac{2y_C}{\sqrt{1+4y_C^2}}\ \tanh\left[\frac{y_B}{2y_C}\ \sqrt{1+4y_C^2}\right]$$

appear with various corrections to this form displayed. Since $|\mu^*(L)-\mu^*| \le e^{-(\tau-O(1))L}$, the bound (2.18) follows from Theorem A and the definition of ξ_L. This completes the proof of Theorem 2.1. The bound (2.27) follows from (2.3), Proposition 2.4 and Proposition 2.5. ■

Proof of Proposition 2.2. The proof is based on the bounds

$$\left|\frac{d}{d\mu}\ R_{+-}\right| \le \begin{cases} O(L)|R_{+-}|\left(1+\frac{1}{2}|f_+-f_-|e^{O(L)}\right)\ , & \nu=1 \\ O(L^\nu)|R_{+-}|\ , & \nu\ge 2\ , \end{cases} \tag{2.42}$$

$$\left|\frac{d^k}{d\mu^k}\ R_{+-}\right| \le e^{O(L)}|R_{+-}| \tag{2.43}$$

proven in [9] under the assumption that τ is large, $k \leq 4$ and $|\mu - \mu^*|L^\nu \leq O(1)$.

For $\nu \geq 2$ we now replace R_{+-} with $\widetilde{R}(\mu)$ in (2.42); the derivatives of $e^{\frac{1}{2}(\tilde{f}_+ + \tilde{f}_-)L^\nu}$ merely contribute to the $O(L^\nu)$. Integrating the bound from $\mu^*(L)$ to μ we obtain

$$\widetilde{R}(\mu) = \widetilde{R}(\mu^*(L))(1 + O(\mu - \mu^*(L))L^\nu) \tag{2.44}$$

which is just (2.29) without the last term.

In order to prove (2.29) for $\nu = 1$ we note that the results of Section 5 of [9], in particular Proposition 5.2 (ii) and Proposition 5.3, (5.6b), imply that

$$|R_{+-}(\mu)| \leq |R_{+-}(\mu^*(L))| e^{O(L)} \tag{2.45}$$

provided $|\mu - \mu^*|L \leq O(1)$. Combined with (2.43) (for $k = 2$) and rephrased in terms of $\widetilde{R}$, we get

$$\left| \frac{d^2}{d\mu^2}\, \widetilde{R}(\mu) \right| \leq \left| \widetilde{R}(\mu^*(L)) \right| e^{O(1)L} \,. \tag{2.46}$$

On the other hand,

$$\left| \frac{d}{d\mu}\, \widetilde{R}(\mu^*(L)) \right| \leq O(L)(\widetilde{R}(\mu^*(L)))\,, \tag{2.47}$$

due to (2.42) and the fact that $|f_+(\mu^*(L)) - f_-(\mu^*(L))| \leq e^{-(\tau - O(1))L}$. Then, applying the second order Taylor's formula for $\widetilde{R}(\mu)$ in powers of $\mu - \mu^*(L)$, we obtain (2.29) for $\nu = 1$. ■

Proof of Lemma 2.3. The best bound on $d\widetilde{R}/d\mu$ is obtained from (2.42) and (2.44) if $\nu > 1$ and (2.46), (2.47) if $\nu = 1$. We obtain

$$L^{-\nu} \left| \frac{d\widetilde{R}}{d\mu}(\mu) \right| \leq O(1)\xi_L^{-1}(1 + |\mu - \mu^*(L)|L^\nu e^{O(L)}) \,.$$

Hence for $|\mu - \mu^*(L)| \leq e^{-\tau L/2}$ the bound (2.34) holds. For larger values S cannot be too small, and so by using (2.29) also we obtain

$$\left| L^{-\nu}\widetilde{R}\frac{d\widetilde{R}}{d\mu}(S^2 + \widetilde{R}^2)^{-1/2} \right| \leq e^{(\tau/2 + O(1))L}\xi_L^{-2} \leq \xi_L^{-1} \,,$$

which completes the proof. ∎

In order to prove Theorem B, which covers the whole region $|\mu-\mu^*|\le O(1)$, we recall the definition of high and low energy phases introduced in [9]. If $|\mu-\mu^*|$ is so small that

$$\beta|f_+(\mu)-f_-(\mu)|L^\nu \le \tfrac{13}{16}\tau\ , \tag{2.48}$$

the set $Q_s(L)$ of low energy phases is just the whole set $\{+,-\}$, while $Q_s(L)$ contains only the phase m with $f_m(\mu)=f(\mu)\equiv\min_{\tilde m} f_{\tilde m}(\mu)$ if the condition (2.48) is violated. In [9] the concept of high and low energy phases was introduced to distinguish between phases which (for a given cross-section L^ν) are stable against perturbations with bubbles of all other phases (and hence may be analyzed by convergent cluster expansions), and phases which are so heavily suppressed that they do not contribute to the leading asymptotics of $Z_{\rm per}$; see Section 2 of [9] for details. As a net result, one obtains the following generalization of Theorem A:

Theorem A$'$. *Let τ be sufficiently large, $t\ge\nu\log L$, let $N(L)\equiv|Q_s(L)|$ and define*

$$\tau^*\equiv\min\{\tau,\min_{m\notin Q_s(L)}(f_m(\mu)-f(\mu))\}\ . \tag{2.49}$$

Then there is a $N(L)\times N(L)$ matrix R, such that the statements (i) through (iv) of Theorem A remain valid, with τ replaced by τ^* in the bound (1.5)*.*

Remark: If the condition (2.48) is valid, $Q_s(L)=\{+,-\}$, $\tau^*=\tau$ and the bounds of Theorem A$'$ are just the bounds of Theorem A. If, on the other hand, (2.48) is violated, $|Q_s(L)|=1$ and Theorem A$'$ states that there exists a function $\widetilde f(L,\mu)$ with

$$\left|\frac{d^k}{d\mu^k}\beta\left(\widetilde f(L,\mu)-f(L)\right)\right|\le O(e^{-(\tau-O(1))}) \tag{2.50}$$

such that

$$\left|\frac{d^k}{d\mu^k}\left[Z_{\rm per}(V,\mu)-e^{-\beta\widetilde f(\mu)|V|}\right]\right|\le e^{-\beta\widetilde f(L,\mu)|V|}e^{-(\tau^*-O(1))t}\ . \tag{2.51}$$

Proof of Theorem B. Since Theorem B covers the whole region $|\mu-\mu^*|\le O(1)$, we must piece together the cases covered by the theorems of this section.

(i) $|\mu-\mu^*|L^\nu \le 1$. We apply Theorem 2.1, noting the changes $O(e^{-(\tau-O(1))L})$ between $f_\pm$, M_0, ΔM and their L-dependent versions. There is a similar change in ξ_L between the two theorems if $\nu \ge 2$. But it can be checked that the changes

$$y_B \to y_B(1+O(e^{-(\tau-O(1))L})), y_C \to y_C(1+O(e^{-(\tau-O(1))L}))$$

affect the scaling function in a manner which can be written as

$$Y(y_B, y_C) \to Y(y_B, y_C)(1+O(e^{-(\tau-O(1))L})) \ .$$

Furthermore, since $|Y(y_B, y_C)| \le 1$, this change and the other terms in (2.27) fall within the bound desired in Theorem B:

$$M_{\rm per}(V,m) = M_0 + \Delta M\ Y(y_B,y_C) + O(e^{-(\tau-O(1))L}) + O(e^{-(\tau-O(1))t}) + O(\mu-\mu^*) \ . \quad (1.14')$$

(ii) $1 \le |\mu-\mu^*|L^\nu \le \frac{13\tau}{32}(\Delta M)^{-1}$. In this case $y_C \ge \exp(O(\tau)L^\nu)$ and

$$Y(y_B, y_C) = (\tanh y_B)(1+\exp(-O(\tau)L^\nu)) \ . \quad (2.52)$$

We may apply Theorem A′ with $N(L) = 2$, obtaining the following matrix for the eigenvalue calculation:

$$R = e^{-fL^\nu} \begin{pmatrix} 1+e^{-O(\tau)L} & R_0 \\ R_0 & e^{-(f_- - f_+)L^\nu}(1+e^{-O(\tau)L}) \end{pmatrix} ,$$

with $R_0 = \exp(-O(\tau)L^\nu)$. Here we take the case $f_+ < f_-$, in which case $(f_- - f_+)L^\nu \ge O(1)$ because $|\mu-\mu^*|L^\nu \ge 1$. Thus $|R_{++} - R_{--}|^{-1} \le O(1)$ and R_0 perturbs the diagonal part of R with no small denominator. Hence the eigenvalues are

$$\lambda_\pm(L) = e^{-f_\pm L^\nu}(1+e^{-O(\tau)L}) \ .$$

Proceeding to $M_{\rm per}(V,\mu)$, we have

$$M_{\rm per}(V,\mu) = \frac{M_+(L,\mu)\lambda_+(L)^t + M_-(L,\mu)\lambda_-(L)^t}{\lambda_+(L)^t + \lambda_-(L)^t} + O(e^{-(\tau-O(1))t}) \ ,$$

where $M_\pm$ are defined by (2.4). Letting $M_0(L,\mu) \pm \Delta M(L,\mu) = M_\pm(L,\mu)$, this becomes

$$
\begin{aligned}
M_0(L,\mu) + \Delta M(L,\mu) \tanh\left[\frac{t}{2}(\log\lambda_+(L) - \log\lambda_-(L))\right] + e^{-O(\tau)t} \\
= M_0 + \Delta M \tanh\left[\frac{t}{2}(f_+L^\nu - f_-L^\nu)\right] + e^{-O(\tau)L} + e^{-O(\tau)t} + O(\mu-\mu^*) \\
= M_0 + \Delta M \tanh y_B + e^{-O(\tau)L} + e^{-O(\tau)t} + O(\mu-\mu^*) \ .
\end{aligned}
$$

Together with (2.51) we get (1.14).

(iii) $\frac{13\tau}{32}(\Delta M)^{-1} \le |\mu-\mu^*|L^\nu \le O(1)L^\nu$. In this case $y_C \ge \exp(O(\tau)L^\nu)$ and $y_B \ge O(\tau)t$ so

$$
Y(y_B,y_C) = 1 + \exp(-O(\tau)L^\nu) + \exp(-O(\tau)t) \ . \tag{2.53}
$$

Theorem A$'$ applies with $N(L)=1$ and $R=\lambda_1(L) = e^{-fL^\nu}(1+e^{-O(\tau)L})$. Taking again the case $f_+ < f_-$ we find

$$
M_{\rm per}(V,\mu) = M_0 + \Delta M + e^{-O(\tau)L} + e^{-O(\tau)t} + O(\mu-\mu^*) \ ,
$$

and together with (2.53) this completes the proof. ■

3. Crossover Finite-Size Scaling for Potts Models.

In this section, we consider the q-state Potts model, which is a spin model with spin variable $\sigma_x \in \mathbf{Z}_q := \{1, e^{2\pi i/q}, \ldots, e^{2\pi i(q-1)/q}\}$ and Hamiltonian

$$H = -\tfrac{1}{2} \sum_{\substack{x,y \\ |x-y|=1}} \delta(\sigma_y, \sigma_y) \ , \tag{3.1}$$

where δ is the Kronecker delta. As the inverse temperature β is varied, the model undergoes a phase transition from a disordered high temperature region $\beta < \beta_t$ with a unique infinite volume phase to an ordered region $\beta > \beta_t$ where q different low temperature phase coexist. If q is sufficiently large, this transition is first order, and the model is an example of a temperature driven first order transition where q ordered low temperature phases and one disordered high temperature phase coexist at the transition point β_t.

For sufficiently large q and cubic boxes V, or more generally for cylinders V which obey the condition (1.2), finite-size scaling of the internal energy

$$E_{\text{per}}(V, \beta) := -\frac{1}{|V|} \frac{d}{d\beta} \log Z_{\text{per}}(V, \beta) \tag{3.2}$$

and of the specific heat

$$C_{\text{per}}(V, \beta) := -k\beta^2 \frac{d}{d\beta} E_{\text{per}}(V, \beta) \tag{3.3}$$

can be derived from the ansatz

$$Z_{\text{per}}(V, \beta) = e^{-\beta f_d(\beta)|V|} + q e^{-\beta f_o(\beta)|V|} + O(q^{-b \min\{t, L\}}) \tag{3.4}$$

for the partition function, see [3]. Here $|V|$ is the volume of the box V, β is the inverse temperature, $b > 0$ is a constant which depends only on the dimension $\nu + 1$, and $f_m(\beta)$ $(m = o, d)$ is some sort of metastable free energy of the phase m. It may be chosen as a C^6 function of β such that $f_o(\beta)$ is equal to the free energy and $f_d(\beta) > f(\beta)$ if $\beta > \beta_t$, while $f_d(\beta)$ is equal to the free energy and $f_o(\beta) > f(\beta)$ if $\beta < \beta_t$.

Here we derive the finite-size scaling (FSS) of $E_{\text{per}}(V, \beta)$ for cylinders which obey a condition

$$t \geq \nu \log L \ . \tag{3.5}$$

To this end we need a suitable version of Theorem A for the Potts model. Using a combination of the methods of [9] and [3], such a theorem has been proven in [17]. For the convenience of the reader we restate this theorem below as Theorem 3.1. Our notation is as follows: $Z_{\rm per}(V,\beta)$ is the periodic partition function in the cylinder V, $|V| = L^\nu t$, β is the inverse temperature, β_t is the transition point, σ_{od} is the infinite volume surface tension between the disordered phase and the ordered phases, and $f_o(\beta)$, $f_d(\beta)$ are the metastable free energies introduced above. Throughout this section we will use b, b_0, b_1, etc. for constants $b > 0$, $b_0 > 0$, $b_1 > 0$ which depend on nothing but the dimension $\nu + 1$.

Theorem 3.1. *Let q and L be sufficiently large and assume that $|f_d(\beta) - f_o(\beta)|L^\nu \le \frac{7}{8}\tau_1$, where $\tau_1 = \left(\frac{1}{2\nu+2} - \frac{1}{4\nu+2}\right)\log q$. Then there are real valued functions $f_o(L,\beta)$, $f_d(L,\beta)$, $\Gamma_{oo}(L,\beta)$, $\Gamma_{dd}(L,\beta)$ and $\Gamma_{od}(L,\beta)$, forming $(q+1)\times(q+1)$ symmetric matrices F and Γ, as follows: F is the diagonal matrix with matrix elements $F_{00} = \exp(-\beta f_d(L,\beta)L^\nu)$, $F_{mm} = \exp(-\beta f_o(L,\beta)L^\nu)$ $(m = 1,\cdots,q)$ and Γ is the matrix with matrix elements $\Gamma_{00} = \Gamma_{dd}(L,\beta)$, $\Gamma_{0m} = \Gamma_{m0} = \Gamma_{od}(L,\beta)$ and $\Gamma_{mn} = \Gamma_{oo}(L,\beta)$, $(m,n = 1,\cdots,q)$. The following statements hold for $k \le 6$ and some $b > 0$.*

(i) *Let $t \ge \nu\log L$. Then*

$$\left|\frac{d^k}{d\beta^k}\left[Z_{\rm per}(V,\beta) - tr\,(F + F^{1/2}\Gamma F^{1/2})^t\right]\right| \le e^{-\beta f|V|}q^{-bt}\ . \tag{3.6}$$

(ii) *Let $\tau = \frac{1}{2\nu+2}\log q = \sigma_{od} + O(q^{-b})$. Then*

$$\left|\frac{d^k}{d\beta^k}\Gamma_{oo}(L,\beta)\right| \le e^{-(2\tau - O(1))L^\nu}\ , \tag{3.7a}$$

$$\left|\frac{d^k}{d\beta^k}\Gamma_{dd}(L,\beta)\right| \le qe^{-(2\tau - O(1))L^\nu}\ , \tag{3.7b}$$

$$\left|\frac{d^k}{d\beta^k}\Gamma_{od}(L,\beta)\right| \le e^{-(\tau - O(1))L^\nu}\ . \tag{3.7c}$$

(iii)
$$\left|\frac{d^k}{d\beta^k}\left(\beta f_i(L,\beta) - \beta f_i(\beta)\right)\right| \le q^{-bL} \tag{3.8}$$

(iv) *There is a (q-dependent) constant $C_{od} > 0$ such that*

$$\Gamma_{od}(L,\beta) = \begin{cases} C_{od}\ L^{-1/2}e^{-\beta\sigma_{od}L}(1 + O(L^{-1}))\ , & \nu+1 = 2\ , \\ e^{-\beta\sigma_{od}L^\nu}(1 + O(q^{-bL}))\ , & \nu+1 \ge 3\ , \end{cases} \tag{3.9}$$

provided $|\beta - \beta_t| \le q^{-bL/2}$.

Remarks:

i) The leading contribution to Γ_{oo} and Γ_{dd} are terms involving two interacting interfaces. This explains the fact that Γ_{oo} and Γ_{dd} are roughly given by $(\Gamma_{od})^2$. The additional factor of q in (3.7b) comes from the fact that these interfaces enclose an ordered region (which corresponds to q different ordered phases) if the outer region is disordered.

ii) The reader may have noticed that the above condition that L is sufficiently large is not present in Theorem A. In [17], this restriction is used as a technical tool at several places, *e.g.* in the proof of the decay condition (2.7) of Section 2 of [17]. It is clear, however, that this condition is not a purely technical condition because the transfer matrix $\mathcal{T}$ for $L = 1$ has rank q, which would not be compatible with (3.6) if $L = 1$ were an allowed value for Theorem 3.1 (recall that F and Γ are matrices of rank $q + 1$).

Computation of eigenvalues. The first step in deriving the scaling form for the Potts model is a computation of the eigenvalues of the $(q + 1) \times (q + 1)$ matrix

$$R = F + F^{1/2}\Gamma F^{1/2} \; .$$

By Theorem 3.1, $Z_{\text{per}}(V, \beta)$ is well approximated by tr T^t.

The calculation is simplified by noting that any vector of the form $(0, v_1, \ldots, v_q)$ with $\sum v_i = 0$ is an eigenvector with eigenvalue

$$\lambda_\perp = \exp(-\beta f_0(L, \beta) L^\nu) \; . \tag{3.10}$$

Thus $\lambda_\perp$ is $(q - 1)$-fold degenerate. On the remaining subspace of vectors of the form $(v_0, v, \ldots, v)$, the eigenvalues are obtained by diagonalizing the effective 2×2 matrix

$$\hat{R} = \begin{pmatrix} (1 + \Gamma_{dd}) e^{-\beta f_d(L,\beta) L^\nu} & \sqrt{q}\,\Gamma_{od} e^{-(\beta/2)(f_0(L,\beta) + f_d(L,\beta)) L^\nu} \\ \sqrt{q}\,\Gamma_{od} e^{-(\beta/2)(f_0(L,\beta) + f_d(L,\beta)) L^\nu} & (1 + q\Gamma_{oo}) E^{-\beta f_0(L,\beta) L^\nu} \end{pmatrix} \; , \tag{3.11}$$

If we define

$$\beta\tilde{f}_0(L,\beta) = \beta f_0(L,\beta) - L^{-\nu}\log(1+q\Gamma_{oo})\ , \tag{3.12a}$$

$$\beta\tilde{f}_d(L,\beta) = \beta f_d(L,\beta) - L^{-\nu}\log(1+q\Gamma_{dd})\ , \tag{3.12b}$$

$$\tilde{x} = \frac{1}{2}(\beta\tilde{f}_d(L,\beta) - \beta\tilde{f}_0(L,\beta))L^{\nu}\ , \tag{3.13}$$

$$A = \exp\left(-\frac{\beta}{2}(\tilde{f}_0(L,\beta) + \tilde{f}_d(L,\beta)\right)L^{\nu}\ , \tag{3.14}$$

$$\widetilde{\Gamma}_{od} = \frac{\Gamma_{od}}{\sqrt{1+\Gamma_{dd}}\sqrt{1+q\Gamma_{oo}}}\ , \tag{3.15}$$

then $\hat{R}$ can be written in a form familiar from the two-phase case:

$$\hat{R} = A\begin{pmatrix} e^{-\tilde{x}} & \sqrt{q}\,\widetilde{\Gamma}_{od} \\ \sqrt{q}\,\widetilde{\Gamma}_{od} & e^{\tilde{x}} \end{pmatrix}\ . \tag{3.16}$$

Fig. 1. *The avoiding crossing region for the first three eigenvalues of* $-\log\hat{R}$*. The eigenvalue* $\lambda_{\perp}$ *is* $q-1$ *fold degenerate. To make the figure better readable, we have subtracted a term* $\frac{\beta\tilde{f}_o+\beta\tilde{f}_d}{2}L^{\nu}$ *from all curves.*

Thus the remaining two eigenvalues may be computed as

$$\lambda_{\pm} = A\left(\cosh\tilde{x} \pm \sqrt{\sinh^2\tilde{x} + q\widetilde{\Gamma}_{od}^2}\right) . \tag{3.17}$$

The degenerate eigenvalue can be rewritten as

$$\lambda_{\perp} = Ae^{\tilde{x}}(1 + q\Gamma_{oo})^{-1} . \tag{3.18}$$

The eigenvalues are plotted in Fig. 1.

Definition of scaling variables. We define an L-dependent "transition point" $\beta^*(L)$ by the equation

$$\tilde{f}_d(L, \beta^*(L)) = \tilde{f}_o(L, \beta^*(L)) , \tag{3.19}$$

i.e., where $\tilde{x} = 0$. A "correlation length" ξ_L may be defined by the relation

$$\xi_L^{-1} = \sqrt{q}\,\widetilde{\Gamma}_{od}(\beta^*(L)) . \tag{3.20}$$

The true correlation length in the time direction is

$$\xi_{\|} = [\log(\lambda_+/\lambda_{\perp})]^{-1} ,$$

since λ_+ and $\lambda_{\perp}$ are the two largest eigenvalues. However, at $\beta^*(L)$, $\xi_{\|}^{-1}$ and ξ_L^{-1} differ by only $O(q\widetilde{\Gamma}_{od}^2) + O(\Gamma_{oo}) = O(\xi_L^{-(2-\epsilon)})$ so that $\xi_{\|} = \xi_L(1 + O(\xi_L^{-(1-\epsilon)}))$. Thus, there is no harm in using the more convenient definition.

Next we define the L-dependent internal energies

$$\widetilde{E}_{o,d}(L) = \frac{d}{d\beta}\left(\beta\tilde{f}_{o,d}(L, \beta^*(L))\right) , \tag{3.21}$$

and write

$$\widetilde{E} = \tfrac{1}{2}(\widetilde{E}_d(L) + \widetilde{E}_o(L)) , \qquad \widetilde{\Delta E} = \tfrac{1}{2}(\widetilde{E}_d(L) - \widetilde{E}_o(L)) .$$

By (3.7), (3.8), and (3.12),

$$|E - \widetilde{E}|,\ |\Delta E - \widetilde{\Delta E}| \le q^{-bL} , \tag{3.22}$$

where E, ΔE are the corresponding $L = \infty$ quantities. Similarly, we have $|\beta_t - \beta^*(L)| \le q^{-bL}$, which verifies (1.16) of Theorem C. Finally, we define scaling variables

$$y_B = tL^\nu(\beta - \beta^*(L))\,\widetilde{\Delta E} , \tag{3.23a}$$

$$y_C = \xi_L L^\nu(\beta - \beta^*(L))\,\widetilde{\Delta E} . \tag{3.23b}$$

Derivation of the scaling function. As in the two-phase case it is worthwhile deriving the scaling form heuristically before carefully going over the approximations involved. We approximate the eigenvalues for small $\tilde{x}$, Γ as

$$\lambda_\pm = A\left(1 \pm \sqrt{\tilde{x}^2 + \xi_L^{-2}}\right) , \qquad \lambda_\perp = A(1 + \tilde{x}) . \tag{3.24}$$

Theorem 3.1(i) implies that for $k \le 5$

$$\left| \frac{d^k}{d\mu^k} \left[E_{\rm per}(V,\beta) - \sum_i E_i(L,\beta)\, P_i(V,\beta) \right] \right| \le O(q^{-bt}) , \tag{3.25}$$

where i runs over $q+1$ values corresponding to the $q+1$ eigenvalues $\lambda_\pm$, $\lambda_\perp$, and

$$E_i(L,\beta) = -L^{-\nu} \frac{d}{d\beta} \log \lambda_i(L) , \tag{3.26}$$

$$P_i(V,\beta) = \lambda_i(L)^t \left[\sum_j \lambda_j(L)^t \right]^{-1} . \tag{3.27}$$

Approximating $\tilde{x}$ as

$$(\beta - \beta^*(L))L^\nu \frac{d}{d\beta} \left(\frac{\beta \tilde{f}_d - \beta \tilde{f}_o}{2} \right)\Bigg|_{\beta^*(L)} = (\beta - \beta^*(L))L^\nu \left(\frac{\widetilde{E}_d - \widetilde{E}_o}{2} \right) = y_c/\xi_L ,$$

we find that

$$
\begin{aligned}
E_\pm(L,\beta) &= \widetilde{E} \mp L^{-\nu} \frac{\tilde{x}\tilde{x}'}{\sqrt{\tilde{x}^2+\xi_L^{-2}}} = \widetilde{E} \mp \frac{\tilde{x}\xi_L \widetilde{\Delta E}}{\sqrt{1+(\tilde{x}\xi_L)^2}} \\
&= \widetilde{E} \mp \frac{y_C \widetilde{\Delta E}}{\sqrt{1+y_C^2}} \ , \\
E_\perp(L,\beta) &= \widetilde{E} - \widetilde{\Delta E} \ .
\end{aligned}
$$

We ignore the β-dependence in ξ_L and work to first order about $\beta = \beta^*(L)$. Note that

$$
\begin{aligned}
\lambda_\pm(L)^t &\sim A^t \exp\left(\pm \frac{t}{\xi_L} \sqrt{(\tilde{x}\xi_L)^2+1}\right) \ , \\
\lambda_\perp(L)^t &\sim A^t \exp\left(\frac{t}{\xi_L} (\tilde{x}\xi_L)\right) \ ,
\end{aligned}
$$

and since $t/\xi_L = y_B/y_C$, this becomes

$$
\begin{aligned}
\lambda_\pm(L)^t &\sim A^t \exp\left(\pm \frac{y_B}{y_C}\sqrt{1+y_C^2}\right), \\
\lambda_\perp(L)^t &\sim A^t \exp y_B \ .
\end{aligned}
$$

Putting these computations into (3.25), we obtain

$$
\begin{aligned}
E_{\rm per} &\approx \widetilde{E} - \widetilde{\Delta E} \left[\frac{\left[\exp(\frac{y_B}{y_C}\sqrt{1+y_C^2}) - \exp(-\frac{y_B}{y_C}\sqrt{1+y_C^2})\right] \frac{y_C}{\sqrt{1+y_C^2}} + e^{y_B}(q-1)}{\exp(\frac{y_B}{y_C}\sqrt{1+y_C^2}) + \exp(-\frac{y_B}{y_C}\sqrt{1+y_C^2}) + e^{y_B}(q-1)} \right] \\
&= \widetilde{E} - \widetilde{\Delta E}\, Y(y_B, y_C) \ ,
\end{aligned}
$$

where

$$
Y(y_B,y_C) = \frac{(q-1)e^{y_B} + y_C(1+y_C^2)^{-1/2} 2\sinh\left(\frac{y_B}{y_C}\sqrt{1+y_C^2}\right)}{(q-1)e^{y_B} + 2\cosh\left(\frac{y_B}{y_C}\sqrt{1+y_C^2}\right)} \ .
$$

The following theorem, analogous to Theorem 2.1 in the two-phase case, gives a precise picture (without errors q^{-bL}) near $\beta^*(L)$.

Theorem 3.2. *Let q and L be sufficiently large and assume that $|\beta - \beta_t| L^\nu \le 1$. The eigenvalues of the matrix $F + F^{1/2}\Gamma F^{1/2}$ obey the following estimates:*

$$\lambda_\pm(L) = A \exp\left(O(\xi_L^{-2}) \pm \xi_L^{-1} \sqrt{1 + y_C^2 (1 + O(\beta - \beta^*(L)))} \right) , \tag{3.28a}$$

$$\lambda_\perp(L) = A \exp\left(O(\xi_L^{-(2-\epsilon)}) + \xi_L^{-1} y_C \left(1 + O(\beta - \beta^*(L))\right) \right) , \tag{3.28b}$$

Furthermore, in the cylindrical volume $V = L^\nu t$ with $t \ge \nu \log L$, the internal energy is described by

$$\begin{aligned} E_{\text{per}}(V,\beta) =& \widetilde{E} - \widetilde{\Delta E}\, Y(y_B, y_C) + O(q^{-bt}) \\ &+ O(\xi_L^{-(1-\epsilon)}) \min\{1 + |y_C|, y_B/y_C\} + O(q|\beta - \beta^*(L)|) . \end{aligned} \tag{3.29}$$

Finally,

$$\xi_L = \begin{cases} C(q) L^{1/2} e^{\beta \sigma_{od} L} (1 + O(L^{-1})) , & \nu = 1 , \\ q^{-1/2} e^{\beta \sigma_{od} L^\nu} (1 + O(q^{-bL})) , & \nu \ge 2 . \end{cases} \tag{3.30}$$

Proof. We shall need estimates analogous to Proposition 2.2 and Lemma 2.3 on the variation of $\widetilde{\Gamma}_{od}$ as a function of β. The situation here is somewhat simpler due to the fact that bounds on the logarithmic derivative of Γ_{od} are available. In 17] it is shown (Theorems 2.1 and 2.2) that

$$\left| \frac{d^k}{d\beta^k} \Gamma_{oo} \right| , \quad \left| \frac{d^k}{d\beta^k} \Gamma_{dd} \right| \le e^{-(2\tau - O(1)) L^\nu} , \tag{3.31a}$$

$$\left| \frac{d^k}{d\beta^k} \Gamma_{od} \right| \le O(L^{k\nu}) \Gamma_{od} , \tag{3.31b}$$

provided $k \le 6$ and $a := \beta |f_o(\beta) - f_d(\beta)| \le \frac{7}{8} \tau_1 L^{-\nu}$. With $\widetilde{\Gamma}_{od} = \Gamma_{od}(1 + \Gamma_{dd})^{-1/2}(1 + q\Gamma_{od})^{-1/2}$, it is immediate that $\left| \frac{d\widetilde{\Gamma}_{od}}{d\beta} \right| \le O(L^\nu) \widetilde{\Gamma}_{od}$. Hence for $|\beta - \beta^*(L)| L^\nu \le 1$ we have

$$\begin{aligned} \sqrt{q}\, \widetilde{\Gamma}_{od}(\beta) &= \sqrt{q}\, \widetilde{\Gamma}_{od}(\beta^*(L)) \exp(O(|\beta - \beta^*(L)| L^\nu)) \\ &= \xi_L^{-1} (1 + O(|\beta - \beta^*(L)| L^\nu)) , \end{aligned} \tag{3.32}$$

$$L^{-\nu} \left| \frac{d\widetilde{\Gamma}_{od}}{d\beta} \right| \le O(\xi_L^{-1}) . \tag{3.33}$$

Rather than expand λ_i in terms of $\beta - \beta^*(L)$ to produce a result like (2.15), we analyze $\log \lambda_i$. With $C = \cosh \tilde{x}$, $S = \sinh \tilde{x}$ we have

$$\frac{\lambda_+\lambda_-}{A^2} = \left(C + \sqrt{S^2 + q\widetilde{\Gamma}_{od}^2}\right)\left(C - \sqrt{S^2 + q\widetilde{\Gamma}_{od}^2}\right) = 1 - q\widetilde{\Gamma}_{od}^2 \ ,$$

so by (3.32) it follows that

$$\sqrt{\lambda_+\lambda_-} = A\exp(O(\xi_L^{-2})) \ . \tag{3.34}$$

Proceeding as in the proof of Proposition 2.5, we find that

$$\begin{aligned}\tfrac{1}{2}\log(\lambda_+/\lambda_-) &= \sqrt{\tilde{x}^2 + q\widetilde{\Gamma}_{od}^2}(1 + O(\xi_L^{-2})) \\ &= \sqrt{\tilde{x}^2 + \xi_L^{-2}(1 + O(\tilde{x})}(1 + O(\xi_L^{-2})) \\ &= \sqrt{\tilde{x}^2 + \xi_L^{-2}}\left(1 + O(\xi_L^{-2}) + \frac{O(\tilde{x}\xi_L^{-2})}{\tilde{x}^2 + \xi_L^{-2}}\right) \\ &= \sqrt{\tilde{x}^2 + \xi_L^{-2}} + O(\xi_L^{-2}) \ . \end{aligned} \tag{3.35}$$

Recall that

$$\begin{aligned}\tilde{x} &= \tfrac{1}{2}(\beta\tilde{f}_d(L,\beta) - \beta\tilde{f}_0(L,\beta))L^\nu \\ &= \widetilde{\Delta E}(\beta - \beta^*(L))L^\nu(1 + O(\beta - \beta^*(L))) \ , \end{aligned} \tag{3.36}$$

so in terms of the scaling variable $y_C = \xi_L L^\nu(\beta - \beta^*(L))\widetilde{\Delta E}$,

$$\tfrac{1}{2}\log(\lambda_+/\lambda_-) = \xi_L^{-1}\sqrt{1 + y_C^2(1 + O(\beta - \beta^*(L)))} + O(\xi_L^{-2}).$$

Taken together with (3.34), this proves (3.28a). The bound (3.28b) on $\lambda_\perp$ follows immediately from (3.18); we can bound $q\Gamma_{oo}$ by a power of ξ_L^{-1} using Theorem 3.1.

In order to compute $E_{\rm per}(V,\beta)$ we follow the prescription given in (3.25)–(3.27). The calculation of $E_\pm(L,\beta)$ is virtually the same as the one for $M_{1,2}$ in the proof of Proposition 2.4. We state the result:

$$\frac{E_+ + E_-}{2} = \widetilde{E}(L,\beta) + O(\xi_L^{-1}) \ , \tag{3.37a}$$

$$\frac{E_+ - E_-}{2} = -\widetilde{\Delta E}(L,\beta)\,\frac{y_C}{\sqrt{1 + y_C^2}} + O(\xi_L^{-1}) \ . \tag{3.37b}$$

Here

$$\widetilde{E}(L,\beta) = \frac{d}{d\beta}\left(\frac{\beta\tilde{f}_d(L,\mu)+\beta\tilde{f}_o(L,\mu)}{2}\right) ,$$

$$\widetilde{\Delta E}(L,\beta) = \frac{d}{d\beta}\left(\frac{\beta\tilde{f}_d(L,\mu)-\beta\tilde{f}_o(L,\mu)}{2}\right) = L^{-\nu}\,\frac{d\tilde{x}}{d\beta} .$$

The remaining internal energy is

$$\begin{aligned} E_\perp(L,\beta) &= -L^{-\nu}\,\frac{d}{d\beta}\,\log\lambda_\perp(L) \\ &= \widetilde{E}(L,\beta) - L^{-\nu}\,\frac{d}{d\beta}\,\log(1+q\Gamma_{oo}) - \widetilde{\Delta E}(L,\beta) \\ &= \widetilde{E}(L,\beta) - \widetilde{\Delta E}(L,\beta) + O(\xi_L^{-(2-\epsilon)}) . \end{aligned} \tag{3.37c}$$

The other part of the formula for $E_{\rm per}(V,\beta)$ is the relative weightings P_i. Using (3.18), (3.34), and (3.35) we obtain

$$P_+ - P_- = \frac{2\sinh(t(\sqrt{\tilde{x}^2+\xi_L^{-2}}\ + O(\xi_L^{-2})))}{2\cosh(t(\sqrt{\tilde{x}^2+\xi_L^{-2}}\ + O(\xi_L^{-2}))) + (q-1)\exp(t(\tilde{x}-x_0))} , \tag{3.38a}$$

$$P_\perp = \frac{\exp(t(\tilde{x}-x_o))}{2\cosh(t(\sqrt{\tilde{x}^2+\xi_L^{-2}}\ + O(\xi_L^{-2}))) + (q-1)\exp(t(\tilde{x}-x_o))} , \tag{3.38b}$$

where

$$x_0 = \log\left[(1+q\Gamma_{od})\sqrt{1-q\widetilde{\Gamma}_{od}^2}\right] = o\left(\xi_L^{-(2-\epsilon)}\right) .$$

We would like to pull out x_0 and $O(\xi_L^{-2})$ as additive corrections to $P_+ - P_-$ and $P_\perp$. To this end we rewrite

$$P_+ - P_- = \frac{1-(\lambda_-/\lambda_+)^t}{1+(\lambda_-/\lambda_+)^t+(\lambda_\perp/\lambda_+)^t} , \qquad \textit{and} \qquad P_\perp = \frac{(\lambda_\perp/\lambda_+)^t}{1+(\lambda_-/\lambda_+)^t+(\lambda_\perp/\lambda_+)^t}$$

and prove the following

Lemma 3.3. *Let q and L be sufficiently large and assume that $|\beta-\beta_t|\,L^\nu \le 1$. Then*

$$\left|(\lambda_-/\lambda_+)^t - e^{-2t\sqrt{\tilde{x}^2+\xi_L^{-2}}}\right| \le O(\xi_L^{-1}) \tag{3.39a}$$

and

$$\left|(\lambda_\perp/\lambda_+)^t - e^{-t(\sqrt{\tilde{x}^2+\xi_L^{-2}}-\tilde{x})}\right| \le O(\xi_L^{-(1-\epsilon)}) \min\left\{1+|y_C|, \frac{y_B}{y_C}\right\} \tag{3.39b}$$

Proof: The bound (3.39a) is trivial. In order to prove (3.39b) we may assume without loss of generality that

$$\frac{y_B}{y_C}\xi_L^{-(1-\epsilon)} = t\xi_L^{-(2-\epsilon)} \le 1 \tag{3.40a}$$

or

$$\xi_L^{-(1-\epsilon)}|y_C| \le 1 \tag{3.40b}$$

because the r.h.s. of (3.39b) is just $O(1)$ if both (3.40a) and (3.40b) are violated. We then use the bound $e^\delta - 1 \le \delta e^\delta$ (with $\delta = O(t\xi_L^{-2}) + tx_0 = o(t\xi_L^{-(2-\epsilon)})$) to bound the l.h.s. of (3.39b) by

$$O(t\xi_L^{-(2-\epsilon)})e^{-t\left(\sqrt{\tilde{x}^2+\xi_L^{-2}}-\tilde{x}-o(t\xi_L^{-(2-\epsilon)})\right)}$$

If the bound (3.40a) is fulfilled, we conclude that the l.h.s. of (3.39b) is bounded by

$$\begin{aligned}
&O(t\xi_L^{-(2-\epsilon)})e^{-t\left(\sqrt{\tilde{x}^2+\xi_L^{-2}}-\tilde{x}\right)} \\
&\quad = O(\frac{y_B}{y_C}\xi_L^{-(1-\epsilon)})e^{-O(y_B)\left(\sqrt{1+y_C^{-2}}-1\right)} \\
&\quad \le O(\xi_L^{-(1-\epsilon)}) \min\left\{\frac{y_B}{y_C}, \frac{1}{|y_C|(\sqrt{1+y_C^{-2}}-1)}\right\} \\
&\quad \le O(\xi_L^{-(1-\epsilon)}) \min\left\{\frac{y_B}{y_C}, 1+|y_C|\right\}.
\end{aligned}$$

We have used that

$$t\tilde{x} = y_B(1+O(\beta-\beta^*(L)))\ , \tag{3.41a}$$

which follows from (3.36). If (3.40b) is valid, we use the fact that $\tilde{x} = O(y_C\xi_L^{-1})$ to bound $\xi_L^{-(2-\epsilon)}|\tilde{x}|$ by $O(\xi_L^{-2})$. As a consequence,

$$\sqrt{\tilde{x}^2+\xi_L^{-2}} \ge |\tilde{x}| + b\xi_L^{-(2-\epsilon)}$$

provided $b > 0$ is chosen small enough. We conclude that

$$o(t\xi_L^{-(2-\epsilon)}) \leq \tfrac{1}{2}\left(\sqrt{\tilde{x}^2+\xi_L^{-2}} - |\tilde{x}|\right) \leq \tfrac{1}{2}\left(\sqrt{\tilde{x}^2+\xi_L^{-2}} - \tilde{x}\right)$$

provided L is large enough. Using this bound we may continue as before. ■

Combining Lemma 3.3 with (3.27) and (3.37), we obtain

$$\begin{aligned} E_{\mathrm{per}}(V,\beta) =& \widetilde{E}(L,\beta) + O(\xi_L^{-(1-\epsilon)}) \min\{1+|y_C|, y_B/y_C\} + O(\xi_L^{-1}) + O(q^{-bt}) \\ &- \widetilde{\Delta E}(L,\beta)\frac{2\sinh(\sqrt{(t\tilde{x})^2+(y_B/y_C)^2})y_C(1+y_C^2)^{-1/2} + (q-1)e^{t\tilde{x}}}{2\cosh(\sqrt{(t\tilde{x})^2+(y_B/y_C)^2}) + (q-1)e^{t\tilde{x}}} \ . \end{aligned}$$

Finally, we expand in $\beta - \beta^*(L)$ using (3.41a) and

$$\widetilde{\Delta E}(L,\beta) = \widetilde{\Delta E} + O(\beta - \beta^*(L)) \ , \tag{3.41b}$$

$$\widetilde{E}(L,\beta) = \widetilde{E} + O(\beta - \beta^*(L)) \ . \tag{3.41c}$$

Once again there is a problem with pulling out the correction. After dividing through numerator and denominator, the only tricky term is the derivative of

$$(q-1)\exp\left(t\tilde{x}(1+\delta) - \sqrt{(t\tilde{x}(1+\delta))^2 + (y_B/y_C)^2}\right) \tag{3.42}$$

in δ (which stands for $O(\beta-\beta^*(L))$. The logarithmic derivative of the exponent is bounded by a constant, so the derivative of (3.42) is bounded by $O(q)$. Hence we may replace $t\tilde{x}$ with y_B if we add an error $O(q|\beta-\beta^*(L)|)$. Bounding $O(\xi_L^{-1})$ by $O(q^{-bL})$, this completes the proof of (3.29).

The last statement of Theorem 3.2 follows immediately from Theorem 3.1(ii), (iv). (Recall that $\xi_L^{-1} = \sqrt{q}\,\Gamma_{od}(1+\Gamma_{dd})^{-1/2}(1+q\Gamma_{oo})^{-1/2}$.) ■

Proof of Theorem C. We consider three cases:

(i) $|\beta-\beta_t|L^\nu \leq 1$. By (3.22), $\frac{1}{2}(E_d \pm E_0)$ differ from $\widetilde{E}$, $\widetilde{\Delta E}$ by $q^{-O(1)L}$. This induces changes

$$y_B \to y_B(1+O(q^{-O(1)L})), \quad y_C \to y_C(1+O(q^{-O(1)L})),$$

going from Theorem 3.2 to the simpler definitions (1.18), (1.19). Note that y_B/y_C is not changed. Checking the effect of these changes on $P_+ - P_-$ and $P_\perp$ as before (see (3.42)), and observing that

$$\frac{y_C(1+\delta)}{\sqrt{1+y_C^2(1+\delta)^2}} = \frac{y_C}{\sqrt{1+y_C^2}} + O(\delta)$$

(with $\delta = q^{-O(1)L}$), we obtain

$$\begin{aligned} E_{\rm per}(V,\beta) = & \frac{(E_o+E_d)}{2} + \frac{(E_o-E_d)}{2} Y(y_B,y_C) + q^{-O(1)L} + q^{-O(1)t} + O(q|\beta-\beta^*(L)|) \\ & + O(\xi_L^{-(1-\epsilon)}) \min\{1+|y_C|, y_B/y_C\} \ . \end{aligned} \tag{1.21'}$$

(ii) $1 \le |\beta-\beta_t| L^\nu \le \frac{13}{32}(\Delta E)^{-1}\tau_1$. In this case $y_C \ge O(\xi_L)$ and we may perturb away y_C^{-2} in

$$Y(y_B,y_C) = \frac{(q-1)e^{y_B} + \alpha^{-1}(e^{\alpha y_B} - e^{-\alpha y_B})}{(q-1)e^{y_B} + (e^{\alpha y_B} + e^{-\alpha y_B})} \ ,$$

where $\alpha = \sqrt{1+y_C^{-2}} = 1 + O(\xi_L^{-2})$. We distinguish two cases: either $|y_B| \le \log \xi_L$, which implies $|\alpha y_B - y_B| = O(\xi_L^{-(2-\epsilon)})$ and hence

$$\begin{aligned} Y(y_B,y_C) &= \frac{qe^{y_B} - e^{y_B}}{qe^{y_B} + e^{-y_B}} + O(q\xi_L^{-(2-\epsilon)}) \\ &\equiv T(y_B) + O(q\xi_L^{-(2-\epsilon)}) \ . \end{aligned} \tag{3.43}$$

Or $|y_B| \ge \log \xi_L$, in which case both $Y(y_B,y_C)$ and $T(y_B)$ are equal to $\operatorname{sgn} y_B + O(q\xi_L^{-2}) = \operatorname{sgn} y_B + O(\xi_L^{-(2-\epsilon)})$, which gives again the bound (3.43). By Theorem 3.1, the matrix, $F + F^{1/2}\Gamma F^{1/2}$ governs the behavior in the region (ii), and its eigenvalues (3.17), (3.18) can be approximated as

$$\lambda_\pm = Ae^{\pm\tilde{x}}(1+O(\xi_L^{-2})) \qquad \lambda_\perp = Ae^{\tilde{x}}(1+O(\xi_L^{-(2-\epsilon)})) \ . \tag{3.44}$$

Noting that we have good bounds on $\frac{d\Gamma_{ij}}{d\beta}$, a calculation shows that

$$\begin{aligned} E_\pm(L,\beta) &= -L^{-\nu}\frac{d}{d\beta}\log\lambda_\pm = \widetilde{E}(L,\beta) \mp \widetilde{\Delta E}(L,\beta) + O(\xi_L^{-1}) \ , \\ E_\perp(L,\beta) &= -L^{-\nu}\frac{d}{d\beta}\log\lambda_\perp = \widetilde{E}(L,\beta) - \widetilde{\Delta E}(L,\beta) + O(\xi_L^{-1}) \ . \end{aligned}$$

(The error term in $E_\pm$ is essentially the third term in (2.33) and is easily bounded.) Putting these results together we obtain

$$E_{\rm per}(V,\beta) = \widetilde{E}(L,\beta) - \widetilde{\Delta E}(L,\beta)\frac{2\sinh t(\tilde{x}-x_0) + (q-1)e^{t(\tilde{x}-x_1)}}{2\cosh t(\tilde{x}-x_0) + (q-1)e^{t(\tilde{x}-x_1)}} + O(\xi_L^{-1}) + O(q^{-bt}),$$

where $x_0 = O(\xi_L^{-2})$, $x_1 = O(\xi_L^{-(2-\epsilon)})$. If $|\tilde{x}|t \geq \log\xi_L$, $e^{-2t|\tilde{x}-x_0|}$ and $e^{-2t|\tilde{x}-x_1|}$ are $O(\xi_L^{-(2-\epsilon)})$ and

$$\begin{aligned} E_{\rm per}(V,\beta) &= \widetilde{E}(L,\beta) - \widetilde{\Delta E}(L,\beta)(1 + O(\xi_L^{-(2-\epsilon)})) + O(\xi_L^{-1}) + O(q^{-bt}) \\ &= \widetilde{E}(L,\beta) - \widetilde{\Delta E}(L,\beta)T(\tilde{x}t) + O(\xi_L^{-1}) + O(q^{-bt})\ . \end{aligned}$$

If $|\tilde{x}|t < \log\xi_L$, we pull out a correction $O(q)(t|x_1| + |x_0|) \leq O(q\,\xi_L^{-(2-\epsilon)}\log\xi_L) = O(\xi_L^{-(2-\epsilon)})$. Again we find that

$$E_{\rm per}(V,\beta) = \widetilde{E}(L,\beta) - \widetilde{\Delta E}(L,\beta)T(\tilde{x}t) + O(\xi_L^{-1}) + O(q^{-bt})\ . \tag{3.45}$$

Combining (3.45) with (3.41) and (3.43), we obtain that

$$E_{\rm per}(V,\beta) = E(L) - \Delta E(L)Y(y_B,y_C) + O(\xi_L^{-1}) + O(q^{-bt}) + O(q(\beta-\beta^*(L))\ . \tag{1.21$''$}$$

(iii) $\frac{13}{32}(\Delta E)^{-1}\tau_1 \leq |\beta-\beta_t|L^\nu$. Here $|y_C| \geq e^{O(\tau_1)L^\nu}$, $|y_B| \geq O(\tau_1)t$ so that

$$Y(y_B,y_C) = \mathrm{sgn}(\beta-\beta_t) + q^{-O(L^\nu)} + q^{-O(t)}\ , \tag{3.46}$$

We need a replacement for Theorem 3.1 when the ordered and disordered states are widely separated in energy. The following theorem, proven in 17], provides the necessary information.

Theorem 3.4. *Let q and L be sufficiently large, and assume that $\frac{3}{4}\tau_1 \leq |f_d(\beta)-f_o(\beta)|L^\nu \leq O(1)L^\nu$. Then the following statements hold for $k \leq 6$ and some $b > 0$.*

(i) *If $\beta < \beta_t$, then there exists $\Gamma'_{dd}(L,\beta)$ satisfying (3.7b) such that*

$$\left|\frac{d^k}{d\beta^k}\left[Z_{\rm per}(V,\beta) - \left((1+\Gamma'_{dd}(L,\beta))e^{-\beta f_d(L,\beta)L^\nu}\right)^t\right]\right| \leq e^{-\beta f|V|}q^{-bt}.$$

(ii) *If $\beta > \beta_t$, then there exists $\Gamma'_{oo}(L,\beta)$ satisfying (3.7a) such that*

$$\left| \frac{d^k}{d\beta^k} \left[Z_{\mathrm{per}}(V,\beta) - \mathrm{tr}(F + F^{1/2}\Gamma F^{1/2})^t \right] \right| \le e^{-\beta f|V|} q^{-bt} \ ,$$

where Γ, F are $q \times q$ matrices with matrix elements $\Gamma_{mn} = \Gamma'_{oo}$ and $F_{mn} = \delta_{mn} e^{-\beta f_0(L,\beta)L^\nu}$.

Recall that $E_{\mathrm{per}}(V,\beta)$ is approximated as a convex combination of $E_i = -L^{-\nu} \frac{d}{d\beta} \log \lambda_i$, where λ_i are the eigenvalues of $F + F^{1/2}\Gamma F^{1/2}$. If $\beta < \beta_t$ there is only one λ_i, and the corresponding energy is

$$E_i = \frac{d}{d\beta}(\beta f_d(L,\beta)) + O(\xi_L^{-(2-\epsilon)}) = E_d + O(\xi_L^{-(2-\epsilon)}) + O(\beta - \beta_t) \ .$$

If $\beta > \beta_t$, the eigenvalues are $\exp(-\beta f_o(L,\beta)L^\nu)$ and $\exp(-\beta f_o(L,\beta)L^\nu)(1 + q\Gamma'_{oo}(L,\beta))$, the former with multiplicity $q-1$. All of the energies, however, obey the same estimate:

$$E_i = E_o + O(\xi_L^{-(2-\epsilon)}) + O(\beta - \beta_t) \ .$$

Putting these facts together with (3.46) we obtain (1.21), and the proof of Theorem C is complete. ■

4. Crossover Finite-Size Scaling for Free Boundary Conditions.

In this section we consider volumes where we impose free boundary conditions in the directions transversal to the time direction. We therefore take volumes of the form $V = A \times T$ where A is the ν-dimensional box $\{1, 2, \dots, L\}^\nu$ and T is the torus $\mathbf{Z}/(t\mathbf{Z})$. In order to avoid technical complications we only consider the standard Ising model. For this model, the partition function with free boundary conditions is just

$$Z_{\text{free}}(V, \mu) := \sum_{\sigma_V} \exp\left(-\beta \sum_{\langle xy \rangle \in V_1} |\sigma_x - \sigma_y| + \mu \sum_{x \in V} \sigma_x \right) , \tag{4.1}$$

where the first sum goes over all configurations $\sigma_V \ : \ V \to \{-\frac{1}{2}, +\frac{1}{2}\}$, while the second sum goes over the set V_1 of all nearest neighbor pairs $\{x, y\}$ for which both x and y are in V. We recall that the infinite volume transition takes place as μ crosses the point $\mu^* = 0$ due to the $\pm$ symmetry of the model. We use σ to denote the infinite volume surface tension, $f(L)$ to denote the free energy in the infinite cylinder $V_\infty := A \times \mathbf{Z}$,

$$-\beta f(L) := \lim_{V \to V_\infty} \frac{1}{|V|} \log Z_{\text{free}}(V, \mu) , \tag{4.2}$$

and $f_\pm = f_\pm(\mu)$ to denote the metastable free energies introduced in (1.1) (their existence is guarantied by Theorem A). Our main result for free boundary conditions is then summarized in the following theorem.

Theorem 4.1. *Let β be large and $|\mu| L^\nu \le 1$. Then there exists a 2×2 symmetric matrix $R = R(L, \mu)$ with strictly positive entries, such that the following statements are true.*

(i) *For $t \ge \nu \log L$ and for $0 \le k \le 4$,*

$$\left| \frac{d^k}{d\mu^k} (Z_{\text{free}}(V, \mu) - \operatorname{Tr} R^t) \right| \le e^{-\beta f(L)|V|} e^{-(\beta - O(1))t} . \tag{4.3}$$

(ii)
$$R_{++}(L, \mu = 0) = R_{--}(L, \mu = 0)$$

(iii)
$$\left| \frac{d^k}{d\mu^k} \left(L^{-\nu} \log R_{mm} + \beta f_m(\mu) \right) \right| \le O(L^{-1}) , \qquad m \in \{-, +\} \tag{4.4}$$

(iv)
$$\left| \frac{d^k}{d\mu^k} \ R_{+-} \right| \le e^{-\beta f(L) L^\nu} e^{-(\beta - O(1)) L^\nu} \tag{4.5}$$

(v) *There are constants* $b_0, \ldots, b_{\nu-1}$ *such that*

$$\frac{R_{+-}(L,\mu=0)}{R_{++}(L,\mu=0)} = e^{-\beta\sigma L^\nu} \exp\left(-\sum_{i=0}^{\nu-1} b_i L^i\right)(1+O(e^{-(\beta-O(1))L})) \tag{4.6}$$

provided $\nu+1 \geq 2$.

Remarks:

i) If one defines

$$\beta\tilde{f}_+(L,\mu) = -L^{-\nu}\log R_{++}\ , \tag{4.7}$$

$$\beta\tilde{f}_-(L,\mu) = -L^{-\nu}\log R_{--}\ , \tag{4.8}$$

$$x = \frac{\beta}{2}(\tilde{f}_+(L,\mu) - \tilde{f}_-(L,\mu))L^\nu \tag{4.9}$$

$$\Gamma = \Gamma(L,\mu) = e^{\frac{\beta}{2}(\tilde{f}_+(L,\mu)+\tilde{f}_-(L,\mu))L^\nu} R_{+-}(L,\mu)\ , \tag{4.10}$$

then the two eigenvalues of R (and hence the two lowest eigenvalues of the transfer matrix $\mathcal{T}$) are

$$\lambda_\pm = e^{-\frac{\beta}{2}(\tilde{f}_+(L,\mu)+\tilde{f}_-(L,\mu))L^\nu}\left(\cosh x \pm \sqrt{\sinh^2 x + \Gamma^2}\right)\ . \tag{4.11}$$

As a consequence, the spectral gap ξ_L^{-1} in the infinite cylinder V_∞ at $\mu = 0$ is related to the surface tension σ by the equation

$$\xi_L := \left[\frac{1}{\log(\lambda_+/\lambda_-)}\right]_{\mu=0} = D(L)e^{\beta\sigma L^\nu}\ , \tag{4.12}$$

where

$$D(L) = \frac{1}{2}\exp\left(\sum_{i=0}^{\nu-1} b_i L^i\right)(1+O(e^{-(\beta-O(1))L}))\ . \tag{4.13}$$

Note that $D(L) = O(1)$ for $\nu+1=2$, in accordance with the results of [18,19,20].

ii) As in the periodic case, the finite volume magnetization is given by an equation of the form (2.3), *i.e.*

$$\left|\frac{d^k}{d\mu^k}\left[M_{\text{free}}(V,\mu) - \sum_i M_i(L,\mu)P_i(V,\mu)\right]\right| \leq e^{-(\beta-O(1))t} \tag{4.14}$$

if $k \leq 3$, $t \geq \nu \log L$ and $|\mu| L^\nu \leq 1$. Here

$$M_\pm(L,\mu) \equiv \frac{1}{L^\nu} \frac{d}{d\mu} \log \lambda_\pm \ , \tag{4.15}$$

$$P_\pm(V,\mu) \equiv \lambda_\pm^t \left[\lambda_+^t + \lambda_-^t\right]^{-1} \ . \tag{4.16}$$

We leave it to the reader to use the methods of Section 2 to obtain an analog of Theorem B for free boundary conditions.

We now sketch the main ideas of the proof of Theorem 4.1, putting some of the more technical details to the appendix. As usual we define the contours corresponding to a configuration σ_V as the connected components of $\partial\sigma_V$, where $\partial\sigma_V$ is the set of ν dimensional faces dual to the bonds $\langle xy\rangle \in V_1$ for which $\sigma_x \neq \sigma_y$. We distinguish between *long contours* which wind around the cylinder in time direction, and short contours which do not. For short contours we distinguish between *interfaces* which are those short contours which are perforated by all time-like loops[3] in V_1 and *ordinary contours* which are those short contours Y for which it is possible to find a time-like loop in V_1 which does not perforate Y.

Neglecting configurations σ_V for which $\partial\sigma_V$ contains long contours (as shown in the appendix, these configurations only contribute to the error term in (4.3)), we then consider the partition function $Z_{\text{res}}(V,\mu)$ which is obtained from $Z_{\text{free}}(V,\mu)$ by restricting the sum in (4.1) to those configurations for which $\partial\sigma_V$ is only made of interfaces and ordinary contours. If the condition $|\mu| L^\nu \leq 1$ is fulfilled — as we assume from now on — the gain in energy resulting from the insertion of an ordinary contour with interior $\operatorname{Int} Y$ into an unstable phase is bounded by $|\mu|\,|\operatorname{Int} Y| \leq |\mu| L^\nu\,|Y| \leq |Y|$, leaving an effective decay $\exp(-(\beta\,|Y| - |\mu|\,|\operatorname{Int} Y|)) \leq \exp(-(\beta-1)|Y|)$. As a consequence, we can use a convergent cluster expansion to resum the ordinary contours in $Z_{\text{res}}(V,\mu)$. This leads to effective free energies $f_\pm(\mu,L)$ for the regions between interfaces, an interaction term $e^{g(Y,Y')}$ for neighboring interfaces, and a modified weight $\kappa(Y)$ for the interfaces. As a consequence,

$$\begin{aligned} Z_{\text{res}}(V,\mu) =& e^{-\beta f_+(L,\mu)|V|} + e^{-\beta f_-(L,\mu)|V|} \\ &+ \sum_{n=1}^\infty \frac{1}{n} \sum_{Y_1,\cdots,Y_n} \prod_i \kappa(Y_i)\, e^{-\beta f_i(L,\mu)|V_i|}\, e^{g(Y_i,Y_{i+1})} \ , \end{aligned} \tag{4.17}$$

[3] We call a closed line in V *time-like* if its closed via the periodicity of V.

where the second sum goes over interfaces $Y_1, \dots, Y_n$ that are chronologically ordered, V_i is the region between Y_i and Y_{i+1}, $f_i = f_+$ if V_i is in the + phase and $f_i = f_-$ otherwise. The factor $1/n$ in the above sum counts for the fact that cyclic permutations of $Y_1, \dots, Y_n$ correspond to the same configuration in $Z_{\rm res}(V, \mu)$.

Comparing (4.17) to the corresponding expansion for periodic boundary conditions, we note two main differences: first, the L-dependence of $f_\pm(L, \mu)$ is much stronger then before. For the periodic case, we had a bound $|f_\pm(L, \mu) - f_\pm(\mu)| \le e^{-(\beta - O(1))L}$, while now

$$f_\pm(L, \mu) - f_\pm(\mu) = O(L^{-1}) \tag{4.18}$$

due to the presence of the free boundary. Second, the sum over interfaces is now a sum over interfaces with free boundaries, while the interfaces in the periodic case had to match at the boundary (it is this restriction which is responsible for the power law correction $O(L^{-1/2})$ in (1.8), see Section 5 of [9] for details).

Keeping these differences in mind, we continue as in the periodic case: we assign a time $t(Y) \in T_{1/2} := \{1/2, 3/2, \dots, t - 1/2\}$ to each interface Y (roughly speaking, $t(Y)$ is the middle point of the smallest interval $I(Y)$ such that $Y \subset A \times I(Y)$) and define an activity

$$r(Y) = \kappa(Y) e^{-\beta f_{m_-}(L,\mu)[\,|V_-| - L^\nu |I_-|\,]} e^{-\beta f_{m_+}(L,\mu)[\,|V_+| - L^\nu |I_+|\,]}\ , \tag{4.19}$$

where I_+ (I_-) is the part of $I(Y)$ above (below) $t(Y)$, V_+ (V_-) is the part of $A \times I(Y)$ above (below) Y and m_+ (m_-) is the label of the phase above (below) Y. With these definitions, the partition function $Z_{\rm res}(V, \mu)$ can be rewritten as

$$\begin{aligned} Z_{\rm res}(V, \mu) =& e^{-\beta f_+(L,\mu)|V|} + e^{-\beta f_-(L,\mu)|V|} \\ &+ \sum_{n=1}^{\infty} \frac{1}{n} \sum_{Y_1, \cdots, Y_n} \prod_i r(Y_i)\, e^{-\beta f_i(L,\mu)(t(Y_i+1) - t(Y_i))L^\nu}\ e^{g(Y_i, Y_{i+1})}\ . \end{aligned} \tag{4.20}$$

If we neglect the interaction between neighboring interfaces and approximate the non overlap constraint between Y_i and Y_{i+1} by the constraint $t(Y_i) < t(Y_{i+1})$, the right-hand side of (4.17) can be written as a trace

$$Z_{\rm res}(V, \mu) \cong \mathrm{tr}(F(1 + \Gamma^{(0)}))^t = \mathrm{tr}(F + F^{1/2} \Gamma^{(0)} F^{1/2})^t\ . \tag{4.21}$$

Here F is the diagonal matrix

$$F = \mathrm{diag}\left(\exp(-\beta f_-(L,\mu)L^\nu), \exp(-\beta f_+(L,\mu)L^\nu)\right) \ , \tag{4.22}$$

and $\Gamma^{(0)}$ is the 2×2 matrix with matrix elements

$$\Gamma^{(0)}_{m_- m_+} = \lim_{V \to V_\infty} \sum_{Y \,:\, t(Y)=t_0} r(Y) \tag{4.23}$$

where the sum goes over interfaces describing a transition from the phase m_- below Y to the phase m_+ above Y. Note that $\Gamma^{(0)}$ does not depend on the choice of t_0 in (4.23) due to the translation invariance in time direction.

Taking into account the interaction between interfaces requires the use of the methods of [9], Section 4. There is, however, no difference in this part of the proof. We therefore only state the result, which is the existence of a matrix Γ, with matrix elements

$$\Gamma_{m_- m_+} = \Gamma^{(0)}_{m_- m_+} + O(e^{-(2\beta - O(1))L^\nu}) \ , \tag{4.24}$$

such that

$$\left| \frac{d^k}{d\mu^k} \left[Z_{\mathrm{res}}(V,\mu) - tr(F + F^{1/2}\Gamma F^{1/2})^t \right] \right| \le e^{-\beta \min\{f_-(L,\mu), f_+(L,\mu)\}|V|} e^{-(\beta - O(1))t} , \tag{4.25}$$

$$\left| \frac{d^k \Gamma_{m_- m_+}}{d\mu^k} \right| \le e^{-(\beta - O(1))L^\nu} \ , \tag{4.26}$$

provided β is large enough, $k \le 4$ and $|\mu| L^\nu \le 1$. Up to the difference between $Z_{\mathrm{free}}(V,\mu)$ and $Z_{\mathrm{res}}(V,\mu)$ (which is bounded in the appendix) and the difference between $f(L)$ and $\min\{f_-(L,\mu), f_+(L,\mu)\}$ (which is $O(e^{-(\beta-O(1))L^\nu})$ and therefore harmless) this already proves the bounds (4.3) through (4.5) of Theorem 4.1 (use (4.18) and its generalizations to derivatives to prove (4.4)), while (4.24) reduces the proof of (4.6) to the proof of the relation

$$\Gamma^{(0)}_{+-}(\mu = 0) = e^{-\beta\sigma L^\nu} \exp\left(- \sum_{i=0}^{\nu-1} b_i L^i \right) (1 + O(e^{-(\beta - O(1))L})) \ . \tag{4.27}$$

Note that the right-hand side of this equation is typical for the partition function $\tilde{Z}$ of a dilute lattice gas in a volume $A = \{1, \dots, L\}^\nu$, where $\log \tilde{Z}$ contains a volume term proportional to L^ν, a surface term proportional to $L^{\nu-1}$, ... , a corner term $O(1)$ and finally exponential corrections due to the finite correlation length of the model. We therefore have to find a suitable representation of $\Gamma_{+-}^{(0)}(\mu = 0)$ as a dilute lattice gas with free energy density σ.

In order to present the main ideas let us neglect, for the moment, the fact that the resummation of ordinary contours also changes the activity of an interface. In this approximation,

$$
\begin{aligned}
Z_{\mathrm{res}}(V, \mu = 0) &\cong e^{-\beta f_+(L,0)|V|} \left(1 + 1 + \sum_{n=1}^{\infty} \frac{1}{n} \sum_{Y_1, \cdots, Y_n} \prod_i e^{-\beta |Y_i|} \, e^{g(Y_i, Y_{i+1})} \right) , \\
\Gamma_{+-}^{(0)} &\cong \sum_{Y : t(Y) = t_0} e^{-\beta |Y|} ,
\end{aligned}
\tag{4.28}
$$

where we used the fact that $f_+(L, 0) = f_-(L, 0)$. Note that the leading contribution to the r.h.s. of (4.28) comes from the completely flat surface Y_0, with $|Y_0| = L^\nu$

Following an idea originally appearing in [10] we now decompose each interface into *flat pieces* (defined as those parts of Y which are parallel to the minimal surface Y_0 and which are simple in the sense that all straight lines in time direction which intersect a flat piece of Y have only one intersection with Y) and its *walls* $W_1, \dots, W_n$ (defined as the connected components of the part Y^* of Y which is not flat). We then introduce the *floating walls* $[W_1], \dots, [W_n]$ of Y by introducing, for each wall W of Y, the equivalence class $[W]$ of walls W' which are obtained from W by a translation in the time direction. It is then an easy geometric exercise (see, *e.g.* [10]) to show that the orthogonal projections, $\pi(W_1), \dots, \pi(W_n)$, of $W_1, \dots, W_n$ onto the flat surface Y_0 do not overlap, and that two surfaces Y and Y' with the same set of floating walls are identical up to a global translation in time direction. Given, on the other hand, a set $\{[W_1], \dots, [W_n]\}$ of floating walls such that $\pi(W_i)$ and $\pi(W_j)$ do not overlap for $i \neq j$ (we call such a set an *allowed set of floating walls*) one may actually always construct an interface Y such that $[W_1], \dots, [W_n]$ are the floating walls of Y.

We therefore have a one-to-one correspondence between interfaces with fixed time $t(Y) = t_0$ and allowed sets of floating walls. Observing finally that $|Y| = |\pi(Y)| +$

$\sum_{i=1}^n [|W_i| - |\pi(W_i)|] = L^\nu + \sum_{i=1}^n [|W_i| - |\pi(W_i)|]$ we find that the r.h.s. of (4.28) can be rewritten as

$$\sum_{Y:t(Y)=t_0} e^{-\beta|Y|} = e^{-\beta L^\nu} \sum_{n=0}^{\infty} \sum_{\{[W_1],\dots,[W_n]\}} \prod_{i=1}^{n} z(W_i) =: e^{-\beta L^\nu} \tilde{Z}(A) , \tag{4.29}$$

where the second sum goes over allowed sets of floating walls and

$$z(W) := e^{-\beta[|W_i| - |\pi(W_i)|]} . \tag{4.30}$$

In the approximation (4.28), the r.h.s. of (4.29) is the desired representation of $\Gamma_{+-}^{(0)}$ as the partition function of a dilute lattice gas, with "molecules" which are just the excitations of the flat surface Y_0 . This function can be brought to the standard form of a polymer partition function, with polymers which are just the connected subsets of Y_0, by resumming, for each set $\{P_1, \dots, P_n\}$, all floating walls for which $\pi(W_1) = P_1, \dots, \pi(W_n) = P_n$. After this resummation, $\tilde{Z}(A)$ is just a sum over subsets $P_1, \dots, P_n$ of Y_0 which are mutually nonoverlapping, with a weight $\tilde{z}(P_i) \leq e^{-(\beta - O(1))|P_i|}$ for the polymer P_i. The Mayer expansion for the logarithm of the polymer partition function $\tilde{Z}(A)$, which is absolutely convergent if β is large enough, then gives an expansion of the form (4.27). If one adds the corrections coming from the resummation of ordinary contours, using *e.g.* the methods described in Section 5 of [9], the expansion for the free energy of the lattice gas is exactly the same as the usual expansion (see, *e.g.* [10]) for the surface tension σ. Since both expansions are convergent, the bound (4.24) is proven. ∎

It is instructive to compare the above situation to the periodic case. In this case it is no longer true that each allowed set of floating walls $\{[W_1], \dots, [W_n]\}$ leads to an allowed surface Y because the surface constructed from $\{[W_1], \dots, [W_n]\}$ may violate the periodicity conditions imposed by the periodic lattice. If $\nu + 1 \geq 3$, this can only happen if one of the walls is so large that $|W| - |\pi(W)| \geq L$; the contribution of these configurations therefore only enters into the error term in (1.8), see Section 5 of [9] for the proof. But for $\nu + 1 = 2$, this effect leads in fact to the $1/\sqrt{L}$ correction in (1.8), and hence to $w = 1/2$. Heuristically, this can be easily understood by considering only surfaces without overhangs. The sum over surfaces is then just a sum over closed random walks. Since a random walk without restriction on its endpoint walks just an average distance $\sqrt{L}$ in a time L, it gets a $1/\sqrt{L}$ correction if it is forced to return to its endpoint.

We do want to make this more precise, however, taking at the same time the opportunity to explain the main idea of the proof of $w = 1/2$ in the periodic case. To this end, we introduce for each wall W_j, the height difference h_j between its right and left endpoint. The surface constructed from an allowed set of floating walls then fulfills the required periodicity condition if and only if the heights h_j add up to zero. Following [21], we then introduce the partition function

$$\tilde{Z}(p) = e^{-\beta L^\nu} \sum_{n=0}^{\infty} \sum_{\{[W_1],\ldots,[W_n]\}} \prod_{j=1}^{n} z(W_j) e^{iph_j} \ , \tag{4.31}$$

where the sum goes over all allowed sets of floating walls. The restriction $\sum h_j = 0$ is now obtained by integrating over p, so that the sum over periodic interfaces is just

$$\sum_{Y:t(Y)=t_0} e^{-\beta|Y|} = \frac{1}{2\pi} \int_{-\pi}^{\pi} dp\, \tilde{Z}(p) \ . \tag{4.32}$$

Since $\tilde{Z}(p)$ can again be rewritten as the partition function of a dilute lattice gas (note that the activities of the walls are multiplied by a complex number of modulus one, which doesn't affect the about absolute convergence), its logarithm is again of the form

$$\log \tilde{Z}(p) \cong -L\tilde{f}(p) \ . \tag{4.33}$$

For large L, the integration over p in (4.32) can then be analyzed by a saddle point approximation and we obtain

$$\sum_{Y:t(Y)=t_0} e^{-\beta|Y|} \cong \frac{1}{2\pi} \int_{-\pi}^{\pi} dp \ \exp\left(-L\tilde{f}(0) - \frac{p^2}{2} L\tilde{f}''(0)\right) = \frac{1}{\sqrt{2\pi L\tilde{f}''(0)}} e^{-L\tilde{f}(0)} \tag{4.34}$$

in accordance with the heuristic random walk argument.

It is interesting to introduce boundary conditions which interpolate between free and periodic boundary conditions by adding a term

$$\sum_{\{x,y\}} g|\sigma_x - \sigma_y| \tag{4.35}$$

to the Hamiltonian, where the sum runs over all pairs of points x, y which lie on opposite sides of the boundary of V. The value $g = 0$ then corresponds to free and the value $g = 1$ to periodic boundary conditions. For the transverse quantum Ising model in one dimension, such b.c. have been considered by Cabrera and Julien [18] and by Barber and Cates [19]. While Cabrera and Julien present exact calculations on small lattice which suggest that $\xi_L \sim O(L^w)e^{\beta\sigma L}$ where w varies smoothly as g goes from 1 to 0, Barber and Cates give random walk arguments which explain this effect as a crossover phenomenon, suggesting that $w = 1/2$ for all $g > 0$. For the classical Ising model considered here, Abraham, Ko and Svracic [20] gave exact transfer matrix expressions for the spectral gap, which again give $w = 1/2$ for all $g > 0$ in $\nu + 1 = 2$. We think that these results can actually be proven (and at the same time be extended to a large class of two phase systems with a symmetry relating h to $-h$) if one uses the methods developed in Section 5 of [9]. In order to explain the main idea, we again leave off the corrections coming from the resummation of ordinary contours. In this approximation, $\Gamma^{(0)}_{+-}$ is now given as a sum of the form (4.29), with an extra factor $e^{-g\beta\sum_i h_i}$ on the r.h.s. correcting for the fact that we have left out the contribution of (4.35) to the energy of an interface. Rewriting

$$e^{-g\beta\sum_i h_i} = \frac{1}{2\pi}\int_{-\pi}^{\pi} dp\, G(p) e^{ip\sum_i h_i} \ ,$$

where

$$G(p) = \sum_{m=-\infty}^{\infty} e^{ipm} e^{-g\beta|m|} \ , \tag{4.36}$$

we obtain that

$$\Gamma^{(0)}_{+-} \cong \sum_{Y: t(Y)=t_0} e^{-\beta|Y|} e^{-g\beta\sum_i h_i} = \frac{1}{2\pi}\int_{-\pi}^{\pi} dp\, G(p)\tilde{Z}(p) \ . \tag{4.37}$$

Except for $g = 0$, where $G(p) = 2\pi\delta(p)$ and hence

$$\Gamma^{(0)}_{+-}\Big|_{g=0} \cong \frac{1}{2\pi}\tilde{Z}(0) = O(1)e^{-L\tilde{f}(0)} \ ,$$

$G(p)$ is regular at $p = 0$. As a consequence, the integral in (4.37) may again be analyzed by a saddle point approximation, leading to

$$\Gamma^{(0)}_{+-} \cong O(1)\int_{-\pi}^{\pi} dp\, G(0) \exp\left(-L\tilde{f}(0) - \frac{p^2}{2}L\tilde{f}''(0)\right) = O(1)\frac{G(0)}{\sqrt{L\tilde{f}''(0)}} e^{-L\tilde{f}(0)} \tag{4.38}$$

for all $g > 0$. Using the methods of [9], Section 5, it should be possible to actually prove that this behavior persist when the corrections coming from the resumming over ordinary contours are taken into account. We therefore conjecture that the following Quasi-Theorem is in fact a Theorem

Quasi-Theorem 4.2. *Let β be large, $\nu + 1 = 2$ and $\mu = 0$. Let $\xi_L^{-1}(g)$ be the spectral gap in the infinite cylinder V_∞ with boundary conditions g as defined above. Then*

$$\xi_L = D(L) e^{\beta\sigma L} , \tag{4.39}$$

where

$$D(L) \sim \text{const.}\, L^w \qquad \text{as} \qquad L \to \infty \tag{4.40}$$

and $w = 0$ for $g = 0$, while $w = 1/2$ for all g in the range $0 < g \leq 1$.

Note that (4.40) is only an asymptotic statement for large L, and that the answer to the question how large is large may depend on g. Heuristically, one just should compare the average walking distance of the random walk $l(L) = O(L^{1/2})$ to the length scale $l(g) = O(1/g)$ on which the term $e^{-g\beta \sum_i h_i}$ starts to suppress large height differences between the two end points of the surface Y, see also [19]. If $l(L) < l(g)$, the insertion of $e^{-g\beta \sum_i h_i}$ should not have a great influence, so that effectively w is still 0, while for $l(L) > l(g)$ we expect the onset of the asymptotic behavior (4.40). Note that this heuristic arguments can actually be made more quantitative by calculating the next to leading orders in the approximation (4.38). One obtains that

$$\Gamma_{+-}^{(0)} \cong \frac{c_0}{\sqrt{L}} \left(1 + c_1 L^{-1} + O(L^{-2})\right) , \tag{4.41}$$

where both c_0 and c_1 depend on g. For small g, $c_1 \sim g^{-2}$, which gives a crossover if $L = O(g^{-2})$.

Remark: It would be interesting to prove Theorem 4.1 and the above Quasi-Theorem for asymmetric models. For these models, we expect a shift $O(1/L)$ in the free boundary finite volume transition point (defined, *e.g.*, as the point $\mu^*(L)$ where $f_+(L, \mu^*(L)) =$

$f_-(L, \mu^*(L))$, or, more naturally, as the point where the splitting between the two lowest eigenvalues of the transfer matrix is minimal). It is clear, however, that the proof of the analog of Theorem 4.1 requires a substantial extension of the methods used so far, since the *a priori* assumption $|\mu - \mu^*|L^\nu \le O(1)$ which was used to resum ordinary contours is not valid anymore. Note, however, that such a condition is only needed for ordinary contours which touch the boundary, while ordinary contours not touching the boundary may in fact be resummed as long as $|\mu|L \le b\beta$ for some $b < 1$. Using a procedure of inductively defining suitable finite-L free energies $f_\pm(L, \mu)$ (as sketched in the appendix just before equation (A.2)) should then make it possible to actually resum the ordinary contours which touch the boundary if $|\mu - \mu^*(L)|L^\nu \le O(1)$ (where $\mu^*(L)$ is now inductively defined as well).

Appendix

In this appendix we fill in the technical details left out in the last section. In order to avoid lengthy repetitions, we assume that the reader has some familiarity with [9] and only comment on the differences which appear due to the presence of free boundary conditions (b.c).

For preciseness, we distinguish between the lattice $V = A \times T$, the set V_1 of nearest neighbor (n.n.) bonds in V, their duals V^* and V_1^*, and the continuum cylinder $\overline{V} := [1/2, L+1/2]^\nu \times (\mathbf{R}/t\mathbf{Z})$. We introduce contours, long contours, interfaces and ordinary contours as in Section 3 of this note, considering the set $\partial\sigma_V$ as a subset of $\overline{V}$ by taking the closed union of all faces dual to a bond $\langle xy\rangle$ for which $\sigma_x \neq \sigma_y$. Observing that each short contour may be embedded into the infinite cylinder $\overline{V}_\infty := [1/2, L+1/2]^\nu \times \mathbf{R}$, we define, for each contour Y which is either an interface or an ordinary contour, the interior Int$Y$ of Y as the union of all finite components of $\overline{V}_\infty \setminus Y$. Note that the interior of a contour may have several connected components with our definitions where we did not include a "rounding of edges" procedure to produce contours with connected interiors[4].

First, we want to comment on the consequences of the condition $|\mu| L^\nu \leq 1$ on the resummation of ordinary contours. To this end we recall that the resummation of ordinary contours involves activities $K(Y)$ (see equation (3.4) of [9]) which contain ratios of partition functions

$$\frac{Z_-(W,\mu)}{Z_+(W,\mu)} \qquad \text{or} \qquad \frac{Z_-(W,\mu)}{Z_+(W,\mu)}$$

where W is a connected component of Int$Y$ and $Z_\pm(W,\mu)$ is defined as

$$Z_\pm(W,\mu) := \sum_{\sigma_W}{}' \exp\left(-\beta \sum_{\langle xy\rangle \in W_1} |\sigma_x - \sigma_y| + \mu \sum_{x \in W_0} \sigma_x\right) , \qquad (A.1)$$

where the sum goes over all configurations $\sigma_W : W_0 \to \{-\frac{1}{2}, \frac{1}{2}\}$ which are perturbations of the plus ground state (or of the minus ground state, if the sign - is chosen) by ordinary contours (see below), $W_0 = V \cap W$ is the set of lattice points which lie in W, and W_1 is the set of nearest neighbor bonds $\langle xy\rangle \in V_1$ for which both x and y lie in W_0. Here — and in the following — σ_W is called a perturbation of a ground state $m \in \{-\frac{1}{2}, \frac{1}{2}\}$ by ordinary

[4] For the same reasons, interfaces may also have an interior with several components.

contours if all contours corresponding to σ_W are ordinary contours, if none of them touches $\partial W \setminus \partial \overline{V}$, and if $\sigma_x = m$ for all points x in the set Ext $:= W \setminus \cup_i \mathrm{Int} Y_i$ (where the union runs over all contours Y_i of σ_W).

In order to bound the activities $K(Y)$, we have to bound the above ratios of partition functions. Following the strategy used for periodic b.c., we would assume inductively that $K(Y) \leq e^{-(\beta - O(1))|Y|}$ and then use this assumption to bound

$$|\log Z_\pm(W,\mu) + |W|\beta f_\pm(\mu)| \leq |\partial W| O(e^{-\beta})$$

in the next step. Assuming $|\mu| L^\nu \leq 1$, which implies that $\beta|f_+(\mu) - f_+(\mu)|\,|\mathrm{Int}Y| \leq \beta|f_+(\mu) - f_+(\mu)|\, L^\nu |Y| \leq O(1)|Y|$, we then get

$$|K(Y)| \leq e^{-(\beta - O(1))|Y|} \prod_W e^{|\partial W| O(e^{-\beta})} ,$$

where the product goes over the connected components of Int$Y$. Unfortunately, this bound is not good enough, since $|\partial W|$ may now have huge parts which are made of the free boundary $\partial \overline{V}$, so that $|\partial W|$ may be much larger then $|Y|$ (the ratio may in fact be as large as $O(L^{\nu-1})$).

One should therefore try to inductively construct an L-dependent free energy $f_\pm(L,\mu)$ which takes the boundary effects with the free boundary into account, leaving only an error term $|\partial W \cap Y| O(e^{-\beta})$. Fortunately, we do not have to follow this strategy in the present case, where the $+/-$ symmetry implies that

$$Z_-(W, \mu = 0) = Z_+(W, \mu = 0) . \qquad (A.2)$$

Combined with the fact that

$$\left| \frac{d^k Z_\pm(W,\mu)}{d\mu^k} \right| \leq (|W|/2)^k Z_\pm(W,\mu) \qquad (A.3)$$

since the sum in (A.1) is a sum of positive terms and $|\sigma_x| = \frac{1}{2}$, we conclude that

$$\left| \frac{Z_-(W,\mu)}{Z_+(W,\mu)} \right| \leq e^{|W||\mu|} \qquad \text{and} \qquad \left| \frac{Z_+(W,\mu)}{Z_-(W,\mu)} \right| \leq e^{|W||\mu|} .$$

Bounding now $|\mathrm{Int}Y| \leq |I(Y)|L^\nu \leq |Y|L^\nu$, where $I(Y)$ denotes the smallest interval such that $Y \subset [1/2, L+1/2]^\nu \times I(Y)$, we find that the activities $K(Y)$ may be bounded by

$$K(Y) \leq e^{-(\beta-|\mu|L^\nu)|Y|} \ . \tag{A.4}$$

The condition $|\mu|L^\nu \leq 1$ therefore guaranties that the resummation of the ordinary contours in Z_{res} can be analyzed by a convergent expansion.

In order to obtain a representation of the form (4.17), we now use that the resummation of ordinary contours brings $Z_{\mathrm{res}}(V,\mu)$ into the form

$$\begin{aligned} Z_{\mathrm{res}}(V,\mu) =& Z_+(V,\mu) \ + Z_-(V,\mu) \\ &+ \sum_{n=1}^{\infty} \frac{1}{n} \sum_{Y_1,\cdots,Y_n} \prod_i \left[e^{-\beta|Y_i|} \prod_{W\subset \mathrm{Int}Y} Z_{m_W}(W,\mu) \right] \prod_i Z_{m_i}(V_i,\mu) \ , \end{aligned} \tag{A.5}$$

where the sum over $Y_1, \ldots, Y_n$ goes over interfaces $Y_1, \ldots, Y_n$ that are chronologically ordered, the product $\prod_{W\subset \mathrm{Int}Y}$ runs over the connected components of $\mathrm{Int}Y$, and V_i is the region between Y_i and Y_{i+1}; $Z_\pm(\cdot,\mu)$ are the partition functions introduced in (A.1), $m_i = +$ if V_i is in the $+$ phase and $m_i = -$ otherwise, and, in the same way, $m_W = \pm$, depending on whether W is in the phase $+$ or $-$. The factor $1/n$ in the above sum counts for the fact that cyclic permutations of $Y_1, \ldots, Y_n$ correspond to the same configuration in $Z_{\mathrm{res}}(V,\mu)$.

Using W^* and V_i^* to denote the set of cubes dual to the lattice points in W and V_i, respectively, we now use the fact that $Z_\pm(\cdot,\mu)$ can be analyzed by a convergent cluster expansion, to write its logarithm in the form

$$\log Z_\pm(W,\mu) = \pm\mu|W^*| + \sum_{X\subset W^*} k_\pm(X) \ , \tag{A.6}$$

where the sum goes over connected subsets X of W^*, and $|k_\pm(X)| \leq e^{-(\beta-O(1))|X|}$. We then rewrite

$$\log Z_\pm(W,\mu) = \sum_{c\in W^*} \left[\pm\mu + \sum_{\substack{X\subset W^* \\ X\ni c}} \tilde{k}_\pm(X) \right] \ ,$$

where $\tilde{k}_\pm(X) = k_\pm(X)/|X|$, and introduce position dependent free energies

$$\beta f_{c\pm} := \mp\mu - \sum_{\substack{X \subset V_\infty^* \\ X \ni c}} \tilde{k}_\pm(X) \,, \tag{A.7}$$

noting that

$$\beta f_{c\pm} = \beta f(\mu) + O(e^{-(\beta - O(1))\mathrm{dist}(c, \partial V_\infty^*)} \,. \tag{A.8}$$

Using these free energies, $\log Z_\pm(W,\mu)$ may be written as $\beta \sum_{c\in W^*} f_{x\pm}$ plus a sum of the form (A.6), where X now goes over sets $X \subset V_\infty^*$ which intersect $\partial W \setminus \partial V_\infty^*$. As a consequence, $Z_{\mathrm{res}}(V,\mu)$ may be rewritten as

$$\begin{aligned} Z_{\mathrm{res}}(V,\mu) &= e^{-\beta f_+(L,\mu)|V|} + e^{-\beta f_-(L,\mu)|V|} \\ &+ \sum_{n=1}^\infty \frac{1}{n} \sum_{Y_1,\cdots,Y_n} \prod_i \tilde{\kappa}(Y_i)\, e^{g(Y_i,Y_{i+1})} \exp\big(-\sum_{c\in V_i^*} \beta f_{xm_i}\big) \,, \end{aligned} \tag{A.9}$$

where

$$\begin{aligned} f_\pm(L,\mu) &= \frac{1}{tL^\nu} \sum_{c\in V^*} f_{c\pm} \,, \\ \tilde{\kappa}(Y) &= e^{-\beta|Y| + g(Y)} \prod_{W\subset \mathrm{Int} Y} \exp\big(-\sum_{c\in W^*} \beta f_{cm_W}\big) \,. \end{aligned}$$

Here $g(Y)$ may be rewritten as a sum of terms X intersecting Y and hence can be bounded by $|Y|O(e^{-\beta})$, and $g(Y,Y')$ can be written as a sum of terms intersecting both Y and Y', and hence can be bounded by $\min\{|Y|,|Y'|\}e^{-\mathrm{dist}(Y,Y')(\beta - O(1))}$.

In order to bring (A.9) into the form (4.17), we note that

$$V_i = (\bar{A}\times I) \setminus \big[(\bar{A}\times I(Y_i)) \setminus V_+(Y_i) \cup (\bar{A}\times I(Y_{i+1})) \setminus V_-(Y_{i+1})\big] \,, \tag{A.10}$$

where $\bar{A} = [1/2, L+1/2]^\nu$, $I(Y)$, $V_-(Y)$ and $V_+(Y)$ are the smallest interval such that $Y \subset \bar{A}\times I(Y)$, the part of $I(Y)$ which lies below Y and the part of $I(Y)$ which lies above Y, respectively. Finally I is the interval which extends from the lowest endpoint of $I(Y_i)$ to the highest endpoint of $I(Y_{i+1})$. Using (A.10) and the fact that the translation invariance in the time direction implies that

$$\sum_{c\subset \bar{A}\times\tilde{I}} f_{c\pm} = |\bar{A}\times\tilde{I}| f_{\pm}(L,\mu)$$

for $\tilde{I}=I$, $I(Y_i)$ and $I(Y_{i+1})$, we now rewrite (A.9) as

$$\begin{aligned} Z_{\rm res}(V,\mu) =& e^{-\beta f_{+}(L,\mu)|V|} + e^{-\beta f_{-}(L,\mu)|V|} \\ &+ \sum_{n=1}^{\infty} \frac{1}{n} \sum_{Y_1,\cdots,Y_n} \prod_i \kappa(Y_i)\, e^{-\beta f_i(L,\mu)|V_i|}\, e^{g(Y_i,Y_{i+1})}\ , \end{aligned} \qquad (A.11)$$

where, for an interface Y which describes the transition from a state m_- below Y to a state m_+ above Y,

$$\kappa(Y) := \tilde{\kappa}(Y)\exp\left(-\beta\sum_{c\in V_+^*}(f_{cm_+} - f_{m_+}(L,\mu)) - \beta\sum_{c\in V_-^*}(f_{cm_-} - f_{m_-}(L,\mu))\right)\ . \quad (A.12)$$

In order to bound $\kappa(Y)$, we note that

$$\kappa(Y) = e^{g(Y)-\beta|Y|} e^{-\beta\Delta F(Y)} \prod_{W\subset {\rm Int}Y} e^{-\beta f_{m_W}(L,\mu)|W|}\ , \qquad (A.13a)$$

where

$$\begin{aligned} \Delta F(Y) =& \sum_{c\in V_+^*}(f_{cm_+} - f_{m_+}(L,\mu)) + \sum_{c\in V_-^*}(f_{cm_-} - f_{m_-}(L,\mu)) \\ &+ \sum_{W\subset {\rm Int}Y}\sum_{c\in W^*}(f_{cm_W} - f_{m_W}(L,\mu))\ . \end{aligned} \qquad (A.13b)$$

Using the fact that $|d\Delta F(Y)/d\mu| \le |I(Y)| L^{\nu} O(e^{-\beta})$ and that $\Delta F(Y)=0$ if $\mu=0$, we conclude that

$$|\kappa(Y)| \le e^{-\beta|Y|} e^{O(1)(|Y|+|I(Y)|)} \le e^{-(\beta-O(1))|Y|}\ , \qquad (A.14)$$

provided $|\mu| L^\nu \leq 1$.

Given the representation (A.10), the bound (A.14) and its generalization to derivatives, and the fact that the derivatives of $f_\pm(L,\mu)$ are bounded by $O(1)$, the results of Section 4 of [9] immediately give (4.24) through (4.26). In order to prove (4.27), we note that

$$L^\nu |I_+(Y)| + L^\nu |I_-(Y)| - |V_+(Y)| - |V_-(Y)| = |\mathrm{Int} Y| \ ,$$

where $I_\pm(Y)$ are the parts of $I(Y)$ which lie above and below the point $t(Y)$ defined in the last section. Combined with the fact that $\Delta F(Y) = 0$ if $\mu = 0$, we obtain that

$$r(Y)\big|_{\mu=0} = e^{g(Y) - \beta|Y|} \ ,$$

and hence

$$\Gamma_{+-}^{(0)}\Big|_{\mu=0} = \lim_{V \to V_\infty} \sum_{Y : t(Y) = t_0} e^{g(Y) - \beta|Y|} \ .$$

Using the fact that $g(Y)$ is a sum over connected sets $X \subset V^*$ which intersect the surface Y, the methods introduced in [21] (see also [22]) then allow us to rewrite $\Gamma_{+-}^{(0)}$ as the partition function $\tilde{Z}(Y_0)$ of a dilute gas of excitations over the flat surface Y_0, where an excitation is now a connected cluster made of the walls introduced in Section 3 and the subsets $X \subset V^*$ appearing in the cluster expansion for $g(Y)$. Expanding $\log \tilde{Z}(Y_0)$ into volume terms, surface terms, etc., we obtain equation (4.27).

We finally bound the difference $Z_{\mathrm{free}}(V,\mu) - Z_{\mathrm{res}}(V,\mu)$. Resumming ordinary contours, we rewrite this difference as

$$Z_{\mathrm{free}}(V,\mu) - Z_{\mathrm{res}}(V,\mu) = \sum_{n=1}^\infty \sum_{\{Y_1,\cdots,Y_n\}} \prod_i e^{-\beta|Y_i|} \prod_W Z_{m_W}(W,\mu) \ ,$$

where the second sum goes over sets $\{Y_1, \cdots, Y_n\}$ of long contours in V such that $Y_i \cap Y_j = \emptyset$, the product over W runs over the connected components of $\overline{V} \setminus \cup_i Y_i$, m_W is the label of the state in W and $Z_{m_W}(W,\mu)$ are the partition functions introduced in (A.1). Using the bound (A.3) and the symmetry (A.2) we then bound

$$|Z_{\mathrm{free}}(V,\mu) - Z_{\mathrm{res}}(V,\mu)| \leq e^{|\mu/2||V|} \sum_{n=1}^\infty \sum_{\{Y_1,\cdots,Y_n\}} \prod_i e^{-\beta|Y_i|} \prod_W Z_+(W,0) \ .$$

We then note that the last product in this sum can be rewritten as

$$\prod_W Z_+(W,0) = \sum_{\sigma_V}{}' \prod_{\langle xy\rangle \in V_1} e^{-\beta|\sigma_x - \sigma_y|} \ ,$$

where the sum goes over configurations which are small perturbations of the plus ground state by ordinary contours obeying the additional constraint that $\sigma_x = \sigma_y = +1/2$ for all bonds $\langle xy\rangle$ which are dual to a face in $\cup Y_i$. Summing over all configurations which are small perturbations of the plus ground state by ordinary contours without any additional constraints gives an upper bound, and we obtain that

$$\begin{aligned} |Z_{\text{free}}(V,\mu) - Z_{\text{res}}(V,\mu)| &\le e^{|\mu/2||V|} Z_+(V,0) \sum_{n=1}^{\infty} \sum_{\{Y_1,\cdots,Y_n\}} \prod_i e^{-\beta|Y_i|} \\ &\le e^{|\mu||V|} Z_+(V,\mu) \sum_{n=1}^{\infty} \sum_{\{Y_1,\cdots,Y_n\}} \prod_i e^{-\beta|Y_i|} \ . \end{aligned} \qquad (A.15)$$

Using the fact that each contour in the sum over $\{Y_1,\ldots,Y_n\}$ is long, and hence larger then t, and bounding $Z_+(V,\mu)$ by $e^{-\beta\min\{f_+(L,\mu),f_-(L,\mu)\}|V|} e^{|V|\exp(-(\beta-O(1))t)}$, we obtain that

$$|Z_{\text{free}}(V,\mu) - Z_{\text{res}}(V,\mu)| \le e^{-\beta\min\{f_+(L,\mu),f_-(L,\mu)\}|V|} e^{-(\beta-O(1))t} \ , \qquad (A.16)$$

provided $|\mu|L^\nu \le 1$. At this point we use the bound (4.26) to bound the smallest eigenvalue λ_0 of the matrix $(F + F^{1/2}\Gamma F^{1/2})$ from below

$$\begin{aligned} \lambda_0 &\ge e^{-\beta\min\{f_+(L,\mu),f_-(L,\mu)\}L^\nu}(1 - \exp(-(\beta - O(1))L^\nu)) \\ &\ge e^{-\beta\min\{f_+(L,\mu),f_-(L,\mu)\}L^\nu} e^{-O(1)} \ . \end{aligned} \qquad (A.17)$$

Combining the bounds (4.25) and (A.16) with (A.17) and the fact that $|V| = tL^\nu$ we obtain that

$$\left| \frac{d^k}{d\mu^k} (Z_{\text{free}}(V,\mu) - \text{Tr}\,(F + F^{1/2}\Gamma F^{1/2})^t) \right| \le \lambda_0^t e^{-(\beta-O(1))t} \ . \qquad (A.18)$$

provided $t \ge \nu\log L$, $|\mu|L^\nu \le 1$ and $0 \le k \le 4$. Since this bound implies that $-\log\lambda_0/(\beta L^\nu)$ is actually the free energy $f(L)$ defined in (4.2), the bound (4.3) is finally proven. ∎

IV. References

[1] Privman, V. (ed.), *Finite-Size Scaling and Numerical Simulation of Statistical Systems.* Singapore 1990: World Scientific.

[2] Borgs, C., Kotecký, R.: Finite-size effects at asymmetric first-order phase transitions, to appear in *Phys. Rev. Lett.* A rigorous theory of finite-size scaling at first order phase transitions; *Jour. Stat. Phys.* **61**, 79 (1990).

[3] Borgs, C., Kotecký, R., Miracle-Sole, S.: Finite-size scaling for Potts models. *Jour. Stat. Phys.* **62**, 529 (1991).

[4] Blöte, H. W. J., Nightingale, M. P.: Critical behavior of the two dimensional Potts model with a continuous number of states; a finite size scaling analysis. *Physica* **112A**, 405–465 (1981).

[5] Privman, V., Fisher, M. E.: Finite-size effects at first-order transitions. *Jour. Stat. Phys.* **33**, 385–417 (1983).

[6] Brézin, E., Zinn-Justin, J.: Finite size effects in phase transitions. *Nucl. Phys.* **B257**, 867–893 (1985).

[7] Münster, G.: Tunneling amplitude and surface tension in ϕ^4-theory. *Nucl. Phys.* **324**, 630–642 (1989). Interface tension in three-dimensional Systems from field theory. *Nucl. Phys.* **340**, 559–567 (1990).

[8] Privman, V., Svrakic, N. M.: Asymptotic degeneracy of the transfer matrix spectrum for systems with interfaces: Relation to surface stiffness and step free energy. *Jour. Stat. Phys.* **54**, 735–754 (1989).

[9] Borgs, C., Imbrie, J. Z.: Finite-size scaling and surface tension from effective one dimensional systems. Harvard-reprint 1991, to appear in *Commun. Math. Phys.*

[10] Dobrushin, R. L.: Gibbs states describing the coexistence of phases for a three-dimensional Ising model. *Theor. Prob. Appl.* **17**, 582–600 (1972). Investigation of Gibbsian states for three-dimensional lattice systems. *Theor. Prob. Appl.* **18**, 253–271 (1973).

[11] Jansen, K., Jersak, J., Montway, I., Münster, G., Trappenberg, T. Wolf, U.: Vacuum tunneling in the four-dimensional Ising model. *Phys. Lett.* **213**, 203 (1988).

[12] Jansen, K., Shen, Y.: Tunneling and energy splitting in Ising models. UCSD/PTH 92-02, preprint.

[13] Wu, F. Y., *Rev. Mod. Phys.* **54** (1982); 55 (E) (1983).

[14] Kotecký, R., Shlosman, S. B.: First order phase transitions in large entropy lattice models. *Commun. Math. Phys.* **83**, 493 (1982).

[15] Lanait, L., Messager, A., Miracle-Solé, S., Ruiz, J., Shlosman, S.: Interfaces in the Potts model I: Pirogov-Sinai theory of the Fortuin-Kasteleyn representation. *Commun. Math. Phys.* **140**, 81-91 (1991).

[16] Cabrera, G. G., Julien, R., Brézin, E., Zinn-Justin, J.: Test of finite-size scaling in first order phase transitions. *J. Physique* **47**, 1305–1313 (1986).

[17] Borgs, C.: Finite-Size Scaling for Potts Models in Long Cylinders. FUB-preprint 1992.

[18] Cabrera, G. G., Julien, R.: Role of boundary conditions in finite-size Ising model. *Phys. Rev.* **B35**, 7062–7072 (1987).

[19] Barber, M. N., Cates, M. E.: Effect of boundary conditions on finite-size transverse Ising model. *Phys. Rev.* **B36**, 2024–2029 (1987).

[20] Abraham, D. B., Ko, L. F., Svrakic, N. M.: Transfer matrix spectrum for the finite -width Ising model with adjustable boundary conditions: exact solution. *J. Stat. Phys.* **56**, 563–587 (1989).

[21] Bricmont, J., Fröhlich, J.: Statistical mechanical methods in particle structure analysis of lattice field theories II: Scalar and surface models. *Commun. Math. Phys.* **98**, 553–578 (1985).

[22] Holichy, P., Kotecký, R., Zahradnik, M.: Rigid interfaces for lattice models at low temperatures. *Jour. Stat. Phys.* **50**, 755–812 (1988).