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FINITE-SIZE SCALING FOR POTTS MODELS IN LONG CYLINDERS

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ABSTRACT

Using a recently developed method to rigorously control the finite-size behaviour in long cylinders near first-order phase transitions, I calculate the finite-size scaling of the first q+1 eigenvalues of the transfer matrix of the q states Potts model in a d dimensional periodic box of volume $L \times \ldots \times L \times t$ (assuming that $d \geq 2$ and that q is sufficiently large). I find two simple eigenvalues $\lambda_\pm$ corresponding to the trivial representation of the global symmetry and an $q-1$ fold degenerate eigenvalue $\lambda_\perp$ corresponding to the remaining irreducible representations of the global symmetry group. The finite-size scaling of the gap $\xi^{-1}(L,\beta) = \log(\lambda_+/\lambda_\perp)$ and of the gap $\xi_{\text{sym}}^{-1}(L,\beta) = \log(\lambda_+/\lambda_-)$ in the symmetric subspace, and their relation to the surface tension, as well as the finite-size scaling of the internal energy $E_{\text{cyl}}(L,\beta) = -L^{-(d-1)} d \log \lambda_+ / d\beta$ are discussed. As a final application, I discuss the finite-size scaling of the derivative of $\xi(L,\beta)$. I prove that $1/\nu(L) := \log[-Ld\xi(L,\beta)/d\beta]_{\beta=\beta_t(L)} / \log L$ converges to the renormalization group eigenvalue $y_T = d$, if $\beta_t(L)$ is chosen as the point where $\xi_{\text{sym}}^{-1}(L,\beta)$ is minimal. I also propose other definitions of a finite volume exponent $\nu(L)$ which should be more suitable for numerical considerations.

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1. Introduction

In the last years, the Potts model, a spin model with spin variables $\sigma_x \in \mathbf{Z}_q := \{1, e^{2\pi i/q}, \ldots, e^{2\pi i(q-1)/q}\}$ and Hamiltonian

$$H = -\tfrac{1}{2} \sum_{\substack{x,y \\ |x-y|=1}} \delta(\sigma_y, \sigma_y) \ , \tag{1.1}$$

(where δ is the Kronecker delta) has gained more and more popularity. One of the reasons for this popularity is the fact that the Potts model may be understood as a simple model for the confinement/deconfinement transition in QCD, another one is the possibility of tuning the model from a model with a second-order transition via a model with a weak first-order transition to a model with a very strong first-order transition by varying the number of states q. This, together with the fact that many physical quantities like the transition temperature or the latent heat at the transition are exactly known in $d = 2$, makes the model an ideal testing ground for numerical simulations.

Since numerical studies are performed in finite volumes, a detailed analysis of the numerical data requires finite-size scaling (FSS), see e.g. [1] or [2] for recent reviews of FSS theory. For cubic boxes V with periodic boundary conditions, and for values of q for which the transition is first-order, the finite-size scaling of the Potts model can be derived from the ansatz

$$Z_{\text{per}}(V, \beta) \cong e^{-\beta f_d(\beta)|V|} + q e^{-\beta f_o(\beta)|V|} \tag{1.2}$$

for the partition function. Here $|V|$ is the volume of the cubic box V, β is the inverse temperature, and $f_m(\beta)$ $(m = o, d)$ is some sort of meta-stable free energy of the phase m. It is equal to the free energy $f(\beta)$ if m is stable, and strictly larger than $f(\beta)$ if m is unstable. If q is large enough, a formula of the form (1.2) can actually be proven, together with a bound $O(|V| q^{-b \text{diam} V})$ for the error term [3]. Here $\text{diam} V$ 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 d dimensional cylinder with $L \times \cdots \times L \times t$ points, provided

$$|V| e^{-\min(L,t)} \leq 1 \ . \tag{1.3}$$

Even though (1.2) is only proven for large enough q, it is plausible that it holds for any q larger than q_c (where q_c is the value of q where the transition becomes second-order[1]), provided L is large with respect to the correlation length of the infinite system. Numerically this has been tested for various values of q (see e.g. [5-8]).

For long cylinders, however, the effects neglected in the approximation (1.2) 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 have developed a heuristic theory [9] of finite-size scaling in long cylinders. A little bit later, Privman and Fisher developed an alternative theory [10], starting from the observation that the periodic partition function of a spin system may be written as

$$Z_{\text{per}}(V) = \sum_{i=1}^{\infty} \lambda_i(L)^t \tag{1.4}$$

if the model in consideration has a positive transfer matrix. Here $\lambda_1(L) \geq \lambda_2(L) \geq \cdots$ are the eigenvalues of the transfer matrix. They then argue, for models like the low temperature Ising model where two phases related by a symmetry coexist at the transition, that only λ_1 and λ_2 are important for the asymptotic behaviour of $Z_{\text{per}}(V)$, 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

$$\xi_L = D(L) \exp(\beta\sigma L^{d-1})$$

where σ is the surface tension between the two phases and $D(L)$ is a "slowly varying function of L".

In [11], Borgs and Imbrie developed a rigorous theory of first-order FSS in long cylinders, generalizing the results of [10] to a wide class of models with N coexisting phases not necessarily related by a symmetry. Starting from a detailed analysis of the microscopic

[1] For $d = 2$, it is known [4] that $q_c = 4$; for $d \geq 3$ is is believed that $q_c = 2$, see [5] and references therein.

configurations of the system, they constructed an $N \times N$ matrix R which gives the first N eigenvalues of the transfer matrix in the vicinity of the transition point, showing at the same time that the other eigenvalues of the transfer matrix do not contribute to the asymptotic behaviour of $Z_{\text{per}}(V)$. In the Ising case, their results conform with the picture developed in [10]. In addition, Borgs and Imbrie were able to calculate the slowly varying function $D(L)$ for low temperatures, giving $D(L) = O(L^{1/2})$ with a non universal constant in $d = 2$, and $D(L) = \frac{1}{2}(1 + O(e^{-bL}))$ for $d \geq 3$.

Here I apply the methods of [11] to the Potts model. In order to explain the main idea, I assume that the partition function of the Potts model has been rewritten in terms of contours with small activities, so that the configurations of the system are given in terms of ordered and disorderd "ground state region" separated by contours (if q is sufficiently large, such a representation can be obtained from the Fortuin Kasteleyn representation [12] of the Potts model, see e.g. [13,14]). Neglecting for the moment contours which wind around the cylinder in time direction, we 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 don't. Summing the ordinary contours we get an effective weight, $\kappa(Y)$, for the interfaces, a "renormalized" ground state energy, $f_m(L, \beta)$, $m = o, d$ for the regions between interfaces, and an interaction between interfaces.

In a first step, let us neglect the appearance of interfaces. Then $Z_{\text{per}}(V, \beta)$ is just the sum of $q + 1$ terms, a term $\exp(-\beta f_d(L, \beta) L^{d-1} t)$ for the disordered configuration and q times the term $\exp(-\beta f_o(L, \beta) L^{d-1} t)$ for the ordered configurations. Introducing a diagonal matrix F with matrix elements $F_{00} = \exp(-\beta f_d(L, \beta) L^{d-1})$ and $F_{mm} = \exp(-\beta f_o(L, \beta) L^{d-1})$, $m = 1, \cdots, q$, this sum can be rewritten as the trace of the diagonal matrix F^t.

The appearance of interfaces now leads to transitions between ordered and disordered regions. Neglecting the interaction between interfaces, we may take into account the deviations from flat interfaces by using the surface expansions of Dobrushin [15], see Section 5 of [11] for details. As net result, we get an effective system of flat interfaces, with renormalized weight $O(L^{-1/2}) e^{-\beta \sigma_{od} L^{d-1}}$ for $d = 2$ and $(1 + O(e^{-bL})) e^{-\beta \sigma_{od} L^{d-1}}$ for $d > 2$, where σ_{od} is the surface tension between the ordered and the disordered phase. The matrix

F is therefore replaced by a matrix $F + F^{1/2}\Gamma^{(1)}F^{1/2}$, where $\Gamma^{(1)}$ is an off-diagonal matrix with matrix elements $\Gamma^{(1)}_{0m} = \Gamma^{(1)}_{m0} = \Gamma^{(1)}_{od}$, with $\Gamma^{(1)}_{od} = O(L^{-1/2})e^{-\beta\sigma_{od}L^{d-1}}$ for $d = 2$ and $\Gamma^{(1)}_{od} = (1 + O(e^{-bL}))e^{-\beta\sigma_{od}L^{d-1}}$ for $d > 2$. In order to explain the different prefactors of the exponential in $d = 2$ and $d \geq 3$, I recall that the two ends of free interfaces in a two dimensional cylinder of width L are typically at two different heights, with height difference of the order $\sqrt{L}$. Forcing the interface to close, as imposed by the periodic boundary conditions, gives the factor $O(L^{-1/2})$ in $d = 2$. In $d \geq 3$, on the other hand, interfaces are rigid, at least if the surface energy is high enough (small surface energies, like in the Ising model near the transition point, may give rise to roughening), and no power law corrections appear, provided q is sufficiently large[2].

Using the methods of [11], Section 4, we finally take into account the interaction between interfaces. This will replace the matrix $\Gamma^{(1)}$ by a matrix Γ, which describes order-order and disorder-disorder transitions, in addition to the order-disorder transitions already described by $\Gamma^{(1)}$. Putting everything together, one obtains the following Theorem A, where $Z_{\text{per}}(V,\beta)$ is the periodic partition function in the cylinder V, $|V| = L^{d-1}t$, 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, $f = f(\beta)$ is the free energy, and $f_m(\beta)$, $m = o, d$, are "meta-stable" free energies (as constructed, e.g., in [3], where it has been shown that they may be chosen to be smooth functions of β which are at least six times differentiable). I recall 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 $\beta < \beta_t$[3]. Throughout this paper I 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 d.

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[2] It would be in fact interesting to prove that there is a roughening transition for the three dimensional Potts model if q approaches q_c while β is tuned to stay at the transition point $\beta_t = \beta_t(q)$.

[3] In [3] it is actually proven that $\frac{d}{d\beta}(\beta(f_d(\beta) - f_o(\beta))) \geq b_1$ for all $\beta > 0$, with a constant $b_1 > 0$ which does not depend on β.

Theorem A. *Let q and L be sufficiently large and assume that $|\beta-\beta_t|L^{d-1}\le 1$. Then there are real valued function $f_o(L,\beta)$, $f_d(L,\beta)$, $\Gamma_{oo}(L,\beta)$, $\Gamma_{dd}(L,\beta)$ and $\Gamma_{od}(L,\beta)$, forming $(q+1)\times(q+1)$ symmetric matrices F and Γ, where F is the diagonal matrix with matrix elements $F_{00}=\exp(-\beta f_d(L,\beta)L^{d-1})$, $F_{mm}=\exp(-\beta f_o(L,\beta)L^{d-1})$ ($m=1,\cdots,q$) and Γ is the matrix with matrix elements $\Gamma_{00}=\Gamma_{dd}(L,\beta)$, $\Gamma_{0m}=\Gamma_{m0}=\Gamma_{od}(L,\beta)$ and $\Gamma_{mn}=\Gamma_{oo}(L,\beta)$, ($m,n=1,\cdots,q$), such that the following statements hold provided $k\le 6$.*

(i) *Let $t\ge(d-1)\log L$. Then*

$$\left|\frac{d^k}{d\beta^k}\left[Z_{\rm per}(V,\beta)-tr\,(F+F^{1/2}\Gamma F^{1/2})^t\right]\right|\le e^{-\beta f|V|}q^{-bt}\,. \tag{1.5}$$

(ii) *Let $\tau=\frac{1}{2d}\log q$. Then*

$$\left|\frac{d^k}{d\beta^k}\Gamma_{oo}(L,\beta)\right|\le e^{-(2\tau-O(1))L^{d-1}}\,, \tag{1.6a}$$

$$\left|\frac{d^k}{d\beta^k}\Gamma_{dd}(L,\beta)\right|\le qe^{-(2\tau-O(1))L^{d-1}}\,, \tag{1.6b}$$

$$\left|\frac{d^k}{d\beta^k}\Gamma_{od}(L,\beta)\right|\le e^{-(\tau-O(1))L^{d-1}}\,. \tag{1.6c}$$

(iii)
$$\left|\frac{d^k}{d\beta^k}\left(\beta f_i(L,\beta)-\beta f_i(\beta)\right)\right|\le q^{-bL} \tag{1.7}$$

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

$$\Gamma_{od}(L,\beta)=\begin{cases} C_{od}\,L^{-1/2}e^{-\beta\sigma_{od}L}(1+O(L^{-1}))\,, & d=2\,,\\ e^{-\beta\sigma_{od}L^{d-1}}(1+O(q^{-bL}))\,, & d\ge 3\,,\end{cases} \tag{1.8}$$

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

Remarks: i) In the Fortuin-Kasteleyn representation for the Potts model, disorder-disorder and order-order interfaces are always made out of two or more interacting order-disorder interfaces. As a consequence, 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 (1.6b) 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) In the Fortuin-Kasteleyn representation for the Potts model, the constant $\tau = \frac{1}{2d}\log q$ is the leading term for the order-disorder surface tension σ_{od}. Since $\sigma_{od} = \tau + O(q^{-b})$, see [13,14], the bounds (1.6) remain valid if τ is replaced by σ_{od}.

Due to Theorem A, the first $q+1$ eigenvalues of the transfer matrix are just the eigenvalues of the matrix $(F + F^{1/2}\Gamma F^{1/2})$. They are easily calculated, see Section 3. One finds two simple eigenvalues $\lambda_\pm$ corresponding to the trivial representation of the global symmetry and one $q-1$ fold degenerate eigenvalue $\lambda_\perp$ corresponding to the remaining irreducible representations of the global symmetry group. Neglecting the higher order corrections coming from Γ_{oo} and Γ_{dd}, the result of this calculation reads

$$\lambda_\pm \cong e^{-\beta\frac{f_o(L,\beta)+f_d(L,\beta)}{2}L^{d-1}}\left(\cosh x_L(\beta) \pm \sqrt{\sinh^2 x_L(\beta) + q\Gamma_{od}^2}\right) \tag{1.9}$$

and

$$\lambda_\perp \cong e^{-\beta f_o(L,\beta)L^{d-1}} = e^{-\beta\frac{f_o(L,\beta)+f_d(L,\beta)}{2}L^{d-1}}e^{x_L(\beta)}\ , \tag{1.10}$$

where

$$x_L(\beta) = \tfrac{1}{2}(\beta f_d(L,\beta) - \beta f_o(L,\beta))L^{d-1}\ . \tag{1.11}$$

In order to compare these eigenvalues to the eigenvalues $\exp(-\beta f_d(L,\beta)L^{d-1})$ and $\exp(-\beta f_o(L,\beta)L^{d-1})$ of the "unperturbed" matrix F, see Fig. 1, I define $\beta_0(L)$ as the inverse temperature where $f_d(L,\beta)$ and $f_o(L,\beta)$ are equal, approximate $\lambda_\pm$ by

$$e^{-\beta\frac{f_o(L,\beta)+f_d(L,\beta)}{2}L^{d-1}}\exp\left(\pm\sqrt{x_L(\beta)^2 + q\Gamma_{od}^2}\right)$$

and expand $x_L(\beta)$ about the point $\beta_0(L)$. Approximating $x_L(\beta)$ by its leading term in $(\beta - \beta_0(L))$ and ignoring the L dependence of the corresponding taylor coefficient, one finds that

$$x_L(\beta) \cong \frac{E_d - E_o}{2}(\beta - \beta_0(L))L^{d-1}\ ,$$

where $E_o = [d(\beta f_o(\beta))/d\beta]_{\beta=\beta_t}$ and $E_d = [d(\beta f_d(\beta))/d\beta]_{\beta=\beta_t}$ are the infinite volume internal energies at the transition point β_t. Neglecting finally the β dependence of Γ_{od}, one gets

$$\lambda_\pm \cong e^{-\beta \frac{f_o(L,\beta)+f_d(L,\beta)}{2} L^{d-1}} e^{\pm \xi_L^{-1} \sqrt{1+y^2}} \tag{1.12}$$

and

$$\lambda_\perp \cong e^{-\beta \frac{f_o(L,\beta)+f_d(L,\beta)}{2} L^{d-1}} e^{\xi_L^{-1} y} \ , \tag{1.13}$$

where y is the scaling variable

$$y = \xi_L(\beta - \beta_0(L)) L^{d-1} \frac{E_d - E_o}{2} \tag{1.14}$$

and ξ_L^{-1} is the constant

$$\xi_L^{-1} = \sqrt{q}\,\Gamma_{od}(\beta_0(L)) = \sqrt{q}\, e^{-\beta\sigma_{od} L^{d-1}} \begin{cases} C_{od}\ L^{-1/2}(1 + O(L^{-1}))\ , & d = 2\ , \\ (1 + O(q^{-bL}))\ , & d \geq 3\ , \end{cases} \tag{1.15}$$

Note that the gaps $\xi_{\rm sym}^{-1}(L,\beta) = \log(\lambda_+/\lambda_-)$ and $\xi^{-1}(L,\beta) = \log(\lambda_+/\lambda_\perp)$ following from (1.12) and (1.13) are just

$$\xi_{\rm sym}^{-1}(L,\beta) \cong 2\xi_L^{-1}\sqrt{1+y^2} \tag{1.16}$$

and

$$\xi^{-1}(L,\beta) \cong \xi_L^{-1}(\sqrt{1+y^2} - y)\ . \tag{1.17}$$

In Fig.1 I have drawn the eigenvalues $\lambda_\pm$ and $\lambda_\perp$ and the eigenvalues $\exp(-\beta f_d(L,\beta)L^{d-1})$ and $\exp(-\beta f_o(L,\beta)L^{d-1})$ of the "unperturbed" matrix F in the vicinity of the "crossing point" $\beta_0(L)$ where $f_o(L,\beta) = f_d(L,\beta)$. While λ_+ and λ_- show a typical "avoiding crossing behaviour" in the region where $(\beta - \beta_0(L))L^{d-1} = O(\xi_L^{-1}) = O(\sqrt{q}\,\Gamma_{od})$,

$$\log \lambda_\pm \sim \left(\frac{f_d(L,\beta) + f_o(L,\beta)}{2} L^{d-1} \right) \pm \sqrt{q\Gamma_{od}^2 + \left(\frac{f_d(L,\beta) - f_o(L,\beta)}{2} L^{d-1} \right)^2}\ ,$$

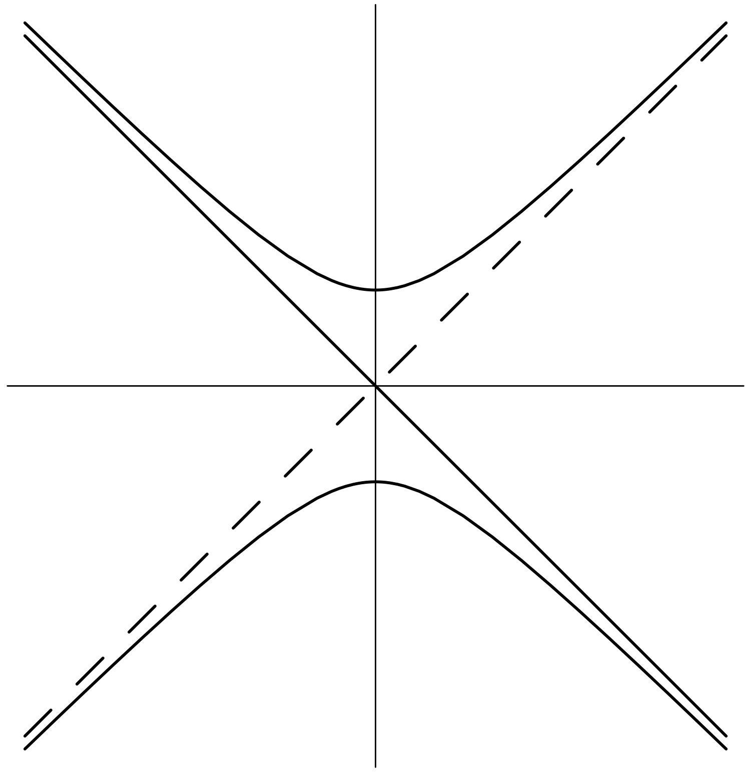

Fig. 1. *The avoiding crossing region for the first three eigenvalues of* $-\log \mathcal{T}$. *The eigenvalue* $\lambda_\perp$ *is* $q-1$ *fold degenerate. To make the figure better readable, I have subtracted a term* $\frac{\beta f_o + \beta f_d}{2} L^{d-1}$ *from all curves.*

the eigenvalue $\lambda_\perp$ is essentially unperturbed and stays very near to $\exp(-\beta f_o(L,\beta)L^{d-1})$ in the whole region $|\beta - \beta_t|L^{d-1} \leq 1$ (in the approximation where the two surface terms Γ_{oo} and Γ_{dd} are neglected, $\lambda_\perp$ is in fact equal to $\exp(-\beta f_o(L,\beta)L^{d-1})$). Outside of the above transition region, the eigenvalues λ_+ and $\lambda_\perp$ are almost degenerate if $\beta > \beta_0(L)$, while λ_- and $\lambda_\perp$ are almost degenerate[4] if $\beta < \beta_0(L)$. In the infinite volume limit, these degeneracies and the $(q-1)$ fold degeneracy of $\lambda_\perp$ combine to give the q fold degeneracy of $f_o(\beta)$. Note that the shift $O(q^{-bL})$ between $\beta_0(L)$ and β_t which is allowed[5] by Theorem

[4] Note that the gap between $\lambda_\perp$ and λ_- may grow again if β leaves the range $|\beta - \beta_t|L^{d-1} \leq 1$ allowed by Theorem A.

[5] It seems natural to conjecture that the actual shift is $O(e^{-L/\xi_o}) - O(e^{-L/\xi_d})$, where ξ_o and ξ_d are of the order of the infinite volume correlation length in the ordered and disordered phase, respectively.

A is much larger than the width of the transition region if $d > 2$. As a last observation, I point out that the gap in the symmetric sector, $\xi_{\rm sym}^{-1}(L,\beta) = \log(\lambda_+/\lambda_-)$, is just two times the gap $\xi^{-1}(L,\beta) = \log(\lambda_+/\lambda_\perp)$ (plus very tiny corrections, see Section 4 for the precise bounds) if $\beta = \beta_0(L)$.

Next, I discuss the FSS of the internal energy

$$E_{\rm cyl}(L,\beta) := -\frac{1}{L^{d-1}}\frac{d}{d\beta}\log\lambda_+ \tag{1.18}$$

in the cylinder $V_\infty = A \times \mathbf{Z}$, where I used A to denote the $d-1$ dimensional periodic cube of side length L. I recall that the infinite volume internal energy $E(\beta) = \lim_{L\to\infty} E_{\rm cyl}(L,\beta)$ jumps from $E_d := E(\beta_t - 0)$ to $E_o := E(\beta_t + 0)$ as β passes through β_t, while the internal energy following from (1.12) is just

$$E_{\rm cyl}(L,\beta) \cong \frac{E_d + E_o}{2} + \frac{E_o - E_d}{2}\frac{y}{\sqrt{1+y^2}}\ , \tag{1.19}$$

where y is the scaling variable introduced in (1.14). Again one finds a transition region of width $O(L^{-(d-1)}\Gamma_{od})$ which is centered at $\beta_0(L)$, this time corresponding to the crossover from $E_{\rm cyl}(L,\beta) \cong E_d$ to $E_{\rm cyl}(L,\beta) \cong E_o$.

Note that the behaviour sketched in (1.16), (1.17) and (1.19) can be made rigorous, provided q and L are sufficiently large, see Section 4 for details. For the convenience of the reader, I summarize the main results in the following theorem.

Theorem B. *Let q and L be sufficiently large and assume that $|\beta - \beta_t| L^{d-1} \le 1$. Let $\beta_t(L)$ be the point where the gap in the symmetric sector, $\xi_{\rm sym}^{-1}(L,\beta)$ is minimal, and let ξ_L be the correlation length at the point $\beta_t(L)$,*

$$\xi_L := \xi(L, \beta_t(L))$$

Then

$$\xi_L^{-1} = \sqrt{q}\, e^{-\beta\sigma_{od}L^{d-1}} \begin{cases} C_{od}\, L^{-1/2}(1 + O(L^{-1}))\ , & d = 2\ , \\ (1 + O(q^{-bL}))\ , & d \ge 3\ , \end{cases} \tag{1.15$'$}$$

$$\xi_{\rm sym}^{-1}(L,\beta) = 2\xi_L^{-1}\sqrt{1+y^2} + O(\xi_L^{-(2-\epsilon)}) \;, \tag{1.16'}$$

$$\xi^{-1}(L,\beta) = \xi_L^{-1}(\sqrt{1+y^2}-y) + O(\xi_L^{-(2-\epsilon)}) \tag{1.17'}$$

and

$$E_{\rm cyl}(L,\beta) = \left\{ \frac{E_d+E_o}{2} + \frac{E_o-E_d}{2}\,\frac{y}{\sqrt{1+y^2}} \right\} (1+O(\beta-\beta_t(L)) + O(q^{-bL})) \;, \tag{1.19'}$$

where

$$y = \xi_L(\beta-\beta_t(L))L^{d-1}\frac{E_d-E_o}{2}(1+O(\beta-\beta_t(L)) + O(q^{-bL})) \tag{1.14'}$$

and $\epsilon = \epsilon(q)$ is a small positive number which goes to zero as $q \to \infty$.

At this point I want to stress that Theorem A and B are only proven if L and q are sufficiently large. Unfortunately, the actual values of q which are needed to make these theorems rigorous are much too large for physical applications[6]. It is therefore important to discuss the validity of Theorem A and B on a more heuristic level. Going back to the derivation of Theorem A as sketched above, we consider several steps:

(i) The resummation of ordinary contours into renormalized "ground state energies": In a region where $|\beta-\beta_t|L^{d-1}$ is small[7], this should always be possible and lead to renormalized "ground state energies" $f_m(L,\beta)$ with $|f_m(L,\beta)-f_m(\beta)| \leq O(e^{-L/\xi_m})$, as long as $L \geq \xi_m$, the infinite volume correlation length of the phase m.

(ii) If one neglects the interaction between interfaces, the resummed weight of all interfaces which correspond to the same flat interface can be considered as the partition function

[6] For $d=2$, where the physically interesting values of q are $q \leq 10$, the methods of [13,14] on which my proof of Theorem A and B is based require $q \gtrsim 250$. Other methods (like [16] for which $q \geq 54$ is enough) might give better bounds, but $q=10$ or smaller is definitely to small for a mathematically rigorous treatment along the lines presented here.

[7] The importance of such a condition is discussed in the paragraph following equation (2.8a) in Sections 2.

of a suitable spin system in $d-1$ dimensions. It seems therefore reasonable to assume that this weight is of the form

$$D(L)e^{-\beta\sigma L^{d-1}} ,$$

where $L^{-(d-1)}\log D(L)$ goes to zero as $L\to\infty$. It is less clear, however, that $D(L)$ is of the form $(1+O(e^{-bL}))$ in $d>2$ if q is small. In fact, for $d=3$, roughening would suggest a different behaviour (a q-dependent constant, for example, or a logarithmic dependence on L with q-dependent prefactor) if q approaches q_c.

(iii) The fact that an order-order interface is always made out of two interacting order-disorder interfaces and the related fact that $\sigma_{oo}=2\sigma_{od}$ is only proven for large q. The question whether this "complete wetting" phenomenon occurs for all values of $q>q_c(d)$ is an interesting open question and a challenging problem for numerical simulations (see, e.g., [17], where complete wetting has numerically been established for the three states Potts model in $d=3$.).

(iv) It seems reasonable to neglect the interaction between interfaces if L is sufficiently large, because the average distance between interfaces is expected to be $O(\xi_L)$, which is much larger than the average height fluctuations within the interfaces, even if the interfaces are rough.

I therefore feel that the theory presented here remains valid for small values of q as well, as long as

$$L \gtrsim L_0 := \max\{\xi_o,\xi_d\} \qquad \text{and} \qquad L^{d-1}\sigma_{mn}\gtrsim 1 \ . \tag{1.20}$$

One should allow, however, for a slightly more general behaviour of the matrix elements Γ_{mn}:

$$\Gamma_{mn}=D_{mn}(L)e^{-\beta\sigma_{mn}L^{d-1}} ,$$

where $D_{mn}(L)$ is a slowly varying function of L, and where σ_{oo} may be different from $2\sigma_{od}$. But as long as σ_{oo} and σ_{dd} are strictly larger than σ_{od} (which is obviously a much weaker assumptions than complete wetting), the dominant contributions to $\lambda_\pm$ and $\lambda_\perp$

still come from Γ_{od}. It therefore seems reasonable to conjecture that Theorem B (with e^{-bL} replaced by $O(e^{-L/L_0})$ and $O(\xi_L^{-(2-\epsilon)})$ replaced by $O(\min\{\Gamma_{oo}, \Gamma_{dd}\}))$ remains valid for small values of q as well if one allows for a slightly more general behaviour of ξ_L^{-1} by inserting a slowly varying function[8] $D(L)$ for $d > 2$.

Outline:

In the next section, I will prove Theorem A and its generalization to values of β which don't fulfil the constraint $|\beta - \beta_t| L^{d-1} \leq 1$, using the results of [11]. In Section 3 I calculate the eigenvalues of the matrix Γ of Theorem A and discuss their correspondence to the irreducible representations of the global symmetry group. The FSS of $\lambda_\pm$, $\lambda_\perp$ and the internal energy $E_{\rm cyl}$ is discussed in Section 4. Section 5 is devoted to the discussion of the gaps $\xi_{\rm sym}^{-1}(L, \beta) = \log(\lambda_+/\lambda_-)$ and $\xi(L, \beta) = 1/\log(\lambda_+/\lambda_\perp)$ and their derivatives, and contains the statement concerning $\nu(L)$ mentioned in the introduction. The appendix contains some material about duality in finite volumes.

While Section 2 and 4 contain the more technical details of this paper, Section 3 and 5 (and this introduction) are probably most interesting for the reader interested in the applications of the ideas presented here.

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[8] It is an interesting problem to determine the small q behaviour of $D(L)$ for $d > 3$. A continuum description of interfaces [18-20] would lead to a powerlaw dependence on L, while the observation that there is no roughening in $d > 3$ suggests a large L behaviour $D(L) = (1 + O(e^{-bL}))$ for all $q > q_c(d)$. Note that there might be a crossover from a small L continuum behavior to an asymptotic large L lattice behaviour.

2. Contours and Interfaces.

In this section I combine the methods of [3] and [11] to prove Theorem A and its generalization to values of β which don't fulfil the constraint $|\beta - \beta_t| L^{d-1} \leq 1$. I start with a review of the main steps which lead from the Fortuin-Kastelyn representation of the Potts model [12] to a contour representation of the Potts model, see [13,14] and [3] for the original treatment. In order to fix the notation used in this section, I define: $\bar{A}$ and $\bar{T}$ are used to denote the continuum torus $(\mathbf{R}/L\mathbf{Z})^{d-1}$ and $(\mathbf{R}/t\mathbf{Z})$, respectively, $\bar{V}$ is the continuum torus $\bar{V} = \bar{A} \times \bar{T}$, A and V are the corresponding lattice analogs $(\mathbf{Z}/L\mathbf{Z})^{d-1}$ and $(\mathbf{Z}/L\mathbf{Z})^{d-1} \times (\mathbf{R}/t\mathbf{Z})$, respectively, and $V_\infty = A \times \mathbf{Z}$ is the infinite cylinder.

Using the symbol V_1 to denote the set of all dtL^{d-1} nearest neighbor bonds in V, the partition function $Z_{\mathrm{per}}(V, \beta)$ of the Potts model is defined as

$$Z_{\mathrm{per}}(V, \beta) = \sum_{\sigma_V} \prod_{\langle xy \rangle \in V_1} e^{\beta \delta(\sigma_x, \sigma_y)} , \tag{2.1}$$

where the sum runs over all possible configurations $\sigma_V \ : \ V \ni x \mapsto \sigma_x \in \mathbf{Z}_q$. The Fortuin-Kasteleyn representation of the Potts model [12] is obtained by expanding $e^{\beta\delta}$ in (2.1) as $1 + (e^\beta - 1)\delta$:

$$Z_{\mathrm{per}}(V, \beta) = \sum_{\sigma_V} \sum_{X \subset V_1} \prod_{\langle xy \rangle \in X} (e^\beta - 1) \delta(\sigma_x, \sigma_y) . \tag{2.2}$$

Interchanging the two sums, the sum over σ_V can be performed exactly, giving a factor q for each connected component of X and for each point $x \in V/S(X)$ (we use the symbol $S(X)$ to denote the set of points $x \in V$ which belong to a bond in X). The partition function $Z_{\mathrm{per}}(V, \beta)$ can therefore be rewritten as

$$Z_{\mathrm{per}}(V, \beta) = \sum_{X \subset V_1} (e^\beta - 1)^{|X|} q^{C(X)} q^{|V \setminus S(X)|} , \tag{2.3}$$

where the summation runs over all sets of bonds $X \subset V_1$, $|X|$ and $C(X)$ are used to denote the number of bonds and connected components of X, respectively, and $|V/S(X)|$ is used to denote the number of points in $V/S(X)$.

Introducing the set of bonds δX which belong to $V_1 \backslash X$ and are connected to X, we note that

$$|S(X)| - \frac{1}{d}|X| = \frac{1}{2d}\|\delta X\| := \frac{1}{2d}\sum_{b\in\delta X} |S(b) \cap S(X)| \,. \tag{2.4}$$

which follows from the fact that $2d$ bonds meet at every site of the lattice As a consequence, the partition function $Z_{\rm per}(V, \beta)$ becomes

$$Z_{\rm per}(V, \beta) = \sum_{X\subset V_1} (e^\beta - 1)^{|X|} q^{\frac{1}{d}|V_1\backslash X|} q^{C(X)} q^{-\frac{1}{2d}\|\delta X\|} \,. \tag{2.5}$$

The formula (2.5) already expresses the fact that (for $(e^\beta - 1) \approx q^{1/d}$) the partition function $Z_{\rm per}(V, \beta)$ describes the coexistence of an ordered phase (small empty islands in a sea of bonds X) and a disordered phase (small oases of X in an empty desert), with excitations suppressed as $q^{-\ell/(2d)}$ where ℓ is the length of their boundary.

In order to define the contours corresponding to a given configuration X, we now introduce the set ∂X of $d - 1$ dimensional faces dual to the bonds in δX. Counting each face dual to a bond in $\delta_2 X := \{b \in \delta X \ : \ |S(b)| = 2\}$ twice, we then decompose ∂X into connected components, say, $Y_1, \ldots, Y_n$, which are called the contours corresponding to the configuration $X \subset V_1$. The contours $Y_1, \ldots, Y_n$ then separate ordered regions (those containing the bonds in X) from disordered regions (those containing the bonds in $V_1 \setminus (X \cup \delta X)$).

To make the above decomposition of ∂X into contours precise, we proceed as follows: Considering the bonds, plaquettes, ... in V as subsets of the continuum torus $\bar{V}$, we define $P(X)$ as the union of all bonds in X and all plaquettes in V which contain 4 bonds of X if $d = 2$. For $d = 3$ the set $P(X)$ contains in addition the cubes whose all 12 bonds are in X, etc. We then consider the neighborhood of $P(X)$ which contains all points of distance less than $1/2 - \epsilon$ from $P(X)$. The boundary of this set (which is non empty except for $X = V_1$ or $X = \emptyset$) splits into connected components (with respect to the usual topology of $\bar{V}$), say, $Y_1, \ldots, Y_n$, which we call the contours corresponding to the configuration $X \subset V_1$. Sending $\epsilon \to 0$, we obtain the desired decomposition of ∂X into contours. Note that two contours can touch on their disordered sides (if this happens, the corresponding bond was a bond in $\delta_2 X$), but not on their ordered side. In a similar way, two plaquettes of a given contour may touch on their disordered sides.

Using the relation (2.4) and the fact that $\|\delta X\| = \sum_{k=1}^n |Y_k|$, where $|Y|$ denotes the number of $d-1$ dimensional faces in Y, we then rewrite

$$Z_{\rm per}(V,\beta) = \sum_{X\subset V_1} (e^\beta - 1)^{|X|} q^{\frac{1}{d}|V_1\setminus X|} q^{C(X)} \prod_Y q^{-|Y|/(2d)} \tag{2.6}$$

This is the desired contour representation of $Z_{\rm per}$. Note the factor $q^{C(X)}$ which accounts for the fact that each ordered region corresponds to the q possibilities $\sigma = 1, \ldots, q$.

Turning to long cylinders, we now define: a contour $Y \subset \bar V = \bar A \times \bar T$ is called *short* iff it is possible to find a closed interval $I \subset \bar T$, $\bar T \setminus I \neq \emptyset$, such that Y lies in $\bar A \times I$. Otherwise Y is called *long*. A short contour can be imbedded in the infinite cylinder $\bar V_\infty = \bar A \times \mathbf{R}$. We therefore may consider the set $\bar V_\infty \setminus Y$ for a given short contour Y. If it contains two infinite components separated by Y, we call Y an *interface* or also a *kink*, otherwise we call Y an *ordinary contour*.

Following [3] we assign an activity $z(Y) = q^{-|Y|/(2d)}$ to each ordinary contour describing a transition from an ordered exterior to a disordered interior, and an activity $z(Y) = q\, q^{-|Y|/(2d)}$ to each ordinary contour describing a transition from a disordered exterior to an ordered interior (the additional factor of q corresponds to the fact that an insertion of such a contour into a disordered region increases $C(X)$ by one). Since the length of the smallest ordinary contour with an ordered interior that may be imbedded into $\mathbf{R}^d$ is $4d-2$,

$$|z(Y)| \leq e^{-\tau_1 |Y|} \qquad \text{with} \qquad \tau_1 := \left(\frac{1}{2d} - \frac{1}{4d-2}\right) \log q\,, \tag{2.7}$$

for all ordinary contours that may be imbedded into $\mathbf{R}^d$. If L is large enough, this bound remains valid for topologically non-trivial ordinary contours as well (obviously, $L \geq 4d-2$ is large enough).

Let us now consider the partition function $\widetilde Z_{\rm res}(V,\beta)$ which is obtained from $Z_{\rm per}(V,\beta)$ by leaving out all configurations which contain interfaces or long contours. Defining the exterior of a configuration as the intersection of the exteriors of its ordinary contours, each configuration X has either an ordered exterior (in this case X is called a perturbation of the completely ordered configuration $X_{ord} = V_1$) or an disordered exterior (in this case X is called a perturbation of the completely disordered configuration $X_{dis} = \emptyset$); collecting the first type of configurations into a partition function $Z_o(V, \beta)$ and the second type into a partition function $Z_d(V, \beta)$, we obtain that $\widetilde{Z}_{\rm res}(V, \beta) = Z_o(V, \beta) + Z_d(V, \beta)$. Assume now that a condition of the form

$$a_o\, L^{d-1} \equiv \beta[f_o(\beta) - f(\beta)]L^{d-1} \leq \tfrac{7}{8}\tau_1 \tag{2.8a}$$

is fulfilled. The gain in energy resulting from the insertion of an ordinary contour with interior $\operatorname{Int} Y$ into the ordered phase can then be bounded by $a_o|\operatorname{Int} Y| \leq a_o L^{d-1}|Y| \leq (7\tau_1/8)|Y|$, leaving an effective decay $\exp(-(\tau_1 - a_o L^{d-1})|Y|) \leq \exp(-(3\tau_1/16)|Y|)$. As a consequence, $Z_o(V, \beta)$ can be analysed by a convergent expansion if L and q are large enough and (2.8a) is fulfilled, see section 3 of [11] for details. One obtains that

$$\log Z_o(V, \beta) = \log q - \beta f_o(\beta, L)|V| + O(|V| e^{-(\tau_1 - O(1) - a_o L^{d-1})t}) \tag{2.9a}$$

where $f_o(\beta, L)$ is a real analytic function of β in the region (2.8a) which obeys a bound

$$\beta|f_o(L, \beta) - f_o(\beta)| \leq e^{-(\tau_1 - O(1) - a_o L^{d-1})L}\ . \tag{2.10a}$$

In a similar way, the condition

$$a_d\, L^{d-1} \equiv \beta[f_d(\beta) - f(\beta)]L^{d-1} \leq \tfrac{7}{8}\tau_1\ , \tag{2.8b}$$

implies that

$$\log Z_d(V, \beta) = -\beta f_d(\beta, L)|V| + O(|V| e^{-(\tau_1 - O(1) - a_d L^{d-1})t}) \tag{2.9b}$$

where $f_d(\beta, L)$ is a real analytic function of β in the region (2.8b) which obeys a bound

$$\beta|f_d(L, \beta) - f_d(\beta)| \leq e^{-(\tau_1 - O(1) - a_d L^{d-1})L}\ . \tag{2.10b}$$

Turning to the actual finite-size scaling in long cylinders, we now consider the partition function $Z_{\text{res}}(V,\beta)$ which contains only interfaces and ordinary contours and resum the ordinary contours. Assume that a condition

$$a\,L^{d-1} \equiv \min\{a_o, a_d\} = \beta|f_o(\beta) - f_d(\beta)|L^{d-1} \leq \tfrac{7}{8}\tau_1 \tag{2.11}$$

is fulfilled. As explained above, the resummation of the ordinary contours can then be controlled by a convergent expansion provided L and q are large enough. As net result one obtains new volume factors $e^{-\beta f_o(L,\beta)|X|/d}$ and $e^{-\beta f_d(L,\beta)|V_1\setminus X|/d}$ for the regions between interfaces, an effective weight $q^{-|Y|/(2d)}e^{g(Y)}$ for the interfaces and an interaction term $e^{g(Y,Y')}$ for neighboring interfaces, see [11], Section 3. If we order the interfaces $Y_1,\cdots,Y_n$ of a configuration X chronologically, this leads to the representation

$$\begin{aligned} Z_{\text{res}}(V,\beta) = &\sum_X e^{-\beta f_o(L,\beta)|X|/d} e^{-\beta f_d(L,\beta)|V_1\setminus X|/d} \times \\ &\times q^{C(X)} \prod_i q^{-|Y_i|/(2d)} e^{g(Y_i)} e^{g(Y_i,Y_{i+1})} \;, \end{aligned}$$

where the sum runs over configurations $X \subset V_1$ for which ∂X contains only interfaces, and $g(Y)$ and $g(Y,Y')$ are functions of β which may be expressed as a convergent sum over ordinary contours. They are analytic in the region (2.11) and and can be bounded by $|Y|O(1)$ and $\min\{|Y|,|Y'|\}O(1)$, respectively. As for $f_i(L,\beta)$, the bound on $g(Y,Y')$ can be sharpened, leading to

$$|g(Y,Y')| \leq \min\{|Y|,|Y'|\} e^{-(\tau_1 - O(1) - a_i L^{d-1})\text{dist}(Y,Y')} \;, \tag{2.12}$$

where $a_i = a_o$ if the region between Y and Y' is ordered and $a_i = a_d$ if it is disordered (see Section 3 of [11]).

Expressing the quantity $|X|$ in the volume factor in terms of $|S(X)|$ and $\|\delta X\|$ and defining

$$\kappa(Y) = e^{-\frac{\beta}{2}(f_d(L,\beta) - f_o(L,\beta))|Y|} e^{g(Y)} q^{-|Y|/(2d)} \;, \tag{2.13}$$

we finally get

$$\begin{aligned} Z_{\rm res}(V,\beta) =& e^{-\beta f_d(L,\beta)|V|} + q\, e^{-\beta f_o(L,\beta)|V|} + \\ &+ \sum_{n=2}^{\infty} \frac{1}{n} \sum_{Y_1,\cdots,Y_n} \prod_i n_i\, \kappa(Y_i)\, e^{g(Y_i,Y_{i+1})} e^{-\beta f_i(L,\beta)|V_i|} \ , \end{aligned} \tag{2.14}$$

where the second sum goes over interfaces $Y_1, \ldots, Y_n$ that are chronologically ordered, V_i is the volume bounded by Y_i and Y_{i+1}, $f_i = f_o$ and $n_i = q$ if V_i is an ordered region, while $f_i = f_d$ and $n_i = 1$ if V_i is a disordered region. Of course, Y_{i+1} must be an interface describing a transition from a disordered state to an ordered state if Y_i describes a transition from an ordered state to a disordered state and vice versa. 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 the sum (2.6).

We finally state two bounds which - together with the bounds (2.10), (2.12), and similar bounds on derivatives - are needed to apply the methods of [11], Section 4 and 5: Assuming that $|\beta - \beta_t| \leq O(1)$ and $t \geq (d-1)\log L$, we have that

$$|\kappa(Y)| \leq e^{-(\tau - O(1))|Y|} \ , \qquad \text{with} \qquad \tau = \frac{1}{2d} \log q \ , \tag{2.15}$$

and

$$|Z_{\rm per}(V,\beta) - Z_{\rm res}(V,\beta)| \leq e^{-\beta f(\beta)|V|} e^{-(\tau_1 - O(1))t} \ . \tag{2.16}$$

While the first bound follows from the fact that we only consider values of β for which $|\beta - \beta_t| \leq O(1)$ (which implies that $\beta|f_d(L,\beta) - f_o(L,\beta)| \leq O(1)$) and the bound $g(Y) \leq O(1)|Y|$, (2.16) is a consequence of the fact that each configuration contributing to $Z_{\rm per}(V,\beta) - Z_{\rm res}(V,\beta)$ contains at least one long contour Y_i. Given the representation (2.14), the bounds (2.10), (2.12), (2.15), (2.16) and the corresponding generalizations to derivatives, we may now apply the methods of Section 4 and 5 of [11]. As a result we obtain the following sharper version of Theorem A, together with several bounds which are needed to prove FSS formula for the internal energy and other quantities of interest.

For the convenience of the reader we state these results in a separate theorem, Theorem 2.2 (below).

Theorem 2.1. *Let q and L be sufficiently large and assume that $aL^{d-1} := \beta|f_o(\beta) - f_d(\beta)|L^{d-1} \leq \frac{7}{8}\tau_1$, where $\tau_1 = (\frac{1}{2d} - \frac{1}{4d-2})\log q$. Then there are real valued function $f_o(L,\beta)$, $f_d(L,\beta)$, $\Gamma_{oo}(L,\beta)$, $\Gamma_{dd}(L,\beta)$ and $\Gamma_{od}(L,\beta)$, forming $(q+1)\times(q+1)$ symmetric matrix F and Γ, where F is the diagonal matrix with matrix elements $F_{00} = \exp(-\beta f_d(L,\beta)L^{d-1})$, $F_{mm} = \exp(-\beta f_o(L,\beta)L^{d-1})$ $(m = 1,\cdots,q)$ and Γ is the matrix with matrix elements $\Gamma_{00} = \Gamma_{dd}(L,\beta)$, $\Gamma_{0m} = \Gamma_{m0} = \Gamma_{od}(L,\beta)$ and $\Gamma_{mn} = \Gamma_{oo}(L,\beta)$, $(m,n = 1,\cdots,q)$, such that the following statements hold provided $k \leq 6$.*

(i) *Assume that $t \geq (d-1)\log L$. Then*

$$\left|\frac{d^k}{d\beta^k}\left[Z_{\rm per}(V,\beta) - tr\,(F + F^{1/2}\Gamma F^{1/2})^t\right]\right| \leq e^{-\beta f|V|}e^{-(\tau_1 - O(1))t}\ . \tag{2.18}$$

(ii) *Let $\tau = \frac{1}{2d}\log q$. Then*

$$\left|\frac{d^k}{d\beta^k}\Gamma_{oo}(L,\beta)\right| \leq e^{-(2\tau - O(1))L^{d-1}}\ , \tag{2.19a}$$

$$\left|\frac{d^k}{d\beta^k}\Gamma_{dd}(L,\beta)\right| \leq qe^{-(2\tau - O(1))L^{d-1}}\ , \tag{2.19b}$$

$$\left|\frac{d^k}{d\beta^k}\Gamma_{od}(L,\beta)\right| \leq e^{-(\tau - O(1))L^{d-1}}\ . \tag{2.19c}$$

(iii) *Let $a_i := f_i(\beta) - f(\beta)$. Then*

$$\left|\frac{d^k}{d\beta^k}\left(\beta f_i(L,\beta) - \beta f_i(\beta)\right)\right| \leq e^{-(\tau_1 - a_i L^{d-1} - O(1))L}\ . \tag{2.20}$$

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

$$\Gamma_{od}(L,\beta)) = \begin{cases} C_{od}\ L^{-1/2}e^{-\beta\sigma_{od}L}(1 + O(L^{-1}))\ , & d = 2\ , \\ e^{-\beta\sigma_{od}L^{d-1}}(1 + O(e^{-b\tau_1 L}))\ , & d \geq 3\ , \end{cases} \tag{2.21}$$

provided $|\beta - \beta_t| \le e^{-\tau_1 L/2}$.

Theorem 2.2. *Let q and L be sufficiently large and assume that $aL^{d-1} := \beta|f_o(\beta) - f_d(\beta)|L^{d-1} \le \frac{7}{8}\tau_1$. Then*

$$\left|\frac{d^k\Gamma_{od}(L,\beta)}{d\beta^k}\right| \le O(L^{k(d-1)})\Gamma_{od}(L,\beta)\ . \tag{2.22}$$

provided $k \le 6$.

Remarks: (i) In order to see that the matrix $(\Gamma_{mn})_{m,n=1,\dots,q}$ of Theorem 2.1 has constant entries $\Gamma_{mn} = \Gamma_{oo}$, we note that the inductive expansions of Section 4 of [11] start from a representation of $Z_{\text{res}}(V,\beta)$ which may be rewritten as a sum of terms of the form

$$\sum_{m_1=0}^{q}\cdots\sum_{m_n=0}^{q}\prod_{i=1}^{n} e^{-\beta f_{m_i}|K_i|L^{d-1}} r_{m_i m_{i+1}}(I_i)$$

where $I_1,\dots,I_n$ and $K_1,\dots,K_n$ are intervals which form a partition of T into disjoint intervals, $f_m = f_o(L,\beta)$ if $m \ge 1$ and $f_m = f_d(L,\beta)$ if $m = 0$, and $r_{mn}(I) = r_{mn}(|I|)$ is a function of the form

$$r_{mn}(I) = \begin{cases} r_{oo}(|I|) & \text{if} \quad m \ge 1 \text{ and } n \ge 1, \\ r_{dd}(|I|) & \text{if} \quad m = n = 0, \\ r_{od}(|I|) & \text{else.} \end{cases}$$

The inductive expansions reproduce this form for $Z_{\text{res}}(V,\beta)$, just replacing r_{oo}, r_{od} and r_{dd} by suitable, inductively defined functions $r_{oo}^{(k)}$, $r_{od}^{(k)}$ and $r_{dd}^{(k)}$. In the limit $k \to \infty$, $r_{mn}^{(k)}(|I|)$ then goes to zero unless I is an interval of length 1, leaving an expression of the form $tr\ R^t$, with $(R-F)_{mn} = \lim_{k\to\infty} r_{mn}^{(k)}(|I|=1)$, see Section 4 of [11] for details. The fact that $r_{mn}^{(k)}(I) = r_{oo}^{(k)}(I)$ then immediately implies that the matrix $(\Gamma_{mn})_{m,n=1,\dots,q}$ has constant entries.

(ii) In the more general context of [11], the bounds on the derivatives of Γ in $d=2$ were much more limited than those stated in Theorem 2.2 (see Proposition 2.4 of [11]). The reason that we can prove the stronger statement of Theorem 2.2 for the concrete model considered here is the fact that we have logarithmic bounds on the derivatives of the surface activity $\kappa(Y)$:

$$\left|\frac{d^k\kappa(Y)}{d\beta^k}\right| \le O(|Y|^k)\kappa(Y)\ . \tag{2.23}$$

Recalling that the main input for the bounds on the derivatives of Γ were the corresponding bounds for the derivatives of the one surface term $\Gamma^{(1)}$, we use that $\Gamma^{(1)}_{od}$ is given as a sum of the form

$$\begin{aligned}\Gamma^{(1)}_{od} &= \sum_Y \kappa(Y)\, e^{-\frac{\beta(f_o(L,\beta)-f_d(L,\beta)}{2}\Delta Y} \\ &= \sum_{|Y|\le 3L} \kappa(Y)\, e^{-\frac{\beta(f_o(L,\beta)-f_d(L,\beta)}{2}\Delta Y} + \sum_{|Y|>3L} \kappa(Y)\, e^{-\frac{\beta(f_o(L,\beta)-f_d(L,\beta)}{2}\Delta Y}\ ,\end{aligned} \tag{2.24}$$

where $\Delta(Y)$ is the quantity introduced in equation (5.3) of [11]. Here we only need that $|\Delta(Y)|$ is bounded by L and that $\Delta(Y) = 0$ for flat surfaces. We then use (2.23) to bound the derivatives of the first sum, and the fact that $\kappa(Y)$ and its derivatives may be bounded by $e^{-(\tau-O(1))|Y|}$ to bound the derivatives of the second sum. We obtain that

$$\left|\frac{d^k\Gamma^{(1)}_{od}(L,\beta)}{d\beta^k}\right| \le O(L^k)\Gamma^{(1)}_{od}(L,\beta) + O(e^{-3(\tau-O(1))L})\ . \tag{2.25}$$

Combining this bound with the fact that $\Gamma^{(1)}_{od}$ is bounded from below by the "flat surface term" $\kappa(Y^{flat}) = e^{-(\tau+O(1))L}$ (we recall that $\Delta(Y) = 0$ if Y is a flat surface), we obtain the bound (2.22) for $\Gamma^{(1)}_{od}$. Using Proposition 5.3 of [11] to bound the difference between Γ_{od} and $\Gamma^{(1)}_{od}$ we get Theorem 2.2 for $d = 2$.

(iii) It is sometimes useful to replace a bound of the form $e^{-(2\tau-O(1))L^{d-1}}$ by $\Gamma_{od}e^{-(\tau-O(1))L^{d-1}}$. In fact, such a replacement can be justified since

$$\Gamma_{od}(L,\beta) \ge e^{-(\tau+O(1))L^{d-1}}\ , \tag{2.26}$$

which can, e.g., be deduced from the corresponding bound on $\Gamma^{(1)}_{od}(L,\beta)$ and Proposition 5.3 of [11].

(iv) Due to the bound (2.20), the eigenvalues of the matrix F lie in an interval of the form

$$[e^{-(\beta f L^{d-1}+7\tau_1/8+O(1))}, e^{-(\beta f L^{d-1}-O(1))}] \,, \tag{2.27}$$

provided $aL^{d-1} \leq 7\tau_1/8$. Due to the bounds (2.19), the eigenvalues of the matrix $F + F^{1/2}\Gamma F^{1/2}$ lie in an interval of the form (2.27) as well. Theorem 2.1 therefore implies that the first $q+1$ eigenvalues $\lambda_1 \geq \cdots \geq \lambda_{q+1}$ of the transfer matrix are just the eigenvalues of the matrix $F + F^{1/2}\Gamma F^{1/2}$, together with a bound $\lambda_i \leq e^{-(\tau_1 - O(1))}\lambda_1$ for the remaining eigenvalues of the transfer matrix.

We finally want to comment on the restriction $aL^{d-1} \leq 7\tau_1/8$ in Theorem 2.1. If a condition of this form is not fulfilled, the resummation of the ordinary contours perturbing an unstable phase can no longer be controlled by a convergent expansion. But if aL^{d-1} is big, configurations containing large regions of the unstable phase are heavily suppressed. As a consequence, two surfaces Y_i and Y_{i+1} bounding an unstable region V_i tend to stay very close to each other and hence may be treated as a single, "fat" surface $\tilde{Y} = Y_i \cup V_i \cup Y_{i+1}$ describing a transition between two stable phases. As a consequence, the unstable phases effectively disappear from the right hand side of (2.14), and we obtain a representation of the form

$$Z_{\rm res}(V,\beta) = e^{-\beta f_d(L,\beta)|V|} + \sum_{m=1}^{\infty} \frac{1}{m} \sum_{\tilde{Y}_1,\cdots,\tilde{Y}_m} \prod_i \kappa(\tilde{Y}_i)\, e^{g(\tilde{Y}_i,\tilde{Y}_{i+1})} e^{-\beta f_d(L,\beta)|V_i|} + \\ + O(e^{-(\tau^*-O(1))t}) \tag{2.28a}$$

if $\beta < \beta_t$ and

$$Z_{\rm res}(V,\beta) = q e^{-\beta f_o(L,\beta)|V|} + \sum_{m=1}^{\infty} \frac{q^m}{m} \sum_{\tilde{Y}_1,\cdots,\tilde{Y}_m} \prod_i \kappa(\tilde{Y}_i)\, e^{g(\tilde{Y}_i,\tilde{Y}_{i+1})} e^{-\beta f_d(L,\beta)|V_i|} + \\ + O(e^{-(\tau^*-O(1))t}) \tag{2.28b}$$

if $\beta > \beta_t$. The error term involving the decay constant

$$\tau^* := \min\{\tau_1, aL^{d-1}\} \,, \tag{2.29}$$

corrects for the fact that we left out all configurations which contain only ordinary contours and are perturbations of the unstable phase (corresponding to the terms $qe^{-\beta f_o(L,\beta)|V|}$ and $e^{-\beta f_d(L,\beta)|V|}$, respectively, in the sum (2.14)). Starting from the representations (2.28), we may proceed as before to obtain the following

Theorem 2.3. *Let L and q be sufficiently large, assume that*

$$aL^{d-1} \geq \frac{3}{4}\tau_1 \ ,$$

and let τ^* be the constant defined in (2.29). Then the following statements are true provided $k \leq 6$ and $t \geq (d-1)\log q$ and $|\beta - \beta_t| \leq O(1)$.

(i) *If $\beta < \beta_t$, then there is a function $\Gamma'_{dd}(L,\beta)$ satisfying the bound* (2.19b) *such that*

$$\left| \frac{d^k}{d\beta^k} \left[Z_{\text{per}}(V,\beta) - \left((1+\Gamma'_{dd}(L,\beta)) e^{-\beta f_d(L,\beta) L^{d-1}} \right)^t \right] \right| \leq e^{-\beta f|V|} e^{-(\tau^* - O(1))t} \ . \tag{2.30}$$

(ii) *If $\beta > \beta_t$, then there is a function $\Gamma'_{oo}(L,\beta)$ satisfying the bound* (2.19a) *such that*

$$\left| \frac{d^k}{d\beta^k} \left[Z_{\text{per}}(V,\beta) - tr(F + F^{1/2}\Gamma F^{1/2})^t \right] \right| \leq e^{-\beta f|V|} e^{-(\tau^* - O(1))t} \ , \tag{2.31}$$

where Γ is the $q \times q$ matrix with matrix elements $\Gamma_{mn} = \Gamma'_{oo}$, and F is the $q \times q$ matrix with matrix elements $F_{mn} = \delta_{mn}\, e^{-\beta f_o(L,\beta) L^{d-1}} \quad (m,n = 1,\ldots,q)$.

Remark: The matrix $F + F^{1/2}\Gamma F^{1/2}$ in (2.31) can be easily diagonalized. One finds one simple eigenvalue $(1+q\Gamma'_{oo})e^{-\beta f_o(L,\beta)L^{d-1}}$ and one $q-1$ fold degenerate eigenvalue $e^{-\beta f_o(L,\beta)L^{d-1}}$. As a consequence, the bound (2.31) can be rewritten as

$$\left| \frac{d^k}{d\beta^k} \left[Z_{\text{per}}(V,\beta) - \left((1+q\Gamma'_{oo})^t + (q-1) \right) e^{-\beta f_o(L,\beta)|V|} \right] \right| \leq e^{-\beta f|V|} e^{-(\tau^* - O(1))t} \ . \tag{2.31'}$$

3. The Transfer Matrix and its First Eigenvalues

As a consequence of Theorem A, the first $q+1$ eigenvalues of the transfer matrix $\mathcal{T}$ are just the eigenvalues of the matrix

$$R = F + F^{1/2}\Gamma F^{1/2} \ , \tag{3.1}$$

provided $|\beta-\beta_t|L^{d-1} \leq 1$. In order to calculate these eigenvalues, we consider vectors $\vec{v} = (v_0, v_1, \cdots, v_q) \in \mathbf{C}^{q+1}$ and note that $R\vec{v} = \lambda_\perp \equiv e^{-\beta f_o(L,\beta)L^{d-1}}\vec{v}$ for vectors of the form $\vec{v} = (0, v_1, \cdots, v_q)$, $\sum v_i = 0$. On the remaining two dimensional subspace (where $\vec{v} = (v_0, v, \cdots, v)$), the eigenvalues of R are obtained by diagonalizing the effective 2×2 matrix

$$\hat{R} = \begin{pmatrix} (1+\Gamma_{dd})e^{-L^{d-1}\beta f_d(L,\beta)} & \sqrt{q}\, e^{-\beta\frac{f_o(L,\beta)+f_d(L,\beta)}{2}L^{d-1}}\Gamma_{od} \\ \sqrt{q}\, e^{-\beta\frac{f_o(L,\beta)+f_d(L,\beta)}{2}L^{d-1}}\Gamma_{od} & (1+q\Gamma_{oo})e^{-L^{d-1}\beta f_o(L,\beta)} \end{pmatrix} . \tag{3.2}$$

Defining

$$\beta\tilde{f}_o(L,\beta) = \beta f_o(L,\beta) - L^{-d-1}\log(1+q\Gamma_{oo}) \ , \tag{3.3a}$$

$$\beta\tilde{f}_d(L,\beta) = \beta f_d(L,\beta) - L^{-d-1}\log(1+\Gamma_{dd}) \ , \tag{3.3b}$$

$$\tilde{x} = \tfrac{1}{2}(\beta\tilde{f}_d(L,\beta) - \beta\tilde{f}_o(L,\beta))L^{d-1} \ , \tag{3.3c}$$

and

$$\widetilde{\Gamma}_{od} = \frac{\Gamma_{od}}{\sqrt{1+\Gamma_{dd}}\sqrt{1+q\Gamma_{oo}}} \ , \tag{3.4}$$

we rewrite $\hat{R}$ as

$$\hat{R} = e^{-\beta\frac{\tilde{f}_o(L,\beta)+\tilde{f}_d(L,\beta)}{2}L^{d-1}} \begin{pmatrix} e^{-\tilde{x}} & \sqrt{q}\widetilde{\Gamma}_{od} \\ \sqrt{q}\widetilde{\Gamma}_{od} & e^{\tilde{x}} \end{pmatrix} .$$

Calculating the eigenvalues of $\hat{R}$ and putting everything together we find that the first $q+1$ eigenvalues of the transfer matrix $\mathcal{T}$ are just

$$\lambda_\perp = e^{-\beta f_o(L,\beta) L^{d-1}} = e^{-\beta \frac{\tilde{f}_o(L,\beta)+\tilde{f}_d(L,\beta)}{2} L^{d-1}} \left(\frac{e^{\tilde{x}}}{1+q\Gamma_{oo}} \right) \tag{3.5}$$

and

$$\lambda_\pm = e^{-\beta \frac{\tilde{f}_o(L,\beta)+\tilde{f}_d(L,\beta)}{2} L^{d-1}} \left(\cosh \tilde{x} \pm \sqrt{\sinh^2 \tilde{x} + q\widetilde{\Gamma}_{od}^2} \right) \tag{3.6}$$

where λ_+ and λ_- are simple eigenvalues, while $\lambda_\perp$ is $q-1$ fold degenerate.

Remark: It is sometimes convenient to rewrite $\lambda_\pm$ in a slightly different form. Observing that

$$\left(\cosh \tilde{x} + \sqrt{\sinh^2 \tilde{x} + q\widetilde{\Gamma}_{od}^2} \right) \left(\cosh \tilde{x} - \sqrt{\sinh^2 \tilde{x} + q\widetilde{\Gamma}_{od}^2} \right) = 1 - q\widetilde{\Gamma}_{od}^2 \ ,$$

while

$$\frac{\cosh \tilde{x} + \sqrt{\sinh^2 \tilde{x} + q\widetilde{\Gamma}_{od}^2}}{\cosh \tilde{x} - \sqrt{\sinh^2 \tilde{x} + q\widetilde{\Gamma}_{od}^2}} = \frac{1 + \sqrt{\tanh^2 \tilde{x} + q\widetilde{\Gamma}_{od}^2 / \cosh^2 \tilde{x}}}{1 - \sqrt{\tanh^2 \tilde{x} + q\widetilde{\Gamma}_{od}^2 / \cosh^2 \tilde{x}}} \ ,$$

we introduce the quantity $\hat{x}$ defined by

$$\tanh \hat{x} = \sqrt{\tanh^2 \tilde{x} + q\widetilde{\Gamma}_{od}^2 / \cosh^2 \tilde{x}} \tag{3.7}$$

to rewrite

$$\frac{\lambda_+}{\lambda_-} = \frac{1+\tanh \hat{x}}{1-\tanh \hat{x}} = e^{2\hat{x}} \ . \tag{3.8}$$

Using the variable $\hat{x}$, we then rewrite $\lambda_\pm$ as

$$\lambda_\pm = e^{-\beta \frac{\tilde{f}_o(L,\beta)+\tilde{f}_d(L,\beta)}{2} L^{d-1}} \sqrt{1 - q\widetilde{\Gamma}_{od}^2}\, e^{\pm \hat{x}} \ . \tag{3.9}$$

In order to discuss the relation of the eigenvalues $\lambda_\pm$ and $\lambda_\perp$ to the irreducible representations of the global symmetry, we recall that the transfer matrix may be considered as a bounded operator on the Hilbert space $\mathcal{H}$ of complex valued functions $\psi = \psi(\sigma_A)$ over the configuration space $(\mathbf{Z}_q)^A = \{\sigma_A \,|\, \sigma_A : A \to \mathbf{Z}_q\}$ (recall that $V = A \times T$, where T is the one dimensional torus of length t and A, the spatial lattice, is a $d-1$-dimensional torus of side length L). On this Hilbert space, an element $g = e^{2\pi ik/q}$ $(k = 0, \cdots, q-1)$ of the global symmetry group $\mathbf{Z}_q$ is represented by the unitary operator $U(e^{2\pi ik/q})$,

$$(U(e^{2\pi ik/q})\psi)(\sigma_A) := \psi(e^{-2\pi ik/q}\sigma_A) \;, \tag{3.10}$$

where the configuration $e^{-2\pi ik/q}\sigma_A$ is obtained from the configuration σ_A by multiplying each spin σ_x by $e^{-2\pi ik/q}$. Denoting the irreducible representations of the abelian group Z_q by χ_l, $\chi_l(e^{2\pi ik/q}) = e^{2\pi ikl/q}$, we may then decompose the Hilbert space $\mathcal{H}$ as

$$\mathcal{H} = \bigoplus_{l=0}^{q-1} \mathcal{H}_l \tag{3.11}$$

where $\mathcal{H}_l$ is the subspace of $\mathcal{H}$ on which the unitary operator $U(g)$ is just the multiplication by $\chi_l(g)$.

Due to the global symmetry of the model, the transfer matrix $\mathcal{T}$ commutes with the unitary operators $U(g)$, $g \in \mathbf{Z}_q$. It follows that $\mathcal{T}$ and $U(g)$ can be simultaneously diagonalized, and that

$$Z_{\mathrm{per}}(V, \beta) = \sum_{l=0}^{q-1} \mathrm{Tr}_{\mathcal{H}_l} \mathcal{T}^t \;. \tag{3.12}$$

The following theorem then expresses the fact that the two lowest eigenvalues of $\mathcal{T}$ in the subspace $\mathcal{H}_0$ where the global symmetry is represented trivially are just the eigenvalues $\lambda_\pm$ defined in (3.6), while the lowest eigenvalue of $\mathcal{T}$ in $\mathcal{H}_l$ $(l \neq 0)$ is $\lambda_\perp$. Heuristically, this can be seen by arguing that the action of $\mathbf{Z}_q$ in the effective one dimensional model, where the transfer matrix is just the matrix R on the Hilbert space $\mathcal{H} = \mathbf{C}^{q+1}$, is given by the relation

$$U(e^{2\pi ik/q})(v_0, v_1, \cdots, v_q) := (v_0, v_{1+k}, \cdots, v_{q+k}) \;,$$

where we identified v_{n+q} with v_n, $n = 1, \cdots, q$. Admitting this correspondence, the correspondence between the $q+1$ lowest eigenvalues of $\mathcal{T}$ and the irreducible representations of the global symmetry just follows from the fact that $\lambda_\perp$ corresponds to the subspace where $v = (0, v_1, \cdots, v_q)$ with $\sum v_i = 0$, while $\lambda_\pm$ correspond to the subspace where $v = (v_0, v, \cdots, v)$.

In order to actually prove the above correspondence, we will use the Fortuin-Kasteleyn representation [12] of the Potts model. Using the symbol V_1 to denote the set of all $d|V|$ nearest neighbor bonds in V, the Fortuin-Kastelyn representation of the Potts model is obtained by expanding $e^{\beta\delta}$ in

$$Z_{\mathrm{per}}(V, \beta) = \sum_{\sigma_V} \prod_{\langle xy \rangle \in V_1} e^{\beta\delta(\sigma_x, \sigma_y)} , \tag{3.13}$$

as $1 + (e^\beta - 1)\delta$:

$$Z_{\mathrm{per}}(V, \beta) = \sum_{\sigma_V} \sum_{X \subset V_1} \prod_{\langle xy \rangle \in X} (e^\beta - 1)\delta(\sigma_x, \sigma_y) . \tag{3.14}$$

Interchanging the two sums, the sum over σ_V can be performed exactly, giving a factor q for each connected component of X and for each point $x \in V/S(X)$ (we use the symbol $S(X)$ to denote the set of points $x \in V$ which belong to a bond in X). The partition function $Z_{\mathrm{per}}(V, \beta)$ can therefore be rewritten as

$$Z_{\mathrm{per}}(V, \beta) = \sum_{X \subset V_1} (e^\beta - 1)^{|X|} q^{C(X)} q^{|V \setminus S(X)|} , \tag{3.15}$$

where the summation runs over all sets of bonds $X \subset V_1$, $|X|$ and $C(X)$ are used to denote the number of bonds and connected components of X, respectively, and $|V/S(X)|$ is used to denote the number of points in $V/S(X)$. We stress that the above manipulations are manipulations on finite sums, and therefore do *not* require any assumptions like large q or small β. This is the reason why the first statement of Theorem 3.1 (below) does not contain any restriction on β, q or t.

Theorem 3.1.

(i) *Let* $Z_\perp(V,\beta)$ *be the partition function obtained from* $Z_{\rm per}(V,\beta)$ *by restricting the sum in* (3.15) *to configurations* $X \subset V_1$ *which contain at least one loop closed via the periodicity in time direction. Then*

$$\mathrm{Tr}_{\mathcal{H}_l} \mathcal{T}^t = \frac{1}{q} Z_\perp(V,\beta) \qquad \textit{for all} \qquad l \neq 0\,. \tag{3.16}$$

(ii) *Let* q *and* L *be sufficiently large,* $t \geq (d-1)\log q$*,* $k \leq 6$ *and* $|\beta - \beta_t| L^{d-1} \leq 1$*. Then*

$$\left| \frac{d^k}{d\beta^k} \left[\mathrm{Tr}_{\mathcal{H}_l} \mathcal{T}^t - \lambda_\perp^t \right] \right| \leq e^{-\beta f |V|} q^{-bt} \qquad \textit{for all} \qquad l \neq 0 \tag{3.17}$$

and

$$\left| \frac{d^k}{d\beta^k} \left[\mathrm{Tr}_{\mathcal{H}_0} \mathcal{T}^t - \left(\lambda_+^t + \lambda_-^t \right) \right] \right| \leq e^{-\beta f |V|} q^{-bt}\,. \tag{3.18}$$

Proof. We start with the proof of (i). We note that $\mathcal{H}_l$ may be written as

$$\mathcal{H}_l = P_l \mathcal{H} \qquad \text{where} \qquad P_l := \frac{1}{q} \sum_{g \in \mathbf{Z}_q} \chi_l(g^{-1}) U(g) \tag{3.19}$$

and write the lattice V as $V = \cup_{i=1}^t A_i$, where A_i denotes the i'th time slice of V. Introducing the set B_{12} of nearest neighbor pairs $< xy >$ for which $x \in A_1$ and $y \in A_2$, the partition function

$$Z^{(n)} := \mathrm{Tr}_{\mathcal{H}} U(e^{2\pi i n/q}) \mathcal{T}^t \tag{3.20}$$

is then obtained from $Z_{\rm per}$ by replacing $\delta(\sigma_x, \sigma_y)$ in (3.13) and (3.14) by

$$\delta_{xy}^{(n)}(\sigma_x,\sigma_y) = \begin{cases} \delta(\sigma_x,\sigma_y) & \text{if} \quad < xy > \notin B_{12}\,, \\ \delta(\sigma_x e^{-2\pi i n/q}, \sigma_y) & \text{if} \quad < xy > \in B_{12}\,. \end{cases}$$

For a given $X \subset V_1$ in the sum (3.14), let us consider a component C of X. If C contains a loop $\mathcal{L}$ which is closed via the periodicity in time direction, the product

$$\prod_{\langle xy \rangle \in C} \delta_{xy}^{(n)}(\sigma_x,\sigma_y) \tag{3.21}$$

will be zero for all configurations σ_V if n modulo q is different from zero. If C does not contain such a loop, however, one finds exactly q configurations $\sigma_{S(C)}$ on the set of points $S(C)$ for which the product (3.21) is different from zero (and hence 1!). We therefore find that $Z^{(n)}$ is given by a formula of the form (3.15) as well, with the only difference that the sum over X is restricted to those configurations for which X does not contain a loop which is closed via the periodicity in time direction. With the definitions of the above theorem, this reads

$$Z^{(n)} = Z_{\text{per}}(V,\beta) - Z_{\perp}(V,\beta) =: Z'_{\text{per}}(V,\beta) \qquad \text{if} \qquad n = 1, 2, \cdots, q-1 \; .$$

As a consequence

$$\begin{aligned}
\text{Tr}_{\mathcal{H}_l} \mathcal{T}^t &= \frac{1}{q} \sum_{n=0}^{q-1} e^{-2\pi i n l/q} \, Z^{(n)} \\
&= \frac{1}{q} Z_{\text{per}}(V,\beta) + \frac{1}{q} \sum_{n=1}^{q-1} e^{-2\pi i n l/q} \, Z'_{\text{per}}(V,\beta) \\
&= \frac{1}{q} (Z_{\text{per}}(V,\beta) - Z'_{\text{per}}(V,\beta)) + \frac{1}{q} \sum_{n=0}^{q-1} e^{-2\pi i n l/q} \, Z'_{\text{per}}(V,\beta) \\
&= \frac{1}{q} Z_{\perp}(V,\beta) + \delta_{0l} \, Z'_{\text{per}}(V,\beta)
\end{aligned} \quad ,$$

which proves (i).

In order to prove (ii) we use the contour expansions of the last section. Since the existence of a loop $\mathcal{L} \subset X$ which is closed via the periodicity in time direction implies that the set of contours corresponding to the configuration X contains no interfaces, the partition function $Z_{\perp}(V,\beta)$ is just a sum over configurations X which are perturbations of the completely ordered configuration $X = V_1$ by ordinary contours, plus an error term coming from the configurations which contain long contours. In the language of the last section, this reads $Z_{\perp}(V,\beta) = Z_o(V,\beta) + O(e^{-\beta f|V|} e^{-(\tau_1 - O(1))L})$, where $Z_o(V,\beta)$ is the partition function introduced in the paragraph following (2.7). The results of the last section, in particular (2.9a) and its generalization to derivatives, then imply the bound

(3.17). The bound (3.18) follows from (3.17) and the fact that statement (i) of Theorem A may be rewritten as

$$\left|\frac{d^k}{d\beta^k}\left[Z_{\rm per}(V,\beta)-\left(\lambda_+^t+\lambda_-^t+(q-1)\lambda_\perp^t\right)\right]\right|\leq e^{-\beta f|V|}q^{-bt}\;. \tag{3.22}$$

■

Remarks: i) Up to now, $\lambda_\pm$ and $\lambda_\perp$ are only defined in the region where the "effective transfer matrix" $R = F + F^{1/2}\Gamma F^{1/2}$ is defined. Using the fact that the lowest eigenvalue of the full transfer matrix $\mathcal{T}$ is simple and corresponds to an eigenvector $\psi \in \mathcal{H}_0$ due to the Perron-Frobenious theorem, we may give the following alternative definition which gives $\lambda_\pm$ and $\lambda_\perp$ directly as eigenvalues of $\mathcal{T}$. We define: λ_+ is the largest eigenvalue of $\mathcal{T}$, λ_- is the next eigenvalue of $\mathcal{T}$ in the Hilbert space $\mathcal{H}_0$, and $\lambda_\perp$ is the largest eigenvalue of $\mathcal{T}$ in the Hilbert space $\mathcal{H}_\perp := \bigoplus_{l=1}^{q-1}\mathcal{H}_l$. Note that $\lambda_\perp$ is (at least) $q-1$ fold degenerate due to the above Theorem 3.1.

ii) Introducing $\xi_{\rm sym}^{-1}(L,\beta)$ as the spectral gap of the transfer matrix $\mathcal{T}_{\rm sym} = \mathcal{T}|_{\mathcal{H}_0}$ for the symmetric sector,

$$\xi_{\rm sym}^{-1}(L,\beta) := \log(\lambda_+/\lambda_-)\;, \tag{3.23}$$

and $\xi^{-1}(L,\beta)$ as

$$\xi^{-1}(L,\beta) := \log(\lambda_+/\lambda_\perp)\;, \tag{3.24}$$

the results stated at the beginning of this section, in particular (3.7) through (3.9), imply that

$$\xi_{\rm sym}^{-1}(L,\beta) = 2\hat{x} \tag{3.25}$$

and

$$\xi^{-1}(L,\beta) = (\hat{x}-\tilde{x}) + \tfrac{1}{2}\log(1-q\widetilde{\Gamma}_{od}^2) + \log(1+q\Gamma_{oo})\;, \tag{3.26}$$

provided $|\beta-\beta_t|L^{d-1}\leq 1$.

iii) As shown in the last section, Theorem A can be extended to the wider range

$$aL^{d-1} \equiv \beta|f_o(\beta) - f_d(\beta)|L^{d-1} \le \frac{7\tau_1}{8} \qquad \text{with} \qquad \tau_1 = (\frac{1}{2d} - \frac{1}{4d-2}) \log q \ . \tag{3.27}$$

Outside this region, it is no longer possible to actually calculate all three eigenvalues $\lambda_\pm$ and $\lambda_\perp$ by the methods of [11]. Using an effective matrix R of lower rank, see Theorem 2.3 of the last section, one may prove, however, that

$$\left| \frac{d^k}{d\beta^k} \left(\log \lambda_+ + \beta f(\beta) L^{d-1} \right) \right| \le q^{-bL} \ . \tag{3.28}$$

and

$$\frac{1}{\lambda_+} \left| \frac{d^k \lambda_-}{d\beta^k} \right| \le O(e^{-7\tau_1/8}) \ , \tag{3.29}$$

provided $|\beta - \beta_t|$ is so large that (3.27) is violated. If $\beta < \beta_t$ and (3.27) is violated, the bound (3.29) holds for $\lambda_\perp$ as well,

$$\frac{1}{\lambda_+} \left| \frac{d^k \lambda_\perp}{d\beta^k} \right| \le O(e^{-7\tau_1/8}) \ , \tag{3.30}$$

while

$$\left| \frac{d^k}{d\beta^k} \left(\log \lambda_\perp - \log \lambda_+ \right) \right| \le q e^{-(2\tau - O(1))L^{d-1}} \ , \tag{3.31}$$

if $\beta > \beta_t$ and (3.27) is violated. As in Theorem 2.3, one needs $|\beta - \beta_t| \le O(1)$, q and L sufficiently large, and $k \le 6$.

We close this section with a theorem concerning the behaviour of the ”symmetric part”, $Z_{\text{sym}}(V, \beta) := Tr_{\mathcal{H}_0} \mathcal{T}^t$ of the partition function $Z_{\text{per}}(V, \beta)$ for $d = 2$.

Theorem 3.2. *Assume that $d = 2$, let $\mathcal{H}_0$ be the Hilbert space corresponding to the trivial representation of the global symmetry and define*

$$Z_{\text{sym}}(V, \beta) := Tr_{\mathcal{H}_0} \mathcal{T}^t \ . \tag{3.32}$$

Then

$$Z_{\rm sym}(V,\beta)(e^{\beta}-1)^{-|V|} = Z_{\rm sym}(V,\beta^*)(e^{\beta^*}-1)^{-|V|}\ , \tag{3.33}$$

where β^* and β are related by duality, i.e.

$$(e^{\beta}-1)(e^{\beta^*}-1) = q\ .$$

Remarks: i) Theorem 3.2 follows immediately from the results of [21]. For the convenience of the reader we give an alternative proof in the appendix.

ii) Theorem 3.2 implies that all eigenvalues $\lambda_{\rm sym}$ of the transfer matrix which correspond to the trivial representation of the global symmetry obey the duality relation

$$\lambda_{\rm sym}(L,\beta)(e^{\beta}-1)^{-L^{d-1}} = \lambda_{\rm sym}(L,\beta^*)(e^{\beta^*}-1)^{-L^{d-1}}\ . \tag{3.34}$$

As an immediate consequence, we obtain that

$$\frac{\lambda_+(L,\beta)}{\lambda_-(L,\beta)} = \frac{\lambda_+(L,\beta^*)}{\lambda_-(L,\beta^*)}\ . \tag{3.35}$$

Equation (3.35) is the main input for the statement (iii) of Theorem 4.1 (below).

4. Finite-Size Scaling of $\lambda_\pm$, $\lambda_\perp$ and $E_{\rm cyl}(L,\beta)$.

In this section we derive the finite-size scaling $\lambda_\pm$, $\lambda_\perp$ and of the internal energy

$$E_{\rm cyl}(L,\beta) := -\lim_{t\to\infty}\frac{1}{tL^{d-1}}\frac{d}{d\beta}\log Z_{\rm per}(V,\beta)\ , \tag{4.1}$$

see Theorem 4.2 and 4.3 (below). In a preliminary step, we discuss the definition of a suitable, finite L transition point. We consider two candidates: the point $\tilde\beta_0(L)$ where the L-dependent free energies $\tilde f_o(L,\beta)$ and $\tilde f_d(L,\beta)$ are equal and the point $\beta_t(L)$ where the mass gap in the symmetric sector , $\xi_{\rm sym}^{-1}(L,\beta)=\log(\lambda_+/\lambda_-)$, is minimal. We recall that

τ is the constant $\tau = \frac{1}{2d} \log q$, and that it is related to the order-disorder surface tension σ_{od} by $\sigma_{od} = \tau + O(q^{-b})$.

Theorem 4.1. *Let q and L be sufficiently large. Then the following statements are true.*

(i) *In the range $|\beta - \beta_t| L^{d-1} \leq 1$ where $\tilde{f}_o$ and $\tilde{f}_d$ are defined, there is exactly one point $\tilde{\beta}_0(L)$ such that $\tilde{f}_o(L, \tilde{\beta}_0(L)) = \tilde{f}_d(L, \tilde{\beta}_0(L))$. It obeys a bound*

$$|\tilde{\beta}_0(L) - \beta_t| \leq O(q^{-bL}) \; . \tag{4.2}$$

(ii) *There is exactly one point $\beta_t(L)$ such that*

$$\xi_{\mathrm{sym}}^{-1}(L, \beta) \geq \xi_{\mathrm{sym}}^{-1}(L, \beta_t(L)) \tag{4.3}$$

for all β in the range $|\beta - \beta_t| \leq O(1)$. It obeys the bounds

$$|\beta_t(L) - \beta_t| \leq O(q^{-bL}) \tag{4.4a}$$

and

$$|\beta_t(L) - \tilde{\beta}_0(L)| \leq O(q e^{-(2\tau - O(1)) L^{d-1}}) \; . \tag{4.4b}$$

(iii) *Let $d = 2$. Then $\beta_t(L) = \beta_t$ by duality.*

Proof: (i) The statement (i) of the above theorem follows immediately from the bounds (1.6) and (1.7) of Theorem A and the fact that $f_o(\beta_t) = f_d(\beta_t)$ while

$$\frac{d}{d\beta} \left[\beta f_d(\beta) - \beta f_o(\beta) \right]_{\beta = \beta_t} = E_d - E_o > 0 \; . \tag{4.5}$$

(ii) In a first step we note that

$$\xi_{\mathrm{sym}}^{-1}(L, \tilde{\beta}_0(L)) = \log \left[\frac{1 + \sqrt{q}\, \widetilde{\Gamma}_{od}}{1 - \sqrt{q}\, \widetilde{\Gamma}_{od}} \right] = 2\sqrt{q}\, \widetilde{\Gamma}_{od} + O(q\, \widetilde{\Gamma}_{od}^2) \; .$$

Since $\lambda_+/\lambda_- \geq O(1)$ if $|\beta-\beta_t|L^{d-1} \geq 1$, we may restrict ourselves to the region $|\beta-\beta_t|L^{d-1} \leq 1$. In fact, we may assume the much stronger condition that

$$|\tilde{x}| \leq O(\sqrt{q}\,\widetilde{\Gamma}_{od}) \tag{4.6}$$

since $\lambda_+/\lambda_- = e^{2\hat{x}} \geq e^{2|\tilde{x}|}$ if $|\beta-\beta_t|L^{d-1} \leq 1$, see (3.7) and (3.8). In order to find the minimum of $\xi_{\rm sym}^{-1} = 2\hat{x}$, we now consider the derivatives of

$$\tanh^2\hat{x} = \tanh^2\tilde{x} + \frac{q\widetilde{\Gamma}_{od}^2}{\cosh^2\tilde{x}}\ .$$

Using Theorem A to bound the derivatives of $\widetilde{\Gamma}_{od}$, we find that

$$\begin{aligned}\frac{d^2}{d\beta^2}\tanh^2\hat{x} &\geq \frac{2}{\cosh^4\tilde{x}}\left(\frac{d}{d\beta}\tilde{x}\right)^2 - O(\sqrt{q}e^{-(\tau-O(1))L^{d-1}})\\ &\geq 2\left(\frac{E_d-E_o}{2} - O(q^{-bL})\right)^2 L^{2(d-1)} - O(\sqrt{q}e^{-(\tau-O(1))L^{d-1}})\end{aligned} \tag{4.7}$$

if β lies in the region where (4.6) is fulfilled. (4.7) implies the uniqueness of the point $\beta_t(L)$. Combining (4.7) with the bound

$$\frac{d}{d\beta}\left(\tanh^2\hat{x}\right)\Big|_{\beta=\tilde{\beta}_0(L)} = 2q\widetilde{\Gamma}_{od}\left|\frac{d\widetilde{\Gamma}_{od}}{d\beta}\right| \leq O(qe^{-(2\tau-O(1))L^{d-1}}) \tag{4.8}$$

we obtain the bound (4.4b). The bound (4.4a) follows from (4.4b) and (4.2).

(iii) Combining the fact that $\beta_t(L)$ is unique due to the statement (i) of the above theorem with the relation (3.35) stated at the end of the last section, we conclude that $\beta_t(L) = \beta_t(L)^*$ which implies that $\beta_t(L) = \log(1+\sqrt{q}) = \beta_t$. ∎

Remarks: i) The above theorem shows that $\beta_t(L)$ and $\tilde{\beta}_0(L)$ differ only by an amount $O(qe^{-(2\tau-O(1))L^{d-1}})$, which is much smaller than the width $O(\sqrt{q}\,e^{-(\tau-O(1))L^{d-1}})$ of the transition region.

ii) Using a strategy similar to that which lead to the proof of Theorem 4.1 (ii), one may prove that the point $\beta_{\rm Cmax}(L)$ where the specific heat,

$$C_{\rm cyl}(L,\beta) = -k\beta^2\frac{d}{d\beta}E_{\rm cyl}(L,\beta)\ ,$$

is maximal obeys a bound of the form (4.4) as well. We will not use this statement in this paper, and leave the proof to the interested reader.

The next theorems summarize the main results of this section. We use E_m, C_m, $m = o, d$ to denote the infinite volume internal energy and specific heat of the phase m at $\beta = \beta_t$.

Theorem 4.2. *Let q and L be sufficiently large. Then there are constants ξ_L and $E_o(L)$, $E_d(L)$, $C_o(L)$ and $C_d(L)$ such that the following statements are true.*

(i)
$$E_o(L) = E_o + O(q^{-bL}) \qquad \text{and} \qquad E_d(L) = E_d + O(q^{-bL}) \, , \tag{4.9a}$$
$$C_o(L) = C_o + O(q^{-bL})) \qquad \text{and} \qquad C_d(L) = C_d + O(q^{-bL})) \, , \tag{4.9b}$$

and

$$\xi_L^{-1} = \sqrt{q}\, e^{-\beta\sigma_{od} L^{d-1}} \begin{cases} C_{od}\, L^{-1/2}(1 + O(L^{-1})) \, , & d = 2 \, , \\ (1 + O(q^{-bL})) \, , & d \geq 3 \, , \end{cases} \tag{4.10}$$

(ii) *If $|\beta - \beta_t| L^{d-1} \leq 1$,*

$$\lambda_\pm = e^{-\beta \frac{\tilde{f}_o(L,\beta) + \tilde{f}_d(L,\beta)}{2} L^{d-1}} \exp\left(\pm \xi_L^{-1} \sqrt{1 + y^2 (1 + O(|\beta - \beta_t(L)|^2)} \; + \; O(\xi_L^{-2}) \right) \tag{4.11}$$

and

$$\lambda_\perp = e^{-\beta \frac{\tilde{f}_o(L,\beta) + \tilde{f}_d(L,\beta)}{2} L^{d-1}} \exp\left(q\Gamma_{oo} + \xi_L^{-1} y (1 + O(|\beta - \beta_t(L)|^2) \; + \; O(\xi_L^{-2}) \right) \, , \tag{4.12}$$

where y is the scaling variable

$$y = \xi_L L^{d-1} \left(\frac{E_d(L) - E_o(L)}{2} (\beta - \beta_t(L)) - \frac{C_d(L) - C_o(L)}{4k\beta_t(L)^2} (\beta - \beta_t(L))^2 \right) \, . \tag{4.13}$$

Theorem 4.3. *Let q and L are sufficiently large and assume that $|\beta - \beta_t| L^{d-1} \leq 1$. Then*

$$E_{\rm cyl}(L, \beta) = \bar{E}(L, \beta) - \Delta E(L, \beta) \frac{y}{\sqrt{1 + y^2}} \; + \; O(\xi_L^{-1}) \, , \tag{4.14}$$

where

$$\bar{E}(L,\beta)=\frac{E_d(L)+E_o(L)}{2}-\frac{C_d(L)+C_o(L)}{2k\beta_t(L)^2}(\beta-\beta_t(L))+O(|\beta-\beta_t(L)|^2) \tag{4.15}$$

and

$$\Delta E(L,\beta)=\frac{E_d(L)-E_o(L)}{2}-\frac{C_d(L)-C_o(L)}{2k\beta_t(L)^2}(\beta-\beta_t(L))+O(|\beta-\beta_t(L)|^2)\ . \tag{4.16}$$

Remarks: i) It is possible to eliminate the error terms $O(|\beta-\beta_t(L)|^2)$ in (4.11), (4.12), (4.15) and (4.16) if one introduces the β dependent quantities

$$E_m(L,\beta)=\frac{d}{d\beta}\tilde{f}_m(L,\beta),\qquad m=o,d\ , \tag{4.17}$$

and

$$x=x(L,\beta):=\tilde{x}(L,\beta)-\tilde{x}(L,\beta_t(L))\ , \tag{4.18}$$

where $\tilde{f}_o$, $\tilde{f}_d$ and $\tilde{x}$ are the quantities defined at the beginning of the last section. Then

$$\lambda_\pm=e^{-\beta\frac{\tilde{f}_o(L,\beta)+\tilde{f}_d(L,\beta)}{2}L^{d-1}}\exp\left(\pm\sqrt{\xi_L^{-2}+x^2}\ +\ O(\xi_L^{-2})\right)\ , \tag{4.19}$$

$$\lambda_\perp=e^{-\beta\frac{\tilde{f}_o(L,\beta)+\tilde{f}_d(L,\beta)}{2}L^{d-1}}\exp\left(q\Gamma_{oo}+x\ +\ O(\xi_L^{-2})\right)\ , \tag{4.20}$$

and

$$E_{\rm cyl}(L,\beta)=\frac{E_d(L,\beta)+E_o(L,\beta)}{2}-\frac{E_d(L,\beta)-E_o(L,\beta)}{2}\frac{y}{\sqrt{1+y^2}}+O(\xi_L^{-1})\ . \tag{4.21}$$

Defining $E_m(L)=E_m(L,\beta_t(L))$ and $C_m(L)=-k\beta_t(L)^2(dE_m(L,\beta)/d\beta)(\beta=\beta_t(L))$, the bounds (4.11), (4.12), (4.15) and (4.16) are obtained from (4.19) through (4.21) by expanding x and $E_d(L,\beta)\pm E_o(L,\beta)$ about $\beta_t(L)$. The bounds (4.9) follow from Theorem A and the bound (4.4a).

ii) If one uses Theorem A to bound the two surface term Γ_{oo}, the gaps $\xi^{-1}(L,\beta)$ and $\xi^{-1}_{\rm sym}(L,\beta)$ following from the above bounds are just

$$\xi^{-1}_{\rm sym}(L,\beta) = 2\xi_L^{-1}\sqrt{1+(x\xi_L)^2} \, + \, O(\xi_L^{-2}) \tag{4.22}$$

and

$$\begin{aligned} \xi^{-1}(L,\beta) &= \xi_L^{-1}\left(\sqrt{1+(x\xi_L)^2} - x\xi_L\right) \, + \, O(e^{-(2\tau-O(1))L^{d-1}}) \\ &= \xi_L^{-1}\left(\sqrt{1+(x\xi_L)^2} - x\xi_L\right) \, + \, O(\xi_L^{-(2-\epsilon)}) \, , \end{aligned} \tag{4.23}$$

where $\epsilon = \epsilon(q) \to 0$ as $q \to \infty$.

Proof of Theorem 4.2 and Theorem 4.3. The proof follows the heuristics sketched in the introduction, with $\beta - \beta_0(L)$ replaced by $\beta - \beta_t(L)$. We define

$$\xi_L^{-1} := \sqrt{q}\,\widetilde{\Gamma}_{od}(L,\beta_t(L)) \, , \tag{4.24}$$

and note that ξ_L^{-1} obeys the bound (4.10) by Theorem A. We then use Theorem 2.3 in conjunction with Theorem A to bound the derivative of $\widetilde{\Gamma}_{od}(L,\beta)$,

$$\left|\frac{d^k}{d\beta^k}\widetilde{\Gamma}_{od}(L,\beta)\right| \le O(L^{k(d-1)})\widetilde{\Gamma}_{od}(L,\beta) \, , \tag{4.25}$$

and observe that (4.25) implies that

$$\sqrt{q}\,\widetilde{\Gamma}_{od}(L,\beta) = \xi_L^{-1}(1 + O(L^{d-1}(\beta - \beta_t(L)))) \, . \tag{4.26}$$

Note that (4.25) and (4.26) allow to replace the right hand side of (4.8) by $O(\xi_L^{-2})$, which implies that

$$|\beta_t(L) - \tilde\beta_0(L)|L^{d-1} \le O(\xi_L^{-2}) \, . \tag{4.27}$$

As a consequence,

$$\tilde x = x + O(\xi_L^{-2}) \, . \tag{4.28}$$

Next, we want to approximate

$$\hat{x} = \operatorname{artanh}\left(\sqrt{\tanh^2 \tilde{x} + q\widetilde{\Gamma}_{od}^2/\cosh^2 \tilde{x}}\right) \tag{4.29}$$

by $\sqrt{x^2+\xi_L^{-2}}$. To this end we consider $\hat{x}^2$ as a function of $\tilde{x}^2$ and $q\widetilde{\Gamma}_{od}^2$ and expand in $q\widetilde{\Gamma}_{od}^2$. Using the fact that $|\tilde{x}| \le O(1)$, a straight forward calculation yields

$$\begin{aligned}\hat{x}^2 &= \tilde{x}^2 + \frac{\tilde{x}}{\tanh\tilde{x}} q\widetilde{\Gamma}_{od}^2 + O((q\widetilde{\Gamma}_{od}^2)^2)\\ &= \tilde{x}^2 + q\widetilde{\Gamma}_{od}^2(1+O(\tilde{x}^2)) + O((q\widetilde{\Gamma}_{od}^2)^2)\\ &= (\tilde{x}^2 + q\widetilde{\Gamma}_{od}^2)(1+O(\xi_L^{-2}))\ . \end{aligned} \tag{4.30}$$

Combining this bound with (4.26) and (4.28) and the fact that $(\beta-\beta_t(L))L^{d-1} = O(x)$, we obtain that

$$\begin{aligned}\tilde{x}^2 &= \left(x^2+\xi_L^{-2}+O(x\xi_L^{-2})+O(\xi_L^{-4})\right)\left(1+O(\xi_L^{-2})\right)\\ &\left(x^2+\xi_L^{-2}\right)\left(1+O(\xi_L^{-2})+O\left(\frac{x\xi_L^{-2}}{x^2+\xi_L^{-2}}\right)\right)\ ,\end{aligned}$$

and hence

$$\hat{x} = \sqrt{x^2+\xi_L^{-2}}\left(1+O(\xi_L^{-2})+O\left(\frac{x\xi_L^{-2}}{x^2+\xi_L^{-2}}\right)\right) = \sqrt{x^2+\xi_L^{-2}} + O(\xi_L^{-2})\ . \tag{4.31}$$

Combining (4.31) with the bounds

$$\log(1+q\Gamma_{oo}) = q\Gamma_{oo} + O((q\Gamma_{oo})^2) = q\Gamma_{oo} + O(\xi_L^{-2})\ , \tag{4.32a}$$

$$\log\sqrt{1-q\widetilde{\Gamma}_{od}^2} = \tfrac{1}{2}q\widetilde{\Gamma}_{od}^2 + O((q\widetilde{\Gamma}_{od}^2)^2) = O(\xi_L^{-2})\ , \tag{4.32b}$$

we obtain (4.19) and (4.20) and hence Theorem 4.2. We are left with the proof of (4.21).

We use the results of the last section, in particular equation (3.9), to rewrite the internal energy as

$$E_{\text{cyl}}(L,\beta) = \frac{E_d(L,\beta)+E_o(L,\beta)}{2} - \frac{1}{L^{d-1}}\frac{d\hat{x}}{d\beta} - \frac{1}{L^{d-1}}\frac{d}{d\beta}\log\left(\sqrt{1-q\widetilde{\Gamma}_{od}^2}\right)\ . \tag{4.33}$$

In a first step we calculate the derivative of $\hat{x}$:

$$\frac{d\hat{x}}{d\beta} = \frac{1}{2}\frac{d}{d\beta}\log\left(\frac{\cosh\tilde{x} + \sqrt{\sinh^2\tilde{x} + q\widetilde{\Gamma}_{od}^2}}{\cosh\tilde{x} - \sqrt{\sinh^2\tilde{x} + q\widetilde{\Gamma}_{od}^2}}\right) = \frac{\sinh\tilde{x}}{\sqrt{\sinh^2\tilde{x} + q\widetilde{\Gamma}_{od}^2}}\frac{d\tilde{x}}{d\beta} + \frac{q\widetilde{\Gamma}_{od}}{1 - q\widetilde{\Gamma}_{od}^2}\frac{d\widetilde{\Gamma}_{od}}{d\beta}$$

which gives

$$\frac{1}{L^{d-1}}\frac{d\hat{x}}{d\beta} = \frac{\sinh\tilde{x}}{\sqrt{\sinh^2\tilde{x} + q\widetilde{\Gamma}_{od}^2}}\frac{1}{L^{d-1}}\frac{d\tilde{x}}{d\beta} + O(\xi_L^{-2}) \; . \tag{4.34}$$

We then distinguish between $|x| \leq c\xi_L^{-2}$ and $|x| > c\xi_L^{-2}$, where $c > 0$ is chosen in such a way that $|\tilde{x}(L, \beta_t(L))| \leq c\xi_L^{-2}$. For $|x| > c\xi_L^{-2}$, $\operatorname{sign} x = \operatorname{sign}\tilde{x}$ and

$$\frac{\sinh\tilde{x}}{\sqrt{\sinh^2\tilde{x} + q\widetilde{\Gamma}_{od}^2}} = \frac{x}{\sqrt{x^2 + \xi_L^{-2}}}\left(\frac{1 + q\widetilde{\Gamma}_{od}^2/\sinh^2\tilde{x}}{1 + \xi_L^{-2}/x^2}\right) \; .$$

Using (4.26) and the fact that $\tilde{x} = x + O(\xi_L^{-2}) = x(1 + O(\xi_L^{-2}/x))$ we then expand

$$\frac{1 + q\widetilde{\Gamma}_{od}^2/\sinh^2\tilde{x}}{1 + \xi_L^{-2}/x^2} = \frac{1 + (\xi_L^{-2}/x^2)(1 + O(x) + O(\xi_L^{-2}/x))}{1 + \xi_L^{-2}/x^2} = 1 + O(\xi_L^{-2}/x) \; .$$

We conclude that

$$\frac{\sinh\tilde{x}}{\sqrt{\sinh^2\tilde{x} + q\widetilde{\Gamma}_{od}^2}} = \frac{x}{\sqrt{x^2 + \xi_L^{-2}}}(1 + O(\xi_L^{-2}/x)) = \frac{x}{\sqrt{x^2 + \xi_L^{-2}}} + O(\xi_L^{-1}) \tag{4.35}$$

provided $|x| > c\xi_L^{-2}$.

If $|x| \leq c\xi_L^{-2}$, we bound

$$\left|\frac{\sinh\tilde{x}}{\sqrt{\sinh^2\tilde{x} + q\widetilde{\Gamma}_{od}^2}} - \frac{x}{\sqrt{x^2 + \xi_L^{-2}}}\right| \leq \frac{O(\xi_L^{-2})}{\sqrt{\xi_L^{-2} + O(\xi_L^{-4})}} \leq O(\xi_L^{-1}) \; . \tag{4.36}$$

Combining (4.33) with the bounds (4.25), (4.26), (4.34), (4.35) and (4.36), and the observation that

$$\frac{1}{L^{d-1}}\frac{d\tilde{x}}{d\beta} = \frac{E_d(L,\beta) - E_o(L,\beta)}{2} \; ,$$

we obtain the bound (4.21).

Remarks. i) As a corollary of the above proof and equation (3.25) and (3.26) one obtains that

$$\frac{1}{L^{d-1}}\,\frac{d\xi^{-1}(L,\beta)}{d\beta} = \frac{E_d(L,\beta)-E_o(L,\beta)}{2}\left(\frac{x}{\sqrt{x^2+\xi_L^{-2}}}-1\right)+O(\xi_L^{-1})\ , \tag{4.37}$$

while

$$\frac{1}{L^{d-1}}\,\frac{d\xi_{\mathrm{sym}}^{-1}(L,\beta)}{d\beta} = \frac{E_d(L,\beta)-E_o(L,\beta)}{2}\left(\frac{2x}{\sqrt{x^2+\xi_L^{-2}}}\right)+O(\xi_L^{-1})\ . \tag{4.38}$$

ii) Due to Theorem 4.1, $\beta_t(L)=\beta_t$ if $d=2$ and $|\beta_t(L)-\beta_t|\le O(q^{-bL})$ if $d>2$. In the next section, we need an estimate of the actual shift $\beta_t(L)-\beta_t$ for $d>2$. To this end we first consider the point $\tilde\beta_0(L)$ where the finite volume free energies $\tilde f_o(L,\beta_t)$ and $\tilde f_d(L,\beta_t)$ are equal and recall that $f_o(\beta_t)=f_d(\beta_t)$. Up to power law corrections in L, which may be neglected for the heuristics discussed here, the difference of the finite volume free energies $\tilde f_m(L,\beta_t)$ at the point β_t should then behave like

$$\tilde f_o(L,\beta_t)-\tilde f_d(L,\beta_t)\sim K_o e^{-L/\xi_o}-K_d e^{-L/\xi_d}$$

where ξ_m is of the order of the infinite volume correlation length of the phase m at the transition point β_t and K_m is a constant ($m=o,d$). As a consequence,

$$\tilde\beta_0(L)-\beta_t\sim\frac{1}{E_d(L)-E_o(L)}(K_o e^{-L/\xi_o}-K_d e^{-L/\xi_d})\ .$$

Due to Theorem 4.1, $\beta_t(L)-\beta_t$ shows the same asymptotic behaviour. Assuming now that $\xi_o\neq\xi_d$ for $d>2$, we obtain the asymptotic behaviour

$$\beta_t(L)-\beta_t\sim K e^{-L/L_0}\ , \tag{4.39}$$

where $|K|>0$ and $L_0=\max\{\xi_o,\xi_d\}$.

5. Finite-Size Scaling of the gaps $\xi^{-1}(L,\beta)$ and $\xi_{\rm sym}^{-1}(L,\beta)$.

In this section we discuss the finite-size scaling of the gaps $\xi_{-1}(L,\beta)$ and $\xi_{\rm sym}^{-1}(L,\beta)$ and their derivative with respect to β. For the convenience of the reader we recall the corresponding results derived in the last section. Under the condition that

$$|\beta - \beta_t| L^{d-1} \leq 1 \tag{5.1}$$

we have shown that

$$\xi^{-1}(L,\beta) = \xi_L^{-1} \left(\sqrt{1+(x\xi_L)^2} - x\xi_L \right) + O(\xi_L^{-(2-\epsilon)}) , \tag{5.2}$$

$$\xi_{\rm sym}^{-1}(L,\beta) = 2\xi_L^{-1} \sqrt{1+(x\xi_L)^2} + O(\xi_L^{-2}) , \tag{5.3}$$

$$\frac{d\xi^{-1}(L,\beta)}{d\beta} = \left(\frac{x\xi_L}{\sqrt{1+(x\xi_L)^2}} - 1 \right) \frac{E_d(L,\beta) - E_o(L,\beta)}{2} L^{d-1} + O(L^{d-1}\xi_L^{-1}) , \tag{5.4}$$

and

$$\frac{d\xi_{\rm sym}^{-1}(L,\beta)}{d\beta} = \frac{2x\xi_L}{\sqrt{1+(x\xi_L)^2}} \frac{E_d(L,\beta) - E_o(L,\beta)}{2} L^{d-1} + O(L^{d-1}\xi_L^{-1}) , \tag{5.5}$$

provided L and q are sufficiently large. Here $\epsilon = \epsilon(q) \to 0$ as $q \to \infty$, $E_m(L,\beta) = E_m(L)(1 + O(\beta - \beta_t(L)))$,

$$x = L^{d-1} \frac{E_d(L) - E_o(L)}{2} (\beta - \beta_t(L))(1 + O(\beta - \beta_t(L))) \tag{5.6}$$

and $E_m(L) = E_m + O(q^{-bL})$, ξ_L are the quantities introduced in Theorem 4.2. Finally, $\beta_t(L)$ is defined as the point where the gap in the symmetric sector, $\xi_{\rm sym}^{-1}(L,\beta)$, is minimal. Due to Theorem 4.1, $\beta_t(L) = \beta_t$ if $d = 2$, while $|\beta_t(L) - \beta_t| \leq O(q^{-L})$ if $d > 2$. We also argued that

$$\beta_t(L) - \beta_t \sim K e^{-L/L_0} \qquad \text{if} \qquad d > 2 . \tag{5.7}$$

Fig. 2. *The gaps* $\xi^{-1}(L,\beta)$ *and* $\xi^{-1}_{\rm sym}(L,\beta)$ *in the crossover region* $|\beta-\beta_t(L)|L^{d-1}\le O(\xi_L^{-1})$. *If* $d=2$, $\beta_t(L)=\beta_t$, *while* $|\beta_t-\beta_t(L)|L^{d-1}$ *is expected to be much larger than* ξ_L^{-1} *if* $d>2$ *and* L *is sufficiently large.*

Here K is a non zero constant and L_0 is of the order of the maximum of ξ_o and ξ_d, where ξ_m is the infinite volume correlation length of the phase m.

In Fig.2 we have schematically drawn the behaviour of the gaps $\xi^{-1}(L,\beta)$ and $\xi^{-1}_{\rm sym}(L,\beta)$ as given by (5.2) and (5.3). At the point $\beta_t(L)$, the two gaps just differ by a factor $2(1+O(\xi_L^{-(1-\epsilon)}))$,

$$\xi^{-1}(L,\beta)=\xi_L^{-1}(1+O(\xi_L^{-(1-\epsilon)})) \tag{5.8a}$$

$$\xi^{-1}_{\rm sym}(L,\beta)=2\xi_L^{-1}(1+O(\xi_L^{-1}))\ ; \tag{5.8b}$$

if $x\xi_L$ is large and positive, the gap $\xi^{-1}(L,\beta)$ becomes very small while

$$\xi^{-1}_{\rm sym}(L,\beta)\sim 2x\ ; \tag{5.9}$$

and if $x\xi_L$ is large and negative, both gaps grow proportional to $|x|$,

$$\xi^{-1}(L,\beta)\sim 2|x| \tag{5.10a}$$

$$\xi^{-1}_{\rm sym}(L,\beta)\sim 2|x|\ . \tag{5.10b}$$

The crossover from one region to the other takes place in a region where $|\beta-\beta_t(L)|L^{d-1} = O(\xi_L^{-1})$ and is given by (5.2) and (5.3) with x replaced[9] by $\frac{E_d(L)-E_o(L)}{2}(\beta-\beta_t(L))L^{d-1}$.

Next, we discuss the behaviour of the derivative $d\xi^{-1}(L,\beta)/d\beta$. Let us first sketch the FSS of this derivative in the vicinity of a *second-order* transition point β_c. For a typical second-order transition, the infinite volume correlation length diverges with an exponent ν as β approaches β_c. Phenomenological renormalization group (RG) considerations then imply that the FSS of an observable $P(L,\beta)$ is given by a relation of the form $P(L,\beta)/P(\infty,\beta) = \hat{P}((\beta-\beta_c)L^{\lambda_T})$, with $\lambda_T = 1/\nu$. Since $P(L,\beta)$ must be finite for all β including β_c as long as L stays finite, while $P(\infty,\beta)$ diverges as $\beta \to \beta_c$, consistency then implies that the FSS behaviour of $P(L,\beta_c)$ is given by $P(L,\beta_c) \sim L^{\sigma/\nu}$, if σ is the critical exponent of P (see e.g. [2] for a review of these considerations). For the correlation length and its derivative, we obtain

$$\xi^{-1}(L,\beta_c) \sim L^{-1} \tag{5.11a}$$

and

$$\left.\frac{d\xi^{-1}(L,\beta)}{d\beta}\right|_{\beta=\beta_c} \sim L^{-1+1/\nu} \ . \tag{5.11b}$$

The numerical study of the quantity

$$\frac{1}{\nu(L,\beta)} = \frac{1}{\log L}\log\left(\frac{-dL\xi^{-1}(L,\beta)}{d\beta}\right) \tag{5.12}$$

at the transition point β_c therefore should allow a prediction of the RG eigenvalue $\lambda_T = 1/\nu$. For second-order transitions, this idea, first introduced by Nightingale [22], has been very successful, see e.g. [23] for a recent application.

The above considerations are obviously very doubtful at a first-order transition, where the notion of critical exponents is meaningless. It is nevertheless a legitimate question to ask whether $1/\nu(L,\beta_t)$, as defined in (5.12), converges to the phenomenological RG eigenvalue [24] $\lambda_T = d$. As we will see, this is a delicate question. For first order transitions

[9] In the region $|\beta-\beta_t(L)|L^{d-1} = O(\xi_L^{-1})$, the error resulting from this replacement can be absorbed in to the errors already present in the bounds (5.2) and (5.3).

which describe the coexistence of *two* phases, one which is stable below β_t and one which is stable above β_t, this is in fact *false*, as already observed in [10]. For the case considered here, where $q > 1$ ordered phases coexist with one disordered phase, the answer is positive, at least if β is chosen carefully, see below.

Let us first consider $\xi(L,\beta)$ and its derivative at the finite L transition point $\beta_t(L)$. Using (5.2) one immediately sees that $\xi(L,\beta_t(L))$ diverges *exponentially* with L, in contrast to (5.11a). Nevertheless, $1/\nu(L,\beta_t(L))$ is a *good approximation* for the RG eigenvalue $y_T = d$. Indeed, (5.4) and the fact that $E_m(L,\beta_t(L)) = E_m(1+O(q^{-bL}))$ imply that

$$\frac{1}{\nu(L,\beta_t(L))} = d + \frac{1}{\log L}\left(\frac{E_d - E_o}{2}\right) + O(q^{-bL}) \ . \tag{5.13}$$

Unfortunately, the convergence of $\nu(L,\beta)$ to $1/d$ depends crucially on the right choice of β. If we chose, e.g., β_t instead of $\beta_t(L)$, the answer to the question whether $\nu(L,\beta)$ converges to $1/d$ for $d > 2$ (for $d = 2$, $\beta_t(L) = \beta_t$) will depend on the *sign* of the constant K in (5.7). If the deviation from $\beta_t(L)$ is given by (5.7) with $K < 0$, $(x\xi_L)(\beta = \beta_t)$ will go to $-\infty$ as L goes to ∞[10]. Inserting this behaviour into (5.4) we find that

$$\frac{1}{\nu(L,\beta_t)} = d + \frac{E_d - E_o}{\log L} + O(q^{-bL}) \ . \tag{5.14a}$$

But if the deviation from $\beta_t(L)$ is given by (5.7) with $K > 0$, $(x\xi_L)(\beta = \beta_t)$ will go to $+\infty$ as L goes to ∞, the derivative of $\xi^{-1}(L,\beta)$ at the point β_t goes to zero and

$$\frac{1}{\nu(L,\beta_t)} \sim -\frac{L^{d-1}}{\log L} O(1) \qquad as \qquad L \to \infty \ . \tag{5.14b}$$

The sensitivity of $\nu(L,\beta_t)$ on the *sign* of the exponential small shift (5.7) makes $\nu(L,\beta_t)$ useless for numerical calculations in $d > 2$. But this puts some doubt on the usefulness of $\nu(L,\beta_t(L))$ as well, since β_t and $\beta_t(L)$ might be numerically hard to distinguish.

In the following, I propose to different strategies to avoid this problem. While the second one tries to *avoid* the strong dependence of $\nu(L,\beta)$ on β by slightly modifying its

[10] We recall that $\xi_L \sim e^{\beta\sigma L^{d-1}}$; this obviously overwhelms the exponential decrease of $x \sim L^{d-1}e^{-L/L_0}$.

definition, the first one does in fact *use* this dependence. I start from the observation that $\nu(L,\beta)$ does converge to the right value $1/d$ if $\beta < \beta_t(L)$ and $|\beta-\beta_t|L^{d-1} < 1$. Recalling that the specific heat in a *cubic volume* is maximal for $\beta = \beta_{C_{\max}}(L) = \beta_t - L^{-d}\log q/(E_d - E_o) + O(L^{-2d})$, see e.g. [3], it seems natural to consider $\nu(L,\beta)$ at the point $\beta_{C_{\max}}(L)$. With this choice, $\beta - \beta_t(L) \sim KL^{-d}$ and $x \sim K'L^{-1}$ with *negative* constants $K < 0$, $K' < 0$. As a consequence,

$$\xi^{-1}(L,\beta) \sim L^{-1} \tag{5.15a}$$

and

$$\frac{d\xi^{-1}(L,\beta)}{d\beta} \sim L^{-1+d} \tag{5.15b}$$

provided β is chosen as the point $\beta_{C_{\max}}(L)$ where the specific heat in the corresponding *cubic volume* is maximal. Note the similarity between relations (5.15) and the second-order relations (5.11).

The second strategy starts from the observation that the x dependance of $d\xi_{\text{sym}}^{-1}(L,\beta)/d\beta$ and $d\xi^{-1}(L,\beta)/d\beta$ is of the same form. If one considers the difference $d\xi_{\text{sym}}^{-1}(L,\beta)/d\beta - 2\, d\xi^{-1}(L,\beta)/d\beta$, this dependance cancels out. As a consequence,

$$\frac{1}{\tilde{\nu}(L,\beta)} = \frac{1}{\log L} \log\left(\frac{d}{d\beta}(L\xi_{\text{sym}}^{-1}(L,\beta) - 2L\xi^{-1}(L,\beta))\right) \tag{5.16}$$

has a much weaker β dependance. In fact, as long as β stays in the range (5.1),

$$\frac{1}{\tilde{\nu}(L,\beta)} = d + \frac{E_d - E_o}{\log L} + O(q^{-bL}) + O(\beta - \beta_t)\ . \tag{5.17}$$

This makes the definition (5.17) very promising for numerical simulations.

Remarks: i) None of the considerations in this section depends very strongly on the precise form of ξ_L. A powerlaw correction $O(L^{\omega})$, e.g., would not destroy the results derived in this section. This makes it very plausible that the results of this section remain valid for small q, even though their rigorous proof requires large q.

ii) The reader should be warned, however, to ignore the condition "for L sufficiently large". Taking for example the $q = 5$ Potts model in $d = 2$, which has a correlation length of a few thousand lattice spacings, numerical simulations on lattices as large as 100×100 might quite well give critical exponents, even though the infinite volume transition is first-order.

Appendix.

In this appendix I want to prove Theorem 3.2. In fact, Theorem 3.2 follows immediately from the results of [21]. For the convenience of the reader, I give an independent proof here. I recall that the periodic partition function $Z_{\rm per}(V,\beta)$ is defined as

$$Z_{\rm per}(V,\beta) = \sum_{\sigma_V} \prod_{<xy>\in V_1} e^{\beta\delta(\sigma_x,\sigma_y)} \ , \tag{A.1}$$

where V_1 is the set of all $d|V|$ nearest neighbor bonds in V and $\delta(\cdot,\cdot)$ is the Kronecker delta. Rewriting $Z^{(n)}$ as defined in (3.20) as

$$Z^{(n)} = \sum_{\sigma_V} \prod_{<xy>\in V_1\setminus B_{12}} e^{\beta\delta(\sigma_x,\sigma_y)} \prod_{<xy>\in B_{12}} e^{\beta\delta(\sigma_x e^{-2\pi i n/q},\sigma_y)} \ ,$$

where B_{12} is the set of nearest neighbor pairs $< xy >$ for which x lies in the first and y in the the second time slice of V, the partition function corresponding to the symmetric subspace of $\mathcal{H}$ can be rewritten as

$$Z_{\rm sym}(L,\beta) = \frac{1}{q}\sum_{n=0}^{q-1} Z^{(n)} \ ,$$

see Section 3, equation (3.19) and (3.20). If we introduce

$$\varphi_{xy} = \varphi_{xy}(n) = \begin{cases} 0 & \text{if} \quad < xy > \notin B_{12} \ , \\ 2\pi i n/q & \text{if} \quad < xy > \in B_{12} \ , \end{cases} \tag{A.2}$$

the partition function $Z_{\rm sym}(L,\beta)$ can be expressed as

$$Z_{\rm sym}(L,\beta) = \frac{1}{q}\sum_{n=0}^{q-1}\sum_{\varphi_V} \prod_{<xy>\in V_1} e^{\beta\delta(1,e^{i(\varphi_x-\varphi_y-\varphi_{xy}(n))})} \ , \tag{A.3}$$

where the second sum goes over all configurations $\varphi_V : V \to \{0, 2\pi/q, \cdots, 2\pi(q-1)/q\}$. Note that the sum over n gives the projection onto the symmetric subspace of $\mathcal{H}$.

Equation (A.3) is the starting point of our analysis. Following the usual strategy of duality transformations (see e.g. [25]) , we introduce the the dual inverse temperature β^*,

$$(e^{\beta^*} - 1)(e^{\beta} - 1) = q \, , \tag{A.4}$$

and rewrite the weight $e^{\beta\delta(1,.)}$ as

$$e^{\beta\delta(1,e^{i\varphi})} = 1 + (e^{\beta} - 1)\delta(1, e^{i\varphi}) = 1 + \frac{e^{\beta} - 1}{q}\sum_{p=0}^{q-1} e^{ip\varphi} = \frac{e^{\beta} - 1}{q}\sum_{p=0}^{q-1} e^{ip\varphi} e^{\beta^*\delta(0,p)} \, . \tag{A.5}$$

Inserting (A.5) into (A.3), one finds that

$$\begin{aligned} Z_{\text{sym}}(L,\beta) &= \left(\frac{e^{\beta}-1}{q}\right)^{2|V|} \frac{1}{q} \sum_{n,\varphi_V} \sum_{p_{V_1}} \prod_{<xy>\in V_1} e^{\beta^*\delta(0,p_{xy})} e^{i(\varphi_x - \varphi_y - \varphi_{xy}(n))p_{xy}} \\ &= \left(\frac{e^{\beta}-1}{q}\right)^{2|V|} \sum_{p_{V_1}} \prod_{<xy>\in V_1} e^{\beta^*\delta(0,p_{xy})} \sum_{\varphi_V} e^{i(d\varphi,p)} \frac{1}{q}\sum_{n} e^{-i\frac{2\pi n}{q}\sum_{<xy>\in B_{12}} p_{xy}} \, , \end{aligned}$$

where $(d\varphi, p) = \sum\limits_{<xy>\in V_1} (\varphi_x - \varphi_y)p_{xy}$. After summation by parts,

$$(d\varphi, p) = \sum_x \varphi_x (d^*p)_x \qquad \text{with} \qquad (d^*p)_x = \sum_{y:|y-x|=1} p_{xy} \, ,$$

the sum over φ_V and n in $Z_{\text{sym}}(L,\beta)$ can be carried out, giving a product of δ-functions on $\mathbf{Z}_q$. One obtains

$$Z_{\text{sym}}(L,\beta) = \left(\frac{e^{\beta}-1}{q}\right)^{2|V|} q^{|V|} {\sum_{p_{V_1}}}' \prod_{<xy>\in V_1} e^{\beta^*\delta(0,p_{xy})} \, , \tag{A.6}$$

where the sum is restricted to those configurations $p_{V_1} :< xy > \mapsto p_{xy}$ for which $d^*p = 0 \bmod q$ and $\sum_{<xy>\in B_{12}} p_{xy} = 0 \bmod q$.

At this point, we replace V by the dual lattice V^*, obtaining

$$Z_{\mathrm{sym}}(L,\beta) = \left(\frac{e^{\beta}-1}{q}\right)^{2|V|} q^{|V|} {\sum_{p_{V_1^*}}}' \prod_{<xy>\in V_1^*} e^{\beta^* \delta(0,p_{xy})} \tag{A.7}$$

where the sum goes over all configurations $p_{V_1^*} : V_1^* \to \{0,\cdots,q-1\}$ such that

$$dp = 0 \bmod q \qquad \text{and} \qquad \sum_{<xy>\in B_{12}^*} p_{xy} = 0 \bmod q\ . \tag{A.8}$$

Consider now a function $p_{V_1^*} : V_1^* \to \{0,\cdots,q-1\}$ which obeys the constraints (A.8). We would like to write p as dr, with $r : V^* \to \{0,\cdots,q-1\}$. A minute of reflection shows that this is possible if and only if

$$\sum_{<xy>\in C} p_{xy} = 0 \bmod q \tag{A.9}$$

for all closed loops C. Furthermore, there are exactly q different possibilities to rewrite q as dr if the condition (A.9) is valid. Unfortunately, the relations (A.8) do only guaranty (A.9) for those closed loops which are topologically trivial, or which are closed via the periodicity in the "space" direction[11], while a loop C which is closed via the periodicity in time direction can give rise to a number

$$n(C) = \sum_{<xy>\in C} p_{xy} \neq 0 \bmod q\ .$$

It is an easy exercise, however, to show that this corresponds just to one additional degree of freedom $n \in \{0,\cdots,q-1\}$, and that any p which satisfies the conditions (A.8) can be written as $p = dr + \tilde{n}$, where r is a function $r : V^* \to \{0,\cdots,q-1\}$ and

$$\tilde{n}_{xy} = \tilde{n}_{xy}(n) = \begin{cases} 0 & \text{if} \quad <xy> \notin \tilde{B}_{12}\ , \\ n & \text{if} \quad <xy> \in \tilde{B}_{12}\ . \end{cases}$$

[11] Note that B_{12}^* is such a loop, and that all loops which are closed by the periodicity in the space direction can be build up from topologically trivial loops and B_{12}^*.

Here $\tilde{B}_{12}$ consists of all bonds in V_1^* which are made of a point x in the first and a point y in the second time slice of V_1^*. Finally, r and n are uniquely determined through p, except for the freedom of adding a constant function $(\delta r)_x = s$, $s = 0, \cdots, q-1$ to r. Putting these facts together, we may replace the sum over p in (A.7) by a sum over n and r, obtaining that

$$Z_{\rm sym}(L,\beta) = \left(\frac{e^{\beta}-1}{q}\right)^{2|V|} q^{|V|} \frac{1}{q} \sum_{n=0}^{q-1} \sum_{r_{V^*}} \prod_{<xy>\in V_1^*} e^{\beta^* \delta(1, e^{i(\varphi_x - \varphi_y - \tilde{\varphi}_{xy}(n))})} \ , \qquad (A.10)$$

where $\tilde{\varphi}_{xy}(n)$ is defined by (A.2) with B_{12} replaced by $\tilde{B}_{12}$. Comparing (A.3) and (A.10) and recalling that V and V^* are isomorphic, we obtain the desired equality

$$\begin{aligned} Z_{\rm sym}(L,\beta) &= \left(\frac{e^{\beta}-1}{q}\right)^{2|V|} q^{|V|} Z_{\rm sym}(L,\beta^*) \\ &= \left(\frac{e^{\beta}-1}{e^{\beta^*}-1}\right)^{|V|} Z_{\rm sym}(L,\beta^*) \ . \end{aligned} \qquad (A.11)$$

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