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Series expansions for the q-colour problem on the square and cubic lattices

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Abstract. We apply the finite lattice and cluster expansion methods to evaluate the numbers of q-colourings $\omega(D, q)$ of the square and cubic lattices. In two dimensions, we develop an efficient transfer matrix algorithm to obtain the $1/(q-1)$-expansion of $\omega(D=2, q)$ to order 36, and in three dimensions we construct expansions about the long-range ordered states. We show (for $D=2$) that it is also efficient to use the formulae of the finite-lattice method substituting into them numerical values of the partition functions of finite lattices. Reliable estimates of ω are obtained in all cases.

1. Introduction

This paper deals with the problem of counting the number of ways W to colour a map (sites of a lattice) into q colours subject to the constraint that no two neighbouring sites should be of the same colour, or, equivalently, evaluating the ground-state entropy of the q-state antiferromagnetic (AF) Potts model laid on this lattice [1]. We consider the square and cubic lattices, that is the 2D and 3D hypercubic lattices which split into two sublattices A and B. If the lattice contains $V \to \infty$ sites, then W is of the form $W = \omega^V$ (if $q > 2$ then $1 < \omega < q$). Lieb [2] obtained the exact result $\omega(D=2, q=3) = (4/3)^{3/2} = 1.539\,600\,72\ldots$. Nagle [3] obtained the $z \equiv 1/(q-1)$-expansion of $\omega(D=2,\ q)$ by diagrammatic techniques, and Kim and Enting [4] extended this series to z^{18} using the finite-lattice method (FLM). Mattis [5] proposed a transfer matrix statement of this problem which leads to the estimate for general q and D,

$$\omega(D, q) > 1 + \frac{(q-2)^D}{(q-1)^{D-1}} \tag{1}$$

(the diagrammatic meaning of this formula is that the summation is over the diagrams comprising disjoint unit hypercubes [6]). The Mattis formula is asymptotically exact at $D, q \gg 1$, the error at $D = 2, q = 3$ is 2.6%, and, as we will show, in the cases $D = 2, q = 4$ and $D = 3, q = 3, 4$ it is 0.1%, 13.5%, and 7%, respectively. In addition, for $D = 3$ we only know of the numerical studies of Chen and Pan [7].

We describe series expansions based, for $D = 2$, on the FLM (see [8–12]), which is probably the most efficient and completely automated method for generating series, and, for $D = 3$, on the cluster expansion method [13]. It is believed that the type of low-temperature ordering of the AF Potts model is different in two and three dimensions. The square lattice AF Potts model is disordered at $T = 0$ [14]; in this case we use the FLM with the free

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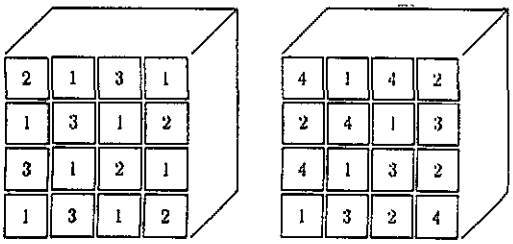

(*a*) (*b*)

Figure 1. Ordering of the cubic lattice AF Potts models: (*a*) BSS for $q = 3$ and (*b*) AF for $q = 4$ [15].

boundary conditions (BC) and z-expansion of ω. We compute this series to order z^{36}, thus adding 18 terms to the result of Kim and Enting [4]. The model laid on the cubic lattice has long-range order [15], see figure 1: the broken symmetry state (BSS) order for $q = 3$ (colour 1 on A, and colours 2 and 3 on B), and 'AF' order for $q = 4$ (1 and 2 on A, and 3 and 4 on B). The z-expansion gives poor results in this case, while the expansions about the BSS or the AF state yield good estimates of ω. This fact lends some additional support to the hypothesis about ordering of the 2D and 3D AF Potts models. We also propose to use the formulae of FLM as a finite-size extrapolation, or optimization. This approach seems to be very accurate, at least for $D = 2$.

2. Finite lattice method

Let W_g be the number of colourings of a finite lattice g

$$W_g = \sum_{\{s_i\}} \prod_{\langle ij \rangle} [1 - \delta(s_i, s_j)] \tag{2}$$

where i enumerates sites of g, $\langle ij \rangle$ is a pair of nearest neighbours, s_i is the colour of site i, $s_i \in \{1, \ldots, q\}$. The colouring number of the square/cubic lattice is equal to the limit

$$w = \lim_{\substack{V_g \to \infty \\ B_g/V_g \to 2}} W_g^{\,1/V_g} \tag{3}$$

where V_g and B_g are the numbers of sites and bonds of g, respectively, and $D = 2$ or 3.

In the 2D case we use the FLM. Let $W_{m,n}$ be the number of colourings of a rectangle consisting of n layers of m sites. It is natural to introduce the quantities

$$W^{c}_{m,n} = q^{-V_{mn}} \left(\frac{q-1}{q} \right)^{-B_{mn}} W_{m,n} \tag{4}$$

which are polynomials in z, [4, 6]. According to the FLM

$$w = q \left(\frac{q-1}{q} \right)^{2} \prod_{m=2}^{\infty} \prod_{n=2}^{\infty} \Phi_{m,n} \tag{5}$$

where $\Phi_{m,n}$ are to be found recursively from the relation

$$W^{c}_{m,n} = \prod_{m'=2}^{m} \prod_{n'=2}^{n} (\Phi_{m',n'})^{(m-m'+1)(n-n'+1)} \tag{6}$$

and have the following asymptotic:

$$\Phi_{m,n} = 1 + O\left(z^{2m+2n-5}\right). \tag{7}$$

Taking into account all the rectangles $m + n \leqslant L + 2$, we have

$$w = \prod_{k=0}^{L} v_k + O(z^{2L+1}) \tag{8}$$

where

$$v_k = \prod_{m=1}^{k+1} \Phi_{m,k+2-m} = 1 + O(z^{2k-1}). \tag{9}$$

As usual, we compute Ws using a transfer matrix algorithm. We find it most efficient to develop a transfer matrix algorithm for $W_{m,n}$ and then reduce it to $W^c_{m,n}$ using (4). If we compute $W^c_{m,n}$ by a transfer matrix algorithm for rectangles with up to m_0 sites in a layer, then in (8) we can put $L = 2m_0 - 1$. (Clearly, when $m > m_0$ and $n \leqslant m_0$ we use the symmetry $W_{m,n} = W_{n,m}$).

In section 4 we consider two lowest-order contributions to v_k (9),

$$v_k = 1 + \alpha_k z^{2k-1} + \beta_k z^{2k} + O(z^{2k+1}). \tag{10}$$

Thus, taking in (10) $k = 2m_0$, in (8) we can put $L = 2m_0$ and receive a z-expansion to order z^{4m_0}.

To calculate the leading terms of v_k we use the connection between the cluster expansion and FLM

$$\Phi_{m,n} = \prod_{g \in G(m,n)} \Phi(g) \tag{11}$$

where $G(m, n)$ is the set of clusters (connected diagrams) for which the minimum rectangle containing the cluster is $m \times n$, and $\Phi(g)$ is defined recursively from the cluster expansion method

$$W_g = \prod_{g' \subseteq g} \Phi(g')^{L(g',g)} \tag{12}$$

where $L(g', g)$ is the number of subgraphs of g equivalent to g'. A cluster g with b bonds and l loops has the asymptotic

$$\Phi(g) = 1 + (-1)^b z^{b-l} + \cdots. \tag{13}$$

The sets of clusters contributing to the leading orders α_k and β_k are simple. We describe them in section 4.

3. 2D transfer matrices

We compute $W_{m,n}$ (we choose $m \leqslant n$) by a transfer matrix algorithm, in which we add one site at each step, so that the rectangle is filled layer by layer and each layer is filled site by site from one edge to another. Suppose that we completely filled $x - 1$ layers, and y sites in layer x. Consider m sites filled last and enumerate them by the index i equal to the ordinal number of a site in its layer (sites $i = 1, \ldots, y$ lie in layer x and the other sites $i = y + 1, \ldots, m$ lie in layer $x - 1$; if $y = m$ we deal with x filled layers). Let us denote a colouring $\{s_i\}_{i=1}^m$ of these sites by $\Psi_{m,y}$. Clearly, we only have to consider colourings such that $s_i \neq s_{i+1}$, $i = 1, \ldots, m - 1$, $i \neq y$. Let $\widetilde{W}_{m,x,y}(\Psi_{m,y})$ be the number of colourings of the filled part of rectangle with fixed $\Psi_{m,y}$. Consider a permutation P of the set of colours $\{1, \ldots, q\}$. It transforms a colouring $\Psi_{m,y}$ into $\Psi'_{m,y} = P\Psi_{m,y}$. We will say that Ψ and Ψ' are equivalent, $\Psi \sim \Psi'$, if there exists a P such that $\Psi' = P\Psi$. Clearly $\widetilde{W}_{m,x,y}(\Psi_{m,y}) = \widetilde{W}_{m,x,y}(\Psi'_{m,y})$ if $\Psi_{m,y} \sim \Psi'_{m,y}$. A colouring $\Psi_{m,y}$ is said to be arranged if

new colours occur consecutively, $s_1 = 1$ and $s_i \leqslant 1 + \max_{1 \leqslant j < i} s_j$, $i = 2, \ldots, m$. Let us denote arranged colourings by $\Psi^{\mathrm{a}}_{m,y}$. For an arbitrary colouring $\Psi_{m,y}$ there exists a unique arranged colouring $\Psi^{\mathrm{a}}_{m,y}$ such that $\Psi_{m,y} \sim \Psi^{\mathrm{a}}_{m,y}$. Let $W_{m,x,y}(\Psi^{\mathrm{a}}_{m,y})$ be the number of colourings of the filled part with $\Psi^{\mathrm{a}}_{m,y}$ such that $\Psi_{m,y} \sim \Psi^{\mathrm{a}}_{m,y}$. We have

$$W_{m,x,y}(\Psi^{\mathrm{a}}_{m,y}) = M(\Psi^{\mathrm{a}}_{m,y})\widetilde{W}_{m,x,y}(\Psi^{\mathrm{a}}_{m,y}) \tag{14}$$

where $M(\Psi^{\mathrm{a}}_{m,y})$ is the number of colourings $\Psi_{m,y}$ equivalent to $\Psi^{\mathrm{a}}_{m,y}$

$$M(\Psi^{\mathrm{a}}_{m,y}) = \prod_{k=1}^{Q(\Psi^{\mathrm{a}}_{m,y})} (q - k + 1) \qquad Q(\Psi^{\mathrm{a}}_{m,y}) = \max_{1 \leqslant i \leqslant m} s^{\mathrm{a}}_i . \tag{15}$$

To begin the transfer matrix algorithm, we fill the first layer

$$W_{m,1,m}(\Psi^{\mathrm{a}}_{m,m}) = M(\Psi^{\mathrm{a}}_{m,m}) \tag{16}$$

and after filling the rectangle completely we sum over arranged colourings

$$W_{m,n} = \sum_{\Psi^{\mathrm{a}}_{m,m}} W_{m,n,m}(\Psi^{\mathrm{a}}_{m,m}) . \tag{17}$$

Let $N_{m,y}$ be the number of arranged colourings $\Psi^{\mathrm{a}}_{m,y}$. To compute them, firstly we note, by considering for $y < m$, the two cases $s_y \neq s_{y+1}$ and $s_y = s_{y+1}$ that

$$N_{m,y} = N_{m,m} + N_{m-1,m-1} \qquad y = 1, \ldots, m-1 . \tag{18}$$

To compute $N_{m,m}$ we use the recurrence

$$\begin{aligned} &\widetilde{N}(0,k) = 1 \qquad k = 1, 2, \ldots \\ &\widetilde{N}(m',k) = (k-1)\widetilde{N}(m'-1,k) + \widetilde{N}(m'-1,k+1) \qquad m', k = 1, 2, \ldots \\ &N_{m,m} = \widetilde{N}(m-1,1) \end{aligned} \tag{19}$$

where $\widetilde{N}(m',k)$ is the number of arranged colourings of the chain such that colours at first $m - m'$ sites are fixed, and $k = \max_{1 \leqslant i \leqslant m-m'} s_i$ ($\widetilde{N}(m',k)$ depend on m only through k). The numbers $\widetilde{N}(m',k)$ allow to define the ordinal number of an arranged colouring $\nu(\Psi^{\mathrm{a}}_{m,y})$. For $y = m$ we put

$$\nu(\Psi^{\mathrm{a}}_{m,m}) = 1 + \sum_{i=3}^{m} [s_i - 1 - \chi(s_i, s_{i-1})]\widetilde{N}(m-i, \max_{1 \leqslant j < i} s_j) \tag{20}$$

where

$$\chi(s_i, s_{i-1}) = \begin{cases} 1 & s_i > s_{i-1} \\ 0 & s_i < s_{i-1} \end{cases} \tag{21}$$

and for $y < m$

$$\nu(\Psi^{\mathrm{a}}_{m,y}) = \begin{cases} \nu(\Psi^{\mathrm{a}}_{m,m}) & s_y \neq s_{y+1} \\ N_{m,m} + \nu(\Psi^{\mathrm{a}}_{m-1,m-1}) & s_y = s_{y+1} \end{cases} \tag{22}$$

where $\Psi^{\mathrm{a}}_{m-1,m-1} = \{s'_i\}_{i=1}^{m-1}$, $s'_i = s_i$, $i \leqslant y$, $s'_i = s_{i+1}$, $i > y$.

There is another way to compute $N_{m,m}$:

$$N_{m,m} = \frac{\mathrm{d}^{m-1}}{\mathrm{d}x^{m-1}} \left(\mathrm{e}^{\mathrm{e}^x - 1}\right)\Big|_{x=0} . \tag{23}$$

The N's we will need in this study are listed in table 1.

Table 1.

m	1	2	3	4	5	6	7	8	9	10
$N_{m,m}$	1	1	2	5	15	52	203	877	4140	21 147
$N_{m,y},\ y < m$	—	2	3	7	20	67	255	1080	5017	25 287

Now we will introduce the transfer matrices $T_{m,y}$ so that

$$\begin{aligned} W_{m,x,1}(\Psi^{a}_{m,1}) &= \sum_{\Psi^{a}_{m,m}} T_{m,1}(\Psi^{a}_{m,1}, \Psi^{a}_{m,m}) W_{m,x-1,m}(\Psi^{a}_{m,m}) \\ W_{m,x,y}(\Psi^{a}_{m,y}) &= \sum_{\Psi^{a}_{m,y-1}} T_{m,y}(\Psi^{a}_{m,y}, \Psi^{a}_{m,y-1}) W_{m,x,y-1}(\Psi^{a}_{m,y-1}) \qquad y = 2, \ldots, m\,. \end{aligned} \tag{24}$$

The transfer matrix element $T_{m,y}(\Psi^{a}_{m,y}, \Psi^{a}_{m,y-1})$ (or $T_{m,1}(\Psi^{a}_{m,1}, \Psi^{a}_{m,m})$ if $y = 1$) is equal to the number of ways to transform a colouring $\Psi^{a}_{m,y-1}$ ($\Psi^{a}_{m,m}$) into $\Psi^{a}_{m,y}$ by means of substituting an arbitrary colour (from $\{1, \ldots, q\}$) for s_y and reducing the obtained colourings to arranged ones. By construction, every non-vanishing element of a transfer matrix $T_{m,y}$ corresponds uniquely to an arranged colouring $\Psi^{a}_{m+1,m+1}$, and we can define sets of non-vanishing elements of transfer matrices as follows.

Let $\Psi^{a}_{m+1,m+1} = \{s_i\}_{i=1}^{m+1}$. Eliminating site y we obtain a colouring $\{s'_i\}_{i=1}^{m}$ such that $s'_i = s_i$ for $i < y$ and $s'_i = s_{i+1}$ for $i > y$. The colouring equivalent to it will be some $\Psi^{a}_{m,y-1}$ ($\Psi^{a}_{m,m}$ if $y = 1$), which we denote by $\Psi^{a}_{m,y-1}(\Psi^{a}_{m+1,m+1})$. (Observe that the function $\Psi^{a}_{m,0}(\Psi^{a}_{m+1,m+1})$ takes on values in the set of colourings $\{\Psi^{a}_{m,m}\}$ but it does not coincide with the function $\Psi^{a}_{m,m}(\Psi^{a}_{m+1,m+1})$ taking on values in the same set.) Now we can list all the non-vanishing transfer matrix elements by the formulae

$$T_{m,y}(\Psi^{a}_{m,y}(\Psi^{a}_{m+1,m+1}), \Psi^{a}_{m,y-1}(\Psi^{a}_{m+1,m+1})) = t_{m,y}(\Psi^{a}_{m+1,m+1}) \qquad y = 1, \ldots, m \tag{25}$$

where

$$t_{m,y}(\Psi^{a}_{m+1,m+1}) = \begin{cases} q + 1 - \max\limits_{1 \leqslant i \leqslant m+1} s_i & s_y \neq s_j \quad \text{for all} \quad j \neq y \\ 1 & \text{otherwise} \end{cases} \tag{26}$$

takes into account that there are $q - k$ equivalent ways to add a new colour to a colouring involving k colours.

Finally, to compute directly $W^{c}_{m,n}$ which are polynomials in z we define

$$W^{c}_{m,x,y}(\Psi^{a}_{m,y}) = q^{-V_{m,x,y}} \left(\frac{q-1}{q}\right)^{-B_{m,x,y}} W_{m,x,y}(\Psi^{a}_{m,y}) \tag{27}$$

where $V_{m,x,y} = mx - m + y$, $B_{m,x,y} = 2mx - 3m - x + 2y$. For the first filled layer, from (16) we get

$$W^{c}_{m,1,m}(\Psi^{a}_{m,y}) = z^{m - Q(\Psi^{a}_{m,y})} \prod_{k=2}^{Q(\Psi^{a}_{m,y})} [1 - (k-2)z]\,. \tag{28}$$

We obtain a transfer matrix algorithm by substituting $W^{c}_{m,x,y}$ and $T^{c}_{m,y}$ for $W_{m,x,y}$ and $T_{m,y}$ in (17) and (24), where

$$T^{c}_{m,1} = zT_{m,1} \qquad T^{c}_{m,y} = (z + z^2)T_{m,y} \qquad y = 2, \ldots, m\,. \tag{29}$$

4. 2D diagrams contributing to two lowest orders of v_k

Using (13) to select clusters contributing to the lowest orders of v_k, we find that the first contribution α_k equals the number of convex polygons of length $2k$ which satisfy the following rule (we will call them C_k-contours):

> if two nearest neighbours on the square lattice i and j belong to a polygon then the bond connecting them also belongs to this polygon.

Guttmann and Enting [11] evaluated the exact generating function of convex polygons; we found that subject to this constraint it takes the form

$$\sum_{k=4}^{\infty}\alpha_k x^{2k} = x^8\frac{2-2x^2-x^2\sqrt{1-4x^2}}{(1-4x^2)(2+x^2)} + x^{12}\frac{3-4x^2-4\sqrt{1-4x^2}}{(1-4x^2)^2}. \tag{30}$$

The second contribution to v_k, β_k, can be calculated as follows. Consider a C_k-contour. Find a site within the domain bounded by C_k which has $p > 1$ nearest neighbours belonging to C_k. The cluster obtained by adding this site to C_k and all bonds connecting it with its nearest neighbours on C_k contribute $p-1$ to β_k. Let $\rho(C_k; p)$ be the number of sites within the domain bounded by C_k which have p nearest neighbours belonging to C_k. Then

$$\beta_k = \sum_{\{C_k\}}\sum_{p=2}^{4}(p-1)\rho(C_k; p). \tag{31}$$

We constructed a transfer matrix to compute β_k. Its dimensionality increases only as k^3. We list several vs:

$$\begin{aligned} v_{18} &= 1 + 356\,923\,968z^{35} + 4281\,819\,554z^{36} + O(z^{37}) \\ v_{19} &= 1 + 1520\,962\,956z^{37} + 18\,999\,367\,420z^{38} + O(z^{39}) \\ v_{20} &= 1 + 6462\,604\,898z^{39} + 83\,924\,203\,204z^{40} + O(z^{41}). \end{aligned} \tag{32}$$

5. Results for the square lattice

We calculated all the $W^{c}_{m,n}$ with $m+n \leqslant 19$ by the transfer matrix algorithm described in section 3, and found from (5) and (9) all the v_ks with $k \leqslant 17$. This computation required 5 Mb CPU memory and 3 minutes CPU time on a IBM PC AT 386 with the Intel 80860 microprocessor (1.6 of the total 5 Mb were used to store the functions $\Psi^{a}_{m,y}(\Psi^{a}_{m+1,m+1})$ and $t_{m,y}(\Psi^{a}_{m+1,m+1})$ only to expedite computations). Then we used two lowest-order terms for v_{18}, (32), and finally obtained

$$\begin{aligned} w(D=2,q) = \frac{(q-1)^2}{q}\big(1 &+ z^3 + z^7 + 3z^8 + 4z^9 + 3z^{10} + 3z^{11} + 11z^{12} + 24z^{13} + 8z^{14} \\ &- 91z^{15} - 261z^{16} - 290z^{17} + 254z^{18} + 1671z^{19} + 3127z^{20} + 786z^{21} \\ &- 13\,939z^{22} - 49\,052z^{23} - 80\,276z^{24} + 21\,450z^{25} + 515\,846z^{26} \\ &+ 1411\,017z^{27} + 1160\,761z^{28} - 4793\,764z^{29} - 20\,340\,586z^{30} \\ &- 29\,699\,360z^{31} + 33\,165\,914z^{32} + 256\,169\,433z^{33} + 495\,347\,942z^{34} \\ &- 127\,736\,296z^{35} - 3068\,121\,066z^{36} + O(z^{37})\big). \end{aligned} \tag{33}$$

Clearly, higher-order coefficients display some regularity. Therefore, for $q = 3$ we factor out several first terms and Pade-approximate the remainder, see table 2. In table 3 we list typical $q = 3$ partition functions for rectangles with free BC. They may be counted

Table 2.

[26,8]	[25,11]	[26,10]
1.539 90	1.539 73	1.539 69

Table 3.

$m \times n$	2×2	3×3	4×4	5×5	6×6	7×7	7×8
$W_{mn}[q=3]$	18	246	7812	580 986	101 596 896	41 869 995 708	1 053 631 126 386
$\omega_{mn}[q=3]$	2.06	1.84	1.75	1.70	1.6688	1.6473	1.6394

Table 4.

L	13	14	15	16	17
ω_L	1.532 9151	1.533 9998	1.534 8392	1.535 5031	1.536 0371
ω'_L	1.539 569	1.539 614	1.539 599	1.539 602	1.539 601

even on an IBM PC by the method of section 3, or, more easily, by constructing allowed impositions of properly coloured straight-line segments. These numerical estimates of ω improve dramatically if we do 'Enting's optimization', that is substitute the exact numerical values of W's into (4), (5) and (6) (table 4). It is also useful to note that the sequence ω_L seems to have the asymptotic limit $\omega_L = \omega(2,3) + C/L^2$, so the sequence

$$\omega'_L = \omega_L - \frac{3}{2}\frac{(\omega_{L+2} - \omega_L)(\omega_L - \omega_{L-2})}{(\omega_{L+2} - 2\omega_L + \omega_{L-2})} \tag{34}$$

converges to $\omega(2,3)$ not worse than as L^{-3}. Finally, we obtain the estimate

$$\omega(D=2, q=3) = 1.539\,601 \pm 0.000\,001\,.$$

For $q = 4$ the Pade-approximants converge very rapidly, and we have the estimate

$$\omega(D=2, q=4) = 2.336\,056\,641 \pm 0.000\,000\,001.$$

6. BSS and AF expansions for the cubic lattice

For $D = 3$ and small q we found that the z-expansion does not give good results, so we used another method. Let us introduce a parameter x so that when $x = 0$ we obtain the pure BSS and AF order for odd and even q, respectively:

$$W(\mathcal{L}; q, x) = \sum_{\{s_i\}} \prod_{i \in A} x^{\alpha_i} \prod_{i \in B} x^{\beta_i} \prod_{(ij) \in \mathcal{L}} \left(1 - \delta(s_i, s_j)\right) \tag{35}$$

where

$$\alpha_i = \sum_{k=[q/2]+1}^{q} \delta(s_i, k) \qquad \beta_i = \sum_{k=1}^{[q/2]} \delta(s_i, k) \tag{36}$$

and $[q/2]$ is for the integer part of $q/2$.

As usual, we define the limit

$$\omega(D, q, x) = \lim_{\substack{V \to \infty \\ B/V \to D}} \left(W(\mathcal{L}; q, x)\right)^{1/V}. \tag{37}$$

Clearly, $\omega(D,q) = \omega(D,q,1)$. A simple duality relation holds: $\omega(D,q,x) = x\omega(D,q,1/x)$.

The zero-order term of this x-expansion is

$$\omega(D,q,0) = \begin{cases} \frac{1}{2}\sqrt{q^2-1} & q \text{ odd} \\ \frac{1}{2}q & q \text{ even} \end{cases} \tag{38}$$

and that of the z-expansion equals $(q-1)^D/q^{D-1}$. Since both of them are lower bounds for $\omega(D,q)$, we suppose, roughly, that the x-expansion yields better results if

$$\omega(D,q,0) > \frac{(q-1)^D}{q^{D-1}}. \tag{39}$$

$D = 3$, $q = 3$ and 4 satisfy this inequality, and for $q \geqslant 5$ it is not valid.

We shall use the method of cluster expansion. To apply it, we impose the appropriate BC. For a finite lattice g we define

$$W_{\mathrm{cl}}(g,x) = \frac{1}{q_A^{V_A(g'\setminus g)}} \frac{1}{q_B^{V_B(g'\setminus g)}} \sum_{\{s_i\}_{i\in g'}} \prod_{i\in A} x^{\alpha_i} \prod_{i\in B} x^{\beta_i} \prod_{\langle ij\rangle \in g'} (1-\delta(s_i,s_j)) \tag{40}$$

where g' is a finite lattice obtained by adding to g all sites $i \in \mathcal{L}$ which have nearest neighbours belonging to g, $V_A(g'\setminus g)$ and $V_B(g'\setminus g)$ are the number of added sites belonging to A and B, respectively, $q_A = [q/2]$ and $q_B = q - q_A$, and we impose the following restriction on the BC spins: $s_i = 1,\ldots,q_A$ if $i \in A \cap (g'\setminus g)$ and $s_i = q_A+1,\ldots,q$ if $i \in B \cap (g'\setminus g)$. If g are cuboids, a unique nearest neighbour in g corresponds to each $i \in g'\setminus g$. Then we can eliminate the summation over s_i with $i \in g'\setminus g$,

$$W_{\mathrm{cl}}(g,x) = \sum_{\{s_i\}_{i\in g}} \prod_{i\in A} \left(\left(\frac{q_B-1}{q_B}\right)^{n_i} x\right)^{\alpha_i} \prod_{i\in B} \left(\left(\frac{q_A-1}{q_A}\right)^{n_i} x\right)^{\beta_i} \prod_{\langle ij\rangle\in g} (1-\delta(s_i,s_j)) \tag{41}$$

where n_i is the number of nearest neighbours of i which do not belong to g. For $q = 3$ ($q_A = 1$) we make the convention that $(((q_A-1)/q_A)^{n_i}x)^{\beta_i}$ equals x^{β_i} if $n_i = 0$, equals 1 if $\beta_i = 0$, and 0 if $\beta_i > 0$ and $n_i > 0$.

A finite lattice g is to be taken into account (is a cluster) if it becomes a connected graph after drawing all the bonds between nearest neighbours and next nearest neighbours on the hypercubic lattice.

For $q = 3$, we obtained

$$\omega(D=3,q=3,x) = \sqrt{2}\left(1 + \frac{x}{32} + 6\left(\frac{x}{32}\right)^2 + 68\left(\frac{x}{32}\right)^3 + 1003\left(\frac{x}{32}\right)^4 + 17\,313\left(\frac{x}{32}\right)^5 + 330\,260\left(\frac{x}{32}\right)^6 + O(x^7)\right)^{1/2}. \tag{42}$$

Pade-approximating this expansion we get

$$\omega(D=3,q=3) = 1.4435 \pm 0.0005.$$

In this case we have a problem: whether the singularity x_0 of the x-expansion about $x = 0$ lying on the real axis is located exactly at $x_0 = 1$, or at $x_0 > 1$. If $x_0 > 1$, then the stable solution for all $x > 1$ is given by the expansion about $1/x = 0$ determined from the duality relation, and in the interval $x \in [1, x_0)$ the expansion about $x = 0$ describes metastable states.

We performed Monte Carlo simulations on the lattice $20 \times 20 \times 20$ with PBC, starting from the pure BSS for $x = 0$. We found that at $x = 1.1$, 1.05, 1.04, 1.035, and 1.03 the

system goes to the neighbourhood of the BSS for $1/x = 0$ after 200, 400, 1000, 4000, and $> 10\,000$ MCS, respectively. These results suggest $1 \leqslant x_0 \leqslant 1.03$.

For $q = 4$ we obtained

$$\omega(D=3,q=4,x) = 2\left(1+\frac{x}{64}+15\left(\frac{x}{64}\right)^2+326\left(\frac{x}{64}\right)^3+9565\left(\frac{x}{64}\right)^4 +316\,014\left(\frac{x}{64}\right)^5+O(x^6)\right) \tag{43}$$

$$\omega(D=3,q=4) = 2.043 \pm 0.001\,.$$

The 3D series can be extended using the FLM. Here we only note that the optimal set G_f in this case are not cuboids but all the convex polyhedrons which can be drawn on the cubic lattice (on the sublattice A if $q = 3$) using bonds between sites which are nearest and next nearest neighbours on the cubic lattice.

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