Large $q$ expansion of the 2D $q$-states Potts model

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Abstract

We present a recursive method to calculate a large $q$ expansion of the 2D $q$-states Potts model free energies based on the Fortuin-Kasteleyn representation of the model. With this procedure, we compute directly the ordered phase partition function up to order 10 in $1/\sqrt{q}$. The energy cumulants at the transition can be obtained with suitable resummation and come out large for $q \lesssim 15$. As a consequence, expansions of the free energies around the transition temperature are useless for not large enough values of $q$. In particular the pure phase specific heats are predicted to be much larger, at $q \lesssim 10$, than the values extracted from current finite size scaling analysis of extrema, whereas they agree very well with recent values extracted at the transition point.

Résumé

Une méthode récursive pour calculer un développement à grand $q$ du modèle de Potts bi-dimensionnel à $q$ états est présentée, sur la base de la représentation de Fortuin-Kasteleyn. Avec cette procédure la fonction de partition dans la phase ordonnée est calculée directement à l’ordre 10 en $1/\sqrt{q}$. Pour $q \lesssim 15$, les cumulants de l’énergie sont trop importants pour rendre utilisable le développement de l’énergie libre au voisinage du point de transition. En particulier les chaleurs spécifiques prédites pour les phases purs sont beaucoup plus grandes que les valeurs extraites des analyses de taille finie d’extrema pour $q \lesssim 10$, alors qu’elles sont en très bon accord avec celles récemment obtenues au point de transition.
1. Introduction

The two-dimensional $q$-states Potts model is a very useful framework for probing numerical algorithms and methods to analyze transitions. The advantage of this model is twofold. First many of its properties, such as the location of its transition temperature $\beta_t^{-1}$ and the internal energy densities in the first order transition regime, are known [1] and put strong constraints on the analysis of any numerical results. Next, its simplicity makes it easy to implement and the existence of the free parameter $q$ (the number of states) allows one to vary the properties of the model, especially the magnitude of the correlation length relative to accessible lattice sizes.

Two recent analytical results are of interest to our purpose. It has been shown [2] that close to $\beta_t$, the partition function $Z$ of the Potts model, in a box of volume $V = L^2$ with periodic boundary conditions, is equal to the sum of the ‘partition functions’ $Z_i = \exp(V F_i)$ of the $q$ ordered and of the disordered pure phases, up to a correction that falls off exponentially faster with $L$. The $i^{th}$ phase free energy $F_i$ is $V$ independent and differentiable many times with respect to the inverse temperature $\beta$ at $\beta_t$. As a consequence of a recent calculation of the disordered correlation length at $\beta_t$[3], the interface tensions also have been analytically predicted [4].

On the numerical side, various simulations have recently been performed for different values of $q$ between 7 and 20, with the main purpose of accumulating more experience on the identification, by numerical means, of the nature and properties of a phase transition. Although the general overview acquired seems quite consistent, there remains some unsatisfactory issues such as slight inconsistencies in finite size scaling analysis of the energy cumulants close to the transition temperature $\beta_t^{-1}$, and some discrepancies between exact results and numerical simulations for the interface tension. A proper understanding of these differences is important since in other cases of physical interest such as the 3D $q = 3$ Potts model or QCD at the deconfinement transition, no good analytic solution exists and one has to resort to similar numerical calculations to determine these quantities.

The problem at hand can be stated as that of disentangling finite size effects coming from adding up the “asymptotic” partition function $Z_i$, and those associated with truly non-asymptotic contributions coming from interfaces between coexisting phases. One way towards the solution of this problem is to learn more
about the pure phase free energies $F_i(\beta)$ in the vicinity of $\beta_t$ and as a function of $q$.

This is our motivation for starting a large $q$ expansion of $F_i$ for $\beta$ near $\beta_t$ based on the Fortuin-Kasteleyn representation [5]. Such an expansion is much in the spirit of the pioneering work by Ginsparg, Goldschmidt and Zuber [6], who pointed out that in d-dimension, at any finite order in $z = q^{-1/d}$, only a finite number of terms contribute in the $\mathbb{Z}_q$ character expansion of the partition function. Low temperature expansions also exist for the same model [7], but the above method seems more adapted to our goal of studying the model close to the transition temperature. A short account of our work has been already published with the free energy expanded in $z = 1/\sqrt{q}$ up to order 9 [8] or 10 [9]. The present paper provides a detailed description of the expansion and an analysis of the behavior in $q$ of the six first energy cumulants. More phenomenological consequences on finite size analysis of numerical data, sketched in [8,9], are fully developed in a separate publication [10].

The organization of the paper is as follows. In section 2 we recall some useful properties of the 2-d $q$-states Potts model and its representation as a model of bonds. Section 3 is devoted to the detailed computation of the partition function. The resulting free energy expansion is given in section 4. Resummation techniques based on Padé approximants are applied in section 5 to the energy cumulants at $\beta_t$. Strong evidence is given that they increase very fast as $q$ is lowered toward 4, the more so their order increases. Quantitative predictions are given down to $q = 6$, some of them being in clear disagreement with values extracted from numerical simulations not analyzed at $\beta_t$. Concluding remarks are presented in section 6.

2. The model and its Fortuin-Kasteleyn representation.

We consider the two-dimensional $q$-state Potts model [11] on a square lattice with $V = L^2$ sites, defined by the partition function

$$Z = \sum_{\{\sigma_i\}} \exp(-\beta H), \quad H = -\sum_{\langle ij \rangle} \delta_{\sigma_i \sigma_j}, \quad (1)$$

where $i$ and $j$ denote the lattice sites, $\langle ij \rangle$ the pairs of nearest neighbors and $\sigma_i = 1, 2, \cdots, q$. The symmetry group of the Hamiltonian is the permutation group of $q$ elements.

There is abundant literature on this model [1], and many of its properties are known exactly. In particular, it possesses a phase transition which, for $q > 4$, is
first order [12] and lies at a coupling

$$\beta_t = \log(\sqrt{q} + 1).$$  \hspace{1cm} (2)$$

At $\beta = \beta_t$, $q + 1$ phases can coexist. One is the disordered phase, the $q$ other ones are degenerate ordered phases. The internal energy densities at $\beta = \beta_t$ in the disordered and ordered phases are $E_d$ and $E_o$ respectively, with

$$E_d + E_o = -2(1 + \frac{1}{\sqrt{q}})$$  \hspace{1cm} (3)$$

and a latent heat

$$\mathcal{L} \equiv E_d - E_o = 2(1 + \frac{1}{\sqrt{q}})\tanh\frac{\theta}{2} \prod_{n>0}[\tanh (n\theta)]^2$$  \hspace{1cm} (4)$$

where $2\cosh\theta = \sqrt{q}$. Duality relates the ordered and disordered free energies

$$F_d(\tilde{\beta}) = F_o(\beta) - 2 \ln((e^\beta - 1)/\sqrt{q}) \quad , \quad (e^{\tilde{\beta}} - 1)(e^\beta - 1) = q. \hspace{1cm} (5)$$

A large $q$ expansion can be obtained through the Fortuin-Kasteleyn [5] representation of the Potts model partition function

$$Z = \sum_X (e^\beta - 1)^{b(X)} q^{c(X)}$$  \hspace{1cm} (6)$$

where $X$ is any configuration of bonds on a square lattice, $b(X)$ is the number of bonds in configuration $X$, and $c(X)$ its number of clusters of sites: two sites bound to each other belong to the same cluster (an isolated site is a cluster).

The completely ordered configuration, $X_o$, has all possible bonds and, hence, corresponds to $c(X_o) = 1$ and $b(X_o) = 2V$. So the partition function of the ordered phase, $Z_o$ can be reorganized as an expansion in $q^{-1/2}$ about $X_o$:

$$Z_o = q(e^\beta - 1)^{2V} \sum_{k\geq0,l\geq0} N_{k,l}^o(V)(\frac{e^\beta - 1}{\sqrt{q}})^{-l} q^{k-l}, \hspace{1cm} (7)$$

where $N_{k,l}^o(V)$ is the number of configurations in a volume $V$ with $l$ bonds removed and comprising $k + 1$ clusters. We made explicit in Eq. (7) the factor $(e^\beta - 1)/\sqrt{q}$ which is 1 at the transition and thus provides an expansion of $Z_o$ in $q^{-1/2}$ near the transition. The enumeration of all the $N_{k,l}^o(V)$ such that $(l - 2k) \leq M$ yields this expansion to order $M$ in $q^{-1/2}$. 

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Similarly, the completely disordered configuration, $X_d$, corresponds to $c = V$ and $b = 0$. Hence we reorganize the expansion of the partition function of the disordered phase about this configuration at temperature $\tilde{\beta}^{-1}$ as

$$Z_d = q^V \sum_{j \geq 0, l \geq 0} N_{j,l}^d(V)(\frac{e^{\tilde{\beta}} - 1}{\sqrt{q}})^l q^{\frac{j}{2}}$$

where $N_{j,l}^d(V)$ is the number of configurations in a volume $V$ with $l$ bonds and $V - j$ clusters. Since the suppression of $j$ clusters requires that at least $j$ bonds are restored, one has $k \equiv l - j \geq 0$. Hence we rewrite $Z_d$ as

$$Z_d = q^V \sum_{l \geq 0, k \geq 0} \tilde{N}_{k,l}^d(V)(\frac{e^{\tilde{\beta}} - 1}{\sqrt{q}})^l q^{k - \frac{1}{2}}$$

where $\tilde{N}_{k,l}^d(V)$ is the number of configurations in a volume $V$ with $l$ bonds and $V - l + k$ clusters. Duality as given in Eq. (5) implies $\tilde{N}_{k,l}^d(V) = N_{k,l}^o(V)$, a trivial geometrical property exemplified later on. Thus, in the following we restrict our calculation to the ordered phase contributions, except for comments on duality.

With a large enough volume $V$ (to eliminate all finite size effects) and periodic boundary conditions (to eliminate edge effects), $N(V)$ are polynomials in $V$ to any given finite order $M$, and all configurations retained correspond to disordered (ordered) islands in a bulk ordered (disordered) phase.

3. Evaluation of the expansion

This simple expansion which computes directly $Z_o$ can be made recursive. To this end we explicitly remove successively up to 8 bonds in sub-section 3.1 where the main properties are exhibited in order to make the general construction in sub-sections 3.2-3.6. To simplify, the number $k$ of clusters added to the bulk ordered cluster will be called in the following the number of cluster.

3.1. Explicit first steps

Starting from the ordered configuration, we have $2V$ ways to remove one bond, the number of clusters remaining 0, so that $N_{0,1}^o(V) = 2V$. Continuing to remove bonds, we obtain $N_{0,2}^o(V) = 2V(2V - 1)/2$ and $N_{0,3}^o(V) = 2V(2V - 1)(2V - 2)/6$. To proceed, let us introduce $C(n, l)$ as the number of ways to remove $l$ identical bonds among $2V - n$ ones

$$C(n, l) = \frac{1}{l!} \prod_{i=0}^{l-1} (2V - n - i),$$

(10)
Thus
\[ N_{0,1}^o(V) = C(0,1), \]
\[ N_{0,2}^o(V) = C(0,2), \]
\[ N_{0,3}^o(V) = C(0,3). \]

A new situation occurs with 4 bonds removed. We have \( C(0,4) \) ways to remove them, but some of them give rise to an isolated 1-site cluster as shown in Fig. 1, when the 4 removed bonds have one site in common. The number of ways to make this figure is \( V \), the number of possible positions for the one site cluster. Thus we have with 4 removed bonds
\[ N_{1,4}^o(V) = V, \]
\[ N_{0,4}^o(V) = C(0,4) - V, \]
where the number of configurations which do not correspond to the specified number of clusters in \( N_{0,4}^o \) is subtracted.

With 5 removed bonds, nothing new happens and one has
\[ N_{1,5}^o(V) = V C(4,1), \]
\[ N_{0,5}^o(V) = C(0,5) - V C(4,1), \]
where the factor \( C(4,1) \) takes into account the number of ways to remove one bond when 4 bonds have already been removed to make the configuration of Fig. 1.

With 6 removed bonds, the new type of configuration shown in Fig. 2 can be made with \( 2V \) possibilities (\( V \) translations and 2 orientations), and its corresponds to one cluster (the 2 sites surrounded by the removed bonds are in the same cluster). Thus we have
\[ N_{1,6}^o(V) = V C(4,2) + 2V, \]
\[ N_{0,6}^o(V) = C(0,6) - V C(4,2) - 2V. \]

Here again the multiplicity \( C(0,6) \) is corrected for all the 1 cluster contributions.
Next with 7 bonds removed, the higher contribution comes from the configuration of Fig. 3 with 2 clusters and with 2V possibilities, and thus $N_{2,7}^0 = 2V$. The contributions to $N_{1,7}^0$ are obtained from the configurations contributing to $N_{1,6}^0$ with one more bond removed. First we have $V C(4,3)$ configurations made of Fig. 1 with 3 more bonds removed, out of which we have to subtract the 4V configurations with 2 clusters as in Fig. 3 (the 3 removed bonds can surround the 4 neighboring sites of the 1-site cluster of Fig. 1 and these configurations do not give new contribution to $N_{2,7}^0$ for which the correct counting is already made). Next we have to remove one bond to the 2V configurations of Fig. 2. If we remove the “internal” bond connecting the two sites of the cluster, we will get 2 clusters. So we only remove bonds of the bulk ordered phase, that is only $2V - 7$ bonds can be removed. Thus we have

\begin{align*}
N_{2,7}^0(V) &= 2V, \\
N_{1,7}^0(V) &= VC(4,3) - 4V + 2VC(7,1), \\
N_{0,7}^0(V) &= C(0,7) - N_{1,7}^0(V) - N_{2,7}^0(V).
\end{align*}

As a last simple example, let us consider 8 removed bonds and discuss the new contributions beside the contributions deduced from $N_{k,7}^0$ with the appropriate changes in the $C$ factors. New configurations with 2 clusters can be made by putting the Fig. 1 twice on the lattice. Once the first figure is put on the lattice (V possibilities), the second one cannot be put at the same site nor at the 4 neighboring sites as shown by open dot in Fig. 4 because a bond ending there has already been removed. Thus the number of such configurations is $V(V - 5)/2$ with the 1/2 factor for symmetry. Concerning the contribution $N_{1,8}^0$, we first correct the contribution coming from Fig. 1 plus 4 removed bonds forming themselves a 1-site cluster, that is a correction $V(V - 5)$ (no 1/2 symmetry factor). Then we add the contribution coming from the configurations shown in Fig. 5 where the cluster extends either

![Fig. 3](image)

*Seven removed bonds (crosses) making two 1-site clusters.*

![Fig. 4](image)

*Sites forbidden (circles) for a second 1-site cluster.*
over 3 sites at left (6V possibilities) or over 4 sites at right (V possibilities). Thus

\[ N_{2,8}(V) = 2V C(7,1) + \frac{1}{2} V(V - 5), \]
\[ N_{1,8}(V) = V C(4,4) - 4V C(7,1) - V(V - 5) + 2V C(7,2) + 6V + V, \]
\[ N_{0,8}(V) = C(0,8) - N_{1,8} - N_{2,8}. \]

In \( N_{1,8} \) we keep the two contributions of Fig. 5 separate because at the next step, as we explained for \( N_{1,8} \) from Fig. 2 with one more removed bond, it is easiest to restrict the removed bond to belong to the bulk ordered phase, that is 2V - 10 and 2V - 12 possibilities respectively.

These examples illustrate the way how a recursive construction of the expansion up to a given order \( M \) can be made. This construction involves 5 steps:

i) Construct the **dominant configurations** made of one connected set of 1-site clusters (two clusters with neighboring sites belong to the same connected set). We note \((k,l)\) the set of configurations with \(k\) connected 1-site clusters and \(l\) removed bonds and they are constructed for all the \(k\) and \(l\) such that \(l - 2k \leq M\). Thus Fig. 1 and Fig. 3 belong respectively to \((1,4)\) and \((2,7)\).

ii) Construct the **sub-dominant configurations** made of one connected set of clusters involving at least one cluster with more than one site (cf. Figs. 2 and 5). They can be obtained by restoring one or several internal bonds of dominant (parent) configurations and we note \((k,l;k^p,l^p)\) the configuration set with \(k\) clusters and \(l \leq M - 2k\) removed bonds inside a parent with \(k^p\) clusters and \(l^p\) removed bonds. Thus the configuration of Fig. 2 belongs to \((1,6;2,7)\), those in Fig. 5 left and right to \((1,8;3,10)\) and \((1,8;4,12)\) respectively.
iii) Construct the **product configurations** which are disconnected sets of clusters. Once we have all the connected sets, we compute the number of ways to put together on the lattice connected sets of clusters with \( l_i \) and \( k_i \) such that \( \sum l_i - 2 \sum k_i \leq M \). For example the contribution \( V(V - 5)/2 \) to \( N_{2,8} \) found above is the product \((1, 4) \times (1, 4)\).

iv) Construct the **correcting contributions** which are obtained from the configurations with \( k \) and \( l \) of steps i) to iii) plus \( n \) removed bonds (\( 1 \leq n \leq M + 2k - l \)) and have a number of clusters higher than \( k \). These correcting contributions will allow to get from the contributions of configurations obtained in steps i) to ii) weighted by \( C(l, n) \) the correct contribution to \( N_{k,l+n}^o \) by suppressing the contributions from higher number of clusters (as the correction \( 4V \) in the contribution to \( N_{1,7}^o \) of Fig. 1 plus 3 removed bonds).

v) **Collect the results** of steps i) to iv) to get all the \( N_{k,l}^o \)'s relevant to order \( M \). In the steps i) to iv) the number of removed bonds is minimal in the sense that they are all necessary to make the clusters. Thus this step collects the preceding contributions with appropriate signs (for correction) and \( C' \) factors.

These different steps are explained in details in the following sub-sections. Of course any configuration drawn on the lattice has \( V \) copies obtained by the lattice translations and two configurations will be said distinct if they are unequivalent upon lattice translation.

**3.2. The dominant configurations**

If we consider all the connected sets of clusters corresponding to \( k \) clusters with \( l \) removed bonds and extending on \( n \) given (connected) sites, the exponent \( l - 2k \) of \( q_{-1/2} \) in \( Z_o \) is minimum for \( k = n \). Hence the name of dominant for a \((k,l)\) set of configuration extending on \( k \) sites and thus made of \( k \) 1-site clusters. All the dominant \((k)\)-configurations as defined by the data of \( k \) connected sites can be obtained recursively from the \((k-1)\)-ones

i) connecting one additional site in all the possible ways to all the \((k-1)\) configurations, keeping only the distinct (upon translation) configurations.

ii) eliminating those configurations which happen to have more than \( k \) clusters (extra sites can be isolated from the bulk ordered ones and these configurations can be identified by a suitable cluster finding algorithm [13] ).

In this construction, a dominant \((k,l)\)-configuration contributing at order \( m = l - 2k \) can be obtained from one or several of the following dominant \( k - 1\)-
configurations

i) \((k - 1, l - 3)\) contributing to order \(m - 1\)

ii) \((k - 1, l - 2)\) contributing to order \(m\)

iii) \((k - 1, l - 1)\) contributing to order \(m + 1\)

An example of case i) is given by Fig. 3 obtained from Fig. 1, while examples of case ii) and iii) are given in Fig. 6 left and right respectively.

![Fig. 6](image-url)

The same \((6,17)\) dominant contribution obtained by connecting a 6th 1-site cluster (open point) to a \((5,15)\) (left, case ii) or to a \((5,16)\) (right, case iii).

Note that in the latter case, the order in \(q^{-1/2}\) decreases in the step \(k - 1 - > k\). Hopefully, the example of Fig. 6 is in fact generic, and one can convince oneself that a \((k,l)\)–configuration obtained via iii) can always be obtained via either ii) or i). This means that, once the maximum order \(M\) of the computation is given, it is never necessary to keep contributions to a higher order in the iterative process.

Once all the distinct dominant configurations with \(k\) 1-site clusters are obtained, they can easily be classified according to the number \(l\) of removed bonds. Thus a \((k,l)\) set is given by a set of \(2k\) data, the \(x\) and \(y\) positions of the \(k\) 1-site clusters. Their number is given in Table 1 and represents the corresponding contribution to \(N_{k,l}^0/V\). At order \(M = 10\), 59 \((k,l)\) set are contributing, the largest size to be considered being a \((25,50)\) configuration, a \(5 \times 5\) square of 1–site clusters.

### 3.3. The sub-dominant configurations

Sub-dominant configurations correspond to connected set of clusters involving at least one cluster extending over more than one site. They can be obtained from the dominant configurations by restoring some of their \(4k - l\) internal links.
Let us start from a \((k^p, l^p)\) dominant set, the parent of a family of sub-dominant \((k, l; k^p, l^p)\) configurations. If one interior bond is restored, the two sites it links now belong to the same (2-sites) cluster. Then \(k = k^p - 1\) and \(l = l^p - 1\) and the exponent is one unit less that the parent one \((m = l - 2k = m^p - 1)\). Hence the name subdominant. For example Fig. 2 can be obtained from Fig. 3 by restoring the interior bond (only one possibility), leading to a 2-site cluster.

These sub-dominant configurations are obtained from the dominant \((k^p, l^p)\) configurations by restoring the interior bonds one after the other in all possible distinct ways, looking at the \(k\) and \(l\) values of the generated configurations. In fact, it is not necessary to keep memory of the restored bonds and for each \((k^p, l^p)\) configuration it is enough to count the number of distinct \((k, l; k^p, l^p)\) configurations obtained. Thus a \((k, l; k^p, l^p)\) set is given by a set of \(2k^p + 1\) data, the \(x\) and \(y\) positions of the parent \(k^p\) 1-site clusters and their multiplicity.

Restoring systematically bonds among the \(4k^p - l^p\) interior ones can be time consuming for large clusters. However restoring up to 5 bonds can be implemented easily because there is a classification according to the number of \(4\) 1-site clusters making a plaquette, with the property that all the parent configuration give rise to the same multiplicity.

For the order \(M = 10\) considered here, we had to construct 146 sets \((k, l; k^p, l^p)\) from the 59 dominant \((k, l)\).

### 3.4. The product configurations

Let us now consider disconnected configurations. They are made of components which are either dominant or subdominant configurations. In fact for components which are sub-dominant configuration, the corresponding result is the same as given by the ‘parent’ component, and thus we can only consider product of dominant contributions. Here “disconnected” implies that two requirements must be fulfilled

i) no overlap between links of any two of the connected component;

ii) no site of the surrounding bulk ordered phase become a cluster.

According to these requirements, the values of \(k\) and \(l\) of a product are the sums of the \(k_i\)’s and \(l_i\)’s of the factors (its components). The method used is first to count all the possible ways the components can be put on the lattice with requirement i) satisfied, then subtract the number of configurations which do not satisfy \(k = \sum k_i\).
For the product of two configurations given by the sets $F_1$ and $F_2$ of occupied sites, once the first configuration $F_1$ is put on the lattice with $V$ possibilities, we have to search all the possibilities to put the second one. For that purpose let us define as $F_{12}$ the set of sites around $F_1$ where a given site of $F_2$ taken as origin cannot be put according to requirement i). If $v_{12}$ is the number of sites in $F_{12}$, then we have $V(V - v_{12})$ configurations for the product $F_1 \star F_2$ (divide by 2 for identical configurations). An example is the product $(1,4) \star (1,4)$ as already been given in subsection 3.1.

This process can be generalized to product of more figures. For the product of $F_1 \star F_2 \star F_3$ let us first define the protected areas $F_{12}$, $F_{13}$ and $F_{23}$ with $F_{ij}$ the set of $v_{ij}$ sites around $F_i$ which cannot be occupied by an origin site of $F_j$ according to requirement i). Once $F_1$ is on the lattice ($V$ possibilities) let us first put $F_2$ far enough from $F_1$ such that $F_3$ can be put every where except on $F_{13}$ or $F_{23}$. This will be the case when $F_2$ is every where except in a region $F_{12,23}$ for which there will be overlap of sites of $F_{13}$ and $F_{23}$. If $v_{12,23}$ is the number of sites of $F_{12,23}$, we get a first number of possible configurations which is

$$n_a = V(V - v_{12,23})(V - v_{13} - v_{23}).$$

Next we consider all the possible positions of $F_2$ inside $F_{12,23}$ but outside $F_{12}$ ($v_{13,23} - v_{12}$ possible positions). For each such position there is a protecting region $F_{(12)3}$ with $v_{(12)3}$ sites forbidden for $F_3$ according to rule i) ($v_{(12)3} < v_{13} + v_{23}$) and we have to add to $n_a$

$$n_b = V \sum_{i=1}^{v_{13,23} - v_{12}} (V - v_{(12)3}).$$

This method can be extended to products of more factors and implemented on computer. As an example the resulting polynomials in $V$ for the powers of $(1,4)$ needed at order $M = 10$ are

$$(1, 4)^2 = \frac{1}{2} V(V - 5),$$

$$(1, 4)^3 = \frac{1}{6} V(V^2 - 15V + 62),$$

$$(1, 4)^4 = \frac{1}{24} V(V^3 - 30V^2 + 323V - 1254),$$

$$(1, 4)^5 = \frac{1}{120} V(V^4 - 50V^3 + 995V^2 - 9370V + 35424).$$

(11)
Finally we have to fulfill requirement ii), and thus subtract to the above configurations those which do not correspond to the specified number of clusters, \( \sum k_i \). Two examples are given in Fig. 7, with at left a peculiar configuration of \((1, 4)^4\) contributing to a 5 clusters contribution and at right a product \((3, 10)^2\) contributing to 7 clusters.

![Fig. 7](image_url)

Product of configurations giving rise to extra cluster number.

These corrections can be obtained by trying to cast dominant or subdominant configurations with \( l = \sum l_i \) into the corresponding products (see next subsection).

3.5. Correcting configurations

In the three preceding sub-sections, it was assumed that the number of removed bonds was minimum to make a definite configuration of clusters. In other words there is no “free” links, that is removed bonds not belonging to any cluster. Thus the number \( n_{(k,l)} \) of configurations \((k, l)\) gives directly its contribution to \( N_{k,l} \)

\[
\text{[contrib. } (k, l) \text{ to } N_{k,l}] = n_{(k,l)}.
\]

(For simplicity we consider only dominant configurations). We now wish to get its contribution to \( N_{k,l+i}, 1 \leq i \leq M + 2k - l \). This contributions is \( n_{(k,l)} C(l, i) \) up to corrections from the configurations corresponding to a higher value of cluster number. These corrections are twofold. First these \( i \) removed bonds can make a cluster and the corresponding corrections can be computed as in the preceding subsection. Or the configuration \((k, l)\) with \( i \) removed bonds can make connected sets of clusters which can be considered as inside dominant configurations. Thus
in Fig. 8 a (2,7) configurations with 5 more removed bonds can make connected sets of clusters inside a (4,12) at right or inside a (4,13) at left. The distinction between the different possible parent dominant configurations is necessary for further removing of bonds.

**(2,7) configuration plus 5 removed bonds making connected sets of clusters inside a (4,12) at right or a (4,13) at left.**

If \( n_{((k,l)+i;k^p_r,l^p_r)} \) is the number of these \( r \) configurations, then

\[
[\text{contrib. } (k, l) \text{ to } N_{k,l+i}] = n_{(k,l)}C(l, i) - n_{((k,l)+i;k^p_r,l^p_r)},
\]

with eventual summation on \( r \). This process has to be continued and let us suppose that the configuration \(((k,l)+i;k^p_r,l^p_r)\) plus \( j \) removed bonds can make higher configurations \(((k,l)+i;k^p_s,l^p_s)\). Then there is also higher configurations obtained directly from \((k,l)\) plus \( i + j \) removed bonds inside the same parents. The proper correction which take correctly the \( i + j \) bonds symmetrization is the direct one. This means that we have to correct the correction itself on the form

\[
[\text{contrib. } (k, l) \text{ to } N_{k,l+i+j}] = n_{(k,l)}C(l, i + j) - \left[ (n_{((k,l)+i;k^p_r,l^p_r)}C(l^p_r, j) - n_{((k,l)+i+k^p_s,l^p_s) + j;k^p_s,l^p_s)} \right] - n_{((k,l)+i+j;k^p_s,l^p_s)}.
\]

with eventual summation on \( r \) and \( s \).

Clearly this computation apply to dominant or sub-dominant contribution as well as to product of connected sets of clusters and for all the configurations from subsections 3.2 to 3.4 characterized by \( k \) and \( l \), we have in this step to compute recursively all the connected sets of clusters obtained with \( l_f \) more removed links.
The recursive process means that we start from all the already obtained configurations with \((k,l)\) plus \(l'_f\) removed bonds \((0 \leq l'_f < l_f)\) and add \(l_f - l'_f\) removed bonds.

Such configurations will be in the list of dominant or sub-dominant contributions. So as in section 3.3, we have to search all the possibilities to found a starting configuration plus the removed links inside the dominant configurations in such a way that all the exterior links match. In the example of a \((2,7)\) configuration and 5 removed bonds, we know from the sub-dominant configuration analysis that a connected set of clusters with 12 removed bonds and more than 2 clusters can be inside a \((4,12)\) or a \((4,13)\). For the \((4,12)\) there is 2 possibilities to found the \((2,7)\) configuration of Fig. 9. For the \((4,13)\) configurations, we have to search the possibilities to put Fig. 9 inside the \((4,13)\) with one restored interior link and found that 3 \((4,13)\) configurations give rise to 2 possibilities and 8 other ones to 1 possibility.

3.6. Collecting the contributions to \(N_{k,l}\).

In computing the partition function from Eq. (7), we need the value of \(N_{k,l}\) for each values of \(k\) and \(l\). The contributions to \(N_{k,l}\) comes from the dominant, sub-dominant and product configurations obtained in subsections 3.2-3.4 and corresponding to a number \(k_c\) of clusters and a number \(l_c\) of removed bonds such that \(k_c = k\), \(l_c \leq l\), up to corrections as explained in subsection 3.5. The whole procedure is better understood on a particular example and let us consider the computation of the \(N_{2,12}\) coefficient. Its contributions comes from dominant, sub-dominant and product configurations with \(k = 2\) and \(l \leq 12\) which can be

- \((2,7)\) dominant configurations,
- \((2,9), (2,10), (2,11)\) and \((2,12)\) sub-dominant configurations,
- \((1,4)\ast(1,4), (1,4)\ast(1,6), (1,4)\ast(1,8)\) and \((1,6)\ast(1,6)\) product configurations.

For each of them, we have to correct their naive weight (number of configurations times the appropriate \(C\) factor of Eq. Eq. (10) for the extra links) for the configurations corresponding to a higher number of clusters. The various contributions building up the final value of \(N_{2,12}/V\) are given in the first column of Table 2, along with its corresponding set of cluster in column 2 (the last column labels the lines). Note that when a \(C\) factor is present, its second argument gives the number of free links, that is the number of removed bonds not belonging to a cluster.

The first contribution (line 1) comes from the dominant \((2,7)\) configurations
(two such configurations weighted by \( C(7, 5) \), the number of ways to removed 5 bonds among \( 2V - 7 \) ones. Its corresponding corrections (contributions corresponding to a number of cluster higher than 2) are given in the lines 2 to 7. First in line 2, 4 removed bonds can isolate a 1-site cluster as in Fig. 1. For each \((2,7)\) configuration there is \((V - 8)\) such possibilities (the product \((2,7) \ast (1,4)\) with 1 link remaining free among \(2V - 11\). Lines 3-6 concern clusters obtained with \((2,7)\) and 3 to 5 removed bonds. We made a distinction between different possible parents in lines 5 and 6 because they imply different \( C \) factor for their corresponding contributions at \( N_{2,13} \). Furthermore these \((2,7)+5\) corrections represent the whole contribution to higher cluster numbers obtained with \((2,7)\) and 5 extra removed bonds such that all the 5 extra links belong to the clusters. However in the line 3 such corrections are included and should not have been subtracted. Line 7 provides this “correction to the correction” of line 3, and thus with a positive sign.

Lines 8 and 11 to 15 concerns contributions of sub-dominant contributions. They are characterizes by their parent distribution in order to determine the number of frozen links which give the arguments of the \( C \) coefficients. Only line 8 needs subtraction in line 9 and 10, either 2 or 3 extra links giving rise to \( k > 2 \) configurations. Let us note that there is two ways to have a 2 clusters inside a dominant \((5,15)\), one in line 14 when restoring 3 bonds, one in line 13 when restoring the four bonds of a loop.

We finally start with The possible products of dominant or sub-dominant \( k = 1 \) configurations (lines 16,23,25-27). First in the product \((1,4) \ast (1,4)\) we consider the two \((1,4)\) as different in such a way that all the corresponding contributions (lines 16-22) have an explicit \( 1/2 \) factor. The first correction concern the 4 extra removed bonds making a \((1,4)\) cluster. This product \((1,4)^3\) have no extra symmetry factor, the third \((1,4)\) factor being formed by the extra links distinctly from the two other (identical) factors. The connected cluster corrections are in line 18-21, with again a “correction to the correction” with a positive sign in line 21. We have also to make a disconnected cluster correction in line 22, when 3 of the extra links are making a 2 clusters with each of the product configurations. For the other products only one of them need to be corrected.

All these computations have been made automatic on workstation.

4. Results

We have computed the series for \( Z_o \) up to order \( M = 10 \) in \( q^{-1/2} \), which
involves contributions up to $N_{60,25}(V)$, that is up to 60 removed bonds and 25 clusters. This series exponentiates in $V$ to give $F_o$ to order $M$ in the form

$$F_o(\beta) \equiv \frac{1}{V} \ln Z_o = 2 \ln(e^\beta - 1) + \sum_{m \geq 1, l \geq 1} A_{l,m} \left( \frac{e^\beta - 1}{\sqrt{q}} \right)^{-l} q^{-m/2} + O(q^{-11/2}), \quad (12)$$

where the non-zero coefficients $A_{l,m}$ are given in Table 3 up to $m = 10$.

One may notice, at the top of the columns, the appearance of stable sequences with decreasing $l$. For $k$ even, the $m/2$ higher $l$ values are in the sequence 1, 6, 22, 68, 187, ... that is as long as the contributions are coming from removing a corner (case ii) when starting from a square of size $m/2 \times m/2$. For $m$ odd, the series is 2, 8, 30, 88, ... for the $(m-1)/2$ higher $l$ values for the same reason when starting from a rectangle $(m+1)/2 \times (m-1)/2$. In contrast the bottom of each column is totally alternating.

Our series truncated at $l = 20$ can be compared to the result of Ref. [7]. Up to order 9 in $q^{-1/2}$, the two series are in agreement. At order 10, some coefficients, missing in [7], cannot be compared, but we disagree with the coefficient of $r_3 u_{17}$ of Ref. [7] (we find 3822 instead of 3818) and of $r_2 u_{16}$ (6269 instead of 6265).

Our result is obtained for the ordered phase. Then the disordered free energy can be obtained using the duality relation given in Eq. (5). As already mentioned our geometrical construction must comply with duality, and this can be explicitly verified on an example as shown in Fig. 10 for a dominant configuration $(5,15)$.

![Fig. 10](image)

(5,15) dual configurations in the ordered and disordered phase

a ) At left, 15 bonds removed from the fully ordered phase increases the number of clusters by 5 and contributes to $N_{15,5}^O(V)$ of Eq. (7).
b) At right, 15 bonds restored from the fully disordered phase make one cluster only out of 11 sites, reducing the number of clusters by 10, and thus contributing to $N_{10,15}^d(V)$ of Eq. (8), or $\tilde{N}_{5,15}^d(V)$ of Eq. (9). The open dots in the disordered figure (at right) are the centers of the bond plaquettes. They coincide with sites of the dual lattice, reproducing the same figure as in the left. Thus the contribution to $N_{5,15}^o(V)$ and $\tilde{N}_{5,15}^d(V)$ of such figures are the same as a priori stated from duality.

The expansion of the free energy gives similar series for the $n^{th}$ derivative with respect to $\beta$, $F_{o}^{(n)}(\beta)$. At $\beta = \beta_t$ we write the energy cumulants as

$$F_{o}^{(n)} = F_{o}^{(n)}(\beta_t) = (\ln(q) + 2z)\delta_{n0} + 2\delta_{n1} + (-)^n \sum_{m=2}^{10} C_{m}^{n} z^m + O(z^{11}), \quad (13)$$

for

$$z = \frac{1}{\sqrt{q}}$$

where the $C_{m}^{n}$ coefficients are given in Table 4 for $n$ varying from 0 to 6.

The corresponding disordered cumulants can be obtained from the ordered ones by use of the duality relation Eq. (5). The relation for the energies ($E_i = -F_{i}^{(1)}$) is given in Eq. (3). For higher cumulants up to $n = 5$ we can write

$$F_{d}^{(2)} - F_{o}^{(2)} = -\frac{1}{q^{1/2}} [F_{d}^{(1)} - F_{o}^{(1)}]$$

$$F_{d}^{(3)} - F_{o}^{(3)} = \frac{q^{1/2} - 1}{q} \left[ F_{d}^{(1)} + F_{o}^{(1)} \right] - \frac{3}{q^{1/2}} \left[ F_{d}^{(2)} + F_{o}^{(2)} \right]$$

$$F_{d}^{(4)} - F_{o}^{(4)} = \frac{6 - q}{q^{3/2}} \left[ F_{d}^{(1)} - F_{o}^{(1)} \right] - \frac{6}{q^{1/2}} \left[ F_{d}^{(3)} - F_{o}^{(3)} \right]$$

$$F_{d}^{(5)} + F_{o}^{(5)} = \frac{q^{3/2} + q + 24q^{1/2} - 24}{q^2} \left[ F_{d}^{(1)} + F_{o}^{(1)} \right] - \frac{5(q - 12)}{q^{3/2}} \left[ F_{d}^{(2)} + F_{o}^{(2)} \right]$$

$$-\frac{10}{q^{1/2}} \left[ F_{d}^{(4)} + F_{o}^{(4)} \right]. \quad (14)$$

The $n = 0$ (free energy) and $n = 1$ (internal energy) series match the exact results [12] up to $M = 10$. The next section is devoted to a study of the series $n \geq 2$.  

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5. Resummation of the large $q$ series

We start from the result Eq. (13) which gives the cumulants $F^{(n)}_o$ of the ordered free energy $F_o(\beta)$, taken at $\beta_t$, as series expansions to order 10 in the variable $z = 1/\sqrt{q}$. The coefficients $C^m_n$ of $q^{-m/2}$ in $F^{(n)}$ are given in Table 4 up to $n = 6$. We want to explore the behavior in $q$ of $F^{(n)}$, $n \geq 2$ as $q$ is decreased towards $q = 4$. The first cumulants $F_o(\beta_t)$ and $F^{(1)}_o = -E_o$ are known exactly. For later convenience we write $F^{(1)}_o$ as

$$F^{(1)}_o = (1 + z) + \frac{1}{2} L,$$

where the latent heat $L$ is given by Eq. (4), with $\theta$ defined through

$$2 \cosh \theta = \sqrt{q}.$$

At first glance to Table 4, the task of resumming the series $F^{(n)}$ (from now on we omit the index $o$) looks quite discouraging: not only increase all the (known) $C^m_n$’s very fast with $m$, the more so $n$ is large, but also they are all positive for $n \geq 2$. We will undertake this task, however, with the help of a few assumptions on the singularities in $q$ of the $F^{(n)}$’s, and after checking that the techniques used work well for the known case of $L$.

From Eq. (4), we known that the radius of convergence of the series in $q^{-1/2}$ of $L$ is $1/2$ ($q = 4$). We will assume that it is so for all the $F^{(n)}$’s. Furthermore, the leading singularity of $L$ at $q = 4$ is given by

$$L \sim (1 + z) \tanh(\frac{\theta}{2}) \frac{2\pi}{\theta} x^{-1/2}, \quad (15)$$

where

$$x = \exp(\frac{\pi^2}{2\theta}) \quad (16).$$

A similar singularity at $q \to 4$ occurs in the disordered phase correlation length [3,4]

$$\xi_d \sim \frac{1}{8\sqrt{2}} x.$$

Our second assumption will be that for $n \geq 2$, $F^{(n)}$ diverges at $q \to 4$ like a power of $x$, up to a smooth factor. Arguments for that have been given in [8,10], where we proposed that $F^{(n)}/x^{3n/2-2}$ is a slowly varying function of $x$. 18
Relative difference to the latent heat exact result of 4/6, 5/5 and 6/4 Padé’s applied to \( \mathcal{L}^{-1} \) (dotted lines), to the logarithmic of \( \mathcal{L}^{-1} \) (dashed lines) and to the regularized logarithmic (solid lines). The 4/6 simple Padé has a pair of pole and zero near the real axis giving a spurious spike near \( q = 20 \).

According to the above results and assumptions, we now experiment resummation techniques by Padé approximants on the series for \( \mathcal{L}^{-1} \), which diverges as \( x^{1/2} \), Eq. (15). Truncating it at order 10, we want to compute \( \mathcal{L}^{-1} \) from

\[
2\mathcal{L}^{-1} = 1 + z + 5z^2 + 7z^3 + 27z^4 + 41z^5 + 143z^6 + 225z^7 + 737z^8 + 1187z^9 + 3713z^{10} + \cdots
\]

(17)
a series which does exhibit the same qualitative aspect as \( F^{(n)} \), \( n \geq 2 \). In the absence of any further information on the behavior of \( \mathcal{L}^{-1} \), we would try a Padé resummation (P). With the knowledge we have, a better attempt is to apply the Padé resummation to the logarithm of \( \mathcal{L}^{-1} \) (Pln). But \( \log \mathcal{L}^{-1} \sim 1/\theta \) is still singular at \( q = 4 \); its leading singularity is a pole at 1 in the variable

\[
u = \frac{2z}{(1 + \sqrt{1 - 4z^2})} = \frac{2}{\sqrt{q + \sqrt{q - 4}}},
\]

(18)
and \( u \) is expandable in \( z \) around 0. So an even better Padé technique in this case is to construct Padé approximants for the less singular function \((1-u) \log(2L^{-1})\).

Using \(2L^{-1}\) rather than any other constant times \(L^{-1}\) is arbitrary, but happens to be very convenient as avoiding logarithms of numerical constants. Therefore we will construct, for any series \(S(z)\) whose lowest order term is \(C_{k_{\text{min}}} z^{k_{\text{min}}}\) and which is assumed to be dominantly a power of \(x\) as \(q \to 4\), the regularized logarithmic Padé approximant as

\[
(\text{Pln}_R) : \quad S = C_{k_{\text{min}}} z^{k_{\text{min}}} \exp \left[ \frac{1}{1-u} \text{Padé} \left[ (1-u) \log \frac{S}{C_{k_{\text{min}}} z^{k_{\text{min}}}} \right] \right].
\]

(19)

The Padé \([f(z)]\)'s are \(P_M/Q_N\) ratios of polynomials of degrees \(M\) and \(N\), their Taylor expansion matches that of \(f(z)\) up to order \(M+N\). Of course, with regards to the Padé techniques here applied, a series \(S\) or its inverse \(S^{-1}\) leads to the same set of approximants and the purpose of considering \(L^{-1}\) was just to illustrate its similarities with the series at hand.
The results for $M/N = 4/6, 5/5, \text{ and } 6/4$ of the techniques (P), (Pln) and (PlnR) applied to $\mathcal{L}$ are shown in Fig. 11, where the error $\Delta(\mathcal{L})/\mathcal{L} = \frac{\mathcal{L}_{\text{approx}} - \mathcal{L}_{\text{exact}}}{\mathcal{L}_{\text{exact}}}$ is plotted against the variable $x$. Typical $q$ values are also shown. As expected, (PlnR) gives the best result while (P) is worse by far (the 4/6 approximant is even ill behaved around $q = 20$). The precision reached is still less than 3% with (PlnR) at $q$ values as “small” as 5. We adopt this technique throughout the rest of this paper. An idea of the convergence of this resummation with the length of the series is given by Fig. 12 showing various results for $\Delta(\mathcal{L})/\mathcal{L}$ using the series truncated at 8, 9, 10 and 12 (the 11th term is zero). The convergence is fast; the diagonal and near diagonal Padé’s lead to comparable results.

We now turn to the study of the $F^{(n)}$’s with $n \geq 2$ for which the series are known to order 10 in $z$. Because their lowest term is $\sim z^2$, the maximum value of $M + N$ available in (PlnR) is 8. For $F^{(2)}$ we find consistently that it behaves nearly linearly with $x$ for $x \gtrsim 100$ ($q \lesssim 10$) as well exposed by the plot of Fig. 13.

![Fig. 13](image_url)

*Regularized logarithmic Padé resummations for $F^{(2)}$.\*
Fig. 14

Regularized logarithmic Padé resummations for $F^{(3)}$.

showing various estimates of $F^{(2)}/x$. If we assume that this quantity is indeed asymptotically constant, its limit is very close to

$$F^{(2)}/x \sim \alpha = 7.610^{-2}. \quad (20)$$

In any case, there is a clear cross-over around $x = 100$ between the large $q$ regime and a very different low $q - 4$ behavior. Because the various Padé’s lead to very stable results for $q \geq 7$, our result also provides accurate predictions for the specific heat (see below).

Since we have a good control on $F^{(2)}$ behavior, we next analyze $F^{(3)}$ by the ratio $F^{(3)}/F^{(2)}$, a slightly better series than that of $F^{(3)}$ itself. With the prejudice that $F^{(3)} \sim x^{5/2}$ describes the leading behavior and with $F^{(2)} \sim x$, it is convenient to consider the positive quantity $-F^{(3)}/xF^{(2)}$ as a function of $x$, as shown in Fig. 14. The four curves correspond to the Padé’s 3/5, 4/4, 5/3 and 6/2. Note that although $F^{(3)}$ varies by 4 orders of magnitude in the $x$ interval shown, the above ratio stays between $\sim .1$ and .25. If now we assume that $F^{(3)}/(F^{(2)}x^{3/2})$
has a finite limit at large $x$, a reasonable estimate is

$$\frac{F^{(3)}}{x^{3/2} F^{(2)}} \sim \beta = 0.17$$

indicated by the dashed line in Fig. 14.

Given the estimates $\alpha$ and $\beta$ for the supposed limits of $F^{(2)}/x$ and $F^{(3)}/(x^{3/2} F^{(2)})$, the ansatz proposed in [8,10] for the free energy of the ordered phase gives a prediction for all the higher cumulants

$$F^{(n)}(x) \approx (-)^n \alpha \left( \frac{3\beta}{2} \right)^{n-2} \frac{\Gamma\left(\frac{2}{3} + n - 2\right)}{\Gamma\left(\frac{2}{3}\right)} x^{\frac{3}{2} n - 2}$$

We have compared direct ($\text{Pln}_R$) estimates of $F^{(n)}$, $n = 2, \cdots, 6$ with the above parametrization where $\alpha$ and $\beta$ have been fixed to their guessed values. The results for $(-)^n F^{(n)}$ as a function of $x$ is shown in Fig. 15. For each $n$, four curves are drawn, one showing the ansatz (dotted lines), the three other ones resulting from $4/4$, $5/3$ (solid lines) and $6/2$ (dashed lines) Padé’s. The $3/5$ Padé gives non-sense answers for $n = 5$ and $6$, for which case the $6/2$ approximant tends to blow up at small $q$. Nothing convincing can be extracted for $n > 6$, where the series become really too short.

With this in mind, we consider the results of Fig. 15 as a manifest evidence for an indefinite increase with $x$ of all the $F^{(n)}$’s, $n > 1$ and a good indication that the ratios $F^{(n)}/x^{3n/2-2}$ become smooth functions of $x$ at $x$ large enough, with relative ratios close to that of Eq. (22) (note that although $F^{(6)}$ varies by $\sim 7$ orders of magnitude when $x$ increases from 10 to 100, its value differs by less than a factor 2 from Eq. (22)).

Independently of any prejudice on the behavior of the cumulants, our analysis finally provides a quantitative prediction for the values of the first cumulants at fixed (not too small) values of $q$. Their knowledge may be of great help in understanding better the way how the thermodynamical limit is reached in the Potts model case, so accumulating experience on the use of finite size effects in other studies of phase transitions. We give in Table 5, for the ordered phase, the value of the specific heat at the transition point ($C_o = \beta^2 F_o^{(2)}$) and of the two next moments $F^{(3)}$ and $F^{(4)}$, together with results on $C_o$ from existing numerical simulations. The uncertainties quoted contain some arbitrariness, as often when Padé techniques are involved. To be specific, we quote as central values the results
Energy cumulants $(-)^n F^{(n)}$ from 4/4, 5/3 (solid lines) and 6/2 Padé resummation and comparison to the ansatz Eq. (22) (dotted lines).

from 4/4 Padé (for $F^{(3)}$ it is the 4/4 result of $F^{(3)}/F^{(2)}$ times the 4/4 result of $F^{(2)}$). The uncertainty in each case is the mean distance to the 4/3 and 3/4 results. We clearly contradict values recently obtained from low temperature series [14]. As already noticed [8], there is strong discrepancies for $q \leq 10$ with $C_o$ values extracted from earlier numerical simulations [15–18]. Let us note that we quote two $C_o$ values from [16], the value 12.7 from an analysis at the maximum of the specific heat and the value 18 from an analysis at the transition temperature, and this inconsistency was the starting point of the present work.

In contrast our predictions agree very well with the most recently published values [16–21]. These data correspond to higher $q$ value [16] or to analysis at the transition point in the disordered phase [20] and in the ordered phase [21]. The third momentum have been measured in these two last references and agree also very well with our predictions.

The discrepancies are observed with data obtained from FSS analysis at the
maximum of the specific heat. In fact the corresponding analysis are neglecting energy cumulants higher than \( n = 2 \) in the expansions in \( 1/V \) as made in [15]. Thus the discrepancies observed can be understood from the large values of the higher energy cumulants as we have shown, and we can try to be more quantitative by introducing them in the \( 1/V \) expansions. For example the \( \beta \) value at which the second moment is maximum expands as

\[
\beta_{\max F^{(2)}} = \beta_t + \frac{1}{V} \ln q - \frac{1}{V^2} \frac{12}{2} \frac{F^{(2)}}{F^{(1)^3}}
\]

\[ - \frac{1}{V^3} \frac{1}{6F^{(1)^2}} \left[ -24F^{(3)}_+ F^{(1)}_- + (\ln^3 q - 36 \ln q)(F^{(1)}_- F^{(3)}_- - 3F^{(2)^2}_- ) \right] \]

\[ - \frac{1}{V^4} \frac{1}{24F^{(1)^2}} \left[ -1152F^{(1)}_- F^{(2)}_- F^{(3)}_- + 1728F^{(2)^3}_- \right] \]

\[ + 96 \ln q (4F^{(3)}_+ F^{(1)}_- F^{(2)}_- - F^{(4)}_+ F^{(1)^2}_-) \]

\[ + (\ln^4 q - 72 \ln^2 q)(F^{(1)^2}_- F^{(4)}_+ - 10F^{(1)}_- F^{(2)}_- F^{(3)}_- + 15F^{(3)^3}_+) \]

\[ + \ldots \]

where \( F_\pm = F_o \pm F_d \) and \( F^{(n)}_d \) are obtained from \( F^{(k)}_o, \) \( k = 1 \) to \( n, \) with the duality relation. At \( q = 10 \) we obtain

\[
\beta_{\max F^{(2)}} = \beta_t - \frac{3.3}{V} - \frac{2.2}{V^2} + \frac{1.9 \cdot 10^5}{V^3} - \frac{1.5 \cdot 10^8}{V^4} + \ldots
\]

It is clear that this expansion is useless in practice as well as that of the maximum of the specific heat.

Detailed comparisons between data and consequences of our results on energy distributions can be found in [10].

6. Conclusions

We have explored the properties of the 2D-Potts model free energy \( F(\beta) \) in the region \( q \geq 4 \) where the model has a temperature driven first order transition. This was achieved by a series expansion of \( F(\beta) \), close to the transition temperature, in powers of \( 1/\sqrt{q} \), performed to order 10 from the Fortuin-Kasteleyn representation of the partition function. At each order \( m \) in \( q^{-1/2} \), we compute the number of lattice configurations of \( l \) bonds enclosing \( k \) clusters of sites such that \( l - 2k = m \).

The results obtained were translated into similar series in \( q^{-1/2} \) for the derivatives \( F^{(n)} \) of the free energy taken at the transition temperature, that is for the
energy cumulants of the model. These series truncated at order 10 provide strong
evidence for highly divergent behaviors at a low \( q \) value, the more so \( n \) increases.
We assumed that this value is \( q = 4 \), and conjectured that these singular behav-
iors are dominantly embodied in powers of the variable \( x(q) \) of Eq. (16), known
to accurately describe the latent heat and the largest correlation length in a wide
region of \( q > 4 \). Then, Padé techniques adapted to such behaviors were applied to
the \( F^{(n)} \) series, leading to quantitative predictions for \( n \lesssim 4 \), \( q \gtrsim 6 \), confirming
severe divergences of all \( F^{(n)} \)'s and in semiquantitative agreement, for \( n \) up to 6
at least, with an ansatz [8–10] which prescribes the divergence rates.

First these results enlarge our analytical knowledge of the 2D-Potts model, so
providing useful additional tests on methods for analyzing numerical data on finite
lattices. Next they illustrate the possible occurrence in first order transitions of
properties widely influenced by a nearby continuous transition point. This may be
the case as well for field driven phase transitions just below the critical temperature
when the correlation is still large [22,23].

One may think of other applications of our analytical approach to the free
energy of the Potts model. An interesting ones would be a study of the analytic
structure of \( F_o(\beta) \) ( or \( F_d(\beta) \) ) at fixed \( q > 4 \) around \( \beta = \beta_t \), where an essential
singularity is expected [24,25].

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Table 1

Number $N$ of unequivalent (upon lattice translations) dominant configurations.
| Contribution | Cluster set                                      |   |
|--------------|-----------------------------------------------|---|
| +2 $C(7, 5)$ | (2, 7)                                        | 1 |
| -(2$V - 16$) $C(11, 1)$ | (2, 7) × (1, 4)                                  | 2 |
| -12 $C(10, 2)$ | ((2, 7) + 3; 3, 10)                            | 3 |
| -4 $C(12, 1)$ | (2, 7) + 4; 4, 12                              | 4 |
| -4          | (2, 7) + 5; 4, 12                              | 5 |
| -28         | (2, 7) + 5; 4, 13                              | 6 |
| +8          | (((2, 7) + 3; 3, 10) + 2; 4, 12)                | 7 |
| +12 $C(10, 3)$ | (2, 9; 3, 10)                                  | 8 |
| -8 $C(12, 1)$ | ((2, 9; 3, 10) + 2; 4, 12)                     | 9 |
| -80         | ((2, 9; 3, 10) + 3; 4, 13)                     | 10|
| +6 $C(12, 2)$ | (2, 10; 4, 12)                                 | 11|
| +48 $C(13, 1)$ | (2, 11; 4, 13)                                 | 12|
| +8 $C(15, 1)$ | (2, 11; 5, 15)                                 | 13|
| +80         | (2, 12; 5, 15)                                 | 14|
| +12         | (2, 12; 6, 17)                                 | 15|
| +1/2($V - 5$) $C(8, 4)$ | (1, 4) × (1, 4)                                  | 16|
| -1/2($V^2 - 15V + 62$) | (1, 4) × (1, 4) × (1, 4)                      | 17|
| -12/2 $C(10, 2)$ | ((1, 4) × (1, 4) + 2; 3, 10)                  | 18|
| -4/2        | ((1, 4) × (1, 4) + 4; 4, 12)                  | 19|
| -52/2       | ((1, 4) × (1, 4) + 4; 4, 13)                  | 20|
| +8/2        | (((1, 4) × (1, 4) + 2; 3, 10) + 2; 4, 12)     | 21|
| -2/2($4V - 32$) $C(11, 1)$ | (1, 4) × ((1, 4) + 3; 2, 7)                  | 22|
| +(2$V - 16$) $C(11, 2)$ | (1, 4) × (1, 6; 2, 7)                           | 23|
| -28         | ((1, 4) × (1, 6; 2, 7) + 2; 4, 13)             | 24|
| +(6$V - 62$) | (1, 4) × (1, 8; 3, 10)                         | 25|
| +(V - 12)   | (1, 4) × (1, 8; 4, 12)                         | 26|
| +1/2($4V - 46$) | (1, 6; 2, 7) × (1, 6; 2, 7)                 | 27|

Table 2

Detailed contributions to $N_{2,12}/V$ in column 1 (with $C(i,j)$ as given in Eq. (10)) of the different cluster sets in column 2.
| \(l\) | \(m = 2\) | \(m = 4\) | \(m = 6\) | \(m = 8\) | \(m = 10\) | \(l\) | \(m = 1\) | \(m = 3\) | \(m = 5\) | \(m = 7\) | \(m = 9\) |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| 60  | 1   |     |     |     |     | 59  |     |     |     |     |     |
| 58  | 6   |     |     |     |     | 57  |     |     |     |     |     |
| 56  | 22  |     |     |     |     | 55  |     |     |     |     |     |
| 54  | 68  |     |     |     |     | 53  |     |     |     |     |     |
| 52  | 187 |     |     |     |     | 51  |     |     |     |     |     |
| 50  | 328 | 49  |     |     |     | 2   |     |     |     |     |     |
| 48  | 600 | 47  |     |     |     | 8   |     |     |     |     |     |
| 46  | 610 | 45  |     |     |     | 30  |     |     |     |     |     |
| 44  | 4   | 43  |     |     |     | 88  |     |     |     |     |     |
| 42  | -1352 | 41 |     |     |     | 178 |     |     |     |     |     |
| 40  | 1   | -2896 | 39 |     |     | 252 |     |     |     |     |     |
| 38  | 6   | -5198 | 37 |     |     | 204 |     |     |     |     |     |
| 36  | 22  | 2612 | 35 |     |     | -532 |     |     |     |     |     |
| 34  | 68  | -5863 | 33 |     |     | -722 |     |     |     |     |     |
| 32  | 89  | 24485 | 31 |     |     | 2   | -2618 |     |     |     |     |
| 30  | 112 | -16014 | 29 |     |     | 8   | 620 |     |     |     |     |
| 28  | -229 | 28035 | 27 |     |     | 30  | 894 |     |     |     |     |
| 26  | -570 | -38351 | 25 |     |     | 48  | 7334 |     |     |     |     |
| 24  | 1   | -1749/2 | 100263 | 23 |     | 14  | -6054 |     |     |     |     |
| 22  | 6   | 1182 | -379348 | 21 |     | -244 | 71360/3 |     |     |     |     |
| 20  | 22  | 233 | 3321646/5 | 19 |     | -208 | -78920 |     |     |     |     |
| 18  | 6   | 6704 | -625246 | 17 |     | 2   | -138 | 106586 |     |     |     |
| 16  | -63 | -65917/4 | 351774 | 15 |     | 8   | 2156 | -226216/3 |     |     |     |
| 14  | -201 | 15532 | -119493 | 13 |     | 6   | -3000 | 29954 |     |     |     |
| 12  | 1   | 1555/3 | -7365 | 21723 | 11 | -72 | 1762 | -6066 |     |     |     |
| 10  | 6   | -406 | 1686 | -6431/5 | 9 | 88  | -468 | 3422/9 |     |     |     |
| 8   | -33/2 | 131 | -459/4 | 7 |     | 2   | -38 | 254/7 |     |     |     |
| 6   | 12  | -37/3 |     |     | 5 | -4  | 22/5 |     |     |     |     |
| 4   | 1   | -3/2 |     |     | 3 | 2/3 |     |     |     |     |     |
| 2   | -1 |     |     |     | 1 | 2 |     |     |     |     |     |

**Table 3**

*Non zero coefficients \(A(l,m)\) contributing to \(F_o\) in Eq. (12)*
|     | 0    | 1    | 2    | 3    | 4    | 5    | 6    |
|-----|------|------|------|------|------|------|------|
| 2   | 0    | 4    | 16   | 64   | 256  | 1024 | 4096 |
| 3   | -4/3 | -2   | 34   | 430  | 3778 | 29518| 218914|
| 4   | 1    | 2    | 114  | 2654 | 41778| 556382| 6813714|
| 5   | -8/5 | -6   | 254  | 12186| 322670| 6773994| 126069374|
| 6   | 2    | 4    | 882  | 57018| 2210982| 67122114| 1774583142|
| 7   | -12/7 | -16  | 1944 | 224732| 12819264| 546094604| 19774354944|
| 8   | 5/2  | 6    | 6128 | 888024| 68657204| 3918393456| 187361651588|
| 9   | -4/9 | -38  | 13550| 3164682| 333583598| 25037212842| 1545876302510|
| 10  | 0    | 0    | 39698| 11243178| 1532324246| 146961943266| 11451708807878|

Table 4

Coefficients $C_m^n$ of the expansion of $F_o^{(n)}$ in Eq. (13).

| $q$ | $C_o$   | $-F_o^{(3)}$ | $F_o^{(4)}$ | $C_o^{\text{exp}}$ | $-F_o^{(3)\text{exp}}$ | Ref. |
|-----|---------|--------------|-------------|--------------------|-------------------------|-----|
| 30  | 3.41294(5) | 16.74(2)    | 7.00(5) $10^2$ | 5.2(2)            | 55.8(9)                | [19] |
| 20  | 5.3612(4) | 56.9(4)      | 5.0(1) $10^3$ | 5.38(4)           | 57.0(13)               | [20] |
|     |          |              |             | 5.351(15)         |                        | [21] |
| 15  | 7.999(3) | 179(.4)      | 3.1(2) $10^4$ | 8.04(4)           | 175(5)                 | [20] |
|     |          |              |             | 8.016(21)         | 180.5(31)              | [21] |
| 10  | 17.98(2) | 1.9(2) $10^3$| 1.3(2) $10^6$ | 10.6(11)          | 18.0(2)                | [15] |
|     |          |              |             | 12.7(3)           | 2066(81)               | [16] |
|     |          |              |             | ~18.              | 1979(87)               | [16] |
|     |          |              |             | 18.0(2)           |                        | [20] |
|     |          |              |             | 17.95(13)         |                        | [21] |
| 8   | 36.9(2)  | 1.4(4) $10^4$| 2.7(8) $10^7$ | 22.8(30)          |                        | [15] |
| 7   | 69.6(5)  | 7.(3) $10^4$ | 3.4(13) $10^8$ | 47.5(25)          | 50.10                   | [17] |
|     |          |              |             | 44.22              |                        | [18] |

Table 5

Results for the first energy cumulants at some $q$ values and comparison to numerical data.