LARGE ENERGY CUMULANTS IN THE 2D POTTS MODEL AND THEIR EFFECTS IN FINITE SIZE ANALYSIS

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ABSTRACT

We develop an ansatz for expressing the free energy of the two dimensional $q$-states Potts model for $q > 4$ near its first order phase transition point. We notice that for the moderate values of $q \lesssim 15$, the energy profile at the phase transition is not expressible as a sum of gaussians. We discuss how this affects the traditional finite size analysis of this phase transition. In particular, the dominant length scale governing the finite size corrections turns out to be much ($\sim 6$ times) larger than the largest correlation length in the problem.
1. INTRODUCTION

There has been a lot of recent interest in the numerical study of first order transitions. Though these systems are undeniably of great phenomenological importance, a purely analytical study has often been beyond the reach of current methods. The two-dimensional $q$-states Potts model is, in this arena, a very useful model: for, on the one hand, a lot is known about this model analytically [1- 6]; on the other, a number of numerical simulations [8- 18] have been performed on this model.

Unfortunately, the finite size scaling behaviour of the numerical data are often not satisfactorily explained by the exact analytical results at hand. Small discrepancies also appear when the numerically measured surface tensions are compared to their theoretical estimates.

In an attempt to clarify these issues, we tried to condense the analytically known results into an ansatz which might correctly incorporate the leading singularities of the free-energy near the transition point as function of $q$ and $\beta$, the inverse temperature. This allowed us to investigate all moments of the energy distribution function at the transition point. As expected from our previous analysis of a high $q$ expansion in this model [19,20] and contrary to popular expectations, we discovered that the higher moments are very large at moderate values of $q \sim 10$. As a result, the energy distribution cannot be satisfactorily expressed as a sum of gaussian distributions; and the usual methods of finite size analysis may have to be revised.

In addition to this, the finite volume corrections appear to follow a simple scaling relation, where, however, the relevant length scale turns out to be much larger than the correlation lengths in the model. In fact only the simulations performed at a $q$ value as large as 20 seem to have been in the truly asymptotic regime [16]. We believe that these non-negligible finite size effects (and proper accounting of the large energy cumulants) may have caused the apparent discrepancies in the numerical analyses.

The organization of this paper is as follows. In section 2, we summarize the analytically known properties of the model. In the next section, we show how numerical methods allow to isolate finite volume effects directly in the free energy. We develop our ansatz in section 4, and use it to predict a set of scaling relations. We apply this ansatz to study the available numerical data in section 5. We end with a short discussion of the main results of our paper in section 6.

2. KNOWN PROPERTIES OF THE MODEL AND PRELIMINARIES

The $q$-states 2-D Potts model is defined by the Hamiltonian

$$H = -\sum_{(ij)} \delta_{\sigma_i,\sigma_j}, \quad (2.1)$$

where the $\sigma_i$ variables, attached to the $V = L^2$ sites $i$ of a square lattice, take $q$ distinct values; the summation extends to all the $2V$ pairs $(ij)$ of neighbouring sites. We shall refer to $V$ as the lattice volume. Many properties of this model have been known for a long time and can be found in the review by Wu[3].

Throughout this paper, we shall call

$$F = \lim_{V \to \infty} \left( \frac{1}{V} \ln Z \right) \quad (2.2)$$
the free energy of the system, where $Z$ is its partition function. The model has a temperature driven phase transition which occurs at a value of the inverse temperature $\beta$ given by

$$\beta_t = \ln \left[ \sqrt{q} + 1 \right]$$ (2.3)

This value separates the region where the system is in either one of the $q$ possible ordered phases ($\beta > \beta_t$) from the disordered region ($\beta < \beta_t$). When necessary, the quantities in an ordered or in the disordered phase will be labeled by a subscript $\varphi = o$ or $d$, respectively.

The transition is second order for $q \leq 4$, where the critical properties are described by known, $q$ dependent, indices. In particular, the specific heat and correlation length exponents $\alpha$ and $\nu$ are the same in all phases and are given by

$$\alpha(q) = \frac{2(1-2u)(1-u)}{3(1-u)}$$ (2.4)

$$\nu(q) = \frac{(2-u)(1-u)}{3(1-u)} ,$$ (2.5)

where $\cos \left( \frac{\pi}{2} u \right) = \sqrt{q}/2$. Note in particular that at $q = 4$, $\alpha$ and $\nu$ coincide:

$$\alpha(4) = \nu(4) = \frac{2}{3}.$$ (2.6)

For each phase $\varphi$, we observe that although the correlation length $\xi_\varphi$ and the specific heat $C_\varphi$ both diverge for $q \leq 4$ when $\beta - \beta_t \to 0$ as

$$\xi_\varphi \propto \lambda_\varphi |\beta - \beta_t|^{-\alpha(q)} + ...$$

$$C_\varphi \propto \mu_\varphi |\beta - \beta_t|^{-\nu(q)} + ...$$ (2.7)

their ratio remains finite at $q = 4$ in the neighbourhood of $\beta_t$. In the expression above, the dots stand for (unknown) less singular and regular terms at $\beta = \beta_t$.

The phase transition at $\beta = \beta_t$ is first order for $q > 4$. The internal energies of the pure phases, $E_\varphi$, are exactly known at $\beta = \beta_t$ [1]. The latent heat $\mathcal{L} = E_d - E_o$, finite for any $q > 4$, vanishes as $q \to 4+$; so that this quantity is continuous at the (second order) point $q = 4$. Various expressions and properties of the $E_\varphi$'s are given in Appendix A for completeness and further reference.

In this first order region, the specific heats $C_\varphi$ and correlation lengths $\xi_\varphi$ are finite at any value of $\beta$. The difference $C_d - C_o$ is known at $\beta_t$:

$$C_d - C_o = \beta_t^2 \mathcal{L}/\sqrt{q} ,$$ (2.8)

which shows that it vanishes in the same way as $\mathcal{L}$ when $q \to 4+$. However, their sum is unknown. Exact expressions for various correlation lengths have been obtained in the recent years [5,6] and details are collected in Appendix A. Here we quote only those results which are relevant to us. According to these calculations, and to their interpretation [6,7] in terms of the pure phase $\xi_\varphi$'s, the disordered phase correlation length $\xi_d$ has the following divergent behaviour as $q \to 4+$:

$$\xi_d \simeq \frac{1}{8\sqrt{2}} x ,$$ (2.9)
where \( x \) is given by

\[
x = \exp \left[ \frac{\pi^2}{(2\theta)} \right]
\]

\[
\theta = \ln \left[ \sqrt{q} + \sqrt{q - 4} \right].
\]

The behaviour (2.9) was anticipated by Black and Emery a long time ago using renormalization group techniques [2]. Only very recently numerical simulations were able to produce data in agreement with this result [18].

When \( q \to 4^+ \), \( 2\theta \) tends to 0 as \((q - 4)^{1/2}\) so that \( x \) diverges quite strongly. On the other hand, as \( q \) increases away from 4, \( \theta \) increases very slowly, growing only logarithmically as \( q \to \infty \), so that \( x \) stays very large over a very broad range of \( q \)-values. As a consequence, the approximation (2.9) of \( \xi_d \) remains valid over an equally large domain [7] (see Appendix A for the size of the corrections to (2.9)). For this reason, the variable \( x \) happens to be relevant to our forthcoming analysis of the phase transition above \( q = 4 \). We note in particular that it also controls the leading behaviour of the latent heat, which vanishes as \( x^{-1/2} \) at \( q = 4 \).

So, the correlation length at \( \beta = \beta_t \) in the disordered phase becomes infinite as \( q \to 4^+ \) as it does at \( q = 4 \) when \( \beta \to \beta_{t-} \). Less is known about \( \xi_o \), but it has been conjectured by Borgs and Janke [7] that

\[
\xi_o = \xi_d / 2
\]

which is consistent with numerical estimates of \( \xi_o \) at \( q = 10 \) [9,11].

If \( \xi_o \) diverges at \( q \to 4^+ \), it is not unexpected that the specific heat does so as well, since the latter is related to the integral of the energy-energy correlation function over the whole lattice:

\[
C_o = \lim_{V \to \infty} \frac{\beta^2}{4} \sum_{\ell} \left( \langle E_{\ell_0} E_\ell \rangle_\varphi - \langle E_{\ell_0} \rangle_\varphi \langle E_\ell \rangle_\varphi \right)
\]

(2.12)

Here \( \ell_0 \) is a fixed link, \( E_\ell \) (0 or 1) is the energy carried by the link \( \ell \), \( \langle \rangle_\varphi \) denotes the average inside the phase \( \varphi \); and the thermodynamical limit \( V \to \infty \) is taken before the limit \( \beta \to \beta_t \). As it generically does at a 2\(^{nd} \) order point, the sum in (2.12) most probably diverges along with the correlation length, the major contribution coming from the region of large \( \ell_0 - \ell \) separation. Since \( \xi_d \) is known to diverge as \( q \to 4^+ \), \( C_o \) should also diverge. Further, since \( C_d - C_o \) is bound to vanish in the same limit, \( C_o \) also must go to infinity, consistent with the Borgs-Janke conjecture (Eq. 2.11).

We continue this review of known properties by writing down the consequence of duality for the free energy \( F(\beta) \) of this model. At \( \beta \geq \beta_t \) (respectively \( \beta \leq \beta_t \)), \( F(\beta) \) coincides with the ordered (disordered) free energy \( F_o \) (\( F_d \)). Duality relates \( F(\beta) \) to \( F \left( \tilde{\beta} \right) \), where \( \beta \) is related to \( \tilde{\beta} \) by

\[(e^\beta - 1) \left( e^{\tilde{\beta}} - 1 \right) = q , \]

(2.13)
and we have
\[
F_d(\tilde{\beta}) - \ln \left[ \frac{\exp(\tilde{\beta}) - 1}{\sqrt{q}} \right] = F_0(\beta) - \ln \left[ \frac{\exp(\beta) - 1}{\sqrt{q}} \right].
\]  
Equation (2.14)

It is convenient to parametrize the distance to \( \beta = \beta_t \) (the transition point, where \( \beta = \tilde{\beta} \)) by defining a variable \( b \) through
\[
e^b = \frac{e^\beta - 1}{\sqrt{q}}.
\]  
Equation (2.15)

As \( \beta \to \beta_t \), \( b \) vanishes as \((1 + 1/\sqrt{q}) (\beta - \beta_t)\), the interchange \( \beta \leftrightarrow \tilde{\beta} \) is just \( b \leftrightarrow -b \), and duality is the statement that the free energies of the model can be written
\[
F_0(\beta) = F_t + b + g(b)
\]  
Equation (2.16)
\[
F_d(\beta) = F_t + b + g(-b).
\]
Here \( F_t \) is \( F_0(\beta_t) = F_d(\beta_t) \), \( b \) is defined by (2.15), and \( g(b) \), which vanishes at \( b = 0 \), contains all the essential information about \( F(\beta) \). It follows the \( n \)th energy cumulants at \( \beta = \beta_t \)
\[
F^{(n)}_\phi \equiv \frac{d^n}{d\beta^n} F_\phi(\beta) \bigg|_{\beta=\beta_t}.
\]  
Equation (2.17)

once expressed in terms of the derivatives \( g^{(p)}(0), p \leq n, \) of \( g(b) \) have the same form for \( \phi = o \) and \( d \), up to the change \( g^{(p)}(0) \leftrightarrow (-)^p g^{(p)}(0) \). Thus, the combination \( F^{(n)}_o - (-)^n F^{(n)}_d \) is completely determined by the knowledge of the cumulants of order lower than \( n \). Equation (2.8) and the relation
\[
E_d + E_o = -2 (1 + 1/\sqrt{q})
\]  
Equation (2.18)

are two well known examples of this general statement of duality.

Up to now we only considered properties of the model in the thermodynamical limit; in particular the limit \( V \to \infty \) was always taken before the limit \( \beta \to \beta_t \), which allowed us to properly define \( F(\beta) \). We now turn to the properties of the system in a finite box with periodic boundary conditions, and recall the result obtained in Ref. [4] for the corresponding finite volume partition function \( Z_V(\beta) \):
\[
Z_V(\beta) = q \exp[V F_o(\beta)] + \exp[V F_d(\beta)] + R(L, \beta).
\]  
Equation (2.19)

The first two terms represent the \( q \) ordered and the disordered phase contributions to the total partition function respectively, and the essential statement is that the rest \( R(L, \beta) \) is bounded by the inequality
\[
|R(L, \beta)| < c_1 \times q^{-c_2 L} \times \exp(V F(\beta)),
\]  
Equation (2.20)

where \( c_1 \) and \( c_2 > 0 \) are constants. Similar statements hold for the logarithmic derivatives of \( Z_V(\beta) \), that is for the cumulants of the energy distribution. We refer to \( R(L, \beta) \) as a “true” finite size effect, and to the first two terms in Eq. (2.19) as the asymptotic ordered and disordered contributions.
We also recall that

\[ F(\beta) \equiv F_o(\beta) \quad \text{for} \quad \beta \geq \beta_t \]

\[ F(\beta) \equiv F_d(\beta) \quad \text{for} \quad \beta \leq \beta_t , \]

so that \( F = \text{Max}(F_o, F_d) \). Strictly speaking, the result holds for \( q \) “large enough”. We will ignore this caveat, and consider that (2.20) is valid for \( q > 4 \).

Eqs. (2.19,2.20) are very interesting since they control the size of any deviation of the partition function at finite size from the familiar two component representation \( Z = qZ_o + Z_d \). For this reason, we are going to demonstrate in the next section how \( F(\beta) - F_t \), close to \( \beta = \beta_t \) can, in principle, be extracted from very precise numerical data on the energy distribution, supplemented by the duality property (2.16).

3. NON ASYMPTOTIC PURE PHASE FREE ENERGIES FROM NUMERICAL DATA

By definition, the partition function is given by

\[ Z_V(\beta) = \sum_E \Omega_V(E)\exp[-\beta V E] \quad (3.1) \]

where \( V E \) is the energy of a configuration, and \( \Omega_V(E) \) (which is independent of \( \beta \)), the number of configurations with that energy in the given volume. The current numerical simulations measure the energy probability distribution at some value of \( \beta \), say \( \beta_0 \):

\[ P_{V,\beta_0}(E) = \frac{\Omega_V(E)\exp[-\beta_0 V E]}{Z_V(\beta_0)}. \quad (3.2) \]

It follows from the two above equations that

\[ \frac{Z_V(\beta)}{Z_V(\beta_0)} = \sum_E P_{V,\beta_0}(E)\exp[-V E(\beta - \beta_0)], \quad (3.3) \]

which yields the \( \beta \) dependence of \( Z_V(\beta) \) up to a constant factor \( Z_V(\beta_0) \), and thus, an effective free energy via

\[ F^{\text{eff}}(L, \beta) - F^{\text{eff}}(L, \beta_0) = \frac{1}{V} \ln \left[ \frac{Z_V(\beta)}{Z_V(\beta_0)} \right]. \quad (3.4) \]

This is true for any lattice system, but, in such generality, is not very useful for finite size studies because the \( V \) dependence of the constant (i.e. \( \beta \)-independent) \( F^{\text{eff}}(L, \beta_0) \) remains unknown.

It becomes more interesting in the case of a system which has a first order transition at \( \beta = \beta_t \), with, as in the Potts model, a duality property relating the \( q \) ordered phases to the disordered phase coexisting around \( \beta_t \) in a finite volume. Consider the “asymptotic” form \( Z_{\text{as}}(\beta) \) given by (2.19) when the remainder \( R(L, \beta) \) is dropped and \( F_o, F_d \) are represented in the form (2.16). Then we construct the quantity

\[ X(b) \equiv \frac{Z_{\text{as}}(\beta)}{Z_{\text{as}}(\beta_t)}\exp(-bV) = \frac{q \exp[V g(b)] + \exp[V g(-b)]}{q + 1}. \quad (3.5) \]
with $b$ given by (2.15) as a function of $\beta$. As explained above, the function $X(b)$ can be measured from numerical simulations in the vicinity of $b = 0$ (that is of $\beta = \beta_t$). The function $g(b)$ then follows from the knowledge of $X$ at $b$ and $-b$:

$$g(b) = \frac{1}{V} \ln \left[ \frac{qX(b) - X(-b)}{q - 1} \right],$$

(3.6)

and corresponding $F^\text{eff}_o$ and $F^\text{eff}_d$ can be reconstructed from Eq. 2.16. By construction, $g(b)$ should be independent of the lattice size in the limit where the remainder $R(L, \beta)$, bounded by (2.20), can be neglected. In turn, any $V$ dependence is a direct measure of “true” finite size effects, and these effects, as opposed to the situation of the energy distribution (see our discussion in the next sections), are under theoretical control [4].

Let us now show that this extraction of finite size effects in the pure phase free energies is indeed feasible. For this purpose, we use the numerical data of Ref. [12], for the $q = 10$ Potts model with linear lattice sizes $L = 16, 20, 24, 36, 44$ and 50. Details on the runs can be found in the reference. We just recall that a multi-spin coding was used, allowing for the simultaneous generation of 16 independent Monte Carlo histories and that at each lattice size, a very long run was made near the maximum of the specific heat. We use the data from these long runs and all the errors quoted below are computed from the observed dispersion about their mean of the 16 corresponding results. Because it turns out that the finite size effects are very small, a plot of $g(b)$ itself as given by Eqs.(3.6, 3.5 and 3.3) does not show any $L$ dependence. For clarity, we choose to show, as a function of $\beta$, and for the various lattice sizes, the quantity

$$W_o[L, \beta] = F^\text{eff}_o(L, \beta) - F_t + E_o(\beta - \beta_t),$$

(3.7)

which differs from the measured effective free energy $F_o(L, \beta) - F_t$ by the known asymptotic linear term. Then the finite size effects clearly show up, as exhibited in Figs. (1a) and (1b). On the largest lattices ($L = 50$ and 44), because of important statistical errors, the quantity $W_o$ is available in a limited range of $\beta$ only. Below $\beta = \beta_t$, this is due to the large cancellations occurring in the argument of the log in Eq.(3.6). At large positive values of $V (\beta - \beta_t)$, the errors become large again since we have to extrapolate data far away from the $\beta$ values where they were measured [12]. Fig. (1a) shows $W_o(L, \beta)$ for $L = 50, 44$ and 36. From this figure, we conclude that, within the present errors, there is no sizable $L$ dependence for $L \geq 36$, in the accessible $\beta$ range, as was observed in Ref. [12] for $\langle E \rangle_{\beta_t}$.

On the contrary, finite size effects are clearly exposed (see Fig. 1b) on lattices of linear size $L < 36$. In particular, the slope of $W_o(L, \beta)$ at $\beta = \beta_t$ is not zero showing that the ordered phase internal energy is not $E_o$ (but it does tend rapidly to $E_o$ as $L$ increases). This finite size effect should not be confused with that observed for the location of the peak in the energy distribution: as will be emphasized later on, a peak displacement must be present even in the asymptotic regime (i.e. even when $R(L, \beta)$ is negligible). A closer look at Fig. 1b also reveals that the curvature (specific heat) at $\beta_t$ (as well as the higher derivatives with respect to $\beta$) do exhibit $L$ dependence.
The precision reached in the simulation used here does not allow for a quantitative study of the \( \beta \) and \( L \) dependence of the “non asymptotic” part, \( R(L, \beta) \), of the partition function, at least in the absence of some model for these effects. What is demonstrated is the feasibility of measuring the non-asymptotic contributions to the Potts model free energies. We now turn to a theoretical study of the asymptotic ordered phase free energy \( F_o(\beta) \), which the above numerical determination could be compared with.

4. A THEORETICAL ANSATZ WHICH ACCURATELY DESCRIBES THE POTT S MODEL FREE ENERGY

We start from the observation made in Section 2 that the correlation length of the model tends to infinity when the point \( q = 4, \beta = \beta_t(4) \) is reached along either of the following two paths in the \( q, \beta \) plane:

(i) \( q = 4, \beta \rightarrow \beta_t(4) \) (Temperature driven 2nd order transition)

(ii) \( \beta = \beta_t(q), q \rightarrow 4_+ \) (along the 1st order line).

In case (i) we know furthermore that in each of the two phases \( \varphi = (o, d) \) the ratio of the specific heat to the correlation length tends to a constant (Eq.(2.7)).

For case (ii), we argued that since \( \xi_o \) diverges, it looks reasonable to believe that \( C_{\varphi} \) also diverges.

We now conjecture that in fact \( C_{\varphi}/\xi_o \) is finite also along path (ii), and formulate our ansatz as a generalization of this kind of continuity of \( C_{\varphi}/\xi_o \) at \( q = 4, \beta = \beta_t(4) \). (To be specific, we discuss the ordered phase \( (\beta \rightarrow \beta_t) \), using duality afterwards to determine the free energy in the other phase.)

In situation (i) the known specific heat exponent implies that the most singular part of the second derivative of the free energy with respect to \( \beta \) is

\[
F^{(2)}_o(\beta) \sim A (\beta - \beta_t)^{-2/3} ,
\]

so that the corresponding \((p + 2)\)th derivative is

\[
F^{(p+2)}_o(\beta) \sim A (-)^p \frac{\Gamma(p+2/3)}{\Gamma(2/3)} (\beta - \beta_t)^{-2/3 - p} .
\]

On the other hand, we use our knowledge of the correlation length exponent:

\[
\xi_o \sim \lambda_o (\beta - \beta_t)^{-2/3} ,
\]

to eliminate \((\beta - \beta_t)\) and obtain the relation

\[
F^{(p+2)}_o(\beta) \sim A (-)^p \frac{\Gamma(p+2/3)}{\Gamma(2/3)} (\xi_o/\lambda_o)^{3p+1} ,
\]

between the order \((p + 2)\) cumulant of the energy distribution and the correlation length.

Our ansatz consists in boldly continuing Eq.(4.4), from situation (i) to situation (ii), where we know the behaviour of \( \xi_o \) (Eqs.(2.11,2.9)) as a function of \( q \) at \( \beta = \beta_t \). Hence we have

\[
F^{(p+2)}_o(\beta_t) \sim A (-)^p \frac{\Gamma(p+2/3)}{\Gamma(2/3)} (Bx)^{1+3p/2} ,
\]
where \( x \) is defined in Eq.(2.10). The constant \( B \) includes the proportionality constants occurring in \( \xi_o \) as a function of \( \beta \) or of \( x \). Let us add a few comments.

a) All these relations express the leading behaviour as either \( \beta \rightarrow \beta_t \) at \( q = 4 \), or \( q \rightarrow 4^+ \) at \( \beta = \beta_t \). In particular, subdominant terms in the basic equation (4.5) arise from less singular or regular terms in both \( F^{(2)}_o \) and \( \xi_o \) at the second order point \( q = 4, \beta = \beta_t(4) \), neglected above. Including the (known) corrections to the low \((q-4)\) behaviour of \( \xi_o \) alone would thus have been inconsistent.

b) We recall that \( x \) is very large over a wide range of values of \( q > 4 \). Accordingly, all the energy cumulants \( F^{(p+2)}_o (\beta_t) \), which behave like \( x^{(1+3p/2)} \), become extremely large if \( p \geq 0 \). If we set \( p = -1 \), Eq.(4.5) yields a vanishing contribution of \( O(x^{-1/2}) \) to the internal energy \( E_o \). Though this must be neglected in comparison with other contributions to \( F^{(1)}_o (\beta) \) which do not vanish at \( q = 4, \beta \rightarrow \beta_t(4) \), we note that the known result

\[
E_o = -(1 + 1/\sqrt{q}) - \mathcal{L}/2, \quad (4.6)
\]

shows the presence of this term as the latent heat \( \mathcal{L} \) vanishes as \( x^{-1/2} \) (see Appendix) in the limit \( q \rightarrow 4^+ \).

c) At the leading order in \( x \) we consider here, the energy cumulants \( F^{(p+2)}_d \) in the disordered phase are given by the expression (4.5) with the \((-)^p\) sign dropped. This follows from duality (see Eq.(2.16)) which implies

\[
F^{(p+2)}_d = (-)^p F^{(p+2)}_o + O \left( F^{(p+1)}_o \right), \quad (4.7)
\]

where the corrections are down by \( x^{3/2} \) compared to the leading term.

d) In Eq. (4.5), we call the critical amplitude, \( A \), and the proportionality factor, \( B \), “constants”. What we actually mean is that they are smooth functions of \( q \) when compared with the violent behaviour of \( x(q) \). This is indeed what appears in the latent heat \( \mathcal{L} \) (Appendix), which is \( x^{-1/2} \) times a function of \( q \) which varies smoothly from \( \pi \) at \( q = 4 \) to \( 4\pi/\ln q \) as \( q \rightarrow \infty \).

e) For consistency with duality of our ansatz (4.5), we have the same \( A \) and \( B \) in the ordered and disordered phases cumulants. That \( A_o = A_d \) is no surprise since duality applied directly to (4.1) (which is valid at \( (\beta - \beta_t) \rightarrow 0^+ \)) yields

\[
F^{(2)}_d (\beta) \sim A (\beta_t - \beta)^{-2/3},
\]

which in turn is valid for \( (\beta_t - \beta) \rightarrow 0^+ \). That it is so also for the factor \( B \) may seem more intriguing since \( \xi_o \) is used in deriving (4.5) and is different from \( \xi_d \). What it actually implies is that the ratio \( \xi_d/\xi_o \) at \( q > 4 \), which is two according to (2.11), must also be two at \( q = 4 \) (i.e. it must be continuous at \( q = 4_+ \)).

With the expression (4.5) of the derivative \( F^{(n)}_o (\beta) \) at \( \beta_t, n \geq 2 \), and the knowledge of the first order derivative \( -E_o \), we obtain for \( F_o (\beta) - F_o (\beta_t) \):

\[
F_o (\beta) - F_o (\beta_t) = -E_o (\beta - \beta_t) + \frac{3A}{(Bx)^2} \left[ \frac{3}{4} \left( 1 + (\beta - \beta_t)(Bx)^{3/2} \right)^{4/3} - \frac{3}{4} (\beta - \beta_t)(Bx)^{3/2} \right], \quad (4.8)
\]
For later convenience in exploiting this expression, we rearrange it and rescale its variables. After setting

\[ S^2 = \frac{(Bx)^2}{3A} \]
\[ v = (\beta - \beta_t) \frac{(Bx)^{3/2}}{3} \]

\[ \varepsilon_o = \frac{E_o (Bx)^{1/2}}{3A} \]
\[ \varepsilon_d = \frac{E_d (Bx)^{1/2}}{3A} , \]

and noting that, to the order of accuracy retained, \( F_d \) follows from \( F_o \) by changing \( v \) into \(-v\) and \( E_o \) into \(-E_d,(*)\) we obtain the essential result of this section

\[ S^2 (F_o(\beta) - F_t) = -\frac{3}{4} - v (\varepsilon_o + 1) + \frac{3}{4} (1 + v)^{4/3} \] (4.10o)
\[ S^2 (F_d(\beta) - F_t) = -\frac{3}{4} - v (\varepsilon_d - 1) + \frac{3}{4} (1 - v)^{4/3} \] (4.10d)

These are the expressions we propose as ansätze for the free energies of the model in the first order region. According to the way we established them, we expect their domain of validity to be the region where \( Bx \) is large and \( v \) is finite. Under these conditions, we immediately note that

(i) \( S \) (which is proportional to the correlation length) plays the role of a length scale, to be compared with the linear scale \( L \) of the finite lattice on which we compute the partition function.

(ii) After rescaling the internal energy parameters \( E_o, \ E_d \) according to (4.9) the “asymptotic” partition function

\[ Z = q \exp \left( L^2 F_o(\beta) \right) + \exp \left( L^2 F_d(\beta) \right) \]

depends on \( L \) and \( q \) only through the reduced size \( L/S \) (apart for the multiplicity \( q \)). This statement is true up to residual dependencies of \( A \) and \( B \) upon \( q \) in (4.9) (see comment (d) above).

We repeat that the expressions (4.10o,4.10d) are just ansätze which have been built from the assumed continuity of ratios of energy cumulants at \( q = 4 \) and above, a continuity which we have no theoretical argument for. Hence, we have to justify our approach by explicit comparison of its consequences with results of numerical simulations. This will be done in the next section. However, we already want to point out that Eqs. (4.10o and 4.10d) suffer from the absence of singularity at \( \beta = \beta_t \) (that is \( v = 0 \)). Such a singularity is expected [21] or proven to exist [22] in the similar situation of a field driven first order transition at low temperature (Ising model below \( T_c \) in the limit of a vanishing magnetic field). Here we take the heuristic point of view that this singularity, although probably essential, is numerically mild, so that it does not affect the practical consequences we shall now discuss. A probably related weakness of our ansatz is its singularity at \( v = -1 \) for \( F_o \) (and \( v = +1 \) for \( F_d \)). Indeed \((1 + v)^{4/3}\) is the only analytical function at \( v = 0 \) whis has the required \( F_o^{(n)}(\beta_t) \). But an essential singularity at \( v = 0 \), with a vanishing contribution to all derivatives, may alter the analyticity structure at \( v < 0 \).

* there is a misprint in Ref. 19 where \( \varepsilon_d \) should be changed into \(-\varepsilon_d\) in Eq.(12).
5. APPLICATIONS OF OUR ANSATZ FOR $F(\beta)$

In order to exploit the consequences of the ansatz (4.10), we need to assign numerical values to the “constants” $A$ and $B$ at the value of $q$ we are interested in. As explained in Ref. [19], we are able to do so by comparing the values of the second and third derivatives of $F_o(\beta)$ at $\beta = \beta_t$, given by

\[
\begin{align*}
F_o^{(2)}(\beta_t) &= ABx, \\
F_o^{(3)}(\beta_t) &= -\frac{2}{3}A(Bx)^{5/2},
\end{align*}
\]

to the analytical results of a large $q$ expansion. A full account of the procedure, which includes suitable Padé resummations of series in $1/\sqrt{q}$ now extended to order 10, is given in Ref. [23], together with estimates of $A$ and $B$ for the $q$ values of interest.

5.1. Comparison of $F_o(\beta)$ with numerical data at $q = 10$

As exhibited in Section 3, a simulation measuring the energy distribution in a region of $\beta$ close to $\beta_t$, supplemented by duality, gives access to an estimate, $F_o^{\text{eff}}(L, \beta)$, of the ordered free energy. This estimate should coincide with $F_o(\beta)$ in the asymptotic limit defined by the criterion that $R(L, \beta)$ can be neglected in Eq. (2.19). In Fig. (2), we thus show the difference

\[
\Delta_o = F_o^{\text{eff}}(L, \beta) - F_o^{\text{ansatz}}(\beta).
\]  

The quantity $F_o^{\text{eff}}(L, \beta)$ is the $F_o$ extracted up to its constant term from the $q = 10$ simulation of Ref. [12] using Eqs. (2.16, 3.6, 3.5, and 3.3) while $F_o^{\text{ansatz}}$ is the prediction of Eq. (4.10o), where we used the predetermined values [19]

\[
A = .193 \\
B = .386 \quad \text{at} \quad q = 10
\]

We did not plot the data for $L = 44$ and 50, which are always compatible with those for $L = 36$, with larger errors (see Fig. 1a). Let us now comment on Fig. 2.

The lower limit of the $\beta$ range shown corresponds to the value $-1$ of the scaled variable $v$ of Eq. (4.9), a value below which our ansatz becomes meaningless. The upper limit corresponds to $v$ about 2 and $\beta$ values above which the data at $L \geq 36$ become unreliable. The $\beta$ range can also be expressed in terms of the variable $(\beta - \beta_t)V$, a natural argument for the partition function: it extends from about -4 to about 8 for $L = 36$. In this interval where we can compare the data and the ansatz, the following observations hold:

(i) Although clearly visible, the finite size effects remain tiny: the maximum absolute value of $L^2\Delta_o$ is less than 0.02 for all the data shown.

(ii) For $|v| < 1$, the difference between the $L = 36$ data and the ansatz is less than 1 standard deviation.

(iii) As already mentioned, a quantitative study of the $(L, \beta)$ dependence is difficult to achieve. The slope at $\beta = \beta_t$ is, however, measurable and shows a departure from the asymptotic value $-E_o = 1.66425$. 

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We find respectively at $L = 16, 20, 24$ and $36$

$$10^3 \times (E_o(L) - E_o) = -9.0(8), -5.1(1.0), -1.2(1.0), \text{ and } 1.6(3.0) .$$  \hspace{1cm} (5.4)

This clearly indicates a “fast” decrease of the finite size effect, of the same order of magnitude as the one found in [12] for the total average energy at $\beta = \beta_t$, and compatible with a behaviour $\exp \left( -L/L_o \right)$ with $L_o \sim 7$. Note that this value is intermediate between $\xi_d = 10.6$ which should be relevant to the description of interface effects in $R(L, \beta)$ [7], and $\xi_o = \xi_d/2 = 5.3$ expected to control the finite size effect in the pure ordered phase itself.

We conclude that our ansatz does provide an accurate description of the asymptotic free energies in a substantial range of $\beta$ values around $\beta = \beta_t$. It can be used as a reference model for a quantitative study of finite size effects measured in a high precision numerical study for which the moderate size range $L \lesssim 40$ would be especially suited.

5.2. Energy distributions and finite size effects

Given the free energies $F_o(\beta)$ and $F_d(\beta)$, the corresponding energy distribution can be computed by inverse Laplace transform of Eq. (3.1). As before, we call “asymptotic” the distribution obtained when $R(L, \beta)$ is neglected in (2.19), that is when

$$Z_V(\beta) \simeq Z^\text{as}_V(\beta) \equiv q \exp \left[ V F_o(\beta) \right] + \exp \left[ V F_d(\beta) \right] .$$  \hspace{1cm} (5.5)

The probability distribution at $\beta = \beta_o$ is then given by

$$P^\text{as}_{V,\beta_o}(E) = N \int_{\tilde{\beta} - i\infty}^{\tilde{\beta} + i\infty} d\beta \exp \left[ V (\beta - \beta_o) E \right] \frac{Z^\text{as}_V(\beta)}{Z_V(\beta)} .$$  \hspace{1cm} (5.6)

In this formula, $N$ is a normalization factor fixed for each $V$ and $\beta_o$ by

$$\sum_E P^\text{as}_{V,\beta_o}(E) = 1 ,$$  \hspace{1cm} (5.7)

$\tilde{\beta}$ is suitably chosen according to analyticity properties of $Z(\beta)$. Note that strictly speaking, $F_o$ and $F_d$ should be periodic functions of complex $\beta$ with period $4i\pi V$ since the allowed values of $E$ in Eq. (3.1) on a finite lattice are of the form $E = -k/(2V), k = 0, 1, \ldots, 2V$. Correspondingly, the integration contour in (5.6) should extend over a finite range, e.g., from $\beta - 2i\pi V$ to $eta + 2i\pi V$. We neglect such refinements: any reasonable $Z^\text{as}$ used in computing $P(E)$ should not depend on details of $F(\beta)$ so far away from the real axis. This will be the case in what follows.

Equation (5.6) of course implies that quadratic approximations of $F_o$ and $F_d$ as functions of $(\beta - \beta_t)$ lead to the celebrated two gaussian formula [24] for the probability distribution. Higher terms in $F_o$ and $F_d$ generate size dependent deformations of the two peak structure observed in the vicinity of the first order transition, which should not be misinterpreted as ‘non-asymptotic’ contributions in the partition function. This caveat does not hold [4] if the energy cumulants at $\beta = \beta_t$ only are analyzed.
Because, as we argued in previous sections, the Potts model free energies receive very large non quadratic contributions, \( F_n(\beta_t) \sim x^{3n/2} \) for a broad range of \( q \) values, this model offers a valuable laboratory for studying their effect in measured probability distributions. With this remark in mind we will now compare to numerical data the predictions of (5.6) when \( F_o, F_d \) are given by our ansatz (4.10o,4.10d).

### 5.2.1 Comparison with numerical data

For definiteness, we choose \( \beta_o = \beta_t \) in (5.6). The integral to be computed is thus:

\[
P_{V;\beta}(E) = N \int_{\bar{v}-i\infty}^{\bar{v}+i\infty} dv \times \exp \left[ \left( \frac{L}{S} \right)^2 \varepsilon v \right] \times \\
\times \left\{ \exp \left\{ \left( \frac{L}{S} \right)^2 \left[ -v (\varepsilon_o + 1) + \frac{3}{4}(1 + v)^{4/3} \right] \right\} + \exp \left\{ \left( \frac{L}{S} \right)^2 \left[ -v (+\varepsilon_d - 1) + \frac{3}{4}(1 - v)^{4/3} \right] \right\} \right\}
\]

(5.8)

Here we use the variables \( S, v, \varepsilon_o \) and \( \varepsilon_d \) defined in Eq. (4.9) and also scale the energy \( E \) according to

\[
\varepsilon = E(Bx)^{1/2}/(3A) .
\]

(5.9)

\( N \) is a new normalization factor. This form (5.8) shows explicitly that, apart from the multiplicity \( q \) of the ordered phase contribution, \( P(E) \) depends on \( q \) and \( L \) through \( (L/S) \) alone when expressed as a function of \( \varepsilon \) variables.

At large \( (L/S)^2 \) one may certainly evaluate the integral (5.8) by a saddle point method. The question we are trying to address here is how large should \( L \) be for this to be true. Taking \( q = 10 \) for definiteness, using the numerical values from (5.3) and the expressions (4.9) and (2.10), we find

\[
S_{q=10} = 60.3 ,
\]

(5.10)

about six times larger than the largest correlation length \( \xi_d \). Since we want to compare with distributions measured at \( L \leq 50 \), it is clear that the saddle point method is completely inadequate for this purpose. We shall use it later only for obtaining simple expressions on effectively large lattices. For the time being we have to perform a numerical integration of (5.8).

Up to trivial changes, contributions in the disordered and ordered phase need similar analyses: only the ordered one is considered here. We have to choose \( \bar{v} \) and a convenient path to \( \pm i\infty \). We first remark that the stationary point of the integrand is

\[
v_S(E) = -1 + (\varepsilon_o - \varepsilon + 1)^3 ,
\]

(5.11)
a value for which the integrand is well defined for

\[
\varepsilon_o - \varepsilon + 1 \geq 0 .
\]

(5.12)

In such cases, we take \( \bar{v} = v_S(E) \) and the path \( v = \bar{v} + i\lambda, \lambda \in [-\infty, +\infty] \). The term \( \frac{3}{4}(1 + v)^{4/3} \) insures an exponential fall off of the integrand at large \( |\lambda| \).
For the other case, $\varepsilon \geq \varepsilon_o + 1$, we fix $\bar{v}$ at $-1$ and again choose $v - \bar{v}$ purely imaginary.

Our results for $L = 16, 20, 24, 36, 44$ and $50$ (with no arbitrary adjustable parameters) are shown on Figs. (3a,3b) as continuous curves, together with the data of [12]. (Note the logarithmic scale.) The overall agreement, which continues over nearly three decades for $P(E)$, is very good, it becomes nearly excellent at the largest $L$ values. In particular the non-gaussian character of the peak is very well reproduced.

We already know from our study of Section 3 that non asymptotic contributions are present when $L < 36$. We see their manifestation in Fig. (3a). Since the curves have unit area, the discrepancies between theory and numerical data are concentrated in the largest (the ordered) peak region, and are emphasized by plotting $P(E)$ in that region on a non-logarithmic scale (Fig. 4a): the predicted peak looks too narrow. However, this does not mean that, at such $L$ values, the effective ordered specific heat, or $F_o^{(2)}(L, \beta)$, is larger than its asymptotic value: in fact Fig. 2 shows that the converse is true. At least for $L = 16$ and $20$, the effective broadening of the peak arises from large asymmetries ($|F_o^{(3)}(L, \beta)|$ larger at low $L$ values), whereas $F_o^{(2)}$ is actually smaller (the curves in Fig. 2 are concave around $\beta_t$). Hence, when seen in energy distributions, the nature of finite size effects can easily be misidentified. At the lower right corner of Fig. (4a), our curves level up; this unphysical feature is due to the tail of the ordered (left) peak. It disappears exponentially in $L^2$ and is due to the singularity at $v = -1$ in (4.10o) (see below the evolution of the ordered contribution far away from the peak).

At larger $L$ values (Fig. 3b), the agreement is considerably improved; in particular the absolute prediction for the ordered peak at $L = 50$ is perfect (Fig. 4b). However, a new effect tends to become sizable: a small discrepancy appears in the dip region between the two peaks at $L = 50$. This is the region where interface effects are expected to emerge [8], eventually yielding a flat plateau in $E$ at $\beta = \beta_t$. We shall soon discuss the effective $L$ dependence of the dip depth, of direct physical interest for interface tension determinations.

In order to understand better what is significant and what is not in finite size effects observed in the energy distributions, we now examine what the expected shape of $P_V(E)$ is when $L$ becomes actually large compared with the scale $S$ ($\sim 6 \xi_d$ at $q = 10$) introduced in Section 4.

5.2.2. Effective $L$ dependence and large $(L/S)$ limit of energy distributions

Amongst the quantities which have been extracted, and tentatively interpreted, from numerically determined energy distributions, are the peak locations $E_{o,d}^{\text{max}}(L)$ (asymptotically $E_{o,d}$) and widths (asymptotically related to $C_{o,d}$), and the quantity

$$2\sigma_{o,d}^{\text{eff}} = \frac{1}{L} \ln \left[ \frac{P_V(E_{\text{max}})}{P_V(E_{\text{dip}})} \right],$$

(asymptotically twice the ordered-disordered interface tension [8]). For definiteness, we discuss these quantities at $\beta = \beta_t$.

Let us start with a study of the integral (5.8) via a saddle point method at large $\ell = L/S$. Since by duality one peak is trivially deduced from the knowledge of the other, we again focus on the ordered peak, the first contribution in the integrand of (5.8). The saddle point $v_S(E)$ of (5.11) is useful when it lies above
the singular point of the ansatz, \( v = -1 \), that is in the energy region

\[
R1 : \quad -2 \leq E < E_o + 3A/(Bx)^{1/2}. \tag{5.14}
\]

\( R_1 \) extends above \( E_o \) by a small fraction (about 12% at \( q = 10 \)) of the latent heat. It is the situation of interest for evaluating the asymptotics of the peak structure. It is straightforward to find the saddle point result for the ordered phase energy distribution inside \( R_1 \). We find, up to an energy independent factor, that

\[
\mathcal{P}_{\text{ordered}}(E \in R1) = [1 + \varepsilon_o - \varepsilon] \exp \left\{ -\ell^2 \left[ \frac{(1 + \varepsilon_o - \varepsilon)^4}{4} - (1 + \varepsilon_o - \varepsilon) \right] \right\} \left( 1 + O(1/\ell^2) \right), \tag{5.15}
\]

where we recall that \( \varepsilon - \varepsilon_o = (E - E_o)(Bx)^{1/2}/3A \). Note that \( P \) is asymptotically the exponential of a polynomial of degree 4. The prefactor corrects it by a term \( 1/\ell^2 \) smaller. In order to analyze the approach to asymptotics of this peak, we expand the quantity

\[
p_o(\varepsilon) \equiv -\frac{1}{\ell^2} \ln \mathcal{P}_{\text{ordered}}(E) \tag{5.16}
\]

around its maximum \( \tilde{\varepsilon}_o \), consistently up to \( O(1) \) in \( 1/\ell^2 \). The result is

\[
\tilde{\varepsilon}_o = \varepsilon_o - 1/(3\ell^2) \tag{5.17}
\]

and

\[
p_o(\varepsilon) = \text{cst.} + \frac{3}{2} \left( 1 + \frac{1}{\ell^2} \right) (\varepsilon - \tilde{\varepsilon}_o)^2 - (\varepsilon - \tilde{\varepsilon}_o)^3
+ \frac{1}{4} \left( 1 + \frac{1}{\ell^2} \right) (\varepsilon - \tilde{\varepsilon}_o)^4 + O \left( \frac{1}{\ell^2} (\varepsilon - \tilde{\varepsilon}_o)^5 \right). \tag{5.18}
\]

Corrections of order \( 1/\ell^2 \) are generic to the saddle point method. The above expansion is specific to our ansatz (note the absence of \( 1/\ell^2 \) term in the cubic term, and of any term surviving at \( L = \infty \) at order \( \geq 5 \) in \( \varepsilon - \tilde{\varepsilon}_o \)). It predicts the approach to asymptotics of the ordered phase peak location, of the specific heat (quadratic term) and of the asymmetry (cubic term), and is relevant to a comparison with recent numerical simulations at \( q = 10 \) and 20 where such quantities have been considered [17]. Since \( \ell \) is not large in most cases we also compare the latter results with those of the numerical integration of (5.8), from which we compute for each \( q \) and \( L \) the peak location and curvature at the peak. These comparisons are shown in Figures 5a, 5b, 5c and 5d for \( E_{\text{max}}^o \) and Figures 6a, 6b and 6c for \( C_o \).

Fig. 5a shows \( E_{\text{max}}^o \) for \( q = 10 \) as a function of \( 1/L \) (instead of the natural \( 1/L^2 \)) in order to emphasize once for all how misleading the finite size effects in energy distributions can be. Indeed, the data points of [17] as well as the continuous curve (our ansatz) exhibit an essentially linear behaviour in \( 1/L \) over the whole range \( L = 12 - 100 \). In the absence of the known exact value (square symbol) at \( 1/L = 0 \), a linear fit to the data points would be reasonable, but would predict an asymptotic value wrong by many standard deviations! This is not so for the \( q = 20 \) case (Fig. 5b), which reflects the fact that \( L/S \) is indeed large...
for this case. Hence the apparent $1/L$ behaviour clearly is a finite size artefact, and should not be taken as a significant property of the distributions [10]. Figs. 5c and 5d show the same quantities plotted against $1/L^2$, together with the first order correction (straight line) predicted by Eq.(5.17). The adequacy of this representation is clearly exposed, as well as the strong deviations from asymptotics observed in the data and well (although not perfectly) explained by our ansatz.

We choose to present $C_o$ (as extracted from the curvature at the peak maximum) as a function of $S^2/L^2$, in Figs. (6a) and (6b) for $q = 10$ and 20 respectively. Similar conclusions can be drawn. Note the ranges of $S^2/L^2$ in the graphs are much larger than the domain of applicability of the saddle point method: $S^2/L^2 \ll 1$! As an illustration of the scaling property associated with Eq. (5.8), we finally show, on the same plot for $q = 10$ and 20, the ratio $C_o(L)/C_o(\infty)$ against $S^2/L^2$ (Fig. 6c). We see that the data points fall close to a same curve and to the theoretical prediction, even in regions where the asymptotic expectation is very far away.

Let us now turn to the energy region in between the two peaks, which according to [8] can be (and has been) used for a determination of the interface tension between ordered and disordered phases. Let us recall the argument. At $\beta = \beta_t$ and for sufficiently large linear size $L$, the mixture of a disordered phase in a fraction $\alpha V$ of the volume separated by two walls from an ordered phase occupying the fraction $(1 - \alpha)V$ has a relative weight which is

i) independent of $\alpha$ because $\alpha F_o + (1 - \alpha)F_d = F_t$ at $\beta = \beta_t$.

ii) proportional to $\exp[-2\sigma_{od}L]$ because each wall costs a free energy $\sigma L$. Thus, a plateau in energy is expected, for any $E$ of the form

$$E = \alpha E_o + (1 - \alpha)E_d,$$

whose height with respect to the rest of the distribution is $\exp[-2\sigma_{od}L]$.

The predicted plateau has indeed been seen in recent simulations of the Potts model, either by extending the linear size of a square lattice to many times the correlation length ($q = 20$ in [17]), or by using rectangular lattices, which favour the appearance of separation walls transverse to the large dimension ($q = 7$ in [15, 11]). Such simulations have led to determinations of $\sigma_{od}$ in very good agreement with the predicted $\sigma_{od} = 1/(2\xi_d)$ of Ref. [7].

It is quite remarkable that previous numerical attempts on square lattices with sizes $L \leq 100$, not large enough at $q \lesssim 10$ for the plateau to develop, already led to satisfactory (although not as good) estimates of $\sigma_{od}$ (Ref. [13] for $q = 10$ and Ref. [14] for $q = 7$). Indeed, as we saw above (Fig. 3a,3b) our ansatz is able to reproduce the data for $q = 10$, $L \lesssim 50$ quite correctly, although it totally ignores contributions from mixed phase configurations. We illustrate this fact in Fig. 7a where we show our result and the data of [17] at $q = 10$ for the quantity

$$2f_{od} = \frac{1}{L} \ln \left\{ \frac{P_{max}^{o}P_{max}^{d}}{P_{min}^{d}} \right\}$$

(5.20)
as a function of $1/L$. The curve is computed from the numerical integration leading to the energy distributions already shown. It levels out at low values of $1/L$ (dotted part). This is because in the region

$$R2 : \quad E_o + \frac{3A}{(Bx)^{1/2}} < E < E_d - \frac{3A}{(Bx)^{1/2}}, \quad (5.21)$$

the leading contribution to $P_{o,d}$ as $L/S$ becomes large, as obtained by a saddle point method, is proportional to

$$\exp \left[ -L^2 |E - E_{o,d}| / (Bx)^{3/2} \right], \quad (5.22)$$

so that the right hand side of (5.20) grows as $L$. Only in this regime mixed phase contributions, of relative weight proportional to $\exp(-2\sigma_{od}L)$ may show up, and this is supported by the data. What is puzzling is that for $L \lesssim 40$, our curve accounts for the trend of the data; moreover an extrapolation to $1/L = 0$ of its nearly linear part would accidentally produce a reasonable result. The same remark applies to the case $q = 7$, illustrated in Fig. 7b (There the definition of $f_{od}$ is slightly different: we follow the definition of [14]).

Our conclusion is that it may be misleading to identify $f_{od}$, as defined by (5.13) or (5.20) or as in [14], to the interface tension $\sigma_{od}$ whenever a clear plateau is not seen in between the two peaks.

6. CONCLUSIONS

The main result of this paper can be summarized as that the ansatz for the free energy developed in section 4 is in qualitative and quantitative agreement with available numerical data. Our work indicates that, at least for the Potts model at moderate values of $q$, the energy distribution near a first order transition point cannot be accurately described as a sum of two gaussian contributions. This statement is distinct from the correct statement that, up to exponentially small (what we call non-asymptotic) corrections, the partition function can indeed be written as a sum of the partition function of the pure phases.

These large energy cumulants of the asymptotic distributions call for more careful analysis of the numerical data. In particular, the finite size effects do not seem to be controlled by the correlation lengths of the model: rather, the relevant scale is significantly larger. This implies that numerical work should not assume that any system is sufficiently large: one can (e.g. using Eq. 3.6) and must specifically look for “true” finite size effects in the system (in the sense of Eq. (2.19) ). Especially, one must be careful about interpreting the depth of the minimum of the energy distribution as a measurement of the surface tension: true surface tension effects lead to a flat minimum which does appear on a sufficiently large lattice. In addition, deviations from predictions of the two-gaussian model (e.g. discrepancies in the position and curvature of the peaks in the energy distribution), should not, in itself be considered a finite volume effect: non-quadratic terms in the free energy expansion do lead to such shifts.

The non-gaussian nature of the pure phase energy distributions near the transition point might seem unusual and pathological to the particular model at hand. In reality, our ansatz indicates that this is probably due to the influence of the nearby second order transition starting at $q = 4$. One may conjecture that strong deviations from the gaussian nature are not unusual in systems without a large surface tension between the
phases. Such might also be the case of phenomenologically significant models like QCD, and the results of this paper might be relevant to any numerical simulation of these phase transitions.

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APPENDIX A

For the $q$-states 2D Potts model on a square lattice, the internal energies $E_o$ and $E_d$ in the ordered and disordered phases respectively are given for $q > 4$ by [1]

$$E_d + E_o = -2 \left( 1 + 1/\sqrt{q} \right)$$  \hspace{1cm} (A.1)

$$\mathcal{L} \equiv E_d - E_o = 2 \left( 1 + 1/\sqrt{q} \right) \tanh \frac{\theta}{2} P(\theta)$$  \hspace{1cm} (A.2)

with

$$2 \cosh \theta = \sqrt{q}$$  \hspace{1cm} (A.3)

and

$$P(\theta) = \prod_{n=1}^{\infty} (\tanh n\theta)^2 .$$  \hspace{1cm} (A.4)

Two expressions of $P(\theta)$ [1] are of great interest for accurate numerical estimates of the latent heat $\mathcal{L}$. One is very rapidly converging at large $q$:

$$\sqrt{P(\theta)} = 1 + 2 \sum_{m=1}^{\infty} (-)^m e^{-2m^2 \theta} ,$$  \hspace{1cm} (A.5)

the other one is extremely accurate at small $\theta$

$$\sqrt{P(\theta)} = \left( \frac{2\pi}{\theta} \right)^{1/2} \sum_{m=0}^{\infty} e^{-(m+\frac{1}{2})^2 \pi^2/(2\theta)} .$$  \hspace{1cm} (A.6)

In the paper, we chose to discuss all quantities in the low $q - 4$ regime as functions of the variable $x$ defined as

$$x = \exp \left[ -\pi^2 / 2\theta \right] ,$$  \hspace{1cm} (A.7)

so that in this regime we have

$$\mathcal{L} = h(q)x^{-1/2} \left[ 1 + 2x^{-2} + O \left( x^{-4} \right) \right]$$  \hspace{1cm} (A.8)

with

$$h(q) = 2 \left( 1 + 1/\sqrt{q} \right) \tanh \frac{\theta}{2} \times \left( \frac{2\pi}{\theta} \right) .$$  \hspace{1cm} (A.9)

a smooth function compared to $x$. The corrections to the leading term in (A.8) are extremely small, still less than 3% for $q$ as large as 100. From these properties, we see that there is a very large domain of $q$ values where large $q$ as well as small $(q - 4)$ expansions (A.5) or (A.6) yield very accurate estimates.

Duality relates the specific heat difference to $\mathcal{L}$:

$$C_d - C_o = \beta^2 \frac{\mathcal{L}}{\sqrt{q}} \approx O \left( x^{-1/2} \right) .$$  \hspace{1cm} (A.10)

Since we argue that $C_d$ and $C_o$ are both $\sim x$ at leading order, setting $C_d = C_o$ as implied by the final ansatz implies a relative error of order $x^{-3/2}$, not under control within our approach.
The interest of the $x$ variable also appears in expressions for the correlation lengths [5, 6, 7].

According to the above references, the disordered phase correlation length $\xi_d$ may be accurately computed either at large $q$ using

$$
\frac{1}{\xi_d} = 4 \sum_{m=1}^{\infty} \left[ \frac{(-e^{-\theta})^m}{m} \sinh \left( \frac{m\theta}{2} \right) \tanh(m\theta) + 2 \log \left( \frac{\cosh 3\theta/4}{\cosh \theta/4} \right) \right], \quad (A.11)
$$

or at low $(q - 4)$ using

$$
\frac{1}{\xi_d} = 4 \sum_{m=0}^{\infty} \ln \left( \frac{1 + w_m}{1 - w_n} \right)
$$

$$
w_m = \sqrt{2} \cosh \left( (m + \frac{1}{2}) \frac{\pi^2}{\theta} \right)^{-1}. \quad (A.12)
$$

In particular the latter expression yields

$$
\xi_d = \frac{1}{8\sqrt{2}} x \left[ 1 - \frac{2x^{-2}}{3} + O(x^{-4}) \right], \quad (A.13)
$$

subject to comments similar to those made on Eq. (A.8). The accuracy of (A.13) was already emphasized in Ref. [7].
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(Figure 1a) Graph of $W_o[L, \beta]$ (Eq. 3.7) at various large values of $L$, in an attempt to look for finite size effects at $q = 10$. Data from Ref. [12].

(Figure 1b) Graph of $W_o[L, \beta]$ (Eq. 3.7) for small lattices at $q = 10$. Finite size effects clearly show up. Data from Ref. [12].

(Figure 2) Graph of $\Delta_o$ (Eq. 5.2), the difference of the measured free energy and the free energy predicted by our Ansatz. Data from Ref. [12].

(Figure 3a) Comparison of the energy distribution measured on small lattices against our prediction. Data from Ref. [12].

(Figure 3b) Comparison of the energy distribution measured on large lattices against our prediction. Data from Ref. [12].

(Figure 4a) Enlarged view of the peak region of 3a showing the difference between measured and predicted energy distributions.

(Figure 4b) Enlarged view of the peak region of 3b showing the difference between measured and predicted energy distributions.

(Figure 5a) Plot of the peak of the energy distribution versus $1/L$ at $q = 10$. A linear fit seems good, but predicts the wrong extrapolated value. Data from Ref. [17].

(Figure 5b) Plot of the peak of the energy distribution versus $1/L$ at $q = 20$. Data from Ref. [17].

(Figure 5c) Plot of the peak of the energy distribution versus $1/L^2$ at $q = 10$. Data from Ref. [17].

(Figure 5d) Plot of the peak of the energy distribution versus $1/L^2$ at $q = 20$. Data from Ref. [17].

(Figure 6a) Plot of the specific heat in the ordered phase at transition for $q = 10$ against the scaled lattice size, compared to our prediction. Here $C_o$ is extracted from the peak curvature. Data from Ref. [17].

(Figure 6b) Plot of the specific heat in the ordered phase at transition for $q = 20$ against the scaled lattice size, compared to our prediction. Here $C_o$ is extracted from the peak curvature. Data from Ref. [17].

(Figure 6c) Plot of the the scaled specific heat at transition compared to our prediction for both $q = 10$ and $q = 20$. Here $C_o$ is extracted from the peak curvature. Data from Ref. [17].

(Figure 7b) Comparison of $2f_{od}$ defined in equation 5.20 with our prediction without any mixed phase contribution at $q = 10$. Data from Ref. [17].

(Figure 7a) Comparison of $2f_{od}$ defined and measured in Ref. [14] with our prediction without any mixed phase contribution at $q = 7$. 

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