TOPICS ON FIRST ORDER TRANSITIONS*

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I review a few issues on first order transitions. The motivation arises from unexpected peculiarities encountered in numerical simulations of rather common classical spin systems, and relative to the finite size behaviour of thermodynamical quantities such as the specific heat or higher order energy cumulants. The q-states 2-d Potts model is discussed in some details, in order to state the problems met as well as to propose explanations and to remedy to their consequences in numerical simulation analysis. Emphasis is put on the relationship between the finite size behaviour of the partition function and that of the internal energy distributions.

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1. Introduction

Continuous transitions, mainly because of their universality properties and of the contact with field theory which these allow, have attracted much attention during the last two decades. First order transitions do not present these appealing features. They are present however in nature, not only in condensed matter physics, but also in the context of particle physics. In particular, the problem of the nature of the deconfining or chiral symmetry breaking transition expected in QCD is a still opened question, whose answer is of interest for example within the context of primordial nucleo synthesis after the Big-Bang.

Although this transition is definitely believed to be first order in the case of pure gauge QCD, its nature is still controversial in the realistic case of several light dynamical quarks. At least until now, no other method than

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numerical simulations has been proposed to solve the problem. Hence the need for safe methods allowing to characterize the nature of phase transitions by numerical means. Experimentation on simple classical spin systems reveals to be fruitful, as it will be here illustrated on the case of the 2-d, q-states Potts model.

These notes are organized as follows. Section 2 contains generalities on classical spin systems, the description of their thermodynamical properties from their partition functions and free energies, and the behaviour of the latter in the event of a temperature driven phase transition. The third section discusses the relationship between the free energy of a system, often subject to analytical approaches, and the energy distributions which may be provided by numerical simulations. Section 4 is specifically devoted to the two-dimensional, q-states Potts model. Results of analytical as well as numerical studies are presented and compared to each other. Conclusions are drawn on safe ways to deal with finite size effects in numerical data analysis.

Most of the material presented in these notes results from various works made in collaboration with Bhattacharya, Billoire, and Lacaze.

2. Partition functions and free energies for classical spin systems. Generalities

The typical problem we want to describe is that of a classical spin hamiltonian, where the spin variables σ_i, attached to the sites i of a lattice, have short range interactions. We will consider d-dimensional (hyper-)cubic lattices, with L sites in each of the d directions; periodic boundary conditions will be assumed. The number of sites $V \equiv L^d$ is referred to as the volume.

To be specific, all illustrations of the concepts and properties will be given for the case of the q-states Potts model. A useful review on this model is that by Wu [1]. The Hamiltonian is:

$$H_{\text{Potts}} = -J \sum_{\langle ij \rangle} \delta_{\sigma_i \sigma_j} , \tag{2.1}$$

where the summation extends over the $d \times V$ pairs $\langle ij \rangle$ of nearest neighbour sites. Each spin variable σ_i may take q different values. A pair $\langle ij \rangle$ gives a non vanishing contribution $-J$ iff $\sigma_i = \sigma_j$. We restrict to the ferromagnetic case $J > 0$ where the energy carried by a link $\langle ij \rangle$, namely $-J$ or 0, is non positive. In what follows, J will be taken as the energy unit and will disappear from all equations. The ground state of the system is manifestly q times degenerate; it consists of the q completely "*ordered*" states where the spins take the same value on all sites. Hence in the zero temperature limit,

the system is in either one of these q states of total energy $-dV$. At high enough temperature $T \equiv \beta^{-1}$, the entropy wins and the system becomes "*discordered*". In between, one expects a transition temperature $T_t = \beta_t^{-1}$ and we will focus on the properties attached to this temperature driven phase transition, especially to its nature. Note that for $q = 2$, the model is the standard Ising model. Many q-dependent, properties of the Potts model are exactly known in 2 dimensions (see below), which makes this case ideal for experimenting methods and tools.

2.1. The partition functions

The basic object for studying the thermodynamical properties of a spin system with Hamiltonian H is its partition function at temperature β^{-1}, whose definition is

$$Z_V(\beta) = \mathrm{Tr}[\exp(-\beta H)], \tag{2.2}$$

where the trace extends over all possible states of the system. For a classical system, any spin configuration C specified by the values of the σ_i's over the whole lattice assigns H a well defined value, the energy of the configuration, which is extensive for short range interactions and noted VE_C. Conversely, given E, there is in general a number $\Omega_V(E)$ of configurations which have the same energy density E. So we can rewrite (2.2) either as

$$Z_V(\beta) = \sum_{\text{all configurations}} \exp(-\beta V E_C) , \tag{2.3}$$

or as

$$Z_V = \sum_E \Omega_V(E) \exp(-\beta V E) . \tag{2.4}$$

This latter form is the most suitable to our discussions. Note already that $\Omega_V(E)$ is *independent* of the temperature, which appears only in the Boltzmann factor.

Remark

Other external parameters can be introduced besides the temperature. In particular, adding H a term of the form

$$h \sum_i \sigma_i , \tag{2.5}$$

allows to study the magnetic properties of the system by computing the response of the system to the external magnetic field h. In particular, the magnetization density

$$M = \frac{1}{V} \sum_i \langle \sigma_i \rangle , \tag{2.6}$$

where $\langle\ \rangle$ denotes average over all states of the system, and the magnetic susceptibility

$$\chi = \frac{\partial}{\partial h} M\,, \tag{2.7}$$

can be deduced from the h dependence of the partition function in the presence of (2.5) in H. The magnetization density M and the susceptibility χ play with respect to h the same role as E and the specific heat with respect to β. Hence field driven phase transitions can be studied through the response of the system to h in a way very similar to what follows for T driven transitions. We set h to zero in the rest of these notes.

2.2. Free energy. Energy cumulants. Thermodynamical limit

We *define* the finite volume free energy of the system in a box of volume V as

$$F_V(\beta) = \frac{1}{V} \ln Z_V(\beta)\,. \tag{2.8}$$

Strictly speaking, the free energy is, if it exists, the thermodynamical limit (that is the limit as L, the linear size of the box, goes to infinity) of

$$f_V(\beta) = -\frac{F_V(\beta)}{\beta}\,.$$

Note that for finite V, $Z_V(\beta)$ is a finite sum of exponentials in β; hence $F_V(\beta)$ is an analytic function of β for any real β. It may not be so for its thermodynamical limit (phase transition, see (2.3)).

It follows from Eqs (2.8) and (2.4) that differentiating $F_V(\beta)$ with respect to β yields

$$F_V^{(1)}(\beta) \equiv \frac{\partial F_V(\beta)}{\partial \beta} = -\frac{1}{Z_V(\beta)} \sum_E E\ \Omega_V(E)\ \exp(-\beta V E)\,. \tag{2.9}$$

Equivalently, $-F_V^{(1)}(\beta) = \langle E \rangle_V$ where $\langle E \rangle_V$, the *internal energy density,* appears as the average of E with respect to the energy probability distribution

$$P_{\beta V}(E) = \frac{\Omega_V(E)\ \exp(-\beta V E)}{Z_V(\beta)}\,. \tag{2.10}$$

Numerical simulations of a statistical physics system provide samples of configurations distributed according to this weight [2].

The n^{th} derivative $F^{(n)}(\beta)$ of the free energy with respect to β generates combinations of higher moments of the distribution $P_{\beta V}(E)$, called

n^{th}order energy cumulants, and thus measurable in principle. For example, the specific heat at fixed volume is defined by

$$C(\beta) = \frac{\partial \langle E \rangle}{\partial T} = -\beta^2 \frac{\partial \langle E \rangle}{\partial \beta},$$

and according to (2.9)–(2.10), is given by the familiar expressions

$$C(\beta) = \beta^2 F_V^{(2)}(\beta) = V\beta^2 \left(\langle E^2 \rangle - \langle E \rangle^2 \right). \tag{2.11}$$

They relate the specific heat either to the energy fluctuations or to the second derivative of the free energy. The index V in energy averages is omitted for simplicity, but should not be forgotten. Because the energy dispersion in the r.h.s. of (2.11) is non negative, we recover that the free energy is a convex function of β, wherever the 2^{nd} derivative exists, namely *always* on a finite lattice and, in the thermodynamical limit, away from a phase transition point; this is what we shall immediately discuss.

2.3. The free energy near a phase transition

A temperature driven phase transition is *mathematically* associated with a singularity at β_t, $0 \leq \beta_t$ of the thermodynamical free energy

$$F(\beta) = \lim_{V \to \infty} F_V(\beta). \tag{2.12}$$

The standard classification of phase transitions is as follows

- 1^{st} *order transition*: $F^{(1)}(\beta)$ has a discontinuity at $\beta = \beta_t$; the internal energy jumps at β_t, due to (2.9).
- 2^{nd} *order transition*: $F^{(1)}$ is continuous, but $F^{(2)} \simeq A\,(\beta - \beta_t)^{-\alpha}$, that is the specific heat diverges (for $\alpha > 0$) at β_t (see the first of Eqs (2.11)).
- *Continuous transition*: $F^{(n)}(\beta)$ diverges at $\beta = \beta_t$ for some $n \geq 2$.

In a generic case, a singular point β_t is isolated. According to the heuristic argument given at the beginning of this section, the Potts model does have such a transition point (see Section 4 for details). It follows from the above definition that the order of the limits $\beta \longrightarrow \beta_t$ and $V \longrightarrow \infty$ is relevant to the study of a transition: one should take the thermodynamical limit *first*, and then approach β_t either from above ("low" temperature, ordered, phase) or from below ("high" temperature, disordered, phase).

Because only the opposite situation can be realized in numerical simulations (V is bound by limited computer resources; β can be varied in the vicinity of a known or assumed transition point), the identification and the study of a phase transition by such means requires careful analysis of both

the β and V dependencies of measurable quantities, essentially the energy distribution (2.10). Therefore, we need to explore the relationship between free energies and energy distributions in a given situation. This is done in the next section.

3. Energy distributions and free energies

Let us summarize the problematic at hand.

Analytical investigations of statistical models may often be performed which lead to information on phase transitions. Standard methods are: mean field theory, low or high temperature expansions, large N limits of $O(N)$ symmetric models, large q expansions in the Potts model, Bethe ansatz, conformal theories (in 2 dimensions), *etc.* They often provide exact properties or approximations for the free energy

$$F(\beta) = \lim_{V\to\infty} \frac{1}{V} \ln Z_V(\beta)\,, \tag{3.1}$$

which may be singular at some β_t value.

Conversely, numerical simulations give access to the energy density distributions,

$$P_{\beta,V}(E) = \frac{\Omega_V(E)\ \exp(-\beta V E)}{Z(\beta)}\,,$$

$$\sum_E P_{\beta,V}(E) = 1\,. \tag{3.2}$$

We are interested in answers to two questions.

Question 1: given a measurement of $P_{\beta,V}(E)$, with a given accuracy associated with the size of the configuration sample generated by some stochastic method, what do we learn on $F(\beta)$?

Question 2: assuming a phase transition occurs at $\beta = \beta_t$, what should be expected for the finite volume energy distributions?

3.1. Free energies from measured energy distributions

Suppose that one has measured $P_{\beta_0 V}(E)$, the distribution at some $\beta = \beta_0$ in a volume V, and that we want to construct $Z_V(\beta)$. We start from Eq. (2.4), which we rewrite as

$$Z_V(\beta) = \sum_E \left[\Omega_V(E)\ \exp\left(-\beta_0 V E\right)\right] \times \exp\left(-(\beta-\beta_0)\,VE\right).$$

It immediately follows from (3.2) that the above square bracket is nothing but $P_{\beta_0 V}(E) \times Z_V(\beta_0)$. So we have

$$\frac{Z_V(\beta)}{Z_V(\beta_0)} = \sum_E P_{\beta_0 V}(E) \exp\left(-(\beta - \beta_0) VE\right), \tag{3.3}$$

which shows that up to a β *independent* factor $Z_V^{-1}(\beta_0)$, $Z_V(\beta)$ is nothing but the average of $\exp(-(\beta - \beta_0) VE)$ with respect to the supposedly known distribution. Using Eq. (3.3), we obtain an estimate of the free energy as a function of β, up to a V dependent constant, by

$$F_V(\beta) - F_V(\beta_0) = \frac{1}{V} \log\left[\frac{Z_V(\beta)}{Z_V(\beta_0)}\right]. \tag{3.4}$$

For fixed β, away from any singularity, and measurements of $P_{\beta_0 V}(E)$ for "large enough" lattices, Eq. (3.4) should eventually approach the thermodynamical limit. Here "large enough" means that the linear size L must be substantially larger than the largest correlation length in the system at temperature β^{-1}.

This method has been proposed in the last of Ref. [3] and used to analyze the free energy of the q-states 2 dimensional Potts model from numerical data obtained at $\beta_0 = \beta_t$, $q = 10$ from Ref. [4]. In this case, the exact knowledge of β_t [1]

$$\beta_t(q) = \log(1 + \sqrt{q})$$

and the duality property (in the Potts model, the free energies of the ordered and disordered phases are related to each other, see Section 4) allows to even reach the *ordered phase* free energy $F_o(\beta)$ around β_t. We extract from Ref. [3] (where all details can be found) the results obtained for

$$\Phi(L, \beta) = F_o(\beta) - F_o(\beta_t) + E_o(\beta - \beta_t), \tag{3.5}$$

as a function of β for different L values. Here E_o is the known [5] ordered phase internal energy; due to (2.9) taken at $\beta = \beta_t$, $\Phi(L, \beta)$ has no linear part at $\beta = \beta_t$ in the infinite volume limit, and is thus suitable to illustrate the *shape* of $F_o(\beta)$, and *its approach to the thermodynamical limit.* The data for Φ are shown on Figs 1(a) ($L = 36$ to 50) and 1(b) ($L = 16$ to 36). Within the errors quoted, which reflect the statistical accuracy obtained in the numerical simulation of the energy distributions, there is no finite size effects visible for $L \gtrsim 36$, but they clearly show up below $L = 36$. These results demonstrate the feasibility of an evaluation of the free energy by numerical means, and of a study of the finite size effects for moderate lattice sizes compared to the largest correlation length (known to be around 10 for this case [6–8]).

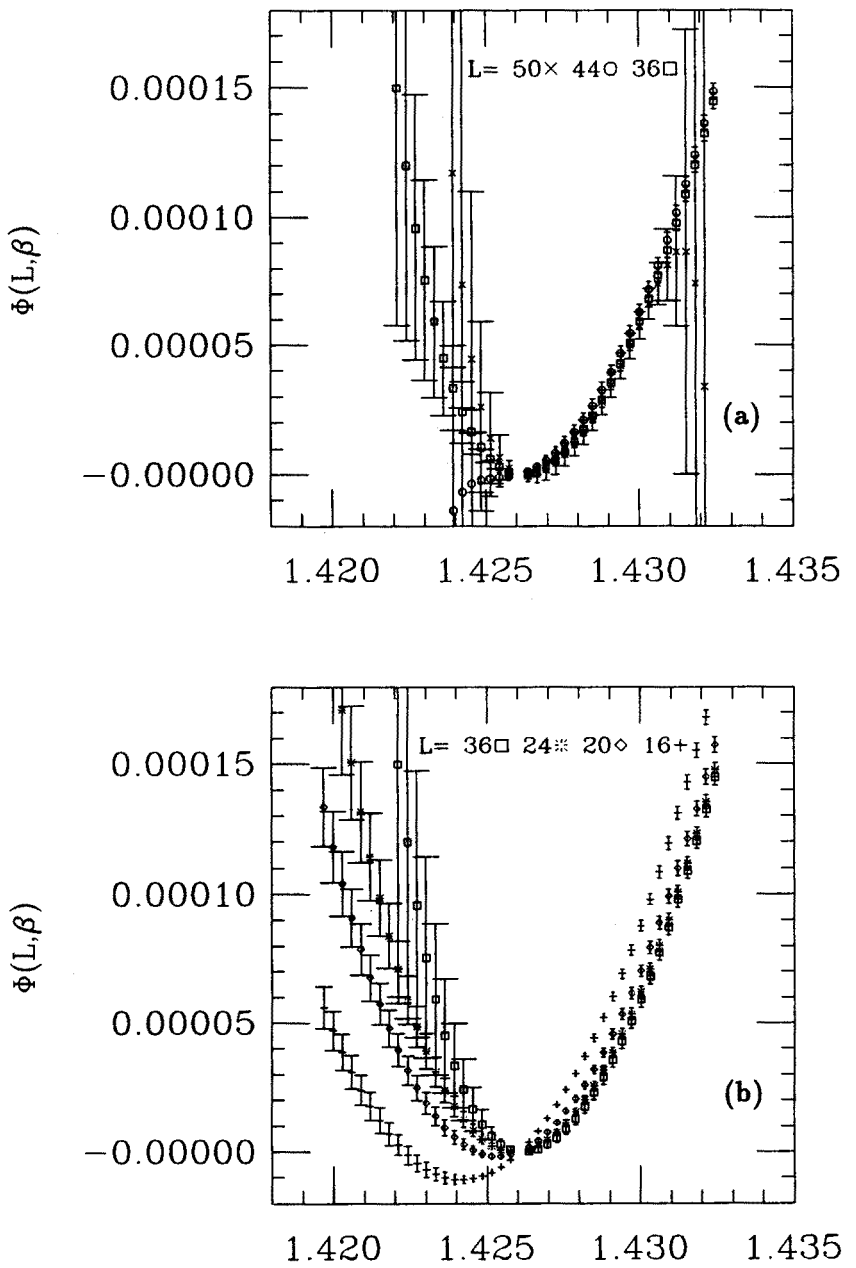

Fig. 1. The quantity Φ of Eq. (3.5) versus β

3.2. Energy distributions from given free energies

We now address the second question raised at the beginning of this section.

We start with an even simpler problem: find $P_{\beta_0 V}(E)$ for a given $F(\beta)$, assuming β_0 is *not* a singular point. Let $F(\beta)$ be the thermodynamical limit (3.1) for some model. If L is large enough with respect to the finite correlation length ξ, it can be shown on very general grounds that the finite V partition function associated with the model can be written

$$Z_V(\beta) = \exp(VF(\beta)) \left(1 + O\left(e^{-L/\xi}\right)\right) .$$

We neglect the exponential corrections, and so assume that the only L dependence of Z is trivially due to the extensivity of the total free energy VF of the system. Due to Eqs (2.4) and (2.10), $P_{\beta_0 V}(E)$ can be obtained by inverse Laplace transform of (2.4), which we write for later convenience

$$P_{\beta_0 V}(E) =$$

$$N \exp\left(VF\left(\beta_0\right)\right) \int_{\bar{\beta}-i\infty}^{\bar{\beta}+i\infty} \frac{V \mathrm{d}\beta}{2\pi} \exp\left(V\left(F(\beta) - F\left(\beta_0\right) + E\left(\beta - \beta_0\right)\right)\right) . \quad (3.6)$$

N is a normalization factor ensuring $\sum_E P(E) = 1$. The value $\bar{\beta}$ is a real value of β in the complex β-plane, suitably chosen in the vicinity of β_0 in order for the integration path to avoid any singular point of $F(\beta)$. Strictly speaking, since the energy values E in (2.4) are discrete (in the reference model, they are of the form $-k/V$, $k = 0, 1, \ldots, 2V$), the function Z_V is periodic in the imaginary direction, with period $2\pi i$, and the integral (3.6) should be truncated accordingly. This has no practical effect however for our purpose.

We now evaluate (3.6) at large V by the saddle point method. Let $\beta_S(E)$ be the solution in β of

$$F^{(1)}(\beta) + E = 0 . \quad (3.7)$$

Since $\mathrm{d}^2F/\mathrm{d}\beta^2$ is positive (Eq. (2.11)), $F^{(1)}(\beta)$ is monotonically increasing and Eq. (3.7) has a unique solution if $-E$ is chosen in the interval $\left[\min_\beta F^{(1)}, \max_\beta F^{(1)}\right]$. The saddle point estimate of (3.6) is then

$$P_{\beta_0 V}(E) \equiv N D(E) \exp\left(VF\left(\beta_0\right)\right)$$

$$D(E) \simeq \left[\frac{2\pi}{V} F^{(2)}\left(\beta_S(E)\right)\right]^{-1/2}$$

$$\times \exp\left(V\left(F\left(\beta_S(E)\right) - F\left(\beta_0\right) + E\left(\beta_S(E) - \beta_0\right)\right)\right) , \quad (3.8)$$

and corrections can be systematically computed as a power expansion in $1/V$.

Although it is trivial, we would like to emphasize that *only if* $F(\beta)$ *is quadratic is* $D(E)$ *a (normalized) Gaussian in* E *for any* β_0.

Furthermore of course (3.8) is exact in this case: no $1/V$ correction, the transform of a Gaussian is a Gaussian. The Gaussian is centered at

$$\bar{E} = -F^{(1)}(\beta_0)$$

and its width σ is given by

$$\sigma^2 = \frac{1}{V} F^{(2)}$$

where $F^{(2)}$ is a constant in β_0.

In non academic cases, F is not quadratic. The $(1/V)$ corrections to (3.8) begin with the $F^{(3)}$ and $F^{(4)}$ derivatives being non zero.

More importantly, and this has been overlooked for a long time in numerical data analysis, the leading order estimate (3.8) differs from a Gaussian shape by two features

(i) the prefactor, proportional to $\left[F^{(2)}(\beta_S(E))\right]^{-1/2}$, is E-dependent,

(ii) the limit

$$\begin{aligned} p(E) &= \lim_{V\to\infty} \frac{1}{V} \log\left[P_{\beta_0 V}(E)\right] \\ &= F(\beta_S(E)) + E(\beta_S(E) - \beta_0) \end{aligned} \tag{3.9}$$

is a function of E as general as $F(\beta)$ can be, only restricted by general analyticity and convexity properties.

In particular, although one may check, using (3.9) and (3.7), that the maximum $\bar{E}$ of $p(E)$ is correctly located at $-F^{(1)}(\beta_0)$, the thermodynamical internal energy, it differs from the maximum $E_{\max}$ of the predicted distribution (3.8) by corrections of order $F^{(3)}/V$. This is a consequence of (i). A corollary of (ii) is that there is no reason why $p(E)$ should be symmetric around $\bar{E}$, and this is *not* a finite size effect. These features will be exemplified in Section 4 on the Potts model.

What remains true is that the infinite volume limit of any average

$$\langle A \rangle = \int \mathrm{d}E\, A(E) P_{\beta V}(E), \tag{3.10}$$

where $A(E)$ is sufficiently regular, is

$$\langle A \rangle = A(\bar{E}).$$

In other words, $P(E)$ acts asymptotically in V as a $\delta\left(E-\bar{E}\right)$ distribution. For $F(\beta)$ analytic, the fluctuations are killed at infinite volume, as expressed in Eq. (2.11) for the quadratic fluctuations: they vanish as $F^{(2)}(\beta)/V$. A Gaussian $P(E)$ is nothing but the first correction to $\delta\left(E-\bar{E}\right)$ which includes the *quadratic* fluctuations.

After this exercise, we examine what happens in the presence of a phase transition at $\beta=\beta_t$, *i.e.* of a singularity of $F(\beta)$ at this point, and focus on the case where the transition is first order. We recall that it corresponds to a discontinuity of the first derivative $F^{(1)}(\beta)$ at β_t. The situation is sketched in Fig. 2: $F(\beta)$ is the maximum of two functions $F_d(\beta)$, $F_o(\beta)$. Below β_t, F coincides with F_d (disordered high temperature phase), above it coincides with F_o (any of the ordered low temperature phases). Hence *for V large enough*, the energy distribution is given by a formula like (3.8) where either $F=F_d$, at β_0 fixed below β_t, and a peak is present around $E_d=-F_d^{(1)}$, or $F=F_o$ at β_0 fixed above β_t, and the peak appears around $E_o=-F_o^{(1)}$. Now the question is: how can one describe the finite V crossover between the two behaviours, in particular in the region $|\beta-\beta_t|\,V$ of order one. Phenomenological analysis [9] and more recent rigorous results, valid for a class of models which includes the q-states Potts model [10], have led to the following prescription for the partition function in the vicinity of a

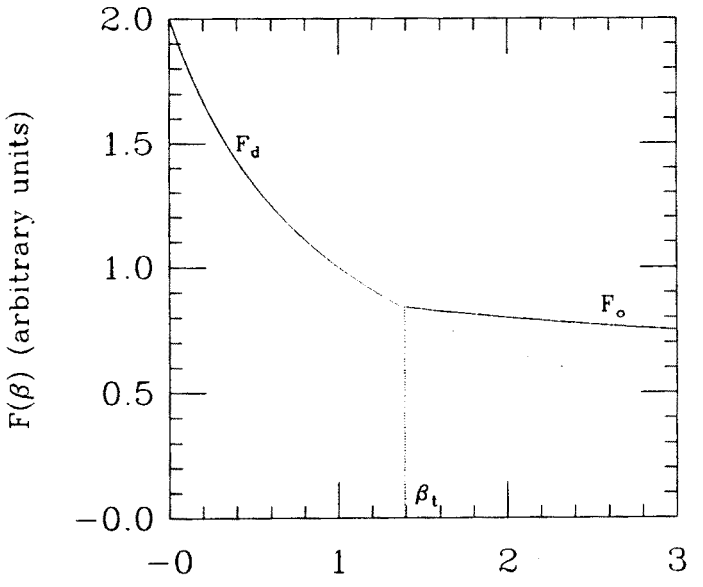

Fig. 2. First order transition $F(\beta)$ versus β (arbitrary units)

1st order point: the full partition function $Z(\beta)$ can be written

$$Z_V(\beta) = \sum_i Z_i(\beta)[1 + \mathcal{O}(\exp(-AL))]$$
$$Z_i(\beta) = \exp(VF_i(\beta)), \tag{3.11}$$

where A is a positive constant, and the sum extends to all phases i which coexist at $\beta = \beta_t$, *i.e.* such that $F_i(\beta_t) = F(\beta_t)$ is independent of i at the transition.

With the prescription (3.11), the corresponding energy distribution

$$P_{\beta_0 V}(V) = N \int_{\bar{\beta}-i\infty}^{\bar{\beta}+i\infty} \frac{V d\beta}{2\pi} Z_V(\beta) \exp(VE(\beta - \beta_0)) \tag{3.12}$$

can be investigated along the same lines as above. We neglect the exponentially small correction in (3.11), the only *true* finite size effect in $Z_V(\beta)$, and assume the functions $F_i(\beta)$ are sufficiently smooth around $\beta = \beta_t$ to allow for a saddle point integration.

Then $P_{\beta V}(E)$ can be written as a normalized sum of contributions

$$P_{\beta V}(E) = N \sum_i Z_i(\beta) D_i(E) \tag{3.13}$$

with each $D_i(E)$ given by an expression similar to $D(E)$ in (3.8) with F replaced by F_i and $\beta_S(E)$ by the solution of

$$F_i^{(1)}(\beta) + E = 0.$$

Suppose there are, as in the Potts model, q ordered phases and one disordered one. Then specializing (3.13) to $\beta = \beta_t$ where all the weights Z_i are equal by definition one obtains,

$$P_{\beta_t V}(E) = \tilde{N} \left[\frac{D_d(E) + qD_o(E)}{q+1} \right] \tag{3.14}$$

The new normalization factor $\tilde{N}$ is 1 in the Gaussian approximation for D_d and D_o. We thus expect, for such a first order transition at β_t, an energy distribution represented by an equal weight sum of more or less Gaussian peaks. The example [4] of the $q = 10$, 2 dimensional Potts model, is displayed in Fig. 3. The two peaks are clear, one is about $q = 10$ times larger that the other in accordance with (3.14); they are clearly non Gaussian

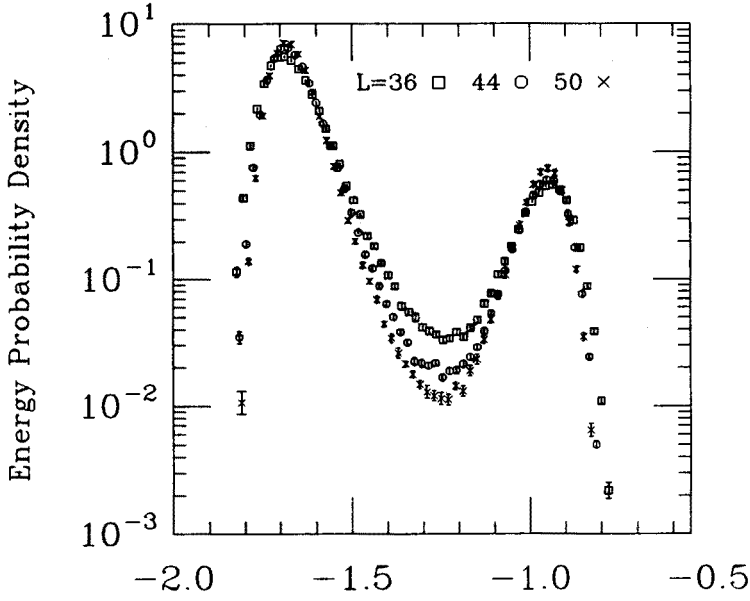

Fig. 3. Energy density for the $q = 10$ $2d$ Potts model at β_t. Data from [4].

shaped (very asymmetric with respect to their maximum). These shapes and their L dependence will be discussed further in the next section.

The specific heat

Since as we saw the asymptotic limits of the $D_i(E)$ distributions are δ functions, it is easy to compute the leading behaviour of the quadratic fluctuations of their weighted sum (3.13). Suppose we have in the vicinity of $\beta = \beta_t$ two phases 1 and 2; we represent the distribution by

$$P(E) = \alpha\, \delta(E - E_1) + (1 - \alpha)\delta(E - E_2)\,.$$

$\alpha = Z_1/(Z_1 + Z_2)$ is the relative weight of phase 1 at β. At $V \longrightarrow \infty$, α varies very rapidly from 0 to 1 as one crosses $\beta = \beta_t$. We have

$$\langle E \rangle = \alpha\, E_1 + (1 - \alpha)E_2\,,$$
$$\langle E^2 \rangle = \alpha\, E_1^2 + (1 - \alpha)E_2^2\,,$$

and hence

$$\langle E^2 \rangle - \langle E \rangle^2 = \alpha(1 - \alpha)(E_1 - E_2)^2\,.$$

We see that although the pure phase fluctuations are neglected, the mixed phase system allowed at $\alpha(1 - \alpha) \neq 0$, fluctuates between energies E_1 and

E_2, leading to a divergent asymptotic specific heat (Eq. (2.11)):

$$C \simeq \alpha(1-\alpha)V\ \beta_t^2\,(E_1 - E_2)^2 + \text{ smaller terms.}$$

This is the well known result that at a *first* order transition the specific heat diverges proportionally to the volume. The proportionality coefficient contains the latent heat squared and is maximum for $\alpha = {}^1/_2$. For the example (3.14), $\alpha = 1/(q+1)$ at $\beta = \beta_t$: C also diverges at β_t, but with a smaller coefficient. Subdominant (constant in V) terms can be computed. Apparent inconsistencies in the analysis of the latter terms, depending of whether it is performed at β_t or at the β value which maximizes the specific heat [4], have been one of the motivations for understanding better the free energy of the Potts model.

4. The q-states 2 dimensional Potts model. Properties and applications

4.1. Known properties

Let us first summarize a few known properties of the model [1]. We recall that its Hamiltonian is

$$H = -\sum_{\langle ij \rangle} \delta_{\sigma_i \sigma_j} \tag{4.1}$$

$\langle ij \rangle$ is a pair of neighbouring sites. The variables σ_i take on q distinct values on each site i of a $L \times L$ lattice. For any q, there is a phase transition at inverse temperature

$$\beta_t = \log(1 + \sqrt{q})\ . \tag{4.2}$$

The transition is second order for $q \leq 4$, with α and ν critical exponents given in the q ordered phases as well as in the disordered phase by

$$\begin{aligned} \alpha(q) &= \frac{2(1-2u)}{3(1-u)}\,, \\ \nu(q) &= \frac{(2-u)}{3(1-u)}\,, \end{aligned} \tag{4.3}$$

where

$$2\cos\frac{\pi}{2}u = \sqrt{q}\,, \qquad 0 \leq u \leq 1\,.$$

Accordingly, the correlation lengths ξ_φ and the specific heats C_φ ($\varphi = o$ or d in the ordered or disordered phase) diverge as $|\beta - \beta_t| \longrightarrow 0$ as

$$\xi_\varphi \sim \lambda_\varphi |\beta - \beta_t|^{-\nu(q)} ,$$
$$C_\varphi \sim \mu_\varphi |\beta - \beta_t|^{-\alpha(q)} . \tag{4.4}$$

We notice that since $\nu(4) = \alpha(4) = {}^2/_3$, the ratio ξ_φ / C_φ remains finite at $q = 4$ when one approaches $\beta = \beta_t$ from either side.

For any $q > 4$, the transition is 1^{st} order, and at $\beta = \beta_t$, exact expressions are known for the internal energies E_φ [5] and the correlation lengths [6 – 8]. If keeping $\beta = \beta_t$, q is extrapolated down to $q = 4$, one finds the following behaviours:

$$\xi_d = \frac{1}{8\sqrt{2}} x \left(1 + O\left(x^{-2}\right)\right) ,$$
$$\xi_o = \frac{\xi_d}{2} , \tag{4.5}$$

where $x = x(q)$ diverges very fast as $q \longrightarrow 4_+$:

$$x = \exp\left(-\frac{\pi^2}{2\theta}\right) ,$$
$$2\cosh\theta = \sqrt{q} , \tag{4.6}$$

and one may check that $\theta \sim \sqrt{q-4}$ at low $q - 4$. In Section 4.2., from a *large q* analysis of the model, we will argue that the pure phase specific heats C_φ also diverge proportionally to the same variable x. In Section 4.3., we shall conjecture from this property an ansatz for the free energies $F_d(\beta)$ and $F_o(\beta)$, discuss its implications for energy distributions, and compare them with results of numerical simulations in the light of the general discussion given before.

4.2. The free energies F_o, F_d from a large q expansion of the partition function

We limit ourselves to sketching the method and giving the main results of a recent investigation whose full account can be found in Ref. [11].

The partition function of the Potts model is

$$Z = \sum_{\{\sigma\}} \exp\left(\beta \sum_{\langle ij \rangle} \delta_{\sigma_i \sigma_j}\right) , \tag{4.7}$$

where $\{\sigma\}$ represents any configuration of spin values on the lattice. Rewriting the exponential as a product over the $2V$ (ij) links,

$$Z = \sum_{\{\sigma\}} \prod_{\text{links}} \Big((\exp(\beta) - 1)\delta_{\sigma_i \sigma_j} + 1 \Big) , \tag{4.8}$$

and performing the spin summation, one arrives at the so-called Fortuin–Kasteleyn representation [12]

$$Z = \sum_{\{X = \text{bond configurations}\}} \Big(\mathrm{e}^{\beta} - 1 \Big)^{b(X)} q^{c(X)} . \tag{4.9}$$

This expression has to be understood as follows. Let X be any subset of links of the lattice. Call bond a link which belongs to X, $b(X)$ the number of bonds of X, and $c(X)$ its number of connected components, with the convention that an isolated site (not at the edge of any bond) is a component. Going from (4.8) to (4.9) proceeds by expanding the product (4.8) before summing over $\{\sigma\}$. One obtains a polynomial in

$$w = \exp(\beta) - 1$$

whose monomials are, up to a combinatorial factor,

$$w^b \delta_{\sigma_{i_1} \sigma_{j_1}} \delta_{\sigma_{i_2} \sigma_{j_2}} \ldots \delta_{\sigma_{i_b} \sigma_{j_b}}$$

if the w term has been taken in b of the $2V$ square bracket factors of (4.8). This is zero unless all links $(i_1 j_1) \ldots (i_n j_n)$ are satisfied (*i.e.* $\sigma_i = \sigma_j$, the links are called bonds). For each *connected* set x of this set X of bonds, one may sum freely over the value of σ common to all sites of x, which yields a factor q. The weight $w^b q^c$ in (4.9) follows. Using (4.9) to compute Z now amounts to count the number $N(c, b)$ of X configurations which correspond to the same values of c and b, leading to

$$Z = \sum_{c,b} N(c, b)(\exp(\beta) - 1)^b q^c . \tag{4.10}$$

This series may be reorganized as a large q expansion in the following sense. The maximum degree in w is $2V$: it corresponds to the fully ordered configurations; *all sites* carry the same value of σ, all links are bonds and the whole lattice form a unique connected set: $N(2V, 1) = 1$, and the contribution to Z is $q\, w^{2V}$. We factor it out and Eq. (4.10) is then rewritten

$$Z = q\, w^{2V} \sum_{l,k} \tilde{N}_{kl} \left(\frac{w}{\sqrt{q}} \right)^{-l} \left(\frac{1}{\sqrt{q}} \right)^{l-2k} . \tag{4.11}$$

Now l is the number of bonds which are *removed* from the fully ordered bulk configuration, k is the number of *additional* connected components (not counting the bulk ordered configuration one starts with), $\tilde{N}_{kl}$ the number of (k,l) configurations. One can easily show that $l-2k$ is ≥ 0, and that a *finite number* of (l,k) pairs contributes at fixed $l-2k$. Hence if one keeps $\left(w/\sqrt{q}\right)$ of order 1 (β in the vicinity of β_t according to (4.2)) as q becomes large, Eq. (4.11) constitutes an expansion of the partition function in powers of $1/\sqrt{q}$. Because it is also an expansion of Z about the fully ordered configuration, a computation of $\tilde{N}_{kl}$ for $l-2k \leq M$ constitutes an approximation to the ordered phase partition function Z_o; at the same order in $1/\sqrt{q}$, $\log(Z_o)/V$ approximates F_o. Computing F_d for the disordered phase needs no new effort because of the duality property of the *two-dimensional* Potts model [1]: if β and $\tilde{\beta}$ are related by

$$\left(e^{\beta}-1\right)\left(e^{\tilde{\beta}}-1\right)=q\,, \tag{4.12}$$

then

$$F_d\left(\tilde{\beta}\right)=F_o(\beta)-2\log\left(\left(e^{\beta}-1\right)/\sqrt{q}\right)\,.$$

The computation of $\tilde{N}_{kl}$ for $l-2k \leq 10$ has been achieved in [11], and we jump to the results directly relevant to our purpose.

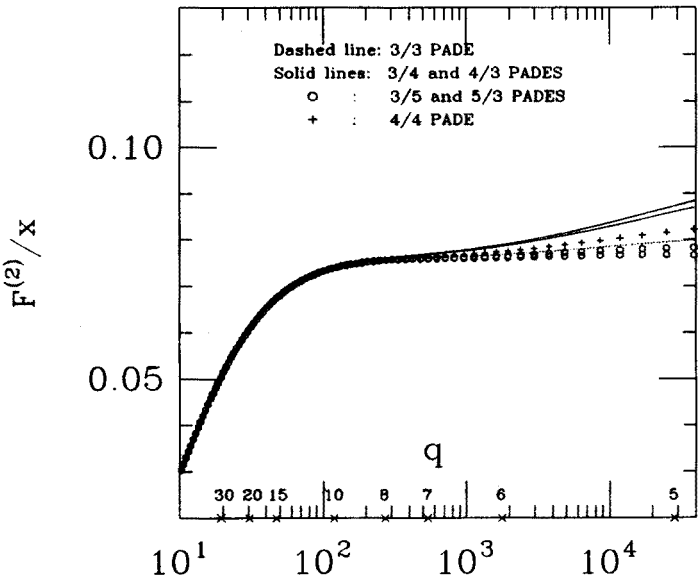

Fig. 4. $F^{(2)}/x$ becomes constant at large x (log abscissa)

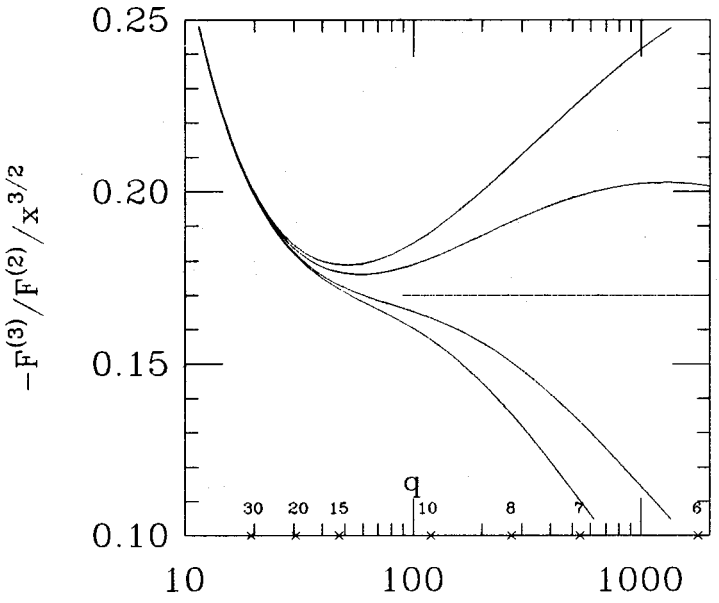

Fig. 5. $-F^{(3)}/F^{(2)}/x^{3/2}$ is smooth at large x (log abscissa)

A series in $1/\sqrt{q}$ of $F_o(q,\beta)$ gives access to the energy cumulants at fixed q

$$F_o^{(n)} = \frac{d^n}{d\beta^n} F_o(q,\beta)\,. \tag{4.13}$$

Their truncated series have been tentatively resumed by Padé techniques adapted to conjectures on their behaviour as q is lowered from large to small values of $q-4$. The basic conjecture is that because the correlation lengths become very large, of order x (see Eqs (4.5) and (4.6)), very large fluctuations, *i.e.* large cumulants, are expected and the relevant scale is the variable x. We reproduce on Figs 4 and 5 evidences that $F^{(2)}$ and $F^{(3)}$ are close to simple powers of x at $q \lesssim 10$, namely $x \gtrsim 100$. Various curves correspond to different Padé resummations. Fig. 4 strongly suggests that $F^{(2)}$ is of order x. In Fig. 5, the dashed straight line is just a guess of what the $q=4$ limit might be (if any) for the positive quantity $-F^{(3)}/\left(x^{3/2}F^{(2)}\right)$; it supports the conjecture that $F^{(3)}$ might be dominantly of order $x^{5/2}$. Higher order cumulants are found not in disagreement with the statement:

$$x^{2-\frac{3\pi}{2}} F^{(n)} \quad \textit{is a smooth function of } q.$$

Apart from bringing evidence for this general trend of the energy cumu-

lants to reveal very large fluctuations, the large q expansion allows a quite precise determination of the pure phase specific heats, via the knowledge we got on $F_o^{(2)}$ down to $q \sim 7$ where numerical simulations have been performed. The origin of discrepancies between different analysis [13, 4, 14–16] can be elucidated, and our analytic result helps in identifying best methods to analyze data when the correlation length becomes of the same size as the box linear size.

4.3. An ansatz for the pure phase free energies in the first order region $q > 4$

The ansatz for F_o and F_d at $q > 4$ which we now present [3] incorporates both the effect of the nearby 2nd order point $q = 4$, $\beta_t = \log 3$ and the information gained from the previous large q expansion.

From Eqs (4.4) taken at $q = 4$, and, for definiteness, at $\beta - \beta_t \gtrsim 0$ (ordered phase), we know that

$$F_o^{(2)}(q = 4, \beta) \simeq A\,(\beta - \beta_t)^{-2/3} + \ldots \tag{4.14}$$

$$\xi_o(q = 4, \beta) \simeq \lambda_o\,(\beta - \beta_t)^{-2/3} + \ldots, \tag{4.15}$$

where the dots stand for less singular or regular terms at $\beta = \beta_t$. We already remarked that this implies that $F_o^{(2)}/\xi_o$ tends to a constant at $q = 4$ fixed, and $\beta \longrightarrow \beta_{t+}$. We extrapolate this result as follows. By differentiating (4.14) p times with respect to β, we have

$$F_o^{(p+2)}(q = 4, \beta) = A(-)^p \frac{\Gamma(p + {}^2/_3)}{\Gamma({}^2/_3)}\,(\beta - \beta_t)^{-2/3-p} + \ldots.$$

We next trade $(\beta - \beta_t)$ for ξ_o using Eq. (4.15), and then set $\beta = \beta_t$:

$$F_o^{(p+2)}(q = 4, \beta_t) = A(-)^p \frac{\Gamma(p + {}^2/_3)}{\Gamma({}^2/_3)} \left(\frac{\xi_o}{\lambda_o}\right)^{3p/2+1} + \ldots.$$

The ansatz consists in wildly continuing this relation above $q = 4$, where we do know the behaviour of ξ_o at $\beta = \beta_t$ via Eq. (4.5). Hence we *conjecture*

$$F_o^{(p+2)}(\beta_t) = A(-)^p \frac{\Gamma(p + {}^2/_3)}{\Gamma({}^2/_3)} (Bx)^{1+3p/2} + \ldots.$$

which we hope is a reasonable approximation wherever x is large, A and B being "constants", at least functions of q smooth compared with the behaviour (4.6) of x. Within this approximation, it is consistent with duality to write

$$F_d^{(p+2)}(\beta_t) = (-)^p F_o^{(p+2)}(\beta_t) + \dots .$$

With (4.15) and the exact knowledge [5] of $F_o^{(0)}(\beta_t)$ and $F_o^{(1)}(\beta_t) = -E_o$, it is straightforward to resum the Taylor series of F_o. The result is:

$$F_o(\beta) - F_o(\beta_t) = -E_o(\beta - \beta_t) + \frac{3A}{(Bx)^2} \times \left\{ \frac{3}{4}\left[1 + (\beta - \beta_t)(Bx)^{3/2}\right]^{4/3} - \frac{3}{4} - (\beta - \beta_t)(Bx)^{3/2} \right\} + \dots \quad (4.16)$$

and duality gives $F_d(\beta)$:

$$F_d(\beta) = F_o[E_o \longleftrightarrow -E_d, (\beta - \beta_t) \longleftrightarrow -(\beta - \beta_t)] + \dots . \quad (4.17)$$

This tentative form of F_o, F_d depends on the two "constants" A and B. These we determine by comparing

$$\frac{F^{(2)}}{x} = AB + \dots \quad \text{and} \quad \frac{F^{(3)}}{F^{(2)}x^{3/2}} = -\frac{2}{3}B^{3/2} + \dots$$

to the values obtained in Subsection 4.2. from the large q expansion (Figs 4 and 5). Once a "best guess" is chosen for A and B, one has a *parameter free prediction* of the partition function of the Potts model around β_t for $q > 4$ [17].

This construction leads to the ansatz

$$Z_V^{\text{ansatz}}(\beta) = \exp(VF_d) + q\exp(VF_o), \quad (4.18)$$

with $F_{o,d}$ given by (4.16), (4.17). If these free energies are good approximations to the true ones, then we know from Eq. (3.11) [10] that (4.18) is a good approximation to the true $Z_V(\beta)$. To test whether it is the case, we compare the energy distributions obtained by (3.13) for $q = 10$ to the data of Ref. [4] taken at $L = 16, 20, 24, 36, 44$ and 50. Because L is not large enough for the saddle point method to be reliable, the integrals of the type (3.6) required by (3.13) are performed numerically. The results are presented in Fig. 6. A good agreement is found. In particular it is quite remarkable that the intermediate region between the two peaks is very well reproduced. Study of the integral (3.13) reveals that this region is especially sensitive to the existence of very large cumulants in the pure phase free energies, and confirms the relevance of interpreting the whole pattern as a consequence of the second order point at $q = 4$, $\beta = \beta_t$ [4]. Other physical issues, such as interface tension measurements [14, 19 – 22] can also be touched upon by reference to the same ansatz [3].

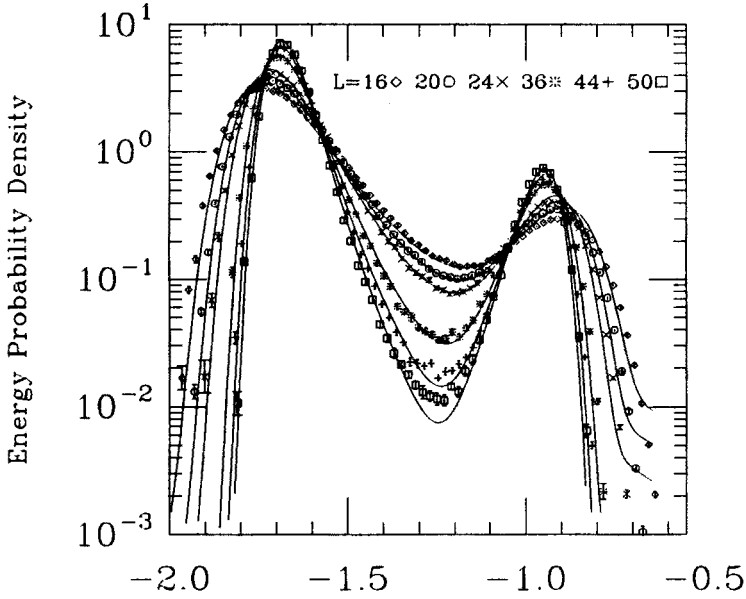

Fig. 6. Solid lines: Densities predicted by Eqs (4.16)–(4.18). Data from [4].

5. Conclusion

The overall lessons one may extract from this general study of first order transitions and from its confrontation to practical cases via the "Potts model laboratory" are two-fold:

- The finite size effects observed in energy density distributions may lead to misinterpretation. Especially when large energy fluctuations are present, standard phenomenology based on "gaussian peaks" attached to pure phases is *not* reliable. In addition, *very large* linear lattice sizes are required before the E-distribution is close to an exponential of V times a function of E.
- A safe point of view is that given (at least for a class of models) by the work of Borgs, Kotecky and Miracle-Sole [10]. Unlike $P(E)$, each phase contributes a term $\exp(V\,F(\beta))$ in the total partition function, up to an exponentially small finite size correction which is of physical interest. In fact, the latter is related to correlation lengths in general, and to interface effects in the vicinity of a first order transition point. Similar situations in cases of field driven first order transitions (*e.g.* in the Ising model below the transition temperature) deserve similar analysis of the magnetization distribution.

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