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Potts model in the many-component limit

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Abstract. The mean-field theory of the q-component Potts model is shown to be exact in the limit $q \to \infty$. This proves a conjecture by Mittag and Stephen.

1. Introduction

In analysing statistical mechanical models it is customary to begin with mean-field theory. Typically, this classical approximation yields incorrect values for critical temperatures and critical exponents. Nevertheless, it usually provides a qualitatively useful phase diagram exhibiting single phase regions, coexistence manifolds, critical manifolds, and so on, with the correct topology. Recently, however, it has been realised that this is not the case for the q-component or q-state Potts model (Potts 1952). This discovery has greatly revitalised theoretical interest in the Potts model and has sparked off a controversy as to the precise nature of its phase transition.

For the two component ($q = 2$) Potts model, that is the Ising model, mean-field theory correctly predicts a continuous phase transition in zero field. For $q > 2$, mean-field theory (Straley and Fisher 1973, Mittag and Stephen 1974) predicts a first-order transition in zero field, independent of the lattice dimension d. Of course, in one dimension, the model has no phase transition for short-ranged interactions. This discrepancy is expected. However, Baxter (1973) has argued convincingly that, in two dimensions, the Potts model in fact exhibits a first-order transition for $q > 4$ and a higher-order transition for $q \leq 4$. His conclusion is also firmly supported by series expansions (Straley and Fisher 1973, Kim and Joseph 1975) though, sadly enough, a proliferation of series expansions (Ditzian and Oitmaa 1974, Straley 1974, Enting 1974, Kim and Joseph 1975) and renormalisation-group calculations (Golner 1973, Rudnick 1975, Zia and Wallace 1975, Burkhardt *et al* 1976, Southern 1977) has not given a definite answer in three dimensions.

Although mean-field theory clearly fails in general, Mittag and Stephen (1974) point out that the theory provides an accurate description of the Potts model transition, in two or higher dimensions, when the number of components is large. Indeed, on the basis of comparison with exact results, they have conjectured that mean-field theory is exact in the limit $q \to \infty$. It is this conjecture that is proved in this paper.

The rest of this section is devoted to a precise statement of the result. In §§ 2 and 3 we obtain upper and lower bounds on the free energy that coalesce with the mean-field free energy in the limit $q \to \infty$. Since the application of the lower bound in § 3 is restricted to finite-range interactions a supplementary argument for long-range interactions is given in § 4.

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The Hamiltonian for the q-state Potts model is

$$H = -\tfrac{1}{2} \sum_{i,j\in\Lambda} J_{ij}\,\delta(\alpha_i, \alpha_j) - h \sum_{i\in\Lambda} \delta(\alpha_i, 1) \tag{1}$$

where the vectors i and j label the sites of a regular infinite lattice $\mathscr{L}$, Λ is a finite subset of $\mathscr{L}$, $\delta(\cdot,\cdot)$ is the Kronecker delta, and the q possible states at each site are given by $\alpha_i = 1, 2, \ldots, q$. The parameters $J_{ij} = J_{ji}$ (we set $J_{ii} = 0$) are pair interaction strengths and h is a symmetry breaking field. The partition function is

$$Z_\Lambda(\beta) = \mathrm{Tr}\exp(-\beta H) \tag{2}$$

where $\beta = 1/kT$ and Tr (trace) denotes a multiple sum over the q states allowed at each site. The free energy per site $\psi(\beta)$ in the thermodynamic limit is given by

$$-\beta\psi(\beta) = \lim_{\Lambda\to\mathscr{L}} |\Lambda|^{-1} \ln Z_\Lambda(\beta) \tag{3}$$

where $|\Lambda|$ is the number of sites in Λ.

We will assume that the interactions are ferromagnetic and translationally invariant,

$$J_{ij} = J(i-j) \geqslant 0, \tag{4}$$

with sufficiently rapid decay that

$$J = \sum_{j\in\mathscr{L}} J_{ij} < \infty. \tag{5}$$

Under these conditions (see Ruelle (1969 ch 2) or Israel (1979 ch 1)) the limiting free energy (3) exists and does not depend on the choice of boundary conditions. We will make use of this freedom by choosing periodic boundary conditions to derive the upper bound on the free energy in § 2, and a different set of boundary conditions to derive the lower bound on the free energy in § 3.

The result we prove is the following.

Theorem. Let $\psi(\beta)$ be the free energy (3) for the Potts model (1), with interactions satisfying (4) and (5) and $h \geqslant 0$. Then in the many-component limit

$$\lim_{q\to\infty} \psi(\beta \ln q) = \lim_{q\to\infty} \psi_{\mathrm{MF}}(\beta \ln q) = \psi_\infty(\beta) \tag{6}$$

where $\psi_{\mathrm{MF}}(\beta)$ is the mean-field free energy and

$$\psi_\infty(\beta) = \begin{cases} -\beta^{-1}, & \beta(\frac{1}{2}J + h) \leqslant 1, \\ -\frac{1}{2}J - h, & \beta(\frac{1}{2}J + h) > 1. \end{cases} \tag{7}$$

The factor $\ln q$ which appears in the argument of ψ in (6) is essential if one is to obtain a non-trivial result in the limit $q \to \infty$. The physical reason for this is that increasing q increases the entropy of the system. To compensate, the interactions (J_{ij} and h) must be increased by factors of $\ln q$ and the free energy decreased by a factor $\ln q$. Equivalently, and more simply, we rescale the inverse temperature β.

In the statement of the theorem we have omitted to write down an expression for the mean-field free energy $\psi_{\mathrm{MF}}(\beta)$. An explicit formula, equivalent to that of Mittag and Stephen (1974), will be derived in the next section. At this juncture it is perhaps also worth mentioning that the mean-field free energy $\psi_{\mathrm{MF}}(\beta)$ can be obtained by solving the equivalent neighbour model. This model, which is defined by setting all the interactions

$J_{ij}=J/|\Lambda|$ in (1), is of course not a genuine statistical mechanical model. With more effort, however, the mean-field free energy can be derived rigorously by starting with the Hamiltonian (1) and taking a long-range interaction limit, or an infinite coordination number limit, after the thermodynamic limit. This approach to mean-field theory has the benefit of avoiding phenomenology, but since these matters do not bear directly on our present considerations, we forego giving the details and refer the interested reader to Thompson (1972 ch 4), Thompson and Silver (1973) and Pearce and Thompson (1978).

2. Mean-field theory as an upper bound on ψ

In this section we use the Gibbs–Bogoliubov variational principle to show that

$$\psi(\beta)\leqslant\psi_{\mathrm{MF}}(\beta) \tag{8}$$

where $\psi_{\mathrm{MF}}(\beta)$ is the mean-field free energy. Although we are specifically concerned here with the Potts model, we remark that the Gibbs–Bogoliubov variational principle (see, for example, Falk 1970) and the arguments leading to (8) are, in fact, quite general and are well known in other contexts.

Let H be defined by (1) and impose periodic boundary conditions so that

$$J^{\Lambda}=\sum_{j\in\Lambda}J_{ij}\rightarrow J \qquad \text{as } \Lambda\rightarrow\mathscr{L} \tag{9}$$

and J^{Λ} does not depend on i. An upper bound (Falk 1970) on the free energy for this system is then given by

$$-\beta^{-1}\ln Z_{\Lambda}(\beta)\leqslant\mathrm{Tr}(\rho H)+\beta^{-1}\,\mathrm{Tr}(\rho\ln\rho) \tag{10}$$

where ρ is any trial probability distribution. One way to obtain the mean-field theory (for example, Blume *et al* 1971) is now to minimise this upper bound with respect to variational parameters in the probability distribution ρ, which is chosen so that the α_i are statistically independent, i.e.

$$\rho=\prod_{i\in\Lambda}\rho_i(\alpha_i). \tag{11}$$

Motivated by symmetry considerations, we choose

$$\rho_i(\alpha_i)=\begin{cases} p & \text{if } \alpha_i=1\\ (1-p)/(q-1) & \text{if } \alpha_i\neq 1\end{cases} \tag{12}$$

where $0\leqslant p\leqslant 1$ and p is independent of i. If we now evaluate the right side of (10), minimise with respect to p and take the thermodynamic limit, using (9), we obtain the desired inequality (8) with

$$\psi_{\mathrm{MF}}(\beta)=\min_{0\leqslant p\leqslant 1}\left\{-\tfrac{1}{2}J\left[p^2+\frac{(1-p)^2}{q-1}\right]-hp+\beta^{-1}\left[p\ln p+(1-p)\ln\left(\frac{1-p}{q-1}\right)\right]\right\}. \tag{13}$$

A convenient order parameter for the mean-field theory turns out to be

$$x=\frac{q}{q-1}\left(p-\frac{1}{q}\right). \tag{14}$$

If we eliminate p in (13), in favour of x, we obtain precisely the Mittag and Stephen expression for the mean-field free energy. In any case, if we replace β by $\beta \ln q$ in (13) and take the limit $q \to \infty$, the minimum over $0 \leqslant p \leqslant 1$ yields the right side of (7).

3. A lower bound on ψ

To obtain an upper bound on the partition function and thus a lower bound on the free energy ψ it is convenient to employ a different set of boundary conditions on the finite set Λ, and to restrict the interactions to finite range. Namely, we shall assume that $\alpha_i = 1$ for all sites i not in Λ, and write

$$H = -\tfrac{1}{2} \sum_{i \in \Lambda} \sum_{j \in \mathscr{L}} J_{ij}^R \, \delta(\alpha_i, \alpha_j) - h \sum_{i \in \Lambda} \delta(\alpha_i, 1) \tag{15}$$

where, for a fixed distance R, we define the truncated interactions

$$J_{ij}^R = \begin{cases} J_{ij} & \text{for } |i-j| < R \\ 0 & \text{otherwise.} \end{cases} \tag{16}$$

The fact that the boundary terms in (15) do not contribute to the free energy ψ in the thermodynamic limit follows by standard arguments (again see Ruelle (1969 ch 2) or Israel (1979 ch 1)).

For $h \geqslant 0$, which we shall henceforth assume is the case, the minimum value of H,

$$H_0 = -|\Lambda|(\tfrac{1}{2}J^R + h), \tag{17}$$

occurs when all α_i (for $i \in \Lambda$ as well as $i \notin \Lambda$) are equal to 1. The basic inequality $H \geqslant H_0$ can now be suitably improved by using graphical methods. With every configuration of the system, i.e. with every choice of the α_i, $i \in \Lambda$, we associate a graph G whose vertices are the sites at which $\alpha_i \neq 1$, with edges connecting the vertices provided $\alpha_i = \alpha_j (\neq 1)$ *and* $|i-j| < R$. We also let μ be the number of connected components in G.

Many configurations may be associated with the same graph G, but it is evident that their number cannot exceed $(q-1)^\mu$, since the α_i are identical in each component. The number of distinct graphs is itself bounded by $2^{\frac{1}{2}|\Lambda| z}$, where z is the number of sites on the lattice within a distance R of a particular site. This estimate holds because a graph is determined by specifying all its edges, and there are at most $\frac{1}{2}|\Lambda| z$ possible edges connecting pairs of sites in Λ separated by a distance less than R.

We now assert that a lower bound to H in (15) is provided by the formula

$$H \geqslant H_0 + \mu(\tfrac{1}{2}J^R + h) \tag{18}$$

where μ is defined for a choice of α_i in the manner described above. To see this, note first that the number of sites with $\alpha_i \neq 1$ is at least μ; this accounts for the μh term in (18). Next, note that for any connected component C in the graph G and for any vector r connecting two sites on $\mathscr{L}$, there will always be *some* site i in C such that the site $i+r$ is *not* in C. Indeed, since C is finite, one can choose any $i \in C$, and if $(i+r) \in C$ one can consider $(i+r)+r$, and so forth, till one finds a site not in C.

Now if $i \in C$ and $(i+r) \notin C$, it follows from the definition of the graph that $\alpha_i \neq \alpha_{i+r}$ provided $|r| < R$, and thus the corresponding term in (15) is zero, rather than $-\frac{1}{2}J^R(r)$ as it is in the case where all $\alpha_i = 1$. Since for *each* component and for *each* r with $|r| < R$ we can identify a corresponding increment in H over H_0, we have established the validity of the J^R term in (18). (The reader concerned about 'double counting' of pairs of sites

$(i, i+r)$, when each belongs to a connected component, should note the corresponding 'double counting' present in (15).)

Combining (18) with the estimates which precede it, we obtain

$$\begin{aligned} Z_\Lambda(\beta) &\leqslant 2^{\frac{1}{2}|\Lambda| z} \exp(-\beta H_0) \sum_{\mu=0}^{|\Lambda|} \{q \exp[-\beta(\tfrac{1}{2}J^R + h)]\}^\mu \\ &\leqslant 2^{\frac{1}{2}|\Lambda| z} \exp(-\beta H_0)\{1 + q \exp[-\beta(\tfrac{1}{2}J^R + h)]\}^{|\Lambda|}. \end{aligned} \tag{19}$$

It then follows from (3) and (17) that

$$\psi(\beta) \geqslant -\tfrac{1}{2}\beta^{-1} z - \beta^{-1} \ln\{q + \exp[\beta(\tfrac{1}{2}J^R + h)]\}. \tag{20}$$

Upon replacing β by $\beta \ln q$ in this expression, and taking the limit $q \to \infty$, one obtains as a lower bound the right side of (7), with J^R in place of J.

4. Interactions of long range

The arguments in §§ 2 and 3 establish the theorem stated in § 1 for interactions of strictly finite range, since in this case we can always choose R large enough so that J_{ij}^R in (16) is identical with J_{ij}. When the interactions are not of strictly finite range, but (5) is satisfied, our arguments yield (7) provided the limit $R \to \infty$ is taken *after* the limit $q \to \infty$, since

$$J^R = \sum_{r:|r|<R} J(r) \to J \qquad \text{as } R \to \infty. \tag{21}$$

If we wish to take the limit $R \to \infty$ first, and then $q \to \infty$, we cannot make direct use of the lower bound (20) because z diverges with R. However, the standard arguments (Ruelle 1969, Israel 1979) noted earlier can be used to show that for any finite q and β,

$$|\psi - \psi^R| \leqslant \sum_{r:|r|\geqslant R} J(r) \tag{22}$$

where ψ^R denotes the free energy (3) for the truncated interaction (16). In view of (21), the convergence of ψ^R to ψ as $R \to \infty$ is uniform in q and β, which means that (7) is also obtained in the case when the limit $q \to \infty$ is taken after the limit $R \to \infty$.

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