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LETTER TO THE EDITOR

Mean-field theory of the many component Potts model

Laurence Mittag† || and Michael J Stephen‡§

† Center for Theoretical Studies, University of Miami, Coral Gables, Florida 33124, USA
‡ Physics Department, Rutgers University, New Brunswick, New Jersey 08903, USA

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Abstract. A mean-field theory of the q-component Potts model is given. The transition is first order for $q \geqslant 3$. For large q the mean-field results agree with all the known exact results in two dimensions for the Potts model. It is conjectured that the mean-field theory provides an accurate description of the transition in two or higher dimensions when the number of components is large.

The Potts (1952) model is a generalization of the Ising model. In the lattice gas representation of this model each site of the lattice is occupied by one of q different types of atoms. Nearest-neighbour atoms have an interaction energy $-\epsilon$ if they are the same and zero if they are different. The system orders at low temperatures into a phase rich in one of the possible types of atoms. The Ising model corresponds to $q = 2$.

Certain exact results are known for the Potts model in two dimensions. On a plane square lattice a dual transformation exists which relates the partition function at high and low temperatures and which determines the critical temperature T_c if it is unique. The dual transformation has been discussed by a number of authors (Potts 1952, Mittag and Stephen 1971). The average energy at T_c can also be obtained from the duality relation. More recently Baxter (1973) has shown that the Potts model on a plane square lattice is equivalent to a staggered ice-type model. From the known properties of this latter model he has obtained the free energy and latent heat at the critical temperature and concluded that for $q > 4$ the Potts model has a first-order transition. For $q \leqslant 4$ the transition is of a higher order. The critical temperatures of the plane triangular and hexagonal lattices may also be determined by a combination of the dual and star–triangle transformations as in the case of the Ising model. A special feature of the star–triangle transformation is that it only exists exactly at T_c (Stephen and Mittag 1972). The critical temperatures of the plane triangular and hexagonal lattices are given by

$$\begin{aligned} \exp\left(\frac{\epsilon}{kT_c}\right) &= 1+\frac{q^{1/2}}{2\cos\theta} && \text{(triangular)} \\ \exp\left(\frac{\epsilon}{kT_c}\right) &= 1+2q^{1/2}\cos\theta && \text{(hexagonal)} \end{aligned} \tag{1}$$

where $2\cos 3\theta = q^{1/2}$ (θ is imaginary for $q > 4$). These results have also been found recently by Kim and Joseph (1974).

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In this letter we present a mean-field treatment of the Potts model. The mean-field approximation leads to a first-order transition for $q \geqslant 3$. The mean-field results agree with all the known exact results for the Potts model on planar lattices when q is sufficiently large and it is conjectured that the mean-field approximation is accurate to leading order in q when q is large. A mean-field treatment of and series expansions for the three-component Potts model have recently been given by Straley and Fisher (1973).

It is convenient to introduce a spin representation for the Potts model (Mittag and Stephen 1971). At each site of the lattice we introduce a spin variable λ which can take on the values $\lambda = 1, \omega, \omega^2, \ldots, \omega^{q-1}$ where $\omega = e^{2\pi i/q}$ is a qth root of unity. The energy of interaction of two nearest-neighbour spins, λ and λ', is

$$E_{\lambda\lambda'} = -\epsilon\delta(\lambda-\lambda') \tag{2}$$

where $\delta(\lambda-\lambda')$ is the Kronecker symbol. Using the relation

$$q^{-1}\sum_{k=1}^{q}\lambda^k\lambda'^{q-k} = \delta(\lambda-\lambda')$$

we write equation (2) in the form

$$E_{\lambda\lambda'} = -q^{-1}\epsilon - q^{-1}\epsilon\sum_{k=1}^{q-1}\lambda^k\lambda'^{q-k}. \tag{3}$$

The fraction of atoms of type $j (j = 1, \ldots, q)$ is n_j and in this spin representation

$$qn_j = 1 + \sum_{k=1}^{q-1}\omega^{q-(j-1)k}\langle\lambda^k\rangle \tag{4}$$

where the angular brackets denote an expectation value.

We first discuss the mean-field treatment of the three-component Potts model. This is generalized to all values of q below. We introduce a complex order parameter $\langle\lambda\rangle = z, \langle\lambda^2\rangle = \langle\lambda^*\rangle = z^*$ which preserves the symmetry of the model†. From equation (4) the three choices (1) $z = R$, (2) $z = \omega R$, (3) $z = \omega^2 R$ where R is real, correspond to an ordered state which is rich in atoms of type 1, 2 and 3 respectively. From equation (3) the effective mean-field hamiltonian for a single spin is

$$H_\lambda = -\tfrac{1}{3}\epsilon n(\lambda z^* + \lambda^* z) \tag{5}$$

where n is the number of nearest neighbours. The first constant term in equation (3) has been omitted. The self-consistency condition determining the order parameter is

$$z = \frac{\mathrm{Tr}\,\lambda\, e^{-\beta H_\lambda}}{\mathrm{Tr}\, e^{-\beta H_\lambda}} \tag{6}$$

where $\beta = (kT)^{-1}$. It can be shown from this equation that z is defined in a triangle on the complex plane with vertices at 1, ω and ω^2. Assuming for simplicity that the order parameter is real corresponding to an ordered state rich in atoms of type 1, equation (6) becomes

$$R = \frac{\exp(\beta\epsilon nR) - 1}{\exp(\beta\epsilon nR) + 2}. \tag{7}$$

† A different representation in terms of two real order parameters was used by Straley and Fisher (1973).

In the mean-field approximation the energy per site is given by $E = -\frac{1}{3}\epsilon n(z^*z+\frac{1}{2})$. The entropy per site is

$$S = -k\sum_{j=1}^{3} n_j \ln n_j. \tag{8}$$

It is of interest to first examine the free energy per site, F, for small values of z. On expanding (8) in powers of z we find

$$-\beta F = \ln 3+\tfrac{1}{6}\beta\epsilon n-(1-\tfrac{1}{3}\beta\epsilon n)z^*z+\tfrac{1}{6}(z^3+z^{*3})-\tfrac{4}{3}(zz^*)^2\ldots. \tag{9}$$

The threefold symmetry of the model gives rise to the cubic terms in z and the presence of these terms forces the transition to be first order. Qualitative features of the transition have been discussed by Straley and Fisher (1973).

As the transition is of first order the expansion leading to (9) is not valid. Introducing the real order parameter in (4) and (8) the exact free energy per site is

$$-\beta F = \ln 3+\tfrac{1}{6}\beta\epsilon n+\tfrac{1}{3}[\beta\epsilon nR^2-(1+2R)\ln(1+2R)-2(1-R)\ln(1-R)]. \tag{10}$$

The equilibrium state is determined by that solution of (7) which minimizes the free energy (10). It is easily verified that, at the critical point, the order parameter jumps to the value $R_c = \frac{1}{2}$ and the critical temperature is given by $kT_c = \epsilon n/4\ln 2$.

The above results are readily generalized to the q-component Potts model. We consider the case where the system orders in a state rich in one type of atom, the other types of atoms being all equivalent. Then we introduce order parameters $\langle\lambda\rangle = R\,e^{i\theta}$, $\langle\lambda^2\rangle = R\,e^{2i\theta}\ldots\langle\lambda^{q-1}\rangle = R\,e^{i(q-1)\theta}$. When $e^{i\theta} = 1, \omega, \ldots, \omega^{q-1}$ we obtain phases rich in atoms of type 1, 2 etc. Without loss of generality we take $\theta = 0$ and then the equation determining the order parameter R is

$$R = \frac{\exp(\beta\epsilon nR)-1}{\exp(\beta\epsilon nR)+q-1}. \tag{11}$$

The free energy per site is

$$-\beta F = \ln q+\frac{\beta\epsilon n}{2q}+q^{-1}\{\tfrac{1}{2}(q-1)\beta\epsilon nR^2-[1+(q-1)R]\ln[1+(q-1)R]$$
$$-(q-1)(1-R)\ln(1-R)\}. \tag{12}$$

The transition is of first order for $q \geqslant 3$ and it is easily verified that at the critical temperature the order parameter jumps to the value $(q-2)/(q-1)$. The critical temperature is given by

$$kT_c = n\epsilon\left(\frac{q-2}{q-1}\right)[2\ln(q-1)]^{-1} \simeq \frac{n\epsilon}{2\ln q}\left(1-\frac{1}{q}+\frac{1}{q\ln q}\ldots\right). \tag{13}$$

Other quantities of interest at the critical point are

$$E_c = -\frac{n\epsilon}{4}\left(\frac{(q-2)^2}{q(q-1)}+\frac{2}{q}\right) \simeq -\frac{n\epsilon}{4}\left(1-\frac{1}{q}\right) \tag{14}$$

$$-\beta_c F_c = \ln q+\frac{q-1}{q(q-2)}\ln(q-1) \simeq \ln q\left(1+\frac{1}{q}\ldots\right) \tag{15}$$

$$L = \frac{n\epsilon}{2}\frac{(q-2)^2}{q(q-1)} \simeq \frac{n\epsilon}{2}\left(1-\frac{3}{q}\ldots\right) \tag{16}$$

where E_c is the average energy, F_c is the free energy per site and L is the latent heat per site. For purposes of comparison we give the exact values of these quantities expanded in powers of q^{-1} for the plane square lattice

$$kT_c = \frac{\epsilon}{\ln(1+q^{1/2})} \simeq \frac{2\epsilon}{\ln q}\left(1-\frac{2}{q^{1/2}\ln q}\cdots\right) \tag{17}$$

$$E_c = -\epsilon\left(1+\frac{1}{q^{1/2}}\right) \tag{18}$$

$$-\beta_c F_c = \ln q + \frac{2}{q^{1/2}} + \cdots \tag{19}$$

$$L = 2\epsilon\left(1-\frac{5}{q^{1/2}}+\cdots\right). \tag{20}$$

For the case $n = 4$, corresponding to the plane square lattice, the mean-field and exact results agree to leading order in q. The transition temperatures for the planar triangular ($n = 6$) and hexagonal ($n = 3$) lattices also agree with the exact results (1) for large q. This leads to the conjecture that the mean-field treatment of the Potts model provides an accurate description of the transition in two or higher dimensions when the number of components q is large. It should be noticed that for large q the transition at T_c is to an almost completely ordered state.

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