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COMMENT

Correlation identities and mean field approximations to the Potts model

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Abstract. Correlation identities for the Potts model are obtained, and the usual mean-field approximation is derived from the identities by neglecting correlations. This derivation is not only clear in its physical meaning but also independent of the representation. These identities may also serve as a starting point for other approximations. As an example, the application of the exponential operator technique is considered.

Recently, there has been much interest in the q-state Potts model (Potts 1952), which is a generalisation of the Ising model, largely because the model has proven to be rich in its contents. It is known that the Potts model is related to a number of outstanding problems in lattice statistics such as vertex models and percolation (for references, see Wu 1982). It has also been recognised that it is possible to realise this model in experiments, for example, ordered adsorbed monolayers. Unfortunately, however, the exact solution of the general q-state Potts model is not yet known except for the celebrated Onsager solution (Onsager 1944) of the $q=2$ (Ising) model in $d=2$ dimensions. Although some information has been obtained through the use of duality relations, series expansions and renormalisation group studies, it is also of some interest to examine the model in the mean-field approximation (Kihara *et al* 1954) which is known to be correct in the $q\to\infty$ limit (Mittag and Stephen 1974).

In this comment, we obtain correlation identities for the Potts model, and show how the usual mean-field approximation can be derived from them. Also, we apply the exponential operator technique (Honmura and Kaneyoshi 1978, 1979, Taggart and Fittipaldi 1982) to those identities.

We start with the Potts Hamiltonian

$$H=-\sum_{i<j} J_{ij}\delta_{\sigma_i\sigma_j}-\sum_i\sum_\lambda \zeta_i^\lambda \delta_{\lambda\sigma_i}, \tag{1}$$

where each spin σ_i $(i=1,2,\ldots,N)$ on lattice sites can take q possible states, δ is the Kronecker delta, J_{ij} is the interaction strength between sites i and j, and ζ_i^λ is the symmetry breaking field on site i. Roman characters (i, j, k, l) and Greek characters (λ, μ, ν) are used for labelling sites and spin states, respectively. Now we consider the ensemble average

$$\langle\delta_{\mu\sigma_k}-\delta_{\nu\sigma_k}\rangle\equiv Z^{-1}\,\mathrm{Tr}(\delta_{\mu\sigma_k}-\delta_{\nu\sigma_k})\,\mathrm{e}^{-\beta H}, \tag{2}$$

where Tr implies the sum over all possible q^N states, i.e., $\mathrm{Tr}\equiv\Sigma_{\{\sigma\}}\equiv\Sigma_{\sigma_1}\Sigma_{\sigma_2}\ldots\Sigma_{\sigma_N}$, and $Z\equiv\mathrm{Tr}\,\mathrm{e}^{-\beta H}$ is the partition function. We note that the Hamiltonian can be separated into two parts

$$H = -\sum_{\lambda} E_k^{\lambda} \delta_{\lambda\sigma_k} - A_k, \tag{3}$$

where E_k and A_k are given by

$$E_k^{\lambda} = \sum_j J_{kj} \delta_{\lambda\sigma_j} + \zeta_k^{\lambda} \qquad A_k = -\sum_{i<j}{}' J_{ij} \delta_{\sigma_i\sigma_j} - \sum_i{}' \sum_{\lambda} \zeta_i^{\lambda} \delta_{\lambda\sigma_i}. \tag{4}$$

In the above equations, primes restrict the summation indices not equal to k. Also we note that neither E_k^{λ} nor A_k contain σ_k. With the notation

$$\mathrm{Tr}' \equiv \sum_{\sigma_1} \cdots \sum_{\sigma_{k-1}} \sum_{\sigma_{k+1}} \cdots \sum_{\sigma_N},$$

the right-hand side of equation (2) becomes

$$\begin{aligned} Z^{-1} \mathrm{Tr}' \sum_{\sigma_k} (\delta_{\mu\sigma_k} - \delta_{\nu\sigma_k}) & \exp[\beta \Sigma_{\lambda} E_k^{\lambda} \delta_{\lambda\sigma_k}] \exp(\beta A_k) \\ &= Z^{-1} \mathrm{Tr}' [\exp(\beta E_k^{\mu}) - \exp(\beta E_k^{\nu})] \exp(\beta A_k) \\ &= Z^{-1} \mathrm{Tr}' \tanh \tfrac{1}{2}\beta (E_k^{\mu} - E_k^{\nu}) [\exp(\beta E_k^{\mu}) + \exp(\beta E_k^{\nu})] \exp(\beta A_k) \\ &= Z^{-1} \mathrm{Tr}' \sum_{\sigma k} (\delta_{\mu\sigma_k} + \delta_{\nu\sigma_k}) \tanh \tfrac{1}{2}\beta (E_k^{\mu} - E_k^{\nu}) \exp(\beta \Sigma_{\lambda} E_k^{\lambda} \delta_{\lambda\sigma_k}) \exp(\beta A_k), \end{aligned}$$

which leads to the desired identity, i.e.,

$$\langle \delta_{\mu\sigma_k} - \delta_{\nu\sigma_k} \rangle = \langle (\delta_{\mu\sigma_k} + \delta_{\nu\sigma_k}) \tanh \tfrac{1}{2} \beta (E_k^{\mu} - E_k^{\nu}) \rangle. \tag{5}$$

It is straightforward to write the above identity in the more general form

$$\langle (\delta_{\mu\sigma_k} - \delta_{\nu\sigma_k}) f_k \rangle = \langle (\delta_{\mu\sigma_k} + \delta_{\nu\sigma_k}) f_k \tanh \tfrac{1}{2} \beta (E_k^{\mu} - E_k^{\nu}) \rangle, \tag{6}$$

where f_k is an arbitrary function of the Potts variables so long as it is not a function of site k. Equation (6) is essentially a generalisation of the identity for the Ising model obtained by Callen (1963) and Suzuki (1965).

By the same procedure, we can obtain other identities, as for example

$$\langle (\delta_{\mu\sigma_k} + \delta_{\nu\sigma_k}) f_k \rangle = \langle (\delta_{\mu\sigma_k} - \delta_{\nu\sigma_k}) f_k \coth \tfrac{1}{2}\beta (E_k^{\mu} + E_k^{\nu}) \rangle \tag{7}$$

$$\begin{aligned} \langle (\delta_{\mu\sigma_k} \delta_{\mu\sigma_1} - \delta_{\nu\sigma_k} \delta_{\nu\sigma_1}) f_{k1} \rangle & \\ = \langle (\delta_{\mu\sigma_k} \delta_{\mu\sigma_1} + \delta_{\nu\sigma_k} \delta_{\nu\sigma_1}) f_{k1} & \tanh \tfrac{1}{2}\beta [E_k^{\mu} + E_1^{\mu} - E_k^{\nu} - E_1^{\nu} \\ & - J_{k1} (\delta_{\mu\sigma_k} + \delta_{\mu\sigma_1} - \delta_{\nu\sigma_k} - \delta_{\nu\sigma_1})] \rangle, \end{aligned} \tag{8}$$

where f_{k1} does not contain sites k and 1. Equation (7) is just the inverse relation of equation (6).

Equation (5) may serve as a starting point for some approximations. The simplest one consists in neglecting correlations and replacing $\delta_{\lambda\sigma_k}$ by its average $\langle \delta_{\lambda\sigma_k} \rangle \equiv x_k^{\lambda}$. We then obtain

$$x_k^{\mu} - x_k^{\nu} = (x_k^{\mu} + x_k^{\nu}) \tanh \tfrac{1}{2}\beta \left[\sum_j J_{kj} (x_j^{\mu} - x_j^{\nu}) + (\zeta_k^{\mu} - \zeta_k^{\nu}) \right],$$

or equivalently,

$$\ln (x_k^{\mu} / x_k^{\nu}) = \beta \left[\sum_j J_{kj} (x_j^{\mu} - x_j^{\nu}) + (\zeta_k^{\mu} - \zeta_k^{\nu}) \right]. \tag{9}$$

This is just the mean-field approximation of the Potts model, which obtains from a minimisation of the mean-field free energy

$$F_{\mathrm{MFA}} = -\sum_{i<j} J_{ij} \sum_{\lambda} x_i^\lambda x_j^\lambda - \sum_{i}\sum_{\lambda} \zeta_i^\lambda x_i^\lambda + \frac{1}{\beta} \sum_{i}\sum_{\lambda} x_i^\lambda \ln x_i^\lambda \tag{10}$$

with the constraint $\Sigma_i \Sigma_\lambda x_i^\lambda = 1$. If $\zeta_k^1 = h$ and $\zeta_k^\lambda \doteq 0$ for $\lambda \neq 1$, then we get equation (9) in the simple familiar form

$$\ln \{[1+(q-1)m]\}/(1-m)] = z\beta J m + \beta h, \tag{11}$$

where we have assumed translational invariance and defined the order parameter m via the relations

$$x_k^1 = [1+(q-1)m]/q \qquad x_k^\lambda = (1-m)/q \qquad (\lambda \neq 1). \tag{12}$$

In deriving equation (11) we have also assumed

$$J_{kj} = \begin{cases} J & \text{for } z \text{ nearest neighbours} \\ 0 & \text{otherwise.} \end{cases} \tag{13}$$

We now use the exponential operator technique, which is based on the identity

$$\tanh A = \mathrm{e}^{A\mathrm{D}} \tanh x|_{x=0} \tag{14}$$

with $\mathrm{D} \equiv \partial/\partial x$. In the absence of the external field, equation (5) becomes

$$\begin{aligned} \langle \delta_{\mu\sigma_k} - \delta_{\nu\sigma_k} \rangle &= \langle (\delta_{\mu\sigma_k} + \delta_{\nu\sigma_k}) \exp[\tfrac{1}{2}\beta D \sum_j J_{kj}(\delta_{\mu\sigma_j} - \delta_{\nu\sigma_j})] \rangle \tanh x|_{x=0} \\ &= < (\delta_{\mu\sigma_k} + \delta_{\nu\sigma_k}) \prod_j \exp[\tfrac{1}{2}\beta D J_{kj}(\delta_{\mu\sigma_j} - \delta_{\nu\sigma_j})] \rangle \tanh x|_{x=0}. \end{aligned} \tag{15}$$

If we note that

$$\exp(\tfrac{1}{2}\beta D J_{kj} \delta_{\mu\sigma_j}) = 1 + \delta_{\mu\sigma_j}[\exp(\tfrac{1}{2}\beta D J_{kj}) - 1],$$

and assume equation (13), we obtain the expression ($k \equiv 0$)

$$\begin{aligned} \langle \delta_{\mu\sigma_0} - \delta_{\nu\sigma_0} \rangle = \langle (\delta_{\mu\sigma_0} + \delta_{\nu\sigma_0}) \prod_{j=1}^{z} [1 - (\delta_{\mu\sigma_j} + \delta_{\nu\sigma_j}) + \delta_{\mu\sigma_j} \exp(\tfrac{1}{2}\beta J D) + \delta_{\nu\sigma_j} \exp(-\tfrac{1}{2}\beta J D/2)] \\ > \tanh x|_{x=0}. \end{aligned} \tag{16}$$

Although equation (16) is exact, it has only a finite number of terms and contains no correlations of order higher than $z+1$. If we assume translational invariance and neglect correlations, through the use of equation (12) we can approximate equation (16) and obtain the expression for the order parameter as a function of temperature

$$m = \sum_{n=1}^{z+1} C_n(z, q; \beta) m^n, \tag{17}$$

where the coefficients $C_n(z, q; \beta)$ can be obtained through the explicit evaluation of equation (16). Since this technique, when applied to the Ising model, gives more precise results than the usual mean-field approximation (Honmura and Kaneyoshi 1978, 1979, Taggart and Fittipaldi 1982), equation (17) is expected to be an improvement over the mean-field result given by equation (11).

In summary, we have obtained correlation identities for the Potts model, and have shown how the mean-field approximation can be derived from them. These arguments, which are physically clear and independent of the representation, can serve as a starting point for some improved approximations.

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