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The Kikuchi approximation: a reformulation and application to the percolation problem

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Abstract. Kikuchi's approximation for describing phase transitions in magnetic systems is reformulated so as to reduce the number of self-consistent equations to be solved and emphasise the analogy with mean field theory. The method is used to calculate the threshold for bond percolation by exploiting the analogy with the Potts model.

1. Introduction

The simplest closed-form approximation for magnetic systems is mean field theory, in which each spin is assumed to lie in an effective field due to its neighbours. A subsequent improvement, due to Bethe and Peierls (see e.g. Huang 1963), is to consider a pair of sites, rather than a single site, as the basic cluster, treat the interaction between the pair exactly and represent the interaction with other spins by an effective field. As originally presented, the method treated a central spin and *all* its neighbours, but identical results are obtained with just a single pair (Kikuchi 1951). Kikuchi also developed a systematic way of extending this approach to larger basic clusters. Choosing, for example, a square as the basic unit one obtains very accurate results for the transition temperature, T_c , of the spin- $\frac{1}{2}$ Ising model on square and simple cubic lattices. For the face-centred cubic lattice, the choice of a tetrahedron as the basic cluster gives excellent results, even predicting the first-order transition in the antiferromagnetic case (Kikuchi and Sato 1974, Phani *et al* 1980). A good review of these methods is Burley (1972).

Kikuchi's method involves enumerating all possible states of the basic unit which have different energies and the deriving self-consistent equations for the corresponding probabilities. This is an extremely laborious process for anything more complicated than a spin- $\frac{1}{2}$ Ising model; as a result, his approach has been used exclusively for this case, as far as we are aware. We report here a reformulation of Kikuchi's approach which avoids these combinatorial preliminaries and which can therefore be more readily applied to other problems. As an illustration we calculate the percolation threshold for the bond percolation problem (Essam 1972) by exploiting the analogy with the Potts model (Fortuin and Kasteleyn 1972, Baxter 1973).

We find it convenient to write the probability of a particular cluster configuration in terms of an effective cluster Hamiltonian. Self-consistent equations for the interactions

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of this Hamiltonian are derived for an arbitrary model of classical spins, thus avoiding the initial problem of delineating all configurations discussed above. The calculations are carried out with a square as the basic cluster for simple cubic lattices of any dimensionality, but there is no difficulty in applying the method to other cases.

This approach also has the advantage of reducing the number of self-consistent equations to be solved. For example, with a square cluster, the effective cluster Hamiltonian does not include next-nearest-neighbour (NNN), three-spin or four-spin couplings if the original Hamiltonian did not have them. Consequently, for the spin- $\frac{1}{2}$ Ising model with nearest-neighbour (NN) forces, three of Kikuchi's five equations are seen to reduce to trivial identities. The only unknowns are firstly a 'molecular field' on each site of the cluster, and secondly an interaction between NN pairs of the cluster, which is different in general from the NN coupling of the original Hamiltonian. If three-spin, four-spin and NNN couplings are present, they have the same value in the effective cluster Hamiltonian as in the original Hamiltonian, so they do not introduce extra self-consistency equations. We therefore feel that our reformulation is a useful simplification and gives some insight into Kikuchi's method by highlighting its similarity to the familiar 'molecular field' approach.

It is also instructive to discuss other closed-form approximations in the framework of an effective cluster Hamiltonian. In the Bethe–Peierls method, which treats a pair, the interaction between the two spins is the *same* as in the original Hamiltonian. This is intuitively reasonable, since contributions to the NN correlation function in addition to the 'direct' contribution from the NN bond involve spins in larger clusters, which are not included at this level of approximation. The Guggenheim–McGlashan (1951) approach lies between those of Bethe–Peierls and Kikuchi, in that it takes a basic cluster of more than two spins but assumes, unlike Kikuchi, that the NN cluster interaction is the same as in the original Hamiltonian. For a cluster of more than two spins the best cluster Hamiltonian, in a variational sense, is Kikuchi's with its modified NN coupling. It is not therefore surprising that Kikuchi's theory leads to the most accurate estimates for T_c .

In § 2 we derive an expression for the free energy of an arbitrary classical spin model on a d -dimensional simple cubic lattice with a square as the basic unit. This is then minimised in § 3 to give self-consistent equations for parameters of the cluster Hamiltonian, while § 4 applies the method to calculate the bond percolation threshold. Our results are summarised in § 5.

2. The free energy

Assume that there is a classical spin at each lattice site which can be in one of M states, specified by a Latin suffix. One can construct a complete set of M operators O^α whose value in state i is given by O_i^α and which satisfy the orthogonality condition

$$\sum_i O_i^\alpha O_i^\beta = A_\alpha \delta_{\alpha\beta} \quad (1)$$

where A_α is an unimportant normalisation constant. One of the operators, with $\alpha = I$, is the identity for which $O_i^I = 1$ so all the other operators are traceless, i.e.

$$\sum_i O_i^\alpha = 0 \quad (\alpha \neq I). \quad (2)$$

For example the spin-1 Ising model would involve the three operators 1, S and $3S^2-2$.

Consider the Kikuchi approximation with a square cluster for a simple cubic lattice of arbitrary dimensionality, d , and coordination number $z (= 2d)$. Denote by w_{ijkl} the probability that the sites around the square are in states i, j, k and l . We shall neglect here the possibility of complicated ordered structures, although they can be treated in our approach, so each site and each bond on the square is equivalent. Therefore w_{ijkl} is invariant under cyclic permutation of the indices. Similarly denote by y_{ij} the probability that an NN pair are in states i and j and by P_i the probability that a single site is in state i , where clearly

$$y_{ij} = \sum_{k,l} w_{ijkl} = \sum_{j,k} w_{ijkl} = \sum_{i,j} w_{ijkl} = \sum_{l,i} w_{ijkl}, \tag{3a}$$

$$P_i = \sum_j y_{ij} = \sum_j y_{ji}. \tag{3b}$$

For the moment neglect possible NNN, three-spin and four-spin interactions, which will be added later. The average energy per site can therefore be written as

$$\frac{U}{N} = \sum_i u_i P_i + \frac{z}{2} \sum_{i,j} u_{ij} y_{ij} \tag{4}$$

where u_i and u_{ij} are single-site and NN pair energies. These are expressed more conventionally in terms of the operators O_i^α , ‘fields’ h^α and ‘interactions’ $J^{\alpha\beta}$ as

$$u_i = \sum_\alpha h^\alpha O_i^\alpha, \tag{5a}$$

$$u_{ij} = \sum_{\alpha\beta} J^{\alpha\beta} O_i^\alpha(l) O_j^\beta(l'), \tag{5b}$$

where l and l' denote a pair of NN sites and the prime on the summation indicates that the identity operator, $\alpha = I$, is not included. Interactions which cannot be fitted into the basic cluster have to be decoupled, just as in mean field theory, e.g. a long-range two-spin interaction \tilde{u}_{ij} would, on averaging, become $\tilde{u}_{ij} P_i P_j$. We shall not, however, include such interactions here.

The expression for the entropy is a little more complicated. In mean field theory it is given by

$$\frac{-S_{MF}}{Nk_B} = \sum_i P_i \ln P_i \tag{6}$$

where N is the number of lattice points and k_B is Boltzmann’s constant. Within the pair (Bethe–Peierls) approximation there is a contribution $\sum_{i,j} y_{ij} \ln y_{ij}$ for each of the $Nz/2$ pairs, but there is a correction to this because different bonds share the same site. In fact, each site is counted z times in the sum over bonds, so it is necessary to subtract off $(z - 1)$ times the single-site contribution

$$\frac{-S_{BP}}{Nk_B} = \frac{z}{2} \sum_{i,j} y_{ij} \ln y_{ij} - (z - 1) \sum_i P_i \ln P_i. \tag{7}$$

It is trivial to check that equation (7) leads to the correct expression when there is no correlation between sites. One proceeds in a similar way to evaluate the entropy with a square cluster. There are $z(z - 2)/8$ squares per site and each bond is counted $(z - 2)$ times in the sum over squares, so one must subtract $(z - 3)$ times the pair contribution, equation (7). This has still counted each site $(-z^2 + 4z)/2$ times, so in addition one has

to add $(z^2 - 4z + 2)/2$ times the right-hand side of equation (6). Putting all this together we have

$$\frac{-S}{Nk_B} = \frac{z(z-2)}{8} \sum_{i,j,k,l} w_{ijkl} \ln w_{ijkl} - \frac{z(z-3)}{2} \sum_{ij} y_{ij} \ln y_{ij} + \frac{(z^2 - 4z + 2)}{2} \sum_i P_i \ln P_i. \quad (8)$$

Further comments on the derivation of the entropy can be found in Kikuchi (1951) and Hijmans and de Boer (1955). The free energy per site is obtained by combining equations (4) and (8) in the usual way, and represents the main result of this section.

3. Self-consistency equations

The free energy obtained from equations (4) and (8) is minimised with respect to the w_{ijkl} , bearing in mind that the pair and single-site probabilities are related to the w 's by equation (3) and that here is an overall constraint

$$\sum_{i,j,k,l} w_{ijkl} = 1 \quad (9)$$

which is readily handled by a Lagrange multiplier. As shown in the Appendix, this leads to the condition

$$\begin{aligned} \frac{1}{8}z(u_{ij} + u_{jk} + u_{kl} + u_{li}) + \frac{1}{4}(u_i + u_j + u_k + u_l) \\ + k_B T \left[\frac{1}{8}z(z-2) \ln w_{ijkl} - \frac{1}{8}z(z-3)(\ln y_{ij} + \ln y_{jk} + \ln y_{kl} + \ln y_{li}) \right. \\ \left. + \frac{1}{8}(z^2 - 4z + 2)(\ln P_i + \ln P_j + \ln P_k + \ln P_l) \right] - \lambda = 0 \end{aligned} \quad (10)$$

where λ is the Lagrange multiplier. Since every term in (10) apart from $\ln w_{ijkl}$ involves only one or two sites, it follows that $\ln w_{ijkl}$ can also be expressed as a sum of one- and two-site terms. It is therefore useful to define a cluster Hamiltonian, H_4 , such that

$$w = (1/Z_4) \exp(-\beta H_4) \quad (11)$$

where Z_4 is the partition function of the cluster and $\beta = (k_B T)^{-1}$. For clarity Latin subscripts will be omitted in equations like (11). H_4 is then expressed as

$$H_4 = u_{ij}^4 + u_{jk}^4 + u_{kl}^4 + u_{li}^4 + u_i^4 + u_j^4 + u_k^4 + u_l^4 \quad (12)$$

where the index '4' denotes an interaction for the square cluster and, analogously to equation (5), one can write

$$u_i^4 = \sum_{\alpha} h_4^{\alpha} O_i^{\alpha}, \quad (13a)$$

$$u_{ij}^4 = \sum_{\alpha, \beta} J_4^{\alpha\beta} O_i^{\alpha}(l) O_j^{\beta}(l'). \quad (13b)$$

Similarly one may define

$$y = (1/Z_2) \exp(-\beta H_2), \quad (14a)$$

$$H_2 = u_{ij}^2 + u_i^2 + u_j^2, \quad (14b)$$

$$P = (1/Z_1) \exp(-\beta H_1), \quad (14c)$$

$$H_1 = u_i^1, \quad (14d)$$

and u_{ij}^2 , u_i^2 and u_i^1 are related to interaction parameters $J_2^{\alpha\beta}$, h_2^{α} and h_1^{α} by expressions

analogous to equation (13). H_2 can be obtained from H_4 by performing a partial trace over a nearest-neighbour pair, i.e.

$$\frac{e^{-\beta H_2}}{Z_2} = \text{Tr}_{\text{sites } 3,4} \frac{e^{-\beta H_4}}{Z_4} \quad (15)$$

and H_1 is obtained from H_4 in a similar way by tracing over three sites.

Equation (10) now becomes

$$\begin{aligned} & \frac{1}{8}z [u_{ij} - (z-2)u_{ij}^4 + (z-3)u_{ij}^2 + 3 \text{ perms } (ij \rightarrow jk \rightarrow kl \rightarrow li)] \\ & + \frac{1}{4}[u_i - \frac{1}{2}z(z-2)u_i^4 + z(z-3)u_i^2 - \frac{1}{2}(z^2-4z+2)u_i^1 \\ & + 3 \text{ perms } (i \rightarrow j \rightarrow k \rightarrow l)] + k_B T [-\frac{1}{8}z(z-2) \ln Z_4 \\ & + \frac{1}{2}z(z-3) \ln Z_2 - \frac{1}{2}(z^2-4z+2) \ln Z_1] - \lambda = 0. \end{aligned} \quad (16)$$

Next sum equation (16) over all i, j, k, l . Since all operators are traceless, most terms vanish and one is left with

$$-\beta\lambda = \frac{1}{8}z(z-2) \ln Z_4 - \frac{1}{2}z(z-3) \ln Z_2 + \frac{1}{2}(z^2-4z+2) \ln Z_1. \quad (17)$$

Summing equation (16) over all k, l leads to

$$u_{ij} - (z-2)u_{ij}^4 + (z-3)u_{ij}^2 = 0 \quad (18)$$

for all pairs (i, j) , while summing over j, k and l gives

$$u_i - \frac{1}{2}z(z-2)u_i^4 + z(z-3)u_i^2 - \frac{1}{2}(z^2-4z+2)u_i^1 = 0 \quad (19)$$

for all i . Equations (5), (8) and (16)–(19) imply that λ is the free energy per site. Expressing u_{ij} in terms of the ‘fields’ h^α through equation (5), and similarly for u_i^4, u_i^2 and u_i^1 , one has

$$\sum_{\beta} [h^\beta - \frac{1}{2}z(z-2)h_4^\beta + z(z-3)h_2^\beta - \frac{1}{2}(z^2-4z+2)h_1^\beta] O_i^\beta = 0. \quad (20)$$

Multiplying (20) by O_i^α , summing on i and using equation (1) gives

$$h^\alpha = \frac{1}{2}z(z-2)h_4^\alpha - z(z-3)h_2^\alpha + \frac{1}{2}(z^2-4z+2)h_1^\alpha \quad (21)$$

for all α . Similarly equation (19) leads to

$$J^{\alpha\beta} = (z-2)J_4^{\alpha\beta} - (z-3)J_2^{\alpha\beta}. \quad (22)$$

Equations (21) and (22) are the self-consistent equations for the parameters in the cluster Hamiltonian and are the main results of this section. They look straightforward because each equation only refers to a single type of interaction. (This is a consequence of choosing *orthogonal* operators O^α .) The variables are not independent, however, because carrying out the partial traces to obtain the pair and single-site couplings from the interactions on the square, one finds that a particular interaction of a smaller cluster depends on all the interactions of the larger one. We emphasise that future applications of the method can *start* with equations (21) and (22), thus avoiding the combinatorial arguments which led up to them.

Carrying out the same manipulations for a cluster of two sites, with the entropy given by equation (7), one finds

$$J^{\alpha\beta} = J_2^{\alpha\beta}, \quad h^\alpha = zh_2^\alpha - (z-1)h_1^\alpha,$$

so the pair interactions are unchanged in the Bethe–Peierls approximation, as mentioned in the Introduction. The expression for the entropy in the Guggenheim–McGlashan (1951) approximation does not involve the pair probabilities y_{ij} , and again the two-site interactions in the cluster are the same as those in the original Hamiltonian. This does not represent the best cluster Hamiltonian if the cluster is larger than a pair.

It is also straightforward to add NNN two-spin terms as well as three-spin and four-spin interactions to the energy and carry out the above manipulations. One finds that their values in the cluster Hamiltonian are the same as in the original Hamiltonian, essentially because corrections to the $\sum w \ln w$ term in the entropy arise from clusters (NN pair and single-site) into which these interactions do not fit.

For a spin- $\frac{1}{2}$ Ising model there is only a single variable, S , so only a single field term hS and a single NN interaction $JS(l)S(l')$ can be constructed, and consequently there are just two self-consistency equations to be solved. In Kikuchi's work there are five, but we now see that, representing the probabilities in terms of the cluster Hamiltonian, three of them become trivial and correspond simply to the vanishing of the NNN two-spin, the three-spin and the four-spin cluster interactions.

4. Application to the bond percolation problem

It has been shown (Fortuin and Kasteleyn 1972, Baxter 1973) that the bond percolation problem corresponds to the limit of the s -state Potts model for $s \rightarrow 1$. In this model the spin on site l can be in one of s states specified by an integer n_l ($n_l = 1, 2, \dots, s$). The interaction between an NN pair depends on whether or not the spins are in the same state, so the Hamiltonian is given by

$$H = -J \sum_{\langle l, l' \rangle} \left(\delta_{n_l n_{l'}} - \frac{1}{s} \right) \quad (23)$$

where the sum includes each NN pair once. In the ordered phase it is necessary to include symmetry breaking terms which single out a particular state, e.g. $n_l = 1$. This means that a single-site term of the form $h^4(\delta_{n_l 1} - 1/s)$ must be included in the cluster Hamiltonian, but one can also have a two-spin term $L^4(\delta_{n_l 1} - 1/s)(\delta_{n_{l'} 1} - 1/s)$ which is allowed by the reduced symmetry. The cluster Hamiltonian for the square is therefore given by

$$H^4 = -J^4 \sum_{\langle l, l' \rangle} \left(\delta_{n_l n_{l'}} - \frac{1}{s} \right) - L^4 \sum_{\langle l, l' \rangle} \left(\delta_{n_l 1} - \frac{1}{s} \right) \left(\delta_{n_{l'} 1} - \frac{1}{s} \right) - h^4 \sum_l \left(\delta_{n_l 1} - \frac{1}{s} \right). \quad (24)$$

In the bond percolation problem one must take the limit $s \rightarrow 1$ and the probability, p , of a bond being occupied is related to J by

$$p = 1 - e^{-\beta J} \quad (25)$$

(Fortuin and Kasteleyn 1972).

Above the critical temperature, which corresponds to p less than the percolation threshold p_c , the symmetry is not broken so one can set $L^4 = h^4 = 0$. One can relate J^2 to J^4 by

$$J^2 = J^4 + \delta J \quad (26)$$

where the factor of J^4 is due to the direct coupling between an NN pair of the square and

δJ is the contribution due to tracing out the other two sites. Equation (22) consequently becomes

$$J = J^4 - (z - 3) \delta J \tag{27}$$

and one can show that δJ is related to J_4 by the equation

$$\frac{e^{\beta \delta J} - 1}{e^{\beta \delta J} + s - 1} = \left(\frac{e^{\beta J_4} - 1}{e^{\beta J_4} + s - 1} \right)^3 \tag{28}$$

This is easily obtained by noting that

$$\exp(K \delta_{n_i n_{i'}}) = \frac{1}{s} (e^K + s - 1) + (e^K - 1) \left(\delta_{n_i n_{i'}} - \frac{1}{s} \right)$$

as well as

$$\sum_{n_{i'}} \left(\delta_{n_i n_{i'}} - \frac{1}{s} \right) = 0,$$

$$\sum_{n_{i'}} \left(\delta_{n_i n_{i'}} - \frac{1}{s} \right) \left(\delta_{n_{i'} n_{i''}} - \frac{1}{s} \right) = \delta_{n_i n_{i''}} - \frac{1}{s},$$

so that

$$\sum_{n_{i'} n_{i''}} \exp[K(\delta_{n_i n_{i'}} + \delta_{n_{i'} n_{i''}} + \delta_{n_i n_{i''}})] = \frac{1}{s} (e^K + s - 1)^3 + (e^K - 1)^3 \left(\delta_{n_i n_{i''}} - \frac{1}{s} \right).$$

For $s \rightarrow 1$, equation (28) becomes

$$\delta p = p_4^3 \tag{29}$$

where p_4 is related to J_4 etc as p is related to J in equation (25). From equations (25), (27) and (29) one readily finds that

$$1 - p = (1 - p_4) / (1 - p_4^3)^{z-3} \tag{30}$$

In this paper we shall restrict ourselves to calculating p_c , which occurs when the symmetry breaking terms L^4 and h^4 tend to zero. It is therefore only necessary to investigate equations (21) and (22) to first order in L^4 and h^4 . Since these terms break the symmetry of the high-temperature phase, they can only induce a second-order change in p_4 , which can be neglected. Consequently equation (30) may be used in estimating p_c , as well as for determining the behaviour for $p < p_c$.

It is convenient to write, analogously to equation (26),

$$L^2 = L^4 + \delta L, \quad h^2 = h^4 + \delta h_2, \quad h^1 = h^2 + \delta h_1, \tag{31}$$

so equations (21) and (22) are equivalent to

$$0 = L^4 - (z - 3) \delta L, \tag{32a}$$

$$0 = h^4 - z(z - 3) \delta h_2 + \frac{1}{2}(z^2 - 4z + 2) \delta h_1. \tag{32b}$$

After some algebra we find that

$$\delta L = \frac{2p_4^3(1 - p_4^2)h_4 + p_4^2(3 - 3p_4 - p_4^2 + 4p_4^3)L_4}{1 + p_4 + p_4^2}, \tag{33}$$

$$\delta h_2 = \frac{p_4(1 + 2p_4 + 2p_4^2 - 2p_4^4)h_4 - p_4(1 + 2p_4 + 3p_4^2 + p_4^3 - 4p_4^4)L_4}{1 + p_4 + p_4^2}, \tag{34}$$

$$\delta h_1 = p_4(2 + 2p_4 + 2p_4^2 - 3p_4^3)h_4 - 2p_4(1 + 2p_4 + 3p_4^2)3p_4^3 L_4. \quad (35)$$

The percolation threshold occurs when the determinant of the coefficients of L^4 and h^4 in equations (32*a,b*) vanishes. This gives p_4 at criticality and p_c is then obtained directly from equation (30). Results for $d = 2$ to 6 are summarised in table 1. They represent a substantial improvement over Bethe–Peierls, although it is perhaps a little disappointing that the two-dimensional value does not approach closer to the exact value of $\frac{1}{2}$.

Table 1. Results for the bond percolation problem for 'simple cubic' lattices of dimensionality d . In the Bethe–Peierls approximation $p_c = (z - 1)^{-1}$ (where $z = 2d$). The results for the Kikuchi approximation are with a square as the basic cluster and are obtained from equations (30) and (32)–(35) of the text. In the last column the references are: ¹ exact result from Sykes and Essam (1964b); ² estimate from series expansions from Sykes and Essam (1964a).

d	p_c (Bethe–Peierls)	p_c (Kikuchi)	p_c (other theories)
2 (square)	0.3333	0.4355	0.5 ¹
3	0.2	0.2358	0.247 ²
4	0.1429	0.1528	—
5	0.1111	0.1154	—
6	0.0909	0.0931	—

5. Conclusions

We have shown how Kikuchi's method can be reformulated in a way which reduces the number of equations to be solved and which brings out more explicitly the analogy with mean field theory. For a square as the basic cluster our principal results are equations (21) and (22), but there is no difficulty in applying the ideas to other clusters. This is straightforward once the coefficients in the entropy expression have been worked out (i.e. the coefficients of $\sum w \ln w$, $\sum y \ln y$ etc). We have illustrated the method by calculating the bond percolation probability for simple cubic lattices of dimensionality between two and six.

Appendix 1

Minimising the free energy given by equations (4) and (8) is complicated slightly by the fact that w_{ijkl} is invariant under cyclic permutation of its indices, and this has already been used in obtaining these equations. The minimisation is more straightforward if we assume initially that the sites and bonds are inequivalent so each w_{ijkl} is distinct. The equivalence of the sites and of the bonds is then imposed *after* minimisation.

Denoting the four bonds by a, b, c, d and the sites by A, B, C and D, where bond a lies between sites A and B (see figure 1), the relationship between the y 's, P 's and w 's is

$$\begin{aligned} y_{ij}^a &= \sum_{k,l} w_{ijkl} & P_i^A &= \sum_{j,k,l} w_{ijkl} \\ y_{jk}^b &= \sum_{i,l} w_{ijkl} & P_j^B &= \sum_{i,k,l} w_{ijkl} \end{aligned}$$

$$\begin{aligned}
 y_{kl}^c &= \sum_{i,j} w_{ijkl}, & P_k^C &= \sum_{i,l} w_{ijkl}, \\
 y_{li}^d &= \sum_{j,k} w_{ijkl}, & P_l^D &= \sum_{i,j,k} w_{ijkl}.
 \end{aligned}
 \tag{A1}$$

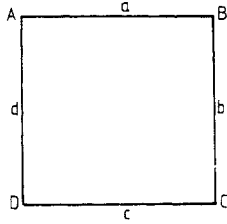


Figure 1. Convention for labelling the bonds and sites on a square. If the spins on sites A, B, C and D are in states i, j, k and l respectively the probability is w_{ijkl} . For the pair probabilities y_{ij}^a is the probability that the spin on site A is in state i , that on site B is in state j , and similarly by cyclic permutation for bonds b, c and d .

In this more general case the free energy is given by

$$\begin{aligned}
 \frac{F}{N} &= \sum \left\{ \frac{1}{4}(u_i P_i^A + u_j P_j^B + u_k P_k^C + u_l P_l^D) + \frac{1}{8}z(u_{ij}y_{ij}^a + u_{ik}y_{jk}^b + u_{kl}y_{kl}^c + u_{li}y_{li}^d) \right. \\
 &\quad + k_B T \left[\frac{1}{8}z(z-2)w_{ijkl} \ln w_{ijkl} - \frac{1}{8}z(z-3) \right. \\
 &\quad \times (y_{ij}^a \ln y_{ij}^a + y_{jk}^b \ln y_{jk}^b + y_{kl}^c \ln y_{kl}^c + y_{li}^d \ln y_{li}^d) + \frac{1}{8}(z^2 - 4z + 2) \\
 &\quad \left. \left. \times (P_i^A \ln P_i^A + P_j^B \ln P_j^B + P_k^C \ln P_k^C + P_l^D \ln P_l^D) \right] \right\}.
 \end{aligned}
 \tag{A2}$$

One can now minimise with respect to the w_{ijkl} , bearing in mind (i) that the y 's and P 's are related to the w 's through equation (A1), and (ii) that there is an overall constraint $\sum_{i,j,k,l} w_{ijkl} = 1$. The second point is easily handled with a Lagrange multiplier, and the first is also straightforward because, now that the equivalence between sites and bonds has been broken, each w_{ijkl} appears at most once in the expression for the y 's and P 's. It is then trivial to obtain equation (10) of the text, where λ is the Lagrange multiplier (apart from an unimportant additive constant of $k_B T(z-2)(z-4)/8$).

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