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A variational approximation for cubic lattice models in statistical mechanics

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Abstract. A variational approximation applicable to three-dimensional isotropic cubic lattice models is formulated. When applied to the simple cubic, face centred cubic and body centred cubic Ising models, the approximation correctly gives the first 14, 19, and 23 terms respectively of the known low-temperature free energy expansion.

1. Introduction

The thermodynamics of many two-dimensional lattice models have been numerically approximated using a variational approximation involving corner transfer matrices (Baxter 1968, 1978, Kelland 1976, Baxter and Tsang 1980). Furthermore the same technique has been applied to obtain series expansions longer than those previously obtained by graphical methods (Baxter and Enting 1979, Baxter *et al* 1980).

It has been previously noted (Baxter 1982) that the variational equations can be extended to three dimensions. Unfortunately, in general, the resulting equations will involve 'corner tensors' with three indices. There being no analogue of matrix diagonalisation for these tensors, the situation is far more complicated than in two dimensions.

However, there is an exception to the general case, which will be investigated in this paper. In two dimensions the lowest-order variational approximation reduces the corner transfer matrices to scalars, and thus matrix diagonalisation is irrelevant. (For the Ising model, the approximation becomes that of Kramers and Wannier (1941).) A similar situation will be shown to occur in three dimensions. The equations defining the lowest-order variational approximation of the type given by Baxter (1978) only involve scalar quantities, and are thus amenable to both numerical and series solution on the computer.

2. Restrictions on the models

Consider a three-dimensional simple cubic lattice of N columns, M rows and P planes. To each site i of the lattice, associate a spin σ_i with values $+1$ or -1 ($+$ or $-$) and impose periodic boundary conditions. To each cube of the lattice associate a Boltzmann weight $W(a|efg|bcd|h)$, the spins $a, b, \ldots, h$ arranged as in figure 1.

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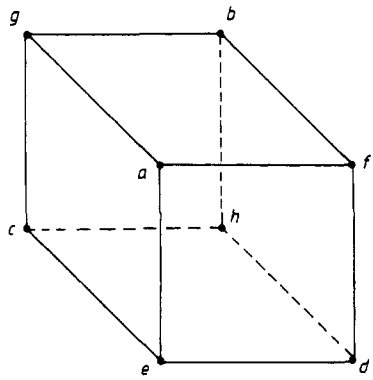

Figure 1. Arrangement of the spins $a, \ldots, h$ on the corner sites of a cube.

We require W to have the reflection symmetries that it be unchanged by interchanging the order of the rows, columns and planes so that

$$W(a|efg|bcd|h) = W(g|cba|feh|d) \tag{2.1a}$$

$$= W(f|dab|ghe|c) \tag{2.1b}$$

$$= W(e|adc|hgf|b). \tag{2.1c}$$

Furthermore we will restrict our attention to isotropic models, so that W is unchanged by rotation through 90°, and thus

$$W(a|efg|bcd|h) = W(e|dac|ghf|b) \tag{2.2a}$$

$$= W(g|abc|hef|d). \tag{2.2b}$$

As a final restriction we require the ground state to have the reflection and rotation symmetries given above, and in addition, to be translation invariant.

The partition function is

$$Z = \sum \prod W(\sigma_i|\sigma_m\sigma_n\sigma_p|\sigma_j\sigma_k\sigma_l|\sigma_q) \tag{2.3}$$

where the product is over all cubes of the lattice, and the sum over all values of the spins. Let $\sigma = \{\sigma_1, \sigma_2, \ldots, \sigma_{NM}\}$ denote the spins in one plane and $\sigma' = \{\sigma'_1, \sigma'_2, \ldots, \sigma'_{NM}\}$ the spins on the plane above. The contribution to the partition function between these two planes is

$$V_{\sigma,\sigma'} = \prod W(\sigma'_i|\sigma_i\sigma'_j\sigma'_k|\sigma'_l\sigma_k\sigma_j|\sigma_l) \tag{2.4}$$

where the product is over all cubes formed between the two planes. Let V denote the $2^{NM} \times 2^{NM}$ plane-to-plane transfer matrix with elements $V_{\sigma,\sigma'}$. Then as usual (Baxter 1982) we have

$$Z = \mathrm{Tr}\ V^P \sim \lambda^P \tag{2.5}$$

where λ is the maximal eigenvalue of V. In statistical mechanics we want to calculate the partition function per site

$$\kappa = Z^{1/NMP} = \lambda^{1/NM}. \tag{2.6}$$

The plane reversal symmetry (2.1c) implies that V is symmetric, so λ can be determined

from the variational principle

$$\lambda = \psi^{\mathrm{T}} V \psi / \psi^{\mathrm{T}} \psi \tag{2.7}$$

where ψ is the 2^{NM}-dimensional vector which maximises the RHS of (2.7), and ψ^{T} is its transpose.

3. The variational approximation

As a variational approximation to λ, we can choose for ψ any trial vector, which will at least reproduce the ground state of the system at zero temperature. By the assumption of the ground state being translation invariant, a choice of ψ which has this feature (this choice is analogous to the lowest-order trial vector given by Baxter (1978)) is

$$\psi(\sigma_1, \sigma_2, \ldots, \sigma_{NM}) = \prod F(\sigma_i, \sigma_j, \sigma_k, \sigma_l) \tag{3.1}$$

where the product is over all faces i, j, k, l (with the sites ordered as in figure 2) of a single plane. Then

$$\psi^{\mathrm{T}}\psi = \sum_{\sigma_1, \sigma_2, \ldots, \sigma_{NM} = \pm 1} \prod_{\text{faces}} F^2(\sigma_i, \sigma_j, \sigma_k, \sigma_l). \tag{3.2}$$

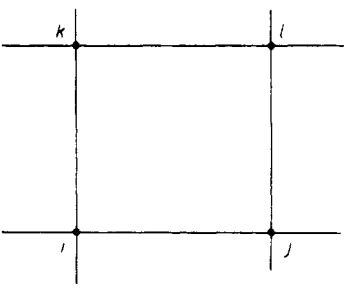

Figure 2. Arrangement of the sites i, j, k and l.

But this is a two-dimensional partition function with face weight $F^2(\sigma_i, \sigma_j, \sigma_k, \sigma_l)$. Choosing F to be invariant under row and column reversal and rotation through 90°, from Baxter (1978) we can write down the variational approximation

$$\psi^{\mathrm{T}}\psi = (s_1 s_3 / s_2^2)^{NM}. \tag{3.3}$$

The quantities s_1, s_2 and s_3 are defined by the equations

$$s_3 = \sum_{a, a', b, b'} F^2(a, b, a', b') y(a, a') y(a, b) y(b', a') y(b, b') x(a) x(a') x(b) x(b'), \tag{3.4}$$

$$s_2 = \sum_{a, b} x^2(a) x^2(b) y^2(a, b), \tag{3.5}$$

$$s_1 = \sum_{a} x^4(a), \tag{3.6}$$

where each independent argument of x and y can take the spin values + or −. The function y satisfies the symmetry requirement $y(a, b) = y(b, a)$, and both x and y are

chosen so that (3.3) is stationary with respect to variations in these functions. Thus

$$\sum_b y^2(a, b)x^2(b) = (s_2/s_1)x^2(a), \tag{3.7}$$

$$\sum_{b, b'} F^2(a, b, a', b')y(a, b)y(b', a')y(b, b')x(b)x(b') = (s_3/s_2)x(a)x(a')y(a, a'). \tag{3.8}$$

Next we have

$$\psi^{\mathrm{T}} V\psi = \sum \prod G(\mu_i, \mu_j, \mu_k, \mu_l) \tag{3.9}$$

where $\mu_i = (\sigma_i, \sigma_i')$ and

$$G(\mu_i, \mu_j, \mu_k, \mu_l) = W(\sigma_i'|\sigma_i\sigma_j'\sigma_k'|\sigma_l'\sigma_k\sigma_j|\sigma_l)F(\sigma_i, \sigma_j, \sigma_k, \sigma_l)F(\sigma_i', \sigma_j', \sigma_k', \sigma_l'). \tag{3.10}$$

The sum in (3.9) is over all allowed spin pair values and the product is over all faces i, j, k, l of a single plane. This is again a two-dimensional partition function, but instead of the spin variable taking on only the values + and −, the allowed values are now the spin pair values (+, +), (+, −), (−, +) and (−, −). Analogous to (3.3) we have the variational approximation

$$\psi^{\mathrm{T}} V\psi = (r_1 r_3/r_2^2)^{NM}. \tag{3.11}$$

The r_j are formally the same as the s_j if we replace F, x, y by $G, \bar{x}, \bar{y}$ respectively, and allow each independent argument of the latter functions to assume the spin pair values given above. Let the analogues of (3.4)–(3.8) thus specified be labelled (3.4)′–(3.8)′ respectively.

We can now give a variational approximation to κ as defined by (2.6). Substituting (3.3) and (3.11) in (2.7) we have

$$\kappa = (r_1 r_3/r_2^2)/(s_1 s_3/s_2^2). \tag{3.12}$$

It remains to maximise (3.12) with respect to F. This gives

$$\begin{aligned}\sum_{\sigma_1, \ldots, \sigma_4} & W(\sigma_1'|\sigma_1\sigma_2'\sigma_3'|\sigma_4'\sigma_3\sigma_2|\sigma_4)F(\sigma_1', \sigma_2', \sigma_3', \sigma_4')\bar{y}(\mu_1, \mu_3)\bar{y}(\mu_1, \mu_2) \\ & \times \bar{y}(\mu_4, \mu_3)\bar{y}(\mu_2, \mu_4)\bar{x}(\mu_1)\bar{x}(\mu_2)\bar{x}(\mu_3)\bar{x}(\mu_4) \\ = {} & (r_3/s_3)F(\sigma_1, \sigma_2, \sigma_3, \sigma_4)y(\sigma_1, \sigma_3)y(\sigma_1, \sigma_2)y(\sigma_4, \sigma_3)y(\sigma_2, \sigma_4) \\ & \times x(\sigma_1)x(\sigma_2)x(\sigma_3)x(\sigma_4).\end{aligned} \tag{3.13}$$

The five equations (3.7), (3.8), (3.7)′, (3.8)′ and (3.13) define a variational approximation for κ. These equations reduce to three if $\bar{x}$, $\bar{y}$ are given by

$$\bar{x}^2(\mu_i) = x(\sigma_i)x(\sigma_i')y(\sigma_i, \sigma_i'), \tag{3.14}$$

$$\bar{y}^2(\mu_i, \mu_j) = y(\sigma_i, \sigma_j)y(\sigma_i', \sigma_j')F^2(\sigma_i, \sigma_j, \sigma_i', \sigma_j'). \tag{3.15}$$

Then $r_1 = s_2$, $r_2 = s_3$, equation (3.7)′ reduces to (3.8), and (3.8)′ reduces to (3.13). Since the equations will now involve square roots of the functions x and y, we define

$$x(\sigma) = A^2(\sigma), \tag{3.16}$$

$$y(\sigma, \sigma') = B^2(\sigma, \sigma'). \tag{3.17}$$

3.1. Final expression for κ and the variational equations

If we denote $r_3 = s_4$, we now have as a three-dimensional variational approximation

$$\kappa = (s_4 s_2^3)/(s_3^3 s_1) \tag{3.18}$$

where, after substituting (3.14)–(3.17) in (3.4)–(3.6) and (3.4)′,

$$s_4 = \sum \left(\prod_{\mathrm{f}} F\right)\left(\prod_{\mathrm{e}} B\right)\left(\prod_{\mathrm{c}} A\right) W, \tag{3.19}$$

$$s_3 = \sum_{a, a', b, b'} F^2(a, b, a', b') B^2(a, a') B^2(a, b) B^2(b', a') B^2(b, b') \times A^2(a) A^2(a') A^2(b) A^2(b'), \tag{3.20}$$

$$s_2 = \sum_{a, b} A^4(a) A^4(b) B^4(a, b), \tag{3.21}$$

$$s_1 = \sum_{a} A^8(a). \tag{3.22}$$

In (3.19) the arguments of F, B, A and W have been omitted. The products f, e and c are over the 8 faces, 12 edges and 8 corners of the cube respectively. The sum is over all 256 allowed spin configurations on the cube.

The variational equations determining κ are, after substituting (3.14)–(3.17) in (3.13), (3.8) and (3.7)

$$\sum \left(\prod_{\mathrm{f}'} F\right)\left(\prod_{\mathrm{e}} B\right)\left(\prod_{\mathrm{c}} A\right) W = (s_4/s_3) F(\sigma_1, \sigma_2, \sigma_3, \sigma_4) B^2(\sigma_1, \sigma_3) B^2(\sigma_1, \sigma_2) B^2(\sigma_3, \sigma_4) B^2(\sigma_2, \sigma_4) \times A(\sigma_1) A(\sigma_2) A(\sigma_3) A(\sigma_4), \tag{3.23}$$

$$\sum_{b, b'} F^2(a, b, a', b') B^2(a, b) B^2(b', a') B^2(b, b') A(b) A(b') = (s_3/s_2) B^2(a, a') A^2(a) A^2(a'), \tag{3.24}$$

$$\sum_{b} B^4(a, b) A^4(b) = (s_2/s_1) A^4(a). \tag{3.25}$$

In (3.23) the products e and c have the same meaning as in (3.19); the product f′ is over all faces of the cube except the top face, and the sum is over all spin configurations of the bottom face only; on the RHS all the spins are in the top face.

3.2. Interpretation of A, B and F

It is clear from (3.19) that the variational quantities A, B and F can be interpreted as face, edge and corner weights respectively. Indeed, if we had considered the three-dimensional analogue of the hierarchy of two-dimensional variational approximations given by Baxter (1978), A, B and F would represent 'corner tensors' for the blocks of spins indicated in figure 3.

In particular A is the three-dimensional analogue of the usual corner transfer matrix. This allows us to write down an expression for the zero-field magnetisation

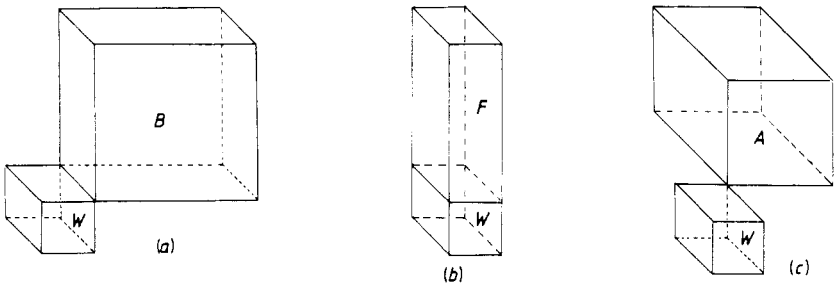

Figure 3. Typical blocks of spin corresponding to the 'corner tensors' A, B and F.

M_0. Consider the three-dimensional cubic lattice divided into eight pieces by three cuts. At the site of the intersection of the three cuts denote the spin σ. In the variational approximation the Boltzmann weight for each cube is $A(\sigma)$. Thus

$$M_0 = \langle\sigma\rangle = (A^8(+) - A^8(-))/(A^8(+) + A^8(-)). \tag{3.26}$$

A direct derivation of (3.26) can also be given. If we impose a magnetic field H on the system the Boltzmann weight becomes

$$W = W_0 \exp\left(h \sum_{k=1}^{8} \sigma_k\right) \tag{3.27}$$

where W_0 denotes the zero-field Boltzmann weight, and h the non-dimensional magnetic field. Define the new variables $\bar{A}$, $\bar{B}$ and $\bar{F}$ by

$$\bar{A}(\sigma) = \mathrm{e}^{-h\sigma} A(\sigma), \tag{3.28}$$

$$\bar{B}(\sigma, \sigma') = \exp[h(\sigma + \sigma')] B(\sigma, \sigma'), \tag{3.29}$$

$$\bar{F}(\sigma_1, \sigma_2, \sigma_3, \sigma_4) = \exp[-h(\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4)] F(\sigma_1, \sigma_2, \sigma_3, \sigma_4). \tag{3.30}$$

Then the expressions for s_4, s_3 and s_2 are formally the same as (3.20), (3.21) and (3.22) if we replace W, A, B, F by W_0, $\bar{A}$, $\bar{B}$ and $\bar{F}$ respectively. The expression for s_1 becomes

$$s_1 = \sum_a \bar{A}^8(a)\, \mathrm{e}^{h\sigma}. \tag{3.31}$$

Thus differentiating the expression for κ, (3.18), logarithmically with respect to h(remembering κ is by definition stationary with respect to $\bar{A}$, $\bar{B}$ and $\bar{F}$), then setting $h = 0$, (3.26) follows immediately.

4. Solving the equations

Inspection of the variational equations (3.23)–(3.25) shows that

$$A(+),\ B(+,+),\ F(+,+,+,+) \text{ and } W(+|+++|+++|+) \tag{4.1}$$

can be taken as normalisations, which we choose to equal unity. There remain 11 equations in 11 unknowns. The equations can be solved both numerically and in series form.

4.1. Series solution

We seek series solutions in powers of a low-temperature parameter u, say, chosen so that the Boltzmann weights W can be written as integer powers of this parameter. This is done by first writing down and solving the equations in the low-temperature limit, which allows the leading term of the series expansion of each to be determined.

In each of the 11 equations there is one term only on the LHS which is of the same order in the low-temperature limit as the single term on the RHS, all other terms on the left being of a lower order. (For the models considered here, the dominant term is the one in which the spins in the summation on the LHS are all +1.) For each equation, we can define the ratio of the RHS to this dominant term as a new variable, and express the original variables as products of powers of these new ones. In the low-temperature limit we can clearly solve the 11 equations for the new variables (each will be one). We can then evaluate (to leading order) the sub-dominant correction terms on the LHS of each equation and re-solve for each of the new variables. Iterating this procedure, we can sequentially expand all variables in powers of the low-temperature variable

$$u = \mathrm{e}^{-4K}, \tag{4.2}$$

where $K = J/k_B T$, J denoting the coupling constant. We can then use (3.18) and (3.26) to obtain the series expansions for κ and M_0.

4.2. Numerical solution

The key to obtaining numerical solutions is to use an accurate initial guess at the solution. For low temperatures the variables are initialised with their leading-order low-temperature expansion term, obtained as described in § 4.1. Explicitly

$$\begin{aligned}
&(s_2/s_1) = (s_3/s_2) = (s_4/s_3) = 1,\\
&A(-) = B(+,-) = F(+,+,+,-) = \bar{W}(+|+++|-++|+),\\
&B(-,-) = F(+,+,-,-) = \bar{W}(+|++-|-++|+),\\
&F(-,+,-,+) = \bar{W}(-|+++|-++|+),\\
&F(-,+,-,-) = \bar{W}(-|++-|-++|+),\\
&F(-,-,-,-) = \bar{W}(-|+--|-++|+),
\end{aligned} \tag{4.3}$$

where the weight functions $\bar{W}$ are defined in terms of W by

$$\bar{W} = W/W(+|+++|+++|+). \tag{4.4}$$

The equations are solved using a Newton–Raphson procedure. The initialisation (4.3) is adequate for sufficiently low temperatures. At higher temperatures, a quadratic extrapolation procedure is used, whereby the solution of the equations for the previous three temperatures is used to construct an initial guess at the solution for the next temperature.

4.3. Determining the critical temperature

By choosing the quantities (4.1) to equal unity, and the initialisations (4.3), the zero-temperature solution of the variational equations thus obtained has $M_0 = 1$. Thus

the ground state of the system with all spins + has been singled out. Assuming the model has spin reversal symmetry, the critical temperature can therefore be determined by plotting the zero-field magnetisation curve (see figure 4). Note that for $u<u_c$, but still close to u_c, there will be three solutions of the variational equations for both $A(+)$ and $A(-)$, and thus three values of M_0. For each solution with $A(+)\neq A(-)$ there will be a solution with the values of $A(+)$ and $A(-)$ interchanged, by spin reversal symmetry. There will also be the symmetric solution $A(+)=A(-)$ which will persist below the critical point, since the equations are only an approximation of real critical behaviour.

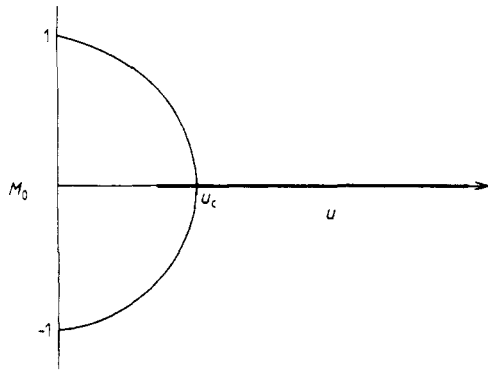

Figure 4. A typical zero-field magnetisation curve obtained from the variational approximation. The critical value of the temperature variable is determined as the intersection of the curve with the axis.

5. Results for the Ising models

In this section the variational approximation will be applied to the simple cubic (SC), face centred cubic (FCC) and body centred cubic (BCC) Ising models. The accuracy of the approximation can then be determined by comparison with the results of Sykes *et al* (1965, 1972, 1973) who used graphical methods.

The models are specified by their Boltzmann weight W. For the SC Ising model

$$W(a|efg|bcd|h)=\exp\tfrac{1}{4}K[a(g+f+e)+b(g+f+h)+c(g+e+h)+d(h+f+e)] \tag{5.1}$$

and for the FCC Ising model

$$W(a|efg|bcd|h)=\exp\tfrac{1}{2}K[a(d+b+c)+b(d+c)+cd+e(f+g+h)+g(f+h)+fh]. \tag{5.2}$$

Note that in the FCC model the spins on the sites a, b, c and d are independent of the spins on the sites e, f, g and h. The partition function on N sites formed by the weight (5.2) can be factored into two non-interacting FCC models on $N/2$ sites. This implies that the variational edge weight $B(a, b)$ can be written as a product of single spin functions

$$B(a, b)=\phi_1(a)\phi_1(b) \tag{5.3}$$

and the face weight in the form

$$F(a, b, c, d)=\phi_2(a, d)\phi_2(b, c). \tag{5.4}$$

In principle the relations (5.3) and (5.4) simplify the solution of the variational equations, however in practice we found it more convenient to use F and B as originally formulated.

There are two ways of formulating the BCC Ising model on a cubic lattice. The first is to use the unit cell with weight function

$$W(a|efg|bcd|h)=\exp K(ah+be+cf+dg), \tag{5.5}$$

which generates four independent BCC lattices. This will be referred to as DBC. In this weight function no spins on an edge or faces of the unit cell interact, and so the variational edge and face weights can be written

$$B(a, b)=\mu_1(a)\mu_1(b), \tag{5.6}$$

$$F(a, b, c, d)=\mu_2(a)\mu_2(b)\mu_2(c)\mu_2(d). \tag{5.7}$$

The variational equations can now be solved exactly. We find

$$\kappa=(1+v^8)[(1-v^{14})/(1-v^{16})]^4. \tag{5.8}$$

This is exactly the formula for κ obtained from the Bethe approximation with coordination number 8 (Domb 1960).

The second method is to begin with a unit cell of the BCC Ising model of $2N$ sites (see figure 5), and then sum over the interior spin. This gives a cubic lattice model on N sites with weight function

$$W(a|efg|bcd|h)=2\cosh K(a+b+c+d+e+f+g+h). \tag{5.9}$$

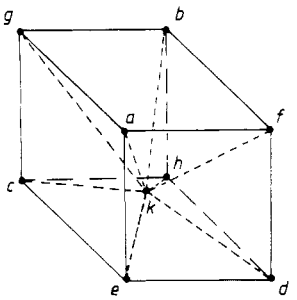

Figure 5. A typical cell of the BCC lattice. In forming the partition function, the spin k is summed over.

This model, to be referred to as BCC, will be more accurate than the DBC, as the unit cell is larger.

Using the method outlined in § 4.3 the critical temperature for the four models (SC, FCC, BCC and DBC) was determined. Following Sykes *et al* (1972) the quantity calculated was

$$v_f=\tanh J/k_B T_c. \tag{5.10}$$

The results, and a comparison with those obtained by Sykes *et al* (1972), are given in table 1.

Series expansions for $\log \kappa$ and M_0 were calculated using the procedure given in § 4.1. The results, and a comparison with those obtained by Sykes *et al* (1965, 1973), are given in table 2. In fact the 23 terms of the BCC Ising model correctly given by

Table 1. v_f^* denotes the value of (5.10) given by the variational approximation, v_f the value given by Sykes *et al* (1972).

Model	v_f^*	v_f	$\lvert(v_f-v_f^*)/v_f\rvert\times100\%$
SC	0.215	0.218 13	1.4%
FCC	0.099	0.101 74	2.7%
BCC	0.154	0.156 12	1.4%
DBC	0.142	0.156 12	9%

Table 2. The column headed 'accuracy' gives the number of terms in the series expansion of both $\log\kappa$ and M_0 correctly given by the variational approximation. The 'next two terms' column gives both the coefficients of the next two terms as given by the variational approximation and, in brackets, the actual coefficients.

Model	Accuracy	Next two terms of $\log\kappa$	Next two terms of M_0
SC	14	$69\,390\frac{1}{5}(69\,393\frac{1}{5})u^{15}$ $-213\,750\frac{1}{2}(-213\,754\frac{1}{2})u^{16}$	$-846\,574(-846\,628)u^{15}$ $2753\,136(2753\,520)u^{16}$
FCC	19	$120(123)u^{20}$ $138(126)u^{21}$	$-960(-984)u^{20}$ $-1104(-1008)u^{21}$
BCC	23	$3832\,715\frac{1}{2}(3832\,961\frac{1}{2})u^{24}$ $-7940\,092(-7941\,796)u^{25}$	$-54\,008\,274(-54012\,882)u^{24}$ $112\,609\,696(112\,640\,896)u^{25}$
DBC	11	$36\frac{1}{3}(48\frac{1}{3})u^{12}$ $252(204)u^{13}$	$-218(-314)u^{12}$ $-2016(-1632)u^{13}$

the variational approximation represent the entire series for this model given by Sykes *et al* (1965) (higher terms in the expansion are given in Sykes *et al* (1973)). Notice that in all cases (the DBC excluded) the deviation from the correct value of the erroneous coefficients is small.

6. Conclusion

A variational approximation applicable to three-dimensional isotropic lattice models has been formulated. It can be regarded as an extension of the two-dimensional Kramers–Wannier approximation, and involves just 11 equations for 11 unknowns, so can be easily handled on a computer (our run times were never more than a few seconds). The approximation gives moderately accurate results when tested on the SC, FCC and BCC Ising models: for the last it correctly gives the first 23 terms of the low-temperature series, and numerically predicts a value of the critical temperature that is in error by only 1.4%.

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