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Triplet order parameters for three-dimensional Ising models

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Abstract. We have derived power series expansions for triplet order parameters of three-dimensional Ising models with pure pair interactions, and pure quartet interactions. We investigate the vanishing of these order parameters and conclude that they become zero at and above the critical temperature, and probably have the same critical exponent as the conventional order parameter $\langle\sigma_i\rangle$.

In a recent publication, Baxter (1975) has obtained an expression for a triplet order parameter $\langle\sigma_1\sigma_2\sigma_3\rangle$ of a planar Ising model with nearest-neighbour pair interactions, where σ_1, σ_2, and σ_3 are the vertices of the mesh triangles on the triangular lattice. This model is an example of types of Ising models which have previously been introduced by the present authors (Wood and Griffiths 1973), having Hamiltonians in the form

$$\mathscr{H} = -J_1 \sum \sigma_m - J_2 \sum \sigma_m\sigma_n - J_3 \sum \sigma_m\sigma_n\sigma_p - J_4 \sum \sigma_m\sigma_n\sigma_p\sigma_q - \dots \quad (1)$$

where the summations of products of m σ-variables are over the smallest s_m simplexes of the underlying lattice structure.

On restricting equation (1) to contain only three coupling constants, we can use the triple-moment power series of the free energy f to form the thermodynamic functions

$$M_i^{j,k}(J_k) = -\lim_{J_i\to 0^+}\left(\frac{\partial f}{\partial J_i}\right)_{J_j=0} \quad (2)$$

which are the expectation values of the s_i simplex product of σ-variables considered to be located in a J_i-type external field. Triplet order parameters can be formed by setting $i=3$ in equation (2), then $M_3^{1,2}$ and $M_3^{2,4}$ are both parameters which one expects to vanish at high temperatures, independently of lattice type. Specific lattice types can also yield other examples which should possess the characteristic features of an order parameter, thus $M_2^{3,4}$ for the FCC lattice vanishes at high temperatures but is positive at low enough temperatures. Such results are readily established through the term structure of the high- and low-temperature expansions of f (see Wood and Griffiths 1973).

For the plane triangular lattice, $M_1^{3,2}$ and $M_3^{1,2}$ are known exactly (Potts 1952, Baxter 1975), both functions possess the same critical exponent value of $\beta = \frac{1}{8}$ and vanish above T_c. Highly plausible exact forms have been conjectured for $M_1^{2,3}$ and $M_2^{1,3}$ (Baxter *et al* 1975); here, also, the same critical exponents are found at T_c, i.e.

$\beta_M = \beta_P = \frac{1}{12}$, however, no proof of such an exponent equality has yet been given. As power series expansions of both $M_1^{2,3}$ and $M_2^{1,3}$ were instrumental in 'guessing' these exact solutions, it is therefore of interest to derive further examples of such series.

We note, in passing, that the technique of using a pole–residue plot for the Padé approximants (PA) to the logarithmic derivative of a function with a *known* singular point can be effective in refining an exponent estimate. This point is tested and verified in figure 1, where twelve terms in the expansion of $M_3^{1,2}$ and $M_2^{1,3}$ (Baxter *et al* 1975) have been used; in this way a wide scatter on such approximations can be ordered to form a much improved estimate of a critical exponent (Griffiths and Wood 1975, Ritchie and Essam 1975).

The present authors have developed low-temperature power series of f for three-dimensional Ising models on the FCC and BCC lattices (Griffiths and Wood 1972, 1974), which have Hamiltonians in the form of equation (1). The new order parameters considered here are the triplet functions $\langle\sigma_1\sigma_2\sigma_3\rangle$ for pure pair and pure quartet

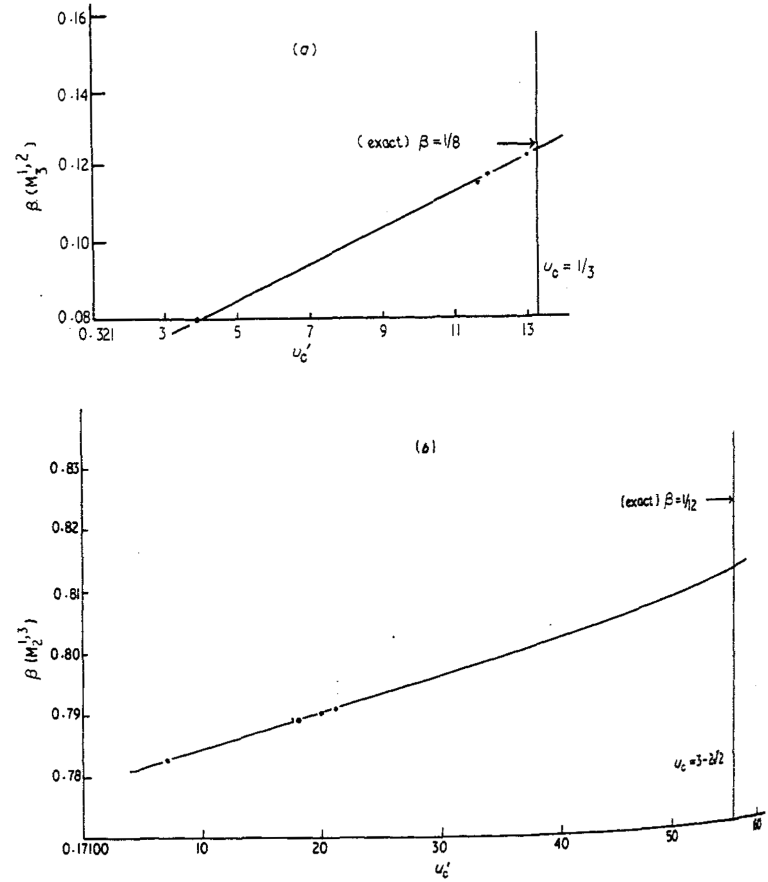

Figure 1. Residue–pole plots of the PA estimates of the critical point (u_c') against the exponent estimates of β for (a) the triplet order parameter $M_3^{1,2}$ and (b) the polarization $M_2^{1,3}$ of the triangular lattice using 12 terms in the expansions; the exact values are $\frac{1}{8}$ and $\frac{1}{12}$ respectively.

interactions in a *triplet external field*, where σ_1, σ_2, and σ_3 are at the vertices of the elementary triangles of each lattice. We quote the expansions

$$M_3^{1,2}=1-6u_2^6-60u_2^{11}+78u_2^{12}-104u_2^{15}-588u_2^{16}+1920u_2^{17}-1298u_2^{18}-384u_2^{19}$$
$$-2088u_2^{20}-2068u_2^{21}+32496u_2^{22}-52932u_2^{23}+13818u_2^{24}-16500u_2^{25}$$
$$+65010u_2^{26}+369136u_2^{27}-1308588u_2^{28}+1185348u_2^{29}-269108u_2^{30}$$
$$+1670220u_2^{31}+\ldots \qquad (\text{FCC lattice}) \qquad (3)$$

$$M_3^{2,4}=1-6u_4^4-60u_4^6-694u_4^8-8988u_4^{10}-125196u_4^{12}-\ldots \qquad (\text{FCC lattice}) \qquad (4)$$

$$M_3^{1,2}=1-6u_2^7-72u_2^{13}+90u_2^{14}-160u_2^{18}-806u_2^{19}+2608u_2^{20}-1680u_2^{21}$$
$$-96u_2^{22}-696u_2^{23}-3448u_2^{24}-2852u_2^{25}+51656u_2^{26}-80344u_2^{27}$$
$$+29394u_2^{28}-15036u_2^{29}-28080u_2^{30}+130060u_2^{31}+679112u_2^{32}$$
$$-2338588u_2^{33}+\ldots \qquad (\text{BCC (1,2) lattice (Dalton and Wood 1969)}) \qquad (5)$$

and

$$M_3^{2,4}=1-6u_4^{12}-40u_4^{18}-32u_4^{20}-294u_4^{24}-352u_4^{26}-422u_4^{28}-2152u_4^{30}-3720u_4^{32}$$
$$-7720u_4^{34}-\ldots \qquad (\text{BCC (1,2) lattice}) \qquad (6)$$

where $u_i=\exp(-4J_i/kT)$ is the usual low-temperature expansion variable. The conventional order parameter expansions ($\langle\sigma_i\rangle$) corresponding to equations (3) and (5) are listed by Domb (1974).

In the case of equation (4), the quartet interactions over the s_4 simplexes of the FCC lattice give the model a self-dual property (Wood 1972, Griffiths and Wood 1972) and both $M_1^{2,4}$ and $M_3^{2,4}$ have expansion coefficients of constant sign, hence the closest singularity to the origin in these functions is real. Simple ratio calculations on very short series clearly indicate that the zero-field specific heat and susceptibility, and the functions $M_1^{2,4}$ and $M_3^{2,4}$ all yield power series with the *same* radius of convergence $u_R^{-2}\simeq 18\pm 1$. It is doubtful in this instance, however, whether u_R forms a 'critical point' (Griffiths and Wood 1972†), because the self-duality ensures that the radii of convergence of the high-temperature and low-temperature expansions of C_v overlap. Thus the 'physical' specific heat probably has a cusp singularity at the intersection of the high-temperature and low-temperature curves leading to a first-order transition before the singular point at u_R is reached. None the less, the above thermodynamic functions appear to have a *real* singularity at u_R whose above value is confirmed by PA which yield estimates of u_R in the range $u_R^2=0{\cdot}057$–$0{\cdot}061$ for $M_1^{2,4}$ and $M_3^{2,4}$. The series are too short to say much on the exponents, but a small exponent, probably in excess of 0·025, is indicated by PA.

The series (6) also appears to yield coefficients of constant sign. Here the coefficients are not smooth enough for the ratio methods; however, the expansions are long enough to yield a useful PA analysis on $(d/du_4)\ln M_3^{2,4}$. All the PA clearly indicate that the closest singularity to the origin is *real* with at least one complex singularity lying close to the physical disc. Typical results from the $[m, n]$ PA are given here for the case $m+n=16$.

† The inequality relating to equations (18) and (19) should be reversed, see acknowledgment at end of paper.

Exponent	0·0675	0·0654	0·0658	0·0650	0·0645	
u_c^2	0·424	0·423	0·423	0·423	0·422	(7)
m	6	7	8	9	10	

On this basis, we estimate $u_c = 0{\cdot}423 \pm 0{\cdot}001$ (compare this with our previous, much less accurate estimate using the magnetization $\langle\sigma_i\rangle$; $u_c = 0{\cdot}40 \pm 0{\cdot}02$, Griffiths and Wood 1974). We conjecture that the exponent in (7) is $\frac{1}{16}$, which may also hold for $\langle\sigma_i\rangle$, and for the corresponding behaviour of $M_3^{2,4}$ and $M_1^{2,4}$ for the FCC lattice at u_R above.

The two series (3) and (5) offer a more substantial basis for a PA analysis; if the two-dimensional result of Baxter (1975) is any guide, we should find evidence that $M_3^{1,2}$ has a zero at the critical temperature, and that the critical exponent takes the same value as β, which is thought to be 0·3125 (Domb 1974). In both pair models relating to equations (3) and (5), the critical point u_c is known with some accuracy; thus for the FCC lattice $u_c = 0{\cdot}6647$ (Sykes *et al* 1972), and, with less certainty, $u_c = 0{\cdot}709$ for the BCC (1,2) lattice (Dalton and Wood 1969). Assuming that the triplet order parameters vanish at u_c, we can attempt to evaluate the exponent using the function $(u_2 - u_c)(d/du_2) \ln M_3^{1,2}$ (Hunter and Baker 1973). We list here some results from the $[m, n]$ PA for $m + n = N$.

(i) FCC lattice, $M_3^{1,2}$:

Exponent	0·321	0·328	0·341	0·337	0·313	0·319	(N=30) (8)
m	13	14	15	16	17	18	
Exponent	0·305	0·346	0·308	0·323	0·303		(N=29) (9)
m	12	13	14	15	17		

(ii) BCC (1,2) lattice:

Exponent	0·331	0·326	0·327	0·367	0·333	0·326	(N=32) (10)
m	13	14	15	16	17	18	
Exponent	0·316	0·317	0·325	0·324			(N=29) (11)
m	13	14	15	16			

The scatter of the above PA estimates is fairly typical of lengthy irregular low-temperature series such as equations (3) and (5) for lattices of high coordination number, where the expansions of $M_3^{1,2}$ and $M_1^{3,2}$ do not converge up to the physical singularity. Direct estimates of the physical singularity in the above triplet order parameters $M_3^{1,2}$ using the PA to the logarithmic derivatives yield estimates of u_c which are usually in excess of the accepted values quoted above by anything up to 7%.

Overall we feel that the numerical position supports the conjecture that the exponents in triplet order parameters will be the same as the magnetization exponent β and that the parameters vanish at T_c.

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