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Triplet order parameters in triangular and honeycomb Ising models

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Abstract. It is shown that the ratios of certain triplet order parameters to magnetisation in honeycomb and diamond lattice Ising models can be easily calculated. Applying the star–triangle transformation reproduces the result obtained by Baxter on the triangular lattice. The new derivation indicates that exact solutions for triplet order parameters are of only limited use as checks on series expansions.

1. Introduction

There have recently been several investigations of three-spin order parameters in Ising models with two-spin interactions (Baxter 1975, Wood and Griffiths 1976, Barber 1976), largely as a parallel to investigations of two-spin order parameters in Ising models with three-spin interactions (Baxter *et al* 1975). The most general result is that in two-spin interaction ferromagnetic Ising models, any three-spin expectation will vanish at the critical point with the same critical exponent as the magnetisation (Barber 1976). Special cases are the exact result of Baxter (1975) (for three neighbour spins on a triangular lattice) and the series expansion work of Wood and Griffiths (1976) on BCC and FCC lattices. On the triangular lattice the three-site order parameter is of interest as it is related to clustering properties of the Ising model as described in appendix 2.

Baxter (1975) obtained the solution for $M_3 = \langle\sigma_{00}\sigma_{10}\sigma_{11}\rangle$ on the triangular lattice by using the method of Pfaffians to obtain the large-n limit of

$$\langle\sigma_{00}\sigma_{10}\sigma_{11}\sigma_{nn}\rangle/\langle\sigma_{11}\sigma_{nn}\rangle \rightarrow \langle\sigma_{00}\sigma_{10}\sigma_{11}\rangle/\langle\sigma_{11}\rangle = R.$$

The main result of the present paper is that this ratio, $R = M_3/M$ can be calculated in a simple direct manner and that on honeycomb and diamond lattices, similar ratios can be found for two distinct triplet order parameters. The method used is related to conditional probability characterisations of the Ising model used by statisticians and is also related to the method of partial generating functions used by Sykes *et al* (1973) to obtain series expansions. One consequence of this latter connection is that exact solutions for M_3 and M cannot be regarded as being independent tests of series expansions obtained using the method of partial generating functions.

The following section contains the algebraic form of the derivation of triplet order parameters. The connection with the method of partial generating functions is sketched briefly in the final section. Appendix 1 gives an interpretation of the calculations in terms of probability distributions defined on Ising models. Appendix 2 derives the connection between M_3 and triangular lattice cluster properties.

2. Calculation of triplet order parameters

The simplified derivation of triplet order parameters relies heavily on the fact that certain crystal lattices can be divided into two sublattices A and B such that A sites have only B sites as neighbours. This approach leads us to express the Hamiltonian of the honeycomb lattice Ising model as

$$E_{\mathrm{H}} = \sum_{\boldsymbol{r}\in \mathrm{A}} E_{\mathrm{H}}(\boldsymbol{r})$$
$$= \sum_{\boldsymbol{r}\in \mathrm{A}} (L_1\sigma(\boldsymbol{r})\sigma(\boldsymbol{r}+\boldsymbol{a}) + L_2\sigma(\boldsymbol{r})\sigma(\boldsymbol{r}+\boldsymbol{b}) + L_3\sigma(\boldsymbol{r})\sigma(\boldsymbol{r}+\boldsymbol{c})). \tag{1}$$

To calculate spin expectation values we use the expressions

$$\langle f(\{\boldsymbol{\sigma}\})\rangle = Z^{-1}\sum_{\{\sigma\}} f(\{\boldsymbol{\sigma}\}) \exp(-E_{\mathrm{H}}/kT) \tag{2}$$

where the sum is over all configurations of all spins $\sigma(\boldsymbol{r})$ in the system $(\sigma(\boldsymbol{r}) = \pm 1)$.

If one focuses attention on a particular A site, r_0 and its three neighbours and only considers expectations of functions of the four spin variables $\sigma(\boldsymbol{r}_0)$, $\sigma(\boldsymbol{r}_0+\boldsymbol{a})$, $\sigma(\boldsymbol{r}_0+\boldsymbol{b})$, $\sigma(\boldsymbol{r}_0+\boldsymbol{c})$, then the sum in (2) can be rearranged giving

$$\langle f(\{\boldsymbol{\sigma}\})\rangle = \sum_{\sigma(\boldsymbol{r}_0)} \sum_{\sigma(\boldsymbol{r}_0+\boldsymbol{a})} \sum_{\sigma(\boldsymbol{r}_0+\boldsymbol{b})} \sum_{\sigma(\boldsymbol{r}_0+\boldsymbol{c})} [f(\{\boldsymbol{\sigma}\}) \exp(-E_{\mathrm{H}}(\boldsymbol{r}_0)/kT)/G(\boldsymbol{r}_0)$$
$$\times F(\sigma(\boldsymbol{r}_0+\boldsymbol{a}), \sigma(\boldsymbol{r}_0+\boldsymbol{b}), \sigma(\boldsymbol{r}_0+\boldsymbol{c}))] \tag{3}$$

where F and $G(\boldsymbol{r}_0)$ are functions of $\sigma(\boldsymbol{r}_0+\boldsymbol{a})$, $\sigma(\boldsymbol{r}_0+\boldsymbol{b})$, $\sigma(\boldsymbol{r}_0+\boldsymbol{c})$ given by

$$G(\boldsymbol{r}_0) = \sum_{\sigma(\boldsymbol{r}_0)} \exp(-E_{\mathrm{H}}(\boldsymbol{r}_0)/kT) \tag{4}$$

$$F(\sigma(\boldsymbol{r}_0+\boldsymbol{a}), \sigma(\boldsymbol{r}_0+\boldsymbol{b}), \sigma(\boldsymbol{r}_0+\boldsymbol{c})) = \sum_{\{\sigma\}}{}' \exp(-E_{\mathrm{H}}/kT + E_{\mathrm{H}}(\boldsymbol{r}_0)/kT)G(\boldsymbol{r}_0)/Z \tag{5}$$

where the sum Σ' is over all configurations of all spins except $\sigma(\boldsymbol{r}_0)$ and its neighbours.

The various terms in expressions (2), (3) and (5) have natural interpretations in terms of probability distributions. This aspect of the work is discussed in appendix 1.

F is actually independent of $\sigma(\boldsymbol{r}_0)$ as can be seen by inspection of equations (4) and (5). The most general possible form for F is

$$A\sigma(\boldsymbol{r}_0+\boldsymbol{a}) + B\sigma(\boldsymbol{r}_0+\boldsymbol{b}) + C\sigma(\boldsymbol{r}_0+\boldsymbol{c}) + D\sigma(\boldsymbol{r}_0+\boldsymbol{a})\sigma(\boldsymbol{r}_0+\boldsymbol{b})\sigma(\boldsymbol{r}_0+\boldsymbol{c})$$
$$+ g_0 + g_1\sigma(\boldsymbol{r}_0+\boldsymbol{a})\sigma(\boldsymbol{r}_0+\boldsymbol{b}) + g_2\sigma(\boldsymbol{r}_0+\boldsymbol{a})\sigma(\boldsymbol{r}_0+\boldsymbol{c})$$
$$+ g_3\sigma(\boldsymbol{r}_0+\boldsymbol{b})\sigma(\boldsymbol{r}_0+\boldsymbol{c}). \tag{6}$$

Substituting this form of F into (3) gives

$$\langle\sigma(\boldsymbol{r}_0+\boldsymbol{a})\rangle = 8A \tag{7a}$$

$$\langle\sigma(\boldsymbol{r}_0+\boldsymbol{b})\rangle = 8B \tag{7b}$$

$$\langle\sigma(\boldsymbol{r}_0+\boldsymbol{c})\rangle = 8C \tag{7c}$$

$$\langle\sigma(\boldsymbol{r}_0)\rangle = (2\alpha-1)(2A+2B+2C+2D)+(2\beta_1-1)(-2A+2B+2C-2D)$$
$$+(2\beta_2-1)(2A-2B+2C-2D)+(2\beta_3-1)(+2A+2B-2C-2D) \quad (7d)$$

$$\langle\sigma(\boldsymbol{r}_0+\boldsymbol{a})\sigma(\boldsymbol{r}_0+\boldsymbol{b})\sigma(\boldsymbol{r}_0+\boldsymbol{c})\rangle = 8D \quad (8a)$$

$$\langle\sigma(\boldsymbol{r}_0+\boldsymbol{a})\sigma(\boldsymbol{r}_0+\boldsymbol{b})\sigma(\boldsymbol{r}_0)\rangle = (2\alpha-1)(2A+2B+2C+2D)$$
$$+(2\beta_1-1)(-2A+2B+2C-2D)-(2\beta_2-1)(2A-2B+2C-2D)$$
$$-(2\beta_3-1)(+2A+2B-2C-2D) \quad (8b)$$

$$\alpha = 1/(1+z_1z_2z_3) \quad (9a)$$

$$\beta_1 = z_i/(z_i+z_1z_2z_3/z_i) \quad (9b)$$

$$z_i = \exp(-2L_i/kT). \quad (9c)$$

If the four single-spin expectations are known then equations $(7a)$–$(7d)$ can be regarded as four simultaneous equations in the unknowns A, B, C, D, and are applicable to any group of four spins for which $E_{\mathrm{H}}(\boldsymbol{r}_0)$ as given by (1) is the only interaction between $\sigma(\boldsymbol{r}_0)$ and the rest of the system. If we consider the thermodynamic limit of a honeycomb lattice then we can put

$$\langle\sigma(\boldsymbol{r}_0)\rangle = \langle\sigma(\boldsymbol{r}_0+\boldsymbol{a})\rangle = \langle\sigma(\boldsymbol{r}_0+\boldsymbol{b})\rangle = \langle\sigma(\boldsymbol{r}_0+\boldsymbol{c})\rangle = M$$

whence $A = B = C$.

Similarly

$$\langle\sigma(\boldsymbol{r}_0+\boldsymbol{a})\sigma(\boldsymbol{r}_0+\boldsymbol{b})\sigma(\boldsymbol{r}_0+\boldsymbol{c})\rangle = M_3 \quad (10a)$$

and because $A = B = C$ we have the somewhat surprising result that

$$\langle\sigma(\boldsymbol{r}_0)\sigma(\boldsymbol{r}_0+\boldsymbol{a})\sigma(\boldsymbol{r}_0+\boldsymbol{b})\rangle = \langle\sigma(\boldsymbol{r}_0)\sigma(\boldsymbol{r}_0+\boldsymbol{a})\sigma(\boldsymbol{r}_0+\boldsymbol{c})\rangle$$
$$= \langle\sigma(\boldsymbol{r}_0)\sigma(\boldsymbol{r}_0+\boldsymbol{b})\sigma(\boldsymbol{r}_0+\boldsymbol{c})\rangle = M_3^*. \quad (10b)$$

In other words, even on anisotropic honeycomb lattices, triplet order parameters of the forms given in $(10b)$ do not show any anisotropy.

Solving the simultaneous equations gives

$$R = M_3/M = (\beta+3\alpha-5)/(\beta-\alpha-1) \quad (11a)$$

$$R^* = M_3^*/M = (8\alpha\beta-5\beta-15\alpha+9)/3(\beta-\alpha-1) \quad (11b)$$

where

$$\beta = \beta_1+\beta_2+\beta_3. \quad (11c)$$

R can also be written as

$$R = \frac{3\tanh(K_1+K_2+K_3)+\tanh(K_1+K_2-K_3)+\tanh(K_1-K_2+K_3)+\tanh(-K_1+K_2+K_3)+4}{\tanh(K_1+K_2-K_3)+\tanh(K_1-K_2+K_3)+\tanh(-K_1+K_2+K_3)-\tanh(K_1+K_2+K_3)} \quad (12)$$

$$K_i = L_i/kT. \quad (13)$$

There is a well known transformation (the star–triangle transformation) connecting honeycomb lattice Ising models to triangular lattice Ising models. In terms of probability distributions it corresponds to performing a partial sum over the probability distribution for a honeycomb lattice Ising model and showing that the result is the probability distribution for a triangular lattice Ising model. The sum is over all configurations of A sublattice spins so that any expectation of B sublattice spins such as $M = \langle\sigma(\boldsymbol{r}_0+\boldsymbol{a})\rangle$ or M_3 will be left invariant. The three triangular lattice interactions J_1, J_2, J_3 are given by

$$\sinh^2(2J_i/kT) = 4(S_1^2S_2^2S_3^2)/A^4S_i^2 \tag{14a}$$

where

$$A^4 = 4(S_1^2+S_2^2+S_3^2+2C_1C_2C_3+2) \tag{14b}$$

$$S_i = \sinh(2L_i/kT) \tag{14c}$$

$$C_i = \cosh(2L_i/kT) \tag{14d}$$

(see for example Syozi 1972).

The conversion of the expression for R to triangular lattice parameters is most readily accomplished by using the form

$$R = \frac{C_1+C_2C_3}{S_2S_3} + \frac{C_2+C_1C_3}{S_1S_3} + \frac{C_3+C_1C_2}{S_1S_2} - \frac{S_1^2+S_2^2+S_3^2+2C_1C_2C_3+2}{S_1S_2S_3}. \tag{15}$$

The expression for R given by Baxter (1975) can be regained after a moderate amount of algebra.

The whole derivation can be repeated for lattices with two sublattices and a coordination number of four.

The factor F has the form

$$\begin{aligned} F = {} & A_1\sigma(\boldsymbol{r}_0+\boldsymbol{a}) + A_2\sigma(\boldsymbol{r}_0+\boldsymbol{b}) + A_3\sigma(\boldsymbol{r}_0+\boldsymbol{c}) + A_4\sigma(\boldsymbol{r}_0+\boldsymbol{d}) \\ & + \sigma(\boldsymbol{r}_0+\boldsymbol{a})\sigma(\boldsymbol{r}_0+\boldsymbol{b})\sigma(\boldsymbol{r}_0+\boldsymbol{c})\sigma(\boldsymbol{r}_0+\boldsymbol{d}) \\ & \times (D_1\sigma(\boldsymbol{r}_0+\boldsymbol{a}) + D_2\sigma(\boldsymbol{r}_0+\boldsymbol{b}) + D_3\sigma(\boldsymbol{r}_0+\boldsymbol{c}) + D_4\sigma(\boldsymbol{r}_0+\boldsymbol{d})) \\ & + \text{even-spin terms.} \end{aligned} \tag{16}$$

The simultaneous equations are

$$\langle\sigma(\boldsymbol{r}_0+\boldsymbol{a})\rangle = 16A_1 \qquad \text{(and 3 other similar equations)} \tag{17a}$$

$$\langle\sigma(\boldsymbol{r}_0+\boldsymbol{a})\sigma(\boldsymbol{r}_0+\boldsymbol{b})\sigma(\boldsymbol{r}_0+\boldsymbol{c})\rangle = 16D_4 \qquad \text{(and 3 similar equations)} \tag{17b}$$

and, taking the limit so that we can put $A_i = A$ and $D_i = D$ and considering only isotropic lattices:

$$\langle\sigma(\boldsymbol{r}_0)\rangle = (2\alpha-1)(8A+8D) + (2\beta-4)(4A-4D) \tag{17c}$$

$$\langle\sigma(\boldsymbol{r}_0)\sigma(\boldsymbol{r}_0+\boldsymbol{a})\sigma(\boldsymbol{r}_0+\boldsymbol{b})\rangle = (2\alpha-1)(8A+8D) \tag{17d}$$

where

$$\alpha = 1/(1+u^2) \tag{18a}$$

$$\beta = 1/(1+u) \tag{18b}$$

$$u = \exp(-4\beta J) \tag{18c}$$

which leads to the solutions

$$M_3/M = (5-2\alpha-\beta)/(2\alpha-\beta+1) = (1-3u-u^2-5u^3)/(1-u)^3 \tag{19a}$$

$$M_3^*/M = (2\alpha-1)(3-\beta)/(2\alpha-\beta+1) = (1+u)(1-3u)/(1-u)^2. \tag{19b}$$

Results (19*a*) and (19*b*) apply to both square and diamond lattice Ising models. For the square lattice the form of M_3^* is independent of which two neighbours of $\boldsymbol{r}_0$ are indexed by $\boldsymbol{a}$ and $\boldsymbol{b}$, so that we have

$$M_3^*/M = \langle\sigma_{00}\sigma_{01}\sigma_{02}\rangle = \langle\sigma_{00}\sigma_{01}\sigma_{11}\rangle. \tag{20}$$

The solution for M_3^*/M given by (19*b*) agrees with the expression for $\langle\sigma_{00}\sigma_{01}\sigma_{11}\rangle$ obtained by Baxter (1975) by equating M_3^* on the square lattice to M_3 on a triangular lattice with one interaction set to zero. Pink (1968) has calculated $\langle\sigma_{00}\sigma_{01}\sigma_{02}\rangle$ for the square lattice. His expression for this correlation appears to differ from (19*b*), incorrectly including a factor of $\frac{1}{4}$.

The calculations of M_3/M and M_3^*/M for the diamond lattice are quite surprising as none of M_3^*, M_3, M have been calculated exactly in this system.

3. Conclusion

As mentioned in the introduction it is also possible to derive R for the triangular lattice using the method of partial generating functions.

Sykes *et al* (1973) showed how the partition function for the honeycomb Ising model in a field H can be equated to the partition function of an Ising model in a field H' with a nearest-neighbour interaction J and a three-site interaction J_3, i.e.

$$\ln Z_{\mathrm{H}}(L, H) = f(L, H) + \ln Z_{\mathrm{tri}}(H', J, J_3)$$

where explicit expressions for H', J, J_3 as functions of L, H are known.

Differentiating with respect to H gives

$$M_{\mathrm{H}} = +\frac{\partial H'}{\partial H}\cdot\frac{\partial}{\partial H'}\ln Z_{\mathrm{tri}} + \frac{\partial J}{\partial H}\cdot\frac{\partial}{\partial J}\ln Z_{\mathrm{tri}} + \frac{\partial J_3}{\partial H}\cdot\frac{\partial}{\partial J_3}\ln Z_{\mathrm{tri}}.$$

In zero field, $\partial J/\partial H$ vanishes, J_3 vanishes and we have $M_{\mathrm{H}} = M_{\mathrm{tri}}$ by the star–triangle transformation so that

$$M_{\mathrm{tri}} = \frac{\partial H'}{\partial H} M_{\mathrm{tri}} + \frac{\partial J_3}{\partial H} M_3$$

from which M_3/M_{tri} can be calculated.

The fact that M_3/M can be expressed purely in terms of the transformation used in setting up the method of partial generating functions means that M_3 and M cannot be regarded as independent checks of series expansions obtained by this method. To be more precise, if full use is made of the sublattice symmetry either as a check or as 'input' information for the expansion technique (Sykes *et al* 1975) M and M_3 can be regarded as independent checks on the algebraic manipulation but are not independent checks on the input combinatorial information.

It appears that generalisations of these methods to other models will not produce results as simple as those obtained here. Relations for even-spin expectations do not simplify because there is no variable common to both sublattices which can take on the role of M. Extensions to other models such as the Potts models are unlikely to be simple because of the many different order parameters possible (see, for example, the number of different terms involved in partial generating functions, given by Enting 1974a, b).

Appendix 1. Probability distributions on Ising models

The basis of statistical mechanics is that expressions $Z^{-1}\exp(-E/kT)$ are of the correct form of joint probability distribution, Gibbs probability distributions, for calculating thermal averages. The calculations presented in § 2 are based on the possibility of factorising this probability distribution into a probability for $\sigma(\boldsymbol{r}_0+\boldsymbol{a})$, $\sigma(\boldsymbol{r}_0+\boldsymbol{b})$, $\sigma(\boldsymbol{r}_0+\boldsymbol{c})$ and a conditional probability of $\sigma(\boldsymbol{r}_0)$ given its three neighbours. These conditional probabilities are given by

$$P(\sigma(\boldsymbol{r}_0)|\sigma(\boldsymbol{r}_0+\boldsymbol{a})\sigma(\boldsymbol{r}_0+\boldsymbol{b})\sigma(\boldsymbol{r}_0+\boldsymbol{c}))=G(\boldsymbol{r}_0)^{-1}\exp(-E_{\mathrm{H}}(\boldsymbol{r}_0)/kT) \quad \text{(A.1)}$$

which takes values α, $1-\alpha$, β_i, $1-\beta_i$.

There is a converse result that Gibbs probability distributions are the most general self-consistent distributions that can occur in a system defined by a conditional probability structure. This result has been proved (to varying degrees of generality) by Dobruschin (1968), Spitzer (1971), Sherman (1973), Grimmet (1973), Preston (1973), Moussouris (1974) and others.

One point that should be emphasised is the importance of the symmetry constraint on the conditional probabilities. Besag (1974) has considered conditional probability structures on lattices that could be regarded as completely asymmetric. The conditional probabilities are associated with a partial ordering of lattice sites so that probabilities for a given site depend only on predecessor sites. These models have been shown to produce probability distributions equivalent to those of more general Ising models (Enting 1977a). (See also Welberry and Galbraith (1973, 1975), Welberry (1977a, b) for further work on these systems.) Although Enting (1977b) used these 'one-way' models or growth models to investigate the honeycomb–triangle code system, the probability distributions occurring coincide with the zero-field distributions used in §§ 2 and 3 only at infinite temperature.

There is however a closer connection between these growth models and the conditional probability formulation of the honeycomb Ising model. If one sets up a hexagonal close packed lattice with triangular lattice layers one can define a three-dimensional growth model using the order of layers to define the required partial ordering of sites. If one uses probabilities of the form (A.1) as the conditional probabilities of the growth model then pairs of layers of the HCP lattice will have two-dimensional honeycomb Ising model distributions of spins. It was the observation of Ising-like distributions in layers of three-dimensional growth models by Welberry (private communication) and discussions of the connections between layers which suggested the possibility of calculating M_3/M.

Appendix 2

The connection between triplet order parameters and clustering properties of triangular Ising models follows directly from the work of Sykes *et al* (1975). Put

$$M = \frac{1}{N}\sum_{c} (N - 2n)\exp(-E/kT)/Z \tag{A.2}$$

where N is the number of sites on the lattice, c stands for configuration and n is the number of down spins in a configuration.

$$M_3 = \frac{1}{2N}\sum(2N - 12n + 8b - 8t)\exp(-E/kT)/Z \tag{A.3}$$

where b is the number of edges on the lattice with both ends 'down' spins and t is the number of elementary triangles of down spins.

We can define a cluster order parameter, Δ, as the difference between the number of clusters of 'down' spins and the number of clusters of 'up' spins. The up clusters will occur as holes in down clusters. Normalising gives

$$\Delta = \frac{1}{N}\sum(c - h)\exp(-E/kT)/Z. \tag{A.4}$$

Sykes *et al* (1975) show geometrically that

$$c - h = t - b + 12 \tag{A.5}$$

whence

$$\Delta = (M - M_3)/4. \tag{A.6}$$

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