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Two site spin correlation function in Bethe-Peierls approximation for Ising model

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Abstract. Two site spin correlation function for an Ising model above Curie temperature has been calculated by generalising Bethe-Peierls approximation. The results derived by a graphical method due to Englert are essentially the same as those obtained earlier by Elliott and Marshall, and Oguchi and Ono. The earlier results were obtained by a direct generalisation of the cluster method of Bethe, while our results are derived by retaining that class of diagrams, which is exact on Bethe lattice.

Keywords. Spin correlation function; Curie temperature; Bethe-Peierls approximation; Bethe lattice susceptibility.

1. Introduction

The two site spin correlation function has been extensively studied (Elliott and Marshall 1958, Brout 1965, Fisher 1967). This quantity plays an important role in the study of phase transitions (Fisher 1967). The idea of length scaling which is a dominant theme in the present day theories of critical phenomena is associated with the study of spin correlation function. Moreover, this correlation function is directly related to the neutron scattering cross-section from magnetic systems (Elliott and Marshall 1958, Marshall and Lowde 1968, Oguchi and Ono 1966).

The two site spin correlation function has been calculated previously by several authors (Elliott and Marshall 1958, Oguchi and Ono 1966, Mori and Kawasaki 1962, Tahir Kheli and Callen 1964). The first detailed calculations of the spin correlation function valid near critical temperature were done by Elliott and Marshall. Their method consisted in generalising the cluster method of Bethe and Peierls (Hill 1956); subsequently Oguchi and Ono using similar ideas and constant coupling approximation (which in case of Ising model yields identical results to BP approximation) derived a similar result which differed from Elliott and Marshall's result only by an insignificant multiplicative factor of order unity. In this paper, we derive the same result (our result again differs from earlier results by a multiplicative factor) by a graphical method.

In the graphical method, originally due to Englert (1963), we obtain our approximation by including only that set of diagrams which occur on a Bethe lattice of

the same coordination number as the real lattice under consideration. It has been well known for some time that BP approximation is an exact result on the Bethe lattice. Here we show that simple generalisations of the cluster method (BP) can also be obtained by considerations based on Bethe lattice. A further advantage of the present derivation is that it can be easily generalised to disordered system. A study of correlation in random Ising model will be published elsewhere.

Our formulae involve connectivity constant of the lattice. If, instead of using Bethe lattice value of the connectivity constant, we use the exact value deduced numerically, we can improve upon the Elliott-Marshall calculation. The Curie temperatures are reduced by an order of 10%. Further, the constant $r_{\|}^2$ occurring in the formula for longitudinal susceptibility is also reduced, bringing it closer to experimental values.

2. Correlation function on a Bethe lattice

We consider the Hamiltonian

$$H = -\sum_{(ij)} J_{ij}\sigma_i\sigma_j \tag{1}$$

where $\sum_{(ij)}$ denotes summation over all the bonds on the lattice, J_{ij} is the exchange constant, which is taken to be same for all the bonds, and σ_i's are the spin variables which take two values ± 1. We are interested in calculating the correlation function C_{pq} defined as

$$C_{pq} = \frac{\mathrm{Tr}\,(e^{-\beta H}\sigma_p\sigma_q)}{\mathrm{Tr}\,(e^{-\beta H})} . \tag{2}$$

Equation (2) can be recast in a different form in the following manner (Hill 1956)

$$C_{pq} = \frac{\mathrm{Tr}\,[\exp(\beta \sum_{(ij)} J_{ij}\sigma_i\sigma_j)\,\sigma_p\sigma_q]}{\mathrm{Tr}\,[\exp(\beta \sum_{(ij)} J_{ij}\sigma_i\sigma_j)]}$$

$$= \frac{\mathrm{Tr}\,[\prod_{(i\,j)} \cosh\beta J_{ij}\,[1 + \sigma_i\sigma_j \tanh\beta J_{ij}]\,\sigma_p\sigma_q]}{\mathrm{Tr}\,[\prod_{(i,j)} \cosh\beta J_{ij}\,[1 + \sigma_i\sigma_j \tanh\beta J_{ij}]]} \tag{3}$$

$$= \frac{\mathrm{Tr}\,[\prod_{(i,j)} (1 + w_{ij}\sigma_i\sigma_j)\,\sigma_p\sigma_q]}{\mathrm{Tr}\,[\prod_{(i,j)} (1 + w_{ij}\sigma_i\sigma_j)]} \tag{4}$$

where w_{ij} stands for $\tanh\beta J_{ij}$. This expression can be evaluated by means of graph theoretical methods developed by Englert [Englert 1963, Stell 1964]. It can be easily shown that diagrammatically the correlation function is the sum of the contributions of all the connected graphs rooted at points p and q. A bond between two sites occur just once and gives a factor w_{ij} — A vertex at which n

bonds meet gives a contribution $M_n^{(o)}$, where $M_n^{(o)}$ is the cumulant average

$$M_n^{(o)} = \langle \sigma_i^n \rangle_c \tag{5}$$

Above Curie temperature and in the absence of magnetic field,

$$M_1^{(o)} = 0$$

$$M_2^{(o)} = 1. \tag{6}$$

In order to motivate the approximation we shall evaluate eq. (4) for a Bethe lattice of coordination number $Z = K + 1$. Since there are no closed paths in a Bethe lattice and there is only one self-avoiding path between any two sites, we have

$$C_{pq} = w_{pi} w_{ij} w_{jk} \cdots w_{mq} [M_2^{(o)}]^n \tag{7}$$

$$= w^n \tag{8}$$

where n is the number of nearest neighbour bonds required to connect sites p and q on the Bethe lattice. We can now calculate the static susceptibility which is given by the formula

$$\frac{\chi}{\beta N (g\mu_0)^2} = 1 + \sum_{r \neq o} C_r \tag{9}$$

where $g\mu_0\sigma_i$ is the magnetic moment associated at the site i and N is the total number of sites. The sum in eq. (9) can be easily performed by noting that the number of points seperated by n bonds lengths from a given origin is $(K+1)\, K^{n-1}$, where $\bar{z} = K + 1$ is the coordination number of the lattice.
Equation (9) becomes

$$\frac{\chi}{N\beta (g\mu_0)^2} = 1 + \sum_{n=1}^{N} (K+1)\, K^{n-1}\, w^n$$

$$= 1 + (K+1)\, \frac{w\,(1 - (Kw)^{N+1})}{1 - Kw} = \frac{1+w}{1-Kw} \tag{10}$$

Equation (10) leads to the following Curie temperature

$$\frac{kT_c}{J} = \left[\tanh^{-1} \frac{1}{Z-1} \right]^{-1} \tag{11}$$

Both the results in eqs (10) and (11) are identical to those obtained by the usual cluster treatment of Bethe-Peierls approximation.

3. Correlation function for real lattices

For a real lattice, the number of diagrams contributing to C_{pq} increases manifold, and their enumerations become a very difficult problem. Horwitz and Callen (1961) and Englert (1963) have introduced the procedures of vertex renor-

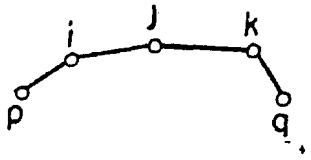

Figure 1. A typical diagram contributing to the correlation function C_{pq}.

malisation and bond renormalisation which considerably reduce the class of diagrams to be considered and ensure the internal consistency of any approximation. However the actual carrying out of these procedures still remains very difficult and has not been gone through. In view of this we propose the following approximation. Even for real lattices, we consider the same set of diagrams that made contribution in Bethe lattice. This set of diagrams is essentially same as was used by Brout for high density expansion of Ising model (Brout 1965). The typical diagram is shown in figure 1. Then we obtain

$$C_{pq} = w_{pq} + \sum_{i}{}' w_{pi}\, w_{iq} + \sum_{ij}{}' w_{pi}\, w_{ij}\, w_{jq} + \cdots \tag{12}$$

where prime on summation indicates that none of the indices being summed can be equal among themselves or equal to p or q. Equation (12) would be a simple iterative equation but for the summation restrictions. We can convert it into an approximate integral equation by multiplying by connectivity constant K, where K^n gives approximately the number of self avoiding walks of n steps for large n. Thus we write

$$C_{pq} = w_{pq} + \frac{K}{Z}\sum_{i} w_{pi}\, C_{iq}. \tag{13}$$

Equation (13) can be solved by taking Fourier transform. It yields the following expression for the correlation function

$$\begin{aligned} C(q) &= \frac{Z\, ws(q)}{1 - Kws(q)} \\ &= \frac{Zs(q)\tanh \beta J}{1 - K\tanh(\beta J)\, s(q)} \end{aligned} \tag{14}$$

when

$$s(q) = \frac{1}{Z}\sum_{\vec{\delta}} e^{iq\vec{\delta}} \tag{15}$$

where δ's denote the nearest neighbour lattice vectors. The wave vector dependent susceptibility $\chi(q)$ is given by

$$\begin{aligned} \chi(q)/\chi_0 &= 1 + C(q) \\ &= \frac{1 + (Z - K)\, s(q)\tanh \beta J}{1 - K\tanh \beta J s(q)} \end{aligned} \tag{16}$$

Here χ_0 denotes $N(g\mu_0)^2\,\beta$.

4. Discussion

Equations (14) and (16) are the main results of this paper. Several points should now be noted. Firstly, for high temperatures, *i.e.*, $\beta J \ll 1$, eq. (14) essentially reduces to Ornstein-Zernike approximation

$$C(q) = \frac{\beta J s(q)}{1 - \beta J s(q)} \tag{17}$$

where we have put $K = Z - 1$. In order to compare our results with the earlier theories, we put our results in the standard form for small wavevectors (Van Hove 1954).

$$\frac{\chi(q)}{\chi_0} = \frac{3}{4 r_{\|}^2} \frac{1}{K_{\|}^2 + q^2} \tag{18}$$

we find

$$a^2 K_{\|}^2 = \frac{Z}{2K} \frac{1 - K \tanh \beta J}{\tanh \beta J} \tag{19}$$

and

$$r_{\|}^2/a^2 = \frac{3K}{2Z} \frac{\tanh \beta J}{1 + (Z - K) \tanh \beta J} \tag{20}$$

where a denotes the lattice constant.
Now if we use for K, the Bethe lattice value $Z - 1$, we get

$$a^2 K_{\|}^2 = \frac{Z}{2(Z-1)} \frac{2 - Z(1 - e^{-2\beta J})}{1 - e^{-2\beta J}} \tag{21}$$

and

$$\frac{r_{\|}^2}{a^2} = \frac{3(Z-1)}{4Z} (1 - e^{-2\beta J}) \tag{22}$$

On the other hand, the results obtained by Oguchi and Ono are

$$a^2 \cdot K_{\|}^2 = \frac{Z}{Z+1} \frac{2 - Z(1 - e^{-2\beta J})}{1 - e^{-\beta J}} \tag{23}$$

and

$$r_{\|}^2/a^2 = \frac{3(Z+1)}{2Z} (1 - e^{-2\beta J}) \tag{24}$$

Though the temperature dependences of the two quantities $r_{\|}$ and $K_{\|}$ are same, the numerical factors differ, by a factor of 2 or so.

We expect that if for real lattices true values of K are used better results will be obtained. Numerical methods give a value $K = 4{\cdot}5$ for simple cubic lattice. Thus, the Curie temperature in our approximation is lowered by 10% for S.C. lattice. In figures 2 and 3, we have plotted our results $(K_{\|}a)^2$ *vs.* T and $r_{\|}^2/a^2$ *vs.* T. On the same diagrams are also plotted the results of Oguchi and Ono. Our results for $r_{\|}^2$ are some-what lower than theirs. Although we have only considered an Ising model of spin $\frac{1}{2}$, our results are in better agreement with the

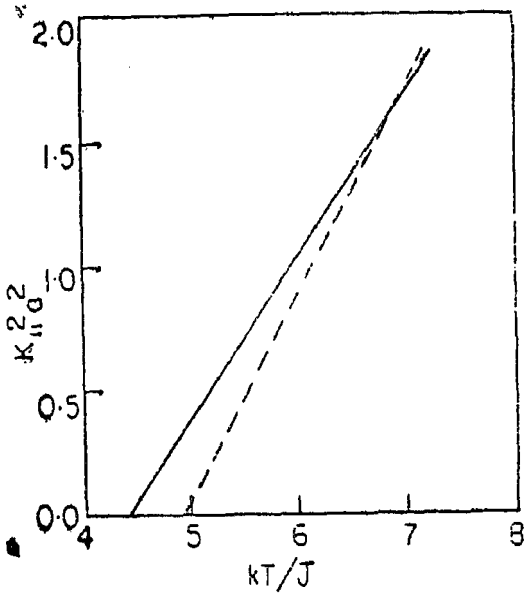

Figure 2. Plot of $(K_{\|}^2\, a^2)^{-1}$ with temperature. For comparison, also shown results due to Oguchi and Ono. Solid line shows our results and dotted line shows Oguchi and Ono's results.

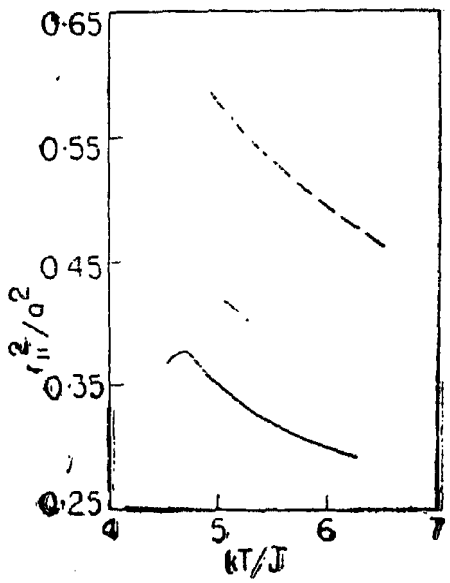

Figure 3. Plot of $r_{\|}^2/a^2$ with temperature. For comparison, also shown are the results of Oguchi and Ono. Solid line shows our results and dotted line shows Oguchi and Ono's results.

neutron scattering measurements on iron. Experimentally measured values for $r_{\|}$ in iron (Marshall and Lowde 1968, Oguchi and Ono 1966) are around 1·4 Å while our theory gives 1·6 Å.

This method can be easily generalised to temperatures below T_c. The only change is that we have to use cumulants $M_2^{(0)}$ which are appropriate in the presence of spontaneous magnetisation. This matter will be pursued and reported separately.

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