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LETTER TO THE EDITOR

Wavevector dependence of fluctuations in the cluster approximation

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Abstract. The self-consistent cluster approximation for the Ising model is extended to obtain the wavevector dependence of the fluctuations. When the method is applied to the one-dimensional Ising model the result for the wavevector-dependent susceptibility is the exact result.

The cluster approximation has been used in recent years to calculate the properties of systems where short-range forces are important (Blinc and Svetina 1966, Tokunaga and Matsubara 1966, Burley 1972, Klein *et al* 1979). To the best of our knowledge, however, the cluster method has been used to calculate only fluctuations in the zero-wavevector limit. In this note the static zero wavevector cluster approximation is extended to nonzero wavevectors. The cluster approximation used was the self-consistent approximation developed by Strieb *et al* (1963) and we apply it in detail to a one-dimensional system. We show that the two-particle cluster approximation for the generalised susceptibility gives results which are identical to the exact one-dimensional Ising solution (Suzuki and Kubo 1968).

We consider a one-dimensional system of interacting Ising spins which are represented by the z-component of the spin variables $\{Z_i = \pm 1\}$. We apply a two-particle cluster approximation to this system and so divide the linear chain into clusters, each containing two spins, when the Hamiltonian of the system is written

$$H = -\sum_{\substack{ji \\ \alpha\beta}} J_{ij}^{\alpha\beta} Z_i^\alpha Z_j^\beta - \mu \sum_{i\alpha} E_i^\alpha Z_i^\alpha \qquad (1)$$

where $\alpha, \beta = 1, 2$ ($\alpha \neq \beta$) represent the two spins in the cluster and i or j are the indices of the different clusters. The field E_i^α is an external field acting on spin α in the ith cluster.

The self-consistent cluster approximation treats the interaction between the spins inside the cluster exactly, but the interaction with spins outside the cluster are averaged in a self-consistent way. Thus the Hamiltonian (1) is approximated by the two-particle cluster Hamiltonian

$$H_2 = -J_{ii}^{\alpha\beta} Z_i^\alpha Z_i^\beta + J_{ij}^{\alpha\beta} Z_i^\alpha \bar{Z}_j^\beta + \mu E_i^\alpha Z_i^\alpha \qquad (2)$$

where the first term in equation (2) represents the exact interaction between the spins

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in the ith cluster, the second term is the interaction of the (i, α) spin with a (j, β) spin outside the cluster and $\bar{Z}_j^\beta$ is the averaged cluster field which is calculated self-consistently. From equation (2) it follows that

$$\langle Z_i^\alpha \rangle_2 \equiv \mathrm{Tr}\, Z_i^\alpha \exp(-\beta H_2)/\mathrm{Tr} \exp(-\beta H_2) - \langle \tanh \beta \bar{E}_i^\alpha \rangle_2 \tag{3}$$

where

$$\bar{E}_i^\alpha = J_{ii}^{\alpha\beta} Z_i^\beta + J_{ij}^{\alpha\beta} \bar{Z}_j^\beta + \mu E_i^\alpha \equiv J_{ii}^{\alpha\beta} Z_i^\beta + \mu F_i^\alpha.$$

The operator in equation (3) can be written in the form

$$\tanh \beta \bar{E}_i^\alpha = X_i + Y_i Z_i^\beta \tag{4}$$

where

$$\begin{aligned} X_i &= \tfrac{1}{2}[\tanh \beta(J_{ii}^{\alpha\beta} + \mu F_i^\alpha) - \tanh \beta(J_{ii}^{\alpha\beta} - \mu F_i^\alpha)] \\ Y_i &= \tfrac{1}{2}[\tanh \beta(J_{ii}^{\alpha\beta} + \mu F_i^\alpha) + \tanh \beta(J_{ii}^{\alpha\beta} - \mu F_i^\alpha]. \end{aligned} \tag{5}$$

Above the transition temperature T_c (here $T_c = 0$) when $E_i^\alpha \to 0$, $F_i^\alpha \to 0$ and therefore

$$X_i \simeq \beta\mu F_i^\alpha/\cosh^2 \beta J \qquad Y_i \simeq \tanh \beta J \tag{6}$$

where we assumed that the interactions between the spins are equal: $J_{ii}^{\alpha\beta} \equiv J$. When equations (4) and (6) are substituted into equation (2) and the result averaged, then

$$\langle Z_i^\alpha \rangle_2 = (\beta/\cosh^2 \beta J)(J_{ij}^{\alpha\beta} \bar{Z}_j^\beta + \mu E_i^\alpha) + \tanh \beta J \langle Z_i^\beta \rangle_2. \tag{7}$$

The determination of $\bar{Z}_j^\beta$ depends on the specific method which is used to make the cluster approximation self-consistent (Strieb *et al* 1963). Here we use the approach proposed and shown to be successful by Blinc and Svetina (1966), namely

$$\langle Z_j^\alpha \rangle_2 = \langle Z_j^\alpha \rangle_1 \tag{8}$$

where $\langle Z_i^\alpha \rangle_1$ is the statistical average calculated by the effective one-spin cluster Hamiltonian, which is given by

$$H_1 = 2J_{ij}^{\alpha\beta} \bar{Z}_j^\beta + \mu E_i^\alpha Z_i^\alpha. \tag{9}$$

From equation (9) it follows that for $T > T_c$

$$\langle Z_i^\alpha \rangle = 2\beta J_{ij}^{\alpha\beta} \bar{Z}_j^\beta + \beta\mu E_i^\alpha. \tag{10}$$

Substituting equations (10) and (8) into (7) gives

$$\langle Z_i^\alpha \rangle_2 = (1/2 \cosh^2 \beta J)(\langle Z_i^\alpha \rangle_2 + \beta\mu E_i^\alpha) + \tanh \beta J (Z_i^\beta \rangle_2. \tag{11}$$

After taking the Fourier transform of equation (11) and averaging, because of symmetry requirements, over the two possible orientations of the cluster (spin Z_i^2 to the right of spin Z_i^1 and Z_i^2 to the left of spin Z_i^1), we obtain

$$\langle Z_q^\alpha \rangle = (1/2 \cosh^2 \beta J)(\langle Z_q^\alpha \rangle + \beta\mu E_q^\alpha) + \tanh \beta J \langle Z_q^\beta \rangle \cos q\pi. \tag{12}$$

If $E_q^1 = E_q^2$, then $\langle Z_q^1 \rangle = \langle Z_q^2 \rangle$ and we get the following expression for the wavevector dependence of the susceptibility

$$\chi_q \equiv (\langle Z_q^\alpha \rangle/\mu E_q^\alpha) = \beta/(\cosh 2\beta J + \sinh 2\beta J \cos \pi q). \tag{13}$$

Equation (13) is the exact result for the one-dimensional Ising model (Suzuki and Kubo

1968). It is interesting to note that, whereas the conventional derivation of this result (Suzuki and Kubo 1968) involves two-spin correlations, the present approach does not.

The above approach can be generalised to two- and three- dimensional systems, but then equation (4) becomes more complicated. It involves either an approximation or higher correlation functions between the spins, which must then be obtained self-consistently. Although the results do not then coincide with the exact results, the surprising success of these methods in one dimension leads us to suggest that the results may give good account of the wavevector-dependent susceptibility. The wavevector dependence of the susceptibility of KD_2PO_4 using a four-cluster approximation will be published soon.

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