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1985 J. Phys. A: Math. Gen. 18 1733

(http://iopscience.iop.org/0305-4470/18/10/026)

J. Phys. A: Math. Gen. **18** (1985) 1733-1740. Printed in Great Britain

New consistency equations for lattice models

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Received 20 July 1984, in final form 20 November 1984

Abstract. New consistency equations involving the internal energy and—when possible—the order parameter are proposed for lattice models; these equations are shown to be very efficient in classical examples such as the two- and three-dimensional Ising model. However, their peculiarity is that they can also be applied to models where the order parameter is unknown and, consequently, any mean-field approach is ruled out. Applications to the self-avoiding walk and surface models are shown to be successful.

1. Introduction

A typical procedure to describe the thermodynamics of lattice models whose phase transition can be characterised by an order parameter amounts to writing down approximate consistency equations involving the order parameter. For instance, in the standard mean-field approximation the original model is approximated by a 'one-body' problem in an effective field, which is determined in a self-consistent way. Improvements can be obtained considering more sophisticated approximate equations of state, which involve clusters with more than 'one body', but they still only include the magnetisation as a fundamental object (Domb 1960).

Much attention has been paid in the literature to the application of these methods to spin and gauge models; in most cases the 'magnetisation' was considered as the order parameter, although for a large variety of statistical lattice models, like the gauge ones, it does not play the role of a true order parameter (for a review and references see Drouffe and Zuber (1983)).

As far as we know there were no previous attempts to improve standard mean-field methods using correlation functions other than the 'magnetisation'.

In this paper we want to propose such an improvement, in particular keeping an eye on models where a local order parameter does not exist, such as the self-avoiding walk and surface models.

The idea is basically the same as the one underlying the mean-field approximation, but now we want to look for more general equations of state, which can include many correlation functions in a cluster of many sites.

0305-4470/85/101733+08$02.25

2. The two- and three-dimensional Ising model

The best way to present this method is to consider the Ising model on a square lattice, whose reduced Hamiltonian is

$$H = K \sum_{\langle i,j \rangle} \sigma_i \sigma_j \qquad \sigma_i = \pm 1 \tag{1}$$

where the sum runs over nearest-neighbour sites and K is the reduced coupling constant.

We are going to approximate this model in a finite 3×3 cluster, with free boundary conditions (figure 1), where the effect of the infinite lattice is taken into account by introducing two different couplings, K' and K'', on the internal and boundary links respectively; in other words we approximate the original model (1) with the Hamiltonian

$$H_0 = K' \sigma_0 \sum_{i=1}^{4} \sigma_{2i} + K'' \sum_{i=1}^{8} \sigma_i \sigma_{i+1} \tag{1a}$$

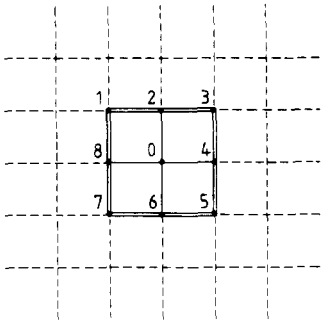

Figure 1. Sublattice considered for the two-dimensional Ising model and for the SAW model. An effective coupling K'' (K') is associated to the bonds drawn with a double (single) line.

where $\sigma_9 \equiv \sigma_1$. The physical idea is to restore translational invariance in a finite cluster without using periodic boundary conditions†. In order to obtain an approximation as simple as the mean-field one, but with the essential ingredients of our main idea, in this paper we restrict ourselves to the simplest case of requiring translational invariance for the internal energy, i.e.

$$\langle \sigma_1 \sigma_2 \rangle_{K',K''} = \langle \sigma_0 \sigma_8 \rangle_{K',K''}. \tag{2}$$

Due to the symmetry of the problem this choice is completely general. Equation (2) allows us to express K' as a function of K'', thus leading to only one free parameter. On clusters of increasing size the natural choice should be to assign the coupling K'' only to the boundary links and to identify the bulk coupling, K', with the original one, K; however, for small clusters another convenient recipe, which we will follow here, is to consider the weighted average of the couplings K' and K'', i.e., for the cluster in figure 1,

$$K = \tfrac{1}{3}(2K'' + K'). \tag{3}$$

† This is reminiscent of the Bethe–Peierls approximation (Huang 1963) where translational invariance is imposed on the magnetisation.

The result is a clear bump in the specific heat at $K_c' = 0.387$ (which, using equation (3), corresponds to $K_c = 0.47$)

$$\frac{C}{k_B N_s} = \frac{N_b}{N_s} K^2 \frac{\partial}{\partial K} U(K) \tag{4}$$

where N_s and N_b are respectively the number of the sites and bonds of the cluster in figure 1, k_B is the Boltzmann constant and $U(K)$ is the common value of the Green functions in equation (2).

As is usual in finite cluster calculations (Ferdinand and Fisher 1969), this bump should be interpreted as a signal of a phase transition at $K_c = 0.47$ (to be compared with the exact critical coupling $K_c = 0.4407$). In this particular case where the order parameter is well defined, one can easily improve the thermodynamics by taking into account a further consistency equation for the magnetic field h acting on the boundary variables in the cluster pictured in figure 1. The Hamiltonian for such a cluster can be written as follows

$$H_1 = K'\sigma_0 \sum_{i=1}^{4} \sigma_{2i} + K'' \sum_{i=1}^{8} \sigma_i \sigma_{i+1} + h \sum_{i=1}^{4} (\sigma_{2i} + 2\sigma_{2i-1}). \tag{5}$$

Now, the consistency equations are

$$U(K) \equiv \langle \sigma_1 \sigma_2 \rangle_{K',K'',h} = \langle \sigma_0 \sigma_8 \rangle_{K',K'',h} \tag{6a}$$

$$m(K) \equiv \langle \sigma_0 \rangle_{K',K'',h} = \tfrac{1}{2}(\langle \sigma_1 \rangle_{K',K'',h} + \langle \sigma_2 \rangle_{K',K'',h}) \tag{6b}$$

where $m(K)$ stands for the magnetisation. (In principle one should use two different fields h_1 and h_2 in the sites (1, 3, 5, 7) and (2, 4, 6, 8), so as to impose $\langle \sigma_0 \rangle = \langle \sigma_1 \rangle = \langle \sigma_2 \rangle$. However we have limited our analysis to equations (6*a*), (6*b*) to avoid the introduction of too many parameters.) The introduction of equation (6*b*) significantly modifies the result previously obtained for the specific heat and furthermore allows us to calculate the magnetisation.

We report in figure 2 the result for the specific heat. The exact and the Bethe-Peierls approximation results are also reported for comparison.

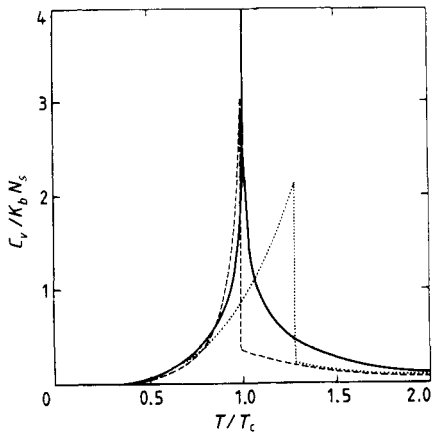

Figure 2. Specific heat for the two-dimensional Ising model obtained in our approximation (broken curve); in the Bethe-Peierls approximation (dotted curve); and in the Onsager solution (full curve).

A comparable improvement with respect to the Bethe-Peierls approximation is also provided by our method for the magnetisation.

We want to point out that these results are definitely better than those obtained by standard consistency equations (Domb 1960).

In particular we obtain a critical coupling $K_c = 0.447$ ($K' = 0.392$) and a jump in the specific heat $(\Delta C/k_B N_s)|_{K=K_c} = 2.7$, whose maximum value is $(C_{max}/K_B N_s)|_{K=K_c} \simeq 3$, which is qualitatively comparable with the results obtained on a periodic 64×64 square sublattice (Ferdinand and Fisher 1969).

It is worthwhile to look at the behaviour of the quantity $R = (1 - K'/K'')$ as a function of K, because one can infer how K'' and h simulate the effect of the spins surrounding the cluster in figure 1. As shown in figure 3, R increases up to $K = K_c$; in this region the effective external coupling K'', which simulates the effect of the surrounding lattice, increases faster than K'; at $K \geqslant K_c$ a spontaneous magnetisation occurs and h is different from zero; R decreases because the ordering effect is now also due to the effective magnetic field h; finally as the spontaneous magnetisation saturates, R increases again.

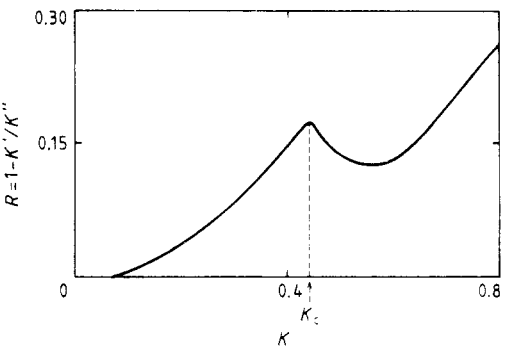

Figure 3. Behaviour of $R = (K'' - K')/K'$ as a function of $K = (2K'' + K')/3$ for the Ising model.

Without complicating the geometry of the cluster, we have also applied this method to the $d = 3$ case, embedding the cluster of figure 1 in a cubic lattice simply adding transverse effective magnetic fields h with proper multiplicity on each site.

The resulting effective Hamiltonian is:

$$H_2 = K'\sigma_0 \sum_{i=1}^{4} \sigma_{2i} + K'' \sum_{i=1}^{8} \sigma_i \sigma_{i+1} + h\left(2\sigma_0 + 3\sum_{i=1}^{4} \sigma_{2i} + 4\sum_{i=1}^{4} \sigma_{2i-1}\right) \qquad (7)$$

and, using equations (6*a*) and (6*b*) and this new Hamiltonian, we have obtained the critical coupling $K_c = 0.218$ ($K_c' = 0.211$) to be compared with the best known estimate, $K_c = 0.221$ (Pawley *et al* 1984). Also in this case the thermodynamic properties are significantly better than the usual mean-field approximation.

It is straightforward to verify that, embedding the cluster of figure 1 in a d-dimensional lattice, by simply adding transverse magnetic fields, in the $d \to \infty$ limit the mean-field result is recovered.

3. The self-avoiding walk model

We think that our method should be more appreciated when one is concerned with models where the order parameter is unknown or probably does not exist.

Let us consider a model which has this typical feature—the well known self-avoiding walk (SAW) (De Gennes 1979). We restrict ourselves to a square lattice and define a two-point correlation function (generating function)

$$G(x, y; K) = \sum_{W: \partial W = \{x,y\}} K^{|W|} \tag{8}$$

where the sum runs over all the non-self-intersecting walks, whose elementary steps link nearest-neighbour sites and whose end points are x and y.

The statistical weight associated to a walk W composed of $|W|$ steps is $K^{|W|}$ where K is the so-called monomer fugacity. From Hammersley theorem (Hammersley 1961) it is known that equation (8) is convergent as far as $0 < K < K_c$, where K_c is some 'critical' value less than 1. Furthermore, if we define in strict analogy with the spin models the 'internal energy'

$$U(K) = K \sum_{\hat{\mu}=1}^{d} G(x, x+\hat{\mu}; K) \tag{9}$$

where $\hat{\mu}$ are the unit vectors in the directions of the lattice axes it is believed that

$$U(K) \underset{K \to K_c}{=} \text{constant} \times (K_c - K)^{1-\alpha} + (\text{regular terms}) \tag{10}$$

where α is a critical index, which is 0.5 in two dimensions (De Gennes 1979).

Now let us apply the method discussed for the Ising model, using only the two-point correlation function. We consider the same cluster as in the previous section (figure 1) and the consistency equation is now

$$G(1, 2; K', K'') = G(0, 8; K', K'') \tag{11}$$

where the effective fugacities K' and K'' refer to the internal and external links respectively. In analogy with the Ising case K' and K'' are connected to the original coupling by the same relation (3).

Fixing K' in equation (11) one obtains the corresponding value of K''; if one follows this solution continuously for increasing values of K', it disappears at $K' \simeq 0.406$.

According to Hammersley theorem this can be interpreted as the transition point, above which equation (9) is not defined; this corresponds to the critical value $K_c = 0.64$. Defining $G(x, x+\hat{\mu}; K)$ in equation (9) as the common value of both sides of equation (11) one obtains $U(K)$ (figure 4), which obeys equation (10) with $\alpha = \frac{1}{2}$. These results are to be compared with the accepted values $\alpha = \frac{1}{2}$ and $K_c = 0.38$ (De Gennes 1979).

Unfortunately, the coincidence of the value of α with the accepted one seems to be quite accidental, because using simple general arguments our method predicts $\alpha = \frac{1}{2}$ in any dimension. Moreover the inaccuracy in the determination of K is due to the poor statistics allowed by our small cluster and by the constraint imposed on the walk to be self-avoiding. There are various recipes to improve this result: one could enlarge the size of the cluster without introducing further consistency equations and/or one could require consistency equations on an enlarged parameter space (Cappelli *et al* 1985).

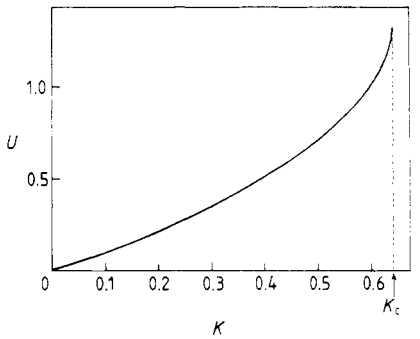

Figure 4. 'Internal energy' for the SAW model obtained by applying our method to the sublattice pictured in figure 1.

Anyway, we want to stress that the important feature of our method is to give a phase transition for the SAW model in qualitative agreement with the expected one. In fact if, for example, one tried to infer some information on this phase transition looking at the specific heat $C = \partial U(K)/\partial K$ using a cluster with periodic boundary conditions (in analogy with the calculations for the Ising model by Ferdinand and Fisher 1969) one could not obtain any signal of a critical point; this is due to the fact that $C(K)$ is a polynomial in K with positive coefficients.

4. Self-avoiding surfaces

A generalisation of the SAW is given by the self-avoiding surfaces (SAS) model.

They are built up by elementary squares (plaquettes) P on a hypercubic lattice with the constraint that each bond b of a surface S is shared by two plaquettes, unless $b \in \partial S$. In this latter case b belongs to only one plaquette. A fugacity K is associated to each plaquette belonging to S; the correlation functions can be defined like in the SAW model. For our purpose we need only the Green function associated to a closed non-intersecting path

$$G(\gamma) = \sum_{S:\partial S=\gamma} K^{|S|} \tag{12}$$

where the sum runs over all the SAS, S, of area $|S|$ and boundary $\partial S = \gamma$†. In particular we are interested in the 'internal energy'

$$U(K) = K \sum_{\hat{\mu}<\hat{\nu}} \sum_{S:\partial S=\partial P_{\mu\nu}} K^{|S|} = \tfrac{1}{2}Kd(d-1)G(\partial P) \tag{13}$$

where $P_{\hat{\mu}\hat{\nu}}$ is a fixed plaquette in the $(\hat{\mu}, \hat{\nu})$ coordinate plane and U is expected to have the same behaviour as described in equation (10).

In order to apply our method to this model in three dimensions we use the cubic cluster pictured in figure 5; K'' and K' represent the effective fugacities of the boundary and internal plaquettes respectively.

† The straightforward generalisation of the Hammersley theorem for this model was given by Durhuus *et al* (1983). It implies that the sum in equation (12) is convergent for $0 < K < K_c < 1$.

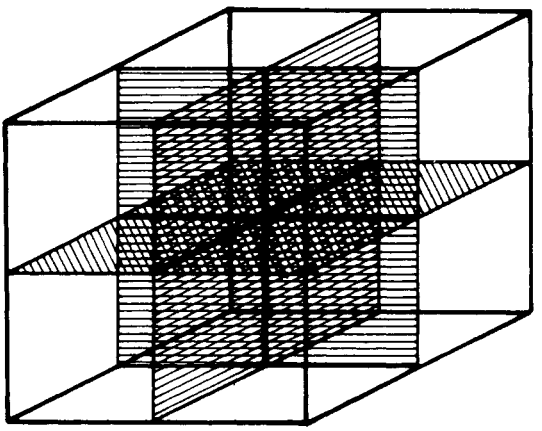

Figure 5. Sublattice used for the three-dimensional SAS model. The effective fugacity $K''(K')$ is associated with the boundary (internal) plaquettes.

In this case we also impose a consistency equation in the form

$$G(\partial P') = G(\partial P) \tag{14}$$

where P' and P are one of the boundary and internal plaquettes respectively. The common value obtained from equation (14) inserted in equation (12) provides the internal energy $U(K)$ (figure 6), where, as usual, K is defined as the weighted average of the effective couplings K'' and K':

$$K = \tfrac{1}{7}(4K'' + 3K'). \tag{15}$$

Also in this case we recover the behaviour described by equation (10) with $\alpha = \frac{1}{2}$ and $K_c = 0.623$, $K_c' = 0.537$ to be compared with the Monte Carlo estimate $K_c = 0.588$ (Greensite and Sterling 1983) and $K_c = 0.62$–0.64 obtained from renormalisation group calculations (Maritan and Stella 1984). Concerning the value of α, as in the SAW case, it does not change with the dimension in our method. The significantly better estimate of K_c with respect to the SAW case is due to the higher statistics allowed in the considered cluster.

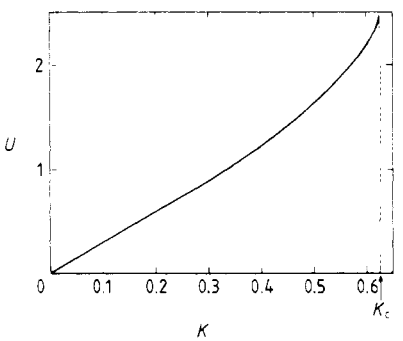

Figure 6. 'Internal energy' for the SAS model obtained by applying our method to the sublattice pictured in figure 5.

5. Conclusions

We have considered new consistency equations for lattice models which present the following main features.

They significantly improve mean-field methods for models where the order parameter is well defined, like in the Ising model; but, what is more relevant, they are also able to predict in a simple way a phase transition for those models, like the SAW and SAS, where it is not clear what the order parameter should be.

In these two last cases the non-analyticity in the thermodynamic quantities, like the 'specific heat', is provided just by the self-consistency equation for the two-point Green functions.

We think that the extension of such a technique to frustrated systems and to gauge models should be quite interesting (Capelli *et al* 1985).

Acknowledgments

We are indebted to G Parisi for determinant discussions and for his warm interest in this work.

We acknowledge, moreover, useful discussions with A Cappelli and A Stella.

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