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LETTER TO THE EDITOR

Star lattice constant expansions for magnetic models

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Abstract. It is shown by a direct method that if the free energy of the Ising model of spin $\frac{1}{2}$ is expanded as a function of the magnetization and temperature, only star lattice constants enter in the expansion. It is deduced that the same property holds for the Potts model; there are indications that it also holds for the D spin classical vector models.

In the classical perturbation expansion for a condensing gas there are two successive stages of simplification. The first uses the activity λ, as expansion variable, and obtains a series for the logarithm of the grand partition function whose coefficients are cluster integrals. The second transforms to the density, ρ, as expansion variable, and obtains a corresponding series whose coefficients are irreducible cluster integrals. In graph theory terminology the activity expansion involves *connected* graphs, and the density expansion *star* graphs (see, eg, Uhlenbeck and Ford 1962).

This theory was first applied to the lattice gas or Ising model of spin $\frac{1}{2}$ by Fuchs (1942) and was further developed by Yvon (1945, 1948), Rushbrooke and Scoins (1955) and Domb and Hiley (1962). For a lattice model the terms of the series expansions can be expressed in terms of *lattice constants* or *embeddings* (see, eg, Domb 1974, chap 1). The parallel to the first expansion above uses the magnetic field H as variable (the direct analogue of λ is $\exp(-\beta m_0 H)$, where m_0 is the magnetic moment of a spin, and $\beta = 1/kT$), and it involves connected lattice constants. The parallel to the second expansion uses the magnetization per particle, m, as variable (the direct analogue of ρ is $\frac{1}{2}(1-m/m_0)$), and it involves only star lattice constants (see, eg, Domb 1974, chap 6)

In the classical theory, which is concerned with a point grouping of graphs, the elimination of articulated graphs does not effect a great saving in diagrams. For lattice models which are largely concerned with line grouping of graphs the saving is much greater; this is one of the reasons why series expansions have been extended so much further for lattice models (Domb 1971).

It is our aim in the present letter to give an independent demonstration that changing to the magnetization as variable eliminates all articulated lattice constants. In this way we gain new insight into the reason for the property, and how it can be generalized to other models.

The logarithm of the partition function for any short-range interacting model on a lattice L can be expanded in the form

$$\ln Z(L) = \sum_r w(c_r)(c_r;L), \tag{1}$$

where the c_r are connected graphs. Here $(c_r;L)$ represent weak lattice constants, and $w(c_r)$ are weighting functions depending on c_r but not on L, which can be calculated from the partition functions of c_r and its sub-graphs. Expansion (1) reduces to a star graph expansion

$$\ln Z(L) = \sum_r w(s_r)(s_r;L), \tag{2}$$

where the s_r are star graphs if the weight of any articulated graph is zero; this will be ensured if the partition function of any articulated graph $c_r \circ c_s$ formed by identifying

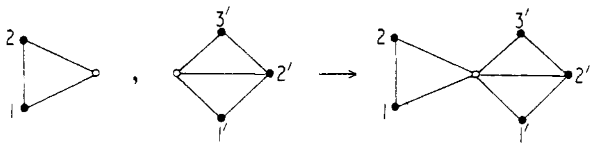

Figure 1.

one vertex on c_r and c_s (see, eg, figure 1) is simply related to the product of the partition functions of the constituents c_r and c_s,

$$Z(c_r \circ c_s) = A\,Z(c_r)Z(c_s), \tag{3}$$

where A depends on the spin at the articulation point O but is independent of the individual c_r and c_s. (The above results will be found in Domb (1974, chap 1) where a number of examples of their application are given.)

Consider now the behaviour of the articulated graph $c_r \circ c_s$ for the Ising model. When $H = 0$ it is clear that relation (3) is satisfied with $A = \frac{1}{2}$. When the *field H* is constant and nonzero the magnetization varies from vertex to vertex and there is no simple relation between the partition function $Z(c_r \circ c_s)$ and the constituents $Z(c_r)$ and $Z(c_s)$. However, let us consider a more general situation in which H is allowed to vary from vertex to vertex but control is exercised on the articulated spin 0 by fixing the probabilities p_+ and p_- of up and down spins. Then it is clear that for any particular set of fields the behaviour of the individual spins in $(c_r \circ c_s)$ is the same as in the original c_r and c_s. In fact it is easy to establish the relation

$$Z(c_r \circ c_s) = \frac{p_+{}^3 + p_-{}^3}{p_-{}^2 + p_-{}^2}\, Z(c_r)Z(c_s) \tag{4}$$

which is of the form (3).

Now p_+ and p_- are uniquely determined by the magnetization m of the spin 0. Thus at constant *magnetization* relation (3) is satisfied A being a function of magnetization. This means that the expansion of the free energy as a function of (m,T) contains only star lattice constants, and likewise the equation of state

$$H = H(m,T). \tag{5}$$

The above property is particularly useful for high temperature expansions of the susceptibility and its derivatives in zero field. Inverting $(\partial H/\partial m)_0$, $(\partial^3 H/\partial m^3)_0$, $(\partial^5 H/\partial m^5)_0$, . . . we find that $1/\chi_0$, $\chi_0{}^{(2)}/\chi_0{}^{(4)}$, $\chi_0{}^{(4)}/\chi_0{}^6 - 10\chi_0{}^{(2)2}/\chi_0{}^7$, . . . all have star lattice constant expansions. Here $\chi_0 = (\partial m/\partial H)_0$ and $\chi_0{}^{(s)} = \partial^s \chi_0/\partial H^s$.

It is clear that the above argument can be generalized to any model with two energy levels, and thus to the q state Potts model (Potts 1952, Mittag and Stephen 1971). For a model with three energy levels, eg the Ising model of spin 1, it is necessary to control the probabilities of occupation of each level and this involves introducing a second density; for a model with t energy levels we need $(t-1)$ densities.

For the D spin classical vector model (eg Stanley 1969) it is easy to show that relation (3) is valid in zero field (Domb 1974, chap 1). We have found empirically that the $1/\chi_0$ expansion contains only star lattice constants, and we suspect that the whole of the above development is also valid for this model. Further investigations are currently being undertaken.

Finally, de Gennes (1972) pointed out that $D = 0$ corresponds to a self-avoiding walk model, and we might therefore expect similar results to hold. Writing the generating function for the number of SAW in the form

$$F(w) = 1 + \sum_{n=1}^{\infty} c_n w^n, \tag{6}$$

and putting

$$\frac{1}{F(w)} = 1 + \sum_{n=1}^{\infty} a_n w^n, \tag{7}$$

we find, using the data of Domb (1960), that

$$\begin{aligned} a_1 &= -q, \qquad a_2 = q, \qquad a_3 = 6p_3 - q, \\ a_4 &= 8p_4 - 18p_3 + q, \\ a_5 &= 10p_5 - 12p_{5a} - 24p_4 + 30p_3 - q, \\ a_6 &= 12p_6 - 12p_{6a} - 12p_{6b} - 30p_5 + 40p_{5a} + 40p_4 - 30p_3 + q. \end{aligned} \tag{8}$$

This is a convenient algorithm for obtaining the c_n in terms of star lattice constants.

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References

Domb C 1960 *Adv. Phys.* **9** 149–361

——1971 *Statistical Mechanics at the Turn of the Decade, Proc. 1969 Evanston Symp. in Honour of G E Uhlenbeck* ed E G D Cohen (New York: Marcel Dekker) p 81

——1974 *Phase Transitions and Critical Phenomena* vol 3, ed C Domb and M S Green (London: Academic Press)

Domb C and Hiley B J 1962 *Proc. R. Soc.* A **268** 506–26

Fuchs K 1942 *Proc. R. Soc.* A **179** 340–61

de Gennes P G 1972 *Phys. Lett.* **38A** 339–40

Mittag L and Stephen M J 1971 *J. math. Phys.* **12** 441–50

Potts R B 1952 *Proc. Camb. Phil. Soc.* **48** 106–9

Rushbrooke G S and Scoins H I 1955 *Proc. R. Soc.* A **230** 74–90

Stanley H E 1969 *J. appl. Phys.* **40** 1272–4

Uhlenbeck G E and Ford G W 1962 *Studies in Statistical Mechanics* vol 1, ed J de Boer and G E Uhlenbeck (Amsterdam: North Holland) pp 123–211

Yvon J 1945 *Cah. Phys.* No 28

——1948 *Cah. Phys.* No 31, 32