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Some Algebraic Techniques for obtaining Low-temperature Series Expansions

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Abstract

It is shown that low-temperature series expansions for lattice models in statistical mechanics can be obtained from a consideration of only connected strong subgraphs of the lattice. This general result is used as the basis of a linked-cluster form of the method of partial generating functions and also as the basis for extending the finite lattice method of series expansion to low-temperature series.

1. Introduction

The techniques of exact series expansions have been some of the most important means of investigating models exhibiting continuous phase transitions. Even though renormalization group techniques have provided a more flexible and unified approach to the study of critical phenomena, there are still a number of problems in which series expansions can prove useful. In many systems, series expansion results are used as the standard against which the results of different approximate realizations of renormalization group transformations are compared. One of the most useful forms of series expansion in lattice models is the high-density or low-temperature expansion (Domb 1974, Section IIB1). These series enable the critical point to be investigated either from the low-temperature regime or from the high-field regime. It is also possible to transform the series into high-temperature series (Domb 1974, Section IIB2).

de Neef and Enting (1977) have pointed out that in recent years techniques of series expansion have, to an increasing degree, involved substituting algebraic complexity for combinatorial complexity. One reason for this trend appears to be the increasing use of digital computers at all stages of series derivation. Algebraic techniques are generally more easily implemented on digital computers than are direct combinatorial techniques. Another reason for using algebraic techniques is the sheer size of the numbers involved. In Ising model high-temperature susceptibility series, for example, successive coefficients grow roughly exponentially. These coefficients correspond to the numbers of embeddings of various classes of subgraphs of the lattice. If direct enumeration of embeddings is used then the amount of computer time must inevitably be determined by this exponential growth. It is, however, possible to obtain high-temperature susceptibility series by an algebraic transformation of enumerations of smaller classes of subgraph embeddings (Sykes 1961). This 'counting theorem' represents probably the earliest of the algebraic techniques of series expansion. Other techniques making extensive use of algebraic manipulation have been described by Sykes et al. (1965, 1975), Wortis (1974) and de Neef and Enting (1977). Enting (1978b) gives a more extensive analysis of algebraic techniques

vis-à-vis combinatorial techniques, using the framework of general theories of computational complexity.

The present paper presents some new algebraic techniques which can be used to obtain low-temperature series expansions for lattice models. When examples are given, the Ising model is considered so as not to obscure the discussion with details which are irrelevant to the general formalism. It must be emphasized that the techniques apply to many other models, that useful applications will be those considering more complicated models than the Ising model and that the gain from using algebraic techniques is likely to be greatest in these more complicated models.

In Section 2 it is shown how low-temperature expansions can be expressed in a form involving only connected 'strong' (or section) subgraphs of the lattice. In particular the grouping properties, that is, the number of series terms which can be obtained from various sets of graphs, are discussed. Section 3 explores the application of these linked-cluster results to the method of partial generating functions (Sykes et al. 1965). In Section 4 resummations of the strong graph expansion are described, showing how it is possible to obtain low-temperature expansions for square lattice systems by combining the partition functions for finite rectangles. This extends the methods of de Neef and Enting (1977) and Enting and Baxter (1977) to low-temperature series. Because algebraic techniques are almost always implemented on digital computers, Section 5 is devoted to considering several technical computational simplifications which should make these series expansion techniques more efficient. One simplification which is used throughout this paper is that the partition function Z is expressed as an infinite product rather than using the conventional technique of expressing $\ln Z$ as an infinite sum. The advantage of working with Z is that usually all the series coefficients are integers.

2. Linked-cluster Expansions for Low-temperature Series

The literature on series expansion techniques contains a number of results which immediately suggest the possibility of obtaining low-temperature series using only connected strong subgraphs of the lattice, but this technique does not appear to have been used in actual calculations.

The combinatorial factors occurring in problems in lattice statistics are given in terms of the number of ways in which various graphs can be embedded in the graph which represents the crystal lattice. There are two classes of embeddings which are important in lattice statistics: weak embeddings which are one-to-one correspondences between the edges and vertices of the embedded graph and the crystal lattice such that the incidence relation is preserved; and strong embeddings which have the additional constraint that if two vertices in the embedded graph map onto a pair of lattice vertices which have a common edge then the two vertices in the embedded graph must have a common edge. Conventionally a less precise terminology is used so that one speaks of strong (weak) subgraphs and the number of strong (weak) subgraphs rather than the number of strong (weak) embeddings of a subgraph.

It is well known that, for Ising and related models, low-temperature expansions for the partition function Z can be expressed in terms of the partition functions of connected weak subgraphs (Sykes *et al.* 1966; Domb 1974, Section IIB3). (In practice it is $\ln Z$ that is expressed as a sum of such contributions but this implies that Z can be expressed as a product.) An examination of the formalism in the light of the results of Sykes *et al.* (1966) shows that one could equally well obtain an expansion

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in terms of partition functions of strong subgraphs. The argument below constitutes an independent proof of this assertion and has the two advantages that (1) the grouping properties, which determine the number of series terms obtained, appear explicitly and (2) by removing any reference to weak embeddings, the arguments can be easily extended to include multisite interactions such as triplet or four-spin interactions. The following proof of the existence of a connected strong graph expansion is written in terms of the Ising model and uses the Ising model variables $\mu = \exp(-2\beta H)$ and $u = \exp(-4\beta J)$. The extension to other lattice models is indicated.

The starting point of the proof is the expression for the reduced partition function $\Lambda = Z/Z(T=0, H=\infty)$ as

$$\Lambda_{G} = \sum_{\{g \subseteq G\}} v^{\nu(g)} x^{e(g)},$$
 (1)

where the set $\{g \subseteq G\}$ is the set of strong subgraphs of G, v(g) is the number of vertices of g and e(g) is the number of edges of g. In terms of conventional Ising model variables, we have $v = \mu u^{\frac{1}{2}q}$ and $x = u^{-1}$, where q is the lattice coordination number. In models such as the Potts (1952) model, x would be replaced by a function of u which would be obtained by summing over decorations of the subgraph g. In other systems, such as the spin-1 Ising model or the Ashkin and Teller (1943) model, this sum may also include higher powers of v.

One now writes, for any graph G,

$$\Lambda_G = \prod_{\{g \subseteq G\}} \left(1 + h(g) \right), \tag{2}$$

where Λ_G is calculated with fixed boundary conditions; that is, we assume G lies within a lattice of coordination number q in which all sites outside G take on the minimum energy configuration. We need to show that the terms h(g) have three properties:

- (i) Equation (2) provides a consistent definition of h(g).
- (ii) h(g) = 0 if g is disconnected.
- (iii) h(g) is at least of order $v^{v(g)}$.

The first of these three properties is easy to prove: One simply defines h(g) by

$$h(g) = -1 + \Lambda_g / \prod_{\{g' \subset g\}} (1 + h(g')),$$
(3)

so that h(g) is, for any graph g, explicitly defined in terms of graphs with a smaller number of vertices.

For disconnected graphs with two connected components g and g' we have

$$\Lambda_{g \cup g'} = \Lambda_g \Lambda_{g'} \tag{4a}$$

$$= \prod_{\{f \subseteq g\}} \left(1 + h(f) \right) \prod_{\{f' \subseteq g'\}} \left(1 + h(f') \right), \tag{4b}$$

so that $\Lambda_{g \cup g'}$ is expressed exactly as a product over proper subgraphs and the formula (3) gives $h(g \cup g') = 0$ (condition (ii) above). Expression (4a) can be regarded as a definition of the term 'connected' in the context of a given lattice model. This definition will correspond to the normal graphical definition if the lattice is drawn so that there is an edge connecting any two sites which interact.

To prove the third property, we generalize the variable v so that, for a graph G with n sites, one has $v_1, v_2, ..., v_n$ associated with vertices $v_1, ..., v_n$. Then

$$\Lambda_G = \Lambda_{G/v_i} + \mathscr{P}(v_i), \tag{5}$$

where $\mathcal{P}(y)$ denotes terms proportional to y.

Equation (5) follows immediately from the condition that all the Λ functions shall be calculated using fixed boundary conditions. If one works inductively and assumes that condition (iii) above is true for all subgraphs of G then

$$\prod_{\{g \subseteq G\}} (1+h(g)) = \left(\prod_{\{g \subseteq G/v_i\}} (1+h(g))\right) \left(1+v_i f(x,v_i)\right)$$
$$= \Lambda_{G/v_i} + \mathscr{P}(v_i)$$
$$= \Lambda_G + \mathscr{P}(v_i).$$
(6)

In the final expression (6) the index i appears only once, so in fact one must have

$$\prod_{\{g \subset G\}} (1+h(g)) = \Lambda_G + \mathscr{P}\left(\prod_{i=1}^n \upsilon_i\right).$$
⁽⁷⁾

Condition (iii) then follows by substituting equation (7) into the formula (3).

3. Application to Method of Partial Generating Functions

The method of partial generating functions (Sykes *et al.* 1965) equates the partition function of a lattice model to the partition function of a related model on a different lattice. If one takes a triangular lattice Ising model with nearest neighbour interactions, a field and a suitably chosen three-spin interaction then the partition function per site will be equal to the square of the partition function per site of a honeycomb Ising model.

On a triangular lattice with N sites we consider the contributions of two subgraphs: a, a single vertex, there being N such subgraphs; and b, a single edge, there being 3N such subgraphs. All other connected subgraphs have three or more vertices, so that to order v^2

$$\Lambda_{\rm TR1} \approx (1 + h(a))^N (1 + h(b))^{3N}, \tag{8}$$

with

$$\Lambda_{(a)} = 1 + \mu u^3 w^3, \qquad \Lambda_{(b)} = 1 + 2\mu u^3 w^3 + \mu^2 u^5 w^4, \tag{9}$$

where μ and u are the conventional Ising model variables and w is the Boltzmann weight associated with the three-site interaction. From equations (3) and (8) we have

$$(\Lambda_{\rm TR1})^{1/N} \approx \Lambda_{(b)}^3 / \Lambda_{(a)}^5$$
 (10a)

$$\approx 1 + \mu u^3 w^3 + 3\mu^2 u^5 w^4 - 3\mu^2 u^6 w^6 + \mathcal{O}(\mu^3), \tag{10b}$$

where $\mathcal{O}(y)$ denotes terms of order y.

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If one has a honeycomb lattice with 2N sites and different fields on each of its two triangular sublattices, with η and λ being the expansion variables for the field and z being the low-temperature expansion variable, then

$$\Lambda_{\rm HC}(\eta,\lambda,z) = (1+\eta z^3)^N \Lambda_{\rm TR1}(\mu,u,w), \qquad (11a)$$

with

$$\mu u^3 w^3 = \lambda (z + \eta z^2)^3 / (1 + \eta z^3)^3, \qquad (11b)$$

$$\mu^2 u^5 w^4 = \lambda^2 (z + \eta z^2)^4 (z^2 + \eta z) / (1 + \eta z^3)^5, \qquad (11c)$$

$$\mu^3 u^6 w^6 = \lambda^3 (z + \eta z^2)^6 (z^3 + \eta) / (1 + \eta z^3)^7.$$
(11d)

In terms of series, the expression for $\Lambda_{\rm HC}$ will be of order n in λ if the expression for Λ_{TR1} is of order *n* in μ but Λ_{HC} will be given exactly as a function of η . Following Sykes et al. (1965) we can use the fact that $\Lambda_{\rm HC}$ has to be symmetric in η and λ to fill in some of the missing coefficients. Thus

$$\begin{split} \Lambda_{\rm HC}^{1/N} &\approx (1+\eta z^3) [1+\lambda(z+\eta z^2)^3/(1+\eta z^3)^3 + 3\lambda^2(z+\eta z^2)^4(z^2+\eta z)/(1+\eta z^3)^5 \\ &\quad -3\lambda^2(z+\eta z^2)^6/(1+\eta z^3)^6 + \dots] \end{split} \tag{12a} \\ &= 1+\eta z^3+\lambda z^3+\eta\lambda(3z^4-2z^6)+(\eta\lambda^2+\lambda\eta^2)(3z^5-6z^7+3z^9) \\ &\quad +\lambda\eta^3(z^6-6z^8+9z^{10}-4z^{12})+\lambda^2\eta^2(12z^6-39z^8+42z^{10}-15z^{12})+\dots. \tag{12b}$$

The knowledge that the coefficient of $\lambda^3 \eta$ will be equal to the coefficient of $\lambda \eta^3$ enables us to find all the terms of fourth order in the field variables, and setting $\lambda = \eta$ gives

$$\Lambda_{\rm HC}^{1/N} = 1 + 2\eta z^3 + \eta^2 (3z^4 - 2z^6) + \eta^3 (6z^5 - 12z^7 + 6z^9) + \eta^4 (14z^6 - 51z^8 + 60z^{10} - 23z^{12}) + \dots.$$
(13)

This result can be checked against the series for $\frac{1}{2}N^{-1}\ln \Lambda_{\rm HC}$ quoted by Sykes *et al.* (1965). It is in fact possible to expand equation (12a) further and obtain the terms of fifth order in the field variable.

4. Finite Lattice Method

For models defined on a square lattice there have been a number of descriptions of techniques for obtaining high-temperature series by using only the partition functions for rectangular subgraphs (de Neef 1975; de Neef and Enting 1977; Enting and Baxter 1977; Enting 1978a). The advantage of such a formulation is that the finite lattice partition function can be easily calculated by transfer matrix techniques. These techniques can be regarded as re-summations of finite cluster expansions. The basic combinatorial results are given by Hijmans and de Boer (1955). Enting (1978a) has given explicit expressions for the combinatorial factors in place of the implicit expressions given in earlier work.

In the Ising and Potts models the existence of a high-temperature expansion in terms of rectangles immediately suggests the existence of a similar low-temperature

(12b)

expansion. This is because duality relations in these models show that the graphcounting problems are the same for both models if the high-temperature systems have free boundaries and the low-temperature systems have fixed boundaries.

For more general systems it is necessary to use the results of Section 2 to demonstrate the existence of a connected strong graph expansion and then formally re-sum this expansion into contributions from rectangles. The combinatorial arguments given by de Neef (1975) and de Neef and Enting (1977) then show that there is a combination of contributions from rectangles which brings in each connected graph with its correct combinatorial weight.

There are two types of finite lattice methods which have been described. The first (de Neef 1975) includes all rectangles whose perimeter (in units of the lattice spacing) is less than or equal to P. In fact only rectangles with perimeters P, P-2, P-4 and P-6 actually contribute (Enting 1978*a*). The second technique (Enting and Baxter 1977) uses only three rectangles of dimensions $n \times n$, $n \times (n-1)$ and $(n-1) \times (n-1)$. In each method the number of series terms is obtained by looking at the h(g) factors of connected graphs which are *not* subgraphs of the largest rectangle used. If one is interested in the field grouping then the order of the first series coefficient that is given incorrectly will be the number of vertices of the smallest connected graph not obtained in the largest rectangle (because of property (iii) of Section 2). The number of terms in the temperature grouping will depend on the particular model. For Ising and Potts models it is most easily determined by considering the duality relation connecting the high-temperature and low-temperature forms of the finite lattice method.

5. Computational Simplifications

As remarked in the Introduction, one important simplification is to express Z as a product of factors rather than to express $\ln Z$ as a sum. From the recursive definition of the h(g) (equation 3) it is clear that if all the Z(g) have integer coefficients then so will the h(g). The advantage of working with integers is that many algebraic techniques involve numbers greater than the maximum number that can be manipulated directly with standard computer hardware, and techniques for extending the precision of arithmetic are more straightforward if only integers are involved. One particularly simple technique is to perform all arithmetic calculations modulo a suitable large prime number and then repeat the calculations modulo other primes. If one has a calculation in which the number of intermediate variables used is much greater than the number of variables required in the final answer, then this technique can bring a considerable reduction in the use of computer memory. This method was used by Kim and Enting (1978) in calculating series for the limit of chromatic polynomials. Product expansions have been used in graph theoretical problems (Biggs 1974) but do not appear to have been applied to problems in physics.

Another class of simplification applies to calculations of series expansions for the magnetization. If one has

$$Z = \sum u^n \Psi_n(\mu), \qquad (14)$$

where Ψ_n is a polynomial in μ , then one can change variables to $x = 1 - \mu$ and write

$$Z = \sum u^n \Phi_n(x). \tag{15}$$

By investigating the temperature grouping one can determine how many of the Ψ_n or Φ_n would be given exactly and to that order in u one can perform the whole calculation in terms of x and u. If only the x^0 terms are retained then one has series for the zero-field partition function, while terms up to x^1 lead to series for the spontaneous magnetization and terms up to x^2 lead to series for the initial susceptibility. Compared to working with the Ψ_n polynomials, the use of truncated series in powers of x can represent a considerable saving if the full field dependence is not required.

The two simplifications described above are relevant in most techniques for obtaining low-temperature expansions. The following technique is a special simplification which applies only to the finite lattice method. In this method the partition functions of finite rectangles are obtained by transfer matrix techniques. Each possible value of the vector and matrix indices corresponds to one of the possible states of a single column of a rectangular system. The various components of the vectors are constrained partition functions, of rectangles, constrained in the sense that the column at one end is in the state corresponding to the vector index. The unconstrained partition functions are obtained by summing all the components of the vector. Components of the vector for the rectangle with one more column are obtained by taking a weighted sum of the components of the original vector. The weights are the Boltzmann weights for the interactions between the columns, and the weighted sum is equivalent to multiplying the original vector by a matrix of Boltzmann weights, that is, the transfer matrix. (Each element of the product vector must then be multiplied by the Boltzmann weight for the interactions within the column.)

For Ising models, the states of a column of *n* spins can be mapped onto a binary number in the range 0 to $2^n - 1$ by making the +/- states correspond to 0/1 binary digits. The intercolumn interaction energy between states indexed by *j* and *k* will depend on the number of positions in which the digits in *j* and *k* differ. If one performs addition modulo 2 (i.e. a logical exclusive-or) on corresponding digits in *j* and *k* then the intercolumn energy will depend on *j* and *k* only via this exclusive-or function. What this means is that, rather than store a $2^n \times 2^n$ transfer matrix, at most 2^n different elements need be stored. Apart from this major reduction in storage there is the minor advantage that, on computers which provide a bit by bit exclusive-or, calculation of *j*.xor.*k* may actually be faster than the conventional matrix indexing calculation $(j-1) \times M + k$ $(M = 2^n)$.

Since the Ashkin–Teller (1943) model can be represented in terms of Ising spins, the same techniques as above can be used. The two-site interaction weight depends (as in the Ising model) on the number of 1s in j.xor.k. The four-site interaction weight depends on the numbers of various pairs of 1s in j.xor.k. Results obtained by these techniques will be published elsewhere.

6. Conclusions

Of all the methods described above the finite lattice method is by far the most powerful for square lattice systems. Even in the earliest calculations (de Neef 1975) a 50% increase in the number of series terms for the three-state Potts model was obtained. From the point of view of attacking new problems, the finite lattice method has the advantage that it does not depend on a large data base of enumerations of subgraph embeddings. The method can be implemented using small self-contained programs. The only sophisticated requirement is the ability to perform large amounts of algebra, possibly using extended precision integers. Following the development of renormalization group techniques it is clear that, if series expansions are to continue to play a useful role in the investigation of critical phenomena, it will be in the study of systems which have traditionally been regarded as 'difficult'. Possible investigations are higher spin Ising models (to test the lattice-lattice scaling theories of Betts *et al.* 1971) or Ashkin-Teller models (to test the conjectures of Enting 1975 and Kadanoff 1977) or Potts models with the 'number of states per site' taking noninteger values (to investigate the approach to the q = 1 percolation limit). Investigations of some of these problems are currently in progress.

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