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Series expansions from the finite lattice method

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Abstract. The finite lattice method of series expansion provides a powerful technique for deriving series expansions for square lattice models. The formalism of the method is derived and a number of applications are considered.

1. Introduction

The methods of exact series expansions have been some of the most useful tools in the investigation of lattice models in statistical mechanics. These techniques and their successes are reviewed in the collection edited by Domb and Green (1974). The most sophisticated techniques have been applied to the Ising model and the two reviews by Domb (1960, 1974a) trace developments through direct geometrical/combinatorial formalisms (Wakefield 1951), through indirect combinatorial formalisms (Domb 1960, § 5.2.4, Sykes *et al* 1966) to star graph expansions (Sykes and Hunter 1974). This development represents a change from combinatorial complexity to algebraic complexity. The finite lattice method described below is an extreme case of this trend since all the combinatorial information about the graphical expansion can be expressed in an explicit algebraic form and the weight functions can be expressed largely in algebraic terms.

In § 2 we give a simple description of the method, reserving the derivation for § 3. In § 4 we summarize some of the results of applying these techniques and in § 5 we give our evaluation of the strengths of the method. The principle weakness of the method is that full power is achieved only for Ising-like models on square lattices.

2. The finite lattice method

The finite lattice method is primarily a technique for obtaining high-temperature expansions for the zero-field free energy of the Ising model and related models on a square lattice. The existence of duality transformations suggests that the method may be useful in deriving low-temperature expansions but at present this possibility has not been explored.

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The models that we consider are defined as having vertices i connected by edges (i, j) and a q-state variable $t_i = 0, 1, 2, 3, \ldots, q-1$ at each side. Associated with each edge is an energy $E(t_i, t_j)$ which depends only on $(t_i - t_j)$ modulo q. This last constraint on the energy can be taken as our definition of 'zero field'. The model described above includes the Ising model (Ising 1925), the Ashkin–Teller model (Ashkin and Teller 1943) and both the standard and planar Potts models (Potts 1952, Domb 1974b). Domb (1974b) gives a description of the techniques for obtaining expansions of the free energy for this class of model.

For any graph α we define the partition function Z_α by

$$Z_\alpha = \sum_{\substack{\text{configurations} \\ \text{of } t_k}} \exp\Big(\sum_{\text{edges}} -E(t_i, t_j)/kT \Big). \tag{1}$$

The finite lattice method states that for a square lattice of N sites, in the limit of $N \to \infty$,

$$\frac{1}{N} \ln Z_{\text{sq}} = \sum_{\alpha \in A} a_\alpha \ln Z_\alpha \tag{2}$$

(correct to order $g(A)$ in $1/kT$) where the only graphs included in the set A are those section subgraphs (strong subgraphs) of the square lattice defined by rectangular arrays of vertices.

The coefficients a_α and the cut-off order $g(A)$ depend on the set of graphs A that are chosen. For the class of models defined above to have $g(A) = r$, the set A must include all rectangular graphs of $m \times n$ vertices such that $2[(m-1)+(n-1)] \leqslant r$, i.e. the perimeter is less than or equal to r. Given a set A we assign to each graph α a weight $b_\alpha = 1$ for square arrays and $b_\alpha = 2$ otherwise (to account combining the $m \times n$ and the $n \times m$ graphs into one term). We then define $c_{\alpha\beta}$ as the number of ways graph β can be embedded in graph α and $d_{\alpha\beta}$ denotes the inverse of matrix $c_{\alpha\beta}$. Then

$$a_\beta = \sum_\alpha b_\alpha d_{\alpha\beta}. \tag{3}$$

There are at most two contributions to $c_{\alpha\beta}$. If α is $m \times n$ and β is $i \times j$ then the first contribution is $(m-i+1) \times (n-j+1) m \geqslant i$ and $n \geqslant j$ or 0 otherwise.

The second contribution which is added only if $i \neq j$ is $(m-j+1) \times (n-i+1) m \geqslant j$ and $n \geqslant i$ or 0 otherwise.

This matrix $c_{\alpha\beta}$ is what Domb (1974c) calls a T matrix. In the work below we shall use $c_{\alpha\beta}$ to denote matrices of embedding constants defined over larger sets of graphs and $d_{\alpha\beta}$ to be its inverse. The sets defining the range of indices will be determined by the context.

The description above essentially defines the finite lattice method. The combinatorial results are very similar to those used by Hijmans and de Boer (1955) in that given a set of maximal graphs (our graphs of perimeter $g(A)$ or the single maximal graph used by Hijmans and de Boer) the only subgraphs needed to give combinatorially correct contributions to lattice sums are those that can be formed from successive overlaps of existing graphs of A.

The new feature in the formalism is our analysis of the grouping or cut-off factor $g(A)$. The power of the finite lattice method comes from the fact that the partition functions for rectangular graphs can be obtained by using the method of transfer

matrices (Domb 1960, § 3.1). Each non-square array can have Z_α evaluated in two ways and if we always choose the way that uses the smallest matrix then transfer matrices for bands up to n sites wide will be sufficient to give all Z_α for arrays of perimeter less than or equal to $4n-2$. This simplicity in calculating the Z_α is the most powerful feature of the finite lattice method and on other lattices where such efficiency is absent the finite lattice method ceases to be superior to conventional cluster expansions.

3. Derivation of the finite lattice method

The finite lattice method can be regarded simply as a re-summation of the finite cluster method described by Domb (1974c). What we require are the following properties.

For any graph α and any model described by (1) there exists an expansion

$$\ln Z_\alpha = xe(\alpha) + f_\alpha = xe(\alpha) + \sum_{\beta \in B} c_{\alpha\beta} h_\beta \tag{4}$$

where $e(\alpha)$ is the number of edges in α and h_β is of order $e(\beta)$ in $(1/kT)$. The factor x essentially determines the choice of the zero of energy. The factor h_β is zero for disconnected graphs and graphs with vertices of order 1. We now choose a set B that includes all rectangular graphs of perimeter r and all subgraphs of such graphs. Clearly this includes all connected graphs with r or fewer edges and no vertices of order 1, and so the expansion is correct to $(1/kT)^r$. We now invert matrix $c_{\alpha\beta}$ to give

$$h_\alpha = d_{\alpha\beta} f_\beta. \tag{5}$$

For α being the infinite square lattice $c_{\alpha\beta}$ becomes Nb_β so that

$$\frac{1}{N} \ln Z = \sum_{\alpha,\beta \in B} b_\alpha d_{\alpha\beta} f_\beta. \tag{6}$$

We can now use the results of Hijmans and de Boer (1955) to show that $\Sigma_\alpha b_\alpha d_{\alpha\beta}$ ($y^{(\beta)}$ in their notation) is zero unless β is one of the rectangular graphs.

The grouping property for the weights h_α is implicit in the work of Domb (1974b) (see also Sykes and Hunter 1974) where the lowest-order contribution to h_α is that which involves all the bonds of the graph α. This property holds in the case of connected graph expansions and not merely for star graph (multiply connected graph) expansions. The existence of a connected graph expansion follows from the work of Sykes (1966).

Instead of using the results of Hijmans and de Boer (1955), de Neef (1975) achieved the re-summation of the finite cluster expansion by noting that any graph β has a minimal rectangle $\gamma(\beta)$ and that an expansion that counts $\gamma(\beta)$ correctly will count β correctly.

4. Applications

4.1. The three-state Potts model

The zero-field free energy has been obtained to order $(1/kT)^{22}$ (de Neef 1975). Using

the notation of Straley and Fisher (1973) we write the reduced free energy as

$$\ln \Lambda = 2x^4+4x^6+4x^7+4x^8+24x^9+16x^{10}+6x^{11}+172\tfrac{2}{3}x^{12}+128x^{13}+840x^{14}$$
$$+1180x^{15}+2568x^{16}+9204x^{17}+11513\tfrac{1}{3}x^{18}+44700x^{19}+90852\tfrac{2}{5}x^{20}$$
$$+191513\tfrac{1}{3}x^{21}+599012x^{22}+\cdots$$

where because of duality (Potts 1952) x can be either a low-temperature variable $u=\exp(-J/kT)$ or a high-temperature variable, $(1-u)/[1+(q-1)u]$. As indicated by Enting (1977) the x^{16} term disagrees with the general q expansions of Kihara *et al* (1954) and in view of other discrepancies the series above appears to be correct. The series has been analysed by the use of Padé approximants giving estimates of the critical exponent $\alpha=\alpha'\approx 0{\cdot}42\pm 0{\cdot}05$. This value of α is much higher than the earlier estimates given by Straley and Fisher (1973). Enting (1974a,b) has pointed out that the thermodynamic inequalities imply that the Straley and Fisher estimates are indeed too low. A possible set of exponents that satisfy scaling is $\alpha=\alpha'=0{\cdot}4$, $\delta=15$, $\beta=0{\cdot}1$, $\gamma=\gamma'=1{\cdot}4$, values that are not inconsistent with earlier estimates. A more detailed analysis of these series will be given elsewhere.

4.2. Colouring polynomials

The limit of colouring polynomials on lattices corresponds to the 'antiferromagnetic' Potts model at zero temperature. For q-colourings the appropriate expansion variable is $(q-1)^{-1}$. Kim and Enting (1978) have obtained such series to $(q-1)^{-18}$ correcting and extending earlier series of Nagle (1971).

4.3. One-dimensional models

The finite lattice method has been applied extensively by de Neef (1975, chaps 5, 6) to one-dimensional Heisenberg magnets. The derivation given does not include these models as it assumes a finite number of states per site. In any case the finite lattice method is equivalent to the finite cluster method on linear chains. The other innovation made in this work was to use the sum over rectangular graphs as a numerical approximation to the behaviour rather than for producing a truncated series. A sequence of such approximations can then be extrapolated to obtain estimates of the limiting behaviour.

5. An assessment

As remarked in the introduction the finite lattice method represents an extreme example of a trend away from combinatorial complexity towards algebraic complexity. This trend facilitates the use of digital computers in the derivation of series. Algebraic techniques can be readily formalized and a number of symbolic algebra systems exist (Barton and Fitch 1972). In contrast techniques based closely on graphical combinatorics suffer from a number of difficulties when implemented on digital computers. Even the problem of identifying graphs and the related problem of a canonical labelling is non-trivial (Nagle 1966). Most graphical operations, such as finding all subgraphs, are defined recursively leading to great inefficiency unless the results of earlier steps are available in a large graph directory.

The finite lattice method does not eliminate the basic problems of complexity arising in calculations of series expansions because the size of the matrices grows exponentially with the number of terms required. Growth described by c^n or $n!$ is typical of brute-force or exhaustive combinatorial techniques. A direct application of the method described in § 2 would have involved transfer matrices with 541 441 elements, and so the actual calculation was performed essentially by re-calculating individual matrix elements each time they were needed.

In conclusion we mention a simple modification that facilitates the application of standard symbolic algebra routines to these techniques. We take the exponential of (2) to give

$$Z_{\mathrm{sq}}^{1/N} = \prod_{\alpha \in A} Z_\alpha^{a_\alpha}.$$

Since the $c_{\alpha\beta}$ has integer coefficients and all diagonal elements are 1, $d_{\alpha\beta}$ also has integer coefficients so the a_α are integers. With appropriate expansion variables the Z_α can be expressed as series with integer coefficients and so only integers are used in the calculations. It should be emphasized that in many cases the integers involved in intermediate results exceed the maximum FORTRAN integers of most computers necessitating the use of the multi-length integer sections of most symbolic algebra packages or alternative techniques such as modular arithmetic (Knuth 1969, p 248).

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