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LETTER TO THE EDITOR

Boundary conditions and the free energy for statistical mechanical models

P P Martin

Department of Theoretical Physics, University of Manchester, Manchester M13 9PL, UK

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Abstract. We show that the choice of boundary conditions can significantly affect the calculation of the free energy for discrete statistical mechanical models on finite or semi-infinite lattices when the exponentiated coupling is extended into the complex plane. We show, however, that the boundary conditions most consistent with boundary configuration independence in the direction in which a lattice is infinite give a unique analytic function for the free energy. This unique function is the free energy most appropriate for extrapolation to the full thermodynamic limit. We show that such boundary conditions are orthogonal to all but one degenerate ferromagnetic ground states at zero temperature.

There has been much interest recently in the zeros of the partition function, and hence the analytic properties of the free energy, in the complex exponentiated coupling plane for statistical mechanical models (see, for instance, Wood 1985, Baxter 1986, 1987a, Martin and Maillard 1986, Glasser *et al* 1986 and Stephenson 1987 and references therein). In this letter we point out the potential ambiguities associated with boundary conditions in such calculations which are not present if attention is restricted to real coupling values. We resolve these ambiguities.

The n-site transfer matrix T for a discrete statistical mechanical lattice model is the matrix whose i, jth element gives the partition function

$$Z_{n1} = \sum_{\substack{\text{configurations} \\ \{\sigma_k\}}} \exp(\beta H) \tag{1}$$

(where the Hamiltonian H depends on the discrete lattice variables $\{\sigma_k\}$) for an n-site lattice layer when the configuration of the variables at the leading and trailing edges of the layer are given by the row and column positions i and j respectively. Provided that succeeding layers are the same (regular), the partition function for an $n \times m$ lattice is then given by

$$Z_{nm} = \langle \alpha | T^m | \gamma \rangle \tag{2}$$

where the vectors correspond to some boundary conditions (see, for example, Kogut 1979). In a recent paper (Martin 1986, hereafter referred to as I) we showed how the zeros of the partition function (in complex $\exp(\beta)$) for a finite or semi-infinite lattice can give an indication of the global analytic structure of the free energy

$$\lim_{N\to\infty} F_N = \lim_{N,M\to\infty} \frac{\ln(Z_{NM})}{NM}. \tag{3}$$

This is important since it gives the phase structure of the model (Fisher 1965, Pearson 1982 and references therein).

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A consequence of Perron's theorem (see Bellman 1960) is that, provided H and β are real and finite and n is finite, the free energy is described by a single analytic function in $\exp(\beta)$ which is the log of the unique largest eigenvalue of T (compare equations (2) and (3)). In I we showed the need for care over boundary conditions in this context if, as when describing the Potts model in the ice-model representation (Baxter *et al* 1976), H is not always real. In the present letter we explain the need for similar care when H is real but $\exp(\beta)$ is complex.

In general we would like to require that the free energy be independent of the boundary configurations in a direction in which the infinite limit has been taken (when applicable, Perron's theorem alone ensures this). Furthermore, we might expect that the analytic function which gives the free energy on the positive axis should give it on continuation to the complex plane, since (in this context) the properties of this function alone are those relevant to the physical model (again compare (2) and (3)). Finally, if there is any ambiguity in the definition of an extended free energy we want a practical definition appropriate for indicating the analytic structure of the thermodynamic limit function.

However, if not properly interpreted, results in the complex plane appear to depend profoundly on boundary conditions. The procedure for finding zeros of the partition function is, in principle, to identify points of degenerate magnitude of the largest two eigenvalues of T which can contribute to the free energy (see I). In general T has various eigenvalues of largest magnitude in different regions of the plane (consider the point $\beta = \infty$ where most spin models have degenerate ground states), but we will see that these eigenvalues should not necessarily contribute to the partition function. They come in general from different global analytic functions and their contributions may be projected to zero by a choice of boundary condition in equation (2) orthogonal to the corresponding eigenvector (see later).

We will first show that certain physically reasonable boundary conditions (defined below) give a unique global analytic function for the free energy in the whole plane and then show that this result is complementary to the requirement of infinite-limit boundary configuration independence. We will thus describe the prescription for obtaining a finite or semi-infinite lattice approximation to the limiting analytic structure of the free energy.

Consider the block diagonalisation of T using β-independent similarity transformations. Such a partial diagonalisation involves all the various (β-independent) spatial and internal symmetries of the Hamiltonian (see I and, for example, Schultz *et al* 1964). If such symmetries are the only ones manifested in T (as is the case in all known examples; see later) then the diagonalisation can proceed until the eigenvalues of a block are the branches (Hille 1962) of a single global analytic function of $\exp(\beta)$ (consider equation (1)). Further diagonalisation would then require β-dependent transformations, since the initial T is polynomial in $\exp(\beta)$. At worst the eigenvalues in such a block are the branches of a small subset of the set of global analytic functions whose branches constitute the full spectrum of T. In I we then focused on the block containing the largest eigenvalue on the real axis

$$\lambda_1 = \exp(F_n).$$

To see why consider the block diagonalised T at $\beta = 0$. From equation (1) we see that all the eigenvalues except λ_1 are zero at this point. Thus all the blocks except the $l \times l$ block containing λ_1 are zero:

$$T(\beta=0)=\begin{bmatrix} \boxed{\leftarrow l \rightarrow} & & & & \\ & 0 & & & \\ & & 0 & & \\ & & & 0 & \\ & & & & \ddots \\ & & & & 0 \end{bmatrix}. \tag{4}$$

The eigenvector for λ_1 at this point may be written

$$|1\rangle_0=(1,1,1,\ldots,1)^\tau$$

(in this context τ means transpose) in the original basis, or, say

$$|1\rangle_0 \rightarrow (C_1, C_2, C_3, \ldots, C_p)^\tau$$

where p is the total dimension of T, in the block diagonal basis. But since $|1\rangle_0$ is an eigenvector with eigenvalue $\lambda_1 \neq 0$ at $\beta=0$ we have that $C_i=0$ if $i>l$.

Now for general β in this basis we have

$$T=\begin{bmatrix} \boxed{\leftarrow l \rightarrow} & & & 0 \\ & \boxed{} & & \\ & & \boxed{} & \\ & & & \ddots \\ 0 & & & \boxed{} \end{bmatrix}. \tag{5}$$

We can, in principle, move to a basis in which all but the first block is diagonal, and the vector

$$(C_1, C_2, \ldots, C_l, 0, 0, \ldots, 0)$$

is clearly unchanged. It is therefore orthogonal to all eigenvectors associated with eigenvalues outside the λ_1 block for all β, since these vectors have zeros in their first l entries in this (and hence in the block diagonal) basis.

Of course, orthogonality is basis independent, so all eigenvectors associated with eigenvalues outside the λ_1 block are orthogonal to

$$(1,1,1,\ldots,1)$$

for all β in the original spin-configuration basis. That is, writing such a vector as

$$(\gamma_1, \gamma_2, \ldots, \gamma_p)$$

we have that

$$\sum_{i=1}^{p} \gamma_i = 0. \tag{6}$$

Regarded as a boundary vector (in equation (2)) $|1\rangle_0$ corresponds to an unweighted sum over possible boundary configurations. We take this to be a reasonable boundary condition and it should therefore allow a calculation of the free energy using equation (2) and the semi-infinite version of equation (3), F_n. We see from the above that for general β it will project away all but the branch partners of λ_1.

In contrast, any vector sensitive to other eigenvalues (orthogonal to $|1\rangle_0$) corresponds to a weighted sum over boundary configurations with cancelling total weight (from equation (6)). Our requirement that the specific boundary configuration be unimportant in the limit thus implies that we should in any case set such contributions to zero in calculations of the free energy (although they will of course be important in correlation functions). This means, for instance, that we should be careful about the interpretation of results obtained using periodic boundary conditions in the infinite direction in semi-infinite lattices, since they include such unwanted contributions in the trace. Fortunately the $|1\rangle_0$ boundary condition is in general quite easy to implement.

Of course such contributions are unimportant anyway if eigenvalues associated with eigenvectors contributing to $|1\rangle_0$ are already those of largest magnitude in the whole complex plane (as λ_1 is on the positive axis). However, it is easy to see that this is not usually the case. For instance, when $\beta = \pm\infty$ some of the elements T_{ij} are zero, whereupon a condition for Perron's theorem is violated (see Bellman 1960). The largest two or more eigenvalues can then be degenerate, typically corresponding to a global spin change symmetry in H. From equation (1) we see that in general for a ferromagnetic ground state T may then be written, up to irrelevant interchanges in the original spin configuration basis, in the form

$$T(\beta=\infty) \sim \begin{bmatrix} 1 & & & & & & & \\ & 1 & & & & & & \\ & & \ddots & & & & & \\ & & & 1 & & & & \\ & & & & 0 & & & \\ & & & & & 0 & & \\ & & & & & & 0 & \\ & & & & & & & \ddots \\ & & & & & & & & 0 \end{bmatrix}. \tag{7}$$

where the first d diagonal entries are 1 for a d-fold degenerate ground state. The eigenvectors associated with these states take the form

$$|i\rangle_\infty = \sum_{j=1}^{d} k_{i,j} |1, j\rangle \tag{8}$$

where $|1, j\rangle$ is the vector with jth entry 1, all others zero. The coefficients $k_{1,j}$ may be obtained by continuity with finite β. Since the ground state is unique at any finite β it cannot break the symmetry, so one of the eigenvectors must be the symmetric

combination

$$k_{1,j}=1 \qquad \text{for all } j=1,d \tag{9}$$

and the others must then have the property

$$\sum_{j=1}^{d} k_{i,j}=0 \qquad i\neq 1 \tag{10}$$

by orthogonality. But all these other vectors are then orthogonal to $|1\rangle_0$.

Consider for example, the two-dimensional q-state Potts model ($q>2$) with $n=2$. The transfer matrix may be written

$$T=q^{n/2}\prod_{j=1}^{n}(x+U_{2j-1})\prod_{j=1}^{n-1}(I+xU_{2j}) \tag{11}$$

where $x=[(\exp(\beta)-1)/q^{1/2}]I$, I is the $q^n\times q^n$ unit matrix and, in an appropriate basis,

$$U_i\sim\bigoplus_{m=0}^{n}(I_{r_m}\otimes U_i^m) \tag{12}$$

where I_{r_m} is the $r_m\times r_m$ unit matrix with

$$r_m=\prod_{r=1}^{m}\left[-4\cos^2\left(\frac{\pi r}{2m+1}\right)+q\right] \tag{13}$$

and $\{U_i^m\}$ is the mth representation of the Temperley-Lieb algebra (Temperley and Lieb 1971) in the notation of Martin (1987); specifically

$$U^0_{1,2,3}=\begin{pmatrix}\sqrt{q} & 0\\ 0 & 0\end{pmatrix},\frac{1}{\sqrt{q}}\begin{pmatrix}1 & q-1\\ 1 & q-1\end{pmatrix},\begin{pmatrix}\sqrt{q} & 0\\ 0 & 0\end{pmatrix}$$

$$U^1_{1,2,3}=\begin{pmatrix}\sqrt{q} & 1 & 0\\ 0 & 0 & 0\\ 0 & 0 & 0\end{pmatrix},\begin{pmatrix}0 & 0 & 0\\ 1 & \sqrt{q} & 1\\ 0 & 0 & 0\end{pmatrix},\begin{pmatrix}0 & 0 & 0\\ 0 & 0 & 0\\ 0 & 1 & \sqrt{q}\end{pmatrix}$$

and $U^2_{1,2,3}=0$ (Baxter 1982, 1987b). In this block diagonalised basis we have

$$|1\rangle_0\rightarrow(1,0,0,0,\ldots,0)^{\tau}$$

which picks out only the U^0 sub-block. The eigenvalues of this sub-block in T are the branches of F_2 for the Potts model, thus illustrating our first point. When $\beta=\infty$ we have

$$T\sim q^{-1/2}\exp(3\beta)U_2$$

where, in an appropriate basis,

$$U_2^0=\begin{pmatrix}\sqrt{q} & \\ & 0\end{pmatrix} \qquad U_2^1=\begin{pmatrix}\sqrt{q} & & \\ & 0 & \\ & & 0\end{pmatrix}$$

so one of the degenerate ground states comes from the U^0 sub-block and one each from the $(q-1)$ U^1 sub-blocks (see equation (13)) which do not contribute to the free energy. These results may be generalised to larger n as indicated and by the additional use of similarity transformations associated with spatial symmetries.

Now in the full thermodynamic limit we could in principle work equally well with the trace or $|1\rangle_0$ boundary conditions. Since the degenerate eigenvalues above the critical coupling β_c are essentially identical (see, for example, Schultz *et al* 1964) the degeneracy simply gives a vanishingly small additive constant (see equation (3)). However, this means that the free energy has a no more complicated structure in the degenerate region than in the unique region. Thus, from the practical perspective, if we want to extrapolate the analytic structure of the free energy to the infinite limit (see I) the smoothest extrapolation will in any case come using the unique function F_n.

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