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J. Phys. A: Math. Gen. 23 (1990) 3051–3060. Printed in the UK

An approach to critical phenomena from one subsystem based on the CAM analysis

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Received 30 October 1989

Abstract. Two systematic series of multi-body effective field approximations are constructed and the CAM analyses are performed for the Ising model on the two-dimensional square lattice. In the first series a two-body effective field is introduced in addition to the usual one-body one and a set of strips are used. The critical temperature and the critical index of the susceptibility are estimated as $T_c^* \simeq 2.2697\,J/k_B$ and $\gamma \simeq 1.749$. In the second series only a three-line strip is used and applied with increasing numbers of multi-body effective fields. The expected CAM scaling behaviour has also been observed. It is very interesting conceptually that critical phenomena of an infinite system can be investigated by the multi-body effective field approximation CAM based on one subsystem. Practically using more multi-body effective fields instead of increasing degrees of freedom makes CPU time fairly shorter. A new derivation of the CAM scaling relation is also presented.

1. Introduction

To investigate critical phenomena in second-order phase transitions is one of the most important questions in statistical physics. Since a phase transition takes place usually in a system with an infinite number of degrees of freedom, an exact treatment of it is generally difficult. Thus we need some approximate approaches such as the renormalisation group theory by Wilson [1] and the finite-size scaling approach by Fisher [2]. In Wilson's RG approach we construct a renormalisation procedure, repeat it and investigate its properties such as the fixed point and the eigenvalue of the linear transformation in the limit. In Fisher's approach we investigate a series of finite systems, study the systematic variance in the response functions for these finite systems and extract the asymptotic behaviour for the corresponding infinite system as the limit. One of the common features shared by these two theories is that more and more degrees of freedom have to be treated to extract the property for the corresponding infinite system.

Recently one of the present authors (MS) has developed the so-called coherent-anomaly method (CAM) by generalising the well known mean-field approximation [4]. According to this theory, true critical phenomena can be derived from a series of effective field approximations. As is well known, in effective field approximations for a classical system the long-range order in a second-order phase transition is extracted by effective fields self-consistently determined and all cooperative effects to the relevant subsystem from the remainder can be represented by a complete set of multi-body

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effective fields [5]. It is clarified by the present authors that by choosing some appropriate subsystem the whole set of multi-body effective fields can be determined self-consistently, in principle, by means of the degrees of freedom within the subsystem [6]. In practice, on the other hand, for an infinite system with infinite cross section, the total number of multi-body effective fields becomes infinite and consequently one cannot determine them as a whole set. However, we can apply increasing numbers of multi-body effective fields on one subsystem to construct a series of classical approximations. The limit of this series of approximations gives the exact solution of the infinite system. Then according to the CAM theory with such series of approximations we can investigate the true critical phenomena of the relevant infinite system. Our parameter to specify individual approximation in the series for the CAM analysis is neither the size of the subsystem nor the range of effective fields. It is a softer and more intrinsic quantity, namely the degree of approximation achieved by each individual approximation as will be seen later. This treatment gives a new aspect of the CAM approach.

In the present paper we apply the so-called even–odd parity effective field approximation CAM to Ising ferromagnets on the square lattice to obtain the best numerical results of the CAM theory for the Ising model. Furthermore we perform a multi-body effective field approximation CAM in which the subsystem is fixed to be a $3 \times \infty$ strip. A new derivation of the CAM scaling relation is also proposed.

2. Multi-body effective field approximations and CAM analyses

2.1. A derivation of the CAM scaling relation

By applying multi-body effective fields on the boundary spins and requiring the corresponding self-consistency conditions, we can formulate generalised multi-body effective field approximations for the Ising ferromagnetic system. As larger subsystems are adopted, or as more multi-body effective fields are used, the results thus obtained, say the susceptibility and the critical point, become better. As a matter of fact, the true behaviour of the infinite system should be recovered in the limit, namely when we treat the infinite system or determine the whole set of the multi-body effective fields [6].

It is the essential point of the CAM theory to recover the true critical behaviour from its classical approximations. One phenomenological derivation is given as follows: with any of multi-body effective field approximations we obtain a bifurcating point T_c for the magnetisation $m = \langle S \rangle \mu_B$. The susceptibility to a uniform external field diverges at the very temperature in the form

$$\chi_0 \simeq \frac{\bar{\chi}(T_c)}{(T/T_c - 1)^{\gamma_0}} \tag{1}$$

near and above the approximate critical point T_c with $\gamma_0 = 1$. On the other hand the true critical behaviour is expected as

$$\chi \simeq \frac{\hat{\chi}}{(T/T_c^* - 1)^{\gamma}} \tag{2}$$

near and above the true critical point T_c^* with $\gamma > 1$.

Thus, one cannot count on a single effective field approximation to recover the true critical behaviour, as is well known. However it may be supposed that an approximation does give the correct value of the true response function at one point near the approximate critical point specified by

$$\frac{T - T_c}{T_c - T_c^*} = \lambda. \tag{3}$$

The quantity λ is a characteristic factor for the way to construct the approximation. Then by adopting such a way to construct a series of approximations as keeping λ constant and with an analytical continuation of the approximate critical point we can compose the true critical behaviour. This corresponds to the canonical construction [3] of series of approximations. Thus we may put

$$\frac{\bar{\chi}(T_c)}{(T/T_c - 1)^{\gamma_0}} = \frac{\hat{\chi}}{(T/T_c^* - 1)^{\gamma}} \qquad \text{at} \qquad \frac{T - T_c}{T_c - T_c^*} = \lambda \tag{4}$$

to find the following asymptotic behaviour which should be followed by the effective field critical coefficient $\bar{\chi}(T_c)$:

$$\bar{\chi}(T_c) = \frac{\hat{\chi}\lambda^{\gamma_0}}{(1+\lambda)^{\gamma}}(T_c/T_c^* - 1)^{-\gamma+\gamma_0}. \tag{5}$$

The above asymptote means that when we establish a systematic series of approximations for a critical phenomenon denoted by a critical index (γ) different from its classical value (γ_0), the effective field critical coefficients of the classical approximations will unavoidably show anomalous behaviour as the degree of the approximation is increased. It is the CAM scaling relation.

If the curves (1) and (2) have no cross point in the region $T \geq T_c \geq T_c^*$ we can modify the above argument by supposing that the approximants at temperatures T in (3) are proportional to the true asymptote. A proportional factor $C(\lambda)$ should be included in (4) and (5). In such a case, λ is not unique and the series of approximations should be specified by the function $C(\lambda)$. The factor λ is the scaling variable in the finite-degree-of-approximation scaling [3] and $\lambda = \gamma_0/(\gamma - \gamma_0)$ corresponds to the envelope theory [3].

It is not difficult to see that for both of the two cases a common strategy to estimate the critical point and critical index can be given as follows. Firstly we construct a systematic series of classical approximations and skeletonise them near their critical point to derive classical asymptotes. Then we extract the systematic anomalous behaviour of the effective field critical coefficients and relate it to the true critical index and critical point through (5). As we cannot determine the factor $C(\lambda)$, the true amplitude $\hat{\chi}$ cannot be estimated with the present approach.

It appears that physically naive approximations based on self-consistency conditions belonging to the same class (Weiss-like one, Bethe-like one [7], etc) and subsystems with the same geometry (cluster [3], strip [7], etc) share the common factor λ (or $C(\lambda)$) and thus compose the so-called canonical series [3]. By the phrase of 'physically naive' we mean that one should introduce an anticipated stronger effective field (nearest-neighbour two-body one) rather than an anticipated weaker effective field (next nearest-neighbour two-body one). Of course, odd-body and even-body effective fields are considered separately.

2.2. Odd–even parity effective field approximation CAM

In the first systematic series, an approximation is constructed by applying one-body effective field H_1 on the boundary single spins and two-body effective field H_2 on the boundary nearest-neighbour spin-pairs of an infinitely long spin-strip. The one-body effective fields cause a symmetry breaking and it is expected that the self-consistency condition about the spin correlation functions can bring efficiently the critical point down to approach the true one. As a trick in our calculations we apply ghost fields G_1 and G_2 on the central spins and put them to zero at the end. Then the effective Hamiltonian for an N-line strip with N being odd is

$$\mathcal{H}_{\text{eff}} = -J \sum_{(l,m)\in\text{strip}} S_l S_m - H_1\mu_{\text{B}} \sum_i (S_{i,1} + S_{i,N}) - H_2 \sum_i (S_{i,1}S_{i+1,1} + S_{i,N}S_{i+1,N})$$
$$- G_1\mu_{\text{B}} \sum_i S_{i,(N+1)/2} - G_2 \sum_i S_{i,(N+1)/2}S_{i+1,(N+1)/2} - H\mu_{\text{B}} \sum_{l\in\text{strip}} S_l. \tag{6}$$

The self-consistency conditions are given by

$$\langle S_1^{\text{c}} \rangle = \langle S_1^{\text{b}} \rangle \qquad \langle S_1^{\text{c}} S_2^{\text{c}} \rangle = \langle S_1^{\text{b}} S_2^{\text{b}} \rangle \tag{7}$$

where for abbreviation we have used the superscripts 'b' and 'c' to denote the spins on the boundary lines and the central line, respectively. The order parameters and spin correlation functions can be expressed by the derivatives of the maximum eigenvalue of the transfer matrix with respect to the effective fields as

$$\begin{aligned}
\langle S_1^{\text{c}} \rangle &\simeq \frac{1}{\lambda_{\max}} \left(\frac{\partial^2 \lambda_{\max}}{\partial g_1 \partial h_1} h_1 + \frac{\partial^2 \lambda_{\max}}{\partial g_1 \partial h} h \right) \\
\langle S_1^{\text{b}} \rangle &\simeq \frac{1}{2\lambda_{\max}} \left(\frac{\partial^2 \lambda_{\max}}{\partial h_1^2} h_1 + \frac{\partial^2 \lambda_{\max}}{\partial h_1 \partial h} h \right) \\
\langle S_1^{\text{c}} S_2^{\text{c}} \rangle &= \frac{1}{\lambda_{\max}} \frac{\partial \lambda_{\max}}{\partial g_2} \\
\langle S_1^{\text{b}} S_2^{\text{b}} \rangle &= \frac{1}{2\lambda_{\max}} \frac{\partial \lambda_{\max}}{\partial h_2}
\end{aligned} \tag{8}$$

by using $h_1 = \beta\mu_{\text{B}}H_1$, $g_1 = \beta\mu_{\text{B}}G_1$, $h_2 = \beta H_2$, $g_2 = \beta G_2$ and $h = \beta\mu_{\text{B}}H$ and taking the first-order terms of the one-body effective field and external field. All the derivatives are taken at $h_1 = g_1 = h = g_2 = 0$. Then the approximate critical point is determined by

$$\begin{aligned}
&\frac{\partial^2 \lambda_{\max}}{\partial g_1 \partial h_1} - \frac{1}{2} \frac{\partial^2 \lambda_{\max}}{\partial h_1^2} = 0 \\
&\frac{\partial \lambda_{\max}}{\partial g_2} - \frac{1}{2} \frac{\partial \lambda_{\max}}{\partial h_2} = 0.
\end{aligned} \tag{9}$$

The susceptibility of the one-body magnetisation to the external field diverges at the critical point determined by (9) with an effective field critical coefficient $\bar{\chi}(T_{\text{c}})$ defined in (1) and explicitly given by

$$\bar{\chi}(T_{\text{c}}) = \frac{1}{\lambda_{\max}} \frac{(\partial^2\lambda_{\max}/\partial g_1 \partial h_1)(\frac{1}{2}\partial^2\lambda_{\max}/\partial h_1 \partial h - \partial^2\lambda_{\max}/\partial g_1 \partial h)}{\frac{\mathrm{d}}{\mathrm{d}K}(\partial^2\lambda_{\max}/\partial g_1 \partial h_1 - \frac{1}{2}\partial^2\lambda_{\max}/\partial h_1^2)}. \tag{10}$$

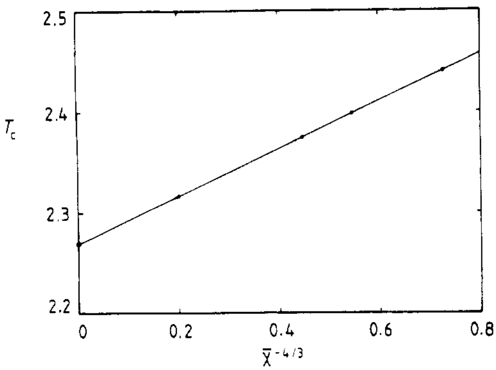

Figure 1. T_c plotted against $\bar{\chi}(T_c)$ in such a way that perfect linearity means $\gamma = 7/4$ and the extrapolation should give the true critical point T_c^*.

Table 1. T_c and $\bar{\chi}(T_c)$ obtained by odd–even parity approximations based on three-line, five-line and seven-line strips. For comparison we also list the results obtained by the so-called Bethe-like approximations [7].

		$T_c[J/k_B]$	$\bar{\chi}(T_c)$
Odd–even	3-line	2.4411	1.2704
	5-line	2.3984	1.5739
	7-line	2.3749	1.8299
Bethe-like	3-line	2.5719	0.81954
	5-line	2.4852	1.0574
	7-line	2.4396	1.2654

Practical calculations are performed with three-line, five-line and seven-line strips. The results are listed in table 1 and plotted in figure 1.

It can be seen clearly that by applying even-body effective fields we have constructed better approximations by using the same subsystems. As a matter of fact, the three-line odd–even parity approximation is nearly equivalent to the seven-line Bethe-like approximation [7].

According to the CAM theory we fit our data from odd–even parity approximations to the asymptotic formula

$$\bar{\chi}(T_c) = A(T_c/T_c^* - 1)^{-\gamma+1}. \tag{11}$$

The results thus obtained are that $A \simeq 0.1834$, $T_c^* \simeq 2.2697 J/k_B$ and $\gamma \simeq 1.749$. They should be compared with the results obtained from the Bethe-like approximation CAM [7] $T_c^* \simeq 2.271 J/k_B$ and $\gamma \simeq 1.749$ and the exact results $T_c^* = \tanh^{-1}(\sqrt{2}-1) J/k_B \simeq 2.2692 J/k_B$ and $\gamma = 1.75$. The estimate about the critical point is improved. The coincidence of the CAM results with the corresponding exact values is very good.

2.3. Multi-body effective field approximation CAM

The second systematic series of approximations is constructed by fixing the subsystem to a three-line strip and applying increasing numbers of multi-body effective fields on its boundary. It can be shown that a three-line strip is necessary and enough, in principle, to obtain exactly local properties, such as magnetisation and susceptibility, of a two-dimensional uniform system [6]. With the CAM approach we can practically estimate the critical point and critical indices. Here in the present paper we investigate the critical phenomenon of the susceptibility above the critical point.

Self-consistency conditions are given in the following way. The expectations of the boundary spin products applied with multi-body effective fields should be equal to the expectations of the corresponding central spin products. Then it is clear that the number of self-consistency equations is always equal to the number of the multi-body effective fields and thus they can be determined without conflict. It has been shown by the present authors [6] that the desired infinite system can be approached by such a set of approximations.

As for the equation which determines the critical point, the LHS of the first equation in (9) becomes the determinant of a matrix whose components are given by the second-order derivatives of the maximum eigenvalue of the transfer matrix with respect to the odd-body effective fields. We have also several additional equations similar to the second equation in (9) for other even-body effective fields. This structure is important for optimising the way to apply multi-body effective fields to save CPU time as will be discussed in appendix 1.

Numerical results are listed in table 2 and plotted in figures 2 and 3. As can be seen from table 2, the effective field critical coefficients estimated with our approximations look irregular at the first sight. However, arranging the data according to the degrees of approximation as plotted in the figures changes the situation, namely the effective field critical coefficients show systematic behaviour according to the degrees of approximation. This is the clearest evidence for the importance of the concept of the degree of approximation [3]. It also shows that the essence of the CAM approach [3] may not be understood from naive finite-size scaling.

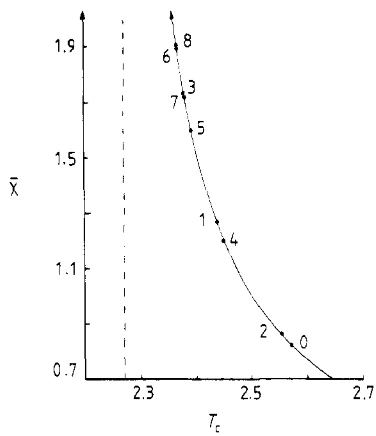

Figure 2. $\bar{\chi}(T_c)$ plotted against T_c. The anomalous behaviour appears clearly. The dashed line denotes the true critical point $T_c^* = \tanh^{-1}(\sqrt{2}-1)[J/k_B]$ where the critical coefficients are supposed to diverge.

From the CAM analysis, namely by fitting the data with (11), we obtain $A \simeq 0.18 \pm 0.01$, $T_c^* \simeq 2.26 \pm 0.02[J/k_B]$ and $\gamma \simeq 1.78 \pm 0.04$ where the errors denote two standard deviations.

The important aspect of the present approach to critical phenomena is that only one subsystem has been used in the investigation of the relevant infinite system.

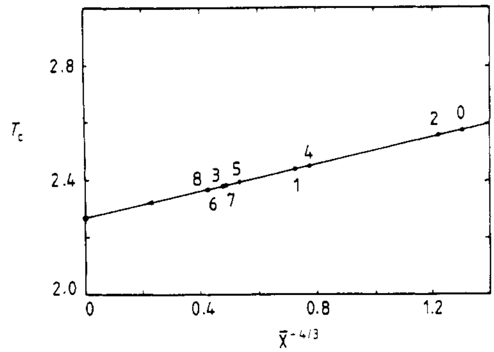

Figure 3. T_c plotted against $\bar{\chi}(T_c)$ as in figure 1.

Table 2. T_c and $\bar{\chi}(T_c)$ obtained by multi-body effective field approximations based on three-line strip. The data are presented in a sequence according to the numbers and the ranges of effective fields: 0: one-body EF; 1: one-body and nearest-neighbour two-body EF; 2: one-body and nearest-neighbour three-body EF; 3: one-body, nearest-neighbour and next-nearest-neighbour two-body EF; 4: one-body, nearest-neighbour two-body and nearest-neighbour three-body EF; 5: one-body, nearest-neighbour, next-nearest-neighbour two-body and nearest-neighbour three-body EF; 6: one-body, nearest-neighbour, next-nearest-neighbour and next-next-nearest-neighbour two-body EF; 7: one-body, nearest-neighbour, next-nearest-neighbour, next-next-nearest-neighbour two-body and nearest-neighbour three-body EF; 8: one-body, nearest-neighbour, next-nearest-neighbour, next-next-nearest-neighbour two-body and nearest-neighbour four-body EF.

No	$T_c[J/k_B]$	$\bar{\chi}(T_c)$
0	2.57192	0.819539
1	2.44107	1.27042
2	2.55743	0.862109
3	2.38131	1.73598
4	2.45009	1.20344
5	2.39328	1.59508
6	2.36753	1.89689
7	2.38135	1.71168
8	2.36719	1.90843

Namely study of the fluctuations coming from the degrees of freedom in a three-line strip (a quasi one-dimensional system) is enough to understand the second-order phase transition in a two-dimensional system. The effects of the fluctuations coming from the other degrees of freedom can be represented by effective fields. It is not difficult to see that a three-line strip is the smallest subsystem to practice the present approach in the present two-dimensional system with nearest-neighbour interactions. Of course, more and more multi-body effective fields are used to express more effects of the remainder. It should, however, be noted that these effective fields are determined with the self-consistency conditions based on the degrees of freedom within the subsystem. Thus it is clearly different from other previous approaches [1, 2].

3. Summary and discussion

We have presented a phenomenological derivation for the CAM scaling relation by adopting a hypothesis that each classical approximation gives (or is proportional to) the correct value of the true asymptote at one temperature point and thus the true asymptote can be composed from a systematic series of approximations. The factor λ corresponds to the scaling factor in the finite-degree-of-approximation scaling [3]. It appears that physically naive approximations based on self-consistency conditions belonging to the same class (Weiss-like one, Bethe-like one [7], etc) and based on subsystems with the same geometry (cluster [3], strip [7], etc) share the common factor λ (or $C(\lambda)$) and thus compose the so-called canonical series [3].

We have constructed two systematic series of approximations. With the first one we have obtained the CAM estimates $T_c^* \simeq 2.2697\,\mathrm{J}/k_\mathrm{B}$ and $\gamma \simeq 1.749$, which should be compared with the exact results $T_c^* = \tanh^{-1}(\sqrt{2}-1)\,\mathrm{J}/k_\mathrm{B} \simeq 2.2692\,\mathrm{J}/k_\mathrm{B}$ and $\gamma = 1.75$. In the second series we have applied more multi-body effective fields but restricted the subsystem to a three-line strip. With one subsystem we have been successful in obtaining the critical behaviour of the relevant infinite system. By practical calculation we have shown that study of the fluctuations coming from the degrees of freedom in a three-line strip (a quasi one-dimensional system) is enough to understand the second-order phase transition in a two-dimensional system. The effects of the fluctuations coming from the other degrees of freedom can be represented by effective fields. We have shown that the essence of the CAM approach may not be understood from naive finite-size scaling. More detailed investigation of the relation between the finite-degree-of-approximation scaling and the finite-size scaling is expected. The relations among the present two CAM analyses, the Bethe-like CAM analysis [7] and the finite-size scaling approach can be shown schematically in figure 4.

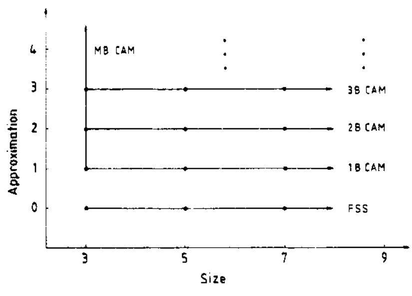

Figure 4. Relations among several CAM analyses and the finite-size scaling approach based on semi-infinite strip systems. The level of the approximation is denoted by the applied multi-body effective fields or the adopted self-consistency conditions and the size denotes the width of the strip used in each approximation. 1B CAM: Bethe-like approximation CAM [7]; 2B CAM: even–odd parity effective field approximation CAM; MB CAM: multi-body effective field approximation CAM; FSS: finite-size scaling approach.

Practically and importantly, by applying more even-body effective fields to construct approximations for the CAM analysis, we have reduced CPU time. As a matter of fact, the CPU time used in the eighth approximation listed in table 2 is one-quarter of that of its equivalent seven-line odd–even approximation listed in table 1. It makes the CAM approach more useful in investigating new problems.

Acknowledgments

One of the present authors (X Hu) appreciates useful discussions with Professor R-B Tao during Hu's visit to Fudan University. The computer calculations were carried out on a HITAC S820 at the Computer Center of the University of Tokyo. This work is partially financed by the Scientific Research Fund of the Ministry of Education, Science and Culture.

Appendix 1. Optimisation of the way to apply multi-body effective fields

In practical application of the CAM approach we have to determine the approximate critical points and the effective field critical coefficients numerically. Thus, as shown in (9) and (10), derivatives of the maximum eigenvalue of transfer matrix with respect to multi-body effective fields should be evaluated in high accuracy. In practical calculations most of the CPU time is spent to compute these derivatives. Then the way to apply the multi-body effective fields should be optimised.

Here we give three points in favour of even-body effective fields. Firstly, the effects from odd-body effective fields are evaluated by second-order derivatives, which in turn, as will be shown in appendix 2, is a sum of N^2 determinants of $N \times N$ matrices (N is the dimension of the transfer matrix), while the effects from even-body effective fields are brought in by first order derivatives and thus N determinants are enough. Secondly, although even-body effective fields do not contribute in causing symmetry breaking, the self-consistency condition determining them bring efficiently the approximate critical point down to approach the true value and enable us to attack the system near its true critical point. Thirdly, the number of derivatives involved in the simultaneous equations to determine the critical point shows a square-power dependence on the number of odd-body effective fields and only a linear dependence on the number of the even-body effective fields.

On the other hand while the number of simultaneous equations does not change when the number of odd-body effective fields is increased, it increases linearly as more even-body effective fields are applied. Then, applying more even-body effective fields will increase the dimensionality of the solution space and thus makes more trials necessary and finally causes further calculation of derivatives.

With these structures in mind we have optimised the method for applying multi-body effective fields. Furthermore in practical computations we have arranged the order of the simultaneous equations so that, according to the algorithm of the computer routine (Brend method), the times of trial of the equation involving the second-order derivatives has been reduced to the minimum. In this way we have reduced CPU time.

Appendix 2. Derivatives of the maximum eigenvalue of the transfer matrix

To guarantee the accuracy of numerical computation we have avoided taking numerical differences in the calculations of the first- and second-order derivatives. The algorithm adopted is as follows. It is easy to see that with a_i denoting the coefficients of the secular equation of the transfer matrix we have, for example,

$$\frac{\partial\lambda_{\max}}{\partial g_2} = -\frac{\sum_{i=0}^{N}(\partial a_i/\partial g_2)\lambda_{\max}^{N-i}}{\sum_{i=0}^{N}(N-i)a_i\lambda_{\max}^{N-i-1}}$$

$$= -\frac{[(\partial/\partial g_2)\det(\boldsymbol{T}-\boldsymbol{E}\lambda_{\max})]_{\lambda_{\max}}}{[(\partial/\partial\lambda_{\max})\det(\boldsymbol{T}-\boldsymbol{E}\lambda_{\max})]_{g_2}}$$

$$= -\frac{\sum_{l=1}^{N}\det\boldsymbol{P}_l}{\sum_{l=1}^{N}\det\boldsymbol{Q}_l} \tag{A2.1}$$

with

$$(\boldsymbol{P}_l)_{ij} = \begin{cases} \partial(\boldsymbol{T})_{ij}/\partial g_2 & \text{if } i = l \\ (\boldsymbol{T}-\boldsymbol{E}\lambda_{\max})_{ij} & \text{otherwise} \end{cases} \tag{A2.2}$$

and

$$(\boldsymbol{Q}_l)_{ij} = \begin{cases} -1 & \text{if } i = j = l \\ 0 & \text{if } i = l \neq j \\ (\boldsymbol{T}-\boldsymbol{E}\lambda_{\max})_{ij} & \text{otherwise} \end{cases} \tag{A2.3}$$

where $\boldsymbol{T}$ denotes the transfer matrix and $\boldsymbol{E}$ the unit matrix. The elements $\partial(\boldsymbol{T})_{ij}/\partial g_2$ can be given analytically and thus with accurate estimate of the maximum eigenvalue, the derivatives can be computed to high accuracy. Similarly we have

$$\frac{\partial^2\lambda_{\max}}{\partial g_1\partial h_1} = -\frac{\sum_{l,m=1}^{N}\det\boldsymbol{P}_{lm}}{\sum_{l=1}^{N}\det\boldsymbol{Q}_l}. \tag{A2.4}$$

Thus an nth order derivative can be evaluated by a sum of N^n determinants of $N \times N$ matrices.

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