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Finite-lattice extrapolation algorithms

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Abstract. Two algorithms for sequence extrapolation, due to van den Broeck and Schwartz, and Bulirsch and Stoer, are reviewed and critically compared. Applications to three-state and six-state quantum chains and to the (2+1)D Ising model show that the algorithm of Bulirsch and Stoer is superior, in particular if only very few finite-lattice data are available.

1. Introduction

Finite-lattice techniques are a useful tool for studying field theories. The numerical diagonalisation of the transfer matrix, combined with finite-size scaling, is a widely applied method for extracting critical properties in statistical mechanics systems (for a review, see Barber (1983)). Studying a specific model, the calculation is done in two steps. First, the highest eigenvalues of the transfer matrix or, using the Hamiltonian formulation (see Kogut 1979), the lowest eigenvalues of the Hamiltonian are computed on some lattices of finite size N. Second, and this will be studied in this paper, one has to extrapolate the finite-size data towards the thermodynamic limit $N \to \infty$.

A common method used to perform this extrapolation is provided by an algorithm proposed by van den Broeck and Schwartz (1979, hereafter referred to as VBS) and first applied to critical phenomena by Hamer and Barber (1981). It allows a reliable determination of critical quantities in the $N \to \infty$ limit, in particular if the original sequence of finite-size data is long enough to allow for an iterative application. This requires sequences of at least five figures. For many two-dimensional systems, it is possible to meet this condition.

For reviews on extrapolation techniques see Smith and Ford (1979) and Joyce (1971). For the applications we have in mind, namely critical phenomena, one usually has to extrapolate a sequence f_N with limit f of the asymptotic form ($N \to \infty$):

$$f_N = f + a_1 N^{-\omega_1} + a_2 N^{-\omega_2} + \dots \tag{1.1}$$

where the ω_i are *non-integer* numbers. It was shown by Barber and Hamer (1982) that the VBS algorithm produces more accurate results than other known algorithms for the sequences (1.1), such as, for example, Levin's (1973) u transform. Levin's u transform gives the best results for linearly converging sequences (Smith and Ford 1979) and also for the logarithmically converging sequence (1.1), provided *all* ω_i are integers (see Barber and Hamer 1982).

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In this work, we explore the characteristics of another algorithm, due to Bulirsch and Stoer (1964, hereafter referred to as BST). A first application to critical phenomena was given by Henkel and Patkós (1987). We shall compare the convergence properties of the VBS and BST algorithms, using as examples the three-state Potts quantum chain (von Gehlen and Rittenberg 1986, Hamer and Barber 1981), a six-state Z_6-symmetric quantum chain (Schütz 1987, 1988, Alcaraz 1987a, b, Zamolodchikov and Fateev 1985) and the (2+1)D Ising model (Hamer 1983, 1987, Hamer and Johnson 1986, Henkel 1984, 1987). We find that, in general, the BST algorithm converges faster and produces more reliable estimates than the VBS algorithm.

The apparent superiority of the BST algorithm becomes more pronounced if there are only very short sequences (with only four entries) available. As a rule, these short sequences occur for three-dimensional models (Hamer 1983), but this situation is also common in studying higher excitations in the Hamiltonian spectrum of quantum chains. The investigation of the higher energy levels, rather than the ground state only, is motivated by the application of conformal invariance to two-dimensional models (for reviews see Cardy (1987a) and Rittenberg (1986)).

The paper is organised as follows. In § 2, we define the VBS and BST algorithms and discuss some of their properties. In § 3, an application to some simple finite rational polynomials is given. In § 4, the algorithms are used to estimate some critical exponents of the Potts and a six-state quantum chain. Emphasis will be laid on the stability and reliability of the estimates. Finally, to illustrate a three-dimensional model, an application to the (2+1)D Ising model is given. Section 5 summarises our conclusions. In the appendix we will briefly consider sequences with logarithmic contributions.

2. The algorithms

In this section, we define the VBS and BST algorithms and give some of their properties.

2.1. VBS algorithm

Consider a sequence f_N ($N = 0, 1, 2, \dots$) which, in the limit $N \to \infty$, converges toward some limit f. It is important that the N are *consecutive*, for example, a sequence like $0, 2, 6, 3, \dots$, or $0, 1, 3, 7, 8, 11, \dots$, should not be taken into consideration, but a sequence like $0, 2, 4, 6, 8, \dots$, can still be used. To obtain the limit f, form approximants $[N, M]$, arranged as a triangular table:

$$\begin{array}{l} [0,0] \\ [1,0]\,[1,1] \\ [2,0]\,[2,1]\,[2,2] \\ [3,0]\,[3,1] \\ [4,0] \end{array} \tag{2.1}$$

where the $[N, M]$ are defined recursively:

$$[N,-1] = \infty \tag{2.2}$$

$$[N,0] = f_N \tag{2.3}$$

$$\begin{aligned} &([N,M+1]-[N,M])^{-1} + \alpha([N,M-1]-[N,M])^{-1} \\ &\quad = ([N+1,M]-[N,M])^{-1} + ([N-1,M]-[N,M])^{-1}. \end{aligned} \tag{2.4}$$

The original sequence $[N, 0]$ is transformed into a new one (e.g. $[N, 1], \ldots$) which is expected to converge faster towards f. The free parameter α is chosen to increase the rate of convergence. Special cases are the Padé table $\alpha = 1$ (Wynn 1966) or the Aitken-Shanks table $\alpha = 0$ (Shanks 1955).

If the original sequence is exactly in geometric progression

$$f_N = [N, 0] = f + gq^N \tag{2.5}$$

then f is found from a single application of the VBS algorithm, with $\alpha = 0$ (Shanks 1955).

On the other hand, if

$$f_N = [N, 0] = f + g_1 N^{-\omega_1} + g_2 N^{-\omega_2} + \ldots \qquad N \to \infty \tag{2.6}$$

when $\omega_1 < \omega_2$, two VBS applications with $\alpha = -1$ give (Hamer and Barber 1981, Barber and Hamer 1982)

$$[N, 2] = f + O(N^{-\omega'}) \tag{2.7}$$

where ω' is the minimum of $\omega_1 + 2$ and ω_2.

2.2. BST algorithm

Consider a sequence h_N $(N = 0, 1, 2, \ldots)$ converging to zero as $N \to \infty$. In many applications, $h_N = 1/N$ where N stands for the length of a finite system. We stress that, in contrast to the VBS algorithm discussed in the last subsection, there is no need to restrict oneself to consecutive sequences and it is even possible to allow N to take non-integer values (which is important for three-dimensional models).

Let $T(h)$ be a function with an expansion

$$T(h) = T + a_1 h^{\omega} + a_2 h^{2\omega} + \ldots . \tag{2.8}$$

The desired limit is obtained from a table of extrapolants:

$$\begin{array}{ccccc} T_0^{(0)} & & & & \\ & T_1^{(0)} & & & \\ T_0^{(1)} & & T_2^{(0)} & & \\ & T_1^{(1)} & & T_3^{(0)} & \\ T_0^{(2)} & & T_2^{(1)} & & \\ & T_1^{(2)} & & & \\ T_0^{(3)} & & & & \end{array} \tag{2.9}$$

and the $T_m^{(N)}$ are computed from

$$T_{-1}^{(N)} = 0 \tag{2.10}$$

$$T_0^{(N)} = T(h_N) \tag{2.11}$$

$$T_m^{(N)} = T_{m-1}^{(N+1)} + (T_{m-1}^{(N+1)} - T_{m-1}^{(N)}) \left[\left(\frac{h_N}{h_{N+m}} \right)^{\omega} \left(1 - \frac{T_{m-1}^{(N+1)} - T_{m-1}^{(N)}}{T_{m-1}^{(N+1)} - T_{m-2}^{(N+1)}} \right) - 1 \right]^{-1} \tag{2.12}$$

where ω is a free parameter. This algorithm arises by approximating the function $T(h)$ of (2.8) by a sequence of rational functions where the degree of the polynomial in the denominator is equal to or larger by one than the degree of the polynomial in the numerator. As for the VBS algorithm, the sequence $T_1^{(N)}$ is expected to converge faster than the original sequence $T_0^{(N)} = T(h_N)$ and so on.

This algorithm was first proposed as a variant of Romberg integration (see BST, Joyce 1971, Stoer 1976) where $\omega = 2$ is known *a priori*. Here, we are going to study the influence of a varying ω on the estimates of the desired limit T.

If the function $T(h)$ has the expansion

$$T(h) = T + g_1 h^{\omega_1} + g_2 h^{\omega_2} + \dots \tag{2.13}$$

instead of (2.8), it follows easily from (2.12) that

$$T_1^{(N+1)} = T + O(h_{N+1}^{\omega'}) \tag{2.14}$$

where ω' is the minimum of ω_2 and $2\omega_1$. This result should be compared with (2.7) for the VBS algorithm, where two instead of one iterations are needed.

Finally, to get some idea about the reliability of the determination of T, define

$$\varepsilon_m^{(i)} = 2(T_m^{(i+1)} - T_m^{(i)}). \tag{2.15}$$

In the limit $i \to \infty$, one should expect $|T_m^{(i)} - T| \leqslant \varepsilon_m^{(i)}$ (see BST, Stoer 1976). Minimising $\varepsilon_m^{(i)}$ gives an intrinsic criterion for choosing ω.

Let us summarise what we have found so far.

(*a*) While the VBS algorithm requires a consecutive sequence of finite-lattice data, there is no requirement for the BST algorithm. This makes the BST algorithm more flexible for applications.

(*b*) Comparing the VBS and BST algorithms, we find that they both will 'absorb' the leading correction(s) to the limit. Since it takes *one* BST application compared to *two* VBS applications to absorb the leading correction (see (2.7) and (2.14)), we can already suspect that the BST should be converging faster. This will become explicit by looking at some examples, as will be done in the next sections.

(*c*) We also note that the BST algorithm is less sensitive to rounding errors than the VBS algorithm.

3. Application to finite rational polynomials

After the description of the two algorithms in § 2, we will apply them to two simple examples. We consider

$$\begin{aligned} f_1(h) &= 1 + \tfrac{1}{4}h^{1/2} \\ f_2(h) &= f_1(h) - \tfrac{1}{3}h^2 \end{aligned} \tag{3.1}$$

and define as 'finite-size sequence' for lattices of length $L = h^{-1}$, $2 \leqslant L \leqslant L_{\max}$:

$$\begin{aligned} &f_N = [N, 0] = \{f_j(\tfrac{1}{2}), f_j(\tfrac{1}{3}), \dots, f_j(1/L_{\max})\} \qquad j = 1, 2 \\ &T_0^{(i)}(h) = f_j(h_i) \qquad h_i = \tfrac{1}{2}, \tfrac{1}{3}, \dots, 1/L_{\max}. \end{aligned} \tag{3.2}$$

Although we are dealing in this paper with problems of statistical physics, where finite-size data are generally given by infinite series expansions, it is interesting to study the behaviour of the algorithms for functions such as (3.1). Before proceeding to realistic examples in § 4, we can study some important characteristics by extrapolating sequences with well known properties.

Table 1 contains the VBS approximants of $f_1(h)$, $L_{\max} = 8$ with $\alpha = -1$. Column 1 shows the initial sequence f_N and the next columns show the Mth approximants $[N, M]$. They converge monotonically and the difference from the limit $f_1(0) = 1$ lies within 1‰ for the last approximants $[N, 2]$ and $[N, 3]$.

Table 1. VBS approximants for the function $f_1(h) = 1 + \frac{1}{4}h^{1/2}$, $h = 1/L$ with $L = 2, 3, \ldots, 8$. The left-hand column gives the sequence $f_1(1/L)$ and columns 1-3 give the approximants with $\alpha = -1$.

M	0	1	2	3
$[N, M]$	1.176 7767			
	1.144 3376	1.096 4582		
	1.125 0000	1.083 4446	1.001 0712	
	1.111 8034	1.074 5987	1.000 5662	1.000 1687
	1.102 0621	1.068 0812	1.000 3444	
	1.094 4911	1.063 0211		
	1.088 3883			

Table 2 gives the corresponding BST approximants $T_m^{(i)}$ for $f_1(h)$ with $\omega = 0.5$. Again we find monotonic convergence, but already after the second iteration the error is less than 10^{-7}. Applying VBS with a longer sequence one obtains this precision in the fifth approximation for at least $L_{\max} = 14$. Comparison shows that both algorithms yield reliable results. However, BST converges much faster and thus shorter sequences are sufficient for approximation. This is of special importance in many applications. Some examples are given below.

Other properties become apparent if one considers $f_2(h)$, $L_{\max} = 10$. Studying tables 3 and 4 we find that convergence is much poorer in both cases. Additionally we find

Table 2. BST approximants for $f_1(h)$, $h = 1/L$ with $L = 2, 3, \ldots, 8$. The left-hand column gives the sequences $f_1(h)$ and columns 1-6 give the approximants with $\omega = 0.5$.

m	0	1	2	3	4	5	6
$T_m^{(i)}$	1.176 7767	1.019 3136	1.000 0000	1.000 0000	1.000 0000	1.000 0000	1.000 0000
	1.144 3376	1.014 2139	1.000 0000	1.000 0000	1.000 0000	1.000 0000	
	1.125 0000	1.011 2996	1.000 0000	1.000 0000	1.000 0000		
	1.111 8034	1.009 4005	1.000 0000	1.000 0000			
	1.102 0621	1.008 0598	1.000 0000				
	1.094 4911	1.007 0607					
	1.088 3883						

Table 3. Same as table 1 for $f_2(h) = f_1(h) - \frac{1}{3}h^2$ with $L_{\max} = 10$.

M	0	1	2	3	4
$[N, M]$	1.093 4434				
	1.107 3005	1.104 7447			
	1.104 1667	1.111 1328	1.107 8104		
	1.098 4701	−0.001 5381	0.359 7862	46.564 6127	
	1.092 8028	1.040 3737	1.048 3093	1.051 4624	1.050 5989
	1.087 6884	1.049 6414	1.050 5584	1.050 2733	
	1.083 1800	1.050 4946	1.050 0514		
	1.079 2181	1.049 4576			
	1.075 7236				

Table 4. Same as table 2 for $f_2(h)$ with $L_{max} = 10$.

m	0	1	2	3	4	5	6	7	8
$T_m^{(1)}$	1.093 4434	1.173 4704	1.101 8985	0.993 0148	0.998 5526	1.002 4037	1.000 5443	1.000 1693	1.000 0000
	1.107 3005	1.084 3293	1.115 6057	0.995 4180	0.999 6346	1.001 0041	1.000 4011	1.000 0987	
	1.104 1667	1.052 4674	1.217 3396	0.996 8926	1.000 0411	1.000 6049	1.000 3257		
	1.098 4701	1.036 7614	0.520 1514	0.997 8105	1.000 2020	1.000 4222			
	1.092 8028	1.027 6617	0.911 0240	0.998 4072	1.000 2613				
	1.087 6884	1.021 8369	0.956 0488	0.998 8114					
	1.083 1800	1.017 8445	0.972 6387						
	1.079 2181	1.014 9674							
	1.075 7236								

approximants which are far off the limit $f_2(0) = 1$. Varying α or ω respectively one observes a pole-like behaviour of the last approximants. These poles result from higher corrections produced by the algorithms and are of width $\Delta\alpha \simeq 0.5$ and $\Delta\omega \simeq 0.05$ respectively (figures 1(a) and (b)).

Furthermore, notice that VBS does not yield the correct value of $f_2(0)$ except in the region of instability near $\alpha = -2$. Examining the differences of the approximants, as well as studying their dependency on α, suggests for the extrapolant $f_2^{\mathrm{VBS}}(0) = 1.050\ (5)$. The number in brackets gives the error in the last digit estimated from the mean value of $[N, 3]$ and $[N, 4]$ for $\alpha = -1$, excluding $[1, 3]$.

The BST extrapolant $T_8^{(1)}$ has a pole-like behaviour, too. However, one obtains $T_8^{(1)} = 1.000\ 0000$ for $\omega = 0.5$ (table 4) which is indeed the leading correction (3.1). The error $T_7^{(2)} - T_7^{(1)}$ (2.15) has a minimum within $0.45 < \omega < 0.51$ (table 5), suggesting $f_2^{\mathrm{BST}}(0) = 1.000\ (2)$. We obtain in a self-consistent way an estimate for $f_2(0)$ and the leading correction. BST is less sensible to the higher correction h^2 than VBS.

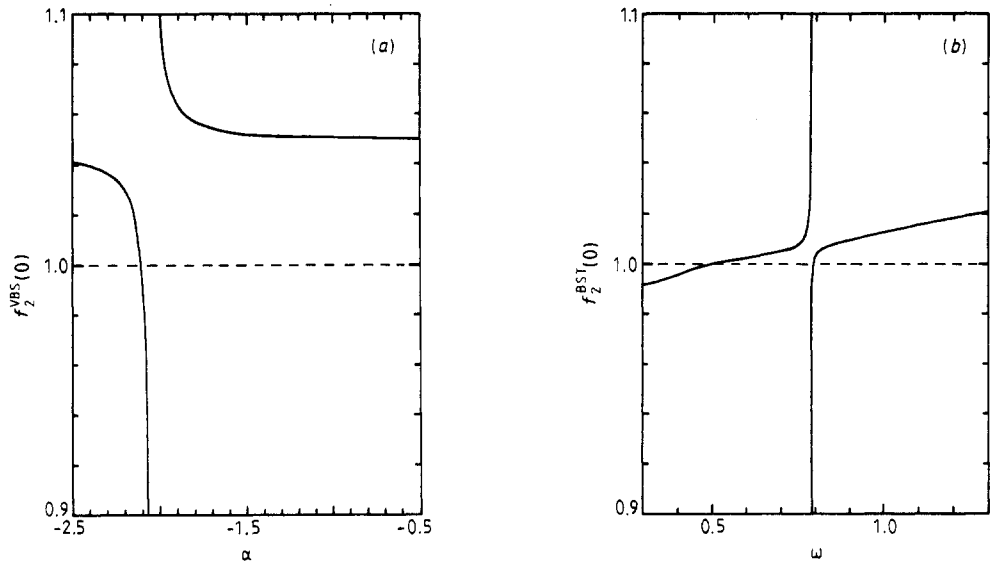

Figure 1. (a) VBS and (b) BST extrapolants for $f_2(h)$ (2.1) as a function of the parameter α or ω, respectively, with limit $f_2(0) = 1$.

Table 5. Last four BST approximants for $f_2(h)$, $L_{max}=10$ with (*a*) $\omega=0.45$, (*b*) $\omega=0.51$ and (*c*) $\omega=1$.

m	5	6	7	8
(*a*) $T_m^{(i)}$	1.001 1319 0.999 3445 0.998 8375 0.998 6571	0.998 3220 0.998 3288 0.998 3915	0.998 3357 0.998 4569	0.998 3205
(*b*) $T_m^{(i)}$	1.002 7250 1.001 3949 1.001 0181 1.000 8368	1.001 0423 1.000 8904 1.000 8368	1.000 5897 1.000 4645	1.000 2573
(*c*) $T_m^{(i)}$	1.023 7363 1.020 6289 1.018 4981 1.016 9281	1.018 3063 1.016 5516 1.015 2271	1.015 4292 1.013 8804	1.012 4736

4. Application to finite-size scaling problems

Having discussed the general properties of the VBS and BST algorithms in § 2 and used both the VBS and BST algorithm in a simple example, we shall apply them to some quantum chains describing continuous phase transitions. The Hamiltonian for the most general critical self-dual Z_n-symmetric quantum chain, defined on N sites, is

$$H=-\xi^{-1}\sum_{i=1}^{n-1}\sum_{k=1}^{N}(a_i\sigma_k^i+a_i\Gamma_k^i\Gamma_{k+1}^{n-i}) \tag{4.1}$$

where $a_i=a_{n-i}$ (to ensure hermiticity) and

$$\sigma_k^n=\Gamma_k^n=1 \tag{4.2}$$

$$\sigma_k\Gamma_l=\delta_{kl}\exp(2\pi\mathrm{i}/n)\Gamma_l\sigma_k+(1-\delta_{kl})\Gamma_l\sigma_k. \tag{4.3}$$

Periodic boundary conditions $\Gamma_{N+1}=\Gamma_1$ are assumed.

H commutes with the operator

$$Q=\sum_{k=1}^{N}q_k \qquad (q)_{ab}=a\delta_{a,b} \bmod n \qquad a,b=1,\ldots,n \tag{4.4}$$

and consequently can be written as a direct sum of block matrices, the blocks being labelled by the eigenvalues of Q. We shall compute the finite-size scaling amplitudes

$$\mathscr{E}_i=\lim_{N\to\infty}\frac{N}{2\pi}(E_i-E_0) \tag{4.5}$$

where E_i is some energy level and E_0 is the energy of the ground state. From the hypothesis of conformal invariance at the 2D critical point, it follows that $\mathscr{E}_i=x_i$ where x_i is a bulk critical exponent describing the power-like decay of the two-point correlation function at the critical point (Cardy 1984).

In the following, we concentrate on two special cases.

(i) The three-state Potts quantum chain with

$$n=3 \qquad a_1=a_2=1 \qquad \xi=\tfrac{3}{2}\sqrt{3} \tag{4.6}$$

(von Gehlen and Rittenberg 1986).

(ii) A six-state quantum chain with

$$n=6 \qquad a_1=a_5=1 \qquad a_2=a_4=1/\sqrt{3} \qquad a_3=\tfrac{1}{2} \qquad \xi=3 \tag{4.7}$$

(Schütz 1987, 1988, Alcaraz 1987a, b, Zamolodchikov and Fateev 1985).

In studying these models, our main interest is not the precise determination of some critical exponents. Rather, these models should be taken as prototypes, illustrating the behaviour of the approximants which is expected to be general in character. For this reason, we have deliberately not included data on the Ising quantum chain (see Henkel and Patkós 1987, Henkel 1988) where the finite-size data are too well behaved to be considered as typical examples. However, we should mention that, in some cases, logarithms are involved in the expansion of the $\mathscr{E}_i$. Then neither of the two algorithms yields good results (see the appendix).

4.1. Three-state Potts quantum chain

As a first example, consider the three-state Potts quantum chain. It is well known that the energy gaps of quantum chains correspond to inverse correlation lengths (see Kogut 1979). Consider the first excitation in the sector $Q=0$, which corresponds to the correlation length of the energy density $\hat{\varepsilon}$. Its critical exponent $x_\varepsilon = 2-y = 0.8$ (see Wu 1982). We computed finite-size estimates for x_ε from (4.5), for $N=2,\ldots,13$. In table 6, we give the VBS approximants, computed with $\alpha=-1$, and in table 7, the BST approximants, obtained with $\omega=0.8$, are shown. The choice of the values for α and ω is motivated by (2.7), which should give optimal convergence for $\alpha=-1$ for the VBS algorithm and the fact that the correction exponent ω_1 (see (2.13)) is known to be $\omega_1=0.8$ for the three-state Potts quantum chain (von Gehlen *et al* 1987). Other values of both α and ω will be considered below.

In both tables 6 and 7, the approximants are seen to converge towards some limit. While for the BST algorithm one obtains a value for x_ε, which deviates from the expected value by less than 2×10^{-4}, the VBS algorithm yields $x_\varepsilon \simeq 0.82$. This phenomenon, namely that the VBS algorithm shows a tendency to converge towards 'wrong' values, is not new. Hamer and Barber (1981) proposed an 'N-shift' technique, which in our

Table 6. VBS approximants for the critical exponent x_ε of the energy density $\hat{\varepsilon}$ of the three-state Potts quantum chain with $\alpha=-1$. The left-hand column gives the finite-lattice results for $N=2$–13.

M	0	1	2	3	4	5
$[N, M]$	0.848 8264					
	0.860 9292	0.858 1640				
	0.857 3452	0.868 5915	0.863 5342			
	0.852 0847	0.791 1769	0.806 3911	0.851 6065		
	0.847 2425	0.818 6550	0.820 6067	0.820 2943	0.820 3593	
	0.843 1016	0.820 6014	0.820 2248	0.820 3765	0.820 3004	0.820 3525
	0.839 6044	0.820 1434	0.820 9847	0.820 5548	0.820 2090	0.820 2817
	0.836 6399	0.819 1898	0.826 5559	0.823 0967	0.807 1675	
	0.834 1059	0.818 1584	0.864 7659	0.847 1675		
	0.831 9193	0.817 1692	0.756 0266			
	0.830 0151	0.816 2560				
	0.828 3423					

Table 7. BST approximants for the critical exponent x_ε of the three-state Potts quantum chain with $\omega = 0.8$.

m	0	1	2	3	4	5	6	7	8	9	10	11
$T_m^{(i)}$	0.848 8264	0.894 2045	0.855 2947	0.799 6336	0.799 4352	0.799 5804	0.799 9590	0.799 9785	0.799 9950	0.799 9963	0.800 0241	0.799 9989
	0.860 9292	0.843 7717	0.877 1901	0.799 5177	0.799 6948	0.796 8101	0.799 9727	0.799 9853	0.799 9958	0.799 9973	0.799 9993	
	0.857 3452	0.826 1483	0.614 7767	0.799 6049	0.799 8099	0.800 0994	0.799 9808	0.799 9890	0.799 9968	0.799 9979		
	0.852 0847	0.817 6524	0.774 4504	0.799 6917	0.799 8705	0.800 0173	0.799 9859	0.799 9913	0.799 9974			
	0.847 2425	0.812 8329	0.788 8735	0.799 7581	0.799 9062	0.800 0000	0.799 9892	0.799 9926				
	0.843 1016	0.809 8089	0.793 7047	0.799 8070	0.799 9290	0.799 9950	0.799 9915					
	0.839 6044	0.807 7750	0.795 9524	0.799 8432	0.799 9444	0.799 9936						
	0.836 6399	0.806 3354	0.797 1856	0.799 8075	0.799 5553							
	0.834 1059	0.805 2757	0.797 9352	0.799 8914								
	0.831 9193	0.804 4710	0.798 4242									
	0.830 0151	0.803 8444										
	0.828 3423											

case amounts to replacing N in (4.5) by $N+\varepsilon$, where ε is a free parameter. There is, however, no prescription how to choose an appropriate value of ε. We conclude that the introduction of ε does not increase the objectivity of the extrapolation procedure.

As a second point, we note that approximants of a higher order can be obtained with the BST than with the VBS algorithm. As a somewhat drastic example, assume that only the first five entries of the first column in tables 6 and 7 had been obtained. Then, we can compute only the second VBS approximant ($\simeq 0.86$), to be compared with the fourth BST approximant ($\simeq 0.799$).

Finally, we note that a single application of both algorithms does not yield very satisfactory results. This can be seen by comparing the first and second columns in both tables 6 and 7. There is some improvement compared to the raw data (and the improvement is larger for the BST algorithm), but the real advantage of using extrapolation algorithms only becomes apparent if the higher approximants are studied.

Having studied the table of approximants for a fixed value of α (or ω), we now examine the consequences of letting these parameters vary freely. In figures 2–4, we give the estimates for x_ε as a function of α or ω, respectively. Chains with a maximal length $N_{\max}$ of 6, 8 or 13 sites are used in figures 2, 3 and 4, respectively. While the longer sequences ($N_{\max}=8, 13$) represent the situation usually encountered studying the lowest excitations of H (for 2D models), the shorter chains are typical for higher excitations and 3D models in general.

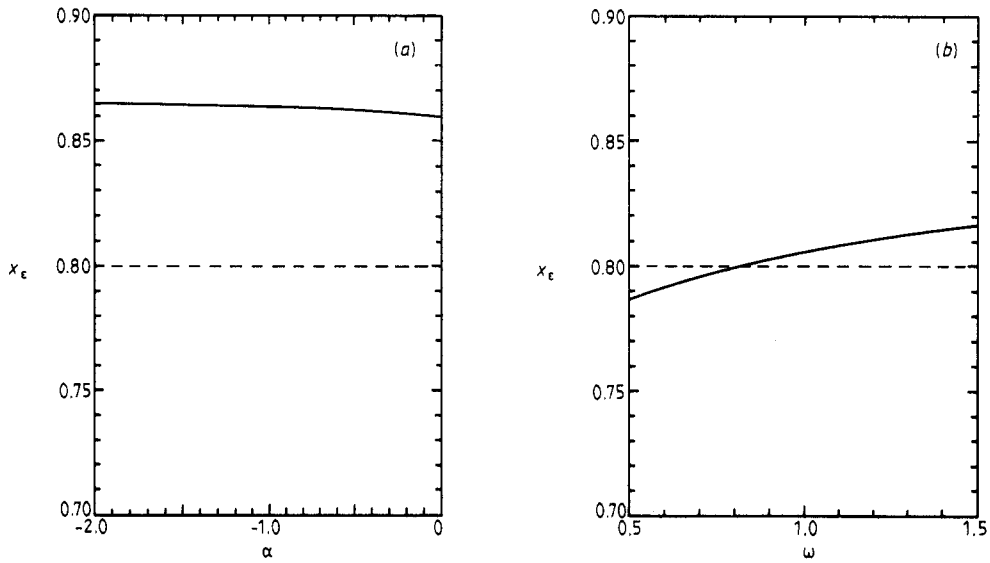

Figure 2. (*a*) VBS and (*b*) BST estimates of the critical exponent x_ε of the energy density $\hat{\varepsilon}$ of the Potts quantum chain as a function of the parameter α or ω, respectively. The theoretical prediction is $x_\varepsilon = 0.8$ (Wu 1982). Chains with $N = 2, 3, \ldots, N_{\max}$ with $N_{\max} = 6$ were used.

The first observation is that there exist broad ranges of values for both α and ω, for which x_ε is *independent* of α (or ω). The regions are separated from each other by poles of the function $x_\varepsilon(\alpha)$ (or $x_\varepsilon(\omega)$). The width of the poles becomes narrower (and the poles more frequent) if the length of the sequence (the size $N_{\max}$ of the largest

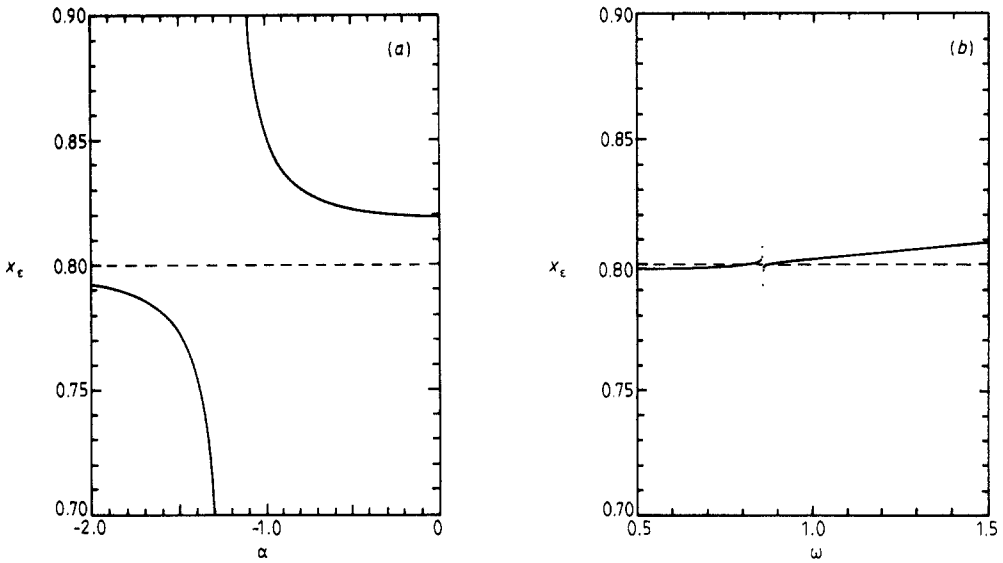

Figure 3. (*a*) VBS and (*b*) BST estimates of the critical exponent x_ϵ of the Potts quantum chain, with $N_{max} = 8$.

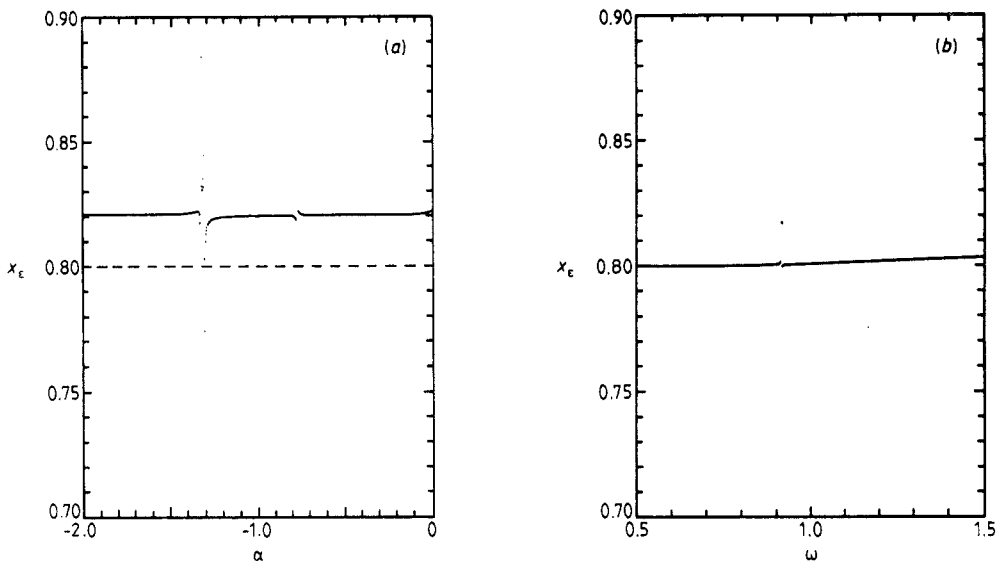

Figure 4. (*a*) VBS and (*b*) BST estimates of the critical exponent x_ϵ of the Potts quantum chain, with $N_{max} = 13$.

lattice used) increases. For the BST algorithm, there are less and much narrower poles than for the VBS algorithm (see also figure 1). This difference is especially pronounced for $N_{max} = 8$ (figure 3) and also clearly visible for $N_{max} = 13$.

It is also apparent that, for almost all values of α inside the stability region, the VBS algorithm yields $x_\epsilon \simeq 0.82$, in disagreement with the expectation $x_\epsilon = 0.8$ (Wu 1982), while the BST algorithm gives $x_\epsilon \simeq 0.80$. As already mentioned, one might use the

'N-shift' technique of Hamer and Barber (1981) to overcome this problem, at the price of having to fix a second free parameter†.

Finally, we note that in the limit $N_{\max} \to \infty$ there is an apparent tendency for the VBS and BST approximants as a function of α (or ω) to behave like a constant plus a sum of derivatives of delta functions. It would be of interest to prove this conjecture rigorously.

4.2. Six-state quantum chain

As a second example, we take the six-state quantum chain defined by (4.7). For a detailed discussion of this model see Schütz (1987, 1988), Zamolodchikov and Fateev (1985) and Alcaraz (1987a, b). In table 8, we give the low-lying spectrum for the sector $Q=2$ ((4.4) and see Schütz (1988) for more details). The states can be characterised by a pair of scaling dimensions $(\Delta, \bar{\Delta})$ and $x = \Delta + \bar{\Delta}$. For the lowest level, the largest lattice has $N_{\max} = 8$ sites, but a correct extrapolation becomes more difficult for the higher levels, as finite-size data could only be obtained for four lattices for the highest energies considered. Comparing the results of the VBS and BST algorithm with the theoretical prediction x_{th} (Zamolodchikov and Fateev 1985), one gets an idea of the reliability of the extrapolation methods applied. In general, the BST algorithm produces more accurate results than the VBS algorithm. We also note that, for the level characterised by $(\Delta, \bar{\Delta}) = (\frac{7}{12}, \frac{7}{12})$, the VBS algorithm yields a result which appears to be extremely stable, yet shows a large deviation from the expected value x_{th}. This phenomenon already occurred in the Potts quantum chain.

Next, we consider the dependence of α and ω. In table 9, we give $x_{\text{VBS}}(\alpha)(x_{\text{BST}}(\omega))$ for both the lowest level of table 8, with a 'magnetic' exponent $x = x_2 = \frac{1}{8}$ and the energy density exponent $x_\epsilon = \frac{1}{2}$ (Zamolodchikov and Fateev 1985) of the six-state quantum chain. The properties of the approximants in table 9 are similar to those of the Potts quantum chain discussed above. Again, we find the BST algorithm to give more reliable

Table 8. Part of the spectrum for $Q=2$ of the six-state chain of (4.7). Δ and $\bar{\Delta}$ are the scaling dimensions and $x_{\text{th}} = \Delta + \bar{\Delta}$. x_{VBS} and x_{BST} are the predictions from the VBS and BST algorithms. The numbers in brackets give the expected uncertainty in the last given digits as estimated from the variation with α or ω and the differences of the highest approximants. If approximants appear several times for one x_{th}, this corresponds to a degeneracy of the state.

$(\Delta, \bar{\Delta})$	x_{th}	x_{VBS}	x_{BST}
$(\frac{1}{12}, \frac{1}{12})$	0.1667	0.167 (1)	0.1667 (3)
$(\frac{7}{12}, \frac{7}{12})$	1.1667	1.2477 (2)	1.170 (5)
$(\frac{5}{6}, \frac{5}{6})$	1.6667	1.66 (2)	1.666 (3)
$(\frac{13}{12}, \frac{13}{12})$	2.1667	2.17 (1)	2.16 (2)
$(\frac{4}{3}, \frac{4}{3})$	2.6667	2.6 (1)	2.68 (2)
$(\frac{19}{12}, \frac{19}{12})$	3.1667	3.1 (1)	3.16 (1)
		3.25 (5)	3.24 (2)
		3.22 (3)	3.22 (2)
$(\frac{11}{6}, \frac{11}{6})$	3.6667	3.65 (3)	3.64 (3)
$(\frac{25}{12}, \frac{25}{12})$	4.1667	3.9 (1)	4.11 (2)

† Although $\alpha = -1$ is the 'correct' value to take for a large class of sequences (Barber and Hamer 1982), the very fact that one does observe a convergence towards a 'wrong' limit indicates that the finite-size data considered here are from a different class of sequences.

Table 9. The last column of the VBS and BST approximants for the critical exponents $x_2 = \frac{1}{6}$ and $x_\varepsilon = \frac{1}{2}$ (defined in the text) of the six-state quantum chain.

	VBS			BST	
α	x_ε	x_2	ω	x_ε	x_2
−2.0	0.6221	0.1827	0.3	0.4915	0.1660
−1.8	0.6324	0.0054	0.4	0.4945	0.1663
−1.6	0.6416	0.1606	0.5	0.4999	0.1665
−1.4	0.6527	0.1840	0.6	0.4981	0.1667
−1.2	0.6703	0.1651	0.7	0.5068	0.1668
−1.0	0.7046	0.1665	0.8	0.5126	0.1670
−0.8	0.8089	0.1670	0.9	0.5178	0.1671
−0.6	−6.6292	0.1674	1.0	0.5230	0.1672
−0.4	0.4083	0.1677	1.2	0.5324	0.1674
−0.2	0.5038	0.1679	1.5	0.5451	0.1679

estimates. For x_ε, as met in two other cases before, the VBS algorithm appears to converge towards a 'wrong' value.

In order to illustrate the selection of ω for the BST algorithm, we show in figure 5 the last difference $\varepsilon_5^{(0)}$ (see (2.15)) for the exponent x_ε as a function of ω. For $\omega \simeq 0.53$, $\varepsilon_5^{(0)}$ shows a well defined minimum with rapidly rising flanks if ω is varied. Usually, the other $\varepsilon_m^{(i)}$, e.g. $\varepsilon_4^{(0)}$ and $\varepsilon_4^{(1)}$, also have a minimum at approximately the same value of ω.

4.3. *(2+1)D Ising model*

As the last example, we take the (2+1)D Ising model (Hamer 1983, 1987, Hamer and Johnson 1986, Henkel 1984, 1987) as an illustration of the increased difficulty of

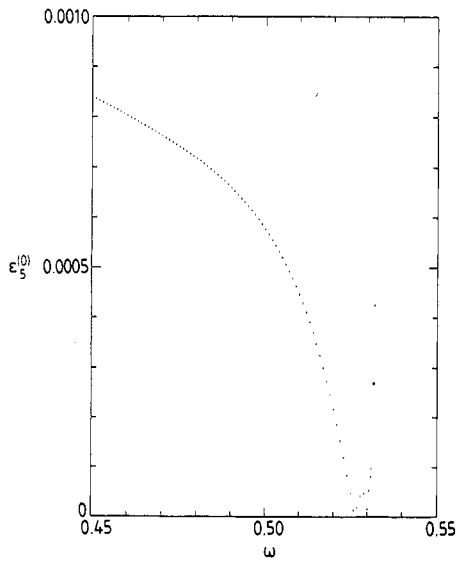

Figure 5. Difference $\varepsilon_5^{(0)}$ for the thermal exponent x_ε of the six-state quantum chain as a function of ω.

obtaining reliable extrapolation estimates in a three-dimensional model. We consider square $N \times N$ lattices with periodic boundary conditions. The notation of (4.1)-(4.4) will be used throughout. Let $|0\rangle$ be the eigenvector of H corresponding to the ground-state energy and $|1\rangle$ and $|2\rangle$ the eigenvectors corresponding to the first excitation in the sectors $Q=1$ and $Q=0$, respectively. With $\sigma_k = \sigma^z(k)$ and $\Gamma_k = \sigma^x(k)$, where σ^x and σ^z are Pauli matrices, we define

$$E = \frac{1}{N^2} \sum_k \sigma^z(k) \tag{4.8}$$

where the sum runs over the whole lattice. One expects that the matrix elements $\langle i|E|i\rangle$, $i=0, 1, 2$, are independent of i (Henkel 1987).

The difficulty in determining $\langle i|E|i\rangle$ comes from the fact that only four lattices are available ($N=5$ needs a Hilbert space of 86 056 states, but for $N=6$, about 10^8 states should be considered, which is out of the question). In table 10, we give the finite-size data for $N=2, 3, 4, 5$ for the $\langle i|E|i\rangle$. It is apparent from the data that these sequences are slowly converging, especially for $i=2$.

Table 10. Finite-size data and first VBS and third BST approximant to the matrix elements $\langle i|E|i\rangle$ in the (2+1)D Ising model. The numbers in brackets for the BST approximant are estimated from the stability with respect to ω.

N	$\langle 0\|E\|0\rangle$	$\langle 1\|E\|1\rangle$	$\langle 2\|E\|2\rangle$
2	0.854 57	0.418 00	0.098 68
3	0.864 73	0.653 66	0.553 34
4	0.874 54	0.743 11	0.697 58
5	0.881 10	0.788 59	0.762 95
VBS	0.894	0.836	0.817
BST	0.892 (2)	0.90 (1)	0.88 (2)

Since there are only four lattices, the VBS algorithm can only be applied once. So the best we can do is to compute the [1, 1] approximant from the lattices with $N=3, 4, 5$ which is given in table 10 in the row labelled VBS. We already saw that it is essential to be able to iterate the VBS algorithm. So it is not surprising to see that the VBS approximants are quite far from each other since finite-size corrections are especially large in this example.

On the other hand, the BST algorithm still allows the computation of the third approximant, which is also given in table 10. We find that the numbers agree within the given uncertainties. It is instructive to compare with the third approximant for the exponent x_e of the Potts quantum chain, in the fourth column of table 7. The BST algorithm is apparently more able to eliminate large finite-size corrections, as was already seen for the example $f_2(h)$ in § 2.

5. Conclusions

In this paper, we have studied the properties of the sequence extrapolation algorithms of van den Broeck and Schwartz (VBS) and Bulirsch and Stoer (BST). Our conclusions are summarised as follows.

(*a*) These algorithms have to be applied iteratively to yield reliable estimates.

(*b*) The BST algorithm allows the computation of higher approximants and consequently more iterations than the VBS algorithm.

(*c*) Both algorithms tend to 'absorb' the leading corrections to the limit (see (2.7) and (2.14)). The first correction is absorbed by the BST algorithm in one iteration and by the VBS algorithm in two iterations.

(*d*) Both algorithms contain a free parameter (α or ω). For a large range of values of $\alpha(\omega)$, the estimates are independent of $\alpha(\omega)$.

(*e*) Comparing the estimates with the theoretical expectations, the BST algorithm in general yields more accurate results than the VBS algorithm.

(*f*) Even in regions of stability with respect to α, the VBS algorithm shows a tendency to converge towards a 'wrong' limit, while there is no sign of such an effect for the BST algorithm.

(*g*) The differences between the BST and VBS algorithms become more pronounced if only very few finite-size data are available.

Appendix

Finite-size sequences do not always have purely power-like corrections: in some cases logarithms are involved (Cardy 1987b). In order to get an idea how VBS and BST work for such sequences we consider

$$f_3(h) = 1 + \frac{1}{\ln h} \qquad f_4(h) = f_3(h) + h \tag{A1}$$

with $2 \leqslant L \leqslant 10$, $h = 1/L$ and, as in (3.2),

$$\left.\begin{aligned} f_N &= \{f_j(\tfrac{1}{2}), f_j(\tfrac{1}{3}), \ldots, f_j(\tfrac{1}{10})\} \\ T_0^{(i)} &= f_j(h_i) \qquad h_i = \tfrac{1}{2}, \tfrac{1}{3}, \ldots, \tfrac{1}{10} \end{aligned}\right\} j = 3, 4. \tag{A2}$$

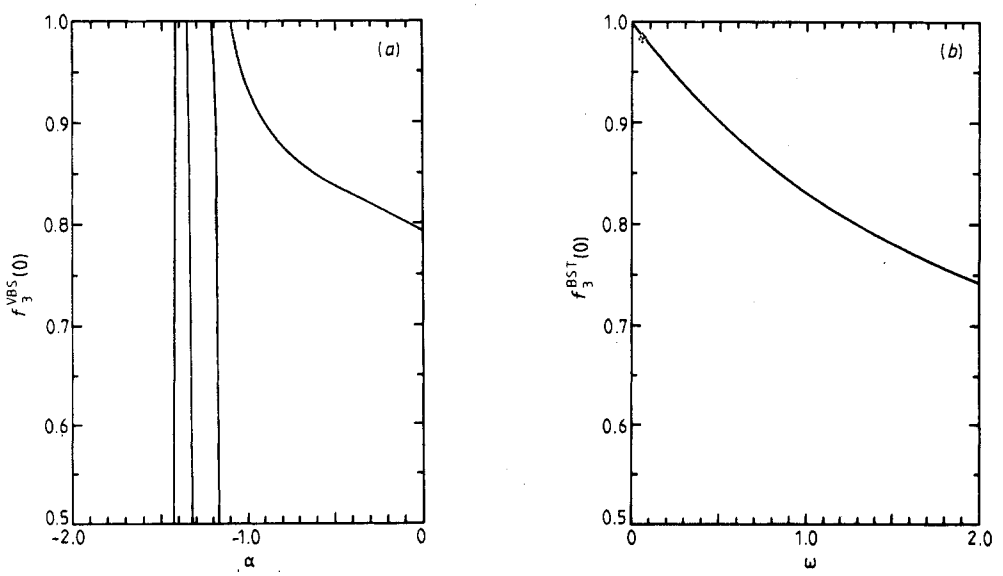

Figure 6. (*a*) VBS and (*b*) BST extrapolants for $f_3(h)$ (A1) as a function of the parameter α or ω, respectively, with limit $f_3(0) = 1$.

Table 11. BST approximants ($\omega = 10^{-4}$) for $f_3(h) = 1 + 1/\ln h$, $h = 1/L$ with $L = 2, 3, \ldots, 10$.

m	0	1	2	3	4	5	6	7	8
$T_m^{(i)}$	−0.442 6950	0.000 0030							
	0.089 7608	−0.000 0038	0.999 9500	0.999 9582					
	0.278 6525	−0.000 0235	0.999 9500	0.999 9583	0.999 9499				
	0.378 6651	−0.000 0483	0.999 9500	0.999 9584	0.999 9499	0.999 9580			
	0.441 8894	−0.000 0749	0.999 9500	0.999 9582	0.999 9500	0.999 9583	0.999 9499	0.999 9583	
	0.486 1067	−0.000 1021	0.999 9500	0.999 9583	0.999 9500	0.999 9583	0.999 9503	0.999 9584	0.999 9502
	0.519 1016	−0.000 1293	0.999 9500	0.999 9583	0.999 9501	0.999 9583	0.999 9502		
	0.544 8804	−0.000 1560							
	0.565 7055								

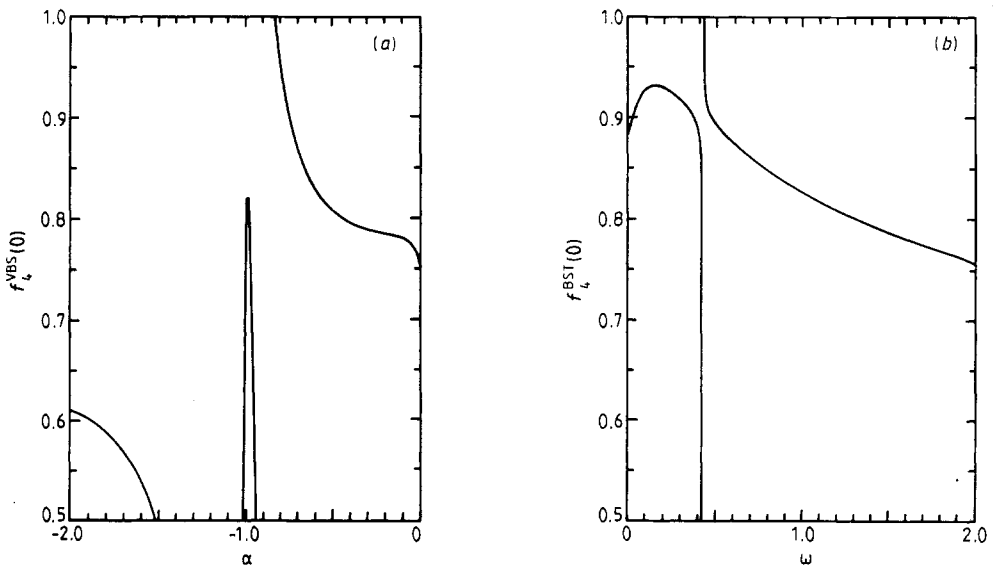

Figure 7. (*a*) VBS and (*b*) BST extrapolants for $f_4(h)$ (A1) as a function of the parameter α or ω, respectively, with limit $f_4(0) = 1$.

Table 12. BST approximants with (*a*) $\omega = 0.2$ and (*b*) $\omega = 2$ for $f_4(h) = f_3(h) + h$, $h = 1/L$ with $L = 2, 3, \ldots, 10$.

m	5	6	7	8
(*a*) $T_m^{(i)}$	1.300 5677			
	1.138 2208	0.965 0513		
	1.080 7591	0.955 8098	0.928 3503	0.929 8626
	1.052 4749	0.951 7173	0.928 7832	
(*b*) $T_m^{(i)}$	0.724 0054			
	0.734 1339	0.758 5244		
	0.742 2349	0.752 2796	0.752 0414	0.755 3730
	0.748 5148	0.758 2919	0.759 3023	

Figure 6 gives the last approximants $f_3^{\mathrm{VBS}}(0) = [1, 5]$ (a) and $f_3^{\mathrm{BST}}(0) = T_8^{(1)}$ (b) dependent on α and ω respectively. Both extrapolants vary strongly with α or ω, respectively. However, BST yields the correct value $f_3(0) = 1$ in the limit $\omega \to 0$. As table 11 shows, the differences of the extrapolants for $\omega = 10^{-4}$ are extremely small.

The situation changes if one adds the piece h to $f_3(h)$ (A1) and applies the algorithm again (figure 7). As above $f_4^{\mathrm{VBS}}(0)$ (figure 7(a)) does not give any information about the limit one wishes to calculate, but BST (figure 7(b)) also exhibits rather poor convergence for all values of ω (see tables 12(a) and (b)). The differences $T^{(i+1)} - T^{(i)}$ (see (2.15)) for $\omega = 0.2$ (table 12(a)) are scarcely better than those for $\omega = 2$ (table 12(b)) and thus we do not have a criterion to choose ω from considering these quantities. However, as for $f_3(h)$, the extrapolants $f_4^{\mathrm{BST}}(0)$ are nearer to $f_4(0)$ for ω small than for large values of ω.

These observations show that both algorithms do not give satisfactory estimates if logarithmic corrections play an important part in the series expansion of a finite-size quantity. The error one has to expect is quite large.

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