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# Estimations for asymptotic series using a modified Romberg algorithm: I. Finite-size scaling calculations

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**Abstract.** A new numerical method for estimating asymptotic properties is proposed. A generalisation of the Romberg algorithm leads to a systematic elimination of higher-order analytical terms in finite-size calculations and determines both the asymptotic value and the leading convergence exponent in a self-consistent way.

## 1. Introduction

One of the most successful methods for calculating critical properties of statistical mechanical models is based on the fact that (at least the most important) physical quantities near the critical point scale with the size of the finite system in a definite way—hence the extrapolation to the infinite system is determined by this finite-size scaling (Fisher and Barber 1972). Connecting this feature with the renormalisation group method (Nightingale 1977) and almost unlimited access to extremely fast computers improved the estimations of the statistical physical critical properties based on finite-size calculations. These new developments have led to a renewed interest in numerical finite-size scaling calculations for a wide range of systems from magnets to gauge field theory and to an extremely powerful method, at least for two- and $(1+1)$-dimensional systems.

However, the most important parameter of this numerical scaling, the critical index, is not known in most cases, and even the scaling can only be described by more than one parameter (confluent singularities). Hence the success of the finite-size calculations greatly depends on the method by which the extrapolation is performed.

This extrapolation is equivalent to the mathematical problem of evaluating asymptotic properties by numerical methods. It is interesting that till now this extrapolation was mostly done by simple qualitative numerical-graphical procedures or with an approximate fitting of the presupposed asymptotic form by non-linear parameter estimation (Hamer 1983).

It was Hamer and Barber (1981) who tried to compare and further develop the usual series transformation methods (Padé approximation, Aitken-Shanks tables, ...) to evaluate their results for $Z_3$ and $Z_5$ symmetric spin models. To get reasonable results they introduced an arbitrary parameter to unite the advantages of the Padé analysis and the power series extrapolation methods. Another correction (the so-called $M$ shift) was needed to avoid the (non-physical) variation of the estimated parameters. The disadvantage of their method is that these two parameters cannot be evaluated from basic principles; they are empirical. In addition, the apparent (numerical) convergence

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of their method is misleading, since the numerical variation is much smaller than the change introduced by the $M$ shift. This shows that the error of these calculations can hardly be estimated from the mathematical procedure itself.

These shortcomings are common for the more simple and subjective graphical and numerical fitting procedures as well.

In this paper a new asymptotic method will be developed which is based on the Romberg algorithm, mostly used for numerical integration. It is shown that the accuracy of this method is comparable to or better than the other known methods; the estimates do not depend on arbitrary parameters and the estimated error can also be given in most cases.

In § 2 the method will be introduced. The applications will be discussed in §§ 3.1-3.4. In the short summary (§ 4) a quick résumé concerning the convergence and other properties of the method is presented.

## 2. Numerical evaluation of limits, the Romberg algorithm

It is a well known problem in numerical analysis (Henrici 1977) to evaluate the limit $a_0$ of a given $q(h)$ function in the $h \to 0$ limit when the $q(h)$ function can be evaluated for given values of $h$, or only given for a set of values $(h_i)$ of which 0 is an accumulation point. The other important case when the limit $N \to \infty$ should be determined can be reduced to the previous case by the substitution $h_i = 1/N_i$.

If the function $q(h)$ has an asymptotic (not necessarily convergent) power series expansion in the $h \to 0$ limit,

$$q(h) = a_0 + a_1 h^1 + a_2 h^2 + \ldots \qquad (h \to 0, h > 0), \tag{1}$$

then without knowing the coefficients $a_i$, an algorithm can be derived which calculates the limiting value $a_0$.

Let the values $q_{i,0}$ be defined by $q_{i,0} = q(h_i)$, for $h_0 > h_1 > h_2 > \ldots$; then the series $q_{i,k}$ are calculated by the following expression:

$$q_{i,k} = (q_{i,k-1} - \rho_i^k q_{i-1,k-1})/(1 - \rho_i^k), \tag{2}$$

where $\rho_i^k = (h_{i-k}/h_i)$.

The ordered set

$$\begin{array}{ccccccc}
q_{0,0} & & & & & & \\
 & \searrow & & & & & \\
q_{1,0} & \rightarrow & q_{1,1} & & & & \\
 & \searrow & & \searrow & & & \\
q_{2,0} & \rightarrow & q_{2,1} & \rightarrow & q_{2,2} & & \\
 & \searrow & & \searrow & & \searrow & \\
q_{3,0} & \rightarrow & q_{3,1} & \rightarrow & q_{3,2} & \rightarrow & q_{3,3} \\
 & \searrow & & \searrow & & \searrow & \\
 & & & & \ldots & &
\end{array} \tag{3}$$

is called a Romberg array (RA), and the arrows show the flow of the calculation of the elements of this array as given by equation (2).

It is known that if all the coefficients $a_i$ are different from zero in expansion (1), then every column of the RA converges faster to $a_0$ than the previous ones.

With very weak restrictions on the asymptotic series (1) it can be proved that the convergence of the diagonal series to $a_0$ is faster than linear. In addition, the error $\varepsilon$

of the numerical estimate of $a_0$ (which is equal to $a_{n,n}$ for a series of $n$ terms) for large enough $k$ is given (Stoer and Bulirsch 1980) by

$$\varepsilon < 2|q_{n,n-1} - q_{n-1,n-1}|. \tag{4}$$

Although the method just reviewed has appealing features it cannot be applied directly for real physical systems since the supposed asymptotic expansion (1) does not exist.

Instead of that, for example the asymptotic form of a singular function at the critical point is determined by the critical indices. With the leading critical index, however, at the critical point, the following expansion always exists:

$$q(H) = a_0 + a_1 H^1 + a_2 H^2 + \ldots, \qquad H = h^\alpha, \tag{5}$$

where $\alpha$ is the (leading) convergence exponent, $h$ is the reduced temperature (concentration ...) and $q(H)$ is the investigated singular physical quantity. The form (5) is different from the usual expressions given by finite-size scaling renormalisation techniques. There, for any estimated quantity, instead of form (5) an expansion exists in which the different terms contain the reduced quantity having exponents combined from the leading and the correction (confluent) exponents (Privman and Fisher 1983). It is not difficult to show that any term of this 'physical' expansion can be expanded in a power series of the variable $H$ for $H > 0$. In what follows, the explicit expansion is not needed; the very existence of this expansion is sufficient to apply the Romberg method as discussed earlier. Naturally, the convergence of this expansion does depend on the actual values of the correction exponents and, in addition, of the coefficients of the correction terms.

Formally the expression (5) with the $h_i^\alpha = H_i$ substitution can be transformed to the form (1). However, without the value of $\alpha$ this transformation is a useless formal transcription.

What we propose in this paper is a consistent, modified Romberg-type procedure by which both $a_0$ and $\alpha$ can be, in principle, determined. If the RA is constructed in some way such that its convergence is 'optimal', then according to the different possible choices, the following cases can be proposed.

*Case A.* If neither the limit $a_0$ nor the critical (expansion) exponent $\alpha$ is known, one should try to minimise the estimated error (equation (4)) with the optimal choice of $\alpha$. (Given the initial data $q_{1,0}$ the further entries of the RA (3) depend only on the parameter $\alpha$ in a non-linear way.)

*Case B.* $a_0$ is known in advance and the 'critical index' $\alpha$ is to be determined. In this case the condition is that the last entry of the RA, $(q_{n,n})$, should agree with the value of $a_0$ within the estimated error. An important and frequent case is when the limit $a_0$ (or the inverse of the limit) is zero. In this case we require that the limit $a_{n,n}$ and the error are simultaneously minimised and have comparable values (case $B_1$). In case B ($B_1$) the value of $\alpha$ is fitted by a non-linear parameter estimation.

*Case C.* If the value $\alpha$ is known in advance either from basic principles or from a conjecture (which might have already been checked by calculations based on case A and/or case B) then the $h_i^\alpha = H_i$ substitutions reduce this case to the standard Romberg procedure.

It is seen that in case C in addition to the required asymptotic value an error estimate is also given (equation (4)). In case A this value has been used to optimise the modified Romberg procedure, hence there is no estimate of the error. The convergence of the procedure can be checked only qualitatively. In case B an error is also given; however, this is biased by the forced convergence to the assumed or known limit.

The programming of all three cases is almost trivial and the subroutines of this modified Romberg algorithm consist of less than 100 lines of plain FORTRAN statements. The time requirements even in cases A and B (when iteration is needed for the determination of the value of $\alpha$) is less than some tenths of a second for calculations with $n$ up to 10 on a medium size IBM computer (IBM 3031).

As in every numerical procedure, the numerical stability of the Romberg algorithm is an important issue. Without going into details it can be seen directly that the $k$th column of the RA contains terms which are higher orders in $h$ than $(h^k)$. It means that the next column is determined by the (usually very small) differences of the right-hand sides of equation (2). The error of this difference is enhanced by the denominator $(1-\rho_i^k)$, which goes to zero if $h_i/h_{i+1}$ goes to one. This is usually the case in finite-size calculations, where the calculation time increases rapidly with $N$, hence the values of $h_i(=1/N_i)$ cannot be chosen arbitrarily.

So the applications of the method require some experience in choosing the accuracy of the original (usually numerical) calculations and the values $N_i$ optimally. We come back to this point in § 3. In the following the order of the calculation is defined as the number of initial different data.

## 3. Applications of the modified Romberg algorithm

### *3.1. Coulomb-type lattice sums*

In quantum mechanical calculations of infinite systems the numerical evaluation of the Coulomb or exchange energy of the many-particle system is often needed. Although in this paper we are dealing mostly with statistical physical problems, a simple one-dimensional Ewald summation could well demonstrate the numerical procedure and it may be more interesting for physicists than the standard mathematical examples.

The infinite sum to be evaluated in suitable units is the following:

$$\sum_{k=1,\text{odd}}^{\infty}\left(\frac{1}{k}-\frac{1}{(k+1)}\right). \tag{6}$$

This is the Coulomb energy of a chain with alternating charges, and it is a special case of the function $\eta(n)$, which is defined by

$$\eta(n)=\sum_{l=1}^{\infty}(-1)^{l+1}(l)^{-n}. \tag{6a}$$

Table 1 contains the results of the calculation of $\eta(1)$ using our method. In the first column the number of pairs in the partial sum of the infinite sum of equation (6) is given, and the corresponding partial sums (or approximate values) are listed in column 2. Since the limit is finite and it is not known, the calculation according to case A is performed. Column 3 contains the calculated limits using partial sums up to the value indicated in column 1. Column 4 lists the resulting 'optimal values' of $\alpha$, too.

Naturally in this case the value of $\alpha$ is known in advance ($\alpha=-1$), and the calculations following case C can also be performed. These results are found in column 5.

It is seen that the calculated limits are extremely accurate. Although the starting approximate values are only about 1% accurate, the relative error of the extrapolated limit with $n=10$ is less than $10^{-8}$ in case A where no *a priori* knowledge has been used.

**Table 1.** Calculation of the one-dimensional Ewald sum ($\eta(1)$) with full accuracy (upper part) and with rounded initial data for six digits (lower part). The first inaccurate digits of the results are underlined.

| | | Case A | | Case C | |
|---|---|---|---|---|---|
| M | Input data | $q_{m,n}$ | $\alpha$ | $q_{n,n}$ | $\lvert\varepsilon\rvert$ |
| 1 | 0.500 000 0000 | — | — | — | — |
| 2 | 0.583 333 3333 | — | — | — | — |
| 3 | 0.616 666 666 666 | 0.721 512 540 353 | −0.680 848 | 0.691 666 666 666 | 0.16E−1 |
| 4 | 0.634 523 809 523 | 0.694 829 949 043 | −0.960 270 | 0.693 253 968 254 | 0.11E−2 |
| 5 | 0.645 634 920 635 | 0.693 056 960 621 | −1.004 931 | 0.693 171 296 296 | 0.66E−4 |
| 6 | 0.653 210 678 210 | 0.693 101 148 953 | −1.003 029 | 0.693 147 847 523 | 0.19E−4 |
| 7 | 0.658 705 183 705 | 0.693 144 578 872 | −1.000 213 | 0.693 146 930 230 | 0.78E−6 |
| 8 | 0.662 871 850 371 | 0.693 147 828 722 | −0.999 919 | 0.693 147 150 468 | 0.19E−6 |
| 9 | 0.666 139 824 228 | 0.693 147 292 025 | −0.999 983 | 0.693 147 181 316 | 0.27E−7 |
| 10 | 0.668 771 403 175 | 0.693 147 179 826 | −1.000 000 | 0.693 147 181 023 | 0.26E−9 |
| ⋮ | | | | | |
| | 0.693 147 180 559 | (exact value) | | | |
| 1 | 0.500 000 | — | — | — | — |
| 2 | 0.583 333 | — | — | — | — |
| 3 | 0.616 666 | 0.721 508 96 | −0.680 858 | 0.691 665 00 | 0.16E−1 |
| 4 | 0.634 523 | 0.694 829 75 | −0.960 251 | 0.693 263 00 | 0.11E−2 |
| 5 | 0.645 634 | 0.693 053 45 | −1.004 995 | 0.693 169 25 | 0.67E−4 |
| 6 | 0.653 210 | 0.693 164 72 | −1.000 196 | 0.693 167 75 | 0.12E−5 |
| 7 | 0.658 705 | 0.693 151 21 | −1.001 069 | 0.693 163 07 | 0.40E−5 |
| 8 | 0.662 871 | 0.691 750 39 | −1.115 117 | 0.692 625 75 | 0.47E−3 |
| 9 | 0.666 139 | 0.696 042 82 | −1.343 242 | 0.695 390 95 | 0.24E−2 |
| 10 | 0.668 771 | 0.689 750 10 | −1.420 047 | 0.688 552 27 | 0.61E−2 |

Calculations based on case C are somewhat more accurate, and in this case the error can also be estimated. These estimates are listed in column 6—in perfect agreement with the calculated values. All these calculations have been done with double precision (~16 digits). It is worth mentioning that in case A an estimate of the 'critical index' has also been obtained. It is seen tha its value for $n = 10$ is accurate for $10^{-6}$!

Since this sum can be calculated easily, the most important features of the proposed algorithm will be demonstrated using data obtained here. As has been discussed in § 2, the accuracy of the estimated limit does depend on the accuracy of the raw input data. If the data in our example are rounded for six digits then the results change as shown in the second part of table 1. It is seen that the estimated limit is best at the intermediate order of 6. What is remarkable is that the estimated error (column 6) clearly indicates this optimum; moreover, it is in agreement with the calculated value. (The estimate of the convergence exponent (column 4) is also optimum in a calculation of type A at the same order, which shows the consistency of the proposed methods.) In agreement with the expectation, the smaller the accuracy, the more the minimal error is shifted towards lower orders.

Hence it is demonstrated that the accuracy of the original calculation (input data) determines the optimal order and the ultimate accuracy of the modified Romberg algorithm. The unique error estimating properties, however, of our method clearly indicate the loss of accuracy, hence the choice of the order is not arbitrary; it is

controlled by this measure of the accuracy of this numerical procedure. Our example indicates even more that the original values could hardly be used for accurate and reliable graphical extrapolation since the data deviate significantly from the straight line corresponding to the asymptotics $1/N$.

### *3.2. Investigation of model $Z_3$*

The finite-size calculation and analysis of the energy gap in the two-dimensional $Z_3$ model have been performed by Roomany *et al* (1980). Their data have been used by Hamer and Barber in their series extrapolation method mentioned earlier. Table 2 reproduces those data which will be used in this section. Column 2 contains the numerical values of the Callan-Symanzik $\beta$ function for the lattice of size $M$. Similarly columns 3 and 4 list the approximate values of the specific heat and the susceptibility.

**Table 2.** Numerical data of the Callan-Symanzik $\beta$ function, specific heat and susceptibility for model $Z_3$ of finite-size calculations (Roomany *et al* 1980).

| $M$ | $\beta_{M/g}$ | $C_M$ | $\chi_M$ |
|---|---|---|---|
| 1 | 1.000 000 000 | 0.000 000 | 0.666 658 |
| 2 | 0.361 661 031 | 0.433 0124 | 2.821 367 |
| 3 | 0.217 322 900 | 0.652 6328 | 5.943 208 |
| 4 | 0.153 075 335 | 0.819 0950 | 9.936 795 |
| 5 | 0.116 976 574 | 0.957 9403 | 14.739 091 |
| 6 | 0.093 994 260 | 1.079 0415 | 20.304 015 |
| 7 | 0.078 156 144 | 1.187 4918 | 26.595 732 |
| 8 | 0.066 623 193 | 1.286 3330 | 33.582 213 |
| 9 | 0.057 876 606 | 1.377 5694 | 41.247 03 |
| 10 | 0.051 032 229 | 1.462 5929 | — |

It is known that the finite-size (mass-) gap scales at the critical point as $1/M$. Other physical quantities scale with the mass-gap in a well defined way more accurately, if $\Psi(\lambda)$ is a quantity which diverges in the infinite system as follows:

$$\Psi(\lambda) = A(\lambda - \lambda_c)^{\Psi}, \qquad |\lambda - \lambda_c| \to 0, \tag{7}$$

then the approximate $\Psi_M(\lambda_c)$ scales with the lattice size $M$ as $M^{\psi/\nu}$. The $\psi/\nu$ numbers will be determined for the quantities listed in table 2.

*3.2.1. The $\beta$ function.* The proposed method can be applied directly to the data in column 2 of table 2. Using the same notation as in § 3.1, in table 3 the results for cases A, B and C are listed. In case B it is used that the limit $a_0$ is zero; in case C, on the other hand, for the critical exponent $1/\nu$, the conjectured value $-1.2$ (den Nijs 1979) is used which is well supported by our calculations (columns 3 and 5).

The error of these calculated critical indices can also be estimated if the known limit $a_0$ is modified with the estimated errors of the calculations. Using this estimation, the suggested value of the critical index from our calculation is

$$1/\nu = -1.198 \pm 0.003.$$

*3.2.2. Susceptibility and specific heat.* In the same way as for the $\beta$ function the data for the (inverse) susceptibility have been analysed. The results are listed in table 4.

**Table 3.** Evaluation of the $\beta$ function by methods A, B and C. For notation see text.

| | | Case A | | Case B | | Case C | | |
|---|---|---|---|---|---|---|---|---|
| $M$ | $\beta_M$ | $1/\nu$ | $\lvert q_{n,n}\rvert$ | $1/\nu$ | $\lvert\varepsilon\rvert$ | $1/\nu$ | $\lvert q_{n,n}\rvert$ | $\lvert\varepsilon\rvert$ |
| 1 | 1.000 000 00 | | | | | | | |
| 2 | 0.361 661 031 | | | | | | | |
| 3 | 0.217 322 900 | −1.664 88 | 0.67E−1 | −1.101 65 | 0.15E 0 | −1.200 | 0.298E−1 | 0.117E 0 |
| 4 | 0.153 075 335 | −1.335 28 | 0.11E−1 | −1.207 05 | 0.24E−1 | −1.200 | 0.648E−3 | 0.247E−1 |
| 5 | 0.116 976 574 | −1.227 39 | 0.18E−2 | −1.187 93 | 0.15E−2 | −1.200 | 0.557E−3 | 0.103E−2 |
| 6 | 0.093 994 260 | −1.173 06 | 0.67E−3 | −1.194 96 | 0.28E−3 | −1.200 | 0.158E−3 | 0.352E−3 |
| 7 | 0.078 156 144 | −1.191 85 | 0.97E−4 | −1.196 29 | 0.37E−4 | −1.200 | 0.816E−4 | 0.693E−4 |
| 8 | 0.066 623 193 | −1.193 66 | 0.57E−4 | −1.197 23 | 0.18E−4 | −1.200 | 0.451E−4 | 0.335E−4 |
| 9 | 0.057 876 606 | −1.195 53 | 0.27E−4 | −1.197 75 | 0.78E−5 | −1.200 | 0.280E−4 | 0.157E−4 |
| 10 | 0.051 032 229 | −1.195 51 | 0.27E−4 | −1.198 35 | 0.69E−5 | −1.200 | 0.162E−4 | 0.110E−4 |

In case C the conjectured value $-1.733$ (which is supported by our calculations as well) has been used. Here in all calculations the values obtained from the data corresponding to $M=9$ significantly deviate from the other (better converged) values. The estimated error also signals some disturbing change. The good quality of the convergence for $M$ values up to 8 and the experience gained from different numerical studies permit us to believe that the last entry in column 3 is either erroneously listed or the original calculation has significantly higher relative error for $M=9$.

Hence using only values up to 8 we obtain

$$\gamma/\nu = -1.734 \pm 0.002.$$

The data for the specific heat could not have been analysed succesfully using this direct approach. With some standard series transformation, however, the critical index could be evaluated. These calculations will be published elsewhere. One possible reason for this is that the estimated value of the exponent is $\alpha/\nu \approx -0.4$, and the convergence in this case is much slower.

Before closing this section it should be mentioned that Hamer and Barber in their calculations gave somewhat smaller errors for their estimates. We repeated their

**Table 4.** Evaluation of the critical exponent $\gamma/\nu$ from the finite-size inverse susceptibility data (column 2) by methods A, B and C. For notation see table 3.

| | | Case A | | Case B | | Case C | | |
|---|---|---|---|---|---|---|---|---|
| $M$ | $\chi_M$ | $\gamma/\nu$ | $\lvert q_{n,n}\rvert$ | $\gamma/\nu$ | $\lvert\varepsilon\rvert$ | $\gamma/\nu$ | $\lvert q_{n,n}\rvert$ | $\lvert\varepsilon\rvert$ |
| 1 | 0.666 656 | | | | | | | |
| 2 | 2.821 367 | | | | | | | |
| 3 | 5.943 208 | −2.216 76 | 0.40E−1 | −1.584 39 | 0.18E 0 | −1.733 | 0.729E−2 | 0.124E 0 |
| 4 | 9.936 795 | −1.595 16 | 0.57E−2 | −1.737 24 | 0.68E−2 | −1.733 | 0.175E−3 | 0.679E−2 |
| 5 | 14.739 091 | −1.740 59 | 0.13E−3 | −1 734 29 | 0.11E−3 | −1.733 | 0.284E−4 | 0.138E−3 |
| 6 | 20.304 015 | −1.733 28 | 0.22E−4 | −1.734 94 | 0.13E−4 | −1.733 | 0.259E−4 | 0.232E−5 |
| 7 | 26.595 732 | −1.734 79 | 0.20E−5 | −1.735 02 | 0.10E−5 | −1.733 | 0.176E−4 | 0.802E−5 |
| 8 | 33.585 213 | −1.734 84 | 0.15E−5 | −1.735 10 | 0.67E−6 | −1.733 | 0.126E−4 | 0.483E−5 |
| 9 | 41.247 030 | −1.766 49 | 0.19E−3 | −1.721 38 | 0.80E−4 | −1.733 | 0.484E−4 | 0.598E−4 |

calculations and found that in all cases the change of their estimates due to different $M$ shifts is larger than their suggested limits, even outside the region where this shift causes some unexplained instability. Moreover, the optimum parameters of these $M$ shifts are different for $1/\nu$ and for $\gamma/\nu$ and their values are chosen arbitrarily. Hence we feel that their errors are underestimated and do not follow from the given data.

### *3.3. One-dimensional quantum Ising model*

There are many quasi-one-dimensional magnetic insulators which can be described by the quantum Ising model with spin values of $\frac{1}{2}$, 1, or higher.

The case $\frac{1}{2}$ can be solved exactly by the Bethe ansatz; the other cases should be investigated numerically. Recently Solyom and Ziman (1984) investigated these models with specific finite-size calculations. To check their numerical procedure they calculated the $\frac{1}{2}$ case, too. Using their data we analysed the energy of the ground state and the value of the gap with our modified Romberg algorithm. Tables 5 and 6 contain the results of this analysis. It is seen that the ground state energy is obtained for five digit accuracy (the exact value is $\ln 2 - 0.25 = 0.443\ 147\ldots$), in spite of the fact that the initial data were given only for six digits! If we use all the calculated data, then the estimated error (column 6) indicates that the inital accuracy does not allow such high-order calculation, in the same way as was noticed in § 3.1. From the estimated error it is seen that the order of about six is optimal. Hence six input data have been chosen such that they span the same interval (2-18) and the ratio of the consecutive $M$ values should be as big as possible. Calculation with one possible choice is presented

**Table 5.** Asymptotic estimates of the ground state energy for the spin-$\frac{1}{2}$ quantum Ising model. Finite-size data are from Solyom and Ziman (1984).

| | | Case A | | Case C | |
|---|---|---|---|---|---|
| $M$ | $E_M$ | $E_0$ | $\alpha$ | $E_0$ | $\lvert\varepsilon\rvert$ |
| 2 | −0.750 000 | | | | |
| 4 | −0.500 000 | | | | |
| 6 | −0.467 129 | −0.449 158 | −2.5649 | −0.443 853 | 0.24E − 1 |
| 8 | −0.456 387 | −0.442 117 | −1.8075 | −0.443 110 | 0·69E − 3 |
| 10 | −0.451 545 | −0.443 166 | −2.0110 | −0.443 138 | 0.26E − 4 |
| 12 | −0.448 949 | −0.443 138 | −2.0002 | −0.443 138 | 0.22E − 6 |
| 14 | −0.447 396 | −0.443 167 | −2.0190 | −0.443 149 | 0.10E − 4 |
| 16 | −0.446 394 | −0.443 203 | −2.0574 | −0.443 168 | 0.19E − 4 |
| 18 | −0.445 708 | −0.443 088 | −2.0426 | −0.443 062 | 0.10E − 3 |

**Table 6.** Same as table 5 with optimal sampling.

| | | Case A | | Case C | |
|---|---|---|---|---|---|
| $M$ | $E_M$ | $E_0$ | $\alpha$ | $E_0$ | $\lvert\varepsilon\rvert$ |
| 2 | −0.750 000 | | | | |
| 4 | −0.500 000 | | | | |
| 8 | −0.456 387 | −0.447 171 | −2.5191 | −0.443 528 | 0.25E − 1 |
| 12 | −0.448 949 | −0.442 782 | −1.8807 | −0.443 131 | 0.38E − 3 |
| 14 | −0.447 396 | −0.443 153 | −2.0073 | −0.443 143 | 0.11E − 4 |
| 18 | −0.445 708 | −0.443 151 | −2.0061 | −0.443 147 | 0.40E − 5 |

in table 6. The results show a steadily improved approximation for the limit as is expected. Other possible choices show the same feature.

From here, the estimated limit is accurate to six digits, which is the true accuracy of the initial data, and the estimated critical index is accurate to three digits. Naturally, one can hardly expect more accurate values and it is significantly better than the values obtained by standard graphical extrapolation.

### *3.4. Mass gap in lattice spectrum calculations*

For the time being the numerical investigations of field theoretical models are the most powerful methods to explore the structure of quantum field theory.

Different numerical approaches have been applied to the quantum spin chains with O(2) symmetry. A new numerical procedure to handle the problem of truncating the (infinite-)dimensional Hilbert space has been investigated by Patkos and Rujan (1985). The finite-lattice mass-gap values from their calculations for different coupling strengths ($x$) are given in table 7.

Figure 1 summarises the analysis of these data using our method. The numerical limiting mass-gap value has a minimum around $x \approx 2$. Since the numerical convergence exponent converges to $-1$, which is the theoretical value at the critical point, the calculations have been performed according to case C too. In this figure only calculations based on method C are displayed. Basically similar results are obtained in the two other cases (A and $B_1$).

In addition figure 2 shows the deviation of the calculated convergence exponent from the theoretical value of $-1$ as a function of the coupling strength. Once again its minimum is minimal around $x \approx 2$.

**Table 7.** Finite-size mass-gap values for coupling strengths ($x$) between 1.6–2.3 (upper part) of the quantum spin chain with O(2) symmetry (Patkos and Rujan 1985). Double interpolated mass-gap values for 1.9, 2.0, 2.1 (lower separated part) of the spline interpolation. The first inaccurate digits of the interpolated values are underlined.

| $x = 1.6$ | 1.7 | 1.8 | 1.9 | 2.0 | 2.1 |
|---|---|---|---|---|---|
| 1.000 000 | 1.000 000 | 1.000 000 | 1.000 000 | 1.000 000 | 1.000 000 |
| 0.520 616 | 0.517 402 | 0.514 738 | 0.512 521 | 0.510 669 | 0.509 115 |
| 0.354 550 | 0.350 640 | 0.347 510 | 0.433.990 | 0.342 960 | 0.341 300 |
| 0.269 822 | 0.265 769 | 0.262 610 | 0.260 134 | 0.258 182 | 0.256 636 |
| 0.218 280 | 0.214 250 | 0.211 180 | 0.208 820 | 0.207 017 | 0.205 604 |
| 0.183 541 | 0.179 612 | 0.176 670 | 0.174 408 | 0.172 773 | 0.171 485 |
| 0.158 508 | 0.154 579 | 0.151 894 | 0.149 812 | 0.148 231 | 0.147 065 |
| 0.139 619 | 0.135 923 | 0.133 234 | 0.131 318 | 0.129 842 | 0.128 747 |
| $x = 2.2$ | 2.3 | | $x = 1.9$ | 2.0 | 2.1 |
| 1.000 000 | 1.000 000 | | 1.000 000 | 1.000 000 | 1.000 000 |
| 0.507 809 | 0.506 706 | | 0.512 52$\underline{5}$ | 0.510 66$\underline{8}$ | 0.509 11$\underline{2}$ |
| 0.339 960 | 0.338 850 | | 0.344 99$\underline{7}$ | 0.342 95$\underline{7}$ | 0.341 300 |
| 0.255 405 | 0.254 421 | | 0.260 14$\underline{1}$ | 0.259 18$\underline{1}$ | 0.256 63$\underline{2}$ |
| 0.204 500 | 0.203 630 | | 0.208 83$\underline{0}$ | 0.207 01$\underline{3}$ | 0.205 60$\underline{2}$ |
| 0.170 497 | 0.169 718 | | 0.174 42$\underline{8}$ | 0.172 76$\underline{1}$ | 0.171 48$\underline{9}$ |
| 0.146 152 | 0.145 300 | | 0.149 81$\underline{8}$ | 0.148 23$\underline{0}$ | 0.147 96$\underline{7}$ |
| 0.127 932 | 0.127 308 | | 0.131 318 | 0.129855 | 0.128 74$\underline{2}$ |

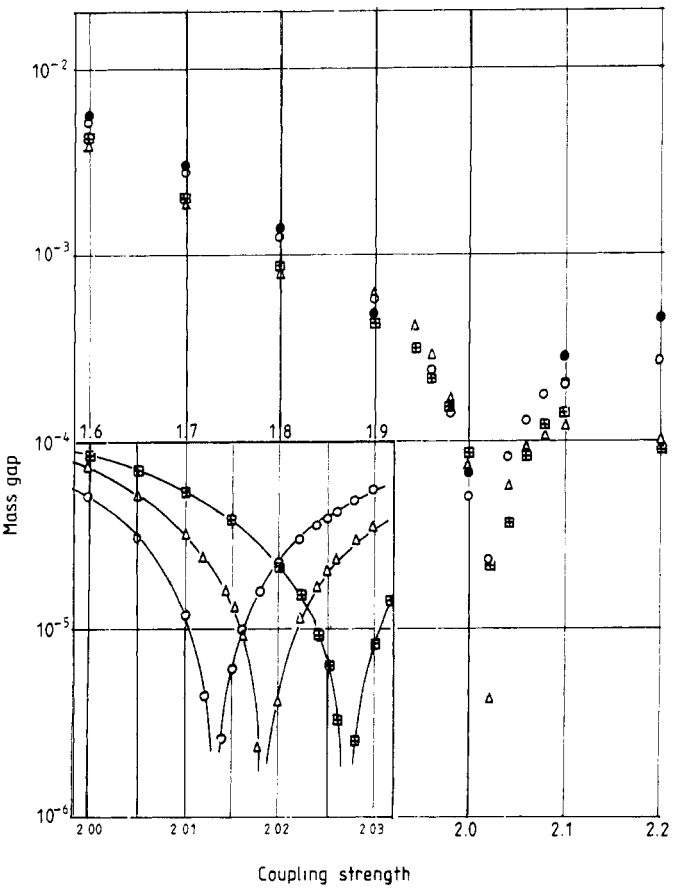


**Figure 1.** Mass-gap values against coupling $x$ from different orders of the modified Romberg algorithm in the O(2) model. △, data with $M = 1, 2, 3, 5, 8$; ○, data with $M = 1, 2, 4, 8$; ⊞, data with $M = 1, 2, 3, 4, 8$; ●, data with $M = 1, 2, 4, 7$.

By standard cubic spline fitting of the $x$ dependence of finite lattice gaps the limiting gap value and its estimated error have been analysed around $x = 2$ in more detail. This analysis is displayed with a finer scale on the insert of figure 1. From this analysis our preferred critical value is $x = 2.02 \pm 0.02$.

Once again the original data are given for six digits, which is the estimated accuracy of the original calculation. With this accuracy the extrapolation can be performed only with some limited order. In figure 1 the different notations correspond to the different choice of the initial data set. However, the calculated limits (and errors) basically do not depend on the actual choice as is seen in the figure.

It is amusing that the gaps obtained at the estimated critical point are consistently of order $10^{-6}$ which is the accuracy of the initial data.

This quasi-zero of the mass gap cannot be obtained, however, for data calculated at the chosen couplings (1.6, 1.7, ..., 2.3) but at some intermediate values generated by the cubic spline interpolation. To check that the singular-looking smooth curves in figure 1 are not an artefact of the interpolation procedure itself, the following test has been performed. First the finite lattice mass-gap data have been interpolated at points 1.65, 1.75, ..., 2.25, using the original data (as given in table 7); then using

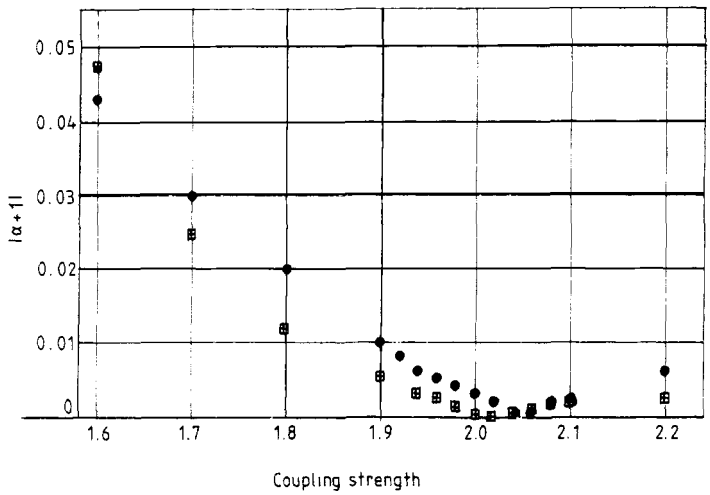


**Figure 2.** Difference of the calculated convergence exponent ($\alpha$) and the theoretical value ($-1$) as a function of the coupling constant in the O(2) model. For notation see figure 1.

these interpolated values a second interpolation is based on these new values and using them again, a cubic spline interpolation has been performed for points 1.9, 2.0, 2.1. These re-interpolated values are listed in the second part of table 7. It is seen that the original data were re-obtained for six digits which proves the consistency and accuracy of the cubic spline interpolation used to generate the finite lattice mass-gap values at the intermediate coupling strengths.

## 4. Summary

A new method is presented to evaluate limiting values of finite-size scaling calculations. This new method is an appropriate modification of the Romberg algorithm, which calculates the 'critical index' consistently (this quantity should be predetermined for the standard Romberg procedures).

For a simple physical problem, for the one-dimensional lattice (Ewald) sum the extraordinary accuracy of the method is demonstrated. This accuracy cannot be reached in standard finite-size calculations, where the input data for this algorithm are usually given with much less accuracy.

However, for a selection of published finite-size data the evaluation of the limits shows accuracy which in a certain sense surpasses the usual expectations.

The ultimate accuracy in some cases seems to reach the accuracy of the raw initial data themselves. This naturally can only be reached if the expansion equation (5) is highly convergent. In the case when a singular expression has confluent singularities as well, a much slower convergence is expected. The results for the quantum Ising problem (at least for $s=\frac{1}{2}$) and for the O(2) model indicate that in these cases the confluent term probably vanishes.

It is important to emphasise that the unique error predicting features of the presented method are very useful to get an objective measure of the quality for the limiting value. As far as we know this is the first method which has this important feature.

In this first paper the method itself is presented and we excluded many possible modifications of it. As it stands the application for the model $Z_3$ allows the evaluation of the critical indices indirectly, hence their error can only be estimated by biased estimation discussed in § 3.2. Naturally if one expresses finite-size approximants for a given exponent from the ratio of the consecutive elements of table 2 as usual (Hamer and Barber 1981), then our Romberg-type calculation (now with $\alpha = -1$) will give critical indices directly and their error estimates as discussed earlier.

One further comment is that any transformation which eliminates some confluent (or antiferromagnetic) term can be applied along with this proposed method. It is, therefore, expected that as a first step the application of the alternating VBS transformation due to Vanden Broeck and Schwartz (1979) which is capable of reducing the 'next' leading correction term would be beneficial in cases where this term is significant. Evaluation of this possibility and a detailed comparison with existing studies for different extrapolation methods (Barber and Hamer 1982, Smith and Ford 1979) will be published elsewhere.

The question of the confluent singularities will be discussed also in the second part of this series of papers with applications to series extrapolations different from the finite-size calculations discussed here.

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