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Accurate calculation of ground-state energies in an analytic Lanczos expansion

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Abstract. An analysis of a general non-perturbative technique for calculating ground-state properties of extensive lattice many-body systems is presented, in order to extract accurate numerical values characterizing the ground-state spectrum. This technique, the plaquette expansion, employs an expansion about the thermodynamic limit of the coefficients that are generated by the Lanczos process. For the ground-state energy this error analysis, using theorems on the error bounds for the Lanczos method and the truncation in the plaquette expansion, allows for an accurate estimate when the approximation is taken to a given order. As an example we analyse the one-dimensional antiferromagnetic Heisenberg model, and find that the best ground-state energy density is within 3×10^{-6} of the exact value, although the systematic error is 10^{-5}. We also find, for this model, systematic improvement with each new order included in the expansion and have not observed any asymptotic tendencies. At equivalent orders of truncation we achieve far better results than for the other moment methods, such as the t-expansion or the connected-moment expansion.

1. Introduction

Recently a number of non-perturbative techniques have been devised for calculating spectral properties of strongly interacting systems, and all share a common background in being based on moment formalisms. The first of these was the t-expansion [1], which in turn led to the connected-moment expansion (CMX) [2], and most recently an analytic Lanczos expansion, the plaquette expansion [3]. These methods are all based essentially on linked-cluster expansions, that is to say connected moments with respect to some trial ground state, and all ground-state averages automatically have size extensivity. However, while these methods have the same starting point they differ in their treatment, and consequently have different properties with regard to accuracy and convergence. Most implementations of these techniques have been numerical ones where the aim was to accurately represent ground-state properties over a wide range of coupling strengths, far beyond any perturbative regime. There have been a number of numerical investigations of the t-expansion and the CMX in all its variants with simple models drawn from a range of problems, e.g. correlation energies in molecules [2] and quantum spin systems [4] to name but a few. Our intention here is to present a theoretical analysis of the errors in the plaquette expansion, and apply this analysis to a specific example of an exactly solvable model thereby demonstrating that this method is capable of yielding accurate ground-state energies. We can also test directly a number of aspects of our analysis against the known exact results of the model.

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The resolvent function,

$$R(z) = \langle\psi_0| \frac{1}{z - H} |\psi_0\rangle \tag{1}$$

plays an important role in describing the spectrum of many-body systems with a Hamiltonian H at zero temperature. Specifically, knowledge of the behaviour and analyticity of the resolvent as a function of complex z yields the ground state and excited states within a given sector, and the density of states from which any physical average may be computed. It has a real Jacobi-fraction continued-fraction form constructed from the Lanczos coefficients α_n, β_n:

$$R(z) = - \underset{n=0}{\overset{\infty}{\mathbf{K}}} - \left(\frac{\beta_n^2}{z - \alpha_n} \right) \tag{2}$$

and its termination after the nth element, termed its nth continuant, defines the nth numerator and nth denominator, $P_n(z)$ and $Q_n(z)$, respectively:

$$R_n(z) \equiv \frac{1}{z - \alpha_0} - \frac{\beta_1^2}{z - \alpha_1} - \frac{\beta_2^2}{z - \alpha_2} - \cdots - \frac{\beta_n^2}{z - \alpha_n} \equiv - \frac{P_n(z)}{Q_n(z)}. \tag{3}$$

Here β_0^2 is taken to be unity. The polynomials $P_n(z)$ and $Q_n(z)$ are orthogonal polynomials defined by the three-term recurrence relation

$$Q_n(z) = (z - \alpha_n) Q_{n-1}(z) - \beta_n^2 Q_{n-2}(z) \tag{4}$$

with the polynomials having the initial terms

$$\begin{aligned} Q_{-2}(z) &= 0 \qquad & Q_{-1}(z) &= 1 \\ P_{-2}(z) &= 1 \qquad & P_{-1}(z) &= 0. \end{aligned} \tag{5}$$

In the more traditional manner the Lanczos coefficients arise from the following recurrence which generates the Lanczos basis $\{|\psi_0\rangle, |\psi_1\rangle \ldots\}$ in which the Hamiltonian becomes tri-diagonal:

$$H|\psi_n\rangle = \beta_n |\psi_{n-1}\rangle + \alpha_n |\psi_n\rangle + \beta_{n+1} |\psi_{n+1}\rangle.$$

The Lanczos coefficients, whose individual terms are ordered with respect to the size of the system, or the number of plaquettes N, were shown [3, 5] to have a simple relationship to the scaled connected moments for arbitrary order:

$$\alpha_n = c_1 N + n \left[\frac{c_3}{c_2} \right] + \frac{1}{2} n(n-1) \left[\frac{3c_3^3 - 4c_2 c_3 c_4 + c_2^2 c_5}{2c_2^4} \right] \frac{1}{N} + \cdots \tag{6}$$

for $n \geqslant 0$, and

$$\begin{aligned} \beta_n^2 = {} & n c_2 N + \frac{1}{2} n(n-1) \left[\frac{c_2 c_4 - c_3^2}{c_2^2} \right] \\ & + \frac{1}{6} n(n-1)(n-2) \left[\frac{-12c_3^4 + 21 c_2 c_3^2 c_4 - 4 c_2^2 c_4^2 - 6 c_2^2 c_3 c_5 + c_2^3 c_6}{2c_2^5} \right] \frac{1}{N} \\ & + \cdots \end{aligned} \tag{7}$$

for $n \geqslant 1$, where the c_n are defined through the connected Hamiltonian moments as $\langle H^n \rangle_c \equiv c_n N$. Here the definitions and notation of reference [5] have been adopted, rather than those in references [3, 6].

The plaquette expansion is a general-purpose non-perturbative method of calculating the spectrum and other ground-state properties of lattice models in the bulk limit. The analytical behaviour and the physical predictions of the first two orders in the plaquette

expansion, referred to as the zeroth level and the first-order level, have been described in previous papers [5, 7]. In all of the analysis presented here we concentrate on the ground-state spectrum, but a formalism has been developed for other ground-state averages by considering modified moments and their modified resolvent operator in reference [8].

For accurate evaluations one needs to take the expansion to higher orders, in fact to arbitrarily large orders, only limited by the practical considerations at hand, such as the maximum number of moments that can be computed. However, there are some delicate questions to consider in applying the plaquette expansion. Assuming that we knew the exact α_n and β_n^2 for all iterations n (which would be tantamount to detailed knowledge of an exactly solvable system), and therefore the derived numerator and denominator polynomials P_n and Q_n, we have two limiting processes to consider:

(i) firstly the limit as the number of Lanczos iterations $n \to \infty$ for a fixed-size, finite system with N sites; and

(ii) the thermodynamic limit $N \to \infty$;

that is,

$$R_\infty(z) = -\lim_{N\to\infty}\left\{\lim_{n\to\infty}\frac{P_n(z;\, N, \{c_k\colon k = 1, 2n+1\})}{Q_n(z;\, N, \{c_k\colon k = 1, 2n+1\})}\right\}. \tag{8}$$

So in practice one would numerically diagonalize the tri-diagonal Lanczos matrix, for a series of finite-sized systems tending to large sizes, where in each case the Lanczos procedure would be applied to construct a sufficiently large matrix for the Lanczos truncation error to become small. But it is immediately apparent that this procedure cannot be applied to the plaquette expansion in general because the error in the truncated coefficients can sometimes grow with Lanczos iteration number, and at a faster rate than the coefficient themselves.

There will be an optimal value n_{opt} at which the Lanczos iteration should be terminated, which will depend on N and the specific model:

$$n < n_{opt}(r, N; \{c_k\})$$

and the plaquette expansion approximation to the resolvent is

$$R_{PE}(z) = -\lim_{N\to\infty}\left\{\frac{P_{n_{opt}}(z;\, N, \{\alpha_k^{(r)}, \beta_k^{(r)}\colon k = 1, 2n_{opt}+1\})}{Q_{n_{opt}}(z;\, N, \{\alpha_k^{(r)}, \beta_k^{(r)}\colon k = 1, 2n_{opt}+1\})}\right\}. \tag{9}$$

In earlier applications of this method [3, 6, 9, 10], these choices of cut-off and termination were made on a plausible although *ad hoc* basis, where the point of inflection of the ground-state energy versus Lanczos iteration number was taken as the cut-off point (assuming there to be a point of inflection, which is not always the case).

The purpose of this paper is to elaborate a theory for the errors arising in the expansion, and therefore to describe an algorithm by which these errors can be controlled, and thus extract the best estimate from numerical data. By way of example we test this analysis on the one-dimensional antiferromagnetic Heisenberg model.

2. Error analysis in the plaquette expansion

We begin by making some definitions and stating some conventions. Firstly we use the Hamiltonian density, that is the Hamiltonian matrix divided by the number of plaquettes, so the Lanczos coefficients are adjusted accordingly. The exact Lanczos coefficients are

denoted by

$$\begin{aligned} &\alpha_n^{(r=\infty)}(N) \\ &(\beta_n^{(r=\infty)})^2(N) \end{aligned} \tag{10}$$

even though they are not known for general n beyond some very low values. The approximated Lanczos coefficients for the Hamiltonian density, accurate to order $r = 0, 1, 2, \ldots$, can be represented as

$$\begin{aligned} \alpha_n^{(r)} &= \sum_{p=0}^{r} \frac{a_p(n)}{N^p} + \mathrm{O}((n/N)^{r+1}) \\ (\beta_n^{(r)})^2 &= \sum_{p=1}^{r+1} \frac{b_p(n)}{N^p} + \mathrm{O}((n/N)^{r+2}) \end{aligned} \tag{11}$$

where a_p and b_p are polynomials of degree p in n. For a given order in the expansion, one has essentially a double asymptotic expansion in $n \to \infty$ and $N \to \infty$.

The Lanczos termination error, for a system of exact Lanczos coefficients, is defined as

$$\delta\epsilon_n^{LT} \equiv \epsilon_n^{(r=\infty)} - \epsilon_\infty^{(r=\infty)} \tag{12}$$

where $\epsilon_\infty^{(r=\infty)}$ is the exact ground-state energy density and $\epsilon_n^{(r=\infty)}$ is the lowest eigenvalue of the nth terminated exact Lanczos matrix. No exact expressions are known for this, except for some simple classical orthogonal polynomials—e.g. the Chebyshev polynomial—although there are results for asymptotic approximations $n \gg 1$ for a larger class of orthogonal polynomial systems. It appears that a universal expression is unlikely to exist. However, there exist bounds on this error [11] of which the simplest form is

$$0 \leqslant \delta\epsilon_n^{LT} \leqslant (\epsilon_{sup} - \epsilon_0) \left(\frac{\tan\theta(\psi_{trial}, \psi_0)}{T_{n-1}(\gamma)} \right)^2 \tag{13}$$

although there are optimized variants of this [12, 13]. Here ϵ_{sup} is the exact supremum to the energy density spectrum, ϵ_0 is the exact ground-state energy density, $\theta(\psi_{trial}, \psi_0)$ is the angle between the trial state ψ_{trial} and the exact ground-state wavefunction ψ_0 computed with the appropriate inner product, and γ is defined by

$$\gamma = 1 + 2\frac{\epsilon_1 - \epsilon_0}{\epsilon_{sup} - \epsilon_1} \tag{14}$$

with the first exact excited-state energy ϵ_1. Finally the n-dependence is controlled through the complex Chebyshev polynomial

$$T_k(z) \equiv \cosh(k \cosh^{-1}(z)). \tag{15}$$

Physically this result means that the rate of convergence of the Lanczos method is determined by the spectrum of the system, controlled in particular by the gap between the first excited state (within the sector defined by the ground state) and the ground state relative to the spectral width. The larger this relative gap, the more rapid the convergence.

We will take this functional form to give the exact Lanczos termination error, and not just the bound to it. There is numerical evidence given in reference [12] that this form quite accurately describes the actual error for $n \gg 1$, at least in its optimized forms. We also have verified that the optimized forms can represent this termination error in the case of exact finite AFH chains for over 12 orders of magnitude. All of the spectral quantities that are unknown will be parametrized and determined from the numerical values of the lowest eigenvalue for a sequence of Lanczos iterations. That is, for large Lanczos iterations,

$$\delta\epsilon_n^{LT} = e_{LT}\lambda^{-n} \tag{16}$$

where e_{LT} and λ are parameters to be determined. From such a simple form there is a simple interpretation of the Lanczos rate of convergence coefficient λ—for large system sizes N we find that the scaled energy gap is given by

$$N^2(\epsilon_1(N) - \epsilon_0(N)) = (\epsilon_{sup} - \epsilon_0)\frac{1}{16}(\lambda - 1)^2 N^2 \tag{17}$$

where $\epsilon_0(N)$, $\epsilon_1(N)$ are the ground-state and first-excited-state energy densities in the particular sector the trial state happens to lie in. We have found that this gap can be successfully extracted from the convergence behaviour of the Lanczos eigenvalue for the exact finite AFH chain using the above simple dependence equation (16). However, it is not possible to identify the gap found using the plaquette expansion data with the exact gap because of plaquette expansion corrections, although there may exist a simple and approximate relationship between them.

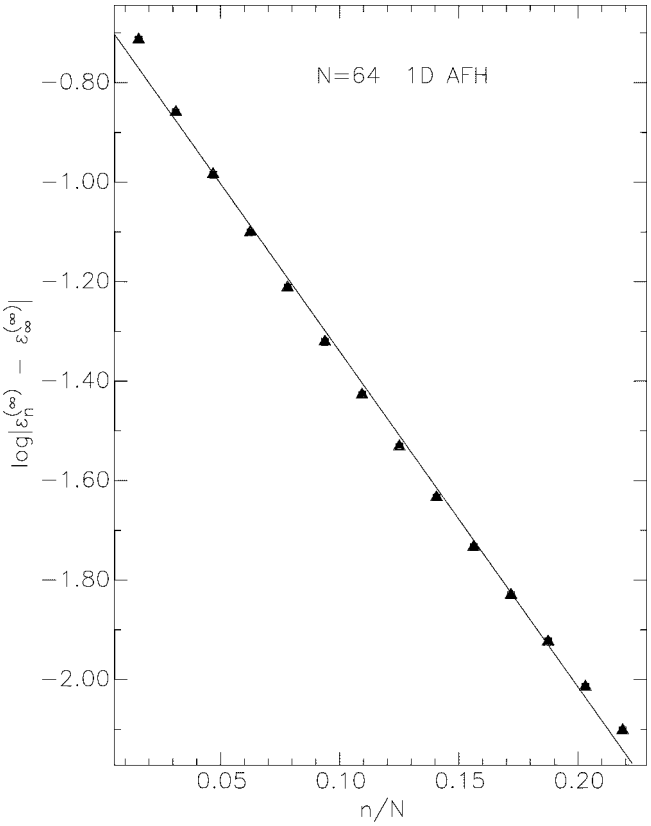

Figure 1. The exact Lanczos termination error $|\delta\epsilon_n^{LT}|$ with Lanczos iteration number $n \leqslant 14$ for the 1D AFH model with $N = 64$ sites.

How accurate this simple form may be can be gauged by examining the exact results for the 1D AFH model. Given that we have moments up to order 28 [14] (see the following section), one can exactly perform the first 14 Lanczos iterations on systems of arbitrary size. In figure 1 we display $\log|\delta\epsilon_n^{LT}|$ versus the Lanczos step n for a system of size $N = 64$. We have taken the exact ground-state energy density for $N = 64$ from the finite-size correction formula of reference [15]. On top of the exact differences we have placed a best-fit straight

line to indicate the extent of the deviations from this simple form. It is clearly not accurate enough in a quantitative sense to follow the local detail, but the deviations are small and regular.

To model the effect of the truncation due to the plaquette expansion taken up to order r we define

$$\delta\epsilon_n^{PE} \equiv \epsilon_n^{(r)} - \epsilon_n^{(r=\infty)} \tag{18}$$

where $\epsilon_n^{(r)}$ is the lowest eigenvalue of the Lanczos matrix truncated to order r and terminated at the nth Lanczos iteration. To arrive at a general form for this error we appeal to three arguments. Firstly, one can utilize theorems for lower bounds on the lowest zeros of members of an orthogonal polynomial system [16] which states $\epsilon_n > B$ where

$$B = \min\{x_k^-\colon 1 \leqslant k < n\} \tag{19}$$

with the simplest bound sequence is given by

$$x_k^- = \frac{1}{2}\left[(\alpha_k + \alpha_{k+1}) - \sqrt{(\alpha_k - \alpha_{k+1})^2 + 16\beta_k^2}\right]. \tag{20}$$

Given that the errors in the Lanczos coefficients are going to be of the order of $(n/N)^{r+1}$, then the error in the bound will be the same, and thus we take this to be the order of the error in the plaquette expansion for the ground-state energy density, at this Lanczos iteration. That is we write

$$\delta\epsilon_n^{PE} = f_1\left(\frac{n}{N}\right)^{r+1} + f_2\left(\frac{n}{N}\right)^{r+3/2} + f_3\left(\frac{n}{N}\right)^{r+2} + \cdots \tag{21}$$

where f_1, f_2 and f_3 are parameters to be determined.

Our second argument arises from the possibility of analytically diagonalizing the Lanczos tri-diagonal Hamiltonian for the first three iterations, with the exact Lanczos coefficients and with the plaquette expansions of them. It is found that the plaquette expansion is exact for the first two iterations: $\delta\epsilon_{1,2}^{PE} = 0$. The first non-zero difference is found to be

$$\delta\epsilon_3^{PE} = \frac{2}{27}\left(\frac{3}{N}\right)^{r+1} + \mathrm{O}(N^{-r-3/2}) \tag{22}$$

which agrees with out first argument.

We also compute the exact plaquette expansion error for Lanczos iterations up to 14 for a system of size $N = 64$, and these are shown in figure 2, in the form of $\log|\delta\epsilon_n^{PE}|$ versus the Lanczos step n for expansion orders $r = 5, 7, 9$ and 11. Clearly the leading-order term is correct, as indicated by the initial point and slope, and the total corrections are reasonably well bounded.

Combining these two forms, and neglecting the small adjustments in the error law for finite Lanczos termination due to the replacement of the exact Lanczos coefficients with the truncated ones (this adjustment can formally be taken into account in the plaquette expansion error law) one has the total error

$$\delta\epsilon_n^{total} \equiv \epsilon_n^{(r)} - \epsilon_\infty^{(r=\infty)} = \delta\epsilon_n^{LT} + \delta\epsilon_n^{PE} \tag{23}$$

or in terms of the introduced parameters

$$\epsilon_n = \epsilon_0 + e_{LT}\lambda^{-n} + f_1\left(\frac{n}{N}\right)^{r+1} + f_2\left(\frac{n}{N}\right)^{r+3/2} + f_3\left(\frac{n}{N}\right)^{r+2}. \tag{24}$$

It is the quantity ϵ_0 that is sought, being the estimate for the ground-state energy. We must emphasize that the above form is not expected to exactly represent the actual variation of

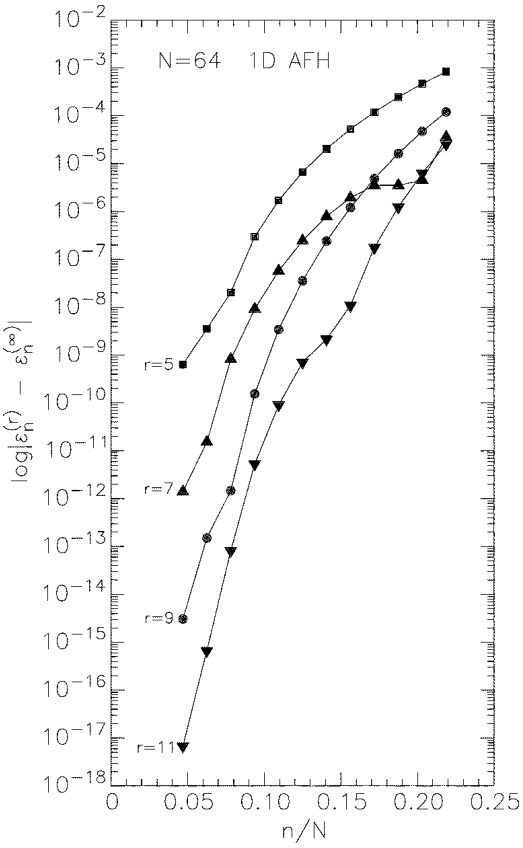

Figure 2. The exact plaquette expansion error $|\delta\epsilon_n^{PE}|$ with Lanczos iteration number $n \leqslant 14$ for the 1D AFH model with $N = 64$ sites. The curves are labelled according to the order r at which the expansion is truncated.

the eigenvalue with the Lanczos iteration number, but that it is the form that most closely represents it for a given small number of free parameters. The actual, or highly accurate but unknown form would be much more complicated and require a greater number of free parameters. In all of the above, the size of the system N had to be finite, although large, for the expansion to work, and we have to extrapolate to the thermodynamic limit via a sequence of systems of increasing size.

3. The method applied to the 1D AFH model

We test these ideas on the one-dimensional isotropic antiferromagnetic Heisenberg model, where the trial state taken in this case was the classical Néel state. The Lanczos coefficients for this model have been calculated, in the plaquette expansion, using connected Hamiltonian moments up to $\langle H^{28}\rangle_c$, which were supplied by Zheng Weihong and colleagues [14]. We have used the product–difference algorithm, obtained within the memory function formalism as given in reference [21, 22], to compute the Lanczos coefficients up to order $r = 11$ from the moments. The cumulants and the Lanczos coefficients are available, upon request, from one of the authors (NSW). With the Hamiltonian matrix constructed in tri-diagonal form the

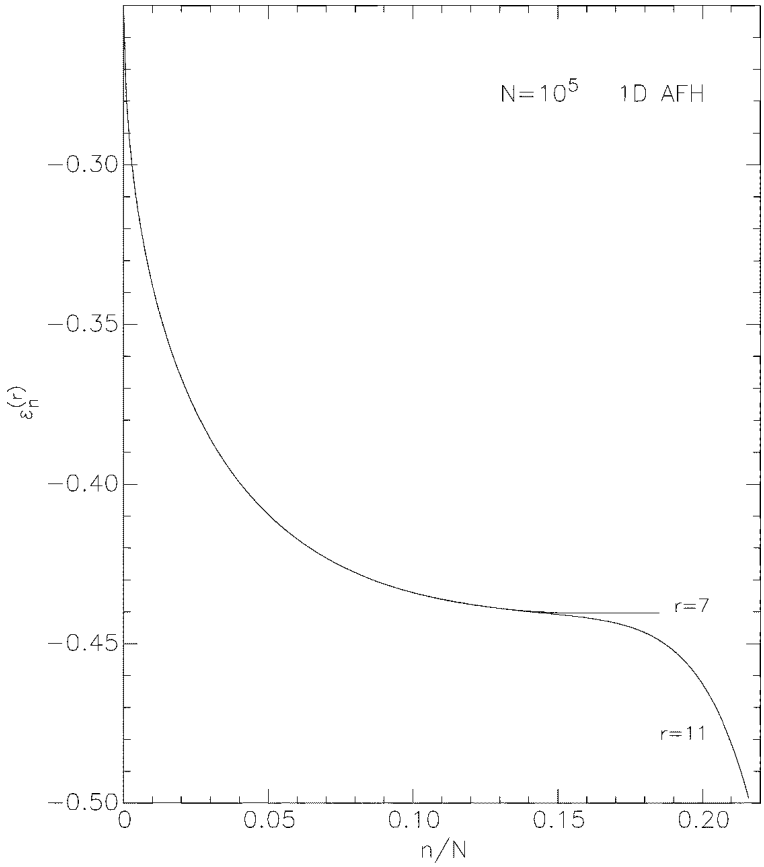

Figure 3. The variation of the lowest eigenvalue in the plaquette expansion $\epsilon_n^{(r)}$ with the Lanczos iteration number n for the two different types of behaviour: the critical case for order $r = 11$; and the non-critical case for $r = 7$ when $N = 10^5$.

lowest eigenvalue for the model was computed for various chain lengths N and at various orders in the plaquette expansion r, all at regular Lanczos iteration numbers. Qualitatively the data were found to exhibit two types of behaviour as the Lanczos iteration number becomes large (of order N):

(i) *critical point* behaviour with at least one point of inflection and where the eigenvalue often diverges through negative values as $n \to \infty$, which applies to orders $r = 4, 5, 6$, and 11; and

(ii) *non-critical point* behaviour without a point of inflection and where the eigenvalue usually tends asymptotically to a fixed value as $n \to \infty$, which occurs for orders $r = 7, \ldots, 10$.

The essential distinction is the existence of a high-order critical point (the slope is always negative), rather than the limiting behaviour of the eigenvalue. For small values of iteration number the two cases have similar rapid decays and flattening-out shapes. Examples of both of these types of behaviour are displayed in figure 3.

There are two possible options for achieving the correspondence of our assumed, but inexact, form with the actual data:

(i) a direct and local approach where the data are transformed under repeated applications of a combined Shanks-type transformation and Richardson extrapolation law constructed according to our assumed form; or

(ii) a global approach whereby the form is fitted to a subset of the data according to some appropriate criteria.

We chose the latter course, as it was more stable and yielded superior accuracy.

Table 1. Ground-state energy density estimates ϵ_0 for the 1D antiferromagnetic Heisenberg chain at various orders r in the plaquette expansion for systems of various sizes N.

ϵ_0	$N = 10^3$	5×10^3	10^4	5×10^4	10^5
Order $r = 4$	−0.442 344 16	−0.443 225 63	−0.443 443 98	−0.443 589 13	−0.443 610 08
5	−0.442 492 69	−0.443 066 96	−0.443 165 26	−0.443 273 09	−0.443 295 76
6	−0.442 623 40	−0.443 017 00	−0.443 102 45	−0.443 205 50	−0.443 227 62
7	−0.442 637 79	−0.443 010 40	−0.443 095 61	−0.443 199 45	−0.443 222 55
8	−0.442 642 86	−0.442 998 29	−0.443 082 67	−0.443 191 29	−0.443 215 84
9	−0.442 681 43	−0.443 020 47	−0.443 097 88	−0.443 199 07	−0.443 221 46
10	−0.442 738 50	−0.443 049 03	−0.443 120 78	−0.443 209 57	−0.443 228 30
11	−0.442 733 78	−0.443 045 10	−0.443 115 35	−0.443 126 23	−0.443 146 09

For the fitting criteria there were two different criteria that we tested, a least-squares and an L_p-norm fit over the residuals for $p = 10$. The latter case should be preferred because the criterion of the fit is then the largest absolute deviation from the chosen law, which is more appropriate for data that have very little random error in comparison to the systematic errors. This was borne out in the analysis, with the least-squares fit giving inferior results. Fitting points were sampled in step sizes of $N/1000$, and a total of 70 points in an interval were taken to be fitted which included at least 41% of the total number of points. Results for fitting intervals containing more than 80 points sometimes failed to yield physical solutions, and those with less than 50 points had little significance. An average of the fitted results for $60 \rightarrow 80$ points changed the most accurate energy by only 1.0×10^{-5}. The fitting interval was moved along the total range of data, and the residuals computed. The fit for the interval where the residual was smallest was the one taken as the best estimate. When the interval includes low-Lanczos-iteration-number data, the form for the termination error is not adequately modelled by a simple exponential decay although the plaquette expansion error is negligible. On the other hand when the interval includes high-Lanczos-number data the termination error is very small but now the plaquette expansion error terms have grown and cannot be adequately represented by three terms. So our fitted residuals were lowest in the intermediate-Lanczos-iteration-number regime, which also happened to be close to an inflection point, where it existed. Generally it was found that the best total residual (not the average residual) was less than 10^{-6}. We used the sequential quadratic programming algorithm to solve the non-linear optimization problem as implemented in the 64-bit packages FSQP Version 3.4 and QLD [17]. This combination was found to be the most robust and efficient amongst the various codes of equivalent accuracy that were available. The intercept parameter, representing the best estimate of the ground-state energy density ϵ_0, is tabulated in table 1.

The first point to note from these data is that the energy density estimates are quite good, the best having a percentage error of 3×10^{-4}%, i.e. better than five decimal digits accuracy. For a given system size it is observed that each new order in the plaquette expansion, amongst the critical data sets, brings about improved accuracy, although this

Table 2. A comparison of ground-state energy density estimates for the 1D antiferromagnetic Heisenberg chain calculated by various methods using Hamiltonian moments.

Method	Ground-state energy density	Notes
t-expansion[a]	−0.441 892	H^8
Plaquette expansion	−0.443 815	$r = 3$, H^8, $N = 10^5$
CMX[b]	−0.434 784	Five orders H^{11}
Plaquette expansion	−0.443 610	$r = 4$, H^{10}, $N = 10^5$
Plaquette expansion	−0.443 144	$r = 11$, H^{24}, $N = \infty$
Exact	−0.443 147 18	

[a] Reference [1].
[b] Reference [18].

improvement is uneven. We do not offer a theoretical justification for the convergence of the expansion on the basis of this. The non-critical data sets follow quite a different trend which arises from the fact that when the eigenvalue approaches a fixed value asymptotically, the Lanczos process has effectively terminated and no further information can be extracted from the eigenvalue, and all of this has occurred before a critical point has been encountered. A second note can be made with regard to the trends in the table 1 with system size. Generally results are better—and more so, with larger systems—when the approximation is taken at a given order. The third point to consider is that the results here systematically considerably improve on the initial employment of the plaquette expansion [3, 6], whereby the eigenvalue at the point of inflection in the Lanczos iterations was taken as the best estimate. Fourthly, these results are considerably better than other related treatments that are based on a moment formalism. We present, in table 2, the best estimates obtained by these methods.

Our approach in analysing the plaquette expansion can be independently appraised by seeing how well the computed energies at a given order in the approximation scale with system size. In figure 4 we display the N-dependence for the highest order and it is clear that there is, within the errors, an analytical dependence of ϵ_0 on $1/N$ about the infinite-system limit. The system sizes that we have used have easily placed us in the regime where a purely linear form can be observed. This form is different from the finite-size scaling for the exact finite systems where one expects [19, 20]

$$-\frac{12N^2}{\pi^2}(\epsilon_0(N) - \epsilon_0(\infty)) = 1 + a_1(\ln N)^{-3} + a_2(\ln N)^{-4} + \cdots. \tag{25}$$

This difference we attribute to the truncation brought about by the plaquette expansion, as there must exist a difference with an order of $1/N$ between the exact finite-system ground-state energy and the plaquette expansion truncated estimate. This result also gives us our most accurate extrapolated energy, which is given in table 2.

It should be noted that we have not attempted to perform an extrapolation from the sequence of energies arising from finite orders in the approximation. This is primarily because we have no theoretical basis for such an extrapolation, and there are not enough unambiguous data for us to make a purely empirical deduction.

There are several sources of error associated with these ground-state energies; some of these cannot be corrected for with our simple analysis but can only remain as part of the final total error, whereas others can be corrected for. In the first instance there is the error associated with the relatively crude form for the Lanczos convergence process, and which is represented by the residuals and the systematic variation with the fitting parameters. We estimate that the residual and the systematic fitting errors are of the order 10^{-6} and 10^{-5}

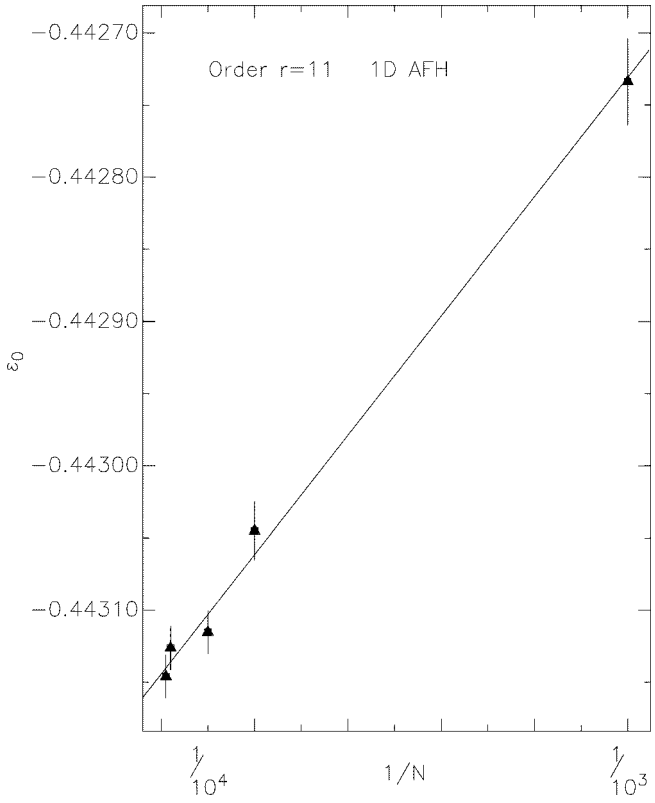

Figure 4. The finite-size scaling of the ground-state energies ϵ_0 at the order $r = 11$, where system sizes range from $N = 10^3$ to 10^5. Also shown is the best-fit straight line.

respectively, in the most accurate case. These cannot be reduced except by the employment of a more refined form for this dependency. Even if these sources of error were negligible or even absent there would still be two remaining errors—those due to the finite size of the system, and the finite order at which the cluster expansion is terminated. These errors can in principle be corrected or compensated for.

4. Conclusion

We have analysed the errors involved in the truncation of the plaquette expansion and the termination of the Lanczos process, and formulated a simple method for extracting accurate estimates for various ground-state spectral quantities of an arbitrary extensive lattice Hamiltonian system. We have shown by dint of the application of such an analysis to the one-dimensional Heisenberg spin chain that this method is capable of producing accurate spectral quantities. By taking the expansion up to the 11th order we have reproduced the known ground-state energy density to better than 10^{-5}. We have used a very simple form in the modelling of the errors in our method, and predict that with refinements in this form, reflecting deeper knowledge of the spectrum of the system and the dynamics of the Lanczos process, better results would be obtained. The effort in obtaining these results is very modest, the computation of the connected moments taking most resources, but even considering this it is modest.

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