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PAPER

Scaling corrections to the ground state energy of the spin-½ isotropic anti-ferromagnetic Heisenberg chain

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Abstract

Solutions to the Bethe Ansatz equations for the ground state of spin-½ isotropic anti-ferromagnetic periodic Heisenberg chains to length $L = 2^{21}$ are obtained by combining Lagrange interpolation with Newton–Raphson iteration. The long chain lengths allow many powers of a renormalization group running coupling constant to be included in fits to the ground state energy and make possible the confirmation of the convergence of the leading logarithmic term. The amplitude of this term is consistent with that expected on the basis of conformal field theory and the connection of the discrete spin-½ system to the continuum Wess–Zumino–Witten model. This resolves a decades old discrepancy based on analysis of shorter chains. An analytical improvement to the Hulthén wave-vector distribution is also provided.

1. Introduction

This paper presents the derivation and asymptotic analysis of the ground state energy of large (even) length L periodic chains of $s = ½$ spins anti-ferromagnetically coupled as defined by the Hamiltonian

$$H = \frac{1}{2}\sum_{i=1}^{L} \vec{\sigma}_i \cdot \vec{\sigma}_{i+1}, \qquad \vec{\sigma}_{L+1} = \vec{\sigma}_1, \tag{1}$$

where i labels both the sites and distance along the chain and the components of $\vec{\sigma}_i$ are the Pauli spin matrices. Eigenstates of (1) can be labelled by total S and S_z; for the ground state $S = S_z = 0$. The motivation for these calculations was an attempt to resolve a long standing apparent failure of universality first noted by Affleck *et al* [1]. More evidence for failure was provided by Nomura [2] in an analysis of spin-½ chains to length $L = 16\,384$.

The history of this model problem dates to 1931 when Bethe [3] (an English translation appears in [4]) conjectured that all eigenstates of (1) could be found based on the solutions of nonlinear algebraic equations that he described. For the ground state these are equations for $L/2$ distinct real wave-vectors, each being associated with one of the $s_z = -½$ spins on the chain. Subsequently Hulthén [5], starting from the Bethe Ansatz, obtained the ground state energy E_L in the limit $L \to \infty$. Hulthén's result is

$$\varepsilon_\infty = \lim_{L\to\infty} \frac{E_L}{L} = \frac{1}{2} - 2\ln(2). \tag{2}$$

The development of conformal field theory (CFT) in the 1980s led to the realization that E_L would approach the Hulthén value $L\varepsilon_\infty$ as $1/L$ with a coefficient constrained by the 'conformal anomaly' of the field theory in the universality class of the spin-½ anti-ferromagnet. Avdeev and Dörfel [6], building on earlier work by de Vega and Woynarovich [7], concluded

$$\lim_{L\to\infty} L(E_L - L\varepsilon_\infty) = -\frac{\pi^2}{6} \tag{3}$$

and confirmed this value by numerical evaluation of E_L for chains to length $L = 256$. Hamer [8] came to the same conclusion independently.

Affleck *et al* [1] argue that the spin-½ anti-ferromagnet is in the universality class of the $k = 1$ Wess–Zumino–Witten nonlinear σ model and use this to identify a marginal operator that will lead to corrections to E_L beyond the conformal anomaly term. Arguments by Cardy [9] specify what form these corrections must take and Affleck *et al* conclude

$$E_L = L\varepsilon_\infty - \frac{\pi^2}{6L}\left(1 + \frac{C}{\ln^3(L)} + o\left(\frac{1}{\ln^3(L)}\right)\right), \qquad C = \frac{3}{8} = 0.375 \quad \text{(CFT)}, \tag{4}$$

C being universal. On the other hand Woynarovich and Eckle [10] had reported an analytic calculation that gave

$$C = 0.3433 \quad \text{(Woynarovich and Eckle)} \tag{5}$$

as the isotropic limit of an anisotropic spin-½ anti-ferromagnet. This clear violation of universality Affleck *et al* recognized but left unresolved. Subsequently, Nomura [2] greatly extended previous numerical calculations of E_L reaching chains of length $L = 16\,384$ and concluded

$$C = 0.365\,16(2) \quad \text{(Nomura)}. \tag{6}$$

In deriving (6), Nomura incorporated Cardy's conclusion that asymptotically the C correction term is proportional to g^3 with g a running coupling that satisfies the renormalization group equation[1]

$$L\frac{\mathrm{d}g}{\mathrm{d}L} = \beta(g) = -g^2 - \frac{g^3}{2} + \ldots \tag{7}$$

with the ellipsis indicating unknown terms. Nomura attributed the difference between (5) and (6) to an invalid reliance by Woynarovich and Eckle on the Euler–Maclaurin sum formula resulting in uncontrolled errors. Of course, even if we accept (5) as unreliable, the apparent failure of universality remains because of the (4) and (6) difference that lies well outside Nomura's error assignment. But this assignment can be faulted because it does not include sensitivity to additional terms in $\beta(g)$ or variation in the constant of integration of (7). The major goal of the present paper is to provide a realistic appraisal of such effects by first generating E_L data for much longer chains.

The outline of the remainder of the paper is as follows. Section 2 expands on the above historical summary by providing formulas useful for subsequent analysis. Particular attention is paid to the approximation necessary to derive (3) from the Hulthén [5] wave-vector distribution. Section 3 is a derivation of an analytic improvement on the Hulthén wave-vector distribution. The approximation that led to (3) can be applied to this improved distribution and leads to a result of the form of (4) but with $C = (3/8)\ln^2(2)$—a roughly factor 2 underestimate from the CFT prediction. Section 4 describes how Lagrange interpolation is combined with Newton–Raphson (NR) iteration for an efficient generator for E_L for large L. Results to a maximum $L = 2^{21}$ are given. Section 5 describes the analysis of the data in section 4 with the conclusion that the CFT result (4) is unambiguously confirmed.

2. E_L alternatives from the Hulthén wave-vector distribution

The ground state is specified by a distinct real wave-vector k_n, $0 < k_n < 2\pi$, for each of the $L/2$ overturned spins from a ferromagnetically aligned state. A convenient change of variable is to the 'rapidity' $\lambda_n = \cot(k_n/2)$; these variables for the ground state satisfy the Bethe ansatz equations (BAE)

$$L\ \mathrm{arccot}(\lambda_n) - \sum_m \mathrm{arccot}\left(\frac{\lambda_n - \lambda_m}{2}\right) - n\,\pi = 0, \qquad n,\, m = \frac{1}{2}, \frac{3}{2}, \ldots, \frac{L-1}{2}, \tag{8}$$

where $\sum_m$ and similar sums hereafter are understood to range over all $L/2$ listed half-integer values. The arccot function is its principal value; i.e. $0 \leqslant \mathrm{arccot}(x) \leqslant \pi$ for $-\infty \leqslant x \leqslant \infty$. The symmetry $\lambda_{L/2-n} = -\lambda_n$ allows reduction to $L/4$ ($(L+2)/4$) independent variables if $L/2$ is even (odd). The BAE (8) with its discrete solutions λ_n can also be interpreted as defining a continuous function

$$n(\lambda) = \frac{1}{\pi}\left(L\ \mathrm{arccot}(\lambda) - \sum\nolimits_m \mathrm{arccot}\left(\frac{\lambda - \lambda_m}{2}\right)\right) \tag{9}$$

with n taking on half-integer values whenever λ is one of the solutions λ_n of (8). This point of view is useful in a number of instances and, for example, allows one to identify $\mathrm{n}(\infty) = 0$ and $\mathrm{n}(-\infty) = L/2$ as the limits on the range of possible n. The energy of the ground state is

[1] The normalization of g in (7) is chosen to make the coefficient of $-g^2$ in $\beta(g)$ equal 1.

$$E_L = \frac{L}{2} - 2\sum_n(1 - \cos(k_n)) = \frac{L}{2} - \sum_n \frac{4}{1+\lambda_n^2}. \tag{10}$$

An exact analytic solution to the BAE (8) is not known for general L. To get solutions of increasing accuracy write an unknown improved estimate $\lambda^{(\ell+1)}$ as a small shift $\delta\lambda^{(\ell+1)}$ from a known ℓth estimate λ^{ℓ}. On substituting $\lambda^{(\ell+1)}$ into the BAE (8) and expanding to first order in $\delta\lambda^{(\ell+1)}$ one obtains the matrix equation $h^{(\ell)} = f^{(\ell)}\,\delta\lambda^{(\ell+1)}$; explicitly,

$$h_n^{(\ell)} = \sum_m (\hat{f}_{nn}^{(\ell)}\,\delta_{nm} + f_{nm}^{(\ell)})\delta\lambda_m^{(\ell+1)}, \quad \lambda_n^{(\ell+1)} = \lambda_n^{(\ell)} + \delta\lambda_n^{(\ell+1)}, \tag{11}$$

where

$$h_n^{(\ell)} = L\ \mathrm{arccot}(\lambda_n^{(\ell)}) - \sum_m \mathrm{arccot}\left(\frac{\lambda_n^{(\ell)} - \lambda_m^{(\ell)}}{2}\right) - n\,\pi, \tag{12}$$

$$f_{nm}^{(\ell)} = \frac{2}{4 + (\lambda_n^{(\ell)} - \lambda_m^{(\ell)})^2}, \quad \hat{f}_{nn}^{(\ell)} = \frac{L}{1+\lambda_n^{(\ell)^2}} - \sum_m f_{nm}^{(\ell)}. \tag{13}$$

The NR solution of (11), $\delta\lambda^{(\ell+1)} = (f^{(\ell)})^{-1}h^{(\ell)}$, converges quadratically but because it requires numerical matrix inversion it is practical in the elementary form given here only to lengths of several thousand. By reparameterizing λ in some appropriate basis, solutions to lengths $L \approx 2 \times 10^6$ have been obtained as described in section 4.

A useful initialization is provided by the Hulthén solution which is based on the approximation $\sum_m \approx \int_0^{L/2} \mathrm{d}m$ in the equation for $\mathrm{d}n/\mathrm{d}\lambda$ obtained by differentiating (9). This equation is of convolution form and can be solved by Fourier transform. Integration then yields $n(\lambda)$ which we identify as the Hulthén approximation $n(\lambda_n^{(0)})$. A summary of equations satisfied by $\lambda_n^{(0)}$ is

$$\begin{aligned} \lambda_n^{(0)} &= -\frac{2}{\pi}\ln(\tan(n\pi/L)), \quad n = \frac{L}{\pi}\arctan\left(\exp(-\pi\lambda_n^{(0)}/2)\right), \\ \frac{\mathrm{d}\lambda_n^{(0)}}{\mathrm{d}n} &= -\frac{4}{L\sin(2n\pi/L)} = -\frac{4}{L}\cosh(\pi\lambda_n^{(0)}/2). \end{aligned} \tag{14}$$

As a consequence of (14), the Hulthén approximation can be written

$$\sum_m \approx \int_0^{L/2} \mathrm{d}m = \frac{L}{4}\int_{-\infty}^{\infty} \frac{\mathrm{d}\lambda_m^{(0)}}{\cosh(\pi\lambda_m^{(0)}/2)} \tag{15}$$

and the final equality, giving the conversion to an integral over $\lambda_m^{(0)}$, is useful in many applications. For example, one can easily check that the middle term in (12) in Hulthén approximation is

$$\begin{aligned} \int_0^{L/2} \mathrm{d}m\ \mathrm{arccot}\left(\frac{\lambda_n^{(0)} - \lambda_m^{(0)}}{2}\right) &= \int_{\lambda_n^{(0)}}^{\infty} \mathrm{d}\mu \int_0^{L/2} \mathrm{d}m \frac{2}{4 + (\mu - \lambda_m^{(0)})^2} \\ &= \int_{\lambda_n^{(0)}}^{\infty} \mathrm{d}\mu \frac{L}{4}\int_{-\infty}^{\infty} \frac{\mathrm{d}\lambda}{\cosh(\pi\lambda/2)} \frac{2}{4 + (\mu - \lambda)^2} \\ &= \int_{\lambda_n^{(0)}}^{\infty} \mathrm{d}\mu \left(\frac{L}{1+\mu^2} - \frac{\pi L/4}{\cosh(\pi\mu/2)}\right) = L\ \mathrm{arccot}(\lambda_n^{(0)}) - n\pi \end{aligned} \tag{16}$$

in which n from (14) has been used for the final equality. This confirms that $h_n^{(0)} = 0$ in Hulthén approximation.

There are ambiguities in the ground state energy of the Hulthén solution depending on the approximations one chooses to make in (10). The integral approximation (15) applied to (10) gives

$$\begin{aligned} E_L(\text{Hulthén}) &= \frac{L}{2} - \int_0^{L/2} \mathrm{d}n \frac{4}{1+\lambda_n^{(0)^2}} = \frac{L}{2} - L\int_{-\infty}^{\infty} \frac{\mathrm{d}\lambda}{\cosh(\pi\lambda/2)} \frac{1}{1+\lambda^2} \\ &= L\left(\frac{1}{2} - 2\ln(2)\right) = L\varepsilon_\infty, \end{aligned} \tag{17}$$

whereas (10) without this approximation is

$$E_L'(\text{Hulthén}) = \frac{L}{2} - \sum_n \frac{4}{1+\lambda_n^{(0)^2}} = L\varepsilon_\infty - \frac{2\pi^2\ln(2)}{\ln^3(L)} + O(1/\ln^4(L)) \tag{18}$$

as derived in the appendix. This last result shows the Hulthén $\lambda_n^{(0)}$ differs significantly from the exact λ_n of the BAE (8) since the periodic boundary condition defining the model (1) allows at most $O(1/L)$ finite size effects as corrections to the extensive $L\varepsilon_\infty$ term. Indeed, the expected energy based on CFT is that given in (4).

A formula equivalent to (10) for E_L was derived by de Vega and Woynarovich [7]. The key identity, restricted here to the isotropic chain (1) and in the present notation, is

$$E_L = L\varepsilon_\infty - \pi\left(\sum_n \frac{1}{\cosh(\pi\lambda_n/2)} - \int_0^{L/2} \mathrm{d}n \frac{1}{\cosh(\pi\lambda_n/2)}\right), \tag{19}$$

where λ_n in the integral in (19) is understood to be the inverse of $n(\lambda)$ from (9). The proof of (19) follows trivially on making the change of integration variable from n to λ using $\mathrm{d}n/\mathrm{d}\lambda$ calculated from (9); explicitly, the last term in (19) is

$$\begin{aligned}\pi\int_0^{L/2} \frac{\mathrm{d}n}{\cosh(\pi\lambda_n/2)} &= \int_{-\infty}^{\infty} \frac{\mathrm{d}\lambda}{\cosh(\pi\lambda/2)}\left(\frac{L}{1+\lambda^2} - \sum_n \frac{2}{4+(\lambda_n-\lambda)^2}\right)\\ &= L\ 2\ln(2) - \sum_n \frac{4}{1+\lambda_n^2} + \pi\sum_n \frac{1}{\cosh(\pi\lambda_n/2)},\end{aligned} \tag{20}$$

where the integrals evaluated for the final equality are those that already appeared in (16) and (17). Substituting (20) into (19) yields (10) and completes the proof. Note that (20) relies only on the functional form of (9) and not that the λ_m in the sum in (9) satisfy the BAE. Thus any approximation to λ_n in (19) (and simultaneously to the λ_m in (9)) has the same effect on E_L as does the approximation when applied directly to (10). In particular (19) reproduces the $O(1)$ error found for the Hulthén approximation E_L' in (18).

On the other hand, different E_L estimates using (19) are possible if one drops the constraint that the analytic continuation from a discrete λ_n list to a continuous λ_n function be via (9). If the approximate λ_n is a known analytic function such as the Hulthén $\lambda_n^{(0)}$ in (14), it would seem more natural to define (19) by the condition that the same analytic λ_n appear in both sum and integral. As an example, if in (19), with the constraining (9) removed, we replace λ_n by the Hulthén $\lambda_n^{(0)}$ in both sum and integral and use the hyperbolic/trigonometric equivalence from (14), we get

$$\begin{aligned}E_L''(\text{Hulthén}) &= L\varepsilon_\infty - \pi\left(\sum_n \sin(2n\pi/L) - \int_0^{L/2} \mathrm{d}n\ \sin(2n\pi/L)\right)\\ &= L\varepsilon_\infty - \pi\left(\frac{1}{\sin(\pi/L)} - \frac{L}{\pi}\right) = L\varepsilon_\infty - \frac{\pi^2}{6L} - \frac{7\pi^4}{360L^3} + O(1/L^5),\end{aligned} \tag{21}$$

a result first obtained by Avdeev and Dörfel [6] and Hamer [8]. The leading correction in (21) agrees with the CFT value in (4) which illustrates the dramatic improvement to an $o(1/L)$ error that has been achieved. This is a surprise since the removal of the constraint (9) has eliminated the justification for (19) to be the formula for E_L. It is of course possible that the dramatic error reduction has just been accidental—which motivates further exploration in the following by observing what changes are induced in (21) when the modified (19) is applied to an analytical improvement on the Hulthén solution (14).

3. An improved wave-vector distribution

Before proceeding with the calculation of such an improvement, it is worth introducing a change of variable $\lambda_n \to \nu_n$ in which we write the exact λ_n as

$$\lambda_n = -\frac{2}{\pi}\ln(\tan((n-\nu_n)\pi/L)), \qquad \nu_n = n - \frac{L}{\pi}\arctan\left(\exp\left(-\frac{\pi}{2}\lambda_n\right)\right), \tag{22}$$

with ν_n satisfying the symmetry condition $\nu_{L/2-n} = -\nu_n$. The unit spacing between n sets the scale for distinguishing ν_n as either small or large. In the case that ν_n is small we find from (22) that

$$\delta\lambda_n = \lambda_n - \lambda_n^{(0)} = \frac{4}{L}\cosh(\pi\lambda_n^{(0)}/2)\nu_n + O(\nu_n^2). \tag{23}$$

By maintaining the functional form of the Hulthén solution (14) we preserve in (22), for example, the hyperbolic/trigonometric equivalence $\cosh(\pi\lambda_n/2) = 1/\sin(2(n-\nu_n)\pi/L)$ and so can write the modified[2] de Vega and Woynarovich energy formula (19) in the doubly subtracted form

$$\begin{aligned}E_L &= L\varepsilon_\infty - \pi\left(\frac{1}{\sin(\pi/L)} - \frac{L}{\pi}\right) - \pi\left(\sum_n s(n,\nu_n) - \int_0^{L/2} \mathrm{d}n\ s(n,\nu_n)\right),\\ s(n,\nu_n) &= \sin(2(n-\nu_n)\pi/L) - \sin(2n\pi/L) = -(2\pi/L)\cos(2n\pi/L)\nu_n + O(\nu_n^2).\end{aligned} \tag{24}$$

The numerical evidence discussed below suggests $|\nu_n|$ is bounded by 0.03 for all n and L and so in the following we use only the linear in ν_n versions of (23) and (24).

Any iteration of (11) to improve on the Hulthén $\lambda_n^{(0)}$ ideally starts with an exact evaluation of the sum contributing to $h_n^{(0)}$ in (12). Fortunately this can be done analytically by complex contour and residue methods

[2] Modified means dropping the constraining (9) as in the discussion leading to (21).

similar to that described in the appendix. The details involve no new concepts but it is useful to first recast the arccot function in the sum in (12) as an integral as was done in the first equality in (16). One can confirm that the singularities in this case at $\lambda_n^{(0)} = \mu \pm 2i$ lie at n < 0 and n > L/2 on the real n axis and thus again outside the chosen contour in the appendix. The final result is

$$h_n^{(0)} = \frac{1}{2\pi}\int_0^\infty \frac{\mathrm{d}y}{1+\exp(2y)} \ln\left(\frac{(\lambda_n^{(0)}-\Lambda(y))^2+1}{(\lambda_n^{(0)}+\Lambda(y))^2+1}\,\frac{(\lambda_n^{(0)}+\Lambda(y))^2+9}{(\lambda_n^{(0)}-\Lambda(y))^2+9}\right), \tag{25}$$

where

$$\Lambda(y) = \frac{2}{\pi}\ln(\tanh(y/L)). \tag{26}$$

(With the substitution $y = \ln(1+e^x) = \operatorname{arcsinh}(e^x(1+e^x/2)/(1+e^x))$, $-\infty < x < \infty$, integrals such as (25) can be done numerically as an equally weighted sum on a uniform grid with exponential convergence both with respect to the large $|x|$ cutoffs and the (inverse) grid spacing.)

To make the right hand side of (11) tractable we employ the Hulthén integral approximation (15). The necessary integral for the sum in $\hat{f}_{nn}^{(0)}$ in (13) already appears in (16) with the result

$$\hat{f}_{nn}^{(0)}\,\delta\lambda_n^{(1)} = \frac{\pi L}{4}\frac{\delta\lambda_n^{(1)}}{\cosh(\pi\lambda_n^{(0)}/2)} = \pi\nu_n^{(1)}, \tag{27}$$

the last equality being the linearized form of (23). The (integral approximated) contribution from $\sum_m f_{nm}^{(0)}\,\delta\lambda_m^{(1)}$,

$$\frac{L}{4}\int_{-\infty}^{\infty}\frac{\mathrm{d}\lambda_m^{(0)}}{\cosh(\pi\lambda_m^{(0)}/2)}\frac{2}{4+(\lambda_n^{(0)}-\lambda_m^{(0)})^2}\delta\lambda_m^{(1)} = \int_{-\infty}^{\infty}\mathrm{d}\lambda_m^{(0)}\frac{2}{4+(\lambda_n^{(0)}-\lambda_m^{(0)})^2}\nu_m^{(1)}, \tag{28}$$

is a convolution. On substituting these (27), (28) values into (11), then taking a Fourier transform and using the explicit $h_n^{(0)}$ from (25), we arrive at[3]

$$\begin{aligned}\pi(1+e^{-2|q|})\int_{-\infty}^{\infty}\mathrm{d}\lambda_n^{(0)}\exp(-\mathrm{i}q\lambda_n^{(0)})\nu_n^{(1)} &= \int_{-\infty}^{\infty}\mathrm{d}\lambda_n^{(0)}\exp(-\mathrm{i}q\lambda_n^{(0)})h_n^{(0)}\\ &= 4\mathrm{i}e^{-2|q|}\frac{\sinh(q)}{q}\int_0^\infty\frac{\mathrm{d}y}{1+\exp(2y)}\sin(q\Lambda(y)).\end{aligned} \tag{29}$$

Inverse Fourier transformation of (29) after dividing out $\pi(1+e^{-2|q|})$ now gives

$$\nu_n^{(1)} = \frac{1}{\pi^2}\int_0^\infty\frac{\mathrm{d}y}{1+\exp(2y)}\left[2\mathrm{i}\int_{-\infty}^{\infty}\frac{\mathrm{d}q}{q}\exp(\mathrm{i}q\lambda_n^{(0)})\frac{e^{-2|q|}}{1+e^{-2|q|}}\sinh(q)\sin(q\Lambda(y))\right]. \tag{30}$$

The [ ] expression in (30) evaluates to

$$\begin{aligned}&-4\int_0^\infty\frac{\mathrm{d}q}{q}\frac{e^{-2q}}{1+e^{-2q}}\sinh(q)\sin(q\Lambda(y))\sin(q\lambda_n^{(0)})\\ &=-2\lim_{K\to\infty}\textstyle\sum_{k=0}^{K}\displaystyle\int_0^\infty\frac{\mathrm{d}q}{q}(e^{-(4k+1)q}-2e^{-(4k+3)q}+e^{-(4k+5)q})\sin(q\Lambda(y))\sin(q\lambda_n^{(0)})\\ &=\lim_{K\to\infty}\textstyle\sum_{k=0}^{K}\displaystyle\Re\ln\left(\frac{(k+g_n^+(y))^2}{(k+g_n^+(y)-\frac12)(k+g_n^+(y)+\frac12)}\,\frac{(k+g_n^-(y)-\frac12)(k+g_n^-(y)+\frac12)}{(k+g_n^-(y))^2}\right),\end{aligned} \tag{31}$$

where

$$g_n^{\pm}(y) = \frac34 + \frac{i}{4}(\lambda_n^{(0)} \pm \Lambda(y)) \tag{32}$$

with $\Lambda(y)$ given in (26). The sum of logarithms in (31) is a logarithm of a product and we get as our final expression

$$\begin{aligned}\nu_n^{(1)} = \frac{1}{\pi^2}\int_0^\infty&\frac{\mathrm{d}y}{1+\exp(2y)}\\ &\times\Re\ln\left(\frac{\Gamma(g_n^+(y)-\frac12)\Gamma(g_n^+(y)+\frac12)}{\Gamma^2(g_n^+(y))}\,\frac{\Gamma^2(g_n^-(y))}{\Gamma(g_n^-(y)-\frac12)\Gamma(g_n^-(y)+\frac12)}\right).\end{aligned} \tag{33}$$

As an example of the accuracy of (33), comparisons of $\nu_n^{(1)}$ with the exact ν_n obtained by NR iteration are shown in figure 1 for $L = 2^{10} = 1024$ and $L = 2^{21} = 2097\,152$. Extrapolation from discrete to continuous n for

[3] The resulting (29) has the structure of the Fourier transform equation that leads to the Hulthén solution (14). The unknown $\nu_n^{(1)}$ in (29) replaces $\mathrm{d}n/\mathrm{d}\lambda_n$ in the Hulthén equation while the known $h_n^{(0)}$ replaces $-L/(1+\lambda_n^2)$.

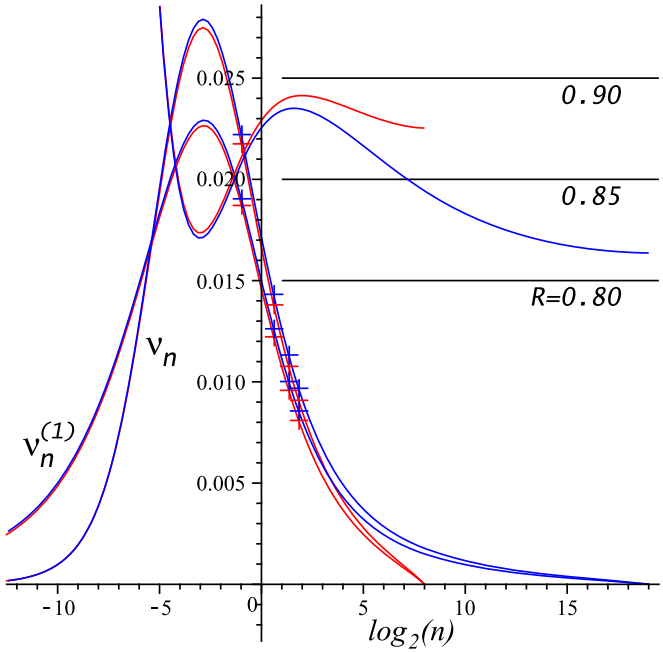

Figure 1. The approximation $\nu_n^{(1)}$ from (33) and the exact ν_n from Newton–Raphson iteration of (11) for chains of length $L = 2^{10}$ (red) and 2^{21} (blue) plotted against $\log_2(n)$ for $n < L/4$. The first four discrete values $\left(n = \frac{1}{2}, \frac{3}{2}, \ldots\right)$ are shown as crosses; the lower pair at each n mark $\nu_n^{(1)}$, the upper pair ν_n. The two curves in the upper part of the graph are the ratios $R = \nu_n^{(1)}/\nu_n$ plotted with respect to the horizontal marker lines indicating ratios of $R = 0.80, 0.85$ and 0.90.

the NR solution is by the use of (9). A single NR iteration starting from the Hulthén solution is graphically almost indistinguishable from the final (multiple iteration) result shown in figure 1 so that the error in $\nu_n^{(1)}$ is inferred to be dominated by the Hulthén integral approximation made in its derivation. The qualitative agreement between $\nu_n^{(1)}$ and the exact ν_n for the lengths L shown in figure 1 suggests we might use (33) to guess how ν_n will approach its $L \to \infty$ limit.

We consider two cases. In the limit $L \to \infty$ with $n = O(1)$, we simplify (33) by first noting

$$g_n^+(y) = \frac{3}{4} + \frac{i}{2\pi}\ln\left(\frac{y}{n\pi}\right) + O(1/L^2), \quad g_n^-(y) = \frac{3}{4} + \frac{i}{\pi}\ln\left(\frac{L}{\sqrt{n\pi y}}\right) + O(1/L^2). \tag{34}$$

The Γ functions involving $g_n^-(y)$ can be expanded in an asymptotic series in $1/\ln(L)$ and the remaining integrals $\int_0^\infty dy\, \ln^i(y)/(1 + \exp(2y))$ can be obtained from the generating function (A.5) in the appendix. The result is

$$\nu_n^{(1)} = \frac{1}{\pi^2}\int_0^\infty \frac{dy}{1+\exp(2y)}\,\Re\ln\left(\frac{\Gamma\left(\frac{1}{4}+\frac{i}{2\pi}\ln\left(\frac{y}{n\pi}\right)\right)\Gamma\left(\frac{5}{4}+\frac{i}{2\pi}\ln\left(\frac{y}{n\pi}\right)\right)}{\Gamma^2\left(\frac{3}{4}+\frac{i}{2\pi}\ln\left(\frac{y}{n\pi}\right)\right)}\right)$$
$$- \frac{\ln(2)}{32\ln^2(L)}\left(1 + \frac{\ln(n\pi/\sqrt{8})}{\ln(L)} + \ldots\right). \tag{35}$$

The first (L independent integral) term in (35) is 0.019 181, 0.012 768, 0.01 0168, … for $n = \frac{1}{2}, \frac{3}{2}, \ldots$ while the remaining term suggests $\nu_n(L) - \nu_n(\infty)$ will be $O(1/\ln^2(L))$ for $n = O(1)$. A second asymptotic result is the slope of $\nu_n^{(1)}$ at the symmetry point $n = L/4$. We have

$$\left.\frac{\partial\nu_n^{(1)}}{\partial\lambda_n^{(0)}}\right|_{\lambda_n^{(0)}=0} = \frac{1}{2\pi^2}\int_0^\infty \frac{dy}{1+\exp(2y)}\,\Im\left(2\psi\left(\frac{3}{4}+\frac{i}{4}\Lambda(y)\right) - \psi\left(\frac{1}{4}+\frac{i}{4}\Lambda(y)\right) - \psi\left(\frac{5}{4}+\frac{i}{4}\Lambda(y)\right)\right)$$
$$= \frac{\pi\ln(2)}{4\ln^3(L)}\left(1 - \frac{9\ln(2)}{2\ln(L)} + \ldots\right) \tag{36}$$

which suggests $\partial\nu_n/\partial\lambda_n$ will be $O(1/\ln^3(L))$ at $\lambda_n = 0$.

The sought for improvement in energy referred to at the end of section 2 comes from the sum minus integral terms in $s(n, \nu_n)$ in (24). Again, working only to linear order in $\nu_n^{(1)}$, this energy correction is

$$\frac{2\pi^2}{L}\left(\sum_n \cos(2n\pi/L)\nu_n^{(1)} - \int_0^{L/2} \mathrm{d}n\, \cos(2n\pi/L)\nu_n^{(1)}\right)$$
$$= \frac{4}{\pi L}\int_0^\infty \frac{\mathrm{d}y'}{1+\exp(2y')}\cosh(2y'/L)\int_0^\infty \frac{\mathrm{d}y}{1+\exp(2y)}$$
$$\times \mathcal{I}\,\ln\left(\frac{\Gamma\left(0^+ + \frac{\mathrm{i}}{2\pi}\ln(t'/t)\right)\Gamma^3\left(\frac{1}{2}+\frac{\mathrm{i}}{2\pi}\ln(t\,'t)\right)\Gamma^3\left(1+\frac{\mathrm{i}}{2\pi}\ln(t'/t)\right)\Gamma\left(\frac{3}{2}+\frac{\mathrm{i}}{2\pi}\ln(t\,'t)\right)}{\Gamma\left(0^+ + \frac{\mathrm{i}}{2\pi}\ln(t'\,t)\right)\Gamma^3\left(\frac{1}{2}+\frac{\mathrm{i}}{2\pi}\ln(t'/t)\right)\Gamma^3\left(1+\frac{\mathrm{i}}{2\pi}\ln(t\,'t)\right)\Gamma\left(\frac{3}{2}+\frac{\mathrm{i}}{2\pi}\ln(t'/t)\right)}\right), \tag{37}$$

where $t' = \tanh(y'/L)$ and $t = \tanh(y/L)$. The equality in (37) is the result of an explicit calculation of the sum minus integral difference by the complex contour method described in the appendix. For the leading terms in (37) in the limit $L \to \infty$ we can set $\cosh(2y'/L) = 1$ and all $\ln(\Gamma(\ldots))$ terms containing the ratio t'/t then vanish because of the anti-symmetry of their imaginary parts under $y' \leftrightarrow y$ interchange. Further reduction analogous to that in (34) followed by asymptotic expansion of the Γ functions gives the energy correction

$$\frac{4}{\pi L}\int_0^\infty \frac{\mathrm{d}y'}{1+\exp(2y')}\int_0^\infty \frac{\mathrm{d}y}{1+\exp(2y)}\,\mathcal{I}\,\ln\left(\frac{\Gamma^3\left(\frac{1}{2}-\frac{\mathrm{i}}{\pi}\ln(L/\sqrt{y'y})\right)\Gamma\left(\frac{3}{2}-\frac{\mathrm{i}}{\pi}\ln(L/\sqrt{y'y})\right)}{\Gamma\left(-\frac{\mathrm{i}}{\pi}\ln(L/\sqrt{y'y})\right)\Gamma^3\left(1-\frac{\mathrm{i}}{\pi}\ln(L/\sqrt{y'y})\right)}\right)$$
$$= -\frac{\pi^2\ln^2(2)}{16L\ln^3(L)}\left(1 - \frac{9\ln(2)}{2\ln(L)} + \ldots\right). \tag{38}$$

By comparison with the expected CFT correction in (4) we see the leading term in (38) has the correct length dependence but is too small by a factor $\ln^2(2)$. Had we used λ_n from (22) with $\nu_n = \nu_n^{(1)}$ from (33) directly in (10) we would only have reduced the error in E_L from its E_L'(Hulthén) value in (18) by an $O(1)$ factor and not the $O(L)$ factor needed to get (38). Thus (38) provides another example besides (21) of the dramatic improvement achieved by changing the analytic continuation prescription in (19). In the absence of any better analytical approximations for ν_n beyond $\nu_n^{(1)}$ in (33) I return to the purely numerical solution of the BAE in section 4.

4. E_L by NR with Lagrange interpolation

The NR procedure for finding the solutions λ_n of the BAE (8) as described in the discussion of equations (11)–(13) is impractical for chains of length L greater than several thousand. To deal with long chains we restrict the number of variables treated by NR to a limited number M of $\lambda_{n_m} > 0, m = 1, 2, \ldots, M$, and use a Lagrange interpolation scheme that accurately and efficiently determines all remaining λ_n in terms of the basis variables λ_{n_m}. In our implementation of the Lagrange interpolation we assume λ_n is a smooth function $\lambda_n(x_n)$ where $x_n = \lambda_n^{(0)}$ as given by (14)[4]. We incorporate the symmetry $\lambda_{L/2-n_m} = -\lambda_{n_m}$ in our basis choice in which case for any n that is distinct from all n_m,

$$\lambda_n = P_n\sum_{m=1}^M \frac{\lambda_{n_m}}{(x_n^2 - x_{n_m}^2)P'_{n_m}}, \qquad P_n = x_n\prod_{m=1}^M (x_n^2 - x_{n_m}^2), \qquad P'_{n_m} = x_{n_m}\prod_{k=1}^M{}'(x_{n_m}^2 - x_{n_k}^2), \tag{39}$$

where the prime on the second product in (39) indicates the term $k = m$ is excluded. NR iteration proceeds as follows. We assume that at the ℓth iteration the M terms $\lambda_{n_m} = \lambda_{n_m}^{(\ell)}$ are known from a previous step. For all other n, (39) serves to define the $\lambda_n^{(\ell)}$. The M array elements $h_{n_m}^{(\ell)}$ in (12), when expressed explicitly in terms of $\lambda_n^{(\ell)} > 0$, are

$$h_{n_m}^{(\ell)} = (L-1)\,\mathrm{arccot}(\lambda_{n_m}^{(\ell)}) - \left(n_m + \frac{1}{2}\right)\pi$$
$$- \sum_{n<\frac{L}{4}}{}'\left(\mathrm{arccot}\left(\frac{\lambda_{n_m}^{(\ell)} - \lambda_n^{(\ell)}}{2}\right) + \mathrm{arc\,cot}\left(\frac{\lambda_{n_m}^{(\ell)} + \lambda_n^{(\ell)}}{2}\right)\right) - \begin{cases} 0 & L/2 \text{ even} \\ \mathrm{arc\,cot}\,(\lambda_{n_m}^{(\ell)}/2) & L/2 \text{ odd}, \end{cases} \tag{40}$$

where the prime on the sum means the term $n = n_m$ is excluded. The M^2 matrix elements $f_{n_m n_{m'}}^{(\ell)}$ are the derivatives $f_{n_m n_{m'}}^{(\ell)} = -\partial h_{n_m}^{(\ell)}/\partial\lambda_{n_{m'}}^{(\ell)}$ and although easy to calculate from (40), result in lengthier analytical expressions than those in (13) because of the dependencies $\lambda_n^{(\ell)}(\lambda_{n_{m'}}^{(\ell)})$ given by (39). Data for a new NR iteration beginning with (39) is obtained by matrix inversion as in the solution of (11), i.e. $\lambda_{n_m}^{(\ell+1)} = \lambda_{n_m}^{(\ell)} + ((f^{(\ell)})^{-1}h^{(\ell)})_{n_m}$. Iteration stops when the M $h_{n_m}^{(\ell)}$ in (40) vanish to our chosen numerical accuracy and we then deem the BAE (8) satisfied—at least within the limitations of the Lagrange interpolation (39).

[4] The choice $x_n = \lambda_n^{(0)}$ obviously makes the interpolation exact for $\lambda_n = \lambda_n^{(0)}$. There might be an advantage to using the improved $x_n = \lambda_n^{(1)}$ from (22) with $\nu_n^{(1)}$ from (33) but this has not been explored.

It remains to discuss the choice of the special $n = n_m$. It is essential that there be a minimum number of $n = n_m = \frac{1}{2}, \frac{3}{2}, \ldots$ with unit gaps since no accurate interpolation is possible near the end-points of the λ interval. Following this are gaps of increasing size between n until a final $n = n_M$ near $L/4$. Because we are interpolating in x it is plausible that the spacing in the corresponding $x_{n_m} = \lambda^{(0)}_{n_m}$ should be nearly uniform. A possible formula to achieve this is a modification of the Hulthén $n(\lambda^{(0)}_n)$ from (14) which we define as

$$N_m(K,\, K') = \frac{L}{\pi}\arctan(\exp(-\pi(2m\, -\, 1)/K)) + \frac{m}{K'}, \tag{41}$$

where the last term has been added to provide extra flexibility and $K,\ K'$ are parameters dependent on L. If we define a crossover integer m_x as the largest (integer) m for which $N_{m-1}(K,\, K') - N_m(K,\, K') > 1$ then the n_m list is

$$n_m = \frac{1}{2} + \begin{cases} \lfloor N_m(K,\, K')\rfloor - \lfloor N_{m_x}(K,\, K')\rfloor + M - m_x, & m = 1,\ 2, \ldots, m_x \\ M - m, & m = m_x + 1,\ m_x + 2, \ldots, M. \end{cases} \tag{42}$$

We can make M and m_x the independent variables in (42) by taking $K,\ K'$ as the solution of the two equations $N_{m_x-1}(K,\, K') - N_{m_x+1}(K,\, K') = 2$ which is an approximation to the defining equation for the crossover m_x and $N_{m_x}(K,\, K') = M - m_x + 1/2$ which makes $n_m \approx N_m(K,\, K')$ for $m \leqslant m_x$ in (42). These two equations can be reduced to

$$\frac{L}{2\pi}\arctan\left(\frac{\sinh(2\pi/K)}{\cosh((2m_x\, -\, 1)\pi/K)}\right) = \frac{1}{m_x}\left(M + \frac{1}{2} - \frac{L}{\pi}\arctan(\exp(-(2m_x\, -\, 1)\pi/K))\right) = 1 + \frac{1}{K'}, \tag{43}$$

where now the first equality determines K after which K' follows trivially. For example, at $L = 2^{21}$ with $M = 92$ and $m_x = 60$, $K = 32.7464$ and $K' = 2.3858$. This is a special case of the parameter choice

$$M = \mathrm{round}(4\log_2(L) + 8), \qquad m_x = \mathrm{round}(3\log_2(L)\, -\, 3) \tag{44}$$

which we have used and have found that for $2^{10} \leqslant L \leqslant 2^{21}$ yields an absolute error in the scaled energy deviation

$$1 + E^{(\mathrm{corr})} = -\frac{6L}{\pi^2}(E_L\, -\, L\varepsilon_\infty) \tag{45}$$

that is less than 10^{-41}. The observed trend suggests this bound will improve slightly for $L > 2^{21}$.

Figure 2 shows for $L = 2^{21}$ both NR/Lagrange error[5] $\delta\lambda_n = \lambda^{\mathrm{NR}/L}_n - \lambda^{\mathrm{exact}}_n$ and the partial sum error

$$\delta E_n = -\sum_{m=n}^{\frac{L}{2}-n}\left(\frac{4}{1 + \lambda^2_m}\bigg|_{\mathrm{NR}/L} - \frac{4}{1 + \lambda^2_m}\bigg|_{\mathrm{exact}}\right) \tag{46}$$

defined such that the energy error $E^{\mathrm{NR}/L}_L - E^{\mathrm{exact}}_L = \delta E_{1/2}$. The oscillatory behaviour of $\delta\lambda_n$ is typical with the decay in amplitude towards large x the (deliberate) result of the large M–m_x choice (44). The decay in amplitude towards small x is not easy to modify given the constraint of the functional form (41) but it is appropriate as it partially compensates for the growth in the number of λ_n terms between adjacent λ_{n_m} at small x and leads to a substantial suppression of the δE_n oscillation amplitude there. The further suppression of these oscillations by about 2 orders of magnitude to a final $\delta E_{1/2}$ (the rightmost point in figure 2) is also typical.

This explicit cancellation in the generation of $\delta E_{1/2}$ implies a loss of significant digits but a more important loss of significance is the cancellation between terms in the sum for λ_n in (39). In total up to 15 digits can be lost which is in addition to the 12 digits lost in cancellation in the scaled energy deviation $1 + E^{(\mathrm{corr})}$ in (45). Significant cancellation between terms in (40) can also occur so in view of this, for all $L > 10^6$, a conservative extended precision arithmetic of 90 digits was used; somewhat less for shorter chains. Finally, if the NR/Lagrange iteration is initialized with $\lambda_{n_m} = \lambda^{(0)}_{n_m}$ about seven iterations are required before reaching the interpolation limiting accuracy. This number can be reduced if instead one starts with $\lambda^{(1)}_{n_m}$ defined by (22) with $\nu^{(1)}_{n_m}$ given by (33) (see the note following (26) for an efficient integration scheme). Whatever initialization is chosen, this must be carried to a precision comparable to that used for a general iteration term—otherwise roundoff noise can lead to failure to converge.

The energies from the NR/Lagrange calculation for $2^{10} \leqslant L \leqslant 2^{21}$ given below are exact to the 40 digits listed. They confirm the Nomura values for $L \leqslant 2^{14}$. The last three columns are the fit deviations $\delta = E^{(\mathrm{corr})}|_{\mathrm{fit}} - E^{(\mathrm{corr})}$ of formulas described in the next section and referenced by their equation numbers.

[5] Error determination is based on comparison with a more accurate calculation using expansion in a 204 Chebyshev polynomial basis set. The Lagrange interpolation scheme described here is easier to implement, much less susceptible to round-off error and instability and, for the same basis size, essentially equivalent in accuracy.

L	$1 + E^{(\mathrm{corr})} = (-6L/\pi^2)(E_L - L\varepsilon_\infty)$	$\delta(53)$	$\delta(54)$	$\delta(55)$
2097152	1.00008105008613531345468866245276352120 6	0	0	0
1835008	1.00008309647492729298927041805073691519 1	$-3.4e-22$	$2.7e-22$	0
1572864	1.00008554623566847645436374687138085162 1	0	0	0
1310720	1.00008857077566705527012952022128255008 4	$1.2e-22$	$-1.0e-22$	$-2.0e-24$
1048576	1.00009247162503170222495346628629442713	0	0	0
917504	1.00009491708226812491391700667492083590 4	$-2.6e-23$	$2.3e-23$	$9.2e-25$
786432	1.00009784963682361762920037177687938185 2	0	0	0
655360	1.00010147773552250946837556036010422049 3	$2.7e-23$	$-2.5e-23$	$-1.5e-24$
524288	1.00010616899635976949929874791142119748 4	0	0	0
458752	1.00010911672031536013559536631083308873 6	$-1.3e-23$	$1.3e-23$	$1.1e-24$
393216	1.00011265832725186602926177794074051212 1	0	0	0
327680	1.00011704993911914811106959634485058019 7	$2.8e-23$	$-2.9e-23$	$-2.9e-24$
262144	1.00012274452739440708425210710693589973 4	0	0	0
229376	1.00012633178306047007140289991034056934 3	$-2.9e-23$	$3.2e-23$	$3.8e-24$
196608	1.00013065088354918207149439674511622590 3	0	0	0
163840	1.00013602017054053201688166952396991843 1	$1.2e-22$	$-1.4e-22$	$-1.9e-23$
131072	1.00014300443151755626987931245431868986 1	0	0	0
114688	1.00014741656248746463465856664412238589 2	$-2.6e-22$	$3.3e-22$	$5.0e-23$
98304	1.00015274135722133672724693236166034654 0	0	0	0
81920	1.00015937962843642488209470026769150147 7	$2.4e-21$	$-3.2e-21$	$-5.4e-22$
65536	1.00016804500873050187882401106026676893 2	0	0	0
57344	1.00017353652874211745996345036941715072 4	$-1.5e-20$	$2.2e-20$	$4.1e-21$
49152	1.00018018156556386212902342515452790015 2	0	0	0
40960	1.00018849218319547330223253349214264302 1	$7.2e-19$	$-1.1e-18$	$-2.2e-19$
32768	1.00019938378602188411713469998060670221 6	$9.2e-18$	$-1.5e-17$	$-3.2e-18$
28672	1.00020631093371656794254521061615507980 1	$3.1e-17$	$-5.2e-17$	$-1.1e-17$
24576	1.00021471838374184749616089964285375732 9	$1.1e-16$	$-1.9e-16$	$-4.2e-17$
20480	1.00022527133800181382309963859280144810 4	$4.2e-16$	$-7.5e-16$	$-1.7e-16$
16384	1.00023916452763612517664842218462602438 6	$1.8e-15$	$-3.4e-15$	$-8.2e-16$
14336	1.00024803705521288394285740035036089415 3	$4.1e-15$	$-8.1e-15$	$-2.0e-15$
12288	1.00025884284830437628182197424265805160 0	$1.0e-14$	$-2.1e-14$	$-5.1e-15$
10240	1.00027246298207532206729212531221558219 9	$2.8e-14$	$-5.9e-14$	$-1.5e-14$
8192	1.00029048865794029307882618472138800367 1	$9.1e-14$	$-2.0e-13$	$-5.3e-14$
7168	1.00030205543834179682409081939567105289 0	$1.8e-13$	$-4.1e-13$	$-1.1e-13$
6144	1.00031619962377879071902145352684368065 1	$3.8e-13$	$-8.9e-13$	$-2.4e-13$
5120	1.00033411561342736513979819967276315296 3	$8.9e-13$	$-2.2e-12$	$-6.1e-13$
4096	1.00035797509699770581543407408143173987 8	$2.4e-12$	$-6.4e-12$	$-1.8e-12$
3584	1.00037337315736373848816731004778873782 4	$4.4e-12$	$-1.2e-11$	$-3.4e-12$
3072	1.00039229457919356796797799355011065900 4	$8.6e-12$	$-2.4e-11$	$-6.9e-12$
2560	1.00041640616681460007342597342764169948 8	$1.9e-11$	$-5.5e-11$	$-1.6e-11$
2048	1.00044876531678210423691602155825373479 8	$4.7e-11$	$-1.4e-10$	$-4.3e-11$
1792	1.00046979897545028785435044833345701140 9	$8.0e-11$	$-2.6e-10$	$-7.6e-11$
1536	1.00049580678729686121432265200558527037 8	$1.5e-10$	$-4.9e-10$	$-1.5e-10$
1280	1.00052920696312763309461718128941092709 2	$3.0e-10$	$-1.1e-09$	$-3.2e-10$
1024	1.00057449060746453188653063328145229877 9	$7.2e-10$	$-2.6e-09$	$-7.9e-10$

(47)

The analysis of the energies (47) described in the following section unambiguously confirms the CFT result (4).

5. Energy scaling analysis

The logarithmic corrections to scaling beyond the conformal anomaly term are contained in $E^{(\mathrm{corr})}$ as defined in (45) and displayed in (47). A fit which includes analytic corrections,

$$E^{(\mathrm{corr})}|_{\mathrm{fit\_1}} = Cg^3 + b/L^2, \tag{48}$$

incorporates the expected CFT asymptotic scaling but treats C as a fitting parameter rather than fixed at the CFT value 3/8. The coupling g in (48) satisfies the renormalization group equation

$$L\frac{\mathrm{d}g}{\mathrm{d}L} = \beta(g), \qquad \beta(g) = -g^2 - \frac{g^3}{2} - g^4\alpha(g), \tag{49}$$

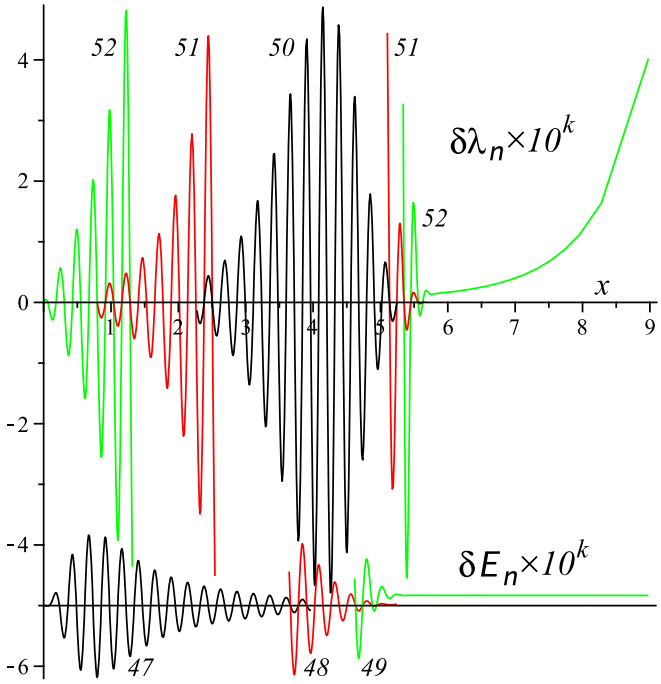

Figure 2. The $L = 2^{21}$ Newton–Raphson/Lagrange (scaled) errors $\delta\lambda_n \times 10^k$ versus $x = \lambda_n^{(0)}$. The integers labelling different coloured segments of the curve are the exponents k. The corresponding (scaled) partial sum error $\delta E_n \times 10^k$ has been shifted to a baseline at –5 for clarity.

which allows for additional terms not present explicitly in (7). Integration of (49) yields

$$\ln\left(\frac{L}{L_0}\right) = \frac{1}{g} - \frac{1}{2}\ln\left(\frac{1}{g} + \frac{1}{2}\right) + \int_{g'=0}^{g} \mathrm{d}g' \frac{\alpha(g')}{\left(1 + \frac{g'}{2}\right)\left(1 + \frac{g'}{2} + g'^2\alpha(g')\right)}, \tag{50}$$

where L_0 is a (model dependent) integration constant. When $\alpha(g) = 0$, (48) combined with (50) with $L_0 = 0.5653$ is the Nomura [2] fit[6]. For long chains the analytic correction b/L^2 in (48) is unimportant and $E^{(\mathrm{corr})}/g(L)^3$, taken as a proxy for C, is shown as squares in figure 3 using the Nomura data for $2560 \leqslant L \leqslant 16\,384$. This is supplemented as crosses using the additional data (47). The trend with increasing L clearly shows Nomura's conclusion $C \approx 0.365$ is no longer tenable.

As the first and most important modification of Nomura, allow L_0 as a free parameter keeping $\alpha(g) = 0$. Determine a sequence of C, b and L_0 from 3-point fits of $E^{(\mathrm{corr})}|_{\mathrm{fit\_1}}$ (48) to $E^{(\mathrm{corr})}$ data (47) at $L = 2^p, 2^{p-1}$ and 2^{p-2}, $12 \leqslant p \leqslant 21$. The results for C for integer p are shown as the lowest diamond sequence in figure 3. The overlapping curve is a (negative) deviation from 3/8 that is proportional to $y^{2/3} = 1/\ln^2(L)$ with an amplitude such that it passes through the point for $L = 2^{21}$. This agreement between the C deviation from 3/8 and a pure $1/\ln^2(L)$ power suggests that we introduce a constant $\alpha(g) = c_0$ into $\beta(g)$ in (49). The resulting added integral term $\approx c_0 g$ in (50) is a relative $O(g^2)$ correction to the leading $1/g$ which in turn is an implicit relative $O(1/\ln^2(L))$ correction to g^3 in the 3-parameter $E^{(\mathrm{corr})}|_{\mathrm{fit\_1}}$ in (48). To check this determine a new sequence of C, b, c_0 and L_0 from 4-point fits to $E^{(\mathrm{corr})}$ (47) at $L = 2^p, \ldots 2^{p-3}$, $13 \leqslant p \leqslant 21$. The results for this new C sequence are shown as the highest cross sequence in figure 3 together with a (positive) deviation curve proportional to $y^{4/3} = 1/\ln^4(L)$. The new agreement between the C deviation and a pure power suggests the process we have started be continued, first with an $\alpha(g) = c_0 + c_2 g^2$ and then with $\alpha(g) = c_0 + c_2 g^2 + c_4 g^4$, resulting in the two remaining cross sequences shown in figure 3. All these fits are plausibly consistent with a deviation pattern of alternating sign and of magnitude proportional to $y^{2\,n/3}$, $n = 1, 2, \ldots$. Although the fits become unstable for n much beyond four, the sequences already shown in figure 3 are impressive evidence that the CFT result (4) is correct and applies to the spin-½ isotropic Heisenberg chain.

As an alternative analysis consider keeping $\alpha(g) = 0$ throughout but changing $E^{(\mathrm{corr})}|_{\mathrm{fit\_1}}$ to include explicit corrections to g^3 of the form g^{5+2n} which are the leading corrections, deduced by power counting, that would be induced by the powers g^{2n} in $\alpha(g)$. Define

[6] It is not clear why Nomura would have considered the non-universal integration constant $L_0 = 0.5653$ he determined from the excited triplet state as a plausible choice for the ground state.

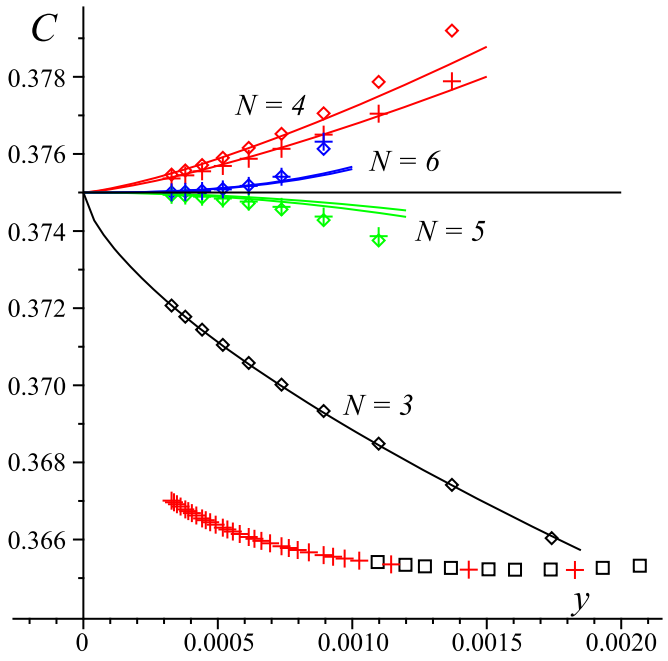

Figure 3. The amplitude C versus $y = 1/\ln^3(L)$ for various fits described in the text. Sequences (and associated curves) are labelled by the number of parameters N used in each fit. Each C from an N-parameter fit to $E^{(\mathrm{corr})}$ at $\mathrm{L} = 2^P, 2^{P-1}, \ldots 2^{P+1-N}$ is displayed as a point at $L = 2^P$. All curves are pure power laws $y^{(2N-4)/3} = 1/\ln^{(2N-4)}(L)$ measured from 3/8 and passing through the $L = 2^{21}$ terminal points of the C fit sequences.

$$E^{(\mathrm{corr})}|_{\mathrm{fit\_2}} = Cg^3 + \sum_{n=0}^{m} a_n g^{5+2n} + b/L^2 \tag{51}$$

and determine C, b, $\{a_n\}$ and L_0 from $N(=m+4)$-point fits of $E^{(\mathrm{corr})}|_{\mathrm{fit\_2}}$ (51) to $E^{(\mathrm{corr})}$ data (47) exactly as done above for C, b, $\{c_n\}$ and L_0. The results are shown as the diamond sequences in the upper part of figure 3 and are a natural extension to $N = 6$ of the $\alpha(g) = 0, N = 3$ diamond sequence. The similarity to the $\alpha(g) \neq 0$ based results supports the conclusion that the CFT result (4) is correct.

The fit sequence using (51) can be carried beyond $N = 6$. The analogs of the last ($L = 2^{21}$) $N = 6$ point in the form $10^5(C-3/8) = 3.31$ are -0.26, 9.95, 1.91, 3.09, -3.66 and -1.11 for $N = 7$ through 12. With increasing N the fits cover a larger range of L and the simple form (51) becomes inadequate. A possible alternative extrapolation to $L \to \infty$ is to use the $N = 6$ sequence from figure 3 and assume that the power law sequence used in the construction of the curves in figure 3 applies to higher order. Some results are given in the Neville-like table

$$\begin{array}{lccccc}
L = 2^{21}: & 3.31 & & & & \\
 & & 0.39 & & & \\
L = 2^{20}: & 4.71 & & 1.11 & & \\
 & & -0.08 & & 0.41 & \\
L = 2^{19}: & 7.14 & & 1.71 & & 0.83 \\
 & & -1.32 & & -0.05 & \\
L = 2^{18}: & 11.72 & & 3.32 & & \\
 & & -4.76 & & & \\
L = 2^{17}: & 21.27 & & & &
\end{array} \tag{52}$$

where the first column entries labelled by L are $N = 6$ diamond estimates $10^5(C-3/8)$. The nth following column entries are the corresponding scaled C_∞ deviations where I take $1/\ln(L)$ as a reasonable proxy for $g(L)$ and use the fitting function $C_L = C_\infty + c_1/\ln^8(L) + \ldots + c_n/\ln^{6+2n}(L)$. The Neville table using the $N = 6$ cross estimates is similar. There is nothing in the extrapolated C_∞ values to suggest any systematic deviation from the CFT $C = 3/8$ but they are disappointing—being at best an order of magnitude improvement on the $N = 6$ fit in figure 3. To see whether more substantial improvement is possible I turn to higher order fits that utilize more of the large L raw data from (47).

An example of a higher order fit that includes $b \rightarrow b(g)$ is

$$\begin{aligned} L_0 &= 0.4834655080, \quad \beta(g) = -g^2 - g^3/2, \\ E^{(\mathrm{corr})}|_{\mathrm{fit}} &= 0.3750032579g^3 + 0.7582000831g^5 + 11.40101912g^7 - 318.0740987g^9 \\ &\quad + 60748.49506g^{11} - 4835298.643g^{13} + 231829573.1g^{15} \\ &\quad + (1.189710255 - 173.8677649g^3 + 3110.122858g^5 - 258835.2988g^7)/L^2. \end{aligned} \tag{53}$$

The coefficients in (53) have been too severely truncated for (53) to be used to determine the fit accuracy but the deviations $\delta = E^{(\mathrm{corr})}|_{\mathrm{fit}} - E^{(\mathrm{corr})}$ calculated directly from the original multiple precision fit are recorded as column $\delta(53)$ in (47). Each zero in that column marks a datum that has been used in the fit to generate (53). The deviation of the C coefficient in (53) from 3/8 is fairly typical of such high order fits and illustrates that, even with data to $L = 2^{21}$, obtaining C to an accuracy better than 1 part in 10^5 does not seem possible. An intriguing observation is the ≈1.19 amplitude of the $1/L^2$ term in (53); this is reasonably close to the $7\pi^2/60 = 1.151\ldots$ Avdeev and Dörfel [6] and Hamer [8] result given in (21) which if exact would be an even greater enigma than suggested in remarks following (21). Another observation regarding (53) is the rapid growth of the coefficients of g^n with increasing n. While this might indicate the exact g series is asymptotic rather than convergent, a more likely reason is that no term in the g series has the exactly correct L dependence. This would imply the higher order terms must in part fit the lower order term errors which necessarily requires a growth in coefficients to compensate the decay in g^n magnitude with increasing n. One can speculate that this error is intrinsic to the single variable approach—a proper renormalization group treatment probably requires a Wilson structure of coupled equations in many variables.

A more accessible numerical question is whether the CFT amplitude $C = 3/8$ can be imposed without a dramatic reduction in the quality of a fit such as (53). The answer is in the affirmative; an example is

$$\begin{aligned} L_0 &= 0.4836300075, \quad \beta(g) = -g^2 - g^3/2 - 0.7920786733g^5, \\ E^{(\mathrm{corr})}|_{\mathrm{fit}} &= (3/8)g^3 + 0.7395919879g^5 + 6.482899058g^7 + 98.44496044g^9 \\ &\quad + 14465.68686g^{11} - 1246508.930g^{13} + 93781125.78g^{15} \\ &\quad + (1.270707901 - 244.5382883g^3 + 14353.69283g^5 - 531957.3542g^7)/L^2 \end{aligned} \tag{54}$$

in which a new term has been introduced into $\beta(g)$ in lieu of a variable C. The fit deviations of (54) are shown as $\delta(54)$ in (47) and are seen to differ little from the $\delta(53)$. Adding another term to $\beta(g)$ and imposing a new fit constraint at $L = 1835\,008$ gives

$$\begin{aligned} L_0 &= 0.4836491910, \quad \beta(g) = -g^2 - g^3/2 - 1.346579559g^5 - 541.9522010g^7, \\ E^{(\mathrm{corr})}|_{\mathrm{fit}} &= (3/8)g^3 + 0.7338448228g^5 - 2.689714940g^7 - 1102.903176g^9 \\ &\quad + 69567.74617g^{11} - 4512379.419g^{13} + 201152072.3g^{15} \\ &\quad + (1.224301918 - 220.6853420g^3 + 9104.234658g^5 - 476403.4388g^7)/L^2. \end{aligned} \tag{55}$$

The deviations $\delta(55)$, shown as the last column in (47), are only a marginal improvement on $\delta(54)$. The effect of eliminating some low order terms in $E^{(\mathrm{corr})}|_{\mathrm{fit}}$ in favour of terms in $\beta(g)$ is illustrated by

$$\begin{aligned} L_0 &= 0.4836482940, \\ \beta(g) &= -g^2 - g^3/2 - 0.6525707300g^4 - 1.314696674g^5 + 9.012883800g^6 - 498.9349125g^7, \\ E^{(\mathrm{corr})}|_{\mathrm{fit}} &= (3/8)g^3 - 1002.089691g^9 + 66725.41067g^{11} - 4268983.752g^{13} + 186770225.8g^{15} \\ &\quad + (1.220515404 - 221.9288813g^3 + 8813.378480g^5 - 487846.3619g^7)/L^2. \end{aligned} \tag{56}$$

The deviations $\delta(56)$ are about 3% smaller than the $\delta(55)$—an inconsequential difference. The effect of other changes such as including a $1/L^4$ term or using only data from the largest chain lengths in the fits are also small. Provided the CFT amplitude $C = 3/8$ is accepted, I estimate from (54)–(56) and other fits that

$$L_0 = 0.48364(2). \tag{57}$$

It is interesting to note that with this value for L_0 rather than the Nomura $L_0 = 0.5653$, the ratio $E^{(\mathrm{corr})}/g(L)^3$ approaches 3/8 from above rather than below. While it is clear that no significance can be attached to any single high order term in the fits, the global quality of the fits as seen in the deviation columns in (47) is good and I estimate that for $L > 2^{21}$, the error in the fits (55) or (56) is bounded by $\approx 10^{-13}$ with the maximum error at $L \approx 10^{21}$.

6. Conclusions

Numerical solutions to the BAE for the ground state of spin-½ isotropic anti-ferromagnetic periodic Heisenberg chains to length $L = 2^{21}$ have been obtained. An analysis of the ground state energy shows unambiguously that the amplitude of the leading logarithmic term is consistent with that expected on the basis of CFT and the

connection of the discrete spin-½ system to the continuum $k = 1$ Wess–Zumino–Witten nonlinear σ model. This resolves a decades old discrepancy based on analysis of shorter chains.

That such exceptionally long chains could be treated depended on the use of a Lagrange interpolation scheme which reduced the number of variables to be iterated by NR from $O(L)$ to $O(\ln(L))$. It is not clear how the method might be best adapted for states for which the Bethe wave-vector distribution does not have the exceptional smoothness of the ground state distribution.

An analytical formula has been derived that is an improvement on Hulthén's wave-vector distribution and while it has the qualitative features of the exact (numerical) distribution it is at best semi-quantitatively useful.

Appendix

This appendix derives the analytic formula (A.4) for the energy difference

$$\Delta = E_L'(\text{Hulthén}) - E_L(\text{Hulthén}), \tag{A.1}$$

where the two energies are defined in (17) and (18). It follows that Δ is the difference between sum and integral of $-4/(1 + \lambda_n^{(0)^2})$ where $\lambda_n^{(0)}$ is defined in (14) and we can use complex contour integral methods to obtain an analytic expression. Specifically, the sum can be expressed, via the residue theorem, as

$$-2i \oint \mathrm{d}n \tan(\pi n)/(1 + \lambda_n^{(0)^2}), \tag{A.2}$$

where the contour is the rectangle with vertices at $(\varepsilon, \pm C)$ and $(L/2-\varepsilon, \pm C)$ with $L/2$ understood to be integer and the limits $\varepsilon \to 0+$ and $C \to \infty$ ultimately to be taken. Note that the integrand singularities at $\lambda_n^{(0)} = \pm\mathrm{i}$ are at $n = \infty$ and not within the (finite) contour. Now $\tan(\pi n)$ rapidly approaches $+\mathrm{i}(-\mathrm{i})$ as one leaves the real axis into the upper(lower) half plane. If we use the asymptotic $+\mathrm{i}(-\mathrm{i})$ everywhere on the upper(lower) contour the integral approximation to the sum is recovered and so we will get the sum minus integral difference expression for Δ by modifying (A.2) by the replacements $\tan(\pi n) \to \tan(\pi n) - \mathrm{i}\,(\tan(\pi n) + \mathrm{i})$ in the upper (lower) half planes. Contributions to this new contour integral on the segments at $\pm C$ vanish as $C \to \infty$ while the limit $\varepsilon \to 0+$ dictates the correct logarithmic branch for $\lambda_n^{(0)}$ on the remaining segments. On the line $n = L/2+\mathrm{iy}$, $\lambda_n^{(0)} = -\mathrm{i}\,\mathrm{sign}(y) + \Lambda(\pi y)$ and on $n = 0+\mathrm{iy}$, $\lambda_n^{(0)} = -\mathrm{i}\,\mathrm{sign}(y) - \Lambda(\pi y)$ where $\Lambda(\pi y) = (2/\pi)\ln(\tanh(\pi|y|/L))$. The result of the contour integration is

$$\Delta = 4\mathrm{i}\int_{y=0}^{\infty} \mathrm{d}y(1 - \tanh(\pi y))\left(\frac{1}{1 + (\mathrm{i} + \Lambda(\pi y))^2} - \frac{1}{1 + (\mathrm{i} - \Lambda(\pi y))^2}\right) \tag{A.3}$$

and a final substitution $\pi y \to y$ and algebraic simplification yields

$$\begin{aligned}\Delta &= 4\pi^2\int_{y=0}^{\infty} \frac{\mathrm{d}y}{1 + \exp(2y)}\,\frac{1}{\ln(\tanh(y/L))}\,\frac{1}{\pi^2 + \ln^2(\tanh(y/L))} \\ &= -\frac{2\pi^2\ln(2)}{\ln^3(L)} + \frac{9\pi^2\ln^2(2)}{\ln^4(L)} + \ldots + \frac{3\pi^2\zeta(3)}{4L^2\ln^4(L)} + \ldots + O(L^{-4}).\end{aligned} \tag{A.4}$$

The terms following the last equality in (A.4) are the start of a double asymptotic expansion. The first block is based on the approximation $\tanh(y/L) = y/L$ followed by expansion in inverse powers of $\ln(L)$ in the integrand in (A.4). All coefficients, $C_i = \int_0^{\infty} \mathrm{d}y\ \ln^i(y)/(1 + \exp(2y))$, in this expansion can be obtained from the generating function

$$\begin{aligned}\sum_{i=0}^{\infty}\frac{a^i}{i!}C_i &= \int_{y=0}^{\infty}\frac{\mathrm{d}y\quad y^a}{1 + \exp(2y)} = \frac{\Gamma(a+1)}{2^{a+1}}\zeta(a+1)\left(1 - \frac{1}{2^a}\right) \\ &= \frac{\ln(2)}{2} - \frac{a}{1!}\frac{3\ln^2(2)}{4} + \frac{a^2}{2!}\frac{\ln(2)}{12}(14\ln^2(2) + \pi^2 - 6\gamma^2 - 12\gamma_1) - \ldots.\end{aligned} \tag{A.5}$$

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