Computer Physics Communications 303 (2024) 109280

Contents lists available at ScienceDirect

Computer Physics Communications

journal homepage: www.elsevier.com/locate/cpc

Computational Physics

Enhanced and generalized one–step Neville algorithm: Fractional powers and access to the convergence rate ☆

Ulrich D. Jentschura [a,*], Ludovico T. Giorgini [b]

[a] Department of Physics and LAMOR, Missouri University of Science and Technology, Rolla, MO 65409, USA
[b] Nordita, Royal Institute of Technology and Stockholm University, Stockholm 106 91, Sweden

ABSTRACT

The recursive Neville algorithm allows one to calculate interpolating functions recursively. Upon a judicious choice of the abscissas used for the interpolation (and extrapolation), this algorithm leads to a method for convergence acceleration. For example, one can use the Neville algorithm in order to successively eliminate inverse powers of the upper limit of the summation from the partial sums of a given, slowly convergent input series. Here, we show that, for a particular choice of the abscissas used for the extrapolation, one can replace the recursive Neville scheme by a simple one-step transformation, while also obtaining access to subleading terms for the transformed series after convergence acceleration. The matrix-based, unified formulas allow one to estimate the rate of convergence of the partial sums of the input series to their limit. In particular, Bethe logarithms for hydrogen are calculated to 100 decimal digits. Generalizations of the method to series whose remainder terms can be expanded in terms of inverse factorial series, or series with half-integer powers, are also discussed.

Contents

☆ The review of this paper was arranged by Prof. W. Jong.

* Corresponding author.
E-mail address: ulj@mst.edu (U.D. Jentschura).

https://doi.org/10.1016/j.cpc.2024.109280
Received 7 March 2024; Received in revised form 25 April 2024; Accepted 8 June 2024
Available online 12 June 2024

1. Introduction

Often in physics, one faces problems connected with slowly convergent, nonalternating series. Examples include angular momentum expansions in both nonrelativistic as well as relativistic atomic physics calculations [1,2], series representations of Bethe logarithms (Chap. 4 of Ref. [3]), or, logarithmic sums over eigenvalues required for the calculation of the functional determinant in $O(N)$ theories [4–6]. The acceleration of the convergence these series is notoriously problematic [7–9]. Traditional methods like the Aitken Δ^2 process [10], the Shanks transformation [11], and Wynn's epsilon algorithm [12] (which calculates Padé approximants), and other methods, all encounter numerical instabilities.

For nonalternating series, the challenge of the convergence acceleration differs significantly from the resummation of a divergent input series. While both scenarios aim to derive meaningful information from the series, the nature of the series and the techniques applied are fundamentally distinct. The latter seeks to assign a finite sum to a series that lacks natural convergence. This process often involves the employment of analytical continuations or summation techniques that go beyond conventional convergence acceleration methods. For example, in Ref. [13], it is shown how, by a suitable resummation procedure, a dissipative effect, namely, a nonperturbative pair creation amplitude in a strong electric background field, can be derived from a nonalternating series that sums the higher-order dispersive terms of the quantum corrections to the Maxwell Lagrangian. These quantum electrodynamic corrections are summarized in a nonalternating divergent perturbative expansion of the Heisenberg–Euler Lagrangian in powers of the electric field strength [3,14–16]. In contrast, summing a slowly convergent series entails enhancing the rate at which an already convergent series approaches its limit.

For alternating series, it is known that nonlinear sequence transformations such as the ones described in Ref. [7], notably, the Weniger–Levin transformation (see Refs. [7,17–21]), can lead both to the acceleration of convergence and also, to efficient convergence acceleration methods. For slowly convergent nonalternating series, the methods described for their resummation (see Ref. [13]) typically differ drastically from those employed for the acceleration of convergence. In Refs. [2,22,23], an algorithm was described which first converts the nonalternating input series to an alternating series, whose convergence is accelerated via nonlinear sequence transformations [2,7,23]. In fact, the first step of the two-step condensation, as described in Ref. [2], consists of the van Wijngaarden transformation [22], which rearranges the nonalternating input series into an alternating series, but it requires the calculation of individual terms of the input series of very high order in the summation indices. It is followed by a nonlinear sequence transformations [7,17–21], leading to what is known as the combined nonlinear-condensation transformation. Sometimes, however, the option of the calculation of terms of very high order in the summation indices is not available. This problem could occur in various contexts, e.g., because, on lattices, we cannot calculate eigenvalues with a high principal quantum number [4–6]. In the following, we will not discuss the combined nonlinear-condensation transformation [2] any further, as it contradicts the main thrust of the method described in the current paper, which pertains to convergence acceleration based on a limited number of terms of the input series.

In these cases, established methods like Aitken Δ^2 process [10] and Wynn's Epsilon Algorithm [12] are often used. One notes, according to Sec. 2.2.7 of Ref. [9], that the Aitken Δ^2 process and Wynn's Epsilon Algorithm are special cases of the general E-algorithm [24,25]. Of course, the Aitken Δ^2 process and Wynn's Epsilon Algorithm constitutes viable and widely used convergence acceleration methods, but numerical instability can be encountered in higher orders of the transformation.

In view of the numerical instabilities encountered in the convergence acceleration of these series, it is desirable to use asymptotic information about the input series to the maximum extent possible, in order to achieve the maximum convergence acceleration already in low orders of the transformation. One possibility to achieve this rapid convergence is to use the Neville algorithm, which, *a priori*, in its most general form, constitutes an interpolation algorithm [26]. It can be used for convergence acceleration, which is tantamount to extrapolation, if one uses the algorithm in order to calculate the interpolating polynomial outside of the domain of interpolation. One first interprets the partial sums of the input series as values of a function at abscissas which tend to a limiting value (say, zero) as the number of terms of the input series is increased. One possibility is to use $x = 1/(i+1)$ for the partial sums s_i of the input series ($i = 0, 1, 2, \dots$). One then calculates the value of the interpolating function at the limiting value of the abscissa (in our example case, at $x = 0$) which is outside of the domain $x \in (1/(n+1), 1)$ used for the interpolation (here, n is the maximum summation index used for the input series in a given order n of the transformation). The Neville algorithm uses information from all partial sums $(s_0, \dots, s_n)$ and hence, about the asymptotic structure of the input series, in order to construct the interpolating polynomial in x and can therefore lead to highly efficient convergence acceleration. Its usual formulation is based on a recursive three-term recursive scheme [see Eq. (12)]. Here, we aim to enhance the Neville algorithm by replacing the three-term recurrence relation with unifying analytic formulas which also give access to subleading asymptotics of the behavior of the partial sums s_n of the input series for large n.

This paper is organized as follows. In Sec. 2, we describe our formulation of the enhanced Neville algorithm. The idea behind our formulation is discussed in Sec. 2.1, while a comparison to the Neville algorithm is presented in Sec. 2.2. We find universal formulas which allow access to the subleading terms for high n, in Sec. 2.3. The performance of the algorithm is compared to other established methods in Sec. 3. Numerical examples are discussed in Sec. 4, generalizations of the algorithm are discussed in Sec. 5, and conclusions are reserved for Sec. 6. Appendix A lists some higher-order coefficients for the subleading asymptotic behavior of the input series, and Appendix C gives numerical values for hydrogen Bethe logarithms obtained using our method.

2. Enhanced Neville algorithm

2.1. Formulation of the algorithm

One starts with the following relations for the partial sums s_n of the input series, and the remainder terms r_n,

$$s_n = \sum_{k=0}^{n} a_k = s_\infty + r_n \,, \qquad r_n = -\sum_{k=n+1}^{\infty} a_k \,. \tag{1}$$

(Here, we start the terms from index $k = 0$, by convention [7].)

Let us assume that the terms of the infinite series possess an asymptotic expansion in inverse integer powers of the summation index,

$$a_k = \frac{A}{k^2} + \frac{B}{k^3} + \mathcal{O}(k^{-4}) \,. \tag{2}$$

The idea is that, if n is sufficiently large, we can use the asymptotic approximation for the remainder term,

$$r_n = -\sum_{k=n+1}^{\infty} a_k = -\sum_{k=n+1}^{\infty} \left[\frac{A}{k^2} + \frac{B}{k^3} + \frac{C}{k^4} + \mathcal{O}(k^{-5}) \right] . \tag{3}$$

One can use the relation

$$\sum_{k=n+1}^{\infty} \frac{1}{k^a} = \frac{(-1)^a}{(a-1)!} \left. \frac{\partial^{a-1}\psi(z)}{\partial z^{a-1}} \right|_{z=n+1} , \tag{4}$$

where $\psi(z)$ is the logarithmic derivative of the Gamma function, to expand the remainder term r_n in inverse power of n. The first terms in this expansion read as follows,

$$r_n = \frac{A}{n} + \frac{B-A}{2n^2} + \frac{A-3B+2C}{6n^3} + \mathcal{O}(n^{-4}) . \tag{5}$$

One then tries to eliminate the asymptotic terms of the remainder function, which are powers of $1/n$. To this end, one interprets the first $(n+1)$ partial sums s_i with $i \in (0, \dots, n)$ as approximations to the values of a function $f(x)$ at the abscissa values $x = x_i = 1/i$,

$$s_i \approx f(x = x_i = 1/(i+1)) , \qquad i \in (0, \dots, n) , \tag{6}$$

so that $\lim_{\epsilon \to 0^+} f(\epsilon) = s_\infty$. If we assume that $f(x)$ can be expanded as a power series, then we can write

$$f(x_i) = \sum_{j=0}^{\infty} c_j (x_i)^j \approx \sum_{j=0}^{n} c_j (x_i)^j = c_0 + \frac{c_1}{(i+1)} + \frac{c_2}{(i+1)^2} + \dots + \frac{c_n}{(i+1)^n} , \tag{7}$$

with $n+1$ unknown coefficients c_j $(j = 0, \dots, n)$. Given $n+1$ partial sums s_i of the input series $\{s_i\}_{n=0}^{\infty}$, the idea of the algorithm is to solve the system of equations

$$s_i = \sum_{j=0}^{n} c_j(n) \left(\frac{1}{i+1} \right)^j , \qquad i, j \in (0, \dots, n) , \tag{8}$$

for the coefficients $c_j(n)$. One then assumes that the value of the infinite series is recovered as n is increased,

$$s = s_\infty = \lim_{n\to\infty} c_0(n) , \tag{9}$$

where $c_0(n)$ is the zeroth-order coefficient of the interpolating polynomial $\sum_{j=0}^{n} c_j(n) x^j$, which, at the abscissas $x = x_i = 1/(i+1)$, coincides with the partial sums s_i of the input series. In view of the fact that $c_0(n)$ is identical to the value of the interpolating polynomial at argument $x = 0$ while all abscissas x_i are positive, the latter step constitutes an extrapolation which can lead to convergence acceleration [9].

To conclude this section, we observe that, in the sense of Eq. (1), the *ansatz* given in Eq. (7) corresponds to an inverse-power behavior of the remainder term,

$$r_n = \sum_{j=1}^{\infty} c_j \left(\frac{1}{n+1} \right)^j = \frac{c_1}{n+1} + \frac{c_2}{(n+1)^2} + \dots . \tag{10}$$

This, in turn, corresponds to Eq. (7.1-2) of Ref. [7].

2.2. Neville algorithm

For the calculation of the coefficient $c_0(n)$ of the interpolating polynomial, one can use the Neville algorithm [26]. Given $n+1$ partial sums s_i of the input series $\{s_i\}_{n=0}^{\infty}$, the Neville algorithm refines the approximation of s_∞ by iteratively interpolating between points defined by the sequence s_i. Recursive schemes have been described in Refs. [27,28]. Adapted to our choice of abscissas $x_i = 1/(i+1)$, one may formulate a lozenge scheme as follows. One starts the recursion with the values

$$s_i^0 = s_i , \qquad i \in (0, \dots, n) , \tag{11}$$

and uses a three-term recursion,

$$s_i^m = \frac{(i+1) s_i^{m-1} - (i+1-m)\, s_{i-1}^{m-1}}{m} , \qquad 1 \le m \le n , \qquad m \le i \le n . \tag{12}$$

One increases m, thereby decreasing the allowable values of i in the process, until, for $m = n$, only one possible value is left for i, namely, $i = m = n$. Finally, the desired coefficient $c_0(n)$ is recovered as follows,

$$c_0(n) = s_n^n . \tag{13}$$

While the recursive scheme is very helpful, it does not establish a direct connection between each term of the partial sums used for extrapolation and the final estimated limit. Hence, no additional information can be derived for the asymptotic behavior of the partial sums s_n for large n. In particular, while the recursive scheme enables the estimation of the limit $\lim_{x_i \to 0^+} f(x_i) = s_\infty$, it does not provide insights into the behavior of the interpolating function $f(x_i)$ near $x_i = 0$, e.g., the rate at which the limit is approached.

Let us briefly clarify a notation used in the following. Our goal is to estimate s_∞ utilizing the initial n terms of the series. We denote the estimate of the limit after the convergence acceleration transformation by the symbol $\mathcal{T}_n$. Let now $\mathcal{T}$ be the transformation which takes as input the partial sums $(s_0, s_1, \dots, s_n)$, and by which one obtains $\mathcal{T}_n$,

$$\mathcal{T}_n = \mathcal{T}(s_0, s_1, \dots, s_n). \tag{14}$$

For example, if $\mathcal{T}$ is the Neville algorithm as given in the adaptation (12), then $\mathcal{T}_n = c_0(n) = s_n^n$. For the other methods discussed here, the definition of $\mathcal{T}_n$ is adapted in the obvious way.

2.3. Universal formula

In order to obtain universal formulas which allow access to subleading terms (that serve to measure the rate of convergence of the input series), it is advantageous to map the problem onto a system of linear equations. One interprets the coefficients $c_j(n)$ of the polynomial as the elements of a vector $\vec{c}(n) = (c_0(n), ..., c_n(n))$ with $n+1$ elements,

$$s_i = \sum_{j=0}^{n} c_j(n) \left(\frac{1}{i+1}\right)^j = \sum_{j=0}^{n} M_{ij}(n)\, c_j(n) \,, \qquad M_{ij}(n) = \left(\frac{1}{i+1}\right)^j \,, \qquad i,j \in (0,\dots,n)\,. \tag{15}$$

The elements $M_{ij}(n)$ can be interpreted as components of a matrix of dimension $(n+1)\times(n+1)$, in which case one has $\vec{s} = \mathbb{M}(n)\cdot\vec{c}(n)$, where $\vec{s} = (s_0, ..., s_n)$ is the vector of the first $n+1$ partial sums of the input series. Therefore, the solution can be obtained by matrix inversion,

$$\vec{c}(n) = [\mathbb{M}(n)]^{-1}\cdot\vec{s}\,, \qquad \vec{c} = (c_0(n), ..., c_n(n))\,. \tag{16}$$

The inversion of the matrix $\mathbb{M}(n)$ can lead to significant numerical instability and loss of accuracy. This is because large numbers can cause overflow or underflow issues in floating-point arithmetic, while the entries of $\mathbb{M}(n)$ span many orders of magnitude, which leads to unfavorable condition numbers for higher n. This can exacerbate rounding errors. For this reason, it is advantageous to derive analytic formulas for the first five rows of the inverted matrix $[\mathbb{M}(n)]^{-1}$, which leads to analytic formulas for the coefficients $c_0(n)$, $c_1(n)$, $c_2(n)$, $c_3(n)$, and $c_4(n)$. We find that

$$c_j(n) = \sum_{i=0}^{n} \frac{(-1)^{n-i}\,(i+1)^n}{\Gamma(i+1)\,\Gamma(n-i+1)}\,\mathcal{P}_j(i,n)\,s_i\,, \qquad j\in(0,1,2,3,4)\,, \tag{17a}$$

$$\mathcal{P}_0(i,n) = 1\,, \tag{17b}$$

$$2\,\mathcal{P}_1(i,n) = 2i - 3n - n^2\,, \tag{17c}$$

$$24\mathcal{P}_2(i,n) = 24i + 24i^2 - 26n - 36in + 9n^2 - 12in^2 + 14n^3 + 3n^4\,, \tag{17d}$$

$$\begin{aligned}48\mathcal{P}_3(i,n) = {} & 48i + 96i^2 + 48i^3 - 48n - 124in - 72i^2n + 26n^2 \\ & - 6in^2 - 24i^2n^2 + 29n^3 + 28in^3 - n^4 + 6in^4 - 5n^5 - n^6\,.\end{aligned} \tag{17e}$$

$$\begin{aligned}5760\mathcal{P}_4(i,n) = {} & 5760i + 17280i^2 + 17280i^3 + 5760i^4 - 5712n - 20640in - 23520i^2n - 8640i^3n \\ & + 3380n^2 + 2400in^2 - 3600i^2n^2 - 2880i^3n^2 + 3660n^3 + 6840in^3 + 3360i^2n^3 \\ & - 385n^4 + 600in^4 + 720i^2n^4 - 888n^5 - 600in^5 - 130n^6 - 120in^6 + 60n^7 + 15n^8\,.\end{aligned} \tag{17f}$$

Results for the coefficients $c_j(n)$ with $j > 4$ are given in Appendix A. The results given in Eq. (17) facilitate the estimation of the functional relationship of the $f(x_i)$ for small abscissas x_i, thereby providing insight the convergence rate of the partial sums of the input series toward its limit. Specifically, one notes the relationship

$$s_n = s_\infty + r_n \approx c_0 + \frac{c_1}{n+1} + \frac{c_2}{(n+1)^2} + \dots\,, \qquad n\to\infty\,, \qquad c_j \equiv \lim_{n\to\infty} c_j(n)\,, \tag{18}$$

$$r_n = s_n - s_\infty \approx \frac{c_1}{n+1} + \frac{c_2}{(n+1)^2} + \dots\,, \qquad n\to\infty\,, \tag{19}$$

where careful attention is given to the sign of the remainder term r_n.

3. Comparison to the other methods

Some remarks may be in order with respect to the comparison of the method outlined above to other established methods like the Aitken's Δ^2 process and Wynn's epsilon algorithm [7–9]. These are two of the most well-known and frequently used algorithms for series convergence acceleration. Both of them are based on the Shanks transformation [11], which produces Padé approximants if the input data are the partial sums of a power series [7]. The former produces an efficient recursive scheme to compute conveniently such transformation. The formula for the epsilon algorithm is given by:

$$\epsilon_{k+1}^{(n)} = \epsilon_{k-1}^{(n+1)} + \frac{1}{\epsilon_k^{(n+1)} - \epsilon_k^{(n)}}, \qquad -1 < k < n-1\,, \tag{20}$$

with k indicating the iteration level and n the position within that level. The initial conditions are $\epsilon_{-1}^{(n)} = 0$ for all n, and $\epsilon_0^{(n)} = s_n$, where s_n is the nth term of the sequence being accelerated. The values for $n = 0$, $\epsilon_k^{(0)}$, describe a sequence of upper-diagonal (odd k) and diagonal (even k) Padé approximants to the input series. The result of the transformation of the partial sums $(s_0,\dots,s_n)$ is written using the diagonal Padé approximants, that is $\mathcal{T}_n = \epsilon^{(0)}_{\lfloor \frac{n}{2}\rfloor}$, with $\lfloor\cdot\rfloor$ denoting the integer part. Aitken's Δ^2 process consists instead of a recursive iteration of the first-order Shanks transformation,

$$A_{k+1}^{(n)} = A_k^{(n)} - \frac{\left(\Delta A_k^{(n)}\right)^2}{\Delta^2 A_k^{(n)}}, \tag{21}$$

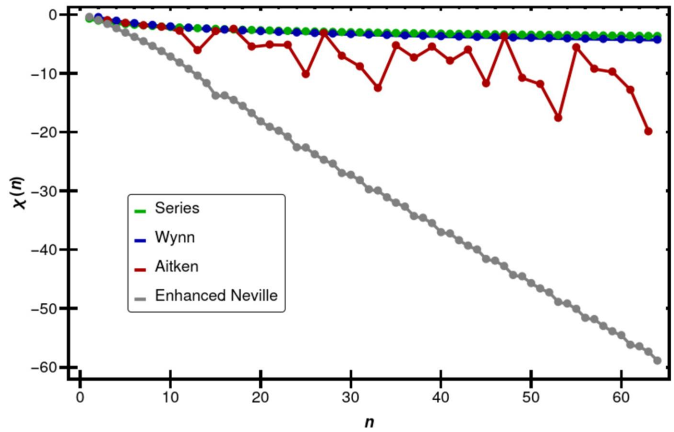

Fig. 1. We investigate the convergence of the enhanced Neville transformation (green curve) for the input series (27), as measured by the quantity $\chi(n)$ defined in Eq. (28). The quantity $\chi(n)$ roughly decreases by unity with every iteration of the algorithm, indicating the gain of roughly one converged decimal with every order of the enhanced Neville transformation. The convergence of the enhanced Neville transformation is compared with the convergence of the Wynn epsilon algorithm (blue curve), of the Aitken Δ^2 process (red curve), and of the series itself (black curve). (For interpretation of the colors in the figure, the reader is referred to the web version of this article. The curves labeled “Series”, “Wynn”, “Aitken” and “Enhanced Neville” are listed from top to bottom both in the figure legend as well as in the figure itself.)

where, as for the epsilon algorithm, k indicates the iteration level and n the position within that level. The initial conditions are $A_0^{(n)} = s_n$, while $\Delta A_k^{(n)} = A_k^{(n+1)} - A_k^{(n)}$ is the first difference of the sequence, and $\Delta^2 A_k^{(n)} = \Delta A_k^{(n+1)} - \Delta A_k^{(n)}$ is the second-order difference of the sequence. The result of the transformation of the partial sums $(s_0, \ldots, s_n)$ then is $\mathcal{T}_n = A^{(0)}_{\lfloor \frac{n-1}{2} \rfloor}$, with $\lfloor \cdot \rfloor$ the integer part. A meaningful iteration of the Δ^2 process, which leads to an improved convergence, therefore is attained when n is increased by two.

Our assumptions, formulated in Eq. (5), imply that the input series exhibits logarithmic convergence. Specifically, one has the asymptotic relation

$$\lim_{n\to\infty} \frac{s_{n+1} - s}{s_n - s} = \lim_{n\to\infty} \frac{r_{n+1}}{r_n} = 1. \tag{22}$$

This observation indicates that the Shanks transform, which is predicated on the assumption that, in the sequence’s tail (for large n), the ratio

$$\frac{s_{n+1} - s}{s_n - s} \approx \frac{s_{n+2} - s}{s_{n+1} - s} \approx \lambda, \tag{23}$$

remains constant, may not yield accurate results. In fact, advantage can be taken in Eq. (23) for a linearly convergent series (i.e., for the case $\lambda < 1$). In this case, the sequence terms are expected to follow

$$s_n = \sigma_0 + \sigma_1 \alpha_1^n + O(\alpha_2^n), \quad |\alpha_2| < |\alpha_1|, \tag{24}$$

indicating that the error in approximating Eq. (23) diminishes geometrically with n. Specifically,

$$\frac{s_{n+1} - s}{s_n - s} - \frac{s_{n+2} - s}{s_{n+1} - s} = \mathcal{O}\left(\frac{\alpha_2}{\alpha_1}\right)^n. \tag{25}$$

However, for a series whose terms are represented by Eq. (7), the error reduction is merely polynomial in n:

$$\frac{s_{n+1} - s}{s_n - s} - \frac{s_{n+2} - s}{s_{n+1} - s} = \mathcal{O}\left(\frac{1}{n}\right), \tag{26}$$

which leads to a much slower rate of convergence for large n as compared to the factor $\lambda = \alpha_2/\alpha_1 < 1$. Consequently, methodologies dependent on such algorithms as Aitken’s Δ^2 process [10], the Shanks transformation [11], or Wynn’s ϵ algorithm [12], demonstrate suboptimal performance for these series. For our particular model example, given in Eq. (27), these statements are illustrated in Fig. 1. A clarifying remark is in order. For the comparison in Fig. 1, we plot the data points as a function of n, where n is the maximum index of the terms of the input series used in order to calculate the convergence acceleration transform. We indicate the error of the extrapolation as a function of n. Some algorithms, such as the Aitken method, only produce a sensible result when n is being increased in steps of two, $n \to n+2$. This explains why there are some apparent “gaps” in the numerical data.

4. Numerical examples

4.1. Slowly convergent model series

We discuss the application of the enhanced Neville algorithm to the infinite series with partial sums

$$s_n = \sum_{k=0}^{n} a_k, \qquad a_k = \frac{4}{\pi (k+1)^2} \arctan\left(\frac{k+2}{k+3}\right), \tag{27}$$

where the prefactor is chosen so that $a_k \approx 1/k^2$ for $k \to \infty$. We calculate the enhanced Neville transformations, up to order $n = 100$, and the determination of the convergence according to the formula

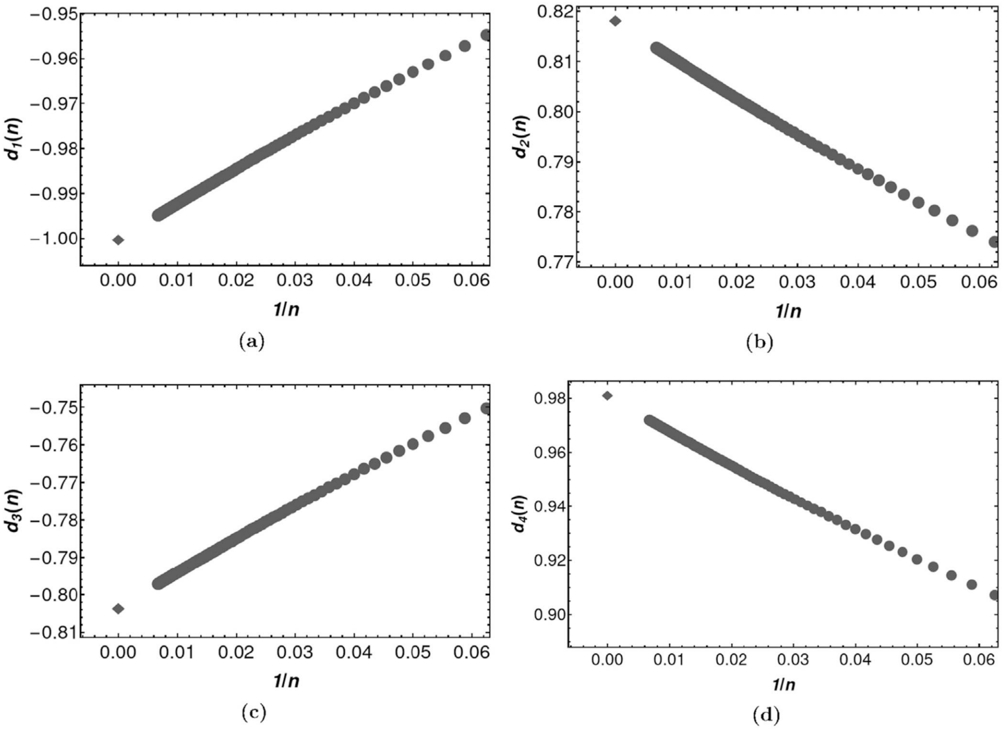

Fig. 2. The figures illustrate the convergence of sequences $d_j(n)$ toward c_j for $j = 1, 2, 3, 4$, according to Eq. (32). The cases $j = 1, 2, 3, 4$ are treated in Fig. (a), (b), (d), and (d), respectively. The first 150 $d_j(n)$ with $n = 0, \ldots, 149$ are compared to the value $c_j = d_j(\infty)$, the latter being denoted by a black diamond. One notes that $c_1 = -1$ is integer-valued, while the first 50 decimals of the coefficients c_2, c_3 and c_4 are given in Eq. (30).

$$\chi(n) = \frac{\ln(|\mathcal{T}_n - \mathcal{T}_{n+1}|)}{\ln(10)}, \tag{28}$$

with $\mathcal{T}_n$ defined in Eq. (14). The quantity $\chi(n)$ measures the apparent convergence of the transforms as the order of the transformation is increased, by calculating the number of apparently converged decimal digits.

In Fig. 1, we compare the convergence of the enhanced Neville transformation to Aitken's Δ^2 process [10], Wynn's epsilon algorithm [12] and alongside the series itself. The enhanced Neville scheme is shown to outperform the other convergence acceleration algorithms, securing approximately one additional decimal of convergence with each transformation order. In contrast, the other methods progress much more slowly. This observation is tied to the asymptotic structure of the input series, according to Eq. (2).

Our analysis, based on the enhanced Neville algorithm, yields a 50-decimal approximation of the series limit:

$$s_\infty = \lim_{n\to\infty} c_0(n) = 1.31279\,49538\,25865\,79196\,34865\,83906\,40442\,73891\,27574\,77554. \tag{29}$$

Furthermore, we obtain the results

$$c_1 = \lim_{n\to\infty} c_1(n) = -1, \qquad c_2 = \lim_{n\to\infty} c_2(n) = \frac{1}{2} + \frac{1}{\pi} = 0.81830\,98861\,83790\ldots, \tag{30a}$$

$$c_3 = \lim_{n\to\infty} c_3(n) = -\frac{1}{6} - \frac{2}{\pi} = -0.80328\,64390\,34248\ldots, \qquad c_4 = \lim_{n\to\infty} c_4(n) = \frac{37}{12\pi} = 0.98145\,54824\,00021\ldots. \tag{30b}$$

The next higher coefficients are $c_5 = \frac{1}{30} - \frac{131}{30\pi}$, $c_6 = \frac{268}{45\pi}$, $c_7 = -\frac{1}{42} - \frac{549}{70\pi}$, $c_8 = \frac{98347}{10000\pi}$, $c_9 = -\frac{1}{30} - \frac{9253}{840\pi}$, and $c_{10} = \frac{66011}{6300\pi}$. These results have been verified to about 100 digits against numerical data obtained with the help of the enhanced Neville algorithm described here. They can be obtained analytically based on the formula

$$s_n = \sum_{k=0}^{n} a_k = s_\infty - \sum_{k=n+1}^{\infty} a_k, \tag{31}$$

while realizing that the terms a_k in the latter sum from $k = n+1$ to $k = \infty$ can be expanded for large summation index k. We define the approximations $d_j(n) \approx c_j$ as follows,

$$d_j(n) = (n+1)^j \left(s_n - \sum_{r=0}^{j-1} \frac{c_r}{(n+1)^r} \right), \qquad \lim_{n\to\infty} d_j(n) = c_j, \qquad j = 1, 2, 3, 4. \tag{32}$$

It is instructive to plot the sequence of the $d_j(n)$ against $1/n$, for $j = 1, 2, 3, 4$, as shown in Fig. 2, for the model series given in Eq. (27). The value at infinite n (where $1/n \to 0$) is given by $\lim_{n\to\infty} d_j(n) = c_j$. The trend of the data presented in Fig. 2 is consistent with the convergence of the approximants $d_j(n) \to c_j$ for $j = 1, 2, 3, 4$, for large n.

4.2. Bethe logarithm

We investigate the series of partial sums s_n, where

$$b_n = \sum_{k=0}^{n} a_k \,, \qquad a_k = \frac{16(k+2)}{(k+1)^2\,(k+3)^2}\,\Phi\left(-\frac{3+k}{1+k}, 1, 2k+4\right), \tag{33}$$

where Φ is the Lerch phi transcendent, with $\Phi(z,s,a) = \sum_{n=0}^{\infty} z^n/(n+a)^s$. According to Chap. 4 of Ref. [3], the limit s_∞ of the input series is related to the Bethe logarithm [29] $\ln k_0(1S)$ of the hydrogen ground-state by the following relation,

$$b_\infty = \ln k_0(1S) - 10\,\ln(2) + 2\,\zeta(2) + 1\,. \tag{34}$$

The sum b_∞ and hence, the Bethe logarithm $\ln k_0(1S)$ of the ground state of hydrogen, is calculated in the same manner as the example treated in Sec. 4.1. The enhanced Neville algorithm obtains the 50-figure result

$$\ln k_0(1S) = 2.98412\,85557\,65497\,61075\,97770\,90013\,79796\,99751\,80566\,17002 \tag{35}$$

in the 58th order of transformation. It is somewhat surprising that the coefficients c_j with $j = 1,2,3,4$ are rational numbers,

$$\begin{aligned} &c_1 = 0, \qquad c_2 = 0, \qquad c_3 = -\frac{4}{3}, \qquad c_4 = \frac{27}{4}, \qquad c_5 = -\frac{703}{30}, \qquad c_6 = \frac{3329}{48}, \\ &c_7 = -\frac{63163}{336}, \qquad c_8 = \frac{184961}{384}, \qquad c_9 = -\frac{569323}{480}, \qquad c_{10} = \frac{7256477}{2560}\,. \end{aligned} \tag{36}$$

The results given in Eq. (36) currently constitute conjectures which we have verified to at least 100 decimals. The result $c_1 = c_2 = 0$ is expected because $\lim_{k\to\infty} a_k \sim \frac{1}{k^4}$, which then leads to $\lim_{k\to\infty} b_k = b_\infty + \mathcal{O}\left(\frac{1}{k^3}\right)$. Values of the Bethe logarithms $\ln k_0(1S)$, $\ln k_0(2S)$ and $\ln k_0(2P)$ accurate to 100 digits are presented in Appendix C. These could be used for the search of possible analytic formulas using the PSLQ algorithm [30–33]. The PSLQ algorithm can be used to search for analytic expressions of accurately known numerical quantities in terms of known constants such as the Euler constant $\gamma_E = 0.57721\ldots$, various Riemann zeta functions, powers of π, and multiplicative combinations of these constants. We can report that we have carried out a limited set of searches with the same constants that were used in Eq. (A11) of Ref. [4] without success.

5. Generalizations of the algorithm

5.1. Generalizations to half–integer–power remainder terms

It is instructive to briefly consider possible generalizations. For example, we may easily adapt the algorithm to series with half-integer powers, which leads to the *ansatz*

$$f(x_i) = \sum_{j=0}^{\infty} c_j^{(1/2)}\, x_{ij}^{(1/2)} \approx \sum_{j=0}^{n} c_j^{(1/2)}\, x_{ij}^{(1/2)} = c_0^{(1/2)} + \frac{c_1^{(1/2)}}{\sqrt{i+1}} + \frac{c_2^{(1/2)}}{i+1} + \ldots + \frac{c_n^{(1/2)}}{(i+1)^{n/2}}\,, \tag{37}$$

where the $x_{ij}^{(1/2)}$ are given as follows,

$$x_{ij}^{(1/2)} = \frac{1}{(i+1)^{j/2}}\,. \tag{38}$$

Our modified remainder term is thus based on half-integer powers,

$$r_n^{(1/2)} = \frac{c_1^{(1/2)}}{(n+1)^{1/2}} + \frac{c_2^{(1/2)}}{(n+1)} + \frac{c_3^{(1/2)}}{(n+1)^{3/2}} + \ldots\,. \tag{39}$$

Given $n+1$ partial sums s_i of the input series $\{s_i\}_{n=0}^{\infty}$, the generalized algorithm aims to solve the system of equations

$$s_i = \sum_{j=0}^{n} c_j^{(1/2)}(n)\, x_{ij}^{(1/2)} \qquad i,j \in (0,\ldots,n)\,, \tag{40}$$

as a function of n, leading to results for the coefficients $c_j^{(1/2)}(n)$ with $j \in (0,\ldots,n)$. In full analogy to Eqs. (9) and (B.6), one then assumes that the value of the infinite series is recovered as n is increased,

$$s = s_\infty = \lim_{n\to\infty} c_0^{(1/2)}(n)\,. \tag{41}$$

Using the half-integer-power Neville scheme, we investigate the acceleration of the convergence of the following series,

$$s_n = \sum_{k=0}^{n} a_k\,, \qquad a_k = \frac{4}{\pi\,(\sqrt{k}+1)^4}\,\arctan\left(\frac{\sqrt{k}+2}{\sqrt{k}+3}\right), \tag{42}$$

where the prefactor is adjusted so that $a_k \approx 1/k^2$ for $k \to \infty$. The transforms $c_0(n \le 203)$ converge to the 100-decimal result

$$\begin{aligned} s_\infty = \lim_{n\to\infty} c_0^{(1/2)}(n) = {}& 0.92316\,76494\,43269\,09201\,53242\,74308\,14908\,92138\,92222\,83308 \\ & 78498\,38145\,30824\,82489\,27413\,45388\,44628\,47523\,62540\,58525\,. \end{aligned} \tag{43}$$

The transforms are calculated by solving the linear system given in Eq. (40) by standard matrix inversion techniques [34]. Furthermore, the following results are obtained,

$$c_1^{(1/2)} = 0\,, \qquad c_2^{(1/2)} = -1\,, \qquad c_3^{(1/2)} = \frac{1}{3}\left(8 + \frac{4}{\pi}\right). \tag{44}$$

These are exact. By contrast, the convergence acceleration method outlined in Sec. 2 has only converged to about nine decimals for $n = 200$.

5.2. Generalizations to fractional–power remainder terms

In Sec. 5.2, we had considered the generalization of the enhanced Neville algorithm to series whose remainder terms comprise half-integer powers. Here, shall generalize the algorithm further, to cases where the remainder terms can be expressed as powers of $n^{-1/s}$. We shall provide an example for the case $s = 3$. The *ansatz* is

$$f(x_i) = \sum_{j=0}^{\infty} c_j^{(1/s)} x_{ij}^{(1/s)} \approx \sum_{j=0}^{n} c_j^{(1/s)} x_{ij}^{(1/s)} = c_0^{(1/s)} + \frac{c_1^{(1/s)}}{(i+1)^{1/s}} + \frac{c_2^{(1/s)}}{(i+1)^{2/s}} + \ldots + \frac{c_n^{(1/s)}}{(i+1)^{n/s}}\,, \tag{45}$$

where the $x_{ij}^{(1/s)}$ are given as follows,

$$x_{ij}^{(1/s)} = \frac{1}{(i+1)^{j/2}}\,. \tag{46}$$

The generalized *ansatz* for the remainder term is

$$r_n^{(1/s)} = \frac{c_1^{(1/s)}}{(n+1)^{1/s}} + \frac{c_2^{(1/s)}}{(n+1)^{2/s}} + \frac{c_3^{(1/s)}}{(n+1)^{3/s}} + \ldots\,. \tag{47}$$

Based on $n+1$ partial sums s_i of the input series $\{s_i\}_{n=0}^{\infty}$, we aim to solve the system of $(n+1)$ equations

$$s_i = \sum_{j=0}^{n} c_j^{(1/s)}(n)\, x_{ij}^{(1/s)} \qquad i, j \in (0, \ldots, n)\,, \tag{48}$$

for the coefficients $c_j^{(1/s)}(n)$ with $j \in (0, \ldots, n)$. In full analogy to Eqs. (9) and (B.6), one then assumes that the value of the infinite series is recovered as n is increased,

$$s = s_\infty = \lim_{n\to\infty} c_0^{(1/s)}(n)\,. \tag{49}$$

Using the fractional-power Neville scheme with $s = 3$, we investigate the acceleration of the convergence of the following series,

$$s_n = \sum_{k=0}^{n} a_k\,, \qquad a_k = \frac{4}{\pi\,(k^{1/3}+1)^6} \arctan\left(\frac{k^{1/3}+2}{k^{1/3}+3}\right), \tag{50}$$

where the prefactor is adjusted so that $a_k \approx 1/k^2$ for $k \to \infty$. The transforms $c_0^{(1/3)}(n \le 402)$ converge to the result

$$s_\infty = \lim_{n\to\infty} c_0^{(1/3)}(n) = 0.79903\,08857\,54877\,20184\,41296\,61307\,30047\,47629\,74541\,71193\,85133\,42481\,37440\,38454\,19813\,14657\,35529\,94968\,85946\,86410\,, \tag{51}$$

which has 100 decimals. The transforms are calculated by solving the linear system given in Eq. (48) by standard matrix inversion techniques [34]. Furthermore, the following results are obtained,

$$c_1^{(1/3)} = c_2^{(1/3)} = 0\,, \qquad c_3^{(1/3)} = -1\,. \tag{52}$$

These are exact. By contrast, the convergence acceleration method outlined in Sec. 2 has only converged to about ten decimals for $n = 400$.

6. Conclusions

For slowly convergent series which possess an asymptotic expansion compatible with Eq. (2), the enhanced Neville algorithm described here harvests the asymptotic structure to eliminate the maximum number of asymptotic terms in the expansion in inverse powers of n, in any given order to the transformation. We take advantage of the asymptotic structure of the terms to be summed, according to Eq. (2). The general structure of the transformation has been described in Sec. 2.1 and compared to the recursive Neville algorithm in Sec. 2.2. Our matrix-based formulation of the problem in Sec. 2.1 enables us to not only derive formulas for the limit of the series, but also for subleading terms, according to Eq. (17).

In Sec. 3, we have compared the performance of the enhanced Neville algorithm to that of Wynn's ϵ algorithm [12], which calculates Padé approximants, and Aitken's Δ^2 process [10], including the iterated Aitken process. We find that our method provides numerically superior results, and harvests the asymptotic structure of the input series, according to Eq. (2). Furthermore, in comparison to the combined nonlinear-condensation transformation, described in Refs [2,23], the enhanced Neville transformation eliminates the need to "sample" the input series at very high orders, which is otherwise necessitated by the van Wijngaarden transformation [22], which is the first step of the combined nonlinear-condensation transformation.

The versatility of the algorithm is demonstrated by considering generalizations to remainder terms involving inverse half-integer powers (Sec. 5.1), general inverse fractional powers (Sec. 5.2), as well as remainder terms constituting inverse factorial series (Appendix B.1), as well as remainder terms containing only even and quartic powers (see Appendix B.2).

For the Bethe logarithm, discussed in Sec. 4.2, we find that the subleading terms of the partial sums b_n of the series given in Eq. (33) can be expressed in terms of rational coefficients,

$$b_n = \ln k_0(1S) - 10\,\ln(2) + 2\,\zeta(2) + 1 - \frac{4}{3(n+1)^3} - \frac{27}{4(n+1)^4} + \mathcal{O}\left(\frac{1}{n^5}\right), \tag{53}$$

for large n. For the definition of b_n, see Eq. (33). The coefficients of the subleading terms ($-4/3$ and $-27/4$) have been determined based on our enhanced Neville algorithm.

Coefficients for the derivation of higher-order subleading asymptotics are given in Appendix A. Furthermore, Bethe logarithms for the $2S$ and $2P$ states are discussed in Appendix C, and numerical results are given to 100 decimal digits. With the enhanced Neville algorithm presented here, the accuracy of the calculation of the Bethe logarithms can easily be enhanced beyond the 100 decimals indicated in Appendix C, facilitating a possible search for analytic representations using the PSLQ algorithm [30–33].

CRediT authorship contribution statement

Ulrich D. Jentschura: Writing – review & editing, Writing – original draft, Software, Conceptualization. **Ludovico T. Giorgini:** Writing – review & editing, Writing – original draft, Software, Conceptualization.

Declaration of competing interest

The authors declare no conflict of interest.

Data availability

No data was used for the research described in the article.

Acknowledgements

This article is inspired by numerous insightful discussions with Ernst Joachim Weniger on related problems, dating back to the years 1999–2012. The authors also acknowledge helpful conversations with Jean Zinn–Justin. UDJ was supported by the National Science Foundation (grant NSF PHY–2110294). LTG gratefully acknowledges support from the Swedish Research Council (Vetenskapsradet) Grant No. 638-2013-9243.

Appendix A. Coefficients for higher–order terms

We report in this Appendix the expressions for the polynomials $\mathcal{P}_k(i,n)$ with $5 \le k \le 10$. For $k = 5$, the result is

$$\begin{aligned} 11520\mathcal{P}_5(i,n) = {} & 11520i + 46080i^2 + 69120i^3 + 46080i^4 + 11520i^5 - 11520n - 52704in - 88320i^2n \\ & - 64320i^3n - 17280i^4n + 6768n^2 + 11560in^2 - 2400i^2n^2 - 12960i^3n^2 - 5760i^4n^2 \\ & + 7652n^3 + 21000in^3 + 20400i^2n^3 + 6720i^3n^3 - 680n^4 + 430in^4 + 2640i^2n^4 + 1440i^3n^4 \\ & - 2085n^5 - 2976in^5 - 1200i^2n^5 - 395n^6 - 500in^6 - 240i^2n^6 + 198n^7 + 120in^7 \\ & + 70n^8 + 30in^8 - 5n^9 - 3n^{10}. \end{aligned} \tag{A.1}$$

For $k = 6$, we have the result

$$\begin{aligned} 2903040\mathcal{P}_6(i,n) = {} & 2903040i + 14515200i^2 + 29030400i^3 + 29030400i^4 + 14515200i^5 + 2903040i^6 \\ & - 2914560n - 16184448in - 35538048i^2n - 38465280i^3n - 20563200i^4n - 4354560i^5n \\ & + 1667232n^2 + 4618656in^2 + 2308320i^2n^2 - 3870720i^3n^2 - 4717440i^4n^2 - 1451520i^5n^2 \\ & + 1942136n^3 + 7220304in^3 + 10432800i^2n^3 + 6834240i^3n^3 + 1693440i^4n^3 - 97020n^4 \\ & - 63000in^4 + 773640i^2n^4 + 1028160i^3n^4 + 362880i^4n^4 - 523446n^5 - 1275372in^5 \\ & - 1052352i^2n^5 - 302400i^3n^5 - 146727n^6 - 225540in^6 - 186480i^2n^6 - 60480i^3n^6 \\ & + 44070n^7 + 80136in^7 + 30240i^2n^7 + 30177n^8 + 25200in^8 + 7560i^2n^8 + 406n^9 \\ & - 1260in^9 - 2205n^{10} - 756in^{10} - 126n^{11} + 63n^{12}. \end{aligned} \tag{A.2}$$

For $k = 7$, the result is

$$\begin{aligned} 5806080\mathcal{P}_7(i,n) = {} & 5806080i + 34836480i^2 + 87091200i^3 + 116121600i^4 + 87091200i^5 + 34836480i^6 \\ & + 5806080i^7 - 5806080n - 38198016in - 103444992i^2n - 148006656i^3n - 118056960i^4n \\ & - 49835520i^5n - 8709120i^6n + 3303936n^2 + 12571776in^2 + 13853952i^2n^2 - 3124800i^3n^2 \\ & - 17176320i^4n^2 - 12337920i^5n^2 - 2903040i^6n^2 + 3783456n^3 + 18324880in^3 \\ & + 35306208i^2n^3 + 34534080i^3n^3 + 17055360i^4n^3 + 3386880i^5n^3 - 147000n^4 \end{aligned}$$

$$\begin{aligned}
&-320040in^4+1421280i^2n^4+3603600i^3n^4+2782080i^4n^4+725760i^5n^4-920780n^5\\
&-3597636in^5-4655448i^2n^5-2709504i^3n^5-604800i^4n^5-313950n^6-744534in^6\\
&-824040i^2n^6-493920i^3n^6-120960i^4n^6+27573n^7+248412in^7+220752i^2n^7\\
&+60480i^3n^7+65187n^8+110754in^8+65520i^2n^8+15120i^3n^8+14457n^9-1708in^9\\
&-2520i^2n^9-5397n^{10}-5922in^{10}-1512i^2n^{10}-1729n^{11}-252in^{11}+273n^{12}+126in^{12}+63n^{13}-9n^{14}.
\end{aligned}\tag{A.3}$$

With $C_8=1393459200$, we have the following formula for $k=8$,

$$\begin{aligned}
C_8\,\mathcal{P}_8(i,n)={}&1393459200i+9754214400i^2+29262643200i^3+48771072000i^4+48771072000i^5+29262643200i^6\\
&+9754214400i^7+1393459200i^8-1387653120n-10560983040in-33994321920i^2n\\
&-60348395520i^3n-63855267840i^4n-40294195200i^5n-14050713600i^6n-2090188800i^7n\\
&+807277824n^2+3810170880in^2+6342174720i^2n^2+2574996480i^3n^2-4872268800i^4n^2\\
&-7083417600i^5n^2-3657830400i^6n^2-696729600i^7n^2+891826560n^3+5306000640in^3\\
&+12871461120i^2n^3+16761669120i^3n^3+12381465600i^4n^3+4906137600i^5n^3+812851200i^6n^3\\
&-67571600n^4-112089600in^4+264297600i^2n^4+1205971200i^3n^4+1532563200i^4n^4\\
&+841881600i^5n^4+174182400i^6n^4-204569280n^5-1084419840in^5-1980740160i^2n^5\\
&-1767588480i^3n^5-795432960i^4n^5-145152000i^5n^5\,49594888n^6-254036160in^6-376457760i^2n^6\\
&-316310400i^3n^6-147571200i^4n^6-29030400i^5n^6-1304520n^7+66236400in^7+112599360i^2n^7\\
&+67495680i^3n^7+14515200i^4n^7+6310455n^8+42225840in^8+42305760i^2n^8+19353600i^3n^8\\
&+3628800i^4n^8+5741280n^9+3059760in^9-1014720i^2n^9-604800i^3n^9+383204n^{10}\\
&-2716560in^{10}-1784160i^2n^{10}-362880i^3n^{10}-825840n^{11}-475440in^{11}-60480i^2n^{11}-76790n^{12}\\
&+95760in^{12}+30240i^2n^{12}+57120n^{13}+15120in^{13}+1260n^{14}-2160in^{14}-1800n^{15}+135n^{16}.
\end{aligned}\tag{A.4}$$

With $C_9=2786918400$ and $\mathcal{P}_9\equiv\mathcal{P}_9(i,n)$, the result can be written, for $k=9$, as the sum of two terms,

$$C_9\,\mathcal{P}_9=\mathcal{T}_1+\mathcal{T}_2\,,\tag{A.5}$$

$$\begin{aligned}
\mathcal{T}_1={}&2786918400i+22295347200i^2+78033715200i^3+156067430400i^4+195084288000i^5\\
&+156067430400i^6+78033715200i^7+22295347200i^8+2786918400i^9-2786918400n\\
&-23897272320in-89110609920i^2n-188685434880i^3n-248407326720i^4n-208298926080i^5n\\
&-108689817600i^6n-32281804800i^7n-4180377600i^8n+1642567680n^2+9234897408in^2\\
&+20304691200i^2n^2+17834342400i^3n^2-4594544640i^4n^2-23911372800i^5n^2-21482496000i^6n^2\\
&-8709120000i^7n^2-1393459200i^8n^2+1839755520n^3+12395654400in^3+36354923520i^2n^3\\
&+59266260480i^3n^3+58286269440i^4n^3+34575206400i^5n^3+11437977600i^6n^3+1625702400i^7n^3\\
&-193851264n^4-359322400in^4+304416000i^2n^4+2940537600i^3n^4+5477068800i^4n^4\\
&+4748889600i^5n^4+2032128000i^6n^4+348364800i^7n^4-486633040n^5-2577978240in^5\\
&-6130320000i^2n^5-7496657280i^3n^5-5126042880i^4n^5-1881169920i^5n^5-290304000i^6n^5\,.
\end{aligned}\tag{A.6}$$

The second term $\mathcal{T}_2$ is given as follows,

$$\begin{aligned}
\mathcal{T}_2={}&-53606320n^6-607262096in^6-1260987840i^2n^6-1385536320i^3n^6-927763200i^4n^6\\
&-353203200i^5n^6-58060800i^6n^6+40638488n^7+129863760in^7+357671520i^2n^7\\
&+360190080i^3n^7+164021760i^4n^7+29030400i^5n^7-6368192n^8+97072590in^8\\
&+169063200i^2n^8+123318720i^3n^8+45964800i^4n^8+7257600i^5n^8-252565n^9+17602080in^9\\
&+4090080i^2n^9-3239040i^3n^9-1209600i^4n^9+5530785n^{10}-4666712in^{10}-9001440i^2n^{10}\\
&-4294080i^3n^{10}-725760i^4n^{10}-77996n^{11}-2602560in^{11}-1071840i^2n^{11}-120960i^3n^{11}\\
&-873524n^{12}+37940in^{12}+252000i^2n^{12}+60480i^3n^{12}+34690n^{13}+144480in^{13}+30240i^2n^{13}\\
&+61670n^{14}-1800in^{14}-4320i^2n^{14}-6212n^{15}-3600in^{15}-1620n^{16}+270in^{16}+315n^{17}-15n^{18}.
\end{aligned}\tag{A.7}$$

Finally, with $C_{10}=367873228800$ and $\mathcal{P}_{10}\equiv\mathcal{P}_{10}(i,n)$, we have the following result for $k=10$,

$$
\begin{aligned}
C_{10}\,\mathcal{P}_{10} = {} & 367873228800i + 3310859059200i^2 + 13243436236800i^3 + 30901351219200i^4 + 46352026828800i^5 \\
& + 46352026828800i^6 + 30901351219200i^7 + 13243436236800i^8 + 3310859059200i^9 + 367873228800i^{10} \\
& - 370660147200n - 3522313175040in - 14917040455680i^2n - 36669077913600i^3n \\
& - 57696244531200i^4n - 60285225369600i^5n - 41842514165760i^6n - 18608254156800i^7n \\
& - 4813008076800i^8n - 551809843200i^9n + 211314216960n^2 + 1435825391616in^2 + 3899225696256i^2n^2 \\
& + 5034352435200i^3n^2 + 1747653304320i^4n^2 - 3762781102080i^5n^2 - 5991990681600i^6n^2 \\
& - 3985293312000i^7n^2 - 1333540454400i^8n^2 - 183936614400i^9n^2 + 252909144576n^3 \\
& + 1879074109440in^3 + 6435076285440i^2n^3 + 12621996288000i^3n^3 + 15516933949440i^4n^3 \\
& + 12257714810880i^5n^3 + 6073740288000i^6n^3 + 1724405760000i^7n^3 + 214592716800i^8n^3 \\
& - 12322523136n^4 - 73018923648in^4 - 7247644800i^2n^4 + 428333875200i^3n^4 + 1111124044800i^4n^4 \\
& + 1349826508800i^5n^4 + 895094323200i^6n^4 + 314225049600i^7n^4 + 45984153600i^8n^4 - 77131325216n^5 \\
& - 404528688960in^5 - 1149495367680i^2n^5 - 1798761000960i^3n^5 - 1666196421120i^4n^5 - 924952089600i^5n^5 \\
& - 286634557440i^6n^5 - 38320128000i^7n^5 - 18618732528n^6 - 87234630912in^6 - 246608991552i^2n^6 \\
& - 349341189120i^3n^6 - 305355536640i^4n^6 - 169087564800i^5n^6 - 54286848000i^6n^6 - 7664025600i^7n^6 \\
& + 13184713168n^7 + 22506296736in^7 + 64354656960i^2n^7 + 94757731200i^3n^7 + 69195962880i^4n^7 \\
& + 25482885120i^5n^7 + 3832012800i^6n^7 + 3778269000n^8 + 11972980536in^8 + 35129924280i^2n^8 \\
& + 38594413440i^3n^8 + 22345424640i^4n^8 + 7025356800i^5n^8 + 958003200i^6n^8 - 2732570786n^9 \\
& + 2290135980in^9 + 2863365120i^2n^9 + 112337280i^3n^9 - 587220480i^4n^9 - 159667200i^5n^9 \\
& - 185879199n^{10} + 114057636in^{10} - 1804196064i^2n^{10} - 1755008640i^3n^{10} - 662618880i^4n^{10} \\
& - 95800320i^5n^{10} + 555823886n^{11} - 353833392in^{11} - 485020800i^2n^{11} - 157449600i^3n^{11} \\
& - 15966720i^4n^{11} - 37142193n^{12} - 110297088in^{12} + 38272080i^2n^{12} + 41247360i^3n^{12} + 7983360i^4n^{12} \\
& - 65980420n^{13} + 23650440in^{13} + 23063040i^2n^{13} + 3991680i^3n^{13} + 9237162n^{14} + 7902840in^{14} \\
& - 807840i^2n^{14} - 570240i^3n^{14} + 3778940n^{15} - 1295184in^{15} - 475200i^2n^{15} - 860970n^{16} - 178200in^{16} \\
& + 35640i^2n^{16} - 48378n^{17} + 41580in^{17} + 29205n^{18} - 1980in^{18} - 2970n^{19} + 99n^{20}.
\end{aligned} \tag{A.8}
$$

Appendix B. Further generalizations

B.1. Generalizations to inverse factorial series

Another obvious generalization of our algorithm would concern the replacement of the abscissas by the terms of an inverse factorial series as opposed to a power series,

$$
f(x_i) = \sum_{j=0}^{\infty} c'_j\, x'_{ij} \approx \sum_{j=0}^{n} c'_j\, x'_{ij} = c'_0 + \frac{c'_1}{(i+1)} + \frac{c'_2}{(i+1)(i+2)} + \ldots + \frac{c'_n}{(i+1)(i+2)\ldots(i+n)}\,, \tag{B.1}
$$

where the x'_{ij} are given as follows,

$$
x'_{ij} = \lim_{\epsilon\to 0} \frac{i+\epsilon}{(i+\epsilon)_{j+1}} = \begin{cases} \dfrac{1}{\Gamma(j+1)} & (i=0) \\[2ex] \dfrac{i}{(i)_{j+1}} = \dfrac{1}{(i+1)(i+2)\ldots(i+j)} & (i \neq 0) \end{cases}\,. \tag{B.2}
$$

We have used the Pochhammer symbol

$$
(i)_{j+1} = \frac{\Gamma(i+j+1)}{\Gamma(i)} = i(i+1)\ldots(i+j)\,. \tag{B.3}
$$

We thus replace the power-like remainder term estimate (10) by a remainder estimate based on an inverse factorial series,

$$
r'_n = \frac{c'_1}{n+1} + \frac{c'_2}{(n+1)(n+2)} + \frac{c'_3}{(n+1)(n+2)(n+3)} + \ldots\,. \tag{B.4}
$$

This, in turn, corresponds to Eq. (8.1-6) of Ref. [7]. Given $n+1$ partial sums s_i of the input series $\{s_i\}_{n=0}^{\infty}$, the generalized algorithm aims to solve the system of equations

$$
s_i = \sum_{j=0}^{n} c'_j(n)\, x'_{ij} \qquad i, j \in (0, \ldots, n)\,. \tag{B.5}
$$

In full analogy to Eq. (9), one then assumes that the value of the infinite series is recovered as n is increased,

$$s = s_\infty = \lim_{n\to\infty} c_0'(n)\,. \tag{B.6}$$

We have performed numerical experiments with the modified Neville scheme based on inverse factorial series, notably, to the series investigated in Secs. 4.1 and (4.2). This is based on the observation that, if the remainder term can be expanded in a series with inverse integer powers of j, it can also be expanded into an inverse factorial series. In general, the performance of the modified algorithm based on inverse factorial series has been observed to be inferior to the inverse-integer-power approach outlined in Sec. 2. For example, for the input series discussed in Sec. 4.1, one obtains just 7-decimal convergence for the inverse-factorial generalized transformation outlined here, for $n = 50$, while the transformation outlined in Sec. 2 leads to 27-decimal convergence in the same order of the transformation. However, one should keep in mind that nonlinear sequence transformations based on remainder estimates with inverse factorials have shown very favorable numerical results for the resummation of divergent series [7,17–21]. The relative performance of the generalized enhanced Neville scheme based on inverse factorial series as compared to inverse power series is expected to significantly depend on the problem under study, and the method outlined in Eq. (B.1)—(B.6) could very well become useful in other contexts.

B.2. Generalizations to quadratic and quartic remainder terms

In this section we present a further generalization of the enhanced Neville algorithm adapted to series involving second and fourth powers:

$$f(x_i) = \sum_{j=0}^{\infty} c_j^{(\alpha)}\, x_{ij}^{(\alpha)} \approx \sum_{j=0}^{n} c_j^{(\alpha)}\, x_{ij}^{(\alpha)} = c_0^{(\alpha)} + \frac{c_1^{(\alpha)}}{(i+1)^{\alpha}} + \frac{c_2^{(\alpha)}}{(i+1)^{2\alpha}} + \ldots + \frac{c_n^{(\alpha)}}{(i+1)^{n\alpha}}, \quad \alpha = 2,4 \tag{B.7}$$

where the terms x_{ij}^{α} are defined as,

$$x_{ij}^{(\alpha)} = \frac{1}{(i+1)^{j\alpha}}. \tag{B.8}$$

Our modified remainder term is thus based on second and fourth powers,

$$r_n^{(\alpha)} = \frac{c_1^{(\alpha)}}{(i+1)^{\alpha}} + \frac{c_2^{(\alpha)}}{(i+1)^{2\alpha}} + \frac{c_3^{(\alpha)}}{(i+1)^{3\alpha}} + \ldots\,, \qquad \alpha = 2,4. \tag{B.9}$$

In these two cases, one may still derive an analytic expression for the coefficient $c_0^{(\alpha)}(n)$, which approaches the value of the infinite series as n approaches infinity:

$$s = s_\infty = \lim_{n\to\infty} c_0^{(\alpha)}(n)\,. \tag{B.10}$$

The coefficients can be explicitly calculated as follows:

$$\begin{aligned} c_0^{(2)}(n) &= \sum_{i=0}^{n} \frac{(-1)^{n-i}2(i+1)^{2n+2}}{\Gamma(i+n+3)\Gamma(n-i+1)}\, s_i, \\ c_0^{(4)}(n) &= \sum_{i=0}^{n} \frac{\pi\,\mathrm{csch}((i+1)\pi)\,(-1)^{n-i}\,4\,(i+1)^{1+4(n+1)}}{\Gamma(n-i+1)\,\Gamma(i+n+3)\,\Gamma(-(i+1)\mathrm{j}+n+2)\,\Gamma((i+1)\mathrm{j}+n+2)}\, s_i\,, \end{aligned} \tag{B.11}$$

where j is the imaginary unit. (The notation j is used in order to clearly distinguish the imaginary unit from the summation index i.) We have performed numerical experiments for the input series discussed in this article, and for other input series, found that the algorithms with $\alpha = 2$ and $\alpha = 4$ typically perform well only in rare cases, in which the remainder term involves only even integer powers of $1/(n+1)$. Such cases are rare. For example, in the conceptually simple case of

$$s_n = \sum_{k=0}^{n} \frac{1}{k^3}\,, \qquad s_\infty = \zeta(3)\,, \qquad r_n = -\sum_{k=n+1}^{\infty} \frac{1}{k^3} = \psi^{(2)}(n+1) = -\frac{1}{2n^2} + \frac{1}{2n^3} - \frac{1}{4n^4} + \ldots\,, \tag{B.12}$$

the remainder term still possesses an expansion, for large n, containing odd powers of n, even if the input series contains only odd powers of k. Its remainder term, under the assumption that summation could be replaced by integration, would be assumed to contain only even powers of n, but this is not the case. Here, $\psi^{(m)}(z) = (\mathrm{d}^{m+1}/\mathrm{d}z^{m+1}) \ln\Gamma(z)$ is the $(m+1)$th logarithmic derivative of the Gamma function. The presence of odd powers in the remainder term persists if the remainder term is written as a function of $n+1$ as opposed to n. Still, for completeness, we believe it is useful to indicate the generalization of the algorithm to series whose remainder terms contain only even inverse powers of $n+1$.

Appendix C. Bethe logarithms for excited states

We supplement the results presented in Sec. 4 with a somewhat more detailed discussion. The Lerch Φ transcendent [35] is defined as

$$\Phi(z,s,a) = \sum_{n=0}^{\infty} \frac{z^n}{(n+a)^s}\,. \tag{C.1}$$

A formula valid in a larger domain of the complex plane is

$$\Phi(z,s,a) = \frac{1}{1-z} \sum_{n=0}^{\infty} \left(\frac{-z}{1-z}\right)^n \sum_{k=0}^{n} \frac{(-1)^k}{(a+k)^s} \binom{n}{k}. \tag{C.2}$$

The Lerch transcendent can be thought of as a generalization of the zeta function, because $\Phi(1,s,1)=\zeta(s)$. The Lerch transcendent, for the case $s=1$, can be written as a hypergeometric function, $\Phi(z,1,a)={}_2F_1(1,a,1+a,z)/a$. According to Chap. 4 of Ref. [3], hydrogenic Bethe logarithms of $1S$, $2S$ and $2P$ states can be written as rather compact sums over Lerch Φ functions, and evaluated to essentially arbitrary accuracy using the convergence acceleration algorithms outlined here. We have for the ground state,

$$\begin{aligned}\ln k_0(1S) &= 10\,\ln(2) - 2\zeta(2) - 1 + \sum_{k=2}^{\infty} \frac{16\,k}{(k-1)^2\,(k+1)^2}\,\Phi\left(\frac{1+k}{1-k},1,2\,k\right)\\ &= 2.98412\,85557\,65497\,61075\,97770\,90013\,79796\,99751\,80566\,17002\\ &\quad 00048\,15926\,13924\,06576\,62306\,75532\,86860\,62013\,30404\,72249\,.\end{aligned}\tag{C.3}$$

This result adds 50 figures to the result communicated in Eq. (35). The logarithmic sum, for the $2S$ state, is given by

$$\begin{aligned}\ln k_0(2S) &= -\frac{545}{36} + \frac{16}{3}\,\ln(2) - 14\,\zeta(2) + 24\,\zeta(3) + \sum_{k=3}^{\infty} \frac{1024\,k\,(k-1)\,(k+1)}{(k-2)^3\,(k+1)^3}\,\Phi\left(\frac{2+k}{2-k},1,2\,k\right)\\ &= 2.81176\,98931\,20563\,51521\,97427\,85941\,63611\,28935\,51470\,29732\\ &\quad 41909\,18696\,96453\,24020\,20118\,89106\,87017\,48612\,02831\,24031\,,\end{aligned}\tag{C.4}$$

whereas for the $2P$ state, it reads

$$\begin{aligned}\ln k_0(2P) &= -\frac{3437}{2916} + \frac{3280}{2187}\,\ln(2) - \frac{14}{3}\,\zeta(2) + \frac{136}{9}\,\zeta(3) - \frac{64}{3}\,\zeta(4)\\ &\quad + \sum_{k=3}^{\infty} \frac{256\,k^3\,(11\,k^2-12)}{3\,(k-2)^4\,(k+2)^4}\,\Phi\left(\frac{2+k}{2-k},1,2\,k\right)\\ &= -\,0.03001\,67086\,30212\,90244\,36757\,10951\,14406\,39409\,33044\,23103\\ &\quad 04668\,98525\,32719\,44796\,89622\,57183\,26244\,10312\,70799\,73828\,.\end{aligned}\tag{C.5}$$

While these formulas do not provide direct, analytic results for Bethe logarithms, they still illustrate that one can think of the Bethe logarithm as a sum of logarithms, zeta functions, and generalized zeta functions.

Appendix D. Supplementary material

Supplementary material related to this article can be found online at https://doi.org/10.1016/j.cpc.2024.109280.

References

[1] U.D. Jentschura, P.J. Mohr, G. Soff, Calculation of the electron self-energy for low nuclear charge, Phys. Rev. Lett. 82 (1999) 53–56.
[2] U.D. Jentschura, P.J. Mohr, G. Soff, E.J. Weniger, Convergence acceleration via combined nonlinear-condensation transformations, Comput. Phys. Commun. 116 (1999) 28–54.
[3] U.D. Jentschura, G.S. Adkins, Quantum Electrodynamics: Atoms, Lasers and Gravity, World Scientific, Singapore, 2022.
[4] L.T. Giorgini, U.D. Jentschura, E.M. Malatesta, G. Parisi, T. Rizzo, J. Zinn-Justin, Two–loop corrections to the large–order behavior of correlation functions in the one–dimensional N–vector model, Phys. Rev. D 101 (2020) 125001.
[5] L.T. Giorgini, U.D. Jentschura, E.M. Malatesta, G. Parisi, T. Rizzo, J. Zinn-Justin, Correlation functions of the anharmonic oscillator: numerical verification of two–loop corrections to the large–order behavior, Phys. Rev. D 105 (2022) 105012.
[6] Ludovico T. Giorgini, Jentschura, D. Ulrich, Enrico M. Malatesta, Tommaso Rizzo, Jean Zinn-Justin, Instantons in ϕ^4 Theories: Transseries, Virial Theorems and Numerical Aspects, arXiv preprint, arXiv:2405.18191, 2024.
[7] E.J. Weniger, Nonlinear sequence transformations for the acceleration of convergence and the summation of divergent series, Comput. Phys. Rep. 10 (1989) 189–371.
[8] C. Brezinski, M. Redivo-Zaglia, Extrapolation Methods, North-Holland, Amsterdam, 1991.
[9] E. Caliceti, M. Meyer-Hermann, P. Ribeca, A. Surzhykov, U.D. Jentschura, From useful algorithms for slowly convergent series to physical predictions based on divergent perturbative expansions, Phys. Rep. 446 (2007) 1–96.
[10] A.C. Aitken, On Bernoulli's numerical solution of algebraic equations, Proc. R. Soc. Edinb. 46 (1926) 289–305.
[11] D. Shanks, Non-linear transformations of divergent and slowly convergent sequences, J. Math. Phys. 34 (1955) 1–42, Cambridge, Mass.
[12] P. Wynn, On a device for computing the $e_m(S_n)$ transformation, Math. Tables Aids Comput. 10 (1956) 91–96.
[13] U.D. Jentschura, Resummation of nonalternating divergent perturbative expansions, Phys. Rev. D 62 (2000) 076001.
[14] W. Heisenberg, H. Euler, Folgerungen aus der diracschen theorie des positrons, Z. Phys. 98 (1936) 714–732.
[15] J. Schwinger, On gauge invariance and vacuum polarization, Phys. Rev. 82 (1951) 664–679.
[16] W. Dittrich, M. Reuter, Effective Lagrangians in Quantum Electrodynamics, Lecture Notes in Physics, vol. 220, Springer, Berlin, Heidelberg, New York, 1985.
[17] A. Sidi, Convergence properties of some nonlinear sequence transformations, Math. Comput. 33 (1979) 315–326.
[18] A. Sidi, Analysis of the convergence of the T-transformation for power series, Math. Comput. 35 (1980) 833–850.
[19] A. Sidi, Borel summability and converging factors for some everywhere divergent series, SIAM J. Math. Anal. 17 (1986) 1222–1232.
[20] E.J. Weniger, Computation of the Whittaker function of the second kind by summing its divergent asymptotic series with the help of nonlinear sequence transformations, Comput. Phys. 10 (1996) 496–503.
[21] A. Sidi, Practical Extrapolation Methods, Cambridge University Press, Cambridge, 2003.
[22] C.W. Clenshaw, E.T. Goodwin, D.W. Martin, G.F. Miller, F.W.J. Olver, J.H. Wilkinson, (National Physical Laboratory), Modern Computing Methods, Notes on Applied Science, vol. 16, 2 ed., H. M. Stationary Office, London, 1961.
[23] S.V. Aksenov, M.A. Savageau, U.D. Jentschura, J. Becher, G. Soff, P.J. Mohr, Application of the combined nonlinear-condensation transformation to problems in statistical analysis and theoretical physics, Comput. Phys. Commun. 150 (2003) 1–20.
[24] C. Brezinski, A general extrapolation algorithm, Numer. Math. 35 (1980) 175–180.
[25] T. Havie, Generalized Neville type extrapolation schemes, BIT 19 (1979) 204–213.
[26] E.H. Neville, Iterative interpolation, J. Indian Math. Soc. 20 (1934) 87–120.
[27] D.S. Gaunt, A.J. Guttmann, in: C. Domb, M.S. Green (Eds.), Phase Transitions and Critical Phenomena 3, Academic Press, London, 1974, p. 181.
[28] A.H. van Tuyl, Acceleration of convergence of a family of logarithmically convergent series, Math. Comput. 63 (1994) 229–246.
[29] H.A. Bethe, The electromagnetic shift of energy levels, Phys. Rev. 72 (1947) 339–341.

[30] H.R.P. Ferguson, D.H. Bailey, A Polynomial Time, Numerically Stable Integer Relation Algorithm, RNR Techn. Rept. RNR-91-032 1992.
[31] D.H. Bailey, S. Plouffe, in: J. Borwein, P. Borwein, L. Jörgenson, R. Corless (Eds.), *Organic Mathematics: Proceedings of the Workshop Held in Burnaby, BC*, American Mathematical Society, Philadelphia, PA, 1997, pp. 73–88.
[32] H.R.P. Ferguson, D.H. Bailey, S. Arno, Analysis of PSLQ, an integer relation finding algorithm, Math. Comput. 68 (1999) 351–369.
[33] D.H. Bailey, D. Broadhurst, Integer relation detection, Math. Comput. 70 (2001) 1719–1736.
[34] W.H. Press, B.P. Flannery, S.A. Teukolsky, W.T. Vetterling, Numerical recipes in C: the art of scientific computing, 2 ed., Cambridge University Press, Cambridge, UK, 1993.
[35] M. Abramowitz, I.A. Stegun, Handbook of Mathematical Functions, 10 ed., National Bureau of Standards, Washington, D. C., 1972.