Convergence accelerator approach for the high-precision evaluation of three-electron correlated integrals

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The standard series expansion that has long been employed to evaluate one-center correlated three-electron integrals is converted into a different form. The alternative expression obtained allows convergence accelerator techniques to be directly applied in a very effective manner. The resulting expansion is found to be numerically stable, in contrast to the series obtained when convergence accelerator techniques are applied to the standard expansion. Using this approach, the increase in computational speed is found to be very significant for the most slowly converging integrals. Some representative values are presented for a number of three-electron correlated integrals calculated using the method suggested herein. [S1063-651X(98)01106-4]

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I. INTRODUCTION

The general one-center three-electron correlated integral takes the form

$$I(i,j,k,l,m,n,\alpha,\beta,\gamma) = \int r_1^i r_2^j r_3^k r_{23}^l r_{31}^m r_{12}^n e^{-\alpha r_1-\beta r_2-\gamma r_3} d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3, \quad (1)$$

where r_i denotes the electron-nuclear distance and r_{ij} designates the electron-electron separation. This integral and a related extension have been well studied in the literature [1–25]. It can be shown that for an energy determination of an S state of a three-electron atomic system, all of the required expectation values can be reduced to integrals of the form given in Eq. (1), when a standard Hylleraas expansion is employed for the wave function. These integrals also arise in the hybrid configuration-interaction Hylleraas approach for the S states of three-electron atoms. It has been shown that a particular group of correlated four-electron integrals can be reduced to a sum of the above I integrals [26]. Since these integrals occur widely in high-precision calculations using correlated basis functions, there is considerable interest in developing improved procedures for the rapid numerical evaluation of these integrals.

It can be shown that an energy determination only requires I integrals with $l \geqslant -1$, $m \geqslant -1$, and $n \geqslant -1$ and, more specifically, only one of the set l, m, $n = -1$, and the other two values are $\geqslant 0$. The analysis presented below will also include cases like $l = -1$, $m = -1$, and $n = -1$. These latter integrals arise in certain applications, such as particular relativistic corrections and lower bound calculations of energy levels. I integrals having arguments with l, m, or $n = -2$ arise in some important applications. These cases have been less extensively investigated [18,19,22,23], in part because of the considerable additional complexities arising from the expansion of r_{ij}^{-2}. They are not considered further in this work.

For the I integral it is straightforward to show that when l, m, and n are not all odd, then the integral simplifies to a finite sum of terms that can be numerically evaluated very quickly. The focus of the present work is the case where l, m, and n are all odd, which gives rise to an infinite series. For an energy determination, the worst-case convergence leads to a series of the form

$$I = \sum_{s=1}^{\infty} \frac{a_s}{s^6}. \quad (2)$$

Using the same type of analysis given by Larsson [11], it is possible to show that the integral $I(0,0,0,-1,-1,-1,1,1,1)$ behaves like

$$I(0,0,0-1,-1,-1,1,1,1) = \sum_{s=1}^{\infty} \frac{a_s}{s^4}. \quad (3)$$

The asymptotic form for the series expansion of the integral $I(i,j,k,l,m,n,\alpha,\beta,\gamma)$ has been given by Drake and Yan [24]. The convergence of each of the preceding two series is dominated by the s^{-p} behavior, although the values of α, β, and γ in Eq. (1) can have an impact on the convergence. It is feasible to numerically evaluate the series in Eq. (2) by direct summation, but the time required to evaluate Eq. (3) directly makes this proposition inefficient.

II. THEORY

From the appearance of the form of the series given in Eq. (2), and particularly that given in Eq. (3), it should be clear that the optimal evaluation of the I integral is governed by how effectively the series expansion can be summed. If the coefficients a_s fall off quickly with increasing s, then direct summation techniques have a chance to be rather effective. However, in a general calculation this behavior is not realized. Direct summation of Eq. (2) is possible, but the CPU requirements are relatively high. For the case of Eq. (3), direct summation is not an efficient strategy if high-precision results are required. In practical calculations, it is essential that the individual integral evaluations be performed at reasonably high precision levels, in order to minimize precision loss that invariably occurs (particularly for very large basis sets) when final expectation values are calculated. There are definite advantages associated with being able to evaluate the

required atomic integrals at close to the limit of machine accuracy, and this is the goal of the present work.

Drake and Yan [24] have suggested an asymptotic approach to avoid the direct summation problem. This approach is closely linked to the well-known Richardson extrapolation technique. These authors also considered direct application of a convergence accelerator technique to the series in Eq. (3). It was found that significant precision loss occurred as they increased the key index in the convergence acceleration method employed. The precision level of their best result using the convergence accelerator approach was rather modest. The problem of precision loss detected by these authors for the convergence accelerator method they employed is not unexpected, and is a well-known difficulty associated with the application of such techniques.

In this paper we show how a convergence accelerator technique can be applied to the calculation of the I integrals, in the process obtaining a much more efficient evaluation process than the classical Öhrn-Nordling analysis. The key idea in our approach is as follows. The first step is to turn the required series into a series whose terms have alternating signs. Generally, this would be a highly undesirable maneuver because of the risk of introducing additional numerical round-off errors. However, the functional form of a number of the more effective convergence accelerator techniques has a mathematical structure that includes an alternating sign behavior. When these techniques are applied to an alternating series, the alternating signs cancel, leading to a much more stable summation method. For discussions of convergence accelerator techniques and applications, see the works by Levin [27], Fessler *et al.* [28], Weniger [29–31], Brezinski and Redivo Zaglia [32], and Smith and Ford [33].

Smith and Ford [33] (see also Ref. [31]) suggested a modification of Levin's t transformation, herein denoted by t', which would normally give superior results for alternating series. The t' transformation takes the form

$$t'_k=\frac{\Sigma_{j=0}^{k} q_j(k,A_{j+1})S_j}{\Sigma_{j=0}^{k} q_j(k,A_{j+1})}, \tag{4}$$

where

$$q_j(k,A_{j+1})=(-1)^j\binom{k}{j}(j+1)^{k-1}{A_{j+1}}^{-1}, \tag{5}$$

and a sequence of partial sums S_j are defined by

$$S_j=\sum_{w=0}^{j} A_w. \tag{6}$$

In Eq. (5), $\binom{k}{j}$ denotes a binomial coefficient.

Perhaps the most widely known technique to accelerate logarithmically convergent series [such as those given in Eqs. (2) and (3)] is the Levin u transformation [27], which was also extensively investigated in this work. The u transformation takes the form

$$u_k=\frac{\Sigma_{j=0}^{k} c_j(k,A_j)S_j}{\Sigma_{j=0}^{k} c_j(k,A_j)}, \tag{7}$$

where

$$c_j(k,A_j)=(-1)^j\binom{k}{j}(j+1)^{k-2}A_j^{-1}. \tag{8}$$

The Levin u transform exhibits the same alternating sign behavior as the t' transformation.

If the individual terms A_j have alternating signs, then clearly Eqs. (4) and (7) are likely to be much more stable for numerical evaluation. The problem with the application of Eq. (7) directly to Eq. (3) is the fact that the coefficients $c_j(k,A_j)$ alternate in sign when $A_j>0$ and grow to a very significant size as k increases, leading to a very substantial loss of precision for u_k for large values of k. For the I integrals of interest in this work, either $A_j>0$ for all j, or this condition on A_j holds true starting at some small value of j. This means that it is impossible to obtain a relative accuracy for the I integrals at precision levels close to machine accuracy via direct application of the u transformation. Application of the t' transformation directly to Eq. (3) is ineffective. This is an expected result as it is well known that this transformation is not capable of accelerating the convergence of series of the form given in Eq. (3) [33].

If the sum of interest

$$S_\infty=\sum_{w=0}^{\infty} A_W \quad \text{for } A_w\geqslant 0 \tag{9}$$

can be converted to a sum of the form

$$S_\infty=\sum_{w=0}^{\infty} (-1)^w B_W \quad \text{for } B_w\geqslant 0, \tag{10}$$

then the loss of precision observed by Drake and Yan can be effectively eliminated. The idea to employ the strategy explicit in Eqs. (9) and (10) seems well known to specialists in numerical applications of convergence accelerator techniques (see, for example, Fessler *et al.* [28]), but often receives no mention in applications papers.

The principal difficulty is whether the functional form of B_w can be determined, and if it can be numerically evaluated in a cost effective manner. We now show how this function can be determined for the I integral. For the case l, m, $n\geqslant -1$, the following result can be derived using the Sack [34] expansion for r_{ij}^p:

$$\begin{aligned} I\equiv& I(i,j,k,l,m,n,\alpha,\beta,\gamma)\\ =&\sum_{w=0}^{\infty}\sum_{w_1=0}^{\infty}\sum_{w_2=0}^{\infty}\int r_1^i r_2^j r_3^k e^{-\alpha r_1-\beta r_2-\gamma r_3} R_{lw}(r_2,r_3)\\ &\times R_{mw_1}(r_3,r_1)R_{nw_2}(r_1,r_2)\\ &\times P_w(\cos\,\theta_{23})P_{w_1}(\cos\,\theta_{31})P_{w_2}(\cos\,\theta_{12})d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3. \end{aligned} \tag{11}$$

where R_{mp} is a Sack radial function. If the functional form of each Sack radial function is substituted into Eq. (11) and integration over the radial and angular coordinates is carried out, then

$$I=\sum_{w=0}^{\infty} A(w), \tag{12}$$

where $A(w)$ is given by

$$A(w)=\frac{64\pi^3}{(2w+1)^2}\sum_{p=0}^{\infty}\sum_{q=0}^{\infty}\sum_{t=0}^{\infty}a_{wlp}a_{wmq}a_{wnt}\{W(i+2+2w+2q+2t,j+2+n+2p-2t,k+2+l+m-2w-2p-2q,\alpha,\beta,\gamma)+W(i+2+2w+2q+2t,k+2+m+2p-2q,j+2+l+n-2w-2p-2t,\alpha,\gamma,\beta)+W(j+2+2w+2p+2t,i+2+n+2q-2t,k+2+l+m-2w-2p-2q,\beta,\alpha,\gamma)+W(j+2+2w+2p+2t,k+2+l+2q-2p,i+2+m+n-2w-2q-2t,\beta,\gamma,\alpha)+W(k+2+2w+2p+2q,i+2+m+2t-2q,j+2+l+n-2w-2p-2t,\gamma,\alpha,\beta)+W(k+2+2w+2p+2q,j+2+l+2t-2p,i+2+m+n-2w-2q-2t,\gamma,\beta,\alpha)\}. \tag{13}$$

The a_{wnt} coefficient is given by

$$a_{wnt}=\frac{\left(\frac{-n}{2}\right)_w\left(w-\frac{n}{2}\right)_t\left(-\frac{1}{2}-\frac{n}{2}\right)_t}{\left(\frac{1}{2}\right)_w t!\left(w+\frac{3}{2}\right)_t}, \tag{14}$$

and $(z)_p$ denotes a Pochhammer symbol. The W function given in Eq. (13) is defined by

$$W(I,J,K,\alpha,\beta,\gamma)=\int_0^{\infty}x^I e^{-\alpha x}dx\int_x^{\infty}y^J e^{-\beta y}dy\int_y^{\infty}z^K e^{-\gamma z}dz. \tag{15}$$

This auxiliary function has been well studied in the literature [1,3,11,15,24,35]. The functional dependence of $A(w)$ on $\{i,j,k,l,m,n,\alpha,\beta,\gamma\}$ is suppressed to simplify the notation.

The principal result employed is

$$\sum_{s=n}^{\infty}A(s)=\sum_{s=1}^{\infty}(-1)^{s+1}\sum_{t=0}^{\infty}2^t A(2^t s+n-1). \tag{16}$$

A concise comment on the origin of this transformation is given in the Appendix. Using Eq. (16) allows the I integral to be expressed as

$$I(i,j,k,l,m,n,\alpha,\beta,\gamma)=-\sum_{v=1}^{\infty}(-1)^v B(v), \tag{17}$$

with

$$B(v)=\sum_{t=0}^{\infty}2^t A(2^t v-1), \tag{18}$$

and $A(2^t v-1)$ is determined from Eq. (13). Equation (17) is the key result of this work. Now the t' transformation is applied directly to Eq. (17). It should be clear from the functional form of the t' transformation that the application of this acceleration technique to Eq. (17) leads to a numerically stable result, provided that $A(2^t v-1)$ can be computed in a numerically stable way, which turns out to be the case for the integrals of interest.

If the first few terms of the series in Eq. (17) have $B(v)$ alternating in sign, then these terms can be separated, and the t' transformation applied to the remaining sum. Some examples were considered where the first few terms alternated in sign, and it was found that the t' transformation could be applied to the entire series without any numerical problems.

It is straightforward to show that for the I integral described in Eq. (1) (with l, m, $n\geqslant -1$), Eq. (18) behaves asymptotically like the power series

$$B(v)=\sum_{t=0}^{\infty}\frac{a_{tv}}{2^{t(l+m+n+9)/2}}, \tag{19}$$

which for the most slowly converging I integral, Eq. (3), leads to

$$B(v)=\sum_{t=0}^{\infty}a_{tv}8^{-t}. \tag{20}$$

$B(v)$ could be evaluated using convergence accelerator techniques. While such an approach would generate characteristic precision loss, the rounding errors would be less severe than those resulting from the application of similar transformations to Eq. (12). However, because the time savings resulting from this additional use of convergence accelerators would be relatively small, and to avoid the introduction of additional precision loss, this approach was not employed. Rather, $B(v)$ was evaluated by direct summation. It is clear from the form of Eq. (19) that this calculation may be performed very rapidly.

III. RESULTS

In Table I we show a comparison of the behavior obtained when the u transformation is applied to Eq. (12) and the t' transformation is applied to Eq. (17) for the case $I(0,0,0,-1,-1,-1,1,1,1)$. The calculations for both tables were carried out using FORTRAN quadruple precision (with a 32-bit word length), which corresponds to approximately 30 digits of precision. The final result reported in Table I using Eq. (17) is in agreement with the results for this integral obtained by other workers [16,24], but is converged to more digits than reported previously. Our calculation is also in agreement with a high-precision arithmetic evaluation of the analytic formula of Remiddi [17]. The advantage of our approach should be readily apparent from these results.

In Table II we report a few representative I integrals obtained using Eq. (17). The tabulated values agree with results obtained using an alternative evaluation employing the Öhrn-

TABLE I. Convergence of the u and t' transforms for the integral $I(0,0,0,-1,-1,-1,1,1,1)$.

Levin index (k)	u transform applied directly to Eq. (12)	t' transform applied to Eq. (17)
0	661.0	702.0
1	681.0	684.3
2	683.8	684.094
3	684.093	684.114 58
4	684.113 0	684.113 374
5	684.113 57	684.113 410 7
6	684.113 43	684.113 412 07
7	684.113 410 8	684.113 411 830
8	684.113 411 5	684.113 411 842 71
9	684.113 411 839	684.113 411 842 668
10	684.113 411 848	684.113 411 842 627 1
11	684.113 411 843 0	684.113 411 842 629 968
12	684.113 411 842 57	684.113 411 842 629 917 7
13	684.113 411 842 622	684.113 411 842 629 911 27
14	684.113 411 842 630 5	684.113 411 842 629 911 853
15	684.113 411 842 630 1	684.113 411 842 629 911 836 99
16	684.113 411 842 629 909	684.113 411 842 629 911 836 066
17	684.113 411 842 629 909 5	684.113 411 842 629 911 836 176 3
18	684.113 411 842 629 911 78	684.113 411 842 629 911 836 172 439
19	684.113 411 842 629 911 87	684.113 411 842 629 911 836 172 321 1
20	684.113 411 842 629 911 838	684.113 411 842 629 911 836 172 341 13
21	684.113 411 842 629 911 835 8	684.113 411 842 629 911 836 172 340 265
22	684.113 411 842 629 911 836 12	684.113 411 842 629 911 836 172 340 253 3
23	684.113 411 842 629 911 836 14	684.113 411 842 629 911 836 172 340 256 9
24	684.113 411 842 629 911 836 3	684.113 411 842 629 911 836 172 340 256 7
25	684.113 411 842 629 911 836 3	684.113 411 842 629 911 836 172 340 256 7
26	684.113 411 842 629 911 835 9	684.113 411 842 629 911 836 172 340 256 7
27	684.113 411 842 629 911 836 7	684.113 411 842 629 911 836 172 340 256 7
28	684.113 411 842 629 911 835	684.113 411 842 629 911 836 172 340 256 7
29	684.113 411 842 629 911 88	684.113 411 842 629 911 836 172 340 256 7
30	684.113 411 842 629 911 86	684.113 411 842 629 911 836 172 340 256 7
31	684.113 411 842 629 911 79	684.113 411 842 629 911 836 172 340 256 7
32	684.113 411 842 629 913	684.113 411 842 629 911 836 172 340 256 7
33	684.113 411 842 629 913	684.113 411 842 629 911 836 172 340 256 7
34	684.113 411 842 629 92	684.113 411 842 629 911 836 172 340 256 7
35	684.113 411 842 629 96	684.113 411 842 629 911 836 172 340 256 7
		684.113 411 842 629 911 836 172 340 256 708 222[a]

[a]Value calculated from the formulas of Remiddi [17].

Nordling scheme [3]. The optimal value of the t' transformation index k is also reported for each I integral in Table II. The optimal value of k stays in a narrow range, and not surprisingly, increases slightly when $l+m+n$ is smaller. The first entry in Table II can be written in a simple compact form as [17]

$$I(-1,-1,-1,-1,-1,-1,1,1,1) = 48\pi^3\left\{2\ln 2\ln 3-[\ln 2]^2-\frac{\pi^2}{6}-2\mathrm{Li}_2\left(-\frac{1}{2}\right)\right\}, \quad (21)$$

where $\mathrm{Li}_2(x)$ is the dilogarithm function. Equation (21) provides a useful check on the precision of the results calculated from Eq. (17).

In addition to the t' transformation described in Eqs. (4) and (5), both the Levin u transformation [Eqs. (7) and (8)] and the Wynn ε algorithm (see Ref. [32]) were applied to Eq. (17). All three transformations were able to produce results converged to machine precision using a relatively small number of partial sums. However, it was found that the t' transformation converged slightly faster (approximately 4–20% for the test cases explored) than the Levin u transformation, which in turn performed noticeably better than Wynn's ε algorithm.

IV. DISCUSSION

The success of the method described in Sec. II is clearly indicated by the results presented in Table I. The transforma-

TABLE II. I integrals calculated using Eq. (17).

i	j	k	l	m	n	α	β	γ	Levin index (k)	I integral
−1	−1	−1	−1	−1	−1	1.0	1.0	1.0	25	$4.382\,174\,441\,144\,904\,256\,316\,255\,864\,0\times10^{2}$
1	2	3	−1	−1	1	2.0	2.0	2.0	24	$3.708\,891\,282\,966\,454\,151\,598\,287\,024\,4\times10^{2}$
1	2	3	−1	1	1	2.7	2.9	0.6	20	$1.578\,902\,278\,992\,620\,564\,949\,557\,089\,8\times10^{5}$
1	1	1	1	1	1	2.7	2.9	0.6	19	$1.040\,856\,004\,718\,114\,742\,772\,502\,350\,0\times10^{5}$
1	2	3	1	3	5	2.7	2.9	0.6	16	$4.835\,593\,508\,551\,350\,528\,836\,141\,841\,9\times10^{11}$
1	1	1	−1	−1	3	2.7	2.9	0.6	23	$5.955\,187\,798\,127\,083\,390\,562\,091\,432\,6\times10^{2}$
1	−1	1	−1	−1	5	2.7	2.9	0.6	20	$4.153\,189\,410\,286\,313\,893\,597\,821\,275\,0\times10^{3}$
1	2	3	−1	3	5	2.7	2.9	0.6	18	$2.586\,142\,496\,244\,587\,259\,912\,015\,456\,2\times10^{9}$
2	3	4	3	3	3	2.7	2.9	0.6	16	$8.916\,498\,620\,151\,390\,527\,629\,386\,520\,9\times10^{14}$
1	2	3	−1	1	5	2.7	2.9	0.6	20	$2.040\,035\,974\,322\,132\,225\,687\,117\,746\,2\times10^{7}$
1	2	3	−1	3	3	2.7	2.9	0.6	19	$1.735\,574\,025\,561\,259\,042\,558\,668\,735\,7\times10^{8}$
1	2	3	1	1	3	2.7	2.9	0.6	18	$1.624\,109\,122\,716\,939\,602\,311\,210\,167\,1\times10^{8}$
1	2	3	1	3	1	2.7	2.9	0.6	18	$3.746\,128\,793\,511\,223\,583\,778\,107\,984\,5\times10^{9}$
2	1	3	−1	3	5	2.7	2.9	0.6	18	$3.148\,008\,255\,555\,465\,945\,427\,369\,006\,7\times10^{9}$
2	3	1	−1	3	5	2.7	2.9	0.6	19	$1.582\,909\,076\,240\,029\,045\,602\,994\,145\,6\times10^{8}$
3	2	1	−1	3	5	2.7	2.9	0.6	19	$2.017\,154\,027\,170\,239\,339\,249\,790\,957\,8\times10^{8}$
3	1	2	−1	3	5	2.7	2.9	0.6	18	$9.359\,166\,057\,879\,182\,911\,239\,528\,248\,0\times10^{8}$

tion given by Eq. (16) has the net effect of transforming a logarithmically converging sequence into an alternating series, with the terms of the transformed series being given by an infinite series that converges linearly. Because of the relatively rapid convergence of the infinite series for $B(v)$, this can be evaluated very efficiently by direct summation.

The Öhrn-Nordling approach amounts to the evaluation of the I integrals as a series of the form

$$\sum_{s=1}^{\infty} a_s s^{-(l+m+n+11)/2}.$$

As $l+m+n$ increases, the Öhrn-Nordling scheme converges more quickly, while the evaluation of Eq. (18) becomes more time-consuming. So an effective computational approach for the I integrals should allow for a combination of the Öhrn-Nordling method and the approach of this paper. Based on calculations of a number of different I integrals, the switchover point in CPU efficiency occurs when $l+m+n\approx7$, although the exact point depends on the values of i, j, k, α, β, γ as well as on the sum $l+m+n$. The smaller the value of $l+m+n$, the larger the CPU savings obtained using the convergence accelerator approach [Eq. (17)]. For the smallest values of $l+m+n$ employed for the entries in Tables I and II, the decrease in evaluation time was several orders of magnitude to produce the precision levels given in the tables. A practical calculation of the energy (particularly for the ground and lowest-lying states) will lead to many more integrals having values of $l+m+n$ of 1 or 3, relative to higher values. Consequently, there will be a very significant gain in computational speed for the entire energy calculation when the technique of the present work is employed.

In this work the focus has been on the most commonly occurring one-center three-electron correlated integrals. The next most important cases have $l=-2$, $m\geqslant-1$, and $n\geqslant-1$. These integrals arise in applications such as certain relativistic corrections, and in applications concerned with finding lower bounds to state energies (see Ref. [36] for a summary on these applications). The possibility of carrying out the series transformation of the type discussed in this work is under investigation for these much more complex integrals. The particular cases of interest are $l=-2$, and m and n both odd, which are extremely difficult to evaluate to high precision by other approaches.

A second application that is about to be investigated concerns the application of the series transformation approach discussed in this work to more complicated many-electron correlated integrals. A target integral for future investigation is the four-electron correlated integral, which involves up to six interelectronic coordinate factors. Although a number of the four-electron correlated integrals have been resolved [26,37,38], there are still a number of important unsolved cases. Convergence accelerator techniques of the type discussed in this work might be particularly well suited for resolving some of the more difficult four-electron correlated integrals.

Evaluation of the I integrals occurs at the innermost level of an atomic energy evaluation. Faster techniques to evaluate these integrals can lead to significant impact on the overall speed of the calculations. This is a particularly important issue in any Hylleraas-type calculation that does extensive optimization of the nonlinear parameters, because the number of I integrals being evaluated becomes enormous when large basis set expansions are employed. The use of global optimization techniques significantly magnifies the number of I integrals that must be evaluated. Future progress in utilizing correlated basis sets for many-electron systems is probably going to be dependent on the judicious application of convergence accelerator techniques.

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APPENDIX

In this appendix a few concise comments are made on the derivation of Eq. (16). By considering separately the two series

$$\sum_{s=1}^{\infty} A(js+m), \quad \sum_{s=1}^{\infty} (-1)^s A(js+m),$$

it is straightforward to show that

$$\sum_{s=1}^{\infty} A(js+m)=\sum_{s=1}^{\infty} (-1)^{s+1}A(js+m)+2\sum_{s=1}^{\infty} A(2js+m). \tag{A1}$$

If Eq. (A1) is used recursively, then it follows that

$$\sum_{s=1}^{\infty} A(js+m)=\sum_{s=1}^{\infty} (-1)^{s+1}\sum_{t=0}^{\infty} 2^t A(2^t js+m). \tag{A2}$$

On setting $m=0$, $j=1$, and $A(s)=s^{-k}$ in Eq. (A2), the well-known result for the Riemann ζ function

$$\zeta(k)=\sum_{s=1}^{\infty} \frac{1}{s^k}=-(1-2^{1-k})^{-1}\sum_{s=1}^{\infty} \frac{(-1)^s}{s^k} \tag{A3}$$

is obtained. Equation (16) follows directly from Eq. (A2) using $j=1$ and $m=n-1$.

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