

Asymptotic series of Generalized Lambert W Function

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Abstract

Herein, we present a sequel to earlier work on a generalization of the Lambert W function. In particular, we examine series expansions of the generalized version providing computational means for evaluating this function in various regimes and further confirming the notion that this generalization is a natural extension of the standard Lambert W function.

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1 Introduction

The Lambert W function satisfying $W(t)e^{W(t)} = t$ provides an exact solution to:

$$e^{-cx} = a_o (x - r_1) \quad (1)$$

with $x = r_1 + \frac{1}{c}W(c e^{-cr_1}/a_o)$. The Lambert W function appears in a myriad number of applications. In particular, it appears in the “lineal” gravity two-body problem [1, 2] as a solution to the Einstein Field equations in $(1 + 1)$ dimensions. The Lambert W function appears as a solution for the case when the two-bodies have exactly the same mass. However, the case of unequal masses required a *Generalization* of Lambert’s function [1, eq.(81)].

$$e^{-cx} = a_o (x - r_1)(x - r_2) \quad (2)$$

This generalization originally appeared from the (quantum-mechanical) Double Well Dirac Delta Potential model [3], a one-dimensional version of a special case of the quantum-mechanical three-body system known as the *Hydrogen Molecular Ion* (and also appears in quantum gravity [2]). For this problem, specifically $r_1 = 1$, $r_2 = \lambda$, $c = 2/R$ where R is the internuclear distance. $a_o = \frac{1}{\lambda}$ and λ was treated formally as real perturbative parameter (the case at $\lambda = 1$ allows eq. (2) to factor into (1) which is solvable in terms of the standard Lambert W function). In its original form, this equation was written in a more complicated form, namely a *pseudo-quadratic*: with two solutions for x [3–6]:

$$x_{\pm}(\lambda) = \frac{1}{2}(\lambda + 1) \pm \frac{1}{2} \left\{ (\lambda + 1)^2 - 4\lambda[1 - e^{-cx_{\pm}(\lambda)}] \right\}^{1/2}$$

where $E_{\pm} = -x_{\pm}/2$ are the quantum state energies (for respectively the two distinct solutions x_{\pm}). All these quantities including the energies were real though we do not rule out a generalization to the complex plane.

A difficulty encountered by Byers-Brown and Scott *et al.* is that Physical Chemists followed a conventional practice of starting with the case $\lambda = 0$ whose solution is $x_0 = 1$ as a starting point and considering a series expansion about x_0 of eq. (1) in powers of λ . This was called the “polarization expansion” for the range $0 < \lambda < 1$ and proves very difficult to sum, necessitating the use of Padé-Hermite Approximants [3]. This slow convergence became aggravated for larger but similar molecular systems like the Hydrogen Molecular Ion requiring much discussion (and calculation) to sort out the convergence of the eigenstates and related quantities once and for all [7, 8].

Subsequently, it was realized that eq. (2) could be further generalized to the case of a rational polynomial [9]:

$$e^{-cx} = \frac{P_N(x)}{Q_M(x)} \quad (3)$$

where $c > 0$ is a constant as before and $P_N(x)$ and $Q_M(x)$ are polynomials in x of respectively orders N and M . Eq. (3) expresses the solution for the energy eigenvalues of the three-dimensional (and realistic) version of the Hydrogen molecular ion. These generalizations were found to express solutions to a huge class of fundamental problems and were found to be natural extensions of the standard W function requiring merely a formal nesting of the standard Lambert W function [10] and thus economical conceptually in terms of mathematical resources. Some exact solutions were even found for some special cases for eq. (2) [10].

Herein, we examine the more pragmatic matter of obtaining series expansions for eq. (2) for analytical and computational purposes. In the process, we will show how closely they relate to the series expansions of the standard W function. We will examine three series expansions which apply to three different regimes. Though eq. (2) is not the full generalization in eq. (3) it already embodies a link between gravity theory and quantum mechanics albeit in lower dimensions [2] and is therefore instructive as a special case beyond the standard W function. Finally, some concluding remarks are made at the end. Since we are dealing with applications in Physics, the input parameters c , a_o and the polynomial roots r_i where $i = 1, 2, \dots$ are assumed to be real.

2 Series Expansions

2.1 Taylor series in r_d

By a series of manipulations, eq. (1) can be brought in the familiar standard form:

$$x_0 = W(x_0)e^{W(x_0)} \quad \text{where} \quad x_0 = \frac{c e^{-cr_1}}{a_o} \quad (4)$$

Using very similar manipulations and defining respectively the mean and difference of the roots r_1 and r_2 :

$$r_m = \frac{r_1 + r_2}{2} \quad \text{and} \quad r_d = \frac{r_1 - r_2}{2}, \quad (5)$$

and by *completing the square* for the quadratic on the right of eq. (2):

$$(x - r_1)(x - r_2) = (x - r_m)^2 - r_d^2$$

and defining $W(r_d) = x - r_m$, eq. (2) can be rewritten as:

$$e^{-c(W(r_d)+r_m)} + a_o r_d^2 = a_o W(r_d)^2. \quad (6)$$

The above can be viewed as the intersection between an exponential of the form Ae^{-cx} and a “simple harmonic oscillator” of the form Bx^2 . Potentially, there can be two and as much as three intersections (in the real plane), in some cases, roots of the same sign. To obtain real solutions, we constrain $a_o > 0$. It is very similar to eq. (1) the equation governing the standard Lambert W function with the mean of the roots r_m playing the role of the r_1 in the monomial on the right side of eq. (1), the difference in the roots r_d representing a departure from the form of eq. (1). This makes perfect sense because when $r_d = 0$, then $r_1 = r_2$ and eq. (2) can be factored into the form of eq. (1) bringing us back to the standard W function. We define:

$$z_0 = \frac{1}{2} \sqrt{\frac{c^2}{a_o}} e^{-cr_m/2} = \frac{1}{2} \frac{c}{\sqrt{a_o}} e^{-cr_m/2} \quad (7)$$

where it is understood that $W(0)$ is/are the solution(s) when $r_d = 0$:

$$W(0) = \frac{2}{c} W(\pm z_0) = \frac{2}{c} W_0 \quad (8)$$

and where $W(\pm z_0)$ on the right side of eq. (8) is the *standard* Lambert W function. For real results, in particular for the parameters mentioned for the Double Well Dirac potential mentioned just below eq. (2), we are interested in real results and make use of the main branch of the standard W function. In this case, $c > 0$ helps ensure $|z_0| < 1/e$ (although $W(-z_0)$ could have a real result on a different branch for c sufficiently small). Implicit differentiation on both sides of eq. (6) yields:

$$\frac{\partial W(r_d)}{\partial r_d} = \frac{2r_d}{\frac{ce^{-c(W(r_d)+r_m)}}{a_o} + 2W(r_d)} = \frac{2r_d}{c W(r_d)^2 - c r_d^2 + 2 W(r_d)} \quad (9)$$

Naturally successive derivatives with respect to r_d yields the Taylor series in r_d . Its radius of convergence will be obtained from the disk about the point of expansion $r_d = 0$ (assuming it is regular at the point of expansion) bounded by the closest singularity or branch point in the complex plane namely when the denominator of this derivative and all successive derivatives is zero, with $W(r_d)$ simultaneously satisfying eq. (6). Note that the expression on the right most side of eq. (9), obtained by virtue of eq. (6), does not formally depend on a_o nor r_m but only on c and r_d . Even though this is a quadratic in $W(r_d)$, only one solution satisfies eq. (6), namely:

$$W(r_{d \text{ crit}}) = \frac{-1 + \sqrt{1 + c^2 r_{d \text{ crit}}^2}}{c} \quad (10)$$

The critical radius in the complex plane is:

$$r_{d \text{ crit}} = \pm \frac{1}{c} \sqrt{2 W(-2 z_0^2) + W(-2 z_0^2)^2}. \quad (11)$$

Here $W_0 = W(\pm z_0)$ is the standard W function and the radius is $|r_{d \text{ crit}}|$. Note that when $z_0 = 0$, $W(z_0) = W(-2z_0^2) = 0$ (on the main branch) and the radius of convergence is also zero even though $z_0 = 0$ is analytic on the main branch for the (standard) Lambert W function. The series in r_d is thus:

$$\begin{aligned} W(r_d) = & 2 \frac{W_0}{c} + \frac{1}{4} \frac{c r_d^2}{W_0(W_0 + 1)} + \frac{1}{64} \frac{c^3 r_d^4 (2 W_0^2 - 1)}{W_0^3(W_0 + 1)^3} \\ & + \frac{1}{1536} \frac{c^5 r_d^6 (8W_0^4 - 12W_0^2 + 3 - 4W_0^3)}{W_0^5(W_0 + 1)^5} \\ & + \frac{1}{49152} \frac{c^7 r_d^8 (48W_0^6 - 132W_0^4 + 90W_0^2 - 15 - 64W_0^5 + 40W_0^3)}{W_0^7(W_0 + 1)^7} + O(c^9 r_d^{10}) \end{aligned} \quad (12)$$

which is a series in r_d^2 for $x = W(r_d) + r_m$ with x governed by eq. (2) and the radius of convergence is provided by the magnitude of (11). Within its radius of convergence, it converges rapidly. Note that when argument of z_0 is such that $W_0 = 0$ (which happens when e.g. $z_0 = 0$ on the main branch) or $W_0 + 1 = 0$ (which happens when $z_0 = -e^{-1}$ which is a branch point on the main branch), the individual series coefficients are confronted with divisions by zero, a result consistent, for the case $W_0 = 0$, with a radius of convergence of zero as given by eq.(11).

The validity of this series is demonstrated with some numerical tests. To reiterate the earlier problem, for a relatively high value of $\lambda = 0.8$ and an internuclear distance near the bond length $R = 2$, we have:

$$a_o = \frac{5}{4}, \quad c = 4, \quad r_d = \frac{1}{10}, \quad r_m = \frac{9}{10}$$

The solution of eq. (2) is $x = 1.0485$ obtained to within 4 decimals using the series in eq. (12) to within and including order $O(r_d^{10})$ using $W_0 = W(z_0)$ as the lead term. Similarly, the other solution $x = 0.6248$ is obtained using $W_0 = W(-z_0)$ as the lead term. The convergence of this series is much more rapid than the original ‘‘polarization expansion’’ mentioned in the introduction. Furthermore, this series is not limited to the real plane. For $\lambda = \frac{9}{10} - \frac{1}{10}i$

$$a_o = \frac{45}{41} + \frac{5}{41}i, \quad c = 4, \quad r_d = \frac{1}{20} + \frac{1}{20}i, \quad r_m = \frac{19}{20} - \frac{1}{20}i$$

The series to (and including) order $O(r_d^{14})$ yields $x = 1.0651408 - 0.0281742i$ to within 7 decimals for $W_0 = W(z_0)$ and similarly $x = 0.72818558 - 0.0876039i$ for $W_0 = W(-z_0)$. This series expansion is valid for small differences in the roots r_d , so clearly an asymptotic expansion valid for large r_d is also needed.

It would seem that in the case of three real roots, that we would only recover at most two out of three solutions. However, when two roots appear for e.g. $x > 0$ and the third root appears for $x < 0$, the latter can be recovered by reflection symmetry on the parameters. Let $x \rightarrow -x$, $c \rightarrow -c$, $r_i \rightarrow -r_i$ and these same formula can be used to recover that third solution.

2.2 Reversion of Power Series

To get an asymptotic series valid for large r_d , we further transform eq. (6) with the following variable transformations:

$$\begin{aligned} W(r_d)^2 &= \left(\frac{2}{c}\right)^2 (U^2 + d^2) \\ d &= c r_d/2 \end{aligned} \quad (13)$$

and $x = W(r_d) + r_m$ as before. Following the procedure for the standard W function [11], we start from:

$$z_0 = f(U) = U e^{\pm \sqrt{U^2 + d^2}} \quad \text{where} \quad z_0 = \frac{1}{2} \frac{c e^{-cr_m/2}}{\sqrt{a_o}} \quad (14)$$

where the sign \pm takes into account that the negative square root is also possible. When $d = 0$, eq. (14) reduces to the form of the standard W function. Eq. (14) has the form:

$$z = f(U)$$

and we seek to reverse the power series to obtain:

$$U = g(z);$$

Defining $\phi(U) = U/f(U) = e^{\mp \sqrt{U^2 + d^2}}$ and noting that $\phi(0) \neq 0$, we use a specialized version of the Lagrange-Bürmann [12] formula:

$$U(z) = z\phi(0) + \sum_{k=1}^{\infty} \frac{z^{k+1}}{(k+1)!} \left. \frac{\partial^k \phi(U)^{k+1}}{\partial U^k} \right]_{U=0} \quad (15)$$

Implicit differentiation of eq. (14) w.r.t. z yields:

$$\frac{\partial U(z)}{\partial z} = \frac{\sqrt{U(z)^2 + d^2} e^{\mp \sqrt{U(z)^2 + d^2}}}{U(z)^2 + \sqrt{U(z)^2 + d^2}} \quad (16)$$

We can see that the square root term dominates the functional form of the derivatives and the branch structure $U(z)$ in the complex plane much in accordance with the findings of Byers-Brown [5, 6]. Note that eq. (16) has no explicit dependence on z and thus there is no need to verify its consistency with (14). To get the radius of convergence, we need to consider both the branch structure of the square root term in the denominator of (16) and values of $U(z)$ in the complex plane about the region $z = 0$ which would make this denominator zero. Thus the radius of convergence is limited by either:

$$|U_{crit}| < |d|$$

or

$$|U_{crit}| < \frac{1}{2} |\sqrt{2 \pm 2\sqrt{1 + 4d^2}}| \quad (17)$$

whichever is smaller. We obtain:

$$U(z) = z e^{\mp d} \mp \frac{1}{2} \frac{z^3 e^{\mp 3d}}{d} \pm \frac{1}{8} \frac{z^5 (\pm 5d + 1) e^{\mp 5d}}{d^3} + O(z^7 e^{\pm 7d}) \quad (18)$$

$$= \frac{1}{2} \frac{c e^{-\frac{1}{2}cr_{\pm}}}{\sqrt{a_o}} \mp \frac{1}{8} \frac{c^2 e^{-\frac{3}{2}cr_{\pm}}}{a_o^{3/2} r_d} \pm \frac{1}{64} \frac{c^2 e^{-\frac{5}{2}cr_{\pm}} (\pm 5c r_d + 2)}{a_o^{5/2} r_d^3} + O(e^{-\frac{7}{2}r_{\pm}c}) \quad (19)$$

where $r_+ = r_1, r_- = r_2, x = r_m + (2/c)\sqrt{U^2 + d^2}$ as x given in eq. (2). This series would have growing exponential terms of the form $\exp(-k*d)$ unless $k > 0$ and consequently this necessitates the requirement that $c r_{\pm} > 0$. Thus, we obtain a valid asymptotic expansion valid for large d or equivalently large r_d .

As in the previous section, we also get two kinds of solutions, respectively for positive and negative d , but they do not necessarily relate at all to the solutions of the previous section. The first section involved a series expansion in r_d^2 where $r_d = (2/c)d$ and invariant with respect to the sign of d . Here we are dealing with a situation where the difference between the roots r_d is very large and thus quite possibly only one intersection between the exponential term on the left side of eq. (2) and its right side namely a quadratic in x , and thus only one solution.

As a numerical check and departing from the earlier physical chemistry problem in the earlier section, consider these particular values:

$$a_o = 1, \quad c = 2, \quad r_1 = 2, \quad r_2 = 1 \quad \Rightarrow \quad d = r_d = \frac{1}{2}, \quad r_m = \frac{3}{2}.$$

The asymptotic series in eq. (19) with only the first 3 terms up to and including $O(1/d^3)$ yields the solution $x = 2.01739$ to within 4 decimals. Another test case, this time with some complex values:

$$a_o = 1, \quad c = 1, \quad r_1 = 2 - i, \quad r_2 = 1 + i \quad \Rightarrow \quad d = \frac{1}{4} - \frac{1}{2}i, \quad r_d = \frac{1}{2} - i, \quad r_m = \frac{3}{2}$$

This same series with only 3 terms gives us $x = 1.9703 - 0.9430i$ to within 4 decimals. Thus, though initially motivated for the case of real numbers, these expansions can be used in the complex plane within certain restrictions.

2.3 Asymptotic series for large argument

The question arises what happens if we decide the left side z_0 of eq. (14) is large? For the principal branch when $z > 0$, taking logs of both sides of the equation governing the standard Lambert W function i.e. $We^W = z$ yields:

$$\ln[W(z)] = \ln(z) - W(z) \quad (20)$$

Recursive substitution yields successively:

$$\begin{aligned} & \ln(z) \\ & \ln(z) - \ln(\ln(z)) \\ & \ln(z) - \ln(\ln(z) - \ln(\ln(z))) \\ & \dots \end{aligned}$$

By taking logs on both sides of eq. (14) for the positive square root case only:

$$\ln(z) - \ln(U) = \sqrt{U^2 + d^2} \quad \text{or} \quad (\ln(z) - \ln(U))^2 = U^2 + d^2 \quad (21)$$

Thus, we consider two types of recursion.

$$U \rightarrow \sqrt{(\ln(z) - \ln(U))^2 - d^2} \quad (22)$$

$$U^2 \rightarrow \frac{1}{4}(-2\ln(z) + \ln(U^2) - 2d)(-2\ln(z) + \ln(U^2) + 2d) \quad (23)$$

The second recursion avoids the square root (and its messy consequences for recursion) and looks like a factored form involving a combination of asymptotic formulae for the standard W function. By successive substitution, we obtain:

$$U \approx \sqrt{\left(\ln(z) - \ln \left(\sqrt{\left(\ln(z) - \ln \left(\sqrt{\dots \ln \left(\ln(z) - \ln \left(\sqrt{(\ln(z) - \ln(U))^2 - d^2}\right)^2 \dots - d^2}\right)^2 - d^2}\right)^2 - d^2} \right) \right)^2 \right)^2 \quad (24)$$

and:

$$\begin{aligned} U^2 \approx & \frac{1}{4} \left(-2\ln(z) + \ln \left(\frac{1}{4} (-2\ln(z) + \ln(\dots \right. \right. \\ & \left. \left. + \ln \left(\frac{1}{4} (-2\ln(z) + \ln(U^2) - 2d)(-2\ln(z) + \ln(U^2) + 2d) \right) + \dots + 2d \right) \right) + 2d \right) \end{aligned} \quad (25)$$

However, we find from experience that the argument z has to be *very large* indeed for these asymptotic formulations to converge. This exercise is more to demonstrate the resemblance with the counterpart expansion for the standard W function, namely eq. (21). For computational value, sections 2.1 and 2.2 are more useful. Nonetheless, the very large z_0 argument is tractable.

Table 1: Non-Linear transformations applied to Taylor series of eq.(12) for $r_d = 0.8$

no. of terms	$W(r_d)$ Taylor Series	Shanks	Levin t
1	-0.9999999996	-0.9999999996	-0.9999999996
2	-1.6400000000	-1.6400000000	-2.7777777780
3	-1.4352000000	-1.4848484850	-1.5213977230
4	-1.6099626670	-1.5294964030	-1.5192810810
5	-1.4421905070	-1.5246574640	-1.5243445560
6	-1.6265161880	-1.5271424650	-1.5267037510
7	-1.4108133840	-1.5280997520	-1.5277557490
\vdots	\vdots	\vdots	\vdots
	-1.528554071	-1.528554071	-1.528554071

Table 2: Non-Linear transformations applied to Taylor series of eq.(12) for $r_d = 1.5$

no. of terms	$W(r_d)$ Taylor Series	Shanks	Levin t
1	0.38889448	0.3888944774	0.3888944774
2	2.81078092	2.8107809190	-0.0743922833
3	-3.02541152	1.0991727410	-5.1438626370
4	24.71693722	1.7964086140	1.7380384290
5	-139.85949420	1.3876539200	1.5296581130
6	953.20098980	1.5894954440	1.5167708910
7	-6823.99405600	1.4791930140	1.5165517370
\vdots	\vdots	\vdots	\vdots
	1.516240428	1.516240428	1.516240428

2.4 Summation techniques

Finally, the series summation can be accelerated even *beyond* the radii of convergence using non-linear transformations as mentioned in the introduction. These transformations are applied to the sequence of partial sums and are capable of accelerating the convergence of a series and even sum divergent series (e.g. see the work of [13, 14]). We take the point of view that a Taylor or asymptotic series has all the desired “information”, getting numbers from the series is a matter of a summation technique. For the series in r_d of the first section for both $W(\pm z_0)$, it was found that the series, when oscillating in r_d , could indeed be extended beyond their radius of convergence. This is demonstrated for the test case:

$$a_o = 1, \quad c = 1, \quad r_m = 1.$$

Here, the asymptotic solution of eq. (19) matches the extrapolated Taylor series of solution about $W_0(z_0)$ of (12) in 4 decimal places. Here $r_{d \text{ crit}} \approx 0.64$ and we consider the regime when $r_d > r_{d \text{ crit}}$, the alternating Taylor series is divergent. This Taylor series to order $O(r_d^{12})$ (6 terms in powers of r_d^2) is used for the t transformation of Levin [15] and the Shanks transformation [16]. To demonstrate agreement between the Taylor series and the outcome of the non-linear transformations, tables 1 and 2 compares the Taylor series of eq. (12) and the outcome of the Shanks and Levin t transformations for respectively $r_d = 0.8$ and $r_d = 1.5$. At the bottom of each table is listed what exact solution to the number of digits shown. The Taylor series of eq. (12) diverges violently when $r_d = 1.5$ but the non-linear transformations converge nicely. Three terms of the asymptotic expansion in eq. (19) for $r_d = 1.5$, yield $x = 1.516240673$ which agrees with the exact solution starting from $W_0(z_0)$ to within 7 decimals. This demonstrates that

the solutions of section 2.2 can match one of the solutions of section 2.1.

3 Conclusions

Previously [10] we had inferred a canonical form for a generalization as expressed by (2) and (3) and given both mathematical and physical justifications for it. Herein, we formulated Taylor series and asymptotic series useful for analysis and computation. We find that the results are similar to those governing the standard W function and represent a natural extension though the branch structure in the complex plane may differ.

This approach could be extended to higher order polynomials fitting the pattern of eq. (3). For example, when the right side of eq. (3) we can *complete the cube* in some special cases, i.e. for

$$x^3 + a x^2 + b x + c = \left(x + \frac{1}{3}\right)^3 - \left(\frac{1}{27} a^3 - c\right)^3 \quad \text{when} \quad b = \frac{a^2}{3}$$

which can allow a special case of eq.(3) and create a cubic relation counterpart of eq. (14):

$$\frac{e^{-cr_m}}{a_o} = Y^3 e^{c(Y^3+d_3)^{1/3}} \quad (26)$$

where $(x - r_m)^3 = Y^3 + d_3$ and $d_3 = \frac{a^3}{27} - c$ and $r_m = -a/3$. However, for larger order polynomials and rational polynomials, this approach is quickly exhausted and one has to rely on numerical techniques which is very feasible.

Finally, the Taylor series summation can be accelerated even *beyond* the radii of convergence using non-linear transformations known as the Levin or Shanks transformations allowing a matching between the Taylor series and the asymptotic series. The resulting series can be converted into FORTRAN or C code using the interface between Maple and these languages [18].

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