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:

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

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)].

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

This generalization also appears in the (quantum-mechanical) Double Well Dirac Delta Potential model [7], 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]. Specifically $r_1 = 1$, $r_2 = \lambda$ and $a_o = \frac{1}{\lambda}$ where $0 < \lambda < 1$, all real quantities and $c > 0$ (the case at $\lambda = 1$ allows eq. (2) to factor into (1) which is solvable in terms of the standard Lambert W function). Subsequently, it was realized that eq. (2) could be further generalized to the case of a rational polynomial:

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

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 [4] and thus economical conceptually in terms of mathematical resources. Some exact solutions were even found for some special cases for eq.!(2) [4].

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 (2) 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 $i = 1, 2, \ldots$ 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:

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

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

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

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:

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

The above can be viewed as the intersection between an exponential of the form $Ae^{-c\,x}$ and a "simple harmomnic 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 since 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:

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

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

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

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 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:

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

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 $r_d = 0$ 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:

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

The critical radius in the complex plane is:

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

With $W_0 = W(\pm z_0)$ is the standard W function and the radius is $|r_{d\ crit}|$. Note that when $z_0 = -e^{-1}$, $W(z_0) = 0$ and this represents a singularity in the denominator of the series terms. However the argument $-2z_0^2 = -2e^{-2}$ of $r_{d\ crit}$ which is smaller in magnitude is still on the right of z_0. Consequently, the series in r_d is thus:

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

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 $W(\pm z_0) = 0$ the individual series coefficients are confronted with divisions by zero, a result confirmed with a radius of convergence of zero as given by eq.(11). This series expansion is valid for small differences in the roots r_d, so cleaarly 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 paramaters. Let $x \to -x$, $c \to -c$, $r_i \to -r_i$ 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:

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

and $x = W(r_d) + r_m$ as before. Following the procedure for the standard W function [5], we start from:

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

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 [6] formula:

$$
U(z) = z\phi(0) + \sum_{k=1}^{\infty} \frac{z^{k+1}}{(k+1)!} \frac{\partial^k \phi(U)^{k+1}}{\partial U^k}\bigg]_{U=0}
\tag{15}
$$

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

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

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 [8,9]. Note that eq. (16) has no explicit dependence on z and thus there is no need to verify its consistency of (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

$$
|U_{crit}| < \frac{1}{2}\left|\sqrt{2 \pm 2\sqrt{1 + 4d^2}}\right|
\tag{17}
$$

whichever is smaller. We obtain:

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

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

where $r_+ = r_1$, $r_- = r_2$, $x = r_m + (2/c)\sqrt{U^2 + d^2}$ as x given in eq. (2). Clearly this is asymptotic series valid for large d or equivalently large r_d. It also needs the requirement $cr_\pm > 0$ for convergence. 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.

2.3 Asymptotic series for large argument

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

$$\ln(z) - \ln(U) = \sqrt{U^2 + d^2} \quad \text{or} \quad (\ln(z) - \ln(U))^2 = U^2 + d^2 \tag{20}$$

Thus, we consider two types of recursion.

$$U \rightarrow \sqrt{(\ln(z) - \ln(U))^2 - d^2} \tag{21}$$

$$U^2 \rightarrow \frac{1}{4}(-2\ln(z) + \ln(U^2) - 2d)(-2\ln(z) + \ln(U^2) + 2d) \tag{22}$$

The second recursion looks like a factored form involving a combination of asymptotic formulae for the standard W function. By successive substitution, we obtain:

$$U \approx \sqrt{\left(\ln(z) - \ln\left(\sqrt{\left(\ln(z) - \ln\left(\sqrt{\ldots \ln\left(\ln(z) - \ln\left(\sqrt{(\ln(z) - \ln(U))^2 - d^2}\right)\right)^2 \ldots - d^2}\right)\right)^2} - d^2\right)\right)^2}$$
$$\tag{23}$$

and:

$$U^2 \approx \frac{1}{4}\left(-2\ln(z) + \ln\left(\frac{1}{4}\left(-2\ln(z) + \ln\left(\ldots\right.\right.\right.\right. \tag{24}$$
$$+ \left.\left.\left.\ln\left(\frac{1}{4}(-2\ln(z) + \ln(U^2) - 2d)(-2\ln(z) + \ln(U^2) + 2d)\right) + \ldots + 2d\right)\right) + 2d\right)$$

We find from experience that the argument z has to be very large indeed for these asympotic formulations to converge. This exercise is more to demonstrate the resemblence with the counterpart expansion for the standard W function.

2.4 Summation techniques

Finally, the series summation can be accelerated even *beyond* the radii of convergence using non-linear transformations known as the Levin or Sidi transformations. The latter involves a series transformation

by which one can accelerate the convergence of a series and even sum divergent series (e.g. see the work of [10, 11]). 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 using a Levin t or Shanks transformation.

3   Conclusions

Previously [4] 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):

$$\frac{e^{-c r_m}}{a_0} \; = \; Y^3 \, e^{c \, (Y^3 + d_3)^{1/3}} \tag{25}$$

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 series summation can be accelerated even *beyond* the radii of convergence using non-linear transformations known as the Levin or Shanks transformations. The resulting series can be converted into FORTRAN or C code using the interface between Maple and these languages [13].

References

[1] R. B. Mann and T. Ohta, *Exact solution for the metric and the motion of two bodies in* $(1 + 1)$-*dimensional gravity*, Phys. Rev. D. **55**, (1997), 4723-4747.

[2] P. S. Farrugia, R. B. Mann, and T. C. Scott, *N-body Gravity and the Schrödinger Equation*, Class. Quantum Grav. **24**, (2007), , 4647-4659.

[3] T. C. Scott, M. Aubert-Frécon and J. Grotendorst, *New approach for the electronic energies of the hydrogen molecular ion*, Chem. Phys. **324**, (2006), 323-338.

[4] T. C. Scott, R. B. Mann and R. E. Martinez II, *General Relativity and Quantum Mechanics: Towards a Generalization of the Lambert W Function*, AAECC, **17**, (2006) 41-47.

[5] (a) R. Corless, G. Gonnet, D. E. G. Hare and D. Jeffrey, *Lambert's W Function in Maple*, MapleTech **9**, ed. T. C. Scott, (Spring 1993); (b) R. Corless, G. Gonnet, D. E. G. Hare, D. Jeffrey and D. Knuth, *On the Lambert W Function*, Advances in Computational Mathematics, **5**, (1996), 329-359.

[6] A. C. Dison, *On Burmann's Theorem*, Proc. London Math. Soc. **34**, pp. 151-153, (1902).

[7] T. C. Scott, J. F. Babb, A. Dalgarno, and J. D. Morgan III, *The Calculation of Exchange Forces: General Results and Specific Models*, J. Chem. Phys. **99**, (1993), 2841-2854.

[8] P. R. Certain and W. Byers Brown, *Branch Point Singularities in the Energy of the Delta-Function Model of One-Electron Diatoms*, Intern. J. Quantum Chem. **6**, (1972), 131-142.

[9] W. N. Whitton and W. Byers Brown, *The Relationship Between the Rayleigh-Schrödinger and Asymptotic Perturbation Theories of Intermolecular Forces*, Int. J. Quantum Chem. **10**, (1976), 71-86.

[10] J. Grotendorst, Comput. Phys. Commun. **67**, pp. 325-342 (1991).

[11] E. J. Weniger, Comput. Phys. Rep. **10**, pp. 189-371 (1989).

[12] B. W. Char, K. O. Geddes, G. H. Gonnet, B. L. Leong, M. B. Monagan and S. M. Watt, *First Leaves: A Tutorial Introduction to Maple V*, Springer-Verlag, New York, (1992).

[13] C. Gomez and T. C. Scott, *Maple programs for generating efficient FORTRAN code for serial and vectorised machines*, Comput. Phys. Commun., Thematic issue: Computer Algebra in Physics Research, **115**, pp. 548-562 (1998).