

Derivatives of Whittaker Functions $W_{K, 1/2}$ and $M_{K, 1/2}$ with Respect to Order K

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Abstract. The Whittaker function derivatives $[\partial W_{\kappa, 1/2}/\partial \kappa]_{\kappa=n}$ and $[\partial M_{\kappa, 1/2}/\partial \kappa]_{\kappa=n}$ which arise in calculations involving the hydrogen atom's generalized Green's functions are computed.

Introduction. Recently, there has been growing interest among chemists and physicists in the analytical properties of the Whittaker functions [1], [6] $W_{\kappa, 1/2}$ and $M_{\kappa, 1/2}$. For example, in quantum mechanics, these functions occur in the hydrogen atom's Green's function [2]. The derivative of these functions with respect to κ occur in the atom's generalized Green's function [4]. The latter Green's functions are of key importance in calculating the second-order physical properties of the atom [5]. In this communication, we wish to report some practical methods of computing the partial derivatives \bar{W}_n and \bar{M}_n , i.e.,

$$(1) \quad \bar{W}_n = [\partial W_{\kappa, 1/2}(Z)/\partial \kappa]_{\kappa=n}, \quad \bar{M}_n = [\partial M_{\kappa, 1/2}(Z)/\partial \kappa]_{\kappa=n}.$$

These quantities have been given [1], [4] only in the case of $n = 0, 1$. We treat the general situation here.

To begin with, we note the infinite series representation [7] for $W_{\kappa, 1/2}$:

$$(2) \quad W_{\kappa, 1/2}(Z) = \frac{e^{-Z/2}}{\Gamma(1 - \kappa)} \times \left\{ 1 - \sum_{k=0}^{\infty} \frac{\Gamma(k + 1 - \kappa) Z^{k+1}}{\Gamma(-\kappa)(k + 1)! k!} \cdot [\psi(k + 1) + \psi(k + 2) - \ln z - \psi(k + 1 - \kappa)] \right\}.$$

Direct differentiation of this form, followed by evaluation at $\kappa = 1$, gives the simple result

$$(3) \quad \bar{W}_1 = e^{-Z/2}(-1 + Z \ln Z),$$

or in terms of Whittaker functions [1], [6]

$$(4) \quad \bar{W}_1 = -W_{0, 1/2}(Z) + W_{1, 1/2}(Z) \ln Z.$$

The other partial derivatives can be obtained from \bar{W}_1 with the use of the "recurrence" formula

$$(5) \quad \bar{W}_{n+1} = -\{Z d\bar{W}_n/dZ + (n - Z/2)\bar{W}_n + W_{n, 1/2}\},$$

Received November 4, 1971, revised June 16, 1972.
 AMS (MOS) subject classifications (1969). Primary 2230.

which is obtained by differentiating a well-known recurrence* relation for the Whittaker function, i.e.,

$$(6) \quad W_{\kappa+1,1/2}(Z) = -\left\{Z \frac{dW_{\kappa,1/2}(Z)}{dZ} + (\kappa - Z/2)W_{\kappa,1/2}(Z)\right\}.$$

Other "recurrence" formulae can be obtained* from Eq. (12a). The first few derivatives are given below.

$$(7) \quad \begin{aligned} \bar{W}_1 &= -W_{0,1/2} + W_{1,1/2} \ln Z, \\ \bar{W}_2 &= W_{0,1/2} - 3W_{1,1/2} + W_{2,1/2} \ln Z, \\ \bar{W}_3 &= -2W_{0,1/2} + 4W_{1,1/2} - 5W_{2,1/2} + W_{3,1/2} \ln Z, \\ \bar{W}_4 &= 6W_{0,1/2} - 10W_{1,1/2} + 9W_{2,1/2} - 7W_{3,1/2} + W_{4,1/2} \ln Z. \end{aligned}$$

An alternate and much less tedious approach to this problem begins by noting that the differential equation defining $W_{\kappa,1/2}$, i.e.,

$$(8) \quad Z^2 W_{\kappa,1/2}'' + \{-Z^2/4 + \kappa Z\} W_{\kappa,1/2} = 0,$$

can be used to obtain the equation

$$(9) \quad Z^2 \bar{W}_n'' + \{-Z^2/4 + nZ\} \bar{W}_n = -Z W_{n,1/2}.$$

Guided by Eqs. (7), we write the solution of the inhomogeneous equation as

$$(10) \quad \bar{W}_n = \sum_{l=0}^{n-1} C_l W_{l,1/2} + W_{n,1/2} \ln Z.$$

Determination of the coefficients in Eq. (10) follows by substituting Eq. (10) into Eq. (9). We get, with the use of Eq. (8),

$$(11) \quad \sum_{l=0}^{n-1} C_l (n-l) Z W_{l,1/2} = (1-Z) W_{n,1/2} - 2Z W_{n,1/2}'$$

which can be simplified with the help of the properties

$$(12a) \quad Z W_{n,1/2} = W_{n+1,1/2} + 2n W_{n,1/2} + n(n-1) W_{n-1,1/2},$$

$$(12b) \quad Z W_{n,1/2}' = (n-Z/2) W_{n,1/2} + n(n-1) W_{n-1,1/2}.$$

Using Eqs. (12a) and (12b), Eq. (5) can be rewritten in terms of the Whittaker functions alone, the linear independence of these functions allowing us to find that

$$C_{n-1} = 1 - 2n, \quad C_{n-2} = (n-1)^2,$$

and

$$(13) \quad (l+1)(l+2)(n-l-2)C_{l+2} + 2(l+1)(n-l-1)C_{l+1} + (n-l)C_l = 0.$$

The solution of the three-term recurrence equation is easily found [3] and is

* Since Whittaker functions satisfy three-term recurrence relations, alternate recurrence formulae can be obtained for \bar{W}_n . Equation (12a) yields the result

$$n(n-1)\bar{W}_{n-1} + (2n-z)\bar{W}_n + \bar{W}_{n+1} = -2W_n - (2n-1)W_{n-1};$$

however, there is no special advantage inherent in this equation over Eq. (5). This is especially true since a closed form for \bar{W}_n is given in Eq. (15).

$$(14) \quad C_l = (-1)^{n+l} \frac{(n-1)! (n+l)}{l! (n-l)},$$

the final expression for \bar{W}_n being

$$(15) \quad \bar{W}_n = (-1)^n (n-1)! \sum_{l=0}^{n-1} \frac{(-1)^l (n+l)}{l! (n-l)} W_{l,1/2} + W_{n,1/2} \ln Z.$$

Finally, we treat the second Whittaker function $M_{\kappa,1/2}$. We proceed as in the case of the W function, i.e., direct differentiation of the infinite series representation

$$(16) \quad M_{\kappa,1/2}(Z) = \frac{e^{-Z/2}}{\Gamma(1-\kappa)} \sum_{k=0}^{\infty} \frac{(k+1-\kappa)Z^{k+1}}{(k+1)! k!},$$

to obtain \bar{M}_1 followed by the use of a recurrence relation. We get, in the case $\kappa = 1$,

$$(17) \quad \bar{M}_1(Z) = M_{0,1/2}(Z) - \{-\gamma + 1 + g(Z)\} M_{1,1/2}(Z),$$

with $g(Z) = \text{Ei}(Z) - \ln Z$, where γ is Euler's constant (.57721. . .) and $\text{Ei}(Z)$ is the exponential integral. The corresponding "recurrence" relation is

$$(18) \quad (n+1)\bar{M}_{n+1} = Z d\bar{M}_n/dZ + (n-Z/2)\bar{M}_n + M_{n,1/2} - M_{n+1,1/2},$$

and follows from the recurrence relation [1], [6]

$$(19) \quad (\kappa+1)M_{\kappa+1,1/2} = Z dM_{\kappa,1/2}/dZ + (\kappa-Z/2)M_{\kappa,1/2}.$$

The first few \bar{M}_n functions are:

$$(20) \quad \begin{aligned} \bar{M}_1 &= M_{0,1/2} - (-\gamma + 1 + g)M_{1,1/2}, \\ 2\bar{M}_2 &= M_{0,1/2} + (3 - e^Z)M_{1,1/2} - (-2\gamma + 3 + 2g)M_{2,1/2}, \\ 3\bar{M}_3 &= M_{0,1/2} + (2 - 3e^Z/2)M_{1,1/2} \\ &\quad + (5 - e^Z)M_{2,1/2} - (-3\gamma + 11/2 + 3g)M_{3,1/2}, \\ 4\bar{M}_4 &= M_{0,1/2} + (5/3 - 5e^Z/3)M_{1,1/2} + (3 - 5e^Z/3)M_{2,1/2} + (7 - e^Z)M_{3,1/2} \\ &\quad - (-4\gamma + 25/3 + 4g)M_{4,1/2}. \end{aligned}$$

Although the differential equation satisfied by \bar{M}_n has the same form as in the \bar{W}_n case

$$Z^2 \bar{M}_n'' + \{-Z^2/4 + nZ\} \bar{M}_n = -ZM_{n,1/2},$$

the solution has the form

$$(21) \quad \bar{M}_n = \sum_{l=0}^{n-1} (a_l + b_l e^Z) M_{l,1/2} - [\psi(n+1) + g(Z)] M_{n,1/2}.$$

As before, we find with help of the recurrence relations [8] for the M functions that the a coefficients are given by

$$a_{n-1} = \frac{2n-1}{n}, \quad a_{n-2} = \frac{n-1}{n},$$

and

$$(22) \quad (n-1-l)a_{l+1} - 2(n-l)a_l + (n+1-l)a_{l-1} = 0.$$

The solution [3] to this equation is just

$$(23) \quad a_l = \frac{1}{n} \frac{(n+l)}{(n-l)}.$$

The b coefficients satisfy the equations

$$b_{n-1} = -\frac{1}{n}, \quad b_{n-2} = \frac{3-2n}{n(n-1)}, \quad b_0 = 0,$$

and

$$(24) \quad 2(l+1)b_{l+2} - (n+5l+1)b_{l+1} + 2(n+2l-1)b_l - (n+l-1)b_{l-1} = 0.$$

This four-term expression can be reduced by the substitution

$$(25) \quad A_l = 2(l+1)b_{l+2} - (n+l+1)b_{l+1},$$

to the simpler three-term form

$$(26) \quad A_{l+1} - 2A_l + A_{l-1} = 0,$$

whose solution [3] is

$$(27) \quad A_l = (n+l+1)/n.$$

The b coefficients are obtained from the inhomogeneous equation

$$(28) \quad 2lb_{l+1} - (n+l)b_l = (n+l)/n,$$

and are given by

$$(29) \quad b_l = -\frac{1}{n} \sum_{k=0}^{n-l-1} \frac{2^k (l)_k}{(l+n)_k}.$$

Acknowledgement. The author would like to thank the referee for his helpful comments; the paper is a better one because of him.

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1. H. BUCHHOLTZ, *The Confluent Hypergeometric Function*, Springer-Verlag, Berlin, 1969.
2. L. HOSTLER, "Runge-Lenz vector and the Coulomb Green's function," *J. Mathematical Phys.*, v. 8, 1967, p. 642.
3. C. JORDAN, *Calculus of Finite Differences*, Chelsea, New York, 1950, p. 543.
4. B. J. LAURENZI, "Green's functions in atomic and molecular calculations," *Chem. Phys. Lett.*, v. 1, 1967, pp. 641-642. MR 41 #4956; also, L. Hostler, *Phys. Rev.*, v. 178, 1969, p. 126.
5. B. J. LAURENZI, "Green's functions in atomic and molecular calculations," *J. Chem. Phys.*, v. 52, 1970, p. 3049.
6. Y. L. LUKE, *The Special Functions and Their Approximations*. Vol. 1, Math. in Sci. and Engineering, vol. 53, Academic Press, New York, 1969, p. 115. MR 39 #3039.
7. I. S. GRADSHTEYN & I. M. RYZHIK, *Tables of Integrals, Sums, Series and Products*, Fizmatgiz, Moscow, 1963; English transl., Academic Press, New York, 1965, p. 1063. MR 28 #5198; MR 33 #5952.
8. Reference [1], p. 81.