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

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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 $\kappa$ 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.,

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

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 $W_{\kappa,1/2}$:

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

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

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

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

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

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

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

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

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

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

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

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

$$Z^2W''_{\kappa,1/2} + \{-Z^2/4 + \kappa Z\}W_{\kappa,1/2} = 0, \tag{8}$$

can be used to obtain the equation

$$Z^2\bar{W}''_n + \{-Z^2/4 + nZ\}\bar{W}_n = -ZW_{n,1/2}. \tag{9}$$

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

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

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

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

which can be simplified with the help of the properties

$$ZW_{n,1/2} = W_{n+1,1/2} + 2nW_{n,1/2} + n(n-1)W_{n-1,1/2}, \tag{12a}$$

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

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

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

and

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

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).

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

the final expression for $\bar{W}_n$ being

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

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

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

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

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

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

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

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

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

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

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

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

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

the solution has the form

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

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

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

and

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

The solution [3] to this equation is just

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

The $b$ coefficients satisfy the equations

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

and

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

This four-term expression can be reduced by the substitution

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

to the simpler three-term form

$$A_{l+1} - 2A_l + A_{l-1} = 0, \tag{26}$$

whose solution [3] is

$$A_l = (n+l+1)/n. \tag{27}$$

The $b$ coefficients are obtained from the inhomogeneous equation

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

and are given by

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

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