Coulomb Green's function and an addition formula for the Whittaker functions

Pavel Šťovíček

Department of Mathematics, Faculty of Nuclear Science, Czech Technical University in Prague, Trojanova 13, 120 00 Praha, Czech Republic

Abstract

A series of the form $\sum_{\ell=0}^{\infty} c(\kappa, \ell) M_{\kappa,\ell+1/2}(r_0) W_{\kappa,\ell+1/2}(r) P_{\ell}(\cos(\gamma))$ is evaluated explicitly where $c(\kappa, \ell)$ are suitable complex coefficients, $M_{\kappa,\mu}$ and $W_{\kappa,\mu}$ are the Whittaker functions, P_{ℓ} are the Legendre polynomials, $r_0 < r$ are radial variables, γ is an angle and κ is a complex parameter. The sum depends, as far as the radial variables and the angle are concerned, on their combinations $r + r_0$ and $(r^2 + r_0^2 - 2rr_0\cos(\gamma))^{1/2}$. This addition formula generalizes in some respect Gegenbauer's Addition Theorem and follows rather straightforwardly from some already known results, particularly from Hostler's formula for Coulomb Green's function. In addition, several complementary summation formulas are derived. They suggest that a further extension of this addition formula may be possible.

I. INTRODUCTION

Green's function of a Hamiltonian is an important object in quantum physics as it contains, in principal, all information about the respective physical system. Particularly the set of singular points of Green's function coincides with the spectrum. Green's function is in fact the integral kernel of the resolvent of the Hamiltonian which is regarded as an integral operator. Sometimes, however, the integral kernel should be interpreted in the distributional sense. Green's function is also closely related to the heat kernel or to the propagator. Namely, Green's function is the Laplace transform of the heat kernel.

Green's function can be explicitly expressed in a compact form for some quantum systems which are usually distinguished by their symmetry properties. As a rule, such systems frequently enjoy rotational symmetry. If so, this also opens the way to an alternative construction of Green's function based on the method of separation of variables. The problem then effectively reduces to a one-dimensional one. Finally one deals with a positive second-order ordinary differential operator of Sturm-Liouville type though on the half-line rather than on a bounded interval. This is a substantial simplification since the construction of Green's function for a Sturm-Liouville operator is commonly known and, in fact, this is a text-book matter. Thus in distinguished solvable cases the radial part of Green's function can be expressed in terms of appropriate special functions. The full Hamiltonian depending on both radial and angle variables is then expressed as a sum with the summation running over eigenmodes of the spherical part of the Hamiltonian. Equaling the compact form of Green's function to the sum obtained via the method of separation of variables leads to an addition formula for the involved special functions.

This procedure can be successfully applied to the Hamiltonian of the hydrogen atom, resulting in an addition formula for the Whittaker functions $M_{\kappa,\mu}$ and $W_{\kappa,\mu}$. The formula turns out to be a generalization of Gegenbauer's Addition Theorem in some respect. To the best of author's knowledge, this possibility has not been exploited yet and still remains overlooked. And this is despite the fact that a compact formula for Coulomb Green's function has been derived by Hostler rather long time ago in [10, 11]. As a companion of the addition formula for the Whittaker functions we further derive another addition formula concerning the Laguerre polynomials. There already exists a well-known addition formula for the Laguerre polynomials but that one reported here is completely different.

From the mathematical point of view, the formula for the Whittaker functions cannot be considered fully satisfactory, however, as the resulting sum involves only the Whittaker functions with the parameter $\mu = 1/2$. A more general formula for arbitrary parameters κ and μ seems to be lacking. Nevertheless here we present some partial results in this direction which indicate that the derived formula could be further generalized. In addition to the parameter κ , with μ being restricted to the values 1/2modulo integers, the formula depends on the radial variables r_0 and r and on an angle γ . In the particular case $\gamma = \pi$ we show that there exists an addition formula admitting general values of both κ and μ . Further we derive a summation formula for the Whittaker functions $W_{\kappa,\mu}$ only and another one for the Whittaker functions $M_{\kappa,\mu}$. Again, in both cases, the parameters κ and μ can take arbitrary values.

The paper is organized as follows. In Section II we summarize some known formulas and results which are essential for the solution of our problem. The main result of the paper, namely a derivation of an addition formula for the Whittaker functions, is the content of Section III. Section IV is devoted to an addition formula for the Laguerre polynomials. Finally, Section V contains some complementary results suggesting that further generalizations could be possible, as discussed above.

II. PRELIMINARIES

First let us recall the definition of the Whittaker functions and summarize several useful formulas related to them [1, 9]. The Whittaker functions are defined in terms of the confluent hypergeometric functions,

$$M_{\kappa,\mu}(r) := e^{-r/2} r^{1/2+\mu} {}_1F_1\left(\mu - \kappa + \frac{1}{2}; 2\mu + 1; r\right), \qquad (1)$$

$$W_{\kappa,\mu}(r) := e^{-r/2} r^{1/2+\mu} U\left(\mu - \kappa + \frac{1}{2}, 2\mu + 1, r\right).$$
(2)

For the derivatives we shall use the notation

$$W'_{\nu,1/2}(x) := \frac{\partial W_{\nu,1/2}(x)}{\partial x}, \ M'_{\nu,1/2}(x) := \frac{\partial M_{\nu,1/2}(x)}{\partial x}$$

The modified Bessel functions K_{ν} , I_{ν} are particular cases of the Whittaker functions,

$$K_{\nu}(z) = \sqrt{\frac{\pi}{2z}} W_{0,\nu}(2z), \ I_{\nu}(z) = \frac{1}{2^{2\nu} \Gamma(\nu+1)\sqrt{2z}} M_{0,\nu}(2z).$$
(3)

Furthermore,

$$M_{0,1/2}(z) = 2\sinh\left(\frac{z}{2}\right), \ W_{0,1/2}(z) = e^{-z/2}.$$
 (4)

For $n \in \mathbb{Z}_+$, the functions $W_{n+(\alpha+1)/2,\alpha/2}$ and $M_{n+(\alpha+1)/2,\alpha/2}$ are linearly dependent,

$$M_{n+(\alpha+1)/2,\alpha/2}(z) = \frac{(-1)^n \Gamma(\alpha+1)}{\Gamma(n+\alpha+1)} W_{n+(\alpha+1)/2,\alpha/2}(z).$$

Moreover, the generalized (associated) Laguerre polynomials are related to the Whittaker functions,

$$L_n^{\alpha}(z) = \frac{(-1)^n}{n!} \, z^{-(\alpha+1)/2} W_{n+(\alpha+1)/2,\alpha/2}(z).$$

Therefore, for $n \in \mathbf{Z}_+$,

$$W_{n,1/2}(z) = (-1)^{n+1} n! M_{n,1/2}(z)$$
(5)

and, for $n \ge 1$,

$$M_{n,1/2}(z) = \frac{1}{n} e^{-z/2} z L_{n-1}^1(z).$$
(6)

Regarding the asymptotic forms, we have

$$e^{r/2} W_{\kappa,\mu}(r) = r^{\kappa} \left(1 + \frac{\left(\mu - \kappa + \frac{1}{2}\right)\left(\mu + \kappa - \frac{1}{2}\right)}{r} + O\left(\frac{1}{r^2}\right) \right), \text{ as } r \to \infty$$
(7)

(see, for example, (2) and equation 13.5.2 in [1]). Furthermore [4, Eqs. 13.20.1, 13.20.2], when $\mu \to \infty$ in \mathbb{C} , $\operatorname{Re}(\mu) > 0$, and $\kappa \in \mathbb{C}$ is fixed,

$$M_{\kappa,\mu}(z) = z^{\mu+1/2} \left(1 + O(\mu^{-1}) \right)$$
(8)

uniformly for z in a bounded region in \mathbb{C} , and

$$W_{\kappa,\mu}(x) = \frac{\Gamma(\kappa+\mu)}{\sqrt{\pi}} \left(\frac{x}{4}\right)^{1/2-\mu} \left(1 + O(\mu^{-1})\right)$$
(9)

uniformly for bounded positive values of x (one can also consult [14, Chap. 7, Sect. 11.1] or [5]).

Next let us shortly recall, without going into all details, a standard construction of Green's function of a Sturm-Liouville operator for it is essential for our purposes. Thus we consider a second-order ordinary differential operator

$$Lf(x) := -(p(x)f'(x))' + q(x)f(x)$$

on an interval which can be bounded or unbounded. Here p(x) > 0 and $q(x) \ge 0$ are sufficiently regular functions. At the finite endpoints one imposes mixed boundary conditions or, if the interval is unbounded, one requires functions from the domain of L to be square integrable on a neighborhood of infinity. One assumes that L with properly chosen boundary conditions is positive definite. To describe Green's function of L one finds two nontrivial solutions v_0 , v_1 of the differential equation

$$-pv_j'' - p'v_j' + qv_j = 0, \ j = 0, 1,$$

on the given interval such that v_0 satisfies the boundary condition at the left endpoint (or minus infinity) only while v_1 satisfies the boundary condition at the right endpoint (or plus infinity) only. Then L^{-1} is an integral operator with the integral kernel

$$\mathcal{G}(x,y) = -\frac{1}{pw} \left(\vartheta(y-x)v_0(x)v_1(y) + \vartheta(x-y)v_0(y)v_1(x) \right)$$

where $w := v_0 v'_1 - v_1 v'_0$ is the Wronskian of v_0 and v_1 . Note that p(x)w(x) is in fact a constant function. Here and in the sequel ϑ denotes the Heaviside step function.

It may be instructive to illustrate the procedure leading to an addition formula, as described in Section I, on the well-known example of the operator $-\nabla^2 + k^2$, k > 0, in \mathbb{R}^2 . Naturally, the partial differential operator is expressed in polar coordinates. Using the method of separation of variables one finds that Green's function can be written in the form

$$G(r,\varphi;r_0,\varphi_0) = \frac{1}{2\pi\sqrt{rr_0}} \left(f_0(r,r_0) + 2\sum_{n=1}^{\infty} f_n(r,r_0)\cos(n(\varphi-\varphi_0)) \right).$$
(10)

The functions $f_n(r, r_0)$ can be obtained as solutions of the Sturm-Liouville problem in the radial variable, as described above, and we get

$$f_n(r,r_0) = \frac{1}{2k(2n)!} \Gamma\left(n + \frac{1}{2}\right) \\ \times \left(\vartheta(r-r_0)W_{0,n}(2kr)M_{0,n}(2kr_0) + \vartheta(r_0 - r)M_{0,n}(2kr)W_{0,n}(2kr_0)\right).$$

The RHS can be also expressed in terms of the modified Bessel functions, see (3). At the same time, a compact formula for Green's function is well known,

$$G(\boldsymbol{r},\boldsymbol{r}_0) = \frac{1}{2\pi} K_0(k|\boldsymbol{r}-\boldsymbol{r}_0|).$$

We can let $\varphi_0 = 0$ and, by comparison, we obtain an addition formula for the modified Bessel functions,

$$I_0(kr_0)K_0(kr) + 2\sum_{n=1}^{\infty} I_n(kr_0)K_n(kr)\cos(n\varphi) = K_0(kR) \text{ for } 0 \le r_0 < r,$$
(11)

where

$$R = R(\varphi) := \sqrt{r^2 + r_0^2 - 2rr_0 \cos(\varphi)}.$$
 (12)

As a matter of fact, formula (11) is a corollary of substantially more general Graf's Addition Theorem [1, Eq. 9.1.79].

Let us rewrite (10) just to have a comparison to Hostler's result (20) which is mentioned below. From (11) we deduce that

$$I_0(v)K_0(u) + 2\sum_{n=1}^{\infty} I_n(v)K_n(u) = K_0(u-v) \text{ for } 0 \le v < u.$$

Let $(r = |\mathbf{r}|, r_0 = |\mathbf{r}_0|)$

$$x := r + r_0 + |\mathbf{r} - \mathbf{r}_0|, \ y := r + r_0 - |\mathbf{r} - \mathbf{r}_0|.$$
(13)

Then

$$2\pi G(\boldsymbol{r}, \boldsymbol{r}_0) = I_0\left(\frac{ky}{2}\right) K_0\left(\frac{kx}{2}\right) + 2\sum_{n=1}^{\infty} I_n\left(\frac{ky}{2}\right) K_n\left(\frac{kx}{2}\right).$$

One can proceed very analogously in case of the operator $-\nabla^2 + k^2$, k > 0, in \mathbb{R}^3 . Doing so one obtains a particular case of Gegenbauer's Addition Theorem. We are not going to discuss this case, however. Instead, in Section III, we will focus on the operator $-\nabla^2 - g/|\mathbf{r}| + k^2$, g > 0 and k > 0, in \mathbb{R}^3 . Nevertheless let us recall what Gegenbauer's theorem claims if specialized to the modified Bessel functions. For $0 \le r_0 < r$ and $\nu \in \mathbb{R}$,

$$\frac{2^{\nu}\Gamma(\nu)}{(rr_0)^{\nu}}\sum_{n=0}^{\infty}(\nu+n)K_{\nu+n}(r)I_{\nu+n}(r_0)C_n^{(\nu)}(\cos(\gamma)) = \frac{K_{\nu}(R)}{R^{\nu}}$$
(14)

with R defined in (12), see [17, §II.4] (and also [1, Eq. 9.1.80]). Here $C_n^{(\nu)}(z)$ are the Gegenbauer polynomials.

Another addition formula which is crucial for our purposes is Spherical Harmonic Addition Theorem, also called Legendre Addition Theorem. Recall that the spherical harmonics are defined for $\ell \in \mathbb{Z}_+$ (the set of non-negative integers), $m \in \mathbb{Z}$, $|m| \leq \ell$,

$$Y_{\ell}^{m}(\theta,\varphi) := \sqrt{\frac{(2\ell+1)(\ell-m)!}{4\pi \,(\ell+m)!}} P_{\ell}^{m}(\cos(\theta))e^{im\varphi}.$$
(15)

Here $\theta \in [0, \pi]$, $\varphi \in [0, 2\pi]$ are coordinates on the unit sphere S^2 and $P_{\ell}^m(z)$ is the associated Legendre polynomial. We have

$$P_{\ell}^{-m}(z) = (-1)^m \frac{(\ell-m)!}{(\ell+m)!} P_{\ell}^m(z).$$
(16)

and

$$Y_{\ell}^{-m}(\theta,\varphi) = (-1)^m \overline{Y_{\ell}^m(\theta,\varphi)}.$$

The spherical harmonics $\{Y_{\ell}^m\}$ form an orthonormal basis in $L^2(S^2, d\Omega)$ and

$$-\nabla^2 Y_{\ell}^m(\theta,\varphi) = \frac{\ell \left(\ell+1\right)}{r^2} Y_{\ell}^m(\theta,\varphi).$$

Spherical Harmonic Addition Theorem tells us that, for every $\ell \in \mathbb{Z}_+$,

$$\sum_{m=-\ell}^{\ell} Y_{\ell}^{m}(\theta,\varphi) \overline{Y_{\ell}^{m}(\theta_{0},\varphi_{0})} = \sum_{m=-\ell}^{\ell} (-1)^{m} Y_{\ell}^{m}(\theta,\varphi) Y_{\ell}^{-m}(\theta_{0},\varphi_{0}) = \frac{2\ell+1}{4\pi} P_{\ell}(\cos(\gamma))$$
(17)

where

$$\cos(\gamma) := \cos(\theta)\cos(\theta_0) + \sin(\theta)\sin(\theta_0)\cos(\varphi - \varphi_0),$$

that is $\cos(\gamma) = \mathbf{n} \cdot \mathbf{n}_0$, $\mathbf{n} := (\sin(\theta) \cos(\varphi), \sin(\theta) \sin(\varphi), \cos(\theta))$ and \mathbf{n}_0 is defined similarly. $P_{\ell}(z) \equiv P_{\ell}^0(z)$ are the Legendre polynomials. Referring to (15) and (16), equation (17) means that

$$P_{\ell}(\cos(\gamma)) = P_{\ell}(\cos(\theta))P_{\ell}(\cos(\theta_0)) + 2\sum_{m=1}^{\ell} \frac{(\ell-m)!}{(\ell+m)!} P_{\ell}^m(\cos(\theta))P_{\ell}^m(\cos(\theta_0))\cos(m(\varphi-\varphi_0)).$$

This is a classical result with a long history [8], and a dozen different proofs of it have been provided, some of them quite intricate [13]. A straightforward derivation, as encountered in physical literature, is based on symmetry considerations and can be briefly rephrased as follows. Observe that

$$\tilde{\mathcal{P}}_{\ell}(\boldsymbol{n},\boldsymbol{n}_{0}) := \sum_{m=-\ell}^{\ell} Y_{\ell}^{m}(\theta,\varphi) \overline{Y_{\ell}^{m}(\theta_{0},\varphi_{0})}$$

is the integral kernel of the orthogonal projection in $L^2(S^2, d\Omega)$ onto the eigenspace of minus the Laplace-Beltrami operator on S^2 (denoted as $-\Delta_{S^2}$) corresponding to the eigenvalue $\ell(\ell+1)$. Thus we have (the differential operator acts in variables θ and φ)

$$-\Delta_{S^2} \tilde{\mathcal{P}}_{\ell}(\boldsymbol{n}, \boldsymbol{n}_0) = \ell(\ell+1) \tilde{\mathcal{P}}_{\ell}(\boldsymbol{n}, \boldsymbol{n}_0).$$
(18)

Owing to rotational symmetry $\tilde{\mathcal{P}}_{\ell}(\boldsymbol{n}, \boldsymbol{n}_0)$ should depend on the distance of the points $\boldsymbol{n}, \boldsymbol{n}_0 \in S^2$ only which in turn is a function of $\boldsymbol{n} \cdot \boldsymbol{n}_0 = \cos(\gamma)$. Writing $\tilde{\mathcal{P}}_{\ell}(\boldsymbol{n}, \boldsymbol{n}_0) = f(\boldsymbol{n} \cdot \boldsymbol{n}_0)$ equation (18) reduces to the ordinary second-order differential equation

$$-(1-z^2)f''(z) + 2zf'(z) - \ell(\ell+1)f(z) = 0.$$

A general solution has the form $f(z) = c_1 P_{\ell}(z) + c_2 Q_{\ell}(z)$. Here $Q_{\ell}(z)$ is the Legendre function of the second kind which is another independent solutions of the differential equation and is known to be singular for $z = \pm 1$. Therefore $\tilde{\mathcal{P}}_{\ell}(\boldsymbol{n}, \boldsymbol{n}_0) = c_1 P_{\ell}(\boldsymbol{n} \cdot \boldsymbol{n}_0)$. The multiplicative constant is easily found to be $c_1 = (2\ell + 1)/(4\pi)$ when letting $\boldsymbol{n} = \boldsymbol{n}_0 = (0, 0, 1)$ and taking into account that $P_{\ell}(1) = 1$ and $P_{\ell}^m(1) = 0$ for $m \neq 0$.

III. THE HYDROGEN ATOM AND AN ADDITION FORMULA FOR THE WHITTAKER FUNCTIONS

Using spherical coordinates $r > 0, \theta \in [0, \pi], \varphi \in [0, 2\pi]$, we denote

 $\boldsymbol{r} = (r\sin(\theta)\cos(\varphi), r\sin(\theta)\sin(\varphi), r\cos(\varphi)).$

We write the Hamiltonian of the hydrogen atom in a dimensionless form as $H = -\nabla^2 - g/r$, g > 0, and we wish to apply the procedure leading to an addition formula, as described in Section I, to the operator

$$H + k^2 = -\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} - \frac{1}{r^2}\left(\frac{1}{\sin(\theta)}\frac{\partial}{\partial\theta}\sin(\theta)\frac{\partial}{\partial\theta} + \frac{1}{\sin^2(\theta)}\frac{\partial^2}{\partial\varphi^2}\right) - \frac{g}{r} + k^2, \quad k > 0.$$

While the continuous spectrum of H coincides with the positive real half-line, the discrete spectrum consists of eigenvalues $E_n = -g^2/4n^2$, $n \in \mathbb{N}$, the multiplicity of E_n equals n^2 . The corresponding normalized eigenfunctions are

$$\psi_{n,\ell,m}(r,\theta,\varphi) = \frac{g^{3/2}}{n^{\ell+2}} \sqrt{\frac{(n-\ell-1)!}{2(n+\ell)!}} (gr)^{\ell} \exp\left(-\frac{gr}{2n}\right) L_{n-\ell-1}^{2\ell+1}\left(\frac{gr}{n}\right) Y_{\ell}^{m}(\theta,\varphi),$$

where $n \in \mathbb{N}$, $\ell \in \mathbb{Z}_+$ and $m \in \mathbb{Z}$ are the principal, the azimuthal and the magnetic quantum number, respectively, and $|m| \leq \ell \leq n-1$.

Application of the method of separation of variables to this operator again leads to the Sturm-Liouville problem in the radial variable whose solution is rather straightforward, as outlined in Section II, and has already been described in the literature [16, 15]. We have

$$\begin{aligned} G(r,\theta,\varphi,r_0,\theta_0,\varphi_0) &= \frac{1}{rr_0} \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \frac{1}{2k (2\ell+1)!} \Gamma\left(\ell+1-\frac{g}{2k}\right) \\ &\times \left(\vartheta(r-r_0) M_{g/(2k),\ell+1/2}(2kr_0) W_{g/(2k),\ell+1/2}(2kr) \right. \\ &\left. + \vartheta(r_0-r) M_{g/(2k),\ell+1/2}(2kr) W_{g/(2k),\ell+1/2}(2kr_0) \right) Y_{\ell}^m(\theta,\varphi) \overline{Y_{\ell}^m(\theta_0,\varphi_0)} \,. \end{aligned}$$

With the aid of (17) this equation can be further simplified,

$$G(r, \theta, \varphi, r_0, \theta_0, \varphi_0) = \frac{1}{8\pi k r r_0} \sum_{\ell=0}^{\infty} \frac{1}{(2\ell)!} \Gamma\left(\ell + 1 - \frac{g}{2k}\right) \\ \times \left(\vartheta(r - r_0) M_{g/(2k), \ell+1/2}(2kr_0) W_{g/(2k), \ell+1/2}(2kr) + \vartheta(r_0 - r) M_{g/(2k), \ell+1/2}(2kr) W_{g/(2k), \ell+1/2}(2kr_0)\right) P_\ell(\cos(\gamma)).$$
(19)

Notably, there exists a remarkable compact formula for Green's function due to Hostler [10, 11],

$$G(r, \theta, \varphi, r_0, \theta_0, \varphi_0) = \frac{1}{4\pi R} \Gamma\left(1 - \frac{g}{2k}\right)$$

$$\times \left(M'_{g/(2k), 1/2}(ky)W_{g/(2k), 1/2}(kx) - M_{g/(2k), 1/2}(ky)W'_{g/(2k), 1/2}(kx)\right)$$
(20)

where in this case we have

$$R := |\boldsymbol{r} - \boldsymbol{r}_0| = \sqrt{r^2 + r_0^2 - 2rr_0 \left(\sin(\theta)\sin(\theta_0)\cos(\varphi - \varphi_0) + \cos(\theta)\cos(\theta_0)\right)},$$

and

$$x := r + r_0 + |\mathbf{r} - \mathbf{r}_0|, \ y := r + r_0 - |\mathbf{r} - \mathbf{r}_0|$$
(21)

(formally the same equations as in (13) but now the dimension is 3 rather than 2).

Comparing (19) to (20) while still using notation (21) we have, for $0 \le r_0 < r$,

$$\frac{1}{krr_0} \sum_{\ell=0}^{\infty} \frac{1}{(2\ell)!} \Gamma\left(\ell + 1 - \frac{g}{2k}\right) M_{g/(2k),\ell+1/2}(2kr_0) W_{g/(2k),\ell+1/2}(2kr) P_\ell(\cos(\gamma))
= \Gamma\left(1 - \frac{g}{2k}\right) \frac{2}{R} \left(M'_{g/(2k),1/2}(ky) W_{g/(2k),1/2}(kx) - M_{g/(2k),1/2}(ky) W'_{g/(2k),1/2}(kx)\right).$$

After substitution $g = 2k\kappa$ and rescaling $r \to r/(2k)$, $r_0 \to r_0/(2k)$ we get an addition formula for the Whittaker functions. Moreover, the parameter κ can be extended to complex values by analyticity.

Theorem 1. For $0 \leq r_0 < r$, $\kappa \in \mathbb{C} \setminus \mathbb{N}$ and $\gamma \in \mathbb{R}$,

$$\frac{1}{rr_0} \sum_{\ell=0}^{\infty} \frac{\Gamma(\ell+1-\kappa)}{\Gamma(1-\kappa)(2\ell)!} M_{\kappa,\ell+1/2}(r_0) W_{\kappa,\ell+1/2}(r) P_\ell(\cos(\gamma)) \\
= \frac{1}{R} \left(M_{\kappa,1/2}'\left(\frac{y}{2}\right) W_{\kappa,1/2}\left(\frac{x}{2}\right) - M_{\kappa,1/2}\left(\frac{y}{2}\right) W_{\kappa,1/2}'\left(\frac{x}{2}\right) \right)$$
(22)

where $R = R(\gamma)$, see (12), and

$$x = r + r_0 + R, \ y = r + r_0 - R.$$
(23)

One has to exclude the values $\kappa \in \mathbb{N}$. As a matter of fact, the equation holds for these values, too, but it should be achieved in the limit after the singular terms in the equation have been combined. For instance, for $\kappa = 1$ we have

$$\frac{1}{rr_0} \sum_{\ell=1}^{\infty} \frac{(\ell-1)!}{(2\ell)!} M_{1,\ell+1/2}(r_0) W_{1,\ell+1/2}(r) P_\ell(\cos(\gamma))$$

= $-\frac{\partial}{\partial \kappa} \left(\frac{1}{R} \left(M_{\kappa,1/2}'\left(\frac{y}{2}\right) W_{\kappa,1/2}\left(\frac{x}{2}\right) - M_{\kappa,1/2}\left(\frac{y}{2}\right) W_{\kappa,1/2}'\left(\frac{x}{2}\right) \right)$
 $-\frac{1}{rr_0} M_{\kappa,1/2}(r_0) W_{\kappa,1/2}(r) \right) \Big|_{\kappa=1}.$

Remark 2. Let us check two particular cases. For $\gamma = 0$ (hence $R = r - r_0$, x = 2r, $y = 2r_0$) we have

$$\frac{1}{rr_0} \sum_{\ell=0}^{\infty} \frac{\Gamma(\ell+1-\kappa)}{(2\ell)!} M_{\kappa,\ell+1/2}(r_0) W_{\kappa,\ell+1/2}(r)
= \frac{\Gamma(1-\kappa)}{r-r_0} \left(M_{\kappa,1/2}'(r_0) W_{\kappa,1/2}(r) - M_{\kappa,1/2}(r_0) W_{\kappa,1/2}'(r) \right),$$
(24)

and for $\gamma = \pi$ (hence $R = r + r_0$, $x = 2(r + r_0)$, y = 0) we have

$$\frac{1}{rr_0} \sum_{\ell=0}^{\infty} (-1)^{\ell} \frac{\Gamma(\ell+1-\kappa)}{(2\ell)!} M_{\kappa,\ell+1/2}(r_0) W_{\kappa,\ell+1/2}(r) = \frac{\Gamma(1-\kappa)}{r+r_0} W_{\kappa,1/2}(r+r_0).$$
(25)

Remark 3. From (25) one can derive a summation formula for Whittaker functions which seems to be also new. For $\kappa \in \mathbb{C} \setminus \mathbb{N}$ and $z \in \mathbb{C}$,

$$\frac{1}{z} \sum_{\ell=0}^{\infty} (-1)^{\ell} \frac{\Gamma(\ell+1-\kappa)}{\Gamma(1-\kappa)(2\ell)!} M_{\kappa,\ell+1/2}(z) = e^{-z/2}$$
(26)

(where the singularity at z = 0 on the LHS is removable). It can be proven by exploring the asymptotic behavior of both sides of (25), as $r \to \infty$. We have, in virtue of (7),

$$\frac{1}{r+r_0}W_{\kappa,1/2}(r+r_0) = e^{-r/2 - r_0/2}r^{-1+\kappa}\left(1 + \frac{\kappa - \kappa^2 - (1-\kappa)r_0}{r} + O\left(\frac{1}{r^2}\right)\right)$$

and

$$\frac{1}{r}W_{\kappa,\ell+1/2}(r) = e^{-r/2}r^{-1+\kappa}\left(1 + \frac{(\ell+1-\kappa)(\ell+\kappa)}{r} + O\left(\frac{1}{r^2}\right)\right).$$

Thus, writing z instead of r_0 , we see that (26) holds for z > 0. But the asymptotic behavior of $M_{\kappa,\ell+1/2}(z)$ for ℓ large, as recalled in (8), which is locally uniform in z implies that the LHS is an entire function of z. Since the same is true for the RHS we conclude that (26) must hold for all $z \in \mathbb{C}$.

Let us point out a relation of Theorem 1 to Gegenbauer's Addition Theorem. Confining ourselves to the value $\kappa = 0$ (corresponding to g = 0) in (22) we obtain a simplified equation

$$\sum_{\ell=0}^{\infty} \frac{2\ell+1}{\sqrt{rr_0}} K_{\ell+1/2}\left(\frac{r}{2}\right) I_{\ell+1/2}\left(\frac{r_0}{2}\right) P_{\ell}(\cos(\gamma)) = \frac{1}{R} e^{-R/2} = \frac{1}{\sqrt{\pi R}} K_{1/2}\left(\frac{R}{2}\right).$$
(27)

This is a particular case of Gegenbauer's Addition Theorem, however, see equation (14) with $\nu = 1/2$. To derive (27) from (22) we have used (3), (4) and also the equation

$$M_{0,1/2}'\left(\frac{y}{2}\right)W_{0,1/2}\left(\frac{x}{2}\right) - M_{0,1/2}\left(\frac{y}{2}\right)W_{0,1/2}'\left(\frac{x}{2}\right) = e^{-R/2} = \sqrt{\frac{R}{\pi}}K_{1/2}\left(\frac{R}{2}\right)$$

Moreover, note that $C_n^{(1/2)}(z) = P_n(z)$.

As for equation (26), letting $\kappa = 0$ we get

$$\sqrt{\frac{\pi}{2r}} \sum_{\ell=0}^{\infty} (-1)^{\ell} (2\ell+1) I_{\ell+1/2}(z) = e^{-z}.$$

This is a particular case of the identity

$$2^{\nu} \Gamma(\nu) \sum_{\ell=0}^{\infty} (\ell+\nu) C_{\ell}^{(\nu)}(\gamma) I_{\ell+\nu}(z) = z^{\nu} e^{\gamma z},$$

which is well known, see [7, §7.15(1)]; note that $C_{\ell}^{(1/2)}(-1) = (-1)^{\ell}$.

IV. AN ADDITION FORMULA FOR THE LAGUERRE POLYNOMIALS

Theorem 4. For $n \in \mathbb{N}$, $0 \leq r_0 < r$ and $\gamma \in \mathbb{R}$,

$$\sum_{\ell=0}^{n-1} \frac{(2\ell+1)(n-\ell-1)!}{(n+\ell)!} (rr_0)^{\ell} L_{n-\ell-1}^{2\ell+1}(r) L_{n-\ell-1}^{2\ell+1}(r_0) P_{\ell}(\cos(\gamma))$$
$$= \frac{1}{2R} \left(x L_{n-1}^1\left(\frac{x}{2}\right) L_n\left(\frac{y}{2}\right) - y L_{n-1}^1\left(\frac{y}{2}\right) L_n\left(\frac{x}{2}\right) \right)$$
(28)

where x, y are defined in (23), with $R = R(\gamma)$, see (12).

Remark. Note that formula (28) is completely different from the well known addition formula for the Laguerre polynomials which claims that [1, Eq. 22.12.6]

$$\sum_{j=0}^{n} L_{j}^{\alpha}(u) L_{n-j}^{\beta}(v) = L_{n}^{\alpha+\beta+1}(u+v).$$

Proof. Recall that

Res
$$\left(\Gamma(z); z = -n\right) = \frac{(-1)^n}{n!}, n \in \mathbb{Z}_+,$$

whence

Res
$$\left(\Gamma\left(1 - g/(2\sqrt{-z})\right); z = E_n\right) = \frac{(-1)^n g^2}{2n! n^2}, n \in \mathbb{N}.$$

If we substitute $k = \sqrt{-z}$ in Hostler's formula (20) then the residue of Green's function at $z = E_n$ equals

$$\frac{(-1)^n g^2}{8\pi n! n^2 R} \left(M'_{n,1/2} \left(\frac{gy}{2n} \right) W_{n,1/2} \left(\frac{gx}{2n} \right) - M_{n,1/2} \left(\frac{gy}{2n} \right) W'_{n,1/2} \left(\frac{gx}{2n} \right) \right).$$
(29)

The residue also equals minus the projection \mathcal{P}_n onto the eigenspace corresponding to eigenvalue E_n . \mathcal{P}_n is an integral operator with the integral kernel

$$\mathcal{P}_n(r,\theta,\varphi,r_0,\theta_0,\varphi_0) = \sum_{\ell=0}^{n-1} \sum_{m=-\ell}^{\ell} \psi_{n,\ell,m}(r,\theta,\varphi) \overline{\psi_{n,\ell,m}(r_0,\theta_0,\varphi_0)}.$$
 (30)

Hence, for $n \in \mathbb{N}$,

$$\frac{(-1)^{n+1}n}{(n-1)!\,gR} \left(M_{n,1/2}'\left(\frac{gy}{2n}\right) W_{n,1/2}\left(\frac{gx}{2n}\right) - M_{n,1/2}\left(\frac{gy}{2n}\right) W_{n,1/2}'\left(\frac{gx}{2n}\right) \right) \\
= \exp\left(-\frac{g\left(r+r_{0}\right)}{2n}\right) \sum_{\ell=0}^{n-1} \frac{(2\ell+1)(n-\ell-1)!}{(n+\ell)!} \left(\frac{g^{2}rr_{0}}{n^{2}}\right)^{\ell} \\
\times L_{n-\ell-1}^{2\ell+1}\left(\frac{gr}{n}\right) L_{n-\ell-1}^{2\ell+1}\left(\frac{gr_{0}}{n}\right) P_{\ell}(\cos(\gamma)).$$
(31)

In regard of (5) and (6), we derive

$$M_{n,1/2}'(z) = \frac{\mathrm{d}}{\mathrm{d}z} \left(\frac{1}{n} e^{z/2} e^{-z} z L_{n-1}^1(z) \right) = \frac{1}{2} M_{n,1/2}(z) + \frac{1}{n} e^{z/2} \frac{\mathrm{d}}{\mathrm{d}z} \left(e^{-z} z L_{n-1}^1(z) \right)$$
$$= \frac{1}{2} M_{n,1/2}(z) + e^{-z/2} L_n(z).$$

Here we have used the formula [12, Eq. (9.12.8)]

$$\frac{\mathrm{d}}{\mathrm{d}z}\left(e^{-z}z^{\alpha}L_{n-1}^{\alpha}(z)\right) = ne^{-z}z^{\alpha-1}L_{n}^{\alpha-1}(z).$$

Furthermore,

$$\frac{(-1)^{n+1}g^2}{8\pi R n! n^2} \left(M'_{n,1/2} \left(\frac{gy}{2n} \right) W_{n,1/2} \left(\frac{gx}{2n} \right) - M_{n,1/2} \left(\frac{gy}{2n} \right) W'_{n,1/2} \left(\frac{gx}{2n} \right) \right) \\
= \frac{g^2}{8\pi R n^2} \left(M_{n,1/2} \left(\frac{gx}{2n} \right) M'_{n,1/2} \left(\frac{gy}{2n} \right) - M_{n,1/2} \left(\frac{gy}{2n} \right) M'_{n,1/2} \left(\frac{gx}{2n} \right) \right) \\
= \frac{g^3}{16\pi R n^4} \exp\left(-\frac{g}{2n} (r+r_0) \right) \left(x L_{n-1}^1 \left(\frac{gx}{2n} \right) L_n \left(\frac{gy}{2n} \right) - y L_{n-1}^1 \left(\frac{gy}{2n} \right) L_n \left(\frac{gx}{2n} \right) \right).$$
(32)

After rescaling $r \to (n/g)r$, $r_0 \to (n/g)r_0$, we get from (31) and (32)

$$\sum_{\ell=0}^{n-1} \frac{(2\ell+1)(n-\ell-1)!}{(n+\ell)!} (rr_0)^\ell L_{n-\ell-1}^{2\ell+1}(r) L_{n-\ell-1}^{2\ell+1}(r_0) P_\ell(\cos(\gamma))$$

$$= \frac{(-1)^{n+1}}{(n-1)!R} \exp\left(\frac{r+r_0}{2}\right) \left(M_{n,1/2}'\left(\frac{y}{2}\right) W_{n,1/2}\left(\frac{x}{2}\right) - M_{n,1/2}\left(\frac{y}{2}\right) W_{n,1/2}'\left(\frac{x}{2}\right)\right)$$

$$= \frac{1}{2R} \left(x L_{n-1}^1\left(\frac{x}{2}\right) L_n\left(\frac{y}{2}\right) - y L_{n-1}^1\left(\frac{y}{2}\right) L_n\left(\frac{x}{2}\right)\right).$$
oncludes the proof.

This concludes the proof.

Let us check two particular cases of (28). For $\gamma = 0$ we have

$$\sum_{\ell=0}^{n-1} \frac{(2\ell+1)(n-\ell-1)!}{(n+\ell)!} (rr_0)^{\ell} L_{n-\ell-1}^{2\ell+1}(r) L_{n-\ell-1}^{2\ell+1}(r_0)$$
$$= \frac{1}{r-r_0} \left(r L_{n-1}^1(r) L_n(r_0) - r_0 L_{n-1}^1(r_0) L_n(r) \right)$$

and for $\gamma = \pi$ we get

$$\sum_{\ell=0}^{n-1} (-1)^{\ell} \frac{(2\ell+1)(n-\ell-1)!}{(n+\ell)!} (rr_0)^{\ell} L_{n-\ell-1}^{2\ell+1}(r) L_{n-\ell-1}^{2\ell+1}(r_0) = L_{n-1}^1(r+r_0),$$

Note that $L_n(0) = 1$ (and $L_n^1(0) = n + 1$).

After the shift $n \to n+1$ one observes, in these two particular cases, that both sides are symmetric polynomials in r and r_0 , and therefore r, r_0 can be replaced by arbitrary complex variables.

Corollary 5. For every $n \in \mathbb{Z}_+$ and all $u, v \in \mathbb{C}$,

$$\sum_{\ell=0}^{n} \frac{(2\ell+1)(n-\ell)!}{(n+\ell+1)!} (uv)^{\ell} L_{n-\ell}^{2\ell+1}(u) L_{n-\ell}^{2\ell+1}(v) = \frac{1}{u-v} \left(u L_{n-1}^{1}(u) L_{n}(v) - v L_{n-1}^{1}(v) L_{n}(u) \right)$$
(33)

and

$$\sum_{\ell=0}^{n} (-1)^{\ell} \frac{(2\ell+1)(n-\ell)!}{(n+\ell+1)!} (uv)^{\ell} L_{n-\ell}^{2\ell+1}(u) L_{n-\ell}^{2\ell+1}(v) = L_n^1(u+v).$$
(34)

As a short digression let us note that the projection \mathcal{P}_n , as introduced in equation (30) in the proof, has already been discussed in the literature [3]. Using expression for the residue of Green's function, see (29) and (32), we get, for $n \geq 1$,

$$\mathcal{P}_n(r,\theta,\varphi,r_0,\theta_0,\varphi_0) = \frac{g^3}{16\pi Rn^4} \exp\left(-\frac{g}{2n}(r+r_0)\right) \\ \times \left(xL_{n-1}^1\left(\frac{gx}{2n}\right)L_n\left(\frac{gy}{2n}\right) - yL_{n-1}^1\left(\frac{gy}{2n}\right)L_n\left(\frac{gx}{2n}\right)\right).$$

The diagonal in fact does not depend on angles and equals

$$\mathcal{P}_n(r,\theta,\varphi,r,\theta,\varphi) = \frac{g^3}{8\pi n^4} \exp\left(-\frac{gr}{n}\right) \\ \times \left(L_n\left(\frac{gr}{n}\right)L_{n-1}^1\left(\frac{gr}{n}\right) - \frac{gr}{n}L_n\left(\frac{gr}{n}\right)L_{n-2}^2\left(\frac{gr}{n}\right) + \frac{gr}{n}L_{n-1}^1\left(\frac{gr}{n}\right)^2\right).$$

 $\mathcal{P}_n(r,\theta,\varphi,r_0,\theta_0,\varphi_0)$ is called the density function in [3], and

$$D_n(r) := 4\pi r^2 \mathcal{P}_n(r,\theta,\varphi,r,\theta,\varphi)$$

is called the radial distribution function. It holds true that

$$4\pi \int_0^\infty \mathcal{P}_n(r,\theta,\varphi,r,\theta,\varphi) r^2 \mathrm{d}r = n^2$$

meaning that

$$\int_0^\infty \exp(-r) \left(L_n(r) L_{n-1}^1(r) - r L_n(r) L_{n-2}^2(r) + r L_{n-1}^1(r)^2 \right) r^2 dr = 2n^3.$$

V. SOME COMPLEMENTARY SUMMATION FORMULAS

The following proposition presents a summation formula for the Whittaker functions $W_{\kappa,\mu}$ and is a straightforward corollary of Theorem 8 below which in turn generalizes the addition formula (25). Nevertheless this proposition should be proven independently because, conversely, it is used in the proof of Theorem 8.

Proposition 6. For every $n \in \mathbb{N}$, r > 0, $\kappa, \mu \in \mathbb{C}$, $2\mu \neq -1, -2, -3, \ldots$,

$$\sum_{\ell=0}^{n} (-1)^{\ell} \binom{n}{\ell} \frac{2\mu + 2\ell}{(2\mu + \ell)_{n+1}} W_{\kappa,\mu+\ell}(r) = (-1)^{n} r^{-n/2} W_{\kappa-n/2,\mu+n/2}(r).$$
(35)

Proof. We shall proceed by induction in n. For n = 0 the equation is trivial. For n = 1 this is a well known identity (for instance, this is a combination of equations 9.234 ad(1) and ad(2) in [9])

$$W_{\kappa,\mu+1}(r) - W_{\kappa,\mu}(r) = \frac{2\mu+1}{\sqrt{r}} W_{\kappa-1/2,\mu+1/2}(r).$$
(36)

Suppose n > 0. Set, for k = 0, 1, ..., n,

$$A(k) := \sum_{\ell=0}^{n-k-1} (-1)^{\ell} {n \choose \ell} \frac{2\mu + 2\ell}{(2\mu + \ell)_{n+1}} W_{\kappa,\mu+\ell}(r) + (-1)^{n+k} {n-1 \choose k} \frac{W_{\kappa,\mu+n-k}(r)}{(2\mu + n - k)_n} \\ - \frac{1}{\sqrt{r}} \sum_{\ell=n-k}^{n-1} (-1)^{\ell} {n-1 \choose \ell} \frac{2\mu + 2\ell + 1}{(2\mu + \ell + 1)_n} W_{\kappa-1/2,\mu+\ell+1/2}(r).$$

In particular,

$$A(0) = \sum_{\ell=0}^{n-1} (-1)^{\ell} {n \choose \ell} \frac{2\mu + 2\ell}{(2\mu + \ell)_{n+1}} W_{\kappa,\mu+\ell}(r) + (-1)^{n} \frac{W_{\kappa,\mu+n}(r)}{(2\mu + n)_{n}}$$
$$= \sum_{\ell=0}^{n} (-1)^{\ell} {n \choose \ell} \frac{2\mu + 2\ell}{(2\mu + \ell)_{n+1}} W_{\kappa,\mu+\ell}(r).$$

Thus A(0) coincides with the LHS of equation (35).

We claim that A(k+1) = A(k) for k = 0, 1, ..., n-1. Suppose $0 \le k < n$. Then

$$\begin{aligned} A(k+1) - A(k) &= (-1)^{n+k} \binom{n}{k+1} \frac{2\mu + 2n - 2k - 2}{(2\mu + n - k - 1)_{n+1}} W_{\kappa,\mu+n-k-1}(r) \\ &+ (-1)^{n+k+1} \binom{n-1}{k+1} \frac{W_{\kappa,\mu+n-k-1}(r)}{(2\mu + n - k - 1)_n} \\ &+ (-1)^{n+k+1} \binom{n-1}{k} \frac{W_{\kappa,\mu+n-k}(r)}{(2\mu + n - k)_n} \\ &+ \frac{1}{\sqrt{r}} (-1)^{n+k} \binom{n-1}{k} \frac{2\mu + 2n - 2k - 1}{(2\mu + n - k)_n} W_{\kappa-1/2,\mu+n-k-1/2}(r) \,. \end{aligned}$$

With the aid of (36) one finds that this expression equals

$$(-1)^{n+k+1} \binom{n-1}{k+1} \frac{(2\mu+2n-k-1)W_{\kappa,\mu+n-k-1}(r)}{(2\mu+n-k-1)_{n+1}} -(-1)^{n+k+1} \binom{n}{k+1} \frac{(2\mu+2n-2k-2)W_{\kappa,\mu+n-k-1}(r)}{(2\mu+n-k-1)_{n+1}} +(-1)^{n+k+1} \binom{n-1}{k} \frac{(2\mu+n-k-1)W_{\kappa,\mu+n-k-1}(r)}{(2\mu+n-k-1)_{n+1}}.$$

Now it is elementary to see that the expression actually equals 0, and therefore A(k+1) - A(k) = 0.

In A(n) we apply substitutions $\kappa' = \kappa - 1/2$, $\mu' = \mu + 1/2$, and obtain, by the induction hypothesis,

$$A(n) = -\frac{1}{\sqrt{r}} \sum_{\ell=0}^{n-1} (-1)^{\ell} {\binom{n-1}{\ell}} \frac{2\mu'+2\ell}{(2\mu'+\ell)_n} W_{\kappa',\mu'+\ell}(r)$$

$$= -\frac{1}{\sqrt{r}} (-1)^{n-1} r^{-(n-1)/2} W_{\kappa'-(n-1)/2,\mu'+(n-1)/2}(r)$$

$$= (-1)^n r^{-n/2} W_{\kappa-n/2,\mu+n/2}(r).$$

Since A(0) = A(n), the identity follows.

Remark 7. From (35) it follows that, for $n \in \mathbb{Z}_+$,

$$\sum_{\ell=0}^{n} (-1)^{\ell} \binom{n}{\ell} \frac{2\mu + 2\ell}{(2\mu + \ell)_{n+1}} = \delta_{n,0}.$$

Indeed, one just has to recall (7) and compare the asymptotic expansions of both sides of (35) as $r \to \infty$.

Here is a generalization of the addition formula for the Whittaker functions (25).

Theorem 8. For $0 \le r_0 < r$, $\kappa, \mu \in \mathbb{C}$, $\operatorname{Re} \mu > 0$,

$$\frac{1}{(rr_0)^{\mu+1/2}} \sum_{\ell=0}^{\infty} (-1)^{\ell} \frac{(\mu-\kappa+1/2)_{\ell}}{(\ell+2\mu)_{\ell} \ell!} M_{\kappa,\ell+\mu}(r_0) W_{\kappa,\ell+\mu}(r) = \frac{1}{(r+r_0)^{\mu+1/2}} W_{\kappa,\mu}(r+r_0).$$
(37)

Remark. The equation for $r_0 = 0$ should be understood as a limiting case of (37), and it is trivial.

Remark 9. Regarding the convergence of the series, it is guaranteed by the assumption $0 \le r_0 < r$. Let us shortly analyze this point. Put

$$t_{\ell} := \left(\frac{r+r_0}{r\,r_0}\right)^{\mu+1/2} \frac{(\mu-\kappa+1/2)_{\ell} M_{\kappa,\ell+\mu}(r_0) W_{\kappa,\ell+\mu}(r)}{(\ell+2\mu)_{\ell} \,\ell! \, W_{\kappa,\mu}(r+r_0)},$$

so that (37) becomes $\sum_{\ell=0}^{\infty} (-1)^{\ell} t_{\ell} = 1$. Referring to (8) and (9), we replace the Whittaker functions in the numerator by their leading asymptotic terms and get

$$t_{\ell} = \frac{2^{2\mu-1}(r+r_0)^{\mu+1/2}}{\sqrt{\pi} r^{2\mu} W_{\kappa,\mu}(r+r_0)} \frac{(\mu-\kappa+1/2)_{\ell} \Gamma(\ell+\kappa+\mu)}{\ell! (\ell+2\mu)_{\ell}} \left(\frac{4r_0}{r}\right)^{\ell} \left(1+O(\ell^{-1})\right).$$

Next we do the same for the factorial and the Pochhammer symbols in the expression while using Stirling's asymptotic formula. We find that for large ℓ ,

$$t_{\ell} = \frac{(r+r_0)^{\mu+1/2}}{\Gamma(\mu-\kappa+1/2) r^{2\mu} W_{\kappa,\mu}(r+r_0)} \,\ell^{2\mu-1} \left(\frac{r_0}{r}\right)^{\ell} \left(1+O(\ell^{-1})\right).$$

This obviously guarantees the convergence.

But on the other hand, the series turns out to be numerically quite unstable for large values of μ . In such a case we can be dealing with an alternating series with many summands in its beginning attaining huge values. Then significant cancellations of the terms necessarily happen. From the numerical point of view this is a troublesome situation. As an example let us consider the case with $\mu = 20$, $\kappa = 1$, $r_0 = 1$, and r = 2. The Computer Algebra System *Mathematica*, as of version 14.0.0, gives the values $t_0 = 1.07239 \times 10^7$, $t_{145} = 3214.65$, and is not capable to compute t_{ℓ} for higher indices. Nonetheless replacing the involved Wittaker functions by their leading asymptotic terms for μ large one finds that the first index for which t_{ℓ} attains a value smaller than 0.1 is $\ell = 168$. This shows that this concrete series starts to rapidly converge to its final sum only for very large summation indices.

Proof. In view of (1) and (2) the equation can be rewritten as

$$\sum_{\ell=0}^{\infty} (-1)^{\ell} \frac{(\mu - \kappa + 1/2)_{\ell}}{(\ell + 2\mu)_{\ell} \ell!} (rr_{0})^{\ell} \times {}_{1}F_{1} \left(\ell + \mu - \kappa + \frac{1}{2}; 2\ell + 2\mu + 1; r_{0}\right) U \left(\ell + \mu - \kappa + \frac{1}{2}, 2\ell + 2\mu + 1, r\right) = U \left(\mu - \kappa + \frac{1}{2}, 2\mu + 1, r + r_{0}\right).$$
(38)

We have [1, Eq. 13.4.21]

$$\frac{\partial^j}{\partial r^j}U(a,b,r) = (-1)^j(a)_j U(a+j,b+j,r), \quad j \in \mathbb{Z}_+.$$

whence

$$U(a, b, r+r_0) = \sum_{n=0}^{\infty} \frac{(-1)^n (a)_n}{n!} U(a+n, b+n, r) r_0^n.$$

Using, in (38), this power expansion as well as the power expansion of ${}_{1}F_{1}$ we get

$$\begin{split} \sum_{\ell=0}^{\infty} (-1)^{\ell} \frac{(1/2+\mu-\kappa)_{\ell}}{(l+2\mu)_{\ell} \,\ell!} & \sum_{j=0}^{\infty} \frac{(\ell+\mu-\kappa+1/2)_{j}}{(2l+2\mu+1)_{j} \,j!} \\ & \times U \bigg(\ell+\mu-\kappa+\frac{1}{2}, 2\ell+2\mu+1, r \bigg) \, r^{\ell} r_{0}^{\ell+j} \\ &= \sum_{n=0}^{\infty} \frac{(-1)^{n} \, (\mu-\kappa+1/2)_{n}}{n!} \, U \bigg(\mu-\kappa+n+\frac{1}{2}, 2\mu+n+1, r \bigg) \, r_{0}^{n}. \end{split}$$

Comparing the coefficients at the same powers of r_0 we obtain an equivalent countable system of equations, with $n \in \mathbb{Z}_+$,

$$\sum_{\ell=0}^{n} (-1)^{\ell} {n \choose \ell} \frac{(2\ell+2\mu)}{(\ell+2\mu)_{n+1}} r^{\ell} U \left(\mu+\ell-\kappa+\frac{1}{2}, 2\mu+2\ell+1, r\right)$$
$$= (-1)^{n} U \left(\mu-\kappa+n+\frac{1}{2}, 2\mu+n+1, r\right).$$

Expressing reversely the confluent hypergeometric function U in terms of the Whittaker function W we get

$$\sum_{\ell=0}^{n} (-1)^{\ell} \binom{n}{\ell} \frac{2\mu + 2\ell}{(2\mu + \ell)_{n+1}} W_{\kappa,\mu+\ell}(r) = (-1)^{n} r^{-n/2} W_{\kappa-n/2,\mu+n/2}(r)$$

This identity has been proven in Proposition 6.

Finally we prove a summation formula for the Whittaker functions $M_{\kappa,\mu}$.

Proposition 10. For $z \in \mathbb{C}$, $\kappa \in \mathbb{C}$, $\mu > 0$ and $c \in [-1, 1]$,

$$\sum_{\ell=0}^{\infty} \frac{(\mu - \kappa + 1/2)_{\ell}}{(2\mu)_{2\ell}} z^{\ell} {}_{1}F_{1}\left(\ell + \mu - \kappa + \frac{1}{2}; 2\ell + 2\mu + 1; z\right) C_{\ell}^{(\mu)}(c)$$

= ${}_{1}F_{1}\left(\mu - \kappa + \frac{1}{2}; \mu + \frac{1}{2}; \frac{1+c}{2}z\right),$ (39)

or, if rewritten in terms of the Whittaker functions, with $\gamma \in [-\pi, \pi]$,

$$z^{-\mu-1/2} \sum_{\ell=0}^{\infty} \frac{(\mu-\kappa+1/2)_{\ell}}{(2\mu)_{2\ell}} M_{\kappa,\ell+\mu}(z) C_{\ell}^{(\mu)}(\cos(\gamma))$$

= $e^{-z/2} {}_{1}F_{1}\left(\mu-\kappa+\frac{1}{2};\mu+\frac{1}{2};\cos^{2}\left(\frac{\gamma}{2}\right)z\right).$ (40)

Remark 11. Here we tacitly assume that $z^{-\mu-1/2}M_{\kappa,\ell+\mu}(z)$ is understood as an entire function – first defined on the positive half-line and then admitting an unambiguous continuation to the entire complex plane as an analytic function.

The particular case $\gamma = 0$ gives

$$\sum_{\ell=0}^{\infty} \frac{(\mu-\kappa+1/2)_{\ell}}{(\ell+2\mu)_{\ell}\,\ell!} \, M_{\kappa,\ell+\mu}(z) = e^{-z/2} \, {}_{1}F_1\left(\mu-\kappa+\frac{1}{2};\mu+\frac{1}{2};z\right),$$

and the particular case $\gamma = \pi$ gives

$$z^{-\mu-1/2} \sum_{\ell=0}^{\infty} (-1)^{\ell} \frac{(\mu-\kappa+1/2)_{\ell}}{(l+2\mu)_{\ell} \ell!} M_{\kappa,\ell+\mu}(z) = e^{-z/2}.$$
 (41)

Note that

$$C_{\ell}^{(\mu)}(1) = \frac{(2\mu)_{\ell}}{\ell!}, \ C_{\ell}^{(\mu)}(-1) = (-1)^{\ell} \frac{(2\mu)_{\ell}}{\ell!}$$

We remark that (41) is a generalization of (26).

Remark 12. Convergence of the series in (40) can be justified by exploring the asymptotic behavior of the summands. Regarding the Gegenbauer polynomials, an elaborate asymptotic expansion for large orders is derived in a recent paper [6]. For our purposes

a comparatively simple approach is sufficient. From equation (3.30) in [2] one infers that

$$\frac{C_{\ell}^{(\nu)}(\cos(\theta))}{C_{\ell}^{(\nu)}(1)} = \frac{2\Gamma\left(\nu + \frac{1}{2}\right)}{\sqrt{\pi}\,\Gamma(\nu)}$$
$$\times \int_{0}^{\pi/2} \cos^{2\nu-1}(\varphi) \cos\left(\ell \arccos\left(\frac{\cos(\theta)}{\sqrt{1 - \sin^{2}(\theta)\cos^{2}(\varphi)}}\right)\right) (1 - \sin^{2}(\theta)\cos^{2}(\varphi))^{\ell/2} d\varphi$$

for $\nu > 0, 0 \le \theta \le \pi$ and $\ell \in \mathbb{Z}_+$. It follows that

$$\frac{|C_{\ell}^{(\nu)}(\cos(\theta))|}{C_{\ell}^{(\nu)}(1)} \le \frac{2\Gamma\left(\nu + \frac{1}{2}\right)}{\sqrt{\pi}\,\Gamma(\nu)} \int_{0}^{\pi/2} \cos^{2\nu - 1}(\varphi) \,d\varphi = 1.$$

Thus for $c \in [-1, 1]$ we have

$$|C_{\ell}^{(\mu)}(c)| \le C_{\ell}^{(\mu)}(1) = \frac{(2\mu)_{\ell}}{\ell!} = \frac{\ell^{2\mu-1}}{\Gamma(2\mu)} \left(1 + O(\ell^{-1})\right) \text{ as } \ell \to \infty.$$

Furthermore, for ℓ sufficiently large, surely for any ℓ such that $\ell + 2\mu + 1 > |\mu - \kappa + 1/2|$, we can estimate

$$\forall n \ge 0, \ \frac{|(\ell + \mu - \kappa + 1/2)_n|}{(2\ell + 2\mu + 1)_n} \le 1,$$

and therefore

$$\left| {}_{1}F_{1}\left(\ell + \mu - \kappa + \frac{1}{2}; 2\ell + 2\mu + 1; z\right) \right| \leq K(\kappa, \mu) e^{|z|}$$

where $K(\kappa, \mu)$ is a constant independent of ℓ and z although it may depend on κ and μ . The convergence now becomes obvious.

These estimates even show that the LHS of (39) is an entire function.

Proof. Using the power series expansion for the hypergeometric series we have to show that

$$\sum_{\ell=0}^{\infty} \sum_{j=0}^{\infty} \frac{(\mu - \kappa + 1/2)_{\ell}}{(2\mu)_{\ell}(l + 2\mu)_{\ell}} \frac{(\ell + \mu - \kappa + 1/2)_{j}}{(2\ell + 2\mu + 1)_{j} j!} C_{\ell}^{(\mu)}(c) z^{\ell+j}$$
$$= \sum_{n=0}^{\infty} \frac{(\mu - \kappa + 1/2)_{n}}{(\mu + 1/2)_{n} n!} \left(\frac{1+c}{2}\right)^{n} z^{n}.$$

Comparing coefficients at the same powers of z we get an equivalent countable set of equations, with $n \in \mathbb{Z}_+$,

$$\sum_{\ell=0}^{n} \frac{(\mu-\kappa+1/2)_{\ell}}{(2\mu)_{2\ell}} \frac{(\ell+\mu-\kappa+1/2)_{n-\ell}}{(2\ell+2\mu+1)_{n-\ell}(n-\ell)!} C_{\ell}^{(\mu)}(c) = \frac{(\mu-\kappa+1/2)_{n}}{(\mu+1/2)_{n}n!} \left(\frac{1+c}{2}\right)^{n}.$$

These equations can be simplified using straightforward manipulations,

$$\sum_{\ell=0}^{n} \frac{(2\mu+2\ell)}{(2\mu)_{n+\ell+1}(n-\ell)!} C_{\ell}^{(\mu)}(c) = \frac{2^{n}(\mu)_{n}}{(2\mu)_{2n} n!} (1+c)^{n}.$$

Recall that [12, Eq. (9.8.19)]

$$C_{\ell}^{(\mu)}(c) = \frac{(2\mu)_{\ell}}{\ell!} {}_{2}F_{1}\left(-\ell, 2\mu + \ell; \mu + \frac{1}{2}; \frac{1-c}{2}\right)$$

After the substitution c = 1 - 2w we get the equation

$$\sum_{\ell=0}^{n} \frac{(2\mu+2\ell)}{(2\mu)_{n+\ell+1}(n-\ell)!} \frac{(2\mu)_{\ell}}{\ell!} {}_{2}F_{1}\left(-\ell, 2\mu+\ell; \mu+\frac{1}{2}; w\right) = \frac{2^{2n}(\mu)_{n}}{(2\mu)_{2n}n!} (1-w)^{n}.$$

And after the power series expansion of the hypergeometric function and interchanging the order of summation we obtain

$$\sum_{j=0}^{n} \left(\sum_{\ell=j}^{n} \frac{(2\mu+2\ell)}{(2\mu)_{n+\ell+1}(n-\ell)!} \frac{(2\mu)_{\ell}}{\ell!} \frac{(-\ell)_{j}(2\mu+\ell)_{j}}{(\mu+1/2)_{j}j!} \right) w^{j} = \frac{2^{2n}(\mu)_{n}}{(2\mu)_{2n}n!} (1-w)^{n}.$$

Comparing coefficients at the same powers of w leads to the equations

$$\sum_{\ell=j}^{n} \frac{(2\mu+2\ell)}{(2\mu)_{n+\ell+1}(n-\ell)!} \frac{(2\mu)_{\ell}}{\ell!} \frac{(-\ell)_j(2\mu+\ell)_j}{(\mu+1/2)_j} = \frac{(-1)^j}{(n-j)!} \frac{2^{2n}(\mu)_n}{(2\mu)_{2n}}, \quad 0 \le j \le n,$$

and this can be further rewritten,

$$\sum_{\ell=j}^{n} \binom{n-j}{\ell-j} \frac{2\mu+2\ell}{(2\mu+\ell+j)_{n-j+1}} = \frac{(\mu+1/2)_j}{(\mu+1/2)_n}, \quad 0 \le j \le n.$$

Shifting the summation index $\ell \to \ell + j$ and applying the substitutions n = N + j, $\nu = \mu + j$, we obtain an identity (equation (42)) which is proven in Lemma 13 below thus concluding this proof.

Lemma 13. For $N \in \mathbb{Z}_+$ and $\nu \in \mathbb{C}$, $\nu \neq 0, -1, -2, \ldots$,

$$\sum_{\ell=0}^{N} \binom{N}{\ell} \frac{2\nu + 2\ell}{(2\nu + \ell)_{N+1}} = \frac{1}{(\nu + 1/2)_N}.$$
(42)

Proof. For $N \in \mathbb{Z}_+$, consider the expression

$$\sum_{\ell=0}^{N} \binom{N}{\ell} \frac{(2\nu+2\ell)(\nu+1/2)_N}{(2\nu+\ell)_{N+1}}$$
(43)

which is regarded as a function of $\nu \in \mathbb{C}$. This is a meromorphic function on \mathbb{C} , and its limit, as $\nu \to \infty$, equals

$$\sum_{\ell=0}^{N} \binom{N}{\ell} \frac{1}{2^{N}} = 1.$$

$$(44)$$

The poles are located at the points $\nu = 0, -1/2, -1, \dots, -(2N-1)/2, -N$, and all of them are of first order.

Owing to the factor $(\nu + 1/2)_N$ the singularities are removable for

$$\nu = -1/2, -3/2, \dots, -(2N-1)/2.$$

Hence it suffices to check the poles at $\nu = 0, -1, \ldots, -N$. The residue at a pole $\nu = -t, 0 \le t \le N$, equals

$$(-t+1/2)_N \sum_{\ell=\max\{2t-N,0\}}^{\min\{2t,N\}} \binom{N}{\ell} \frac{-2t+2\ell}{(-2t+\ell)_{2t-\ell}(1)_{N-2t+\ell}}$$
$$= (-t+1/2)_N \sum_{\ell=\max\{2t-N,0\}}^{\min\{2t,N\}} (-1)^\ell \binom{N}{\ell} \frac{-2t+2\ell}{(2t-\ell)!(N-2t+\ell)!}$$

Further we omit the nonzero factor $2(-t+1/2)_N$. Shifting the summation index $\ell \to t + \ell$, for $t \ge N/2$ we get

$$\sum_{l=2t-N}^{N} (-1)^{\ell} \binom{N}{\ell} \frac{-t+\ell}{(2t-\ell)!(N-2t+\ell)!} = \frac{(-1)^{t}}{N!} \sum_{\ell=t-N}^{N-t} (-1)^{\ell} \binom{N}{t+\ell} \binom{N}{t-\ell} \ell = 0.$$

Just note that the summands are odd in ℓ . For $t \leq N/2$ we similarly get

$$\sum_{\ell=0}^{2t} (-1)^{\ell} \binom{N}{\ell} \frac{-t+\ell}{(2t-\ell)!(N-2t+\ell)!} = \frac{(-1)^{t}}{N!} \sum_{\ell=-t}^{t} (-1)^{\ell} \binom{N}{t+\ell} \binom{N}{t-\ell} \ell = 0$$

Hence all singularities are removable and therefore expression (43) equals 1 identically from (44) and Liouville's Theorem. $\hfill \Box$

ACKNOWLEDGMENTS

The author acknowledges partial support by European Regional Development Fund Project "Center for Advanced Applied Science" No. CZ.02.1.01/0.0/0.0/16_019/0000778. The author is indebted to the reviewer for numerous comments helpful in improving the quality of the paper, and in particular for Remark 9.

References

- ¹ M. Abramowitz, I. A. Stegun: *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables,* (Dover Publications, New York, 1972).
- ² R. Askey: Orthogonal Polynomials and Special Functions, (SIAM, Philadelphia, 1975).
- ³ S. M. Blinder: Generalized Unsöld theorem and radial distribution function for hydrogenic orbitals, J. Math. Chem., **14** (1993), 319-324.
- ⁴ NIST Digital Library of Mathematical Functions. https://dlmf.nist.gov/, Release 1.1.11 of 2023-09-15. F. W. J. Olver, A. B. Olde Daalhuis, D. W. Lozier, B. I. Schneider, R. F. Boisvert, C. W. Clark, B. R. Miller, B. V. Saunders, H. S. Cohl, and M. A. McClain, eds.
- ⁵ T. M. Dunster: Uniform asymptotic expansions for the Whittaker functions $M_{\kappa,\mu}(z)$ and $W_{\kappa,\mu}(z)$ with μ large, Proc. R. Soc. A **477** (2021), 0360.
- ⁶ T. M. Dunster: Uniform asymptotic expansions for Gegenbauer polynomials and related functions via differential equations having a simple pole, Constr. Approx. (2023), https://doi.org/10.1007/s00365-023-09645-1.
- ⁷ A. Erdélyi, W. Magnus, F. Oberhettinger, F. G. Tricomi: *Higher Transcendental Functions. Vol. II.* (McGraw-Hill Book Company, Inc., New York-Toronto-London, 1953).
- ⁸ N. M. Ferrers: An elementary treatise on spherical harmonics and subjects connected with them, (MacMillan, London, 1877).
- ⁹ I. S. Gradshteyn, I. M. Ryzhik: *Table of Integrals, Series, and Products*, Edited by A. Jeffrey and D. Zwillinger, (Academic Press, Amsterdam, 2007).
- ¹⁰ L. C. Hostler: Coulomb Green's function in closed form, Bull. Am. Phys. Soc. 7 (1962), 609.
- ¹¹ L. C. Hostler, R. H. Pratt: Coulomb Green's function in closed form, Phys. Rev. Lett. 10 (1963), 469-470.
- ¹² R. Koekoek, P. A. Lesky, R. F. Swarttouw: *Hypergeometric Orthogonal Polynomials and Their q-Analogues*, (Springer, Berlin, 2010).
- ¹³ K. Maleček, Z. Nádeník: On the inductive proof of Legendre addition theorem, Studia Geophysica et Geodaetica 45 (2001), 1-11.
- ¹⁴ F. W. J. Olver: Asymptotics and Special Functions, (A. K. Peters, Wellesley, 1997).
- ¹⁵ A. Rauh: On the singularities of the nonrelativistic Coulomb Green's function, Adv. Stud. Theor. Phys. **13** (2019), 175-187.

- ¹⁶ S. S. Vasan, M. Seetharaman: The Coulomb Green's function revisited, Pramana J. Phys. 45 (1995), 165-174.
- ¹⁷ G. N. Watson: A Treatise on the Theory of Bessel Functions, 2nd edition, (Cambridge University Press, Cambridge, 1944).