Advanced Studies in Theoretical Physics
Vol. 13, 2019, no. 4, 175 - 187
HIKARI Ltd, www.m-hikari.com
https://doi.org/10.12988/astp.2019.9413

On the Singularities of the Nonrelativistic Coulomb Green's Function

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Abstract

The Green's function of the nonrelativistic Coulomb problem is derived by polar coordinates. The radial part contains the product of the two Whittaker functions M and W; the result is consistent with that of Hostler (1962) who used Lambert coordinates. The function W contains a logarithmic singularity which is related to the continuous energy spectrum. When one goes for numbers, one has to define the physically correct branch of the logarithm, $\ln(z)$, with $z = -2\mathbf{i}\,k\,r_1$, where k is related to the energy parameter $E = k^2/2$ and r_1 is a radial coordinate. The built-in Mathematica function W of Wolfram Research renders the principal value of the logarithm. However, if k is varied in the complex plane, the first singularity, predicted by the Mathematica algorithm for W, appears on the negative imaginary axes which would lead to a negative continuous energy spectrum. By an elementary analysis, it is found that with the complex parameter $k = |k|\exp[\mathbf{i}\,\varphi]$, the logarithm of z should be extended to two sheets of the Riemann surface. We introduce the correction term to the function W of Mathematica in analytical form, such that the singularities of the Green function give the physically correct energy spectrum.

PACS: 02.70.Wz, 03.65.-w

1 Introduction

In an attempt to determine quantum mechanically the time evolution of rectilinear Kepler orbits [17], we studied the method of Green's function (GF)

and checked existing formulas numerically. For this purpose, Mathematica [21] offers useful tools: both, the two Whittaker functions M and W, and the confluent hypergeometric function are implemented. In addition, asymptotic series of these functions can be obtained by key stroke.

After relatively involved integral representations of the GF were achieved, e.g. by Schwinger [18] or bei Meixner [14], it was kind of a sensation when Hostler (1962) derived the Coulomb GF in a compact closed form, basically in terms of a product of the two Whittaker functions [10, 11]. Based on Lambert's theorem [7, 15, 2, 13, 16], Hostler uses a minimal set of two coordinates, namely, $x = r_1 + r_2 + r_{12}$ and $y = r_1 + r_2 - r_{12}$ with $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$. From Hostler's GF, an analytic form of the propagator was derived by Blinder [3]; for special cases of the propagator see, e.g. [12], A different approach to obtain the GF was undertaken by Hameka [8, 9], but remained uncompleted, as to our opinion. Hameka used polar coordinates and Meixner's [14] method which amounts to sum over the eigenstates of the spectral representation of the GF.

In the present article, we partly adopt Hameka's concept but apply Hostler's method which consists in solving the Coulomb differential equation for the GF and in taking into account the proper physical boundary conditions. The configuration space is now three- rather than two-dimensional, with the coordinates r_1, r_2, and $\hat{\mathbf{r}}_1 \cdot \hat{\mathbf{r}}_2$. We, nevertheless, see some advantages of the GF found: When G is represented by spherical harmonics, the radial part G_l (for angular momentum quantum number l), factorizes with respect to the radial coordinates r_1 and r_2; the radial part contains the product of the two Whittaker functions, but has not to be differentiated as in Hostler's work; our GF may also be convenient, if one has to couple with initial, low angular momentum wave packets.

The GF depends parametrically on a complex energy parameter E, which in dimensionless form is set equal to $k^2/2$. As a function of k, the singularities of the GF give the energy spectrum of the Hamiltonian: The poles at $k_n = \mathbf{i}/n$, $n = l+1, l+2, \ldots$ correspond to the discrete spectrum, whereas a branch cut along the negative k axes is related with the continuous positive eigenvalues. In examining the singular structure of the GF found, one immediately observes the Gamma function, as a pre-factor, which produces the poles for the discrete spectrum. The continuous spectrum, on the other hand, is hidden in the non-analytic part of the Whittaker function $W_{\kappa,\nu}(z)$, where $\kappa = \mathbf{i}/k$, $\nu = (2l+1)/2$, and $z = -2\mathbf{i}\,k\,r_1$. To verify the location of the branch cut, we used the Mathematica function "WhittakerW[$\mathbf{i}/k, 1/2, z$]" and produced plots for $k = |k| \exp[\mathbf{i}\,\varphi]$ as a function of the phase φ. Surprisingly, the branch cut had to be located along the negative imaginary axes of k. As far as we know, the Whittaker function W of Mathematica is implemented by the integral representation given in Section $16 \cdot 12$ of Whittaker/Watson [19], for details of the implementation in Mathematica, see [20].

To analyze the discrepancy, the work of Buchholz [4] was most useful: The formula (25a) in §2 explicitly reveals the source of the nonanalyticity of W: the multivalued logarithm $\ln(z) \equiv \ln(-2\mathbf{i}\,k\,r_1)$, which Mathematica renders by the principal value, $\ln(z) = \ln(|z|) + \mathbf{i}\,\phi$ with $-\pi < \phi \leq \pi$. When k is varied in the complex plane, one needs a further sheet of the Riemann surface of $\ln(z)$ to predict the physical energy spectrum. The main conclusions of the article are illustrated by Fig.1 and Fig.2.

In Sec. II., we derive the 3-D Coulomb Green's function by using polar coordinates. In Sec. III., the branch cut of the Whittaker function W is analyzed, followed by Sec. Conclusion. Appendix A gives the definition of the Whittaker functions together with an explicit series representation of W from [4]. In Appendix B, numerical checks are presented on the Wronskian of the two Whittaker functions. The checks also indicate the high precision of the Mathematica algorithms for rendering numbers for M and W. In Appendix C, we comment on the different definitions of the Meixner function F_2.

2 The Green's function in polar coordinates

We are interested in the time evolution of a wave packet Ψ_0 from $t = 0$ to $t > 0$. To this end, we will apply the method of Green functions as follows

$$\psi(\mathbf{r}, t) = \exp\left[-(\mathbf{i}/\hbar)H\,t\right]\Psi_0 = \exp\left[-(\mathbf{i}/\hbar)H\,t\right]\sum_{\nu}|\psi_\nu\rangle\langle\psi_\nu^*|\,\Psi_0, \qquad (1)$$

where we inserted the unit operator in terms of the complete set of eigenfunctions ψ_ν of H with the sum comprising both the discrete and the continuous spectrum. We introduce atomic units a_0, ϵ_0, and T_0 for length, energy, and time, respectively

$$a_0 = \hbar^2/(m\alpha), \quad \epsilon_0 = \alpha/a_0, \quad T_0 = \hbar/\epsilon_0 = \hbar^3/(m\alpha^2); \quad \alpha > 0. \qquad (2)$$

The polar coordinates are defined by $r > 0$, $0 < \theta < \pi$, and $0 \leq \varphi < 2\pi$. We write, for the case of an attractive $(1/r)$ potential,

$$H = -\frac{\hbar^2}{2m}\Delta - \frac{\alpha}{r} \rightarrow \frac{H}{\epsilon_0} = -\frac{1}{2}\left[\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \left(\frac{\mathbf{L}}{\hbar}\right)^2\frac{1}{r^2}\right] - \frac{1}{r}, \quad \alpha > 0, \quad (3)$$

where $\mathbf{L}$ denotes the angular momentum operator and r is in units of a_0. From the eigenfunctions of ψ_ν, we separate off the angle dependence by means of the normalized spherical harmonics $Y_{l,m}$,

$$\psi_\nu = f_{\mu,l}(r)Y_{l,m}(\theta, \phi), \quad \nu = \{\mu, l, m\}, \qquad (4)$$

with

$$(\mathbf{L}/\hbar)^2\, Y_{lm} = l(l+1)Y_{lm}, \quad l = 0, 1, \ldots; \qquad m = -l, (-l+1), \ldots (l-1), l. \tag{5}$$

Using the scaled variables $\mu^2/2 = E_\mu/\epsilon_0$ and $\tau = t/T_0$, we write (1) in terms of the propagator K:

$$K(\mathbf{r}, \mathbf{r}', \tau) = \sum_\nu \exp[-\mathbf{i}\,(\mu^2/2)\tau]\, \psi_\nu(\mathbf{r})\psi_\nu^*(\mathbf{r}')\Theta(\tau), \tag{6}$$

where Θ is the Heaviside function with $\Theta(t) = 1$ if $\tau > 0$ and $\Theta(t) = 0$ if $\tau < 0$:

$$\psi(\mathbf{r}, \tau) = \int \mathrm{d}^3 r'\, K(\mathbf{r}, \mathbf{r}', \tau)\Psi_0(\mathbf{r}') \tag{7}$$

The eigenvalue μ is real in the continuous spectrum and in the discrete part $\mu = \mathbf{i}\,/n$, $n = 1, 2\ldots.$ with $n \geq l + 1$. Eventually, we go to the time Fourier transformed function $\psi_E(\mathbf{r})$

$$\psi_E(\mathbf{r}) = \int \mathrm{d}\tau\, \exp[\mathbf{i}\, E\, \tau]\, \psi(\mathbf{r}, \tau), \quad \psi(\mathbf{r}, \tau) = \frac{1}{2\pi} \int \mathrm{d}E\, \exp[-\mathbf{i}\, E\, \tau]\psi_E(\mathbf{r}). \tag{8}$$

In the first equation of (8), we insert $\psi(\mathbf{r}, \tau)$ from (6) and (7), replace E by $k^2/2$, and take into account that ψ_E is analytic in the upper complex E plane, so that E is defined with a positive imaginary part in the τ integral. We obtain

$$\psi_E(\mathbf{r}) = 2\,\mathbf{i} \int \mathrm{d}^3 r'\, G(\mathbf{r}, \mathbf{r}'; k)\Psi_0(\mathbf{r}'), \tag{9}$$

where, for $\mathrm{Im}(k^2) > 0$, the Green's function is defined by

$$G(\mathbf{r}, \mathbf{r}'; k) \;=\; \frac{1}{2\mathbf{i}} \int_0^\infty \mathrm{d}\tau \exp[\mathbf{i}\,(k^2/2)\tau]K(\mathbf{r}, \mathbf{r}', \tau) = \sum_\nu \frac{\psi_\nu(\mathbf{r})\psi_\nu^*(\mathbf{r}')}{k^2 - \mu^2}. \tag{10}$$

We remark that elsewhere, e.g. in [6], the term Green's function refers to the propagator K which also is called kernel.

From (10), it is seen that, due to the completeness of the functions ψ_ν,

$$H_k G(\mathbf{r}, \mathbf{r}'; k) = \delta(\mathbf{r} - \mathbf{r}'), \quad H_k = k^2 - 2(H/\epsilon_0), \tag{11}$$

which is true independently whether H_k acts on $\mathbf{r}$ or $\mathbf{r}'$. By the product form (4), G is written as follows:

$$G(\mathbf{r}, \mathbf{r}'; k) = \sum_{l=0,1,2,\ldots} G_l(r, r'; k) \sum_{m=-l}^{l} Y_{l,m}(\theta, \phi)\, Y_{l,m}^*(\theta', \phi'). \tag{12}$$

The form (12) implies the rotation symmetry of the problem.

Hameka's work [8] suggests the following ansatz:

$$G_l(r,r';k) = F_l(r;k)\,K_l(r';k)\Theta(r-r') + F_l(r';k)\,K_l(r;k)\Theta(r'-r). \quad (13)$$

Both $F_l(r)$ and $K_l(r)$ obey the Coulomb differential equation

$$H_k(l)\,y(r) = 0, \quad H_k(l) = k^2 + \frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{2}{r}\frac{\mathrm{d}}{\mathrm{d}r} - \frac{l(l+1)}{r^2} + \frac{2}{r}, \quad \mathrm{Im}(k^2) > 0, \quad (14)$$

where the latter condition implies that $k^2/2$ is not an eigenvalue of the Hamiltonian H. The solutions of (14) are written as a linear combination of the Whittaker functions M and W, for definition see Appendix A,

$$y(r) = \frac{1}{r}\left[c_M M_{\kappa,\nu}(z) + c_W W_{\kappa,\nu}(z)\right], \quad \kappa = \frac{\mathbf{i}}{k},\ \nu = \frac{2l+1}{2},\ z = -2\mathbf{i}\,kr. \quad (15)$$

Clearly, both F_l and K_l, can be expressed by means of a suitable linear combination of M and W.

Restrictions result from boundary conditions for $r \to 0$ and $r \to \infty$. Near the origin, one has the following behavior of the Whittaker functions, see Tab.1 of [4],

$$\begin{aligned} M_{\kappa,(2l+1)/2}(z) &= \text{const.}z^{l+1} + \mathcal{O}(z^{l+2}), \quad l = 0,1,2,\ldots & (16)\\ W_{\kappa,(2l+1)/2}(z) &= \text{const.}z^{-l} + O_l, \quad O_0 = \mathcal{O}\left(z\ln(z)\right), \\ &\quad O_l = \mathcal{O}(z^{-l+1}),\ l \geq 1. & (17)\end{aligned}$$

For large $|z|$, the function W behaves asymptotically simpler than M. In the given case with $z = \mathbf{i}\,\zeta$ and $\kappa = \mathbf{i}\,\tau$, where ζ is real, one finds in §7 of [4]

$$\begin{aligned} W_{\kappa,(2l+1)/2}(z) &= z^{\kappa}\exp(-z/2)\left[1+\mathcal{O}(1/z)\right], \quad |\arg(z)| < 3\pi/2, & (18)\\ M_{\kappa,(2l+1)/2}(z) &= a_c\cos[\varphi(\zeta)]\left[1+\mathcal{O}(1/\zeta)\right] - a_s\sin[\varphi(\zeta)]\left[1+\mathcal{O}(1/\zeta)\right], & (19)\\ \varphi(\zeta) &= -\tau\ln(|\zeta|) + \zeta/2 + \delta + \pi/2(l+1)\,\mathrm{sign}(\zeta), \quad z = \mathbf{i}\,\zeta,\ \kappa = \mathbf{i}\,\tau. \end{aligned}$$

For the detailed definition of the constants a_c, a_s, and δ, we refer to [4]. It is inferred that M asymptotically oscillates for large r provided k is real, whereas there is a runaway if k is complex both for positive and negative imaginary parts. This is exemplarily confirmed when plots are produced by the computing system Mathematica [21], where the Whittaker functions belong to the built-in commands. On the other hand, W decays exponentially for large r if k has a positive imaginary part.

Now, let us consider (13) with respect to the boundary conditions stated. If $r > r'$, then the function $K_l(r')$ should behave properly near $r' = 0$ which implies that K_l must not contain the function W:

$$K_l(r;k) = c_K M_{\kappa,\nu}(z)/r, \quad \kappa = \mathbf{i}\,/k,\ \nu = (2l+1)/2,\ z = -2\mathbf{i}\,kr. \quad (20)$$

On the other hand, if $r < r'$, then the proper asymptotic behavior of $F_l(r')$ for $r' \to \infty$ requires that F_l cannot depend on M, in particular, since we assume a positive, non zero, imaginary part of k:

$$F_l(r';k) = c_F W_{\kappa,\nu}(z')/r', \quad \kappa = \mathbf{i}/k, \;\; \nu = (2l+1)/2, \;\; z' = -2\mathbf{i}\,kr'. \tag{21}$$

We now apply the operator $H_k(l)$ to $G_l(r,r';k)$ and take into account that both F_l and K_l are solutions of the differential equation (14). We also use the following properties of the Dirac delta function,

$$\partial_r \Theta(r-r') = -\partial_r \Theta(r'-r) = \delta(r-r'), \quad B(z)\partial_z \delta(z) = -\left[\partial_z B(z)\right]\delta(z), \tag{22}$$

to obtain

$$H_k(l) G_l(r,r';k) = \mathcal{W}\left[K_l(r), F_l(r)\right]\delta(r-r') = \frac{c_K c_F}{r^2}\,\delta(r-r')\,\mathcal{W}_{M,W}, \tag{23}$$

where $\mathcal{W}$ denotes the Wronskian

$$\begin{aligned} \mathcal{W}_{M,W} &= M\frac{\mathrm{d}W}{\mathrm{d}r} - W\frac{\mathrm{d}M}{\mathrm{d}r} = (-2\mathbf{i}\,k)\left[M_{\kappa,\nu}(z)\frac{\mathrm{d}W_{\kappa,\nu}(z)}{\mathrm{d}z} - W_{\kappa,\nu}(z)\frac{\mathrm{d}M_{\kappa,\nu}(z)}{\mathrm{d}z}\right] \\ &= (-2\mathbf{i}\,k)(-1)(2l+1)!/\Gamma(1+l-\mathbf{i}/k). \end{aligned} \tag{24}$$

The latter result is based on the Wronskian (33) on page 25 in [4], where one has to take care of the different definition of M:

$$M^{Buch}_{\kappa,\nu} = M_{\kappa,\nu}/\Gamma(1+2\nu) = M_{\kappa,\nu}/(2l+1)!, \quad \nu = (2l+1)/2. \tag{25}$$

We checked (25) numerically in Appendix B.

In order that

$$H_k(l) G_l(r,r';k) = (1/r^2)\delta(r-r'), \tag{26}$$

we have to set

$$c_K c_F = -\mathbf{i}\,\frac{\Gamma(1+l-\mathbf{i}/k)}{2k(2l+1)!}. \tag{27}$$

By (12) and the completeness of the spherical harmonics, we arrive at the defining relation (11) of G, namely,

$$\begin{aligned} H_k G(\mathbf{r},\mathbf{r}';k) &= \sum_{l=0,1,2,\ldots} \left[H_k(l) G_l(r,r';k)\right] \sum_{m=-l}^{l} Y_{l,m}(\theta,\phi)\, Y^*_{l,m}(\theta',\phi') \\ &= \frac{1}{r^2\sin(\theta)}\delta(r-r')\delta(\theta-\theta')\delta(\varphi-\varphi'), \end{aligned} \tag{28}$$

and

$$\begin{aligned} G_l(r,r';k) &= -\mathbf{i}\,\frac{\Gamma(1+l-\kappa)}{2k(2l+1)!}\left[W_{\kappa,\nu}(-2\mathbf{i}\,k\,r)/r\right]\left[M_{\kappa,\nu}(-2\mathbf{i}\,k\,r')/r'\right], \\ &\quad r > r', \;\; \kappa = \mathbf{i}/k, \;\; \nu = (2l+1)/2; \end{aligned} \tag{29}$$

If $r < r'$, then r and r' have to be interchanged.

In the special case $r' = 0$, we infer from (12), (20), (21), and (A4)

$$\begin{aligned} G_l(r,0;k) &= G_0(r,0;k)\delta_{l,0} = c_K c_F \,[W_{\kappa,\nu}(-2\mathbf{i}\,kr)/r]\,[M_{\kappa,\nu}(-2\mathbf{i}\,kr')/r']_{r'\to 0} \\ &= -2\,\mathbf{i}\,k\,c_K c_F\,\delta_{l,0}\,W_{\kappa,1/2}(-2\mathbf{i}\,kr)/r. \end{aligned} \tag{30}$$

In (30), we used the relation $[M_{\kappa,\nu}(-2\mathbf{i}\,kr')/r']_{r'\to 0} = -2\mathbf{i}\,k\,\delta_{l,0}$ with $\nu = (2l+1)/2 \to 1/2$. Inserting the coefficients $c_K c_F$ for $l = 0$ and taking into account the normalization of the spherical harmonic $|Y_0|^2 = 1/(4\pi)$, we find

$$G(\mathbf{r},0,k) = G_0(r,0;k)/(4\pi) = -\frac{\Gamma(1-\kappa)}{4\pi r} W_{\kappa,1/2}(-2\mathbf{i}\,kr), \quad \kappa = \mathbf{i}\,/k, \tag{31}$$

which agrees with Hostler's result Eq.(9) in [11], up to the different notation $\kappa \to \mathbf{i}\,\nu$.

Asymptotically, for $k\,r \gg 1$, we infer from (18) using $\ln(-\mathbf{i}\,) = -\mathbf{i}\,\pi/2$,

$$G(\mathbf{r},0,k) \to -\frac{\exp\{\mathbf{i}\,[k\,r + (1/k)\ln(2k\,r)]\}}{4\pi r}\exp[\frac{\pi}{2k}]\,\Gamma(1-\mathbf{i}\,/k), \quad k\,r \gg 1. \tag{32}$$

3 The singularities of the Green's function found

The Green's function (29) exhibits simple poles through the factor $\Gamma(1+l-\kappa)$, when the argument of Γ is a negative integer or zero, $\Gamma(-j) = \infty$ for $j = 0, 1, \ldots$. With $\kappa = \mathbf{i}\,/k$, the corresponding k values are

$$k_j = \mathbf{i}\,/(1+l+j), \quad \text{or} \quad k_n = \mathbf{i}\,/n, \;\; n = l+1, l+2, \ldots, \tag{33}$$

and give rise to the well known discrete energy spectrum $E_n = -1/(2n^2)$. The continuous spectrum with $E > 0$ should be related to a branch cut along the negative real axis of k.

In order to detect the branch cut in the Whittaker function W (the function M is regular in k), we performed numerical experiments by setting $k = |k|\exp[\mathbf{i}\,\varphi]$ and by plotting both the real and the imaginary part of the complex parameter k as a function of $0 \le \varphi \le 2\pi$. We used the built-in Mathematica function "WhittakerW[...]". Surprisingly, we observed the discontinuity at $\varphi = 3\pi/2$, rather than at $\varphi = \pi$. A branch cut along the imaginary axes would predict that the continuous spectrum is given by the negative energy values $E < 0$.

The origin of the discrepancy can be located in the logarithm term, $\ln(z)$, which explicitly appears in the definition (A6) for W, as defined by Buchholz [4]. Mathematica renders the principal value of

$$\ln(z) \equiv \ln(|z|\exp(\mathbf{i}\,\phi)) = \ln(|z|) + \mathbf{i}\,\phi \quad \text{with} \quad -\pi < \phi \le \pi. \tag{34}$$

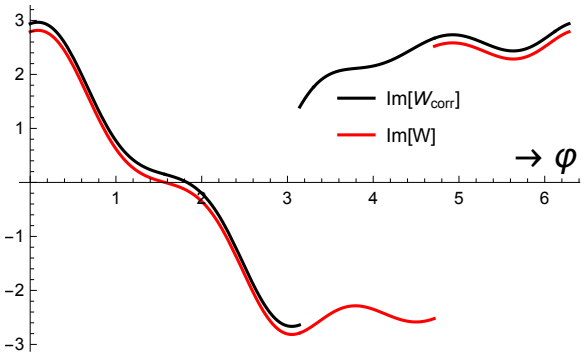

Figure 1: Imaginary part of the Whittaker function W versus the phase φ of the energy parameter $k = |k| \exp[\mathbf{i}\,\varphi]$: red and black lines refer to the Mathematica built-in function WhittakerW$[\mathbf{i}\,/k, 1/2, -2\mathbf{i}\,k\,r]$ and to the corrected version, respectively. The latter takes care of the physically proper Riemann sheet of $\ln(-2\mathbf{i}\,k\,r)$. When k is varied in the complex k plane, starting from $\varphi = 0$, then in the "red" case the first singularity is met at $\varphi = 3\pi/2$ and implies the branch cut along the negative imaginary axes of k with the consequence that the Green's function would predict a negative continuous energy spectrum. When the Mathematica function W is corrected according to (37), then the first singularity occurs at $\varphi = \pi$, and so the Green function predicts the physical, positive, continuous energy spectrum. For the help of the reader, the "black" curve is artificially shifted by a small constant amount. Strictly, the two curves coincide except in the interval $\pi \le \varphi \le 3\pi/2$. The parameters chosen for the plots are $l = 0$, $r = 1$, and $|k| = 1.1$.

Now, when

$$z = -2\mathbf{i}\,k\,r = -2\mathbf{i}\,|k|\,r\exp(\mathbf{i}\,\varphi) = 2|k|\,r\exp[\mathbf{i}\,(\varphi - \pi/2)], \tag{35}$$

then the standard algorithm for rendering $\ln(z)$ projects the k phase into the interval $-\pi/2 < \varphi \le 3\pi/2$ and implies to set the branch cut on the imaginary k axes. In order to obtain the physically correct Riemann sheet of W in the whole complex k plane, we represent $\ln(z)$ as

$$\ln(z) = \ln(-2\mathbf{i}\,r) + \ln(k) \tag{36}$$

and, by (A6), with $\nu = (2l+1)/2$,

$$\begin{aligned} \text{WhittakerW}[\kappa,\nu,z] &\rightarrow \text{WhittakerW}[\kappa,\nu,z] + \frac{1}{\Gamma(-l-\kappa)}\frac{M_{\kappa,\nu}}{(2l+1)!}\,\Delta W, \\ \Delta W &= -\ln(z) + \ln(-2\mathbf{i}\,r) + \ln(k). \end{aligned} \tag{37}$$

As a function of the k-phase φ, Mathematica determines each of the three terms of ΔW modulo 2π with offset at $-\pi$. The result is

$$\Delta W(|k|\exp[\mathbf{i}\,\varphi]) = -2\pi\mathbf{i}\,, \quad \text{if} \quad \pi < \varphi < 3\pi/2, \quad \text{else} \quad \Delta W = 0. \tag{38}$$

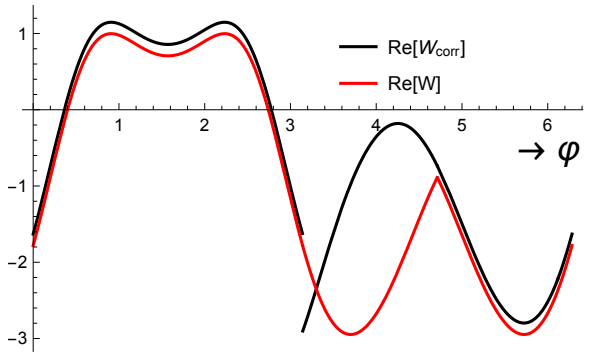

Figure 2: Real part of the Whittaker function W versus the phase φ of the energy parameter k, in full analogy to Fig.1.

For illustration, see Fig.1 and Fig.2. Since ΔW does not depend on the quantum number l, the special case $l = 0$ is sufficient for demonstration.

4 Conclusion

In order that the Green's function predicts the correct physical energy spectrum of the Coulomb Hamiltonian, the multivalued logarithmic term in the Whittaker function W cannot be restricted to the principal value but has to be extended to a further sheet of the Riemann surface. The correction to be considered is restricted to the third quadrant of the complex parameter $k = |k| \exp[\mathbf{i}\,\varphi]$, i.e. to the phase interval $\pi < \varphi < 3\pi/2$. As a consequence, the asymptotic behavior of G in the upper complex k plane with $\mathrm{Im}(k) > 0$, is still fully determined by the Whittaker function W, without admixture of M, and the Mathematica algorithm for W has not to be modified if $\mathrm{Im}(k) > 0$.

Acknowledgements: The author expresses his gratitude to Jürgen Parisi for his support and constant encouragement, and, not at least, for the critical reading of the manuscript.

A The Whittaker functions

The Coulomb differential equation (14),

$$H_k y(r) = 0 \quad \text{with} \quad H_k = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{l(l+1)}{r^2} + \frac{2}{r} + k^2, \tag{A1}$$

is transformed into the Whittaker standard form [19],

$$\frac{\partial^2 w}{\partial z^2} + \left[-\frac{1}{4} + \frac{\kappa}{z} - \frac{l(l+1)}{z^2}\right] w(z) = 0, \tag{A2}$$

which is achieved by the substitutions $r \to z$ and $y(r) \to w(z)$ with

$$y(r) = (1/r)w(z), \quad z = -2\mathbf{i}\,kr, \quad \kappa = \mathbf{i}\,/k. \tag{A3}$$

In the case of a repellent Coulomb potential, one has to set $\kappa = -\mathbf{i}\,/k$, keeping $z = -2\mathbf{i}\,kr$. Two independent solutions of (A2) are the Whittaker functions $M_{\kappa,\nu}(z)$ and $W_{\kappa,\nu}(z)$, $\nu = (2l+1)/2$, where M is connected with the confluent hypergeometric function Φ as

$$M_{\kappa,(2l+1)/2}(z) = z^{l+1} \exp[-z/2]\, \Phi\left(l+1-\kappa, 2+2l, z\right), \quad \kappa = \mathbf{i}\,/k. \tag{A4}$$

In general, W can be defined in terms of M by

$$W_{\kappa,\nu} = \frac{1}{\sin(2\pi\nu)}\left[M_{\kappa,\nu} - M_{\kappa,-\nu}\right]. \tag{A5}$$

However, by the sine function in the denominator, the case needed in the Coulomb problem, where ν is half of an uneven integer, is exceptional and needs either taking limits with the aid of the L'Hospital rule [4] or special contour integration [14].

According to Eqs.(24a) and (25a) in §2 of [4], where we replace the index $\mu/2$ by the symbol $\nu = (2l+1)/2$, $l = 0, 1, \ldots$, the function W reads as follows:

$$\begin{aligned}
W_{\kappa,\nu}(z) &= \frac{(-1)^{2\nu+1}}{\Gamma(1/2-\nu-\kappa)}\left[\frac{M_{\kappa,\nu}}{(2l+1)!}\,\ln(z) + H_{\kappa,\nu}\right], \quad z = -2\mathbf{i}\,k\,r, \quad \kappa = \mathbf{i}\,/k, \\
H_{\kappa,\nu} &= \frac{z^{l+1}\exp[-z/2]}{\Gamma(l+1-\kappa)}\left\{\sum_{j=0}^{\infty}\frac{\Gamma(l+1+j-\kappa)}{(2l+1+j)!}\left[\Psi(l+1+j-\kappa) - \Psi(1+j)\right.\right. \\
&\quad \left.\left. -\Psi(2l+2+j)\right]\,\frac{z^j}{j!} - \sum_{j=1}^{2l+1}\frac{\Gamma(l+1-j-\kappa)}{(2l+1-j)!}\,\frac{(j-1)!}{(-z)^j}\right\},
\end{aligned} \tag{A6}$$

where $\Psi(y) = \partial_y \ln(\Gamma(y)$. The definitions of M and W agree with those given in [1] and [5]; they are also exemplarily numerically confirmed by the built-in Mathematica functions "WhittakerM(W)[...]" [21]. For the implementation of W in Mathematica, see [20].

B Numerical checks of the Wronskian of the Whittaker functions

Mathematica [21] has implemented the Whittaker functions $M_{\kappa,\nu}(z)$ and $W_{\kappa,\nu}(z)$, where in the latter case, the underlying algorithm also applies when ν is half of an uneven positive integer. The differentiations with respect to z are carried out analytically by Mathematica.

The test of the function $T = T(k, l, r)$ refers to (23), without the factor $\delta(r - r')/r^2$. We use (24) and (27) to write

$$\begin{aligned} T_l(k,r) &= c_K c_F \mathcal{W}_{M,W} - 1 = -\mathbf{i}\,(-2\mathbf{i}\,k)\frac{\Gamma(1+l-\mathbf{i}\,/k)}{2k(2l+1)!} \times \\ &\quad [M_{\kappa,\nu}(z)\partial_z W_{\kappa,\nu}(z) - W_{\kappa,\nu}(z)\partial_z M_{\kappa,\nu}(z)] - 1, \end{aligned} \tag{B1}$$

where $\kappa = \mathbf{i}\,/k,\ \nu = (2l+1)/2,\ z = -2\mathbf{i}\,k\,r$. It is noticed that $T(k, l, r)$ strictly is zero independently of $k > 0$, $l = 0, 1, 2, \ldots$, and $r > 0$. The numerical results in Tab.1 are in the order of 10^{-15} to 10^{-14}. The results of Tab.1 also indicate the numerical accuracy of the built-in functions "WhittakerM[...]" and "WhittakerW[...]" of Mathematica.

$\{r, k\}$	=	$\{1,\ 0.6\}$	$\{0.3,\ 1.5\}$	$\{3.3,\ 0.1\}$
$T_0(k,r) \times 10^{15}$	=	$(-0.9 + 2.8\,\mathbf{i}\,)$,	$(0.2 - 2.7\,\mathbf{i}\,)$,	$(8.4 + 19\,\mathbf{i}\,)$,
$T_1(k,r) \times 10^{15}$	=	$(0.7 - 1.9\,\mathbf{i}\,)$,	$(-1.1 + 0.6\,\mathbf{i}\,)$,	$(7.3. - 19.\,\mathbf{i}\,)$,
$T_2(k,r) \times 10^{15}$	=	$(0.5 + 0.2\,\mathbf{i}\,)$,	$(0.2 - 0.2\,\mathbf{i}\,)$,	$(14. + 5.\,\mathbf{i}\,)$

Table 1: Numerical checks of the expression (B1), which strictly is zero for all parameters $k > 0$, $r > 0$ and $l = 0, 1, \ldots$

C Remarks on the second Meixner function

We found inconsistent definitions of the Meixner Function F_2 which is defined in Eq. (32) of [14] for the given Coulomb problem. Meixner's definition differs from that of Buchholz [4], which is given by (2b) on page 214 and reads (notation unchanged)

$$F_2 = 2\Gamma(1+\mu)\exp\left[-\mathbf{i}\,\pi\kappa + z/2\right] z^{-(1+\mu)/2} W_{-\kappa,\mu/2}(-z)/\Gamma\left[(1+\mu)/2 - \kappa\right]. \tag{C1}$$

Here, F_2 depends on the Whittaker function W only, whereas Meixner's F_2 function contains an admixture of the Whittaker function M. Numerical checks of the two versions confirm the discrepancy.

Now, when the Buchholz definition (C1) is inserted into Meixner's Eq.(14) [14], by setting $\mu = 1$, $\kappa = -\mathbf{i}\,/k$, and $z = 2\mathbf{i}\,kr$, one gets the special case $G(\mathbf{r}, 0, E)$, which is equivalent to the result (31). And in this way, Hostler and Pratt [11] quote correctly that their result agrees with that of Meixner.

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Received: April 17, 2019; Published: May 25, 2019