

Zeros of the Whittaker Function Associated to Coulomb Waves

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The zeros in the complex z plane of the Whittaker function $W_{c/z, \mu}(z)$, closely related to spherical waves in the quantum-mechanical Coulomb problem, are investigated for varying real values of the parameters c and μ .

1. Introduction

The solution of the Schrödinger equation for physical systems, like heavy-ions, where the interaction is described via a potential presenting a Coulomb tail requires to match the logarithmic derivative of the regular wavefunction in the internal (nuclear) region with that of the outgoing wavefunction in the external (Coulombian) one (see Grama *et al.*, 1994). The internal function is obtained by numerical integration of the differential equation. The external function is a well known linear combination of the regular and irregular Coulomb wavefunctions (Abramowitz & Stegun, 1965, p. 538), $F_L(\eta, \rho) + iG_L(\eta, \rho)$, which turns out to be proportional to the Whittaker function $W_{\kappa, \mu}(z)$ (Slater, 1960, p. 93), with $\kappa = -i\eta$, $\mu = L + 1/2$, and $z = -2i\rho$. In the physical problem, the angular momentum L is integer, although it is frequent, for large values, to treat it as a continuous real parameter. On the other hand, η and ρ are, respectively, inversely and directly proportional to the square root of the energy. They become complex whenever complex energies are considered, as it happens, for instance, in the case of resonances in a real potential or bound states in a complex (absorptive) one.

Approximate determinations of the eigenvalues of the Schrödinger equation, in the discrete part of the spectrum, and of phase-shifts, in the continuous one, would be facilitated by a chart of modulus and phase of the logarithmic derivative of the external wavefunction. In preparing such a chart, it is crucial to know the location of poles and zeros, since constant-modulus lines surround them and constant-phase lines leave them radially. Obviously, those poles and zeros are respectively the zeros of the wavefunction and those of its derivative.

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Most papers on the zeros of $W_{\kappa,\mu}(z)$, or equivalently of the confluent hypergeometric function $\Psi(a; b; z)$ or $U(a, b, z)$, with $a = \mu - \kappa + 1/2$, $b = 2\mu + 1$, have dealt mainly with the total number of either real or complex zeros for several real values of a and b . References to those papers can be found, for instance, in Erdélyi (1953) and Slater (1960). The purpose of this work is to investigate the zeros of $W_{c/z,\mu}(z)$ in the complex z plane, for real c and μ . Referring to the heavy-ion process mentioned above, the parameters c and μ and the variable z correspond, in appropriate units, respectively to the product of the charges of the interacting ions, the relative angular momentum and the square root of the energy in the center-of-mass reference frame.

The zeros of $F_L(\eta, \rho) + iG_L(\eta, \rho)$ located in the fourth quadrant of the complex ρ plane, that is, in our notation, the zeros of $W_{c/z,\mu}(z)$ in the second quadrant of the z plane for $c \leq 0$, were already considered by Grama *et al.* (1985). Here we obtain the zeros of $W_{c/z,\mu}(z)$ in the whole z plane and discuss their motion as the parameters c and μ vary.

In our subsequent study we consider positive and negative values of c , corresponding, respectively, to opposite and equal signs in the charges of the interacting particles. In view of the relation (Buchholz, 1969, Sect. 2, Eq. (19))

$$W_{\kappa,\mu}(z) = W_{\kappa,-\mu}(z), \quad (1.1)$$

we need to consider only positive values of μ . The variable z will be restricted to the Riemann sheet

$$0 \leq \arg z < 2\pi. \quad (1.2)$$

The complex conjugation property (Buchholz, 1969, Sect. 2.10)

$$W_{\bar{\kappa},\bar{\mu}}(\bar{z}) = \overline{W_{\kappa,\mu}(z)}, \quad \text{for real } \mu, \quad (1.3)$$

allows to extend immediately our results to the sheet

$$-2\pi < \arg z \leq 0. \quad (1.4)$$

Approximate analytical expressions for the location of the zeros for some particular values of the parameters are obtained in Section 2. Different algorithms for the evaluation of the zeros of $W_{c/z,\mu}(z)$ and the behaviour of those zeros in the complex z plane, as the parameters c and μ change, are considered in Section 3. Our results are summarized in Section 4. Finally, an Appendix contains some details of the procedure followed to locate the zeros.

2. Zeros of $W_{c/z,\mu}(z)$ for special values of the parameters

Analytical techniques can be used to determine approximately the location of the zeros of $W_{c/z,\mu}(z)$ for certain values of the parameters c and μ .

2.1 Small values of c

The zeros of $W_{c/z,\mu}(z)$ can be trivially obtained for $c = 0$. In fact, the Whittaker function is in this case closely related (Buchholz, 1969, Sect. 2, Eq. (29)) to a Bessel function

$$\begin{aligned} W_{0,\mu}(z) &= \frac{1}{2} \exp(i(1+\mu)\pi/2) (\pi z)^{1/2} H_{\mu}^{(1)}(e^{i\pi/2} z/2) \\ &= \frac{1}{2} \exp(-i(1+\mu)\pi/2) (\pi z)^{1/2} H_{\mu}^{(2)}(e^{-i\pi/2} z/2). \end{aligned} \quad (2.5)$$

By using the relation between the two Hankel functions (Abramowitz & Stegun, 1965, Eq. 9.1.40), the last equation can be written in the form

$$W_{0,\mu}(z) = \frac{1}{2} \exp(-i(1+\mu)\pi/2) (\pi z)^{1/2} \overline{H_{\mu}^{(1)}(e^{i\pi/2} \bar{z}/2)}. \quad (2.6)$$

The zeros of $H_{\mu}^{(1)}(\xi)$, for varying real μ , have already been discussed and some of them in the Riemann sheet

$$-\frac{3\pi}{2} < \arg \xi \leq \frac{\pi}{2} \quad (2.7)$$

explicitly shown in Cruz & Sesma (1982) and Cruz *et al.* (1991). By identifying

$$\xi \equiv e^{i\pi/2} \bar{z}/2, \quad (2.8)$$

it is immediate to obtain the zeros of $W_{0,\mu}(z)$ in the Riemann sheet

$$0 \leq \arg z < 2\pi. \quad (2.9)$$

The first ones of the infinite set of zeros are shown in Fig. 1, obtained from Fig. 1 of Cruz & Sesma (1982) through complex conjugation followed by a rotation, about the origin, of angle $\pi/2$ and a change of scale by a factor of 2.

As the parameter c increases or decreases from 0, the zeros of $W_{c/z,\mu}(z)$ progressively deviate from their positions for $c = 0$. Obviously, for small $|c|$, the deviations are more important for the zeros not far from the origin, whereas they are negligible for zeros of large modulus. We are interested in the trajectories followed by the zeros for a fixed c and continuously varying real μ . One could expect that, as long as $|c|$ remains sufficiently small, the trajectories of the zeros of $W_{c/z,\mu}(z)$ are close to those of $H_{\mu}^{(1)}(e^{i\pi/2} \bar{z}/2)$. But these trajectories are not *a priori* defined, since the zeros go to infinity for certain critical values of μ . So, one does not obtain a trajectory for each zero, for μ ranging from 0 to $+\infty$, but pieces of trajectories corresponding to values of μ in the interval between two consecutive critical ones. In order to organize this puzzle of pieces in whole trajectories, one needs to give a prescription about which pieces are spliced as μ goes through a critical value. One possibility is to add a small imaginary part to μ , so as to avoid the critical value. If that small imaginary part is taken negative at every critical point, the global trajectories of the zeros of $H_{\mu}^{(1)}$ are those shown in Cruz & Sesma (1982), whereas if it is taken positive, one obtains the trajectories discussed in Cruz *et al.* (1991). Numerical exploration indicates that the trajectories of the zeros of $W_{c/z,\mu}(z)$ tend, as $c \rightarrow 0$, to

FIG. 1. Zeros of $W_{0,\mu}(z)$. The first ones of an infinite set of trajectories, followed by the zeros as μ varies, are shown. The numbers beside the trajectories indicate the values of μ .

the trajectories of those of $H_\mu^{(1)}(e^{i\pi/2}\bar{z}/2)$ with the prescription of adding to μ , at the critical values, a negative small imaginary part if $c \rightarrow 0^+$ (vanishing attractive interaction) and a positive one if $c \rightarrow 0^-$ (vanishing repulsive interaction).

Besides the zeros approaching those of $H_\mu^{(1)}(e^{i\pi/2}\bar{z}/2)$, $W_{c/z,\mu}(z)$ presents another set of zeros that, as $c \rightarrow 0$, go to the origin in such a manner that the quotient c/z remains finite. (Below, in Subsect. 2.2, we report some zeros of $W_{c/z,\mu}(z)$ that go also to the origin, but for c tending to certain finite values and for some particular values of μ .) The position of those zeros for small c can be obtained approximately starting from the expression of the irregular Whittaker function in terms of the

regular one \mathcal{M} (Buchholz, 1969, Sect. 2, Eq. (18a)),

$$W_{\kappa,\mu}(z) = \frac{\pi}{\sin(2\pi\mu)} \left(-\frac{\mathcal{M}_{\kappa,\mu}(z)}{\Gamma(-\mu-\kappa+1/2)} + \frac{\mathcal{M}_{\kappa,-\mu}(z)}{\Gamma(\mu-\kappa+1/2)} \right), \quad (2.10)$$

and using for \mathcal{M} a convergent expansion in terms of Bessel functions (Buchholz, 1969, Sect. 7, Eq. (16)),

$$\mathcal{M}_{\kappa,\mu}(z) = z^{\mu+1/2} \sum_{n=0}^{\infty} \frac{p_n^{(2\mu)}(z)}{2^n} \frac{J_{2\mu+n}(2\sqrt{\kappa z})}{(\sqrt{\kappa z})^{2\mu+n}}, \quad (2.11)$$

that has proved (Abad & Sesma, 1995) to be very convenient to compute the confluent hypergeometric function ${}_1F_1(a; b; z)$ (closely related to $\mathcal{M}_{\kappa,\mu}(z)$, with $\kappa = \frac{1}{2}b - a$, $\mu = \frac{1}{2}b - \frac{1}{2}$) in the case of small z . The symbols $p_n^{(\nu)}(z)$ represent double polynomials in the variables ν and z^2 , the exponents of z ranging from $2 \lfloor \frac{n+1}{2} \rfloor$ to $2n$. Assuming that z and c are both small and of the same order and retaining only the dominant terms in the right hand side of (??), the zeros of $W_{c/z,\mu}(z)$ are given approximately by

$$\begin{aligned} & -\frac{z^{\mu+1/2}}{\Gamma(-\mu-c/z+1/2)} \frac{1}{\Gamma(2\mu+1)} \left(1 - \frac{c}{2\mu+1} \right) \\ & + \frac{z^{-\mu+1/2}}{\Gamma(\mu-c/z+1/2)} \frac{1}{\Gamma(-2\mu+1)} \left(1 - \frac{c}{-2\mu+1} \right) = 0, \end{aligned} \quad (2.12)$$

or, equivalently, by

$$\begin{aligned} \Gamma(\mu-c/z+1/2) = \\ z^{-2\mu} \Gamma(-\mu-c/z+1/2) \frac{\Gamma(2\mu+1)}{\Gamma(-2\mu+1)} \frac{1-c/(-2\mu+1)}{1-c/(2\mu+1)}. \end{aligned} \quad (2.13)$$

This equation suggests, for small z , values of $\mu-c/z+1/2$ in the vicinity of 0 or of negative integers, that is,

$$c/z = n + \mu + 1/2 + \epsilon_n, \quad n = 0, 1, 2, \dots, \quad |\epsilon_n| \ll 1. \quad (2.14)$$

In this case,

$$\begin{aligned} \Gamma(\mu-c/z+1/2) &= \Gamma(-n-\epsilon_n) \\ &\simeq -(-1)^n / \epsilon_n n!, \end{aligned} \quad (2.15)$$

$$\begin{aligned} \Gamma(-\mu-c/z+1/2) &= \Gamma(-n-2\mu-\epsilon_n) \\ &\simeq \Gamma(-n-2\mu) (1 - \epsilon_n \psi(-n-2\mu)). \end{aligned} \quad (2.16)$$

From (??) to (??) one obtains easily

$$z \simeq \frac{c}{n + \mu + 1/2} \left(1 - \frac{\epsilon_n}{n + \mu + 1/2} \right), \quad (2.17)$$

with

$$\epsilon_n \simeq -(-1)^n z^{2\mu} \frac{\Gamma(-2\mu + 1)}{\Gamma(2\mu + 1)\Gamma(-n - 2\mu)}. \quad (2.18)$$

Of course, (??) is not an explicit expression for the location of the zeros, since z enters in the expression of ϵ_n . Nevertheless, consistently with the approximations made, one should replace z in the right hand side of (??) by $c/(n + \mu + 1/2)$.

Equation (??) shows that an infinite set of zeros are located near the origin for sufficiently small c . The zeros approach the origin when either $|c|$ diminishes or the label n increases. Although in the derivation of (??) we have tacitly assumed that the values of μ were different from an integer or a half-integer, continuity suggests the validity of that equation for all real μ . For positive c the zeros lie on the positive real semiaxis. For negative c they are located near the negative real semiaxis and, given c and n , their imaginary parts oscillate, with decreasing amplitude, from positive to negative values and vice versa as μ increases.

2.2 Zeros near the origin for finite values of the parameters c and μ

Let us consider now the possibility of existing zeros at small values of z for finite c and μ . From (??) and (??) one obtains, by retaining only the first terms in the sums,

$$W_{c/z, \mu}(z) \simeq \frac{\pi}{\sin(2\pi\mu)} \left(-\frac{z^{\mu+1/2}}{\Gamma(-\mu - c/z + 1/2)} \frac{J_{2\mu}(2\sqrt{c})}{(\sqrt{c})^{2\mu}} + \frac{z^{-\mu+1/2}}{\Gamma(\mu - c/z + 1/2)} \frac{J_{-2\mu}(2\sqrt{c})}{(\sqrt{c})^{-2\mu}} \right), \quad |z| \ll 1. \quad (2.19)$$

The zeros of $W_{c/z, \mu}(z)$ would then be given approximately by

$$-z^{2\mu} \frac{\Gamma(\mu - c/z + 1/2)}{\Gamma(-\mu - c/z + 1/2)} \frac{J_{2\mu}(2\sqrt{c})}{(\sqrt{c})^{2\mu}} + \frac{J_{-2\mu}(2\sqrt{c})}{(\sqrt{c})^{-2\mu}} = 0. \quad (2.20)$$

Since c/z is now large, one may use (Abramowitz & Stegun, 1965, Eq. 6.1.47)

$$\left(-\frac{z}{c}\right)^{2\mu} \frac{\Gamma(\mu - c/z + 1/2)}{\Gamma(-\mu - c/z + 1/2)} \simeq 1 - \frac{1}{12}\mu(4\mu^2 - 1)(z/c)^2 \quad (2.21)$$

to obtain from (??)

$$J_{2\mu}(2\sqrt{c}) - (-1)^{2\mu} J_{-2\mu}(2\sqrt{c}) \simeq 0. \quad (2.22)$$

Therefore, the existence of zeros of $W_{c/z, \mu}(z)$ in the vicinity of the origin, for finite c and μ , is subordinated to the fulfilment of

$$H_{2\mu}^{(1)}(2\sqrt{c}) = 0. \quad (2.23)$$

This equation cannot be satisfied for real μ and positive values of c . It admits (Cruz & Sesma, 1982), instead, one negative solution, c_n , for $2\mu = 2n - 1/2$, $n = 1, 2, 3, \dots$

TABLE 1
Solutions of Eq. (??) of the text

n	μ_n	c_n
1	3/4	-0.25
2	7/4	-1.348...
3	11/4	-3.325...
4	15/4	-6.180...
\vdots	\vdots	\vdots

We report in Table 1 that solution for the lowest values of n . Zeros of $W_{c/z, \mu}(z)$ near the origin may then be found for values of c and μ in the vicinity of, respectively, c_n and $\mu_n \equiv n - 1/4$. If one considers $\mu = \mu_n + \varepsilon$ and $c = c_n + \delta$, with $|\varepsilon|, |\delta| \ll 1$, keeps terms up to $O(z^2)$ in the series of Bessel functions resulting for $W_{c/z, \mu}(z)$ from (??) and (??), and uses again (??), one has for the approximate location of the zeros, instead of (??),

$$J_{2\mu} - (-1)^{2\mu} J_{-2\mu} - \frac{z^2}{12} \left(\mu(4\mu^2 - 1)c^{-2} J_{2\mu} - c^{-1/2} (J_{2\mu+1} - (-1)^{2\mu} J_{-2\mu+1}) - c^{-1} ((\mu - 1/2)J_{2\mu+2} - (-1)^{2\mu} (-\mu - 1/2)J_{-2\mu+2}) \right) \simeq 0, \quad (2.24)$$

where the value $2\sqrt{c}$ of the variable of all J functions has been omitted. By replacing μ by $\mu_n + \varepsilon$ and c by $c_n + \delta$ and retaining dominant terms, one obtains

$$z^2 \simeq 12 \frac{2c_n A_n \varepsilon + B_n \delta}{D_n}, \quad (2.25)$$

with the notation

$$A_n \equiv \left[\frac{\partial J_\nu}{\partial \nu} \right]_{\nu=2\mu_n} + (-1)^{2\mu_n} \left[\frac{\partial J_\nu}{\partial \nu} \right]_{\nu=-2\mu_n} - i\pi J_{2\mu_n}, \quad (2.26)$$

$$B_n \equiv 2\mu_n J_{2\mu_n} - c_n^{1/2} E_n, \quad (2.27)$$

$$D_n \equiv \left(\frac{4\mu_n^2 - 1}{2c_n} + 1 \right) (2\mu_n J_{2\mu_n} - c_n^{1/2} E_n), \quad (2.28)$$

$$E_n \equiv J_{2\mu_n+1} - (-1)^{2\mu_n} J_{-2\mu_n+1}, \quad (2.29)$$

where the Bessel functions J and their derivative with respect to the order are now particularized for the value $2\sqrt{c_n}$ of the variable.

The approximate expression (??) is valid only for values of ε and δ (and consequently of $|z|$) sufficiently small as to guarantee that terms $O(z^4)$ in the series of Bessel functions are certainly negligible in comparison with those $O(z^2)$. For not so small ε and δ , approximate values of z could be obtained numerically by using for $W_{\kappa, \mu}(z)$ a uniform asymptotic expansion for large κ like, for instance, that given by Dunster (1989). Unfortunately, the intricacy of the expansion makes difficult to obtain an algebraic expression for the values of z .

3. Zeros of $W_{c/z, \mu}(z)$ for general real values of c and μ

In order to have a description of the zeros of $W_{c/z, \mu}(z)$ for arbitrary real values of the parameters, we have obtained numerically the trajectories described by the first zeros for fixed c and changing μ .

Numerical methods to evaluate the regular and irregular Coulomb functions have deserved a considerable attention. The report by Fullerton (1980) collects references to papers on the subject published before 1980. More recently, other algorithms (Aquilanti & Laganà, 1979; Olver, 1980; Martins, 1981; Temme, 1983; Chalbaud & Martin, 1984; Nesbet, 1984; Seaton, 1984; Humblet, 1985; Thompson & Barnett, 1985; Dunster, 1989; Abad & Sesma, 1992; Olde Daalhuis, 1992 and 1993) have been suggested for evaluating Coulomb and/or Whittaker functions. Three methods have been used in our calculations.

The first method makes use of the expression of W in terms of Kummer functions, that are in turn replaced by their power-series expansions. The method works well for $|z| \leq 10$ provided $\mu > |c|$. In the case of μ being smaller than $|c|$, $W_{c/z, \mu}(z)$ can be obtained by previous calculation of $W_{c/z, \mu+n}$ and $W_{c/z, \mu+n+1}$ (n integer such that $\mu + n > |c|$) and repeated application of the recurrence (Buchholz, 1969, Sect. 7, Eq. (11b))

$$W_{\kappa, \mu-1}(z) = \frac{1}{(1+2\mu)(\kappa-1/2+\mu)z} \times ((1-2\mu)(\kappa-1/2-\mu)zW_{\kappa, \mu+1}(z) + 2\mu(2\kappa z+1-4\mu^2)W_{\kappa, \mu}(z)). \quad (3.30)$$

The second method, used for large $|z|$, benefits from the fact that the logarithmic derivative of W , W'/W , can be easily calculated directly, avoiding the slowly convergent series expansions. Obviously, the poles and zeros of the logarithmic derivative are the zeros of, respectively, W and W' . To our knowledge, three different continued fraction procedures can be used in the evaluation of the logarithmic derivative of $W_{\kappa, \mu}(z)$. The first one (Aquilanti and Laganà, 1979) uses the identity

$$W_{\kappa, \mu}(z) \equiv z^{\mu+1/2} e^{-z/2} U(a, b, z) \quad (3.31)$$

to write

$$\frac{W'_{\kappa, \mu}(z)}{W_{\kappa, \mu}(z)} = -\frac{1}{2} + \frac{\mu}{z} + \frac{1}{2z} + \frac{U'(a, b, z)}{U(a, b, z)}, \quad (3.32)$$

Then, the logarithmic derivative of U is related to the quotient of contiguous functions (Abramowitz & Stegun, 1965, Eq. 13.4.25)

$$\frac{U'(a, b, z)}{U(a, b, z)} = 1 - \frac{U(a, b+1, z)}{U(a, b, z)}, \quad (3.33)$$

and the last term is evaluated by means of the two recurrences (Abramowitz & Stegun, 1965, Eqs. 13.4.17 and 13.4.18)

$$U(a, b+1, z) = U(a, b, z) + aU(a+1, b+1, z), \quad (3.34)$$

$$U(a, b, z) = zU(a+1, b+1, z) + (a-b+1)U(a+1, b, z), \quad (3.35)$$

combined to give

$$\frac{U(a, b+1, z)}{U(a, b, z)} = 1 + \frac{a}{z + \frac{a-b+1}{\frac{U(a+1, b+1, z)}{U(a+1, b, z)}}}. \quad (3.36)$$

The second procedure makes use of the relation (Abramowitz & Stegun, 1965, Eq. 13.4.33)

$$\frac{W'_{\kappa, \mu}(z)}{W_{\kappa, \mu}(z)} = \frac{1}{2} - \frac{\kappa}{z} - \frac{1}{z} \frac{W_{\kappa+1, \mu}(z)}{W_{\kappa, \mu}(z)} \quad (3.37)$$

between the logarithmic derivative and the quotient of contiguous Whittaker functions. Then, the asymptotic expansion (Abramowitz & Stegun, 1965, Eq. 13.1.33)

$$W_{\kappa, \mu}(z) = z^{\kappa} e^{-z/2} {}_2F_0(a, a-b+1; ; -1/z) \quad (3.38)$$

is used to get

$$\frac{1}{z} \frac{W_{\kappa+1, \mu}(z)}{W_{\kappa, \mu}(z)} = \frac{{}_2F_0(a-1, a-b; ; -1/z)}{{}_2F_0(a, a-b+1; ; -1/z)} \quad (3.39)$$

and, finally, the right hand side of this expression is calculated by means of the continued fraction expansion deduced from the three term recurrence

$$\begin{aligned} {}_2F_0(\alpha-1, \beta-1; ; t) = \\ (1 - (\alpha + \beta - 1)t) {}_2F_0(\alpha, \beta; ; t) - \alpha\beta t^2 {}_2F_0(\alpha+1, \beta+1; ; t), \end{aligned} \quad (3.40)$$

that can be checked by comparing powers of t in the two sides. The third continued fraction procedure is similar to the second one except for the fact that the right hand side of (??) is written in the form

$$\begin{aligned} \frac{{}_2F_0(a-1, a-b; ; -1/z)}{{}_2F_0(a, a-b+1; ; -1/z)} = \\ \frac{{}_2F_0(a-1, a-b; ; -1/z)}{{}_2F_0(a-1, a-b+1; ; -1/z)} \frac{{}_2F_0(a-b+1, a-1; ; -1/z)}{{}_2F_0(a-b+1, a; ; -1/z)} \end{aligned} \quad (3.41)$$

and then the two quotients in the right hand side of this equation are replaced by their well known (Jones & Thron, 1980) continued fraction expansion.

The third method is especially suited for the case of very low energies, $|z| \ll 1$. It uses, like the first one, the expression of W in terms of Kummer functions, but, these functions are replaced by, instead of a power series, an expansion in terms of Bessel functions given by Buchholz (1969, Sect. 7, Eq. (16)). The resulting algorithm has been thoroughly discussed in Abad & Sesma (1992).

We report, in Figs. 2 to 7, some trajectories of the zeros of $W_{c/z, \mu}(z)$ for several fixed values of c and continuously varying real μ .

FIG. 2. Zeros of $W_{c/z,\mu}(z)$ for $c = 1$. Only the first four trajectories of family I are shown. The values of μ are indicated by the numbers beside the trajectories. All trajectories of family II are contained in the short segment of the real axis drawn

4. Discussion of results

We have already pointed out, in Subsection 2.1, that the zeros can be grouped in two families according to their behaviour as c vanishes: zeros of family I approach the zeros of $H_\mu^{(1)}(e^{i\pi/2} \bar{z}/2)$, whereas those of family II approach the origin. There are, however, important differences between the cases of positive and negative c .

4.1 Positive c (attractive Coulombian interaction)

The case of positive c is exemplified in Fig. 2, where the trajectories of the zeros of $W_{c/z,\mu}(z)$, for $c = 1$ and varying μ , are shown. The zeros of family I appear

FIG. 3. Trajectories of family II zeros of $W_{c/z,\mu}(z)$ for $c = 1$ and $c = 5$. Only the first three members of each family are shown

for $\mu = 0$ regularly spaced along an almost vertical line in the vicinity of the negative imaginary semiaxis. Let us attach a label $s = 1, 2, 3, \dots$ to each zero, in accordance with its increasing modulus, and to its trajectory. As μ increases from 0 to approximately s , the zeros move upwards, their trajectories presenting horizontal oscillations of period one unit in μ . The oscillation amplitude (infinite for $c = 0$) decreases as c increases. For growing μ above s the zeros move in the second quadrant along parabolic-like trajectories approaching those for $c = 0$. The zeros of family II lie on the positive real semiaxis, presenting an accumulation point at the origin. For a given c , these zeros move towards the origin as μ increases; for fixed μ , they move to the right for increasing c . Figure 3 illustrates this behaviour. Of course, these real zeros correspond to the zeros of $U(a, b, x)$ discussed in Slater (1960, Chap. 6). The correspondence, however, is not trivial: the parameters a and b are held constant in the discussion in Slater (1960), whereas in our case a depends on x , $a = \mu + 1/2 - c/x$. Also, those real zeros are in correspondence, in the case of half integer values of μ (integer values of the angular momentum), with the energies of the bound states of a quantum particle of mass m in an attractive Coulombian

potential with a hard core of radius R_0 ,

$$V(r) = \begin{cases} \infty, & \text{for } r \leq R_0, \\ -\frac{\hbar^2}{2mR_0} \frac{c}{r}, & \text{for } r > R_0, \end{cases} \quad (4.42)$$

the energies being given by

$$E = -\frac{\hbar^2}{8mR_0^2} z^2. \quad (4.43)$$

4.2 Negative c (repulsive Coulombian interaction)

In the case of negative c , the distinction between zeros of families I and II is clear only at low values of $|c|$, namely, $-0.25 < c < 0$. Moreover, even for such low values of $|c|$, family I is in fact decomposed in two subfamilies, I.1 and I.2, as can be seen in Fig. 4. The zeros of subfamily I.1, located for $\mu = 0$ at approximately the same positions as in the case of low positive c , move downwards along cycloid-like trajectories, the “radius of the cycle” diminishing with increasing $|c|$. Besides these trajectories, there are others, those of subfamily I.2, coming from the Riemann sheet $2\pi \leq \arg z < 4\pi$, entering into the principal Riemann sheet $0 \leq \arg z < 2\pi$ at finite values of μ , passing from the fourth quadrant to the third and then to the second one, and finally approaching the trajectories for $c = 0$ as μ increases. Zeros of family II are located for $\mu = 0$ in the second quadrant and, for increasing μ , approach the origin as described at the end of Subsection 2.1.

That classification of trajectories in families and subfamilies is no longer valid for c below -0.25 . As c decreases, more and more trajectories undergo a “hybridization” like illustrated in Fig. 5. One trajectory of subfamily I.2, namely the nearest to the origin one, suffers, as c increases, a deformation tending to make it pass through the origin. This happens for $\mu = \mu_n \equiv n - 1/4$, $n = 1, 2, 3, \dots$, and $c = c_n$ such that $H_{2n-1/2}^{(1)}(c_n) = 0$, as discussed in Subsection 2.2. The numerical results suggest that, as c decreases from c_n , that trajectory “collides”, for certain discrete values of c and μ , successively with all trajectories of family II, interchanging “heads” (the parts of the trajectories corresponding to $\mu \simeq 0$) at each collision. In other words, we conjecture that a double zero of $W_{c/z, \mu}(z)$ occurs for an infinity of pairs of values of c and μ respectively below c_n and above μ_n . This infinite sequence of pairs of values (c, μ) should have (c_n, μ_n) as point of accumulation. After the infinite set of collisions, the hybrid trajectory presents the head of the most external trajectory of family II and the “tail” (the part of the trajectory corresponding to $\mu \rightarrow \infty$) of the most internal one of subfamily I.2. In Figs. 6 and 7, corresponding to $c = -1$ and $c = -10$, one can see respectively one and four of those hybrid trajectories.

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FIG. 4. Zeros of $W_{c/z,\mu}(z)$ for $c = -0.1$. Only the first two trajectories of subfamily I.1 and the first four ones of subfamily I.2 are shown. The excursions of the zeros through the Riemann sheet $2\pi \leq \arg z < 4\pi$ are represented by dotted lines. Trajectories of family II concentrate in a small region near the origin and have not been drawn

REFERENCES

- ABAD, J. & SESMA, J. 1992 Computation of Coulomb wave functions at low energies. *Comput. Phys. Comm.* **71**, 110–124.
- ABAD, J. & SESMA, J. 1995 Computation of the Confluent Hypergeometric Function. *The Mathematica Journal* **5** (4), 74–76
- ABRAMOWITZ, M. & STEGUN, I. A. (Eds.) 1965 *Handbook of Mathematical Functions*. Dover, New York.
- AQUILANTI, V. & LAGANÀ, A. 1979 On the computation of eigenenergies for potentials with a Coulomb tail. *Comput. Phys. Comm.* **17**, 113–116.

FIG. 5. Hybridization of the trajectories of the zeros of $W_{c/z, \mu}(z)$. The successive drawings show the evolution, as c varies, of the first two trajectories of family II and the first one of subfamily I.2, and how a hybrid trajectory is created. As in Fig. 4, the dotted lines represent trajectories in the Riemann sheet $2\pi \leq \arg z < 4\pi$. The big dots on the trajectories correspond to the positions of the zeros for $\mu = 3/4$. The arrows beside the trajectories indicate the motion of the zeros as μ increases

- BUCHHOLZ, H. 1969 *The Confluent Hypergeometric Function*. Springer-Verlag, New York/Berlin.
- CHALBAUD, E. & MARTIN, P. 1984 Fractional approximations for the spherically symmetric Coulomb scattering wave functions. *J. Math. Phys.* **25**, 1268–1273.
- CRUZ, A. & SESMA, J. 1982 Zeros of the Hankel function of real order and of its derivative. *Math. Comput.* **39**, 639–645.
- CRUZ, A., ESPARZA, J., & SESMA, J. 1991 Zeros of the Hankel function of real order out of the principal Riemann sheet. *J. Comput. Appl. Math.* **37**, 89–99.
- DUNSTER, T. M. 1989 Uniform asymptotic expansions for Whittaker's confluent hypergeometric functions. *SIAM J. Math. Anal.* **20**, 744–760.
- ERDÉLYI, A. (Ed.) 1953 *Higher Transcendental Functions*. McGraw-Hill, New York. Vol. 2.
- FULLERTON, L. W. 1980 A Bibliography on the Evaluation of Mathematical Functions. Bell Lab. Comp. Sci. Tech. Report No. 86 (unpublished).

FIG. 6. Zeros of $W_{c/z, \mu}(z)$ for $c = -1$. The first two trajectories of subfamily I.1 and the first four ones of subfamily I.2 are shown. The first trajectory of subfamily I.2 is a hybrid one. The trajectories of family II have not been drawn

- GRAMA, C., GRAMA, N., & ZAMFIRESCU, I. 1985 Zeros of the Coulomb wave function $G_L + iF_L$ with respect to the wave number k . Report FT-272-1985, Centr. Inst. of Physics, Bucharest (unpublished).
- GRAMA, C., GRAMA, N., & ZAMFIRESCU, I. 1994 New class of resonant states for potentials with Coulomb barrier: quasimolecular states. *Ann. Phys.* (N. Y.) **232**, 243–291.
- HUMBLET, J. 1985 Bessel function expansions of Coulomb wave functions. *J. Math. Phys.* **26**, 656–659.
- JONES, W. B. & THRON, W. J. 1980 *Continued Fractions*. Addison-Wesley, Reading, Mass.. Sect. 6.1.4.

FIG. 7. Zeros of $W_{c/z,\mu}(z)$ for $c = -10$. Only the first trajectory of subfamily I.1 and the (hybrid) first four ones of subfamily I.2 are shown

- MARTINS, P. DE A. P. 1981 Spherical Coulomb functions: recurrence relations and continued fractions. *J. Comput. Phys.* **41**, 223–230.
- NESBET, R. K. 1984 Algorithms for regular and irregular Coulomb and Bessel functions. *Comput. Phys. Comm.* **32**, 341–347.
- OLDE DAALHUIS, A. B. 1992 Hyperasymptotic expansions of confluent hypergeometric functions. *IMA J. Appl. Math.* **49**, 203–216.
- OLDE DAALHUIS, A. B. 1993 Hyperasymptotics and the Stokes' phenomenon. *Proc. Roy. Soc. Edinburgh* **123 A**, 731–743.
- OLVER, F. W. J. 1980 Whittaker functions with both parameters large: uniform approximations in terms of parabolic cylinder functions. *Proc. Roy. Soc. Edinburgh* **86A**, 213–234.

TABLE 2

Typical output of the Newton's method applied to the location of the zeros of $W_{c/z,\mu}(z)$. This has been expressed in terms of Kummer functions evaluated by means of their power series expansions.

c	μ	$\Re z$	$\Im z$	$\Re W_{c/z,\mu}(z)$	$\Im W_{c/z,\mu}(z)$
1.	3.3	-3.00000000	2.50000000	0.875714E+00	-0.281576E+00
		-3.57179934	2.74660292	0.103602E+00	-0.477182E-01
		-3.65083627	2.80317456	-0.215425E-02	0.342191E-02
		-3.64958986	2.80007334	-0.601440E-05	0.431460E-05
		-3.64958560	2.80006893	0.589522E-09	-0.611905E-09
-1.	3.3	-2.00000000	-3.00000000	0.165103E+01	0.367207E+00
		-2.62966145	-3.37883613	0.298855E+00	-0.143971E+00
		-2.80972002	-3.29837024	-0.886585E-02	0.133178E-01
		-2.80440211	-3.30582657	0.897728E-05	-0.209375E-04
		-2.80440764	-3.30581477	-0.522181E-08	0.794308E-08

SEATON, M. J. 1984 The accuracy of iterated JWKB approximations for Coulomb radial wave functions. *Comput. Phys. Comm.* **32**, 115–119.

SLATER, L. J. 1960 *Confluent Hypergeometric Functions*. Cambridge Univ. Press, Cambridge.

TEMME, N. M. 1983 The numerical computation of the confluent hypergeometric function $U(a, b, z)$. *Numer. Math.* **41**, 63–82.

THOMPSON, I. J. & BARNETT, A. R. 1985 COULCC: a continued-fraction algorithm for Coulomb functions of complex order with complex arguments. *Comput. Phys. Comm.* **36**, 363–372.

Appendix

The trajectories shown in Figures 1 to 7 have been drawn by joining smoothly points corresponding to zeros of $W_{c/z,\mu}(z)$ for a given c and a sequence of values of μ sufficiently close as to guarantee a safe interpolation. The Newton's method was used in the location of each zero. The iterative process was stopped when the distance between two successive approximations was less than 5×10^{-6} , provided that changes of sign in the real and imaginary parts of $W_{c/z,\mu}(z)$ occurred. The typical output in the application of the Newton's method is shown in Tables 2, 3, and 4, corresponding respectively to the three methods mentioned in Sect. 3.

Needless to say, for values of z in the third and fourth quadrants (i. e., out of the generally considered principal Riemann sheet $-\pi < \arg z \leq \pi$) the circuital relation for $W_{\kappa,\mu}$ (Buchholz, 1969, Sect. 2, Eq. (37)) was used.

TABLE 3

The Newton's method applied to the location of the zeros of $W_{c/z,\mu}/W'_{c/z,\mu}$ evaluated by using a continued fraction procedure.

c	μ	$\Re z$	$\Im z$	$\Re(W/W')$	$\Im(W/W')$
1.	3.7	-4.00000000	4.00000000	0.721723E-01	-0.315989E-01
		-3.92296922	3.50513280	0.424731E-03	0.143299E-01
		-3.86920177	3.55319534	-0.381341E-03	0.102098E-02
		-3.86668723	3.55855341	0.776264E-06	-0.365855E-05
		-3.86669846	3.55853655	-0.253726E-11	0.211474E-08
-1.	5.8	-7.50000000	3.50000000	0.594223E-01	0.115845E+00
		-7.29649261	4.23135798	0.423043E-01	0.202296E-01
		-6.87383414	4.22621877	-0.137454E-02	-0.214992E-02
		-6.89175048	4.21679838	-0.310938E-04	-0.947656E-05
		-6.89200499	4.21685707	0.393998E-07	0.694421E-07

TABLE 4

The Newton's method applied to the location of the zeros of $W_{c/z,\mu}(z)$ using an expansion in series of Bessel functions.

c	μ	$\Re z$	$\Im z$	$\Re W_{c/z,\mu}(z)$	$\Im W_{c/z,\mu}(z)$
-0.24	0.3	-0.27000000	0.10000000	-0.258442E-01	0.866761E-03
		-0.27116988	0.10797150	0.135966E-02	-0.311493E-02
		-0.27194158	0.10732012	-0.104012E-04	0.193682E-04
		-0.27193698	0.10732470	0.147868E-08	-0.150984E-08
-1.	0.7	-1.00000000	0.60000000	0.259468E-01	0.110168E+00
		-0.91756919	0.59219225	-0.943648E-03	-0.137193E-02
		-0.91866550	0.59279505	0.350303E-04	0.190672E-04
		-0.91864871	0.59277099	0.197003E-08	0.648940E-09