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Neumann-Type Expansion of Coulomb Functions

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An expansion is derived for the regular (power series) part of the Coulomb function, $G_0(\eta, \rho)$, in terms of Whittaker functions, which are closely related to the regular Coulomb functions $F_l(\eta, \rho)$. The expansion coefficients are given as a sum of three terms; each of the terms obeys a simple three-term recurrence relation. In conjunction with the downward recurrence method for the regular functions (which is also discussed), this expansion is very useful for computing the irregular Coulomb functions $G_l(\eta, \rho)$, in particular for an attractive potential ($\eta < 0$) and for small or moderately large values of ρ © 1994 Academic Press, Inc.

While the Coulomb functions have attracted considerable interest for a rather long time [1], original contributions are still produced nowadays [2]. Apart from their intrinsic value, this research is also motivated by the need for rapid and accurate computations in many branches of physics. In particular, numerical solution of problems with an attractive Coulomb potential in solid-state physics requires special computational care, e.g., using a logarithmic mesh. These solution can be considerably simplified [3] if the Coulomb part of the potential is solved in terms of Coulomb functions. The present note shows that a Neumann-type series representation can be found for the Coulomb functions which finally results in a very elegant and convenient algorithm for their computation.

It is well known that the Neumann functions $Y_n(z)$ can be expressed as a series of Bessel functions $J_n(z)$, usually refered to as a Neumann series [4, p. 67; 5]. For example, for $n = 0$ we have

$$Y_0(z) = \frac{2}{\pi}\left[\log\frac{z}{2} + \gamma\right] J_0(z) - \frac{4}{\pi}\sum_{k=1}^{\infty} \frac{(-1)^k}{k} J_{2k}(z). \quad (1)$$

This series and its generalization for non-integer ν are very useful for computation [6]: they converge fairly rapidly for small or moderately large arguments, and all terms of the series are small because $|J_\nu(z)| \leqslant 1$ for real z and $\nu \geqslant 0$. Therefore no accuracy is lost owing to small numbers being expressed as differences of large numbers. The Bessel functions $J_\nu(z)$ can be computed by the downward recursion method [7–8]. This method yields a sequence of Bessel functions (whose orders differ by unity) times an unknown factor, which can be determined by the normalization relation [4, p. 138]

$$\left(\frac{z}{2}\right)^\mu = \sum_{n=0}^{\infty} (\mu + 2n) \frac{\Gamma(\mu + n)}{n!} J_{\mu+2n}(z),$$
$$\mu \neq -1, -2, -3, \dots \quad (2)$$

It is the purpose of this paper to establish the analog of Eqs. (2) and (1) for the regular and irregular Coulomb functions whose definition [5] we briefly recall here: Any solution of the differential equation

$$\rho^2 \frac{d^2u}{d\rho^2} + [\rho^2 - 2\eta p - l(l+1)]\, u = 0, \quad \eta = \frac{Z}{\sqrt{E}}, \quad \rho = r\sqrt{E} \quad (3)$$

(which is the radial Schrödinger equation in the presence of the Coulomb potential of a charge Z) is called a Coulomb function. Traditionally, the standard fundamental system of solutions $F_l(\eta, \rho)$ and $G_l(\eta, \rho)$ is chosen such that $F_l(\eta, \rho) \approx \sin(\theta_l)$ and $G_l(\eta, \rho) \approx \cos(\theta_l)$ for $\rho \to \infty$, where θ_l contains the Coulomb phase shift [5]. Thus, we want to express the integral powers of ρ as a series of Coulomb functions $F_l(\eta, \rho)$, and to expand the regular part of the irregular solution $G_l(\eta, \rho)$ in terms of the regular solutions.

The first problem can be disposed of very quickly by recalling the connections between Coulomb functions and Whittaker functions [9, p. 213]

$$F_l(\eta, \rho) = A_l(\eta)\, \mathcal{M}_{i\eta, l+1/2}(2i\rho)$$
$$A_0(\eta) = \frac{-i}{\sqrt{2}}\left[\frac{\pi\eta}{\exp(2\pi\eta) - 1}\right]^{1/2} \quad (4)$$
$$A_l(\eta) = -iA_{l-1}(\eta)[l^2 + \eta^2]^{1/2}, \qquad l = 1, 2, 3, \dots$$

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For the Whittaker functions we follow the notation and definition of Buchholz [9],

$$\mathcal{M}_{\kappa,\mu/2}(z)=\frac{z^{(1+\mu)/2}}{\Gamma(1+\mu)}e^{-z/2}\,{}_1F_1\left(\frac{1+\mu}{2}-\kappa;1+\mu;z\right). \quad (5)$$

In Ref. [9, p. 131, Eq. (16b)] one can also find an expansion of the powers of z in terms of regular Whittaker functions,

$$(2i\rho)^{l+1}=\sum_{n=0}^{\infty}(2l+2n+1)(2l+n)!\times P_n^{(l+i\eta,l-i\eta)}(0)\,\mathcal{M}_{i\eta,l+n+1/2}(2i\rho), \quad (6)$$

where the $P_n^{\alpha,\beta}(x)$ are Jacobi polynomials as defined in [5]. Since the $\mathcal{M}_{i\eta,l+1/2}(2i\rho)$ are real (pure imaginary) for odd (even) l, we define the function

$$M_l(\eta,\rho)=i^{l-1}\mathcal{M}_{i\eta,l+1/2}(2i\rho) \quad (7)$$

which is real for real η and ρ. For $l=0$, by using Eq. (6) and the recurrence relation of Jacobi polynomials (Eq. (22.7.1) in [5]), one obtains the following relation for the coefficients of $M_n(\eta,\rho)$:

$$\rho=\tfrac{1}{2}\sum_{n=0}^{\infty}(2n+1)\,p_n^0(\eta)\,M_n(\eta,\rho)$$
$$p_0^0(\eta)=1;\qquad p_1^0(\eta)=\eta; \quad (8)$$
$$p_{n+1}^0(\eta)=(n^2+\eta^2)\,p_{n-1}^0(\eta).$$

The recurrence relation for the Whittaker functions with respect to μ in terms of the functions $M_l(\eta,\rho)$ is given in [9, Eq. (11a), p. 94],

$$-(l+1)\,M_{l-1}(\eta,\rho)=(2l+1)\left[\eta+\frac{l(l+1)}{\rho}\right]M_l(\eta,\rho)+l[(l+1)^2+\eta^2]\,M_{l+1}(\eta,\rho). \quad (9)$$

Equations (8) and (9) are all that are required to compute the functions $M_l(\eta,\rho)$ by the downward recursion method in complete analogy to the well-known method for the Bessel functions. It is then trivial to obtain the regular Coulomb functions by means of Eqs. (4) and (7).

We now derive the expansion of the irregular solution in terms of the regular ones by following the idea of Neumann's original derivation of the Neumann series [4, Eq. (1), p. 67]. Since both $F_l(\eta,\rho)$ and $G_l(\eta,\rho)$ are solutions of Eq. (3), one can then define the Coulomb operators $\nabla^l=\rho^2(d^2/d\rho^2)+[\rho^2-2\eta\rho-l(l+1)]$ having the property

$$\nabla^0 M_l(\eta,\rho)=l(l+1)\,M_l(\eta,\rho). \quad (10)$$

Now we make the following ansatz for a solution $W_0(\eta,\rho)$ of Eq. (3) for $l=0$ which is linearly independent of $M_0(\eta,\rho)$,

$$W_0(\eta,\rho)=M_0(\eta,\rho)\log\rho+C+u(\eta,\rho), \quad (11)$$

where C is a constant and $u(\eta,\rho)$ (which is entire in ρ) will be expressed as a series in $M_n(\eta,\rho)$,

$$u(\eta,\rho)=\sum_{n=1}^{\infty}\alpha_n(\eta)\,M_n(\eta,\rho). \quad (12)$$

The notation $W_n(\eta,\rho)$ was chosen in analogy with $M_l(\eta,\rho)$ because this function is related to the Whittaker function of the second kind, $W_{\kappa,\mu}(z)$. It is evident from Eq. (12) and the definition of $M_n(\eta,\rho)$ (Eqs. (5) and (7)) that $u(\eta,\rho)$ has a second-order zero at $\rho=0$. Since $W_0(\eta,\rho)$ is a solution of Eq. (3), one has

$$\nabla^0 u(\eta,\rho)=-M_0(\eta,\rho)-2\eta\rho M_0(\eta,\rho)-2\rho(1+\eta^2)\,M_1(\eta,\rho)+(2\eta\rho-\rho^2)C, \quad (13)$$

where use was made of the recurrence relation for the derivative of $M_l(\eta,\rho)$ as given by Eq. (42b) on page 47 of [9]. The last term of Eq. (13) can be expanded into a series of $M_n(\eta,\rho)$ by using Eq. (6) with $l=0$ and $l=1$, respectively. Now we choose the constant C such that the first term of the expansion of $2\eta\rho C$ cancels the term $-M_0(\eta,\rho)$ in Eq. (13). It is easily seen that $C=1/\eta$. To expand the remaining terms of Eq. (13) we note that a general three-term recurrence relation, say

$$\rho f_{n-1}(\rho)=(a_n\rho+b_n)f_n(\rho)+c_n\rho f_{n+1}(\rho), \quad (14)$$

can be iterated to obtain formally

$$\rho f_l(\rho)=\sum_{n=1}^{\infty}\sigma_{l+n}f_{l+n}(\rho)$$
$$\sigma_{l+1}=b_{l+1};\qquad \sigma_{l+2}=a_{l+1}b_{l+2}; \quad (15)$$
$$\sigma_{n+1}=b_{n+1}\left(\frac{a_n}{b_n}\sigma_n+\frac{c_{n-1}}{b_{n-1}}\sigma_{n-1}\right).$$

In our particular case, one obtains (from Eqs. (13) and (9))

$$-2\eta\rho M_0(\eta,\rho)-2\rho(1+\eta^2)\,M_1(\eta,\rho)=\sum_{n=1}^{\infty}s_n(\eta)\,M_n(\eta,\rho)$$
$$s_1(\eta)=6\eta;\qquad s_2(\eta)=20-10\eta^2 \quad (16)$$
$$ns_{n+1}(\eta)=-(2n+3)(\eta s_n(\eta)+\frac{n+1}{2n-1}(n^2+\eta^2)\,s_{n-1}(\eta)).$$

It can be shown quite easily that this series converges for all finite values of η and ρ by using the known asymptotic behaviour of the Whittaker functions for $\mu \to \infty$, Eq. (10) on page 94 in [9], and crude estimates of the coefficients which show that there exists a constant c such that $s_n(\eta) = O(\Gamma(n+c))$.

In summary, Eq. (13) now reads

$$\nabla^0 u(\eta, \rho) = \sum_{n=1}^{\infty} q_n(\eta)\, M_n(\eta, \rho)$$
$$q_n(\eta) = s_n(\eta) + (2n+1)\left(p_n^0(\eta) + \frac{1}{4\eta} p_n^1(\eta) \right) \quad (17)$$
$$p_1^1(\eta) = 2; \qquad p_2^n(\eta) = \sigma\eta$$
$$n^2 p_{n+1}^1(\eta) = (2n+1)\, \eta p_n^1(\eta) + (n+1)^2 (n^2 + \eta^2)\, p_{n-1}^1(\eta)$$

which, upon using Eq. (10), produces a solution for $u(\eta, \rho)$, and therefore

$$W_0(\eta, \rho) = M_0(\eta, \rho) \log \rho + \frac{1}{\eta} + \sum_{n=1}^{\infty} \alpha_n(\eta)\, M_n(\eta, \rho);$$
$$\alpha_n(\eta) = \frac{q_n(\eta)}{n(n+1)} \quad (18)$$

is a solution of Eq. (3) for $l = 0$ which is linearly independent of $F_0(\eta, \rho)$. The only remaining problem is to express the standard solution $G_0(\eta, \rho)$ as a linear combination of $W_0(\eta, \rho)$ and $M_0(\eta, \rho)$. The final result is

$$G_0(\eta, \rho) = w(\eta)\, W_0(\eta, \rho) + m(\eta)\, M_0(\eta, \rho)$$
$$w(\eta) = \left(\frac{\eta}{2\pi} (e^{2\pi\eta} - 1) \right)^{1/2}, \quad (19)$$
$$m(\eta) = [\log 2 + \operatorname{Re} \Psi(1 + i\eta) - \Psi(1) - \Psi(2)]\, w(\eta),$$

where $\Psi(z)$ is the logarithmic derivative of the gamma function.

Since we derived this expansion mainly for computational purposes, we now want to discuss some of its practical aspects. The equations derived in this paper are very easily implemented into an algorithm for the computation of $F_l(\eta, \rho)$ and $G_l(\eta, \rho)$ for fixed ρ and η and a sequence of l-values. It is also useful for repeated calculations with the same η and different ρ, since the coefficients which are independent of ρ need only be calculated once. This algorithm comprises the following steps: (i) Assign arbitrary starting values (e.g., zero and one) to M_l and M_{l-1} for sufficiently high l; (ii) Use the recurrence relation Eq. (9) downwards. This gives $M_0, M_1, M_2, \ldots$ times an unknown normalization constant; (iii) Calculate this normalization constant using Eq. (8); (iv) Calculate F_l using Eq. (4); (v) Calculate G_0 from Eqs. (18) and (19); (vi) Calculate G_1 using the Wronskian (as given, e.g., in Ref. [5, Eq. (14.2.4)].); (vii) Calculate $G_2, G_3, \ldots$ by using the recurrence relation as given, e.g., in Ref. [5, Eq. (14.2.3)]. It may seem surprising that the starting values for the calculation of the M_l in (i) are arbitrary. However, this is a consequence of the strong stability of the downward recursion. In the analogous case of the Bessel functions, this is explained in detail in Ref. [10]. For an attractive potential, this algorithm avoids two common sources of numerical error, viz., cancellation errors and unstable recurrence relations. In Table I we present numerical studies of the properties of Eq. (18) compared to the ascending series for $G_0(\eta, \rho)$ (Eq. (14.1.17) in Ref. [5]). As far as efficiency is concerned, Eq. (18) converges somewhat faster, but that is not its major advantage over the ascending series. The important point is that individual terms in our Neumann-type expansion are never significantly larger than the sum. By contrast, for $\eta = -20$ and $\rho = 10$ the largest term in the ascending series is about 16 orders of magnitude larger than the sum: this means that the sum has 16 fewer significant digits than the terms—or no significant digit at all if ordinary floating point arithmetic with about 15 digits is used. The Neumann-type expansion, on the other hand, shows very few cancellation errors even for fairly large values of $|\eta|$ and ρ.

In summary, this method is best suited for small $|\eta|$ and ρ, but gives accurate results even for larger ρ (where methods based on asymptotic expansions and continued fractions are probably more efficient) and for larger $|\eta|$. For very high value $|\eta|$, the Bessel functions expansion of Humblet [2] is recommended instead. We have also verified that no significant cancellation errors occur in any other part of the algorithm, in particular in Eq. (8). (This does not hold for a repulsive potential: for $\eta > 0$, the two terms in Eq. (19)

TABLE I

Numerical properties of (a) the Neumann-type expansion Eq. (23) and (b) the ascending series, Eq. (14.1.17) in Ref. [5], for $G_0(\eta, \rho)$

	$\rho = 1$			$\rho = 2$			$\rho = 5$			$\rho = 10$		
(a)												
$\eta = -1$	14	0	0	17	0	0	24	0	0	34	0	0
$\eta = -5$	16	−1	−1	20	0	−2	27	0	0	36	0	0
$\eta = -10$	17	0	−1	21	−1	−1	28	0	0	38	0	0
$\eta = -20$	20	−1	−2	24	0	0	32	−1	−1	44	−1	0
$\eta = -50$	24	−1	−1	32	−1	−2	42	−1	−1	55	−1	0
(b)												
$\eta = -1$	19	1	0	23	1	0	37	2	0	53	5	0
$\eta = -5$	21	3	0	26	4	0	40	6	0	56	8	1
$\eta = -10$	24	4	0	29	5	1	43	9	0	62	12	0
$\eta = -20$	29	6	1	37	8	−1	50	12	1	69	17	1
$\eta = -50$	40	9	1	51	12	1	70	20	1	92	27	1

Note. For each ρ, the first number is the number of terms required such that the relative truncation error is less than 10^{-15}. The second number is the order of magnitude of the largest term, defined as its decadic logarithm rounded to the nearest integer. The third number is the order of magnitude of the sum of the respective expansions.

are of almost the same magnitude and of opposite sign; this restricts the usefulness of Eq. (18) to attractive potentials.) We have also examined the numerical properties of other expansions, e.g., the expansion of $F_0(\eta, \rho)$ in spherical Bessel functions (Eq. (14.4.5) in [5]). This expansion shows very large cancellation errors for negative η which then severely restricts its usefulness for computational purposes.

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