Analytical evaluation of elastic Coulomb integrals

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(Received 11 June 1991; accepted for publication 11 September 1991)

Indefinite integrals over the product of two Coulomb wave functions and a factor $r^{-\lambda-1}$, $\lambda = 1,2,3,...$, have been evaluated analytically. The results for these multipole integrals could be expressed again in terms of Coulomb wave functions, except for the electric quadrupole ($\lambda = 2$) integral at zero angular momentum in both the incident and final channels.

I. INTRODUCTION

Differential cross sections for atomic or nuclear scattering can be expressed in terms of solutions of a set of radial wave equations. This set is usually written as a set of coupled-channel integral equations, which can be solved numerically.[1-4] For heavy-ion collisions, this is a severe computer-time-consuming calculation, due to the long-range multipole Coulomb interaction. Well outside the nucleus it requires the evaluation of so-called Coulomb integrals, which have the form

$$I_{ll'}^{(\lambda)} = \int_{R_1}^{R_2} dr \frac{X_l(\eta,kr)\, Y_{l'}(\eta',k'r)}{r^{\lambda+1}}. \tag{1.1}$$

The angular momentum quantum numbers l and l' are non-negative integers, and the multipole moment λ has values $\lambda = 1,2,...$ (dipole, quadrupole,...). The wave numbers k and k' are positive, and the Sommerfeld parameters η and η' are real (positive for heavy-ion collisions and negative for electron scattering from a positive ion). These parameters are related by

$$\eta k = \eta' k'. \tag{1.2}$$

Explicitly, $\eta k = q_1 q_2 \mu / 4\pi\epsilon_0 \hbar^2$, with q_1 and q_2 the charges of the collision partners and μ their reduced mass. Functions X_l and $Y_{l'}$ are real-valued Coulomb wave functions, and they are solutions of the Coulomb differential equations

$$\left(\frac{d^2}{dr^2} + k^2 - \frac{2\eta k}{r} - \frac{l(l+1)}{r^2}\right) X_l(\eta,kr) = 0, \tag{1.3}$$

$$\left(\frac{d^2}{dr^2} + k'^2 - \frac{2\eta' k'}{r} - \frac{l'(l'+1)}{r^2}\right) Y_{l'}(\eta',k'r) = 0. \tag{1.4}$$

By making the change of variables $\rho = kr$ in Eq. (1.3), it follows immediately that X_l only depends on k and r through $\rho = kr$. Similarly, $Y_{l'}$ depends only on k' and r through $\rho' = k'r$. The function $X_l(\eta,\rho)$ is taken to be either the regular Coulomb wave function $F_l(\eta,\rho)$ or the irregular Coulomb wave function $G_l(\eta,\rho)$,[5] and similarly $Y_{l'}(\eta',\rho')$ is either $F_{l'}(\eta',\rho')$ or $G_{l'}(\eta',\rho')$. Given l and l', this yields four possible combinations of Coulomb wave functions in the integrand of Eq. (1.1).

For $R_1 = 0$, $R_2 = \infty$, $X_l = F_l$, and $Y_{l'} = F_{l'}$, the Coulomb integral $I_{ll'}^{(\lambda)}$ can be evaluated analytically by contour integration.[6,7] For a finite interval $[R_1,R_2]$ on the positive r axis, the Coulomb integrals can be evaluated numerically through step-by-step integration,[8,9] or with Gaussian quadrature.[10] For heavy-ion collisions at high energies these methods become intractable, because the integrand oscillates too rapidly. Furthermore, for $R_1 \to \infty$ the convergence is extremely slow. In that case, more sophisticated integration routines have to be used.[11,12] The Coulomb wave functions with different l values, but the same η and ρ, are related through recursion relations. This implies recursion relations between Coulomb integrals with different l,l' and λ values.[4,13] Therefore, only a few integrals have to be calculated by direct integration for each set of parameters R_1, R_2, η, k, η', and k'.

In this paper we evaluate analytically the indefinite integral

$$M_{ll'}^{(\lambda)} = \frac{1}{k^\lambda} \int dr \frac{X_l(\eta,kr)\, Y_{l'}(\eta',k'r)}{r^{\lambda+1}} \tag{1.5}$$

for a large class of parameters. The Coulomb integrals can then be found by substituting the integration limits R_1 and R_2,

$$I_{ll'}^{(\lambda)} = k^\lambda M_{ll'}^{(\lambda)} \Big|_{R_1}^{R_2}. \tag{1.6}$$

The factor $k^{-\lambda}$ in Eq. (1.5) makes $M_{ll'}^{(\lambda)}$ dimensionless, and it appears to reduce the number of independent parameters by one [as does the restriction in Eq. (1.2)].

 0022-2488/92/020578-06$03.00

II. BASIC INTEGRAL

When we multiply Eq. (1.3) by $Y_{l'}(\eta',k'r)$, Eq. (1.4) by $X_l(\eta,kr)$, take the difference, use Eq. (1.2), and integrate, we obtain

$$(k'^2-k^2)\int dr\,X_l(\eta,kr)\,Y_{l'}(\eta',k'r)$$

$$+(l-l')(l+l'+1)\int dr\,\frac{1}{r^2}X_l(\eta,kr)\,Y_{l'}(\eta',k'r)$$

$$=Y_{l'}(\eta',k'r)(d/dr)X_l(\eta,kr)$$

$$-X_l(\eta,kr)(d/dr)Y_{l'}(\eta',k'r)+C, \quad (2.1)$$

where C is an arbitrary integration constant. For an elastic Coulomb integral we have $k'=k$, and with Eq. (1.2) we also have $\eta'=\eta$. With $k'=k$, Eq. (2.1) reduces to

$$M_{ll'}^{(1)}=\frac{X_l'Y_{l'}-X_lY_{l'}'}{(l-l')(l+l'+1)}+C, \quad k'=k, \quad l'\neq l, \quad (2.2)$$

which is an electric dipole ($\lambda=1$) integral. Here, all the Coulomb wave functions have argument (η,ρ), and a prime indicates differentiation with respect to the second argument ρ. The derivatives X_l' and $Y_{l'}'$ in Eq. (2.2) can be expressed in terms of Coulomb wave functions (Appendix A). However, subroutines which calculate $F_l(\eta,\rho)$ and $G_l(\eta,\rho)$ also provide their derivatives.[14–16] An interesting point is that such subroutines provide an array of Coulomb functions for $l=0,1,2,\ldots$, up to a certain $l_{\max}$. Therefore, the right-hand side of Eq. (2.2) can be calculated (for given η and ρ) for all l,l' combinations (except $l'=l$) by a single call to such a subroutine. In this way, the highly unstable l,l' recursion of Coulomb integrals can be avoided.

III. DIPOLE INTEGRAL FOR $l'=l$

When we set $\lambda=1$, $l=l'=0$, and $k'=k$ in the recursion relation (A7), we obtain

$$2\eta M_{00}^{(1)}=\frac{X_0Y_0}{(kr)^2}+D_0(\eta)(M_{10}^{(1)}+M_{01}^{(1)})+C, \quad (3.1)$$

where $D_l(\eta)$ is defined by Eq. (A3). With Eq. (2.2) this becomes

$$2\eta M_{00}^{(1)}=\frac{X_0Y_0}{(kr)^2}+\frac{1}{2}D_0(\eta)(X_1'Y_0-X_1Y_0'-X_0'Y_1$$

$$+X_0Y_1')+C, \quad (3.2)$$

which gives $M_{00}^{(1)}$. With Eq. (B4) this can be simplified to

$$M_{00}^{(1)}=\frac{X_0Y_0}{2\eta(kr)^2}-\frac{D_0(\eta)}{2\eta}(X_0'Y_1-X_1'Y_0)+C. \quad (3.3)$$

Notice that the right-hand side of Eq. (3.2) is symmetric in X nd Y, as is $M_{00}^{(1)}$, but that the right-hand side of Eq. (3.3) is not. When we eliminate X_0' and X_1' in Eq. (3.3) with Eqs. (A1) and (A2), respectively, we obtain

$$M_{00}^{(1)}=\frac{X_0Y_0}{2\eta(kr)^2}-\frac{D_0(\eta)}{2\eta}\left(\eta+\frac{1}{kr}\right)(X_0Y_1+X_1Y_0)$$

$$+\frac{D_0(\eta)^2}{2\eta}(X_0Y_0+X_1Y_1)+C, \quad (3.4)$$

which is again symmetric in X and Y.

To find $M_{ll}^{(1)}$ for $l\neq 0$, we set $l'=l$, $\lambda=1$, and $k'=k$ in Eq. (A7). This gives

$$\frac{2l+1}{2l+3}D_l(\eta)M_{ll}^{(1)}-D_l(\eta)M_{l+1,l+1}^{(1)}$$

$$=\frac{2}{2l+3}D_{l+1}(\eta)M_{l+2,l}^{(1)}-\frac{2\eta}{(l+1)(l+2)}M_{l+1,l}^{(1)}$$

$$+\frac{X_{l+1}Y_l}{(kr)^2}, \quad (3.5)$$

where the two integrals on the right-hand side can be expressed in terms of Coulomb wave functions using Eq. (2.2). Solving Eq. (3.5) yields

$$M_{ll}^{(1)}=\frac{1}{2l+1}\left\{M_{00}^{(1)}+\sum_{n=1}^{l}f_n\right\}, \quad k'=k, l=1,2,\ldots, \quad (3.6)$$

in terms of $M_{00}^{(1)}$, given by Eq. (3.3), and the terms

$$f_n=\frac{1}{D_{n-1}(\eta)}\left\{\frac{D_n(\eta)}{2n+1}(X_{n+1}Y_{n-1}'-X_{n+1}'Y_{n-1})\right.$$

$$+\frac{\eta(2n+1)}{n^2(n+1)}(X_n'Y_{n-1}-X_nY_{n-1}')$$

$$\left.-\frac{2n+1}{(kr)^2}X_nY_{n-1}\right\},$$

$$n=1,2,3,\ldots. \quad (3.7)$$

With Wronski relations of the type given in Appendix B, f_n can be written in many different forms.

IV. HIGHER-ORDER MULTIPOLES

The results from Secs. II and III give $M_{ll'}^{(1)}$ for all l,l'. With recursion relations for the Coulomb integrals of the type (A7), we can find $M_{ll'}^{(\lambda)}$ for $\lambda = 2,3,...$. The following scheme generates these higher-order multipole integrals in a symmetric way with respect to l and l'. For $l'=l=0$,

$$(1-\lambda)M_{00}^{(\lambda+1)}=\frac{X_0Y_0}{(kr)^{\lambda+1}}+D_0(\eta)(M_{10}^{(\lambda)}+M_{01}^{(\lambda)}) - 2\eta M_{00}^{(\lambda)}. \quad (4.1)$$

For $l'=l$, $l\neq 0$,

$$(2l+\lambda+1)M_{ll}^{(\lambda+1)}=-\frac{X_lY_l}{(kr)^{\lambda+1}}+D_{l-1}(\eta)\{M_{l-1,l}^{(\lambda)} + M_{l,l-1}^{(\lambda)}\}-\frac{2\eta}{l}M_{ll}^{(\lambda)}. \quad (4.2)$$

For $l'<l$,

$$M_{ll'}^{(\lambda+1)}=\frac{D_l(\eta)}{2l+1}M_{l+1,l'}^{(\lambda)}+\frac{D_{l-1}(\eta)}{2l+1}M_{l-1,l'}^{(\lambda)} -\frac{\eta}{l(l+1)}M_{ll'}^{(\lambda)}. \quad (4.3)$$

For $l'>l$,

$$M_{ll'}^{(\lambda+1)}=\frac{D_{l'}(\eta)}{2l'+1}M_{l,l'+1}^{(\lambda)}+\frac{D_{l'-1}(\eta)}{2l'+1}M_{l,l'-1}^{(\lambda)} -\frac{\eta}{l'(l'+1)}M_{ll'}^{(\lambda)}. \quad (4.4)$$

When we set $\lambda = 1$ in Eq. (4.1) in order to find $M_{00}^{(2)}$ then $M_{00}^{(2)}$ drops out. Therefore, this integral cannot be found by this scheme. Also in other recursion relations, which are not given here, $M_{00}^{(2)}$ always drops out. It appears that this integral cannot be found by recursion, either in an upward or a downward scheme, which is reminiscent of the situation for integrals over products of Bessel functions.[17] After calculating the $\lambda = 1$ integrals for all l,l', $M_{00}^{(2)}$ has to be calculated independently. By expanding X_0 and Y_0 in a power series and integrating term by term, the integral $M_{00}^{(2)}$ can be expressed as an infinite series in r, around $r=0$. Alternatively, $M_{00}^{(2)}$ can be expanded in an asymptotic series around $r=\infty$. After obtaining $M_{00}^{(2)}$, the above scheme yields $M_{ll'}^{(\lambda)}$ for all l, l', and λ.

V. DEFINITE INTEGRALS

Definite integrals over $[R_1,R_2]$ follow from previous results by substituting the limits of integration. For $R_1 = 0$ and $R_2 = \infty$, the results can be simplified with the help of the well-known behavior of Coulomb wave functions around $r=0$ and $r=\infty$.[5] The integral over two regular Coulomb wave functions,

$$P_{ll'}^{(\lambda)}=\frac{1}{k^\lambda}\int_0^\infty dr\frac{F_l(\eta,kr)F_{l'}(\eta',k'r)}{r^{\lambda+1}}, \quad (5.1)$$

converges in the upper limit for all l, l', λ, and converges in the lower limit under the condition $l+l'\geqslant\lambda-1$. Therefore, for $\lambda = 1$ the integral converges for all l and l', and can be found with the results from Secs. II and III.

From Eq. (2.2) and the behavior of $F_l(\eta,\rho)$ for $\rho\to\infty$, we readily find

$$P_{ll'}^{(1)}=\frac{\sin\{\sigma_l(\eta)-\sigma_{l'}(\eta)+(l'-l)\pi/2\}}{(l'-l)(l'+l+1)}, \quad k'=k, \quad l'\neq l, \quad (5.2)$$

where $\sigma_l(\eta)$ is the Coulomb phase shift, defined by

$$\sigma_l(\eta)=\arg\Gamma(l+1+i\eta). \quad (5.3)$$

From the properties of the Γ function we then find

$$\sigma_l(\eta)-\sigma_{l'}(\eta)=\sum_{n=l'+1}^{l}\arctan\left(\frac{\eta}{n}\right), \quad l>l'. \quad (5.4)$$

From Eq. (3.3) we obtain

$$P_{00}^{(1)}=\frac{1}{2\eta}-\frac{\pi}{e^{2\pi\eta}-1}. \quad (5.5)$$

For $\eta\to 0$ this becomes $P_{00}^{(1)}=\pi/2$. From Eq. (3.7) we find $f_n(0)=0$ and $f_n(\infty)=\eta/(\eta^2+n^2)$, which gives

$$P_{ll}^{(1)}=\frac{1}{2l+1}\left\{P_{00}^{(1)}+\sum_{n=1}^{l}\frac{\eta}{\eta^2+n^2}\right\}, \quad k'=k, \quad l=1,2,... . \quad (5.6)$$

Figure 1 shows $P_{ll}^{(1)}$ as a function of η, for $l=0$ and $l=1$. For $l'\neq l$, but l' close to l, the expressions (5.2) and (5.4) can be combined. This gives, for instance,

$$P_{01}^{(1)}=P_{10}^{(1)}=1/2\sqrt{1+\eta^2}, \quad (5.7)$$

which is also shown in Fig. 1.

Integrals with $X_l=F_l$ and $Y_{l'}=G_{l'}$ converge for $l'\leqslant l-\lambda$, and integrals with $X_l=G_l$ and $Y_{l'}=G_{l'}$ diverge for all l, l', λ. Therefore, the only converging definite inte-

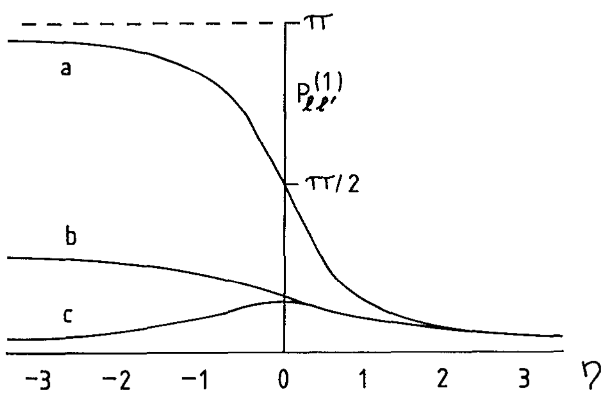

FIG. 1. Curves a, b, and c give the definite integral $P^{(1)}_{ll'}$ for $(l,l') = (0,0)$, $(1,1)$, and $(0,1)$, respectively, as a function of η. The curves are parameter-free.

gral over $[0,\infty]$, for $\lambda = 1$, which involves an irregular Coulomb wave function, is given by

$$\frac{1}{k}\int_0^\infty dr\,\frac{F_l(\eta,kr)G_{l'}(\eta,kr)}{r^2} = \frac{\cos\{\sigma_l(\eta)-\sigma_{l'}(\eta)-(l-l')\pi/2\}}{(l-l')(l+l'+1)},$$

$$k'=k,\quad l'\leqslant l-1, \tag{5.8}$$

as follows from Eq. (2.2).

VI. BESSEL FUNCTIONS

For $\eta\to 0$, the regular and irregular Coulomb wave functions are related to Bessel functions of the first and the second kind, respectively, according to[5]

$$F_l(0,\rho) = \sqrt{\pi\rho/2}J_{l+1/2}(\rho), \tag{6.1}$$

$$G_l(0,\rho) = -\sqrt{\pi\rho/2}N_{l+1/2}(\rho). \tag{6.2}$$

In this fashion, our results for indefinite integrals go over into expressions for indefinite integrals over Bessel functions, some of which were derived recently by Coffey.[17] The definite integral from Eq. (5.5) reduces to

$$\int_0^\infty d\rho\,\frac{J_{l+1/2}(\rho)^2}{\rho} = \frac{1}{2l+1}, \tag{6.3}$$

which is a well-known result.[18] With $\sigma_l(0) = 0$, Eqs. (5.2) and (5.8) become

$$\int_0^\infty d\rho\,\frac{J_{l+1/2}(\rho)J_{l'+1/2}(\rho)}{\rho} = \frac{2\sin\{(l'-l)\pi/2\}}{\pi(l'-l)(l'+l+1)},\quad l'\neq l, \tag{6.4}$$

$$\int_0^\infty d\rho\,\frac{J_{l+1/2}(\rho)N_{l'+1/2}(\rho)}{\rho} = \frac{2\cos\{(l'-l)\pi/2\}}{\pi(l'-l)(l'+l+1)},\quad l'\leqslant l-1, \tag{6.5}$$

respectively.

VII. RELATED INTEGRALS

When we set $l' = l$ in Eq. (2.1), then this equation can be written as

$$k\int dr\,X_l(\eta,kr)\,Y_l(\eta',k'r) = \frac{\alpha^2 X_l'(\eta,kr)\,Y_l(\eta',k'r) - \alpha X_l(\eta,kr)\,Y_l'(\eta',k'r)}{1-\alpha^2} + C,\quad k'\neq k, \tag{7.1}$$

where $\alpha = k/k'$. The left-hand side could be considered to be a Coulomb integral with $\lambda = -1$. Most interesting is that Eq. (7.1) gives an indefinite integral over Coulomb wave functions with $k'\neq k$. It also illustrates that integrals with $k'\neq k$ are essentially different in form than integrals with $k'=k$: for $k'\to k$ we have $1-\alpha^2\to 0$, and this case has to be considered with a limit procedure.

In order to find the limit $k'\to k$ of Eq. (7.1) we expand the right-hand side in a Taylor series in k', around $k'=k$. We expand $Y_l(\eta',k'r)$ as

$$Y_l(\eta',k'r) = Y_l(\eta,kr) + (k'-k)\,[(\partial/\partial k')\,Y_l(\eta',k'r)]_{k'=k} + \mathcal{O}((k'-k)^2). \tag{7.2}$$

In the first term on the right-hand side we have used

$\eta k=\eta' k'$, which implies $\eta'=\eta$ whenever $k'=k$. This relation was also used in the derivation of Eq. (2.1). Therefore, in $Y_l(\eta',k'r)$ both η' and $k'r$ depend on k', and care should be exercised in calculating $\partial/\partial k'$ in Eq. (7.2). When we consider k' as independent variable, then, according to the chain rule, we have

$$\frac{\partial}{\partial k'} Y_l(\eta',k'r)=rY_l'(\eta',k'r)-\frac{\eta'}{k'}\frac{\partial}{\partial\eta'} Y_l(\eta',k'r), \tag{7.3}$$

where the prime on Y_l' indicates differentiation with respect to $k'r$, as before. Then we set $k'=k$ and $\eta'=\eta$ in Eq. (7.3) and substitute the result into Eq. (7.2). For the expansion of Eq. (7.1), we also need $Y_l'(\eta',k'r)$, which is the derivative with respect to $k'r$ of the right-hand side of Eq. (7.2). With Eq. (7.3), this yields a term with Y_l'', and with the differential equation (1.4) for Y_l, this can be expressed in terms of Y_l. When we combine everything and take the limit $k'\to k$, we obtain

$$k\int dr\, X_lY_l=\frac{1}{2}\left[krX_l'Y_l'-X_lY_l'+\left(kr-2\eta-\frac{l(l+1)}{kr}\right)X_lY_l-\eta X_l'\frac{\partial}{\partial\eta}Y_l+\eta X_l\frac{\partial}{\partial\eta}Y_l'\right]+C,\quad k'=k, \tag{7.4}$$

where all Coulomb wave functions have the arguments (η,kr). In deriving Eq. (7.4) we have absorbed a term $X_l'Y_l-X_lY_l'$, the Wronskian of the differential equation, into the integration constant C. The result (7.4) can be verified by differentiation with respect to r.

VIII. CONCLUSIONS

The elastic Coulomb integrals for $\lambda=1$ have been evaluated analytically, and it was shown that higher-order multipole integrals can be obtained from the $\lambda=1$ integrals by recursion. Only the electric quadrupole integral for $l=l'=0$ could not be obtained in closed form (unless expressed as an infinite series). The results can be applied to calculate Coulomb integrals numerically without step-by-step integration and without recursion with respect to the quantum numbers l and l'. In practical applications, the inelastic $(k'\neq k)$ integrals are also needed. Since the values of k' and k are very close, at least for heavy ions, these $k'\neq k$ integrals can be obtained by Taylor expansion of $Y_{l'}(\eta',k'r)$ around $k'=k$.

ACKNOWLEDGMENT

This research was supported in part by the National Science Foundation under Grant No. CHE-9016789.

APPENDIX A: RECURSION RELATIONS

The derivative with respect to ρ of the Coulomb wave function $X_l(\eta,\rho)$ can be expressed in two ways in terms of Coulomb wave functions:[5]

$$X_l'=\left(\frac{\eta}{l+1}+\frac{l+1}{\rho}\right)X_l-D_l(\eta)X_{l+1}, \tag{A1}$$

$$X_l'=-\left(\frac{\eta}{l}+\frac{l}{\rho}\right)X_l+D_{l-1}(\eta)X_{l-1}. \tag{A2}$$

Here we introduced the abbreviation

$$D_l(\eta)=\sqrt{1+(\eta/l+1)^2}. \tag{A3}$$

Either Eq. (A1) or (A2) can be solved for X_l, and the results can be substituted into the integrand in Eq. (1.5). Elimination of X_l' through integration by parts then yields a recursion relation between four Coulomb integrals. A similar procedure can be followed for $Y_{l'}$ in Eq. (1.5). In this fashion, we obtain four recursion relation, three of which are independent. They relate Coulomb integrals with different l, l', and λ values, and by repeated application of these relations an indefinite number of other recursion relations can be obtained.

In Sec. III we need

$$\frac{l+l'-\lambda+2}{2l+3}D_l(\eta)M_{ll'}^{(\lambda)}-\frac{1}{\alpha}D_{l'}(\eta')M_{l+1,l'+1}^{(\lambda)}-\frac{l-l'+\lambda+1}{2l+3}D_{l+1}(\eta)M_{l+2,l'}^{(\lambda)}+\eta\left\{\frac{1}{l'+1}-\frac{l'-\lambda+1}{(l+1)(l+2)}\right\}M_{l+1,l'}^{(\lambda)}=H_{l+1,l'}^{(\lambda)}+C. \tag{A4}$$

Here we introduced the notation

$$\alpha=k/k', \tag{A5}$$

$$H_{ll'}^{(\lambda)}=\frac{X_l(\eta,kr)Y_{l'}(\eta',k'r)}{(kr)^{\lambda+1}}. \tag{A6}$$

Another relation is

$$(l+l'+1-\lambda)M_{ll'}^{(\lambda+1)}-D_l(\eta)M_{l+1,l'}^{(\lambda)}$$
$$-(1/\alpha)D_{l'}(\eta')M_{l,l'+1}^{(\lambda)}$$
$$+\eta\left\{\frac{1}{l+1}+\frac{1}{l'+1}\right\}M_{ll'}^{(\lambda)}=H_{ll'}^{(\lambda)}+C. \qquad \text{(A7)}$$

The easiest way to prove this relation is to differentiate $H_{ll'}^{(\lambda)}$ from Eq. (A6), eliminate X_l' and Y_l', with Eq. (A1), and then integrate the resulting expression. By differentiating $H_{l+1,l'}^{(\lambda)}$, $H_{l,l'+1}^{(\lambda)}$, etc., similar relations can be derived.

APPENDIX B: WRONSKI RELATIONS

The Wronskian of F_l and G_l is

$$F_l'G_l-F_lG_l'=1, \qquad \text{(B1)}$$

and a similar relation is[5]

$$F_lG_{l+1}-F_{l+1}G_l=1/D_l(\eta). \qquad \text{(B2)}$$

Here, all Coulomb wave functions have the same argument (η,ρ). Differentiating Eq. (B2) gives

$$F_l'G_{l+1}+F_lG_{l+1}'-F_{l+1}'G_l-F_{l+1}G_l'=0. \qquad \text{(B3)}$$

If we would replace either F by G or G by F, or interchange F and G, this relation would still hold. Therefore, for arbitrary X and Y we have

$$X_l'Y_{l+1}-X_{l+1}'Y_l=X_{l+1}Y_l'-X_lY_{l+1}', \quad k'=k. \qquad \text{(B4)}$$

A generalization of Eq. (B1) can be found as follows. Write $X_l'(\eta,kr)$ and $Y_l'(\eta',k'r)$ as in Eq., (A1), and calculate $\alpha X_l'Y_l-X_lY_l'$. With $\eta k=\eta'k'$ and $\alpha=k/k'$ we then obtain

$$\alpha X_l'Y_l-X_lY_l'=D_l(\eta')X_lY_{l+1}$$
$$-\alpha D_l(\eta)X_{l+1}Y_l, \quad \text{all } k,k'. \qquad \text{(B5)}$$

For $k'=k$, $X_l=F_l$ and $Y_l=G_l$, this reduces to Eq. (B1).

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