

C. Coulomb functions

Coulomb function is the regular solution of

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + \frac{2Z}{r} + k^2 \right) F_{kl}(z|r) = 0, \quad (C.1)$$

which has asymptotic form

$$F_{kl}(z|r) \underset{r \rightarrow \infty}{\sim} k^{-1/2} \sin[kr - \frac{1}{2}l\pi + \gamma \ln(2kr) + \sigma_l(\gamma)], \quad \gamma = z/k. \quad (C.2)$$

Solution can be expressed through the hypergeometric function

$$F_{kl}(z|r) = \frac{|\Gamma(l+1-i\gamma)|}{2k^{1/2}(2l+1)!} e^{\gamma\pi/2} (2kr)^{l+1} e^{ikr} {}_1F_1(l+1-i\gamma, 2l+2; -2ikr). \quad (C.3)$$

Let introduce Coulomb variables $\rho = zr$ and $\kappa = k/z$. Then

$$\left(\frac{d^2}{d\rho^2} - \frac{l(l+1)}{\rho^2} + \frac{2}{\rho} + \kappa^2 \right) F(\kappa l|\rho) = 0 \quad (C.4)$$

$$F(\kappa l|\rho) = \frac{|\Gamma(l+1-i/\kappa)|}{2\kappa^{1/2}(2l+1)!} e^{\pi/2\kappa} (2\kappa\rho)^{l+1} e^{i\kappa\rho} {}_1F_1(l+1-i/\kappa, 2l+2; -2i\kappa\rho), \quad (C.5)$$

$$F(\kappa l|\rho) \underset{\rho \rightarrow \infty}{\sim} \kappa^{-1/2} \sin[\kappa\rho - \frac{1}{2}l\pi + (1/\kappa) \ln(2\kappa\rho) + \arg \Gamma(l+1-i/\kappa)]. \quad (C.6)$$

It is normalization to the unit flux. Note that normalization to energy differs only by coefficient: $[1/\kappa]^{1/2} \rightarrow [2/(\pi\kappa)]^{1/2}$.

Module of gamma function in (C.5) can be expressed as

$$|\Gamma(l+1+i\eta)| = \eta^l e^{-\pi\eta/2} \left[\frac{2\pi\eta A(\kappa, l)}{1 - e^{-2\pi\eta}} \right]^{\frac{1}{2}}, \quad (C.7)$$

$$A(\kappa, l) = \prod_{m=0}^l (1 + m^2 \kappa^2) \quad (C.8)$$

We can also expand $F(\kappa l|\rho)$ in power series as

$$F(\kappa l|\rho) = C(\kappa, l) \rho^{l+1} \sum_{n=0}^{\infty} a_n \rho^n \quad (C.9)$$

$$C(\kappa, l) = \left\{ \frac{2\pi A(\kappa, l)}{1 - e^{-2\pi/\kappa}} \right\}^{\frac{1}{2}} \frac{2^l}{(2l+1)!} \quad (C.10)$$

$$a_0 = 1, \quad a_1 = -1/(l+1), \quad a_n = -\frac{2a_{n-1} + \kappa^2 a_{n-2}}{n(2l+1+n)} \quad (C.11)$$

C. Coulomb integrals

Let us introduce the integrals

$$I(kl, k'l'; \lambda) = \int_0^{\infty} F_{kl}(r) r^{-\lambda-1} F_{k'l'}(r) dr. \quad (\text{B.1})$$

which play important role in the electron-ion scattering calculations as illustrated in the previous sections. Analytical expressions for integrals (B.1) through the hypergeometric function of the complex arguments are given in several publications (Infeld and Hull 1951, Biedenharn *et al.* 1955, Burgess *et al.* 1970). In particular, Burgess *et al.* 1970 considered the numerical computation of such integrals, expressed through the hypergeometric functions. The corresponding Fortran routine are still using in STGF program. However, only the dipole case $\lambda = 1$ is implemented. Our long experience of using STGF program shows that these subroutines in some cases (especially, for close energies for incident and scattering electron) are numerically unstable and provide unphysical results when top-up procedure is applied. It may distort the final cross sections at the last step of calculations.

Below we suggested more general and computationally more convenient procedure for evaluation of Coulomb integrals (B.1) based only on the recursive relations. This procedure is valid for arbitrary multipole index λ . If use the expansion (C.7) for the Coulomb function $F(\kappa l' | \rho)$, the integral (B.1) is reduces to sum '

$$I(\kappa l, \kappa' l'; \lambda) = C(\kappa', l') \sum_{j=0}^{\infty} a_j^{l'} J_l^{l'+j-\lambda} \quad (\text{B.2})$$

where

$$J_l^m = \int_0^{\infty} \rho^m F(\kappa l; \rho) d\rho. \quad (\text{B.3})$$

Assuming that sum in (B.2) converges, the task then is reduced to determination of the integrals J_l^m . Similar integrals

$$Q_l^m(q) = \int_0^{\infty} \rho^m e^{-qr} F(\kappa l; \rho) d\rho$$

first were considered by Bransden and Dalgarno (1953) in their treatment of helium autoionization in the perturbation approach. Later, their expressions were corrected by Zemtsov (1974). For our

task, we may use their expressions in the limit $q \rightarrow 0$. In this case, all integrals J_l^m can be obtained from the set of following recursive relations.

Depending on the value $l'-\lambda$, we have two branches of the recursion relations:

(i) In the case $l'-\lambda \geq l$ ($m \geq l$) all the necessary values of integrals in (B.x)) are defined according to formulae

$$\begin{aligned} J_l^l &= C(\kappa, l)(2l+1)! \kappa^{-2(l+1)} \exp(-\pi/\kappa), \\ J_l^{l+1} &= -2J_l^l / \kappa^2, \end{aligned} \quad (\text{B.4})$$

with consecutive application of the following recursion relations

$$J_l^m = \{-2J_l^{m-1} - (m+l)(m-l-1)J_l^{m-2}\} / \kappa^2 \quad (\text{B.5})$$

for rising values of the parameter m .

(ii) In the case $l'-\lambda < l$ ($m < l$), the necessary values of integrals J_l^m can be from (B.x) in the opposite direction, i.e.

$$J_l^m = \frac{-2J_l^{m+1} - \kappa^2 J_l^{m+2}}{(m+l+2)(m-l+1)}. \quad (\text{B.6})$$

This procedure, however, is not working for J_l^{l-1} ($m=l-1$). In this case we have to use the additional relations

$$J_l^{l-1} = \frac{l(2l+1)J_{l-1}^{l-2} - J_{l-1}^{l-1}}{(1+\kappa^2 l^2)^{1/2}}, \quad (\text{B.7})$$

$$J_l^l = J_{l-1}^{l-1} \frac{2(1+\kappa^2 l^2)^{1/2}}{\kappa^2}, \quad (\text{B.8})$$

with the initial values of J_0^0 and J_0^{-1} being directly calculated as

$$J_0^0 = C(\kappa, 0) \exp(-2\pi/\kappa^2), \quad (\text{B.9})$$

$$J_0^{-1} = C(\kappa, 0)[1 - \exp(-2\pi/\kappa^2)]. \quad (\text{B.10})$$

We found, that the series (B.x) converges rapidly for $\kappa > \kappa'$, almost independently of the parameters l, l', κ, κ' . However, for the case of small κ, κ' or when κ is close to κ' one inevitably encounters large numerical values of J_l^m . This difficulty can be circumvented rather easily by renormalization of the integrals at each stage of recursive relations.

Appendix A contain the program IKL, the FORTRAN installation of the above expressions.

D. Testing of the programs.

For monopole and dipole cases, $\lambda=0,1$, results agree with accuracy 10^{-6} with values from the Fdip subroutine in the STGF program. This comparison was used as primary test and check the accuracy the programs. Time debugging of the calculations revealed that the present programs make the similar calculations **4 times faster**.

For higher multipole index, the test of programs was based on the recurrence relations and limit case of equal energies, $\kappa \sim \kappa'$.

D.1. The limit $\kappa \sim \kappa'$

If we let $\kappa \sim \kappa'$ the integrals I simplify considerably. The monopole integrals $I(kl, kl; 0)$ diverge, and for $\lambda > 0$ the general formula is given by Alder *et al.* (1956), Eq. II E.74 [note they are working

with integrals $M_{\kappa l \kappa' l'}^{-\lambda-1} = \frac{1}{\kappa \kappa'} I(\kappa l, \kappa' l'; \lambda)$ and using $\eta=1/\kappa$]:

$$\begin{aligned} I(\kappa l, \kappa l + \lambda; \lambda) &= (2)^{\lambda-2} (\kappa)^{\lambda-1} \frac{[(\lambda-1)!]^2}{(2\lambda-1)!} \left| \frac{\Gamma(l+1+i/\kappa)}{\Gamma(l+1+\lambda+i/\kappa)} \right| \\ &= (2)^{\lambda-2} (\kappa)^{2\lambda-1} \frac{[(\lambda-1)!]^2}{(2\lambda-1)!} \left[\prod_{s=l+1}^{l+\lambda} (1+s^2 \kappa^2) \right]^{-\frac{1}{2}} \end{aligned} \quad (\text{B.11})$$

In particular, for the lowest multipole orders, one obtains the following expressions:

$$I(\kappa l, \kappa l + 1; 1) = \frac{1}{2} \kappa [1 + (l+1)^2 \kappa^2]^{-\frac{1}{2}} \quad (\text{B.11})$$

$$I(\kappa l, \kappa l + 2; 2) = \frac{1}{6} \kappa^3 [(1 + (l+1)^2 \kappa^2)(1 + (l+2)^2 \kappa^2)]^{-\frac{1}{2}} \quad (\text{B.11})$$

$$I(\kappa l, \kappa l + 3; 3) = \frac{1}{15} \kappa^5 [(1 + (l+1)^2 \kappa^2)(1 + (l+2)^2 \kappa^2)(1 + (l+3)^2 \kappa^2)]^{-\frac{1}{2}} \quad (\text{B.11})$$

The present program IKL is working for all combinations of the κ, κ' parameters. It allowed us to check the program by comparison with analytical results from the above relations.

D.1. Recursion relations (we switch from notation κ, κ' to κ_1, κ_2)

For monopole integrals, one obtains the three-terms relation (Adler 1956, II B 66):

$$y_1 I(\kappa_1 l + 1, \kappa_2 l + 1; 0) + y_2 I(\kappa_1 l, \kappa_2 l; 0) + y_3 I(\kappa_1 l - 1, \kappa_2 l - 1; 0) = 0$$

with

$$\begin{aligned} y_1 &= 2l[1 + (l+1)^2 \kappa_1^2]^{\frac{1}{2}} [1 + (l+1)^2 \kappa_2^2]^{\frac{1}{2}} \\ y_2 &= -(2l+1)[2 + l(l+1)(\kappa_1^2 + \kappa_2^2)] \\ y_3 &= 2(l+1)[1 + l^2 \kappa_1^2]^{\frac{1}{2}} [1 + l^2 \kappa_2^2]^{\frac{1}{2}}, \quad l > 0 \end{aligned}$$

These relations connect monopole integrals with the two first, with $l=0$.

To do:

Write program to calculate, for the given κ and κ' , all integrals from $l=2$ up to $l=50$ from integrals for $l=0,1$ using the above recursion relations and directly. Compare the results.

For $\lambda=1$, the dipole integrals are most easy obtained from the monopole integrals by (Adler 1956,

II B68, Burgess 1970 A3):

$$2(l+1)I(\kappa_1 l, \kappa_2 l+1; 1) = [1 + (l+1)^2 \kappa_2^2]^{\frac{1}{2}} I(\kappa_1 l, \kappa_2 l; 0) - [1 + (l+1)^2 \kappa_1^2]^{\frac{1}{2}} I(\kappa_1 l+1, \kappa_2 l+1; 0)$$

Check this numerically! Factor 2 above only in Adler 1956.

The above relation is also should be valid for all odd $\lambda=1,3,5,\dots$

$$(\lambda+1)(l+1)I(\kappa_1 l, \kappa_2 l+1; \lambda) = [1 + (l+1)^2 \kappa_2^2]^{\frac{1}{2}} I(\kappa_1 l, \kappa_2 l; \lambda-1) - [1 + (l+1)^2 \kappa_1^2]^{\frac{1}{2}} I(\kappa_1 l+1, \kappa_2 l+1; \lambda-1)$$

Check this numerically for $\lambda=3,5$

For the dipole case also may be written the three-term recursion relation which connects different values of l ((Adler 1956, II B70):

$$y_1 I(\kappa_1 l-1, \kappa_2 l-2; 1) + y_2 I(\kappa_1 l, \kappa_2 l-1; 1) + y_3 I(\kappa_1 l+1, \kappa_2 l; 1) = 0 \quad (\text{X05})$$

with

$$\begin{aligned} y_1 &= 2[1 + (l-1)^2 \kappa_2^2]^{\frac{1}{2}} [1 + l^2 \kappa_1^2]^{\frac{1}{2}} \\ y_2 &= -4 - l(2l+1)\kappa_2^2 - l(2l-1)\kappa_1^2 \\ y_3 &= 2[1 + l^2 \kappa_2^2]^{\frac{1}{2}} [1 + (l+1)^2 \kappa_1^2]^{\frac{1}{2}} \end{aligned}$$

This relation connects all monopole integrals with the two first.

Write the program to calculate, for the given κ and κ' , all integrals $I(\kappa_1 l, \kappa_2 l+1; 1)$ from $l=2$ up to $l=50$ from integrals for $l=0,1$ using the above recursion relations and directly. Compare the results.

SUM RULES (Burgess 1974)

$$\sum_{l=L}^{\infty} \sum_{l'=l \pm 1} l_{>} I^2(\kappa_1 l, \kappa_2 l'; 1) = [I^2(\kappa_1 L, \kappa_2 L - 1; 1) - I^2(\kappa_1 L - 1, \kappa_2 L; 1)] \frac{1 + L^2 \kappa_1^2}{L(\kappa_1^2 - \kappa_2^2)} \quad Z > 0$$

$$\sum_{l=L}^{\infty} \sum_{l'=l \pm 1} l_{>} I_0^2(k_1 l, k_2 l'; 1) = [I_0^2(k_1 L, k_2 L - 1; 1) - I_0^2(\kappa_1 L - 1, \kappa_2 L; 1)] \frac{L k_1^2}{(k_1^2 - k_2^2)} \quad Z = 0$$

These results are of importance in dealing with angular momentum summations of partial collision strengths.

Another expression for the case $Z=0$ (Whelan 1986):

$$\sum_{l=L}^{\infty} \sum_{l'=l \pm 1} l_{>} I_0^2(k_1 l, k_2 l'; 1) = \frac{1}{4} L \left(\frac{k_1}{k_2} \right) (Q_{L-1}^2 - Q_L^2)$$

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