Coulomb integrals - neutral case

For Z=0, the function F_{kl} can be expressed in terms of spherical Bessel functions and the Coulomb integrals has the form

$$I_0(kl,k'l';\lambda)=\sqrt{kk'}\int_0^\infty j_l(kr)r^{-\lambda-1}j_{l'}(k'r)dr.$$

The recurrence relations reduce to

$$(2l+2)k_1k_2I_0(k_1\ l+1,k_2\ l+1;\ 0)-(2l+1)I_0(k_1\ l,k_2\ l;\ 0)+2lI_0(k_1\ l-1,k_2 l-1;\ 0)=0$$

and

$$I_0(k_1l,k_2l+1;\ 1)=k_2I_0(k_1\ l,k_2\ l;\ 0)-k_1I_0(k_1\ l+1,k_2\ l+1;\ 0)$$

The limit k = k' (Whelan 1986)

$$I_0(kl,kl';\ \lambda)=\frac{\pi k^{\lambda-1}\Gamma(\lambda)\Gamma[\frac{1}{2}(l+l'-\lambda+2)]}{2^{\lambda+1}\Gamma[\frac{1}{2}(l-l'+\lambda+1)]\Gamma[\frac{1}{2}(l'-l+\lambda+1)]\Gamma[\frac{1}{2}(l+l'+\lambda+2)]}$$

Direct formulas through the hypergeometric functions (Burgess et al 1970):

$$I_0(k_1\ l,k_2\ l;\ 0)=\frac{4^l(l!)^2(k_1k_2)^{l+\frac{1}{2}}}{(2l+1)!(k_1+k_2)^{2l+2}}\,{}_2F_1\left(l+1,l+1,2l+2;\frac{4k_1k_2}{(k_1+k_2)^2}\right)$$

or

$$I_0(k_1\ l,k_2\ l;\ 0)=\frac{4^l(l!)^2(k_1k_2)^{\frac{1}{2}}}{(2l+1)!k_>^2}\left(\frac{k_<}{k_>}\right)^l\,{}_2F_1\left(l+1,\tfrac{1}{2},l+\tfrac{3}{2};\frac{k_<^2}{k_>^2}\right)$$

where $k_<$ is the smaller of k_1 and k_2, $k_>$ is the greater of k_1 and k_2, which is a more usual form for the integrals I_0 (see Watson 1944, p.401).

Using the above recurrence relations or from Watson (1944) we have

$$I_0(k_1\ l,k_2\ l+1;\ 1)=\frac{2^{2l+p}l!(l+p)!(k_1k_2)^{\frac{1}{2}}}{(2l+1+2p)!k_>}\left(\frac{k_<}{k_>}\right)^{l+p}\,{}_2F_1\left(l+1,-\tfrac{1}{2}+p,l+\tfrac{3}{2}+p;\frac{k_<^2}{k_>^2}\right),$$

where $p = 0$ if $k_1 < k_2$

$p = 1$ if $k_1 > k_2$.

This formula is used in `STGF` program (subroutine `Fdip0`)

More general formula including higher multipoles is given by Chidishimo (1992) (also based on the Watson 1944). The general expressions for $\lambda \geq 1$ has discontinuity at $k = k'$:

$0<k'<k$

$$I_0(kl,k'l';\lambda)=\frac{\pi}{2^{\lambda+1}}\left(\frac{k'}{k}\right)^{l+1/2}k^{\lambda-1}\left[\frac{k^2-k'^2}{k^2}\right]^{-[(l'-l-\lambda)/2]}\frac{\Gamma((l+l'-\lambda+2)/2)}{\Gamma(l'+\frac{3}{2})\Gamma((l-l'+\lambda+1)/2)}$$
$$\times\,{}_2F_1\left(\frac{l'-l+\lambda+1}{2},\frac{l'-l-\lambda+1}{2},l'+\tfrac{3}{2};\frac{k'^2}{k'^2-k^2}\right)$$

$0<k<k'$

$$I_0(kl,k'l';\lambda)=\frac{\pi}{2^{\lambda+1}}\left(\frac{k}{k'}\right)^{l+1/2}k'^{(\lambda-1)}\left[\frac{k'^2-k^2}{k'^2}\right]^{-[(l-l'-\lambda+1)/2]}\frac{\Gamma((l+l'-\lambda+2)/2)}{\Gamma(l'+\frac{3}{2})\Gamma((l'-l+\lambda+1)/2)}$$
$$\times\,{}_2F_1\left(\frac{l-l'+\lambda+1}{2},\frac{l-l'-\lambda+1}{2},l+\tfrac{3}{2};\frac{k^2}{k^2-k'^2}\right).$$

Another expression for $I_0(kl,k'l';\lambda)$ is derived by Whelan (1986) and programmed by Burgess and Whelan (1987):

$$I_0(kl,k'l';\lambda)=\sum_L F_{\lambda L}(k,l,k',l')Q_L(\chi)\left(\frac{\pi}{kk'}\right)^{\frac{1}{2}}\frac{1}{2^{\lambda}\Gamma(\lambda+\frac{1}{2})},$$

where $Q_L(\chi)$ is a Legendre function of the 2nd kind whose argument is given by $\chi=(k^2+k'^2)/2kk'$. These functions satisfy the same recurrence relations as the standard Legendre functions

$$(l+1)Q_{l+1}(\chi)=(2l+1)\chi Q_l(\chi)-lQ_{l-1}(\chi)$$

and

$$Q_0(\chi)=\tfrac{1}{2}\ln\left(\frac{\chi+1}{\chi-1}\right);\qquad Q_1(\chi)=\tfrac{\chi}{2}\ln\left(\frac{\chi+1}{\chi-1}\right)-1.$$

Therefor it would appear that Q_{l+1} could be calculated from Q_l ,Q_{l-1}. However (as noted Burgess and Whelan 1987) for certain values of χ cancellations errors are appreciable and in this case it is more efficient to use the recurrence relations for decreasing l. In general the nearer χ is to 1 the less likely it is to need the decreasing l procedure. To evaluate Q-functions, we will use the DLEGENI program of Gil and Segura (1997).

The coefficients $F_{\lambda L}(k,l,k',l')$ are given by Seaton (1961) and expressed in terms of 3*j* and 6*j* symbols. It is more convenient to use the formula given by Somerville (1963):

$$F_{\lambda L}(k,l,k',l')=(-1)^{(\lambda+l'-l)/2}\frac{2L+1}{2}E(\lambda,l',l)\sum_{\mu=|L-l'|,2}^{\lambda-|L-l|}\frac{k^{\lambda-\mu}(-k')^{\mu}}{E(l,L,\lambda-\mu)E(l',L,\mu)}$$

where

$$E(a,b,c)=\frac{(a+b+c+1)!(\frac{1}{2}(a-b+c))!(\frac{1}{2}(a+b-c))!(\frac{1}{2}(-a+b+c))!}{(a+b-c)!(\frac{1}{2}(a+b+c))!}\ .$$

Parameters a,b,c are restricted by triangle relation $\{a,b,c\}$ and $a+b+c$ must be even. Value L in the above relations is also restricted by the relations (empirically found based on table of Seaton (1961):

$$(l+l'-\lambda)/2\ \le\ L\ \le\ (l+l'+\lambda)/2$$

As programing algorithm, we will use the simplified expression

$$I_0(kl,k'l';\lambda)=(-1)^{(\lambda+l'-l)/2}E(\lambda,l',l)\left(\frac{\pi}{kk'}\right)^{\frac{1}{2}}\frac{1}{2^{\lambda+1}\Gamma(\lambda+\frac{1}{2})}$$
$$\times\sum_{L=(l+l'-\lambda)/2}^{(l+l'+\lambda)/2}(2L+1)Q_L(\chi)\sum_{\mu=0}^{\lambda}\frac{k^{\lambda-\mu}(-k')^{\mu}}{E(l,L,\lambda-\mu)E(l',L,\mu)}$$

where all terms with $E(\ldots)=0$ are dropped.

SUM RULES (Burgess 1974)

$$\sum_{l=L}^{\infty}\sum_{l'=l\pm1}l_{>}I^2(\kappa_1 l,\kappa_2 l';\ 1)=[I^2(\kappa_1 L,\kappa_2 L-1;1)-I^2(\kappa_1\ L-1,\kappa_2 L;1)\frac{1+L^2\kappa_1^2}{L(\kappa_1^2-\kappa_2^2)}\qquad Z>0$$

$$\sum_{l=L}^{\infty}\sum_{l'=l\pm1}l_{>}I_0^2(k_1 l,k_2 l';\ 1)=[I_0^2(k_1 L,k_2 L-1;1)-I_0^2(\kappa_1\ L-1,\kappa_2 L;1)\frac{Lk_1^2}{(k_1^2-k_2^2)}\qquad Z=0$$

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

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

$$\sum_{l=L}^{\infty}\sum_{l'=l\pm1}l_{>}I_0^2(k_1 l,k_2 l';\ 1)=\tfrac{1}{4}L\left(\frac{k_1}{k_2}\right)(Q_{L-1}^2-Q_L^2)$$

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