Here is collected the formulas used in utility programs for calculations of differential cross section.

LS coupling: (utility **dif_sec_LS**)

See also:

1. Salvini A A (1982) CPC 27, 25
2. Griffin D C and Pindzola M S (1990) Phys. Rev. A 42, 248

The scattering amplitude for electron-ion scattering from an initial states

$$\alpha_0 L_0 S_0 M_{L_0} M_{S_0}; \mu_0$$

to a final state

$$\alpha_1 L_1 S_1 M_{L_1} M_{S_1}; \mu_1$$

in LS coupling is given by

$$\begin{aligned} f_{01}(\theta,\varphi) &= f_c + f_m = \delta(all)\frac{(z/k_0)}{2k_0\sin^2(\theta/2)}e^{i2\sigma_0}e^{i(z/k_0)\ln[\sin^2(\theta/2)]} \\ &+ i\sqrt{\frac{\pi}{k_0 k_1}}\sum_{l_0,l_1,L,S,\Pi,M_L,M_S} i^{(l_0-l_1)}\sqrt{(2l_0+1)}e^{i(\sigma_{l_0}+\sigma_{l_1})}C^{L_0 l_0 L}_{M_{L_0} 0 M_L}C^{L_1 l_1 L}_{M_{L_1} m_1 M_L}C^{S_0 \frac{1}{2} S}_{M_{S_0}\mu_0 M_S}C^{S_1 \frac{1}{2} S}_{M_{S_1}\mu_1 M_S} \\ &\times T^{LS\pi}_{l_0 l_1}(\alpha_0 L_0 S_0 \to \alpha_1 L_1 S_1)Y_{l_1 m_1}(\theta,\varphi) \end{aligned}$$

where first term represent purely Coulombic scattering in the elastic channel; k_0 and k_1 are the linear momenta of the incident and scattering electrons, respectively; l_0,m_0,μ_0 and l_1,m_1,μ_1 are the orbital angular momentums, orbital magnetic, and spin magnetic quantum numbers of the incident and scattering electrons, respectively; σ_l is the Coulomb phase shift, $\arg\Gamma(l+1+i\frac{Z}{k})$; $T^{LS\pi}_{l_0 l_1}(\alpha_0 L_0 S_0 \to \alpha_1 L_1 S_1)$ is an element of the T-matrix for a give total angular momentum L, total spin S and parity Π. In the above formula we assume the z axes is chosen along the direction of the incident beam. As consequence, $m_0=0$ and $m_1=M_{L1}-M_L$, are not free parameters.

The DCS is then determined by squaring the scattering amplitude, averaging over the initial states, summing over the final states, and multiplying by the ratio of the final and initial linear momenta:

$$\frac{d\sigma}{d\Omega} = \frac{1}{2(2L_0+1)(2S_0+1)}\frac{k_1}{k_0}\sum_{M_{L_0},M_{L_1},M_{S_0},M_{S_1},\mu_0,\mu_1}|f(\theta,\varphi)|^2$$

with

$$|f(\theta,\varphi)|^2 = |f_c|^2\delta(i,f) + 2\,\mathrm{Re}(f_c^* f_m)\delta(i,f) + |f_m|^2$$

After summation over magnetic numbers, we have:

The first term, purely Coulombic scattering, is

$$\frac{d\sigma_c}{d\Omega} = \frac{(Z/k_0)^2}{4k_0^2 \sin^4 \theta/2}\delta(i,f)$$

The second term, interference term, can be represented as

$$\frac{d\sigma_{\text{int}}}{d\Omega} = \frac{(z/k_0)\delta(i,f)}{4(2L_0+1)(2S_0+1)k_0^2 \sin^2 \theta/2} \mathrm{Re}\left\{ e^{-i(z/k_0)\ln[\sin^2(\theta/2)]})\sum_{l_0} Q_l P_{l_0}(\cos\theta) \right\}$$

where

$$Q_l = \sum_{LS\pi} e^{i2(\sigma_{l_0}-\sigma_0)}(2L+1)(2S+1)T_{l_0 l_1}^{LS\pi}(\alpha_0 L_0 S_0 \to \alpha_0 L_0 S_0)$$

Finally, the third term is given by

$$\frac{d\sigma_m}{d\Omega}(\theta) = \sum_{\lambda} A_\lambda P_\lambda(\cos\theta)$$

where

$$A_\lambda = \frac{1}{8k_0^2(2L_0+1)(2S_0+1\}} \sum_{l_0 l_1 l'_0 l'_1 Sj} e^{i(\sigma_{l_0}+\sigma_{l_1}-\sigma_{l'_0}-\sigma_{l'_1})}(-1)^{j+\lambda}(2j+1)$$

$$(l_0 0 l'_0 | \lambda 0)(l_1 0 l'_1 | \lambda 0)\begin{Bmatrix} l_0 & l_1 & j \\ l'_1 & l'_0 & \lambda \end{Bmatrix}\left(M_{l'_0 l'_1}^{Sj}\right)^* M_{l_0 l_1}^{Sj}$$

$$M_{l_0 l_1}^{Sj} = [l_0, l_1, S]^{1/2} \sum_{L\pi} (-1)^{L_0+L_1+l_0+l_1}(-1)^L(2L+1)\begin{Bmatrix} l_0 & L_0 & L \\ L_1 & l_1 & j \end{Bmatrix} T_{l_0 l_1}^{LS\pi}(\alpha_0 L_0 S_0 \to \alpha_1 L_1 S_1)$$

and j is the momentum transfer, i.e. the angular omentum actually transferred during the collision from the incident electron to the target:

$$j = l_1 - l_0 = L_0 - L_1$$

In neutral case:

ICS: (angle-integrated cross section):

$$\sigma = \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta \frac{d\sigma_m}{d\Omega}(\theta) = -2\pi\int_0^{\pi} d(\cos\theta)\sum_\lambda A_\lambda P_\lambda(\cos\theta) = 2\pi\int_{-1}^{1} dx \sum_\lambda A_\lambda P_\lambda(x) P_0(x) = 4\pi A_0$$

Momentum transfer:

$$\sigma_M = \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta(1-\cos\theta) d\theta \frac{d\sigma_m}{d\Omega}(\theta) = -2\pi\int_0^{\pi} d(\cos\theta)(1-\cos\theta)\sum_\lambda A_\lambda P_\lambda(\cos\theta) =$$

$$= 2\pi\int_{-1}^{1} dx \sum_\lambda A_\lambda P_\lambda(x)(P_0(x)-P_1(x)) = 4\pi(A_0 - \frac{1}{3}A_1) \qquad \text{(we use } P_1(x) = x)$$

JK –coupling: (utilities **sec_dif_JK**, **sec_dif_JK_ampl**)

$$f_{01}(J_0,M_0,\mu_0 \to J_1,M_1,\mu_1;\theta,\varphi) = f_c + f_m = \delta(all)\frac{(z/k_0)}{2k_0\sin^2(\theta/2)} e^{i2\sigma_0} e^{i(z/k_0)\ln[\sin^2(\theta/2)]}$$

$$+ i\sqrt{\frac{\pi}{k_0k_1}} \sum_{\substack{l_0,l_1,K_0,K_1,J,\pi \\ M,m_1\kappa_1}} i^{(l_0-l_1)}\sqrt{(2l_0+1)}e^{i(\sigma_{l_0}+\sigma_{l_1})} C^{J_0 l_0 K_0}_{M_0 0 \kappa_0} C^{J_1 l_1 K_1}_{M_1 m_1 \kappa_1} C^{K_0 \frac{1}{2} J}_{\kappa_0 \mu_0 M} C^{K_1 \frac{1}{2} J}_{\kappa_1 \mu_1 M} \times T^{J\pi}(\alpha_0 J_0 l_0 K_0 \to \alpha_1 J_1 l_1 K_1) Y_{l_1 m_1}(\theta,\varphi)$$

$$\frac{d\sigma}{d\Omega} = \frac{a_0^2}{8(2J_0+1)k^2}\sum_{\lambda>0} A_\lambda P_\lambda(\cos\theta)$$

$$A_\lambda = \sum_{\substack{l_0\ l_1\ K_0\ K_1\ J, \\ l_0'l_1'K_0'K_1'J'}} (-1)^{l_0-l_1} \hat{l}_0 \hat{l}'_0 \hat{l}_1 \hat{l}'_1 \hat{K}_0 \hat{K}'_0 \hat{K}_1 \hat{K}'_1 (2J+1)(2J'+1)$$

$$\times (l_0 0 l'_0 | \lambda 0)(l_1 0 l'_1 | \lambda 0) \begin{Bmatrix} K_0 & K'_0 & \lambda \\ l'_0 & l_0 & J_0 \end{Bmatrix} \begin{Bmatrix} K_1 & K'_1 & \lambda \\ l'_1 & l_1 & J_1 \end{Bmatrix} \begin{Bmatrix} K_0 & K'_0 & \lambda \\ J' & J & \frac{1}{2} \end{Bmatrix} \begin{Bmatrix} K_1 & K'_1 & \lambda \\ J' & J & \frac{1}{2} \end{Bmatrix}$$

$$\times T^{\pi J}(J_0 l_0 K_0 \to J_1 l_1 K_1) T^{*\pi' J'}(J_0 l'_0 K'_0 \to J_1 l'_1 K'_1)$$

(see also MJK program by A.Grum-Grzhimailo, CPC, 152 (2003) 101)

JJ –coupling (utility **sec_dif_JJ_ampl**)

$$f_{01}(J_0,M_0,\mu_0 \to J_1,M_1,\mu_1;\theta,\varphi) = f_c + f_m = \delta(all)\frac{(z/k_0)}{2k_0\sin^2(\theta/2)}e^{i2\sigma_0}e^{i(z/k_0)\ln[\sin^2(\theta/2)]}$$

$$-i\sqrt{\frac{\pi}{k_0k_1}}\sum_{l_0,l_1,j_0,j_1,J,\pi} i^{(l_0-l_1)}\sqrt{(2l_0+1)}e^{i(\sigma_{l_0}+\sigma_{l_1})}C^{l_0\frac{1}{2}j_0}_{0\mu_0 m_{j_0}}C^{l_1\frac{1}{2}j_1}_{m_1\mu_1 m_{j_1}}C^{J_0 j_0 J}_{M_0 m_{j_0} M}C^{J_1 j_1 J}_{M_1 m_{j_1} M}\times T^{J\pi}(\alpha_0 J_0 l_0 j_0 \to \alpha_1 J_1 l_1 j_1)Y_{l_1 m_1}(\theta,\varphi)$$

(relative phase between the Coulomb and potential part ($\pm i$) is different in different publications)

$$Y_l^m(\theta,\varphi) = \Theta_{lm}(\theta)\Phi_m(\varphi)$$

$$\Phi_m(\varphi) = \sqrt{\frac{1}{2\pi}}e^{im\varphi}$$

$$\Theta_{lm}(\theta) = (-1)^m\sqrt{\frac{(2l+1)}{2}\frac{(l-m)!}{(l+m)!}}P_l^m(\cos\theta) = (-1)^m\overline{P}_l^m(\cos\theta), \qquad (m>0)$$

$$\Theta_{l-m}(\theta) = (-1)^m\Theta_{lm}(\theta) = \overline{P}_l^m(\cos\theta)$$

Considering φ=0, we may rewrite expression as

$$f_{01}(J_0,M_0,\mu_0 \to J_1,M_1,\mu_1;\theta,\varphi) = f_c + f_m = \delta(all)\frac{(z/k_0)}{2k_0\sin^2(\theta/2)}e^{i2\sigma_0}e^{i(z/k_0)\ln[\sin^2(\theta/2)]}$$

$$-i\sqrt{\frac{1}{2k_0k_1}}\sum_{l_0,l_1,j_0,j_1,J,\pi} i^{(l_0-l_1)}\sqrt{(2l_0+1)}e^{i(\sigma_{l_0}+\sigma_{l_1})}C^{l_0\frac{1}{2}j_0}_{0\mu_0 m_{j_0}}C^{l_1\frac{1}{2}j_1}_{m_1\mu_1 m_{j_1}}C^{J_0 j_0 J}_{M_0 m_{j_0} M}C^{J_1 j_1 J}_{M_1 m_{j_1} M}\times T^{J\pi}(\alpha_0 J_0 l_0 j_0 \to \alpha_1 J_1 l_1 j_1)\overline{P}_{l_1}^{m_1}(\theta)$$

($\overline{P}_{l_1}^{m_1}(\theta)$ - is given by program ALEGFM)

$$\frac{d\sigma}{d\Omega} = \frac{1}{2(2J_0+1)}\frac{k_1}{k_0}\sum_{M_0,M_1,\mu_0,\mu_1} \left|f(\theta,\varphi)\right|^2$$

So, we may use direct calculation of scattering amplitude for different M's and them sum their modules.

Angle-integrated cross sections (if needed) are then obtain direct integration of $d\sigma$ by angles.

$$\sigma_{ij} = \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta \frac{d\sigma_{ij}}{d\Omega}(\theta) \qquad \sigma_M = \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta(1-\cos\theta)d\theta\frac{d\sigma}{d\Omega}(\theta)$$

JJ –coupling (utility **sec_dif_JJ**)

In neutral case:

$$\frac{d\sigma}{d\Omega}=\frac{a_0^2}{8(2J_0+1)k_0^2}\sum_{\lambda\geq 0}A_\lambda P_\lambda(\cos\theta)$$

$$A_\lambda=\sum_{\substack{l_0 l_1 j_0 j_1 J\\ l'_0 l'_1 j'_0 j'_1 J'}}(-1)^{J_0-J_1}i^{l_0-l_1+l'_0-l'_1}\hat{l}_0\hat{l}'_0\hat{l}_1\hat{l}'_1\hat{j}_0\hat{j}'_0\hat{j}_1\hat{j}'_1(2J+1)(2J'+1)$$

$$\times\left(l_0 0 l'_0\,|\,\lambda 0\right)\left(l_1 0 l'_1\,|\,\lambda 0\right)\begin{Bmatrix} j_0 & j'_0 & \lambda\\ l'_0 & l_0 & \frac{1}{2}\end{Bmatrix}\begin{Bmatrix} j_1 & j'_1 & \lambda\\ l'_1 & l_1 & \frac{1}{2}\end{Bmatrix}\begin{Bmatrix} j_0 & j'_0 & \lambda\\ J' & J & J_0\end{Bmatrix}\begin{Bmatrix} j_1 & j'_1 & \lambda\\ J' & J & J_1\end{Bmatrix}$$

$$\times T^{\pi J}(J_0 l_0 j_0\to J_1 l_1 j_1)\left[T^{\pi' J'}(J_0 l'_0\, j'_0\to J_1 l'_1\, j'_1)\right]^*$$

$$\hat{a}=\sqrt{2a+1};$$

Angle-integrated and momentum-transfer cross section can be express as:

$$\sigma=4\pi\, N\, A_0 \qquad \sigma_{MT}=4\pi\, N\,(A_0-1/3A_1)$$

Coulomb case: We again can express DCS as pure Coulomb scattering, interference term and potential term (first two only for elastic scattering, when initial, i, state equal final, f).

$$\frac{d\sigma_c}{d\Omega}=\frac{(Z/k_0)^2}{4k_0^2\sin^4\theta/2}\delta(i,f)$$

$$\frac{d\sigma_{\text{int}}}{d\Omega}=\frac{(z/k_0)\delta(i,f)}{4(2J_0+1)k_0^2\sin^2\theta/2}\mathrm{Re}\left\{e^{-i(z/k_0)\ln[\sin^2(\theta/2)]})\sum_l Q_l P_l(\cos\theta)\right\}$$

$$Q_l=\sum_{J\pi}e^{i2(\sigma_l-\sigma_0)}(2J+1)T_{ll}^{J\pi}(\alpha_0 J_0\to\alpha_0 J_0)$$

$$\frac{d\sigma_M}{d\Omega}=\frac{a_0^2}{8(2J_0+1)k_0^2}\sum_{\lambda\geq 0}A_\lambda^{Coul}P_\lambda(\cos\theta); \qquad A_\lambda^{Coul}=A_\lambda\times e^{i(\sigma_{l_0}+\sigma_{l_1}-\sigma_{l'_0}-\sigma_{l'_1})}$$