

A Mathematical procedures for the calculation of elastic scattering cross-sections

This appendix reports the mathematical derivations performed to solve the equations for the calculation of the elastic scattering cross-sections. This method can be safely used for any ion. In order to obtain the differential cross-section $\frac{d\sigma_{el}}{d\Omega}$ from equation (13), three steps were necessary:

1. numerically solve equation (18);
2. assure that $\theta(p)$ is an invertible function and consider the inverse numerical relationship $p(\theta)$;
3. numerically calculate the derivative $\frac{dp(\theta)}{d\theta}$, interpolating $p(\theta)$ with a *spline* function to obtain the results at the desired value of θ .

Mathematical derivations are only required for step 1. The approach employed for solving the equation was adapted from the “large angle calculations” approach proposed by Everhart et al.¹. Reporting equations (18) and (19):

$$\theta(p) = \pi - 2 \int_{r_0}^{\infty} [r\phi(r)]^{-1} dr$$

$$\phi(r) = \sqrt{\frac{r^2}{p^2} - 1 - \frac{r^2 V(r)}{p^2 T_{CM}}}$$

By considering equations (15) and (20), we can re-write and manipulate equation (19) as:

$$\phi(r) = \sqrt{\frac{r^2}{p^2} - 1 - \frac{rb}{p^2} F_s \left(\frac{r}{r_s} \right)}$$

$$\phi(r) = \frac{r}{p} \sqrt{1 - \frac{p^2}{r^2} - \frac{b}{r} F_s \left(\frac{r}{r_s} \right)}$$

Substituting $\phi(r)$ in equation (18) we obtain:

$$\theta(p) = \pi - 2 \int_{r_0}^{\infty} \left[\frac{r^2}{p} \sqrt{1 - \frac{p^2}{r^2} - \frac{b}{r} F_s \left(\frac{r}{r_s} \right)} \right]^{-1} dr$$

Conveniently changing variable:

$$z = \frac{r_s}{r} \tag{a1}$$

thus considering $dz = -\frac{r_s}{r^2} dr$:

$$\theta(p) = \pi - 2 \int_{z_0}^0 - \left[\frac{r_s}{p} \sqrt{1 - \frac{p^2}{r_s^2} z^2 - \frac{b}{r_s} z F_s(z^{-1})} \right]^{-1} dz$$

and defining:

$$y(z) = 1 - \frac{p^2}{r_s^2} z^2 - \frac{b}{r_s} z F_s(z^{-1}) \tag{a2}$$

we have:

$$\theta(p) = \pi - 2 \frac{p}{r_s} \int_0^{z_0} y^{-1/2}(z) dz \tag{a3}$$

where z_0 is the largest positive root of equation (a2). To overcome the difficulty in maintaining numerical accuracy at small angles, where the second term of equation (a3) becomes comparable with π , Everhart proposed to write the equation in a more convenient form by introducing the term y_0 so that:

$$y_0(z) = 1 - \frac{p^2}{r_s^2} z^2 - \frac{b}{r_s} z F_s(z_0^{-1}) \tag{a4}$$

and the integral in equation (a3) can be written as

$$\int_0^{z_0} y^{-1/2}(z)dz = \int_0^{z_0} y_0^{-1/2}(z)dz - \int_0^{z_0} \left(y_0^{-1/2} - y^{-1/2}(z) \right) dz$$

where the first integral in the equation can be solved analytically. By defining two constants A and B :

$$\begin{cases} A = \frac{b}{r_s} F_s(z_0^{-1}) \\ B = \frac{p_s^2}{r_s^2} \end{cases} \quad (\text{a5})$$

the visualisation of equation (a4) is simplified:

$$\int_0^{z_0} y_0^{-1/2}(z)dz = \int_0^{z_0} \frac{1}{\sqrt{1-Az-Bz^2}} dz$$

To obtain the analytical solution, the integral should be rewritten in a known integral form. In this case, it is convenient to consider the form $\int \frac{1}{\sqrt{1+C^2x^2}} dx = \frac{1}{C} \sin^{-1}(Cx)$. As the original integral has a first-order term in z , x will be of the form $x = z + D$. In order to obtain a solvable identity, it is useful to introduce a third constant G so that the identity to solve is:

$$\int_0^{z_0} \frac{1}{\sqrt{1-Az-Bz^2}} dz = \frac{1}{G} \int_0^{z_0} \frac{1}{\sqrt{1-C^2(z+D)^2}} dz$$

which reduces to:

$$\begin{aligned} 1 - Az - Bz^2 &= G^2 (1 - C^2(z+D)^2) \\ &= [G^2 - G^2 C^2 D^2] - [2G^2 C^2 D] z - [G^2 C^2] z^2 \end{aligned}$$

Thus

$$\begin{cases} G^2 - G^2 C^2 D^2 = 1 \\ 2G^2 C^2 D = A \\ G^2 C^2 = B \end{cases}$$

which leads to:

$$\begin{cases} C = \frac{2B}{\sqrt{A^2+4B}} \\ D = \frac{A}{2B} \\ G = \frac{\sqrt{B}}{C} \end{cases} \quad (\text{a6})$$

The integral can now be solved:

$$\begin{aligned} \int_0^{z_0} y_0^{-1/2}(z)dz &= \frac{1}{G} \int_0^{z_0} \frac{1}{\sqrt{1-C^2(z+D)^2}} dz \\ &= \frac{1}{G} \int_D^{z_0+D} \frac{1}{\sqrt{1-C^2x^2}} dx \\ &= \frac{1}{GC} [\sin^{-1}(Cx)]_D^{z_0+D} \\ &= \frac{1}{GC} [\sin^{-1}(C(z+D))]_0^{z_0} \\ &= \frac{1}{GC} (\sin^{-1}(C(z_0+D)) - \sin^{-1}(CD)) \end{aligned}$$

Using the identities in equation (a6), the integral becomes:

$$\begin{aligned} \int_0^{z_0} y_0^{-1/2}(z)dz &= \frac{1}{\sqrt{B}} \left(\sin^{-1} \left(\frac{2B}{\sqrt{A^2+4B}} (z_0 + \frac{A}{2B}) \right) - \sin^{-1} \left(\frac{A}{\sqrt{A^2+4B}} \right) \right) \\ &= \frac{1}{\sqrt{B}} \left(\sin^{-1} \left(\frac{2Bz_0 + A}{\sqrt{A^2+4B}} \right) - \sin^{-1} \left(\frac{A}{\sqrt{A^2+4B}} \right) \right) \end{aligned}$$

By definition of z_0 : $1 - Az_0 - Bz_0^2 = 0$. Solving the second-order equation and considering the largest positive root for z_0 :

$$\begin{aligned} z_0 &= \frac{A - \sqrt{A^2 + 4B}}{-2B} \\ &= \frac{\sqrt{A^2 + 4B} - A}{2B} \end{aligned}$$

so

$$2Bz_0 + A = \sqrt{A^2 + 4B}$$

and

$$\begin{aligned} \int_0^{z_0} y_0^{-1/2}(z) dz &= \frac{1}{\sqrt{B}} \left(\sin^{-1}(+1) - \sin^{-1} \left(\frac{A}{\sqrt{A^2 + 4B}} \right) \right) \\ &= \frac{1}{\sqrt{B}} \left(+\frac{\pi}{2} - \sin^{-1} \left(\frac{A}{\sqrt{A^2 + 4B}} \right) \right) \end{aligned}$$

The expression could be further simplified by considering the trigonometric relationship $\sin^{-1}(x) = \cot^{-1} \left(\frac{\sqrt{1-x^2}}{x} \right)$:

$$\begin{aligned} \sin^{-1} \left(\frac{A}{\sqrt{A^2 + 4B}} \right) &= \cot^{-1} \left(\frac{\sqrt{A^2 + 4B}}{A} \sqrt{1 - \frac{A^2}{A^2 + 4B}} \right) \\ &= \cot^{-1} \left(\frac{\sqrt{A^2 + 4B}}{A} \sqrt{\frac{A^2 + 4B - A^2}{A^2 + 4B}} \right) \\ &= \cot^{-1} \left(\frac{2\sqrt{B}}{A} \right) \end{aligned}$$

Finally, considering the definition of A and B in equation (a5), the integral is solved:

$$\int_0^{z_0} y_0^{-1/2}(z) dz = \frac{r_s}{p} \left(\frac{\pi}{2} - \cot^{-1} \left(\frac{2p}{bF_s(z_0^{-1})} \right) \right) \quad (\text{a7})$$

Equation (a3) can now be rewritten:

$$\begin{aligned} \theta(p) &= \pi - 2 \frac{p}{r_s} \left(\int_0^{z_0} y_0^{-1/2}(z) dz - \int_0^{z_0} (y_0^{-1/2} - y^{-1/2}(z)) dz \right) \\ &= \pi - 2 \frac{p}{r_s} \frac{r_s}{p} \left(\frac{\pi}{2} - \cot^{-1} \left(\frac{2p}{bF_s(z_0^{-1})} \right) \right) + 2 \frac{p}{r_s} \int_0^{z_0} (y_0^{-1/2} - y^{-1/2}(z)) dz \\ &= \pi - \pi + \cot^{-1} \left(\frac{2p}{bF_s(z_0^{-1})} \right) + 2 \frac{p}{r_s} \int_0^{z_0} (y_0^{-1/2} - y^{-1/2}(z)) dz \\ \theta(p) &= 2 \cot^{-1} \left(\frac{2p}{b} \frac{1}{F_s(z_0^{-1})} \right) + \frac{2p}{r_s} \int_0^{z_0} (y_0^{-1/2} - y^{-1/2}(z)) dz \quad (\text{a8}) \end{aligned}$$

Equation (a8) shows the final form for the $\theta(p)$ calculation. This derivation brings a fundamental advantage in terms of numerical accuracy with respect of equation (a3). The first term of equation (a8) was found analytically, and the second term can be safely calculated by numerical integration. The integration yields a small quantity $\left(\frac{2p}{r_s} \int_0^{z_0} (y_0^{-1/2} - y^{-1/2}(z)) dz \ll 2 \cot^{-1} \left(\frac{2p}{b} \frac{1}{F_s(z_0^{-1})} \right) \right)$ which is added to the first term, guaranteeing the accuracy of the $\theta(p)$ calculation.

The numerical integration was carried out using the Simpson's rule, being careful to handle the infinity in the integrand at $z = z_0$.

B The analytical functions for the radial dose distribution

This appendix reports the analytical functions for the radial dose profile from the work of Waligorski et al.². The final equation for the radial dose profile $D(r)$ is:

$$D(r) = D_0(r) (1 + K(r)) \quad (\text{a9})$$

where r is the radial distance from the particle track,

$$K(r) = \begin{cases} A \left(\frac{r-B}{C} \right) e^{-\left(\frac{r-B}{C} \right)} & \text{for } r \geq B \\ 0 & \text{for } r < B \end{cases} \quad (\text{a10})$$

with $B = 0.1$ nm, $C = 1.5 + 5\beta$ nm and

$$A = \begin{cases} 8\beta^{1/3} & \text{for } \beta < 0.03 \\ 19\beta^{1/3} & \text{for } \beta \geq 0.03 \end{cases}$$

β is the ratio between the projectile's velocity the speed of light ($\beta = \frac{v}{c}$) and

$$D_0(r) = \frac{Ne^4 Z^{*2}}{\alpha m_e c^2 \beta^2 r} \left[\frac{\left(1 - \frac{r+\theta/\rho}{R+\theta/\rho} \right)^{1/\alpha}}{r + \frac{\theta}{\rho}} \right] \quad (\text{a11})$$

where N is the number of electrons per cm^3 in the medium, m_e is the electron mass, $Z^* = Z \left(1 - e^{-125\beta Z^{-2/3}} \right)$ is the Barkas' effective charge, $\theta = 4.17 \cdot 10^{-8} \text{ g cm}^{-2}$, ρ is the medium's density,

$$\alpha = \begin{cases} 1.079 & \text{for } \beta < 0.03 \\ 1.667 & \text{for } \beta \geq 0.03 \end{cases}$$

and $R = k \left(\frac{2m_e c^2 \beta^2}{1 - \beta^2} \right)^\alpha$ with $k = 6 \cdot 10^{-6} \text{ g cm}^{-2} \text{ keV}^{-\alpha}$. For water, $\frac{2\pi N e^4}{m_e c^2} = 85 \text{ keV cm}^{-1}$. Waligorski's equation is valid for projectile's kinetic energy above approximately 0.5 MeV/u.

References

1. Everhart, E., Stone, G. & Carbone, R. J. Classical calculation of differential cross section for scattering from a coulomb potential with exponential screening. *Phys. Rev.* **99**, 1287–1290, DOI: [10.1103/PhysRev.99.1287](https://doi.org/10.1103/PhysRev.99.1287) (1955).
2. Waligórski, M., Hamm, R. & Katz, R. The radial distribution of dose around the path of a heavy ion in liquid water. *Int. J. Radiat. Appl. Instrumentation. Part D. Nucl. Tracks Radiat. Meas.* **11**, 309–319, DOI: [10.1016/1359-0189\(86\)90057-9](https://doi.org/10.1016/1359-0189(86)90057-9) (1986).