Electromagnetic interaction models for Monte Carlo simulation of protons and alpha particles (supplementary material)

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The present document contains supplementary information to the article of the same title, which is submitted to Nuclear Instruments and Methods. The adopted notation is the same as in the parent article, and the equations in that article are referred to as (a.#).

1 Elastic collisions

The atomic mass of a given isotope, ${}^{A}Z$, is estimated by means of the mass formula (Royer and Gautier, 2006)

$$M({}^{A}Z)c^2 = Zm_{\rm p}c^2 + Nm_{\rm n}c^2 - B_{\rm nuc} + Zm_{\rm e}c^2 - B_{\rm e}, \tag{1}$$

where

$$m_{\rm p} = 1836.15\, m_{\rm e} \qquad \text{and} \qquad m_{\rm n} = 1838.68\, m_{\rm e} \tag{2}$$

are the masses of the proton and the neutron, respectively, $B_{\rm nuc}$ is the binding energy of the nucleus and $B_{\rm e}$ is the binding energy of the Z atomic electrons. These binding energies are approximated by the following empirical expressions, which were determined from fits to available calculated or measured data,

$$B_{\rm e} = (14.4381\ {\rm eV})\, Z^{2.39} + (1.55468 \times 10^{-6}\ {\rm eV})\, Z^{5.35}, \tag{3}$$

and

$$\begin{aligned} B_{\rm nuc} \;=\; & (15.7335 \times 10^{6}\ {\rm eV})\left(1 - 1.6949\, I^2\right) A - (17.8048 \times 10^{6}\ {\rm eV})\left(1 - 1.0884\, I^2\right) A^{2/3} \\ & - \frac{3}{5}\frac{Z^2e^2}{R_0} + E_{\rm pair}, \end{aligned} \tag{4}$$

where $I = (N-Z)/A$ is the charge asymmetry parameter, $R_0 = 1.2181\, A^{1/3}$ fm, and

$$E_{\rm pair} = \begin{cases} -(11 \times 10^{6}\ {\rm eV})\, A^{-1/2} & \text{for nuclei with odd } Z \text{ and odd } N, \\ 0 & \text{for nuclei with odd } A, \\ (11 \times 10^{6}\ {\rm eV})\, A^{-1/2} & \text{for nuclei with even } Z \text{ and even } N. \end{cases} \tag{5}$$

As indicated in the parent article, the formula (1) approximates the experimental atomic masses of naturally occurring isotopes (Coursey *et al.*, 2015) with a relative accuracy better than about 10^{-4}, which is sufficient for the present purposes.

1.1 Nuclear optical-model potentials

The interaction energy of the projectile with a bare nucleus of the isotope ${}^{A}Z$ having atomic number Z and mass number A is described by a phenomenological complex optical-model potential

$$V_{\rm nuc}(r) = V_{\rm opt}(r) + {\rm i}W_{\rm opt}(r). \tag{6}$$

The term $V_{\rm opt}(r)$ is a real potential that reduces to the Coulomb potential at large radii, and ${\rm i}W_{\rm nuc}(r)$ is an absorptive (negative) imaginary potential which should account for the loss of projectiles from the elastic channel caused by inelastic processes. Parameterizations of optical-model potentials have been proposed by various authors (see, *e.g.* Watson *et al.*, 1969; Hodgson, 1971; Koning and Delaroche, 2003; Su and Han, 2015). They are generally expressed as a combination of Woods–Saxon volume terms,

$$f(R,a;r) = \frac{1}{1+\exp[(r-R)/a]}\,, \tag{7a}$$

and surface derivative (d) terms,

$$\begin{aligned} g(R,a;r) &= \frac{\rm d}{{\rm d}r}\, f(R,a;r) \\ &= \frac{1}{a}\, f(R,a;r)\,[f(R,a;r)-1]\,. \end{aligned} \tag{7b}$$

The parameters in these functions are the radius R and the diffuseness a; typically, the radius is expressed as $R = r_0 A^{1/3}$. We consider global model potentials of the type

$$\begin{aligned} V_{\rm nuc}(r) &= V_{\rm v}(E;r) + V_{\rm d}(E;r) + V_{\rm C}(r) + V_{\rm so}(E;r)\, 2\,\mathbf{L}\cdot\mathbf{S} \\ &\quad + {\rm i}\left[W_{\rm v}(E;r) + W_{\rm d}(E;r) + W_{\rm so}(E;r)\, 2\,\mathbf{L}\cdot\mathbf{S}\right] \end{aligned} \tag{8}$$

with the following terms:

1) Real volume potential:

$$V_{\rm v}(E;r) = V_{\rm v}(E)\, f(R_{\rm v}, a_{\rm v}; r). \tag{9a}$$

2) Real surface potential:

$$V_{\rm d}(E;r) = V_{\rm d}(E)\, 4a_{\rm d}\, g(R_{\rm d}, a_{\rm d}; r). \tag{9b}$$

3) Coulomb potential: approximated by the electrostatic potential of a uniformly charged sphere of radius $R_{\rm c}$,

$$V_{\rm c}(r) = \frac{Z_1 Z e^2}{r} \begin{cases} \dfrac{r}{2R_{\rm c}}\left(3 - \dfrac{r^2}{R_{\rm c}^2}\right) & \text{if } r < R_{\rm c}, \\ 1 & \text{if } r \geq R_{\rm c}. \end{cases} \tag{9c}$$

4) Imaginary volume potential:

$$W_{\rm v}(E;r) = W_{\rm v}(E)\, f(R_{\rm w}, a_{\rm w}; r). \tag{9d}$$

5) Imaginary surface potential:

$$W_{\rm d}(E;r) = W_{\rm d}(E)\, 4a_{\rm wd}\, g(R_{\rm wd}, a_{\rm wd}; r). \tag{9e}$$

6) Real spin-orbit potential:

$$V_{\rm so}(E;r) = V_{\rm so}(E) \left(\frac{\hbar}{m_\pi c}\right)^2 \frac{1}{r}\, g(R_{\rm so}, a_{\rm so}; r), \tag{9f}$$

where the quantity in parentheses is the pion Compton wavelength, $\hbar/(m_\pi c) \simeq 1.429\,502$ fm, which is used by convention. For light nuclei, it has been suggested (Watson *et al.*, 1969) that the real spin-orbit term should be multiplied by r to prevent its divergence at $r = 0$.

7) Imaginary spin-orbit potential:

$$W_{\rm so}(E;r) = W_{\rm so}(E) \left(\frac{\hbar}{m_\pi c}\right)^2 \frac{1}{r}\, g(R_{\rm wso}, a_{\rm wso}; r). \tag{9g}$$

The operators **L** and **S** are, respectively, the orbital and spin angular momenta (both in units of $\hbar$) of the projectile. It is worth mentioning that optical model potentials are also used for projectile neutrons, in which case the Coulomb potential vanishes. The spin-orbit terms are null for alpha particles. We have indicated explicitly that the strengths of the potential terms are functions (usually expressed as polynomials) of the kinetic energy E of the projectile in the L frame.

In the calculations for protons (and neutrons) we use the parameterization of the nuclear global optical-model potential given by Koning and Delaroche (2003), which is valid for projectiles with kinetic energies E between 1 keV and about 200 MeV and nuclei with $24 \leq A \leq 209$. Owing to the lack of more accurate approximations, because the potential values vary smoothly with A, Z and E, we use those parameters for all isotopes (except for collisions of protons with isotopes having $A \leq 6$, which are described by means of empirical formulas, see the parent article) and for projectiles with kinetic energies up to 300 MeV, for higher energies the potential parameters at $E = 300$ MeV are employed. For nucleons colliding with target isotopes having $A < 24$ ($Z < 12$), we use the optical-model potential of Watson *et al.* (1969) which is applicable to energies from 10 MeV to 50 MeV; for projectiles with energies higher than 35 MeV the potential of Koning and Delaroche is employed. For alpha particles, the adopted parameterization of the nuclear potential is the one proposed by Su and Han (2015), which is valid for nuclides with $20 \leq A \leq 209$ and projectiles with kinetic energies up to 386 MeV, although we use it for any target atom. For alphas with higher energies, we use the parameter values at $E = 386$ MeV.

The Fortran program PANEL calculates the DCS for elastic collisions of nucleons and alpha particles with nuclei by using the partial-wave expansion method in the CM frame, as described in the parent article. The effect of screening of the nuclear charge by atomic electrons is introduced as a correction factor, which is determined from the DCS obtained from the eikonal approximation (assuming a point nucleus and the analytical approximation to the DHFS self-consistent atomic potential). The program PANEL has been run to produce a complete database of DCSs for elastic collisions of protons, neutrons, and alphas with the elements hydrogen ($Z = 1$) to einsteinium ($Z = 99$), which covers the interval of projectile kinetic energies from 100 keV to 1 GeV. The database files, as well as the program PANEL, are available from the authors under request. The random sampling of the DCS in the CM frame is performed by means of the RITA (rational inverse transform with aliasing) algorithm (García-Toraño *et al.*, 2019) as described by Salvat (2019). This sampling scheme allows restricting the sampling to deflections larger than a given cutoff $\mu_{\rm c}$.

1.2 Derivation of Eq. (a.58)

Our description of elastic collisions is based on the DCS in the CM frame, $\mathrm{d}\sigma_{\rm el}/\mathrm{d}\Omega$, Eq. (a.10), which is a function of the scattering angle θ. In the simulations we need to consider the DCS in the L frame, where the polar scattering angle of the projectile is θ_1. The scattering angles in the two frames are related by Eq. (a.56),

$$\cos\theta = \frac{-\tau\gamma_{\rm CM}^2\sin^2\theta_1 \pm \cos\theta_1\sqrt{\cos^2\theta_1+\gamma_{\rm CM}^2(1-\tau^2)\sin^2\theta_1}}{\gamma_{\rm CM}^2\sin^2\theta_1+\cos^2\theta_1}\,. \tag{10}$$

The DCS in the L frame is

$$\frac{\mathrm{d}\sigma_{\rm el}}{\mathrm{d}\Omega_1} = \left|\frac{\mathrm{d}(\cos\theta)}{\mathrm{d}(\cos\theta_1)}\right|\frac{\mathrm{d}\sigma_{\rm el}}{\mathrm{d}\Omega}\,. \tag{11}$$

To calculate the derivative of $\cos\theta$, we simplify the notation by setting $x=\cos\theta_1$ and $y=\cos\theta$, and writing

$$y = \frac{-\tau\gamma_{\rm CM}^2(1-x^2)\pm x\sqrt{x^2+\gamma_{\rm CM}^2(1-\tau^2)(1-x^2)}}{\gamma_{\rm CM}^2(1-x^2)+x^2}\,.$$

Then

$$\begin{aligned}
\frac{\mathrm{d}y}{\mathrm{d}x} &= \frac{2\tau\gamma_{\rm CM}^2 x \pm \sqrt{x^2+\gamma_{\rm CM}^2(1-\tau^2)(1-x^2)} \pm x\dfrac{1}{2}\dfrac{2x-2\gamma_{\rm CM}^2(1-\tau^2)x}{\sqrt{x^2+\gamma_{\rm CM}^2(1-\tau^2)(1-x^2)}}}{\gamma_{\rm CM}^2(1-x^2)+x^2} \\
&\quad - \frac{-\tau\gamma_{\rm CM}^2(1-x^2)\pm x\sqrt{x^2+\gamma_{\rm CM}^2(1-\tau^2)(1-x^2)}}{\left[\gamma_{\rm CM}^2(1-x^2)+x^2\right]^2}\left[-2\gamma_{\rm CM}^2x+2x\right] \\
&= \frac{2\tau\gamma_{\rm CM}^2 x \pm \sqrt{x^2+\gamma_{\rm CM}^2(1-\tau^2)(1-x^2)} \pm x\dfrac{x-\gamma_{\rm CM}^2(1-\tau^2)x}{\sqrt{x^2+\gamma_{\rm CM}^2(1-\tau^2)(1-x^2)}}}{\gamma_{\rm CM}^2(1-x^2)+x^2} \\
&\quad + \frac{-\tau\gamma_{\rm CM}^2(1-x^2)\pm x\sqrt{x^2+\gamma_{\rm CM}^2(1-\tau^2)(1-x^2)}}{\left[\gamma_{\rm CM}^2(1-x^2)+x^2\right]^2}\,2x\left(\gamma_{\rm CM}^2-1\right)
\end{aligned}$$

Let us define

$$S = \sqrt{x^2 + \gamma_{\rm CM}^2(1-\tau^2)(1-x^2)}$$

and write

$$\begin{aligned}
\frac{\mathrm{d}y}{\mathrm{d}x} &= \frac{1}{\left[\gamma_{\rm CM}^2(1-x^2)+x^2\right]^2 S} \\
&\quad \times \Big\{ \Big(2\tau\gamma_{\rm CM}^2 x S \pm S^2 \pm x^2\left[1-\gamma_{\rm CM}^2(1-\tau^2)\right] \Big) \left[\gamma_{\rm CM}^2(1-x^2)+x^2\right] \\
&\qquad + \left(-\tau\gamma_{\rm CM}^2(1-x^2)S \pm xS^2\right) 2x\left(\gamma_{\rm CM}^2-1\right) \Big\}.
\end{aligned}$$

The quantity in curly braces,

$$\begin{aligned}
\{\cdots\} &= \pm x^2\left[1-\gamma_{\rm CM}^2(1-\tau^2)\right]\left[\gamma_{\rm CM}^2(1-x^2)+x^2\right] \\
&\quad + S\,2\tau x\left\{\gamma_{\rm CM}^2\left[\gamma_{\rm CM}^2(1-x^2)+x^2\right] - \gamma_{\rm CM}^2(1-x^2)\left(\gamma_{\rm CM}^2-1\right)\right\} \\
&\quad \pm S^2\left\{\left[\gamma_{\rm CM}^2(1-x^2)+x^2\right] + 2x^2\left(\gamma_{\rm CM}^2-1\right)\right\},
\end{aligned}$$

can be largely simplified as follows (notice that we add and subtract various quantities to isolate the final result and to leave a residual sum of terms that add to zero)

$$\begin{aligned}
\{\cdots\} &= \pm\gamma_{\rm CM}^2\tau^2x^2 + \gamma_{\rm CM}^2 2\tau x S \pm \gamma_{\rm CM}^2 S^2 \\
&\quad \pm\Big\{\left[x^2-\gamma_{\rm CM}^2(1-\tau^2)x^2\right]\left[\gamma_{\rm CM}^2(1-x^2)+x^2\right] - \gamma_{\rm CM}^2\tau^2x^2 \\
&\qquad + S^2\left[\gamma_{\rm CM}^2(1-x^2)+x^2+2x^2\left(\gamma_{\rm CM}^2-1\right)-\gamma_{\rm CM}^2\right]\Big\} \\
&= \pm\gamma_{\rm CM}^2\left[\tau x \pm S\right]^2 \\
&\quad \pm\Big\{\left[x^2-\gamma_{\rm CM}^2(1-\tau^2)x^2\right]\left[\gamma_{\rm CM}^2(1-x^2)+x^2\right] - \gamma_{\rm CM}^2\tau^2x^2 \\
&\qquad + \left[x^2+\gamma_{\rm CM}^2(1-\tau^2)(1-x^2)\right]\left[-\gamma_{\rm CM}^2x^2+x^2+2x^2\left(\gamma_{\rm CM}^2-1\right)\right]\Big\} \\
&= \pm\gamma_{\rm CM}^2\left[\tau x \pm S\right]^2 \\
&\quad \pm\Big\{\left[x^2-\gamma_{\rm CM}^2(1-\tau^2)x^2\right]\left[\gamma_{\rm CM}^2(1-x^2)+x^2\right] - \gamma_{\rm CM}^2\tau^2x^2 \\
&\qquad + \left[x^2+\gamma_{\rm CM}^2(1-\tau^2)(1-x^2)\right]x^2\left(\gamma_{\rm CM}^2-1\right)\Big\} \\
&= \pm\gamma_{\rm CM}^2\left[\tau x \pm S\right]^2 \\
&\quad \pm\Big\{\gamma_{\rm CM}^2(1-x^2)x^2 + x^4 - \gamma_{\rm CM}^2(1-\tau^2)x^2\left[\gamma_{\rm CM}^2(1-x^2)+x^2\right] - \gamma_{\rm CM}^2\tau^2x^2 \\
&\qquad + \left[x^2+\gamma_{\rm CM}^2(1-\tau^2)(1-x^2)\right]\left(\gamma_{\rm CM}^2x^2-x^2\right)\Big\} \\
&= \pm\gamma_{\rm CM}^2\left[\tau x \pm S\right]^2 \\
&\quad \pm\Big\{\gamma_{\rm CM}^2(1-x^2)x^2 + x^4 - \gamma_{\rm CM}^4(1-\tau^2)x^2(1-x^2) - \gamma_{\rm CM}^2(1-\tau^2)x^4 - \gamma_{\rm CM}^2\tau^2x^2 \\
&\qquad + \gamma_{\rm CM}^2x^4 - x^4 + \gamma_{\rm CM}^4(1-\tau^2)(1-x^2)x^2 - \gamma_{\rm CM}^2(1-\tau^2)(1-x^2)x^2\Big\} \\
&= \pm\gamma_{\rm CM}^2\left[\tau x \pm S\right]^2
\end{aligned}$$

$$\pm\left\{\gamma_{\rm CM}^2 x^2 - \gamma_{\rm CM}^2(1-\tau^2)x^4 - \gamma_{\rm CM}^2\tau^2x^2 - \gamma_{\rm CM}^2(1-\tau^2)(1-x^2)x^2\right\}$$
$$= \pm\gamma_{\rm CM}^2\left[\tau x \pm S\right]^2 \pm \left\{\gamma_{\rm CM}^2 x^2 - \gamma_{\rm CM}^2\tau^2x^2 - \gamma_{\rm CM}^2(1-\tau^2)x^2\right\}$$
$$= \pm\gamma_{\rm CM}^2\left[\tau x \pm S\right]^2 .$$

Hence

$$\frac{{\rm d}y}{{\rm d}x} = \frac{\pm\gamma_{\rm CM}^2\left[\tau x \pm S\right]^2}{\left[\gamma_{\rm CM}^2(1-x^2)+x^2\right]^2 S},$$

or, equivalently,.

$$\frac{{\rm d}(\cos\theta)}{{\rm d}(\cos\theta_1)} = \frac{\pm\gamma_{\rm CM}^2\left[\tau\cos\theta_1 \pm \sqrt{\cos^2\theta_1+\gamma_{\rm CM}^2(1-\tau^2)\sin^2\theta_1}\,\right]^2}{\left(\gamma_{\rm CM}^2\sin^2\theta_1+\cos^2\theta_1\right)^2\sqrt{\cos^2\theta_1+\gamma_{\rm CM}^2(1-\tau^2)\sin^2\theta_1}} . \tag{12}$$

Inserting this result into Eq. (11), the DCS in L is expressed as

$$\frac{{\rm d}\sigma_{\rm el}}{{\rm d}\Omega_1} = \frac{\gamma_{\rm CM}^2\left[\tau\cos\theta_1 \pm \sqrt{\cos^2\theta_1+\gamma_{\rm CM}^2(1-\tau^2)\sin^2\theta_1}\,\right]^2}{\left(\gamma_{\rm CM}^2\sin^2\theta_1+\cos^2\theta_1\right)^2\sqrt{\cos^2\theta_1+\gamma_{\rm CM}^2(1-\tau^2)\sin^2\theta_1}}\,\frac{{\rm d}\sigma_{\rm el}}{{\rm d}\Omega}. \tag{a.58}$$

2 Inelastic collisions

The DDCS for inelastic collisions with the k-th oscillator is split in the form given by Eq. (a.93),

$$\frac{{\rm d}^2\sigma_k}{{\rm d}Q\,{\rm d}W} = \frac{{\rm d}^2\sigma_k^{\rm c}}{{\rm d}Q\,{\rm d}W} + \frac{{\rm d}^2\sigma_k^{\rm dl}}{{\rm d}Q\,{\rm d}W} + \frac{{\rm d}^2\sigma_k^{\rm dt}}{{\rm d}Q\,{\rm d}W} , \tag{a.93}$$

where the terms on the right-hand side account for contributions from close collisions and from distant (resonant) longitudinal and transverse interactions, respectively,

$$\frac{{\rm d}^2\sigma_k^{\rm c}}{{\rm d}Q\,{\rm d}W} = \mathcal{B}\,\frac{1}{W^2}\left(1-\beta^2\,\frac{W}{W_{\rm ridge}}\right)\left[1-g(Q)\right]\delta(W-Q)\,\Theta(W_{\rm ridge}-W)\,, \tag{a.94}$$

$$\frac{{\rm d}^2\sigma_k^{\rm dl}}{{\rm d}Q\,{\rm d}W} = \mathcal{B}\,\frac{1}{W}\,\frac{2m_{\rm e}c^2}{Q(Q+2m_{\rm e}c^2)}\,g(Q)\,\delta(W-W_k)\,\Theta(Q_c-Q), \tag{a.95}$$

and

$$\frac{{\rm d}^2\sigma_k^{\rm dt}}{{\rm d}Q\,{\rm d}W} = \mathcal{B}\,\frac{1}{W}\left\{\ln\left(\frac{1}{1-\beta^2}\right)-\beta^2-\delta_{\rm F}\right\}\delta(W-W_k)\,\delta(Q-Q_-)\,\Theta(Q_c-Q). \tag{a.98}$$

The quantity $\delta_{\rm F}$ is the density-effect correction to the stopping power, Eq (a.99).

The energy-loss DCS for collisions with the k-th oscillator,

$$\frac{{\rm d}\sigma_k}{{\rm d}W} = \int_{Q_-}^{Q_+}\frac{{\rm d}^2\sigma_k}{{\rm d}Q\,{\rm d}W}\,{\rm d}Q\,, \tag{13}$$

splits into the corresponding contributions,

$$\frac{\mathrm{d}\sigma_k}{\mathrm{d}W} = \frac{\mathrm{d}\sigma_k^{\mathrm{c}}}{\mathrm{d}W} + \frac{\mathrm{d}\sigma_k^{\mathrm{dl}}}{\mathrm{d}W} + \frac{\mathrm{d}\sigma_k^{\mathrm{dt}}}{\mathrm{d}W}\,, \tag{14}$$

where

$$\frac{\mathrm{d}\sigma_k^{\mathrm{c}}}{\mathrm{d}W} = \mathcal{B}\,\frac{1}{W^2}\left(1 - \beta^2\,\frac{W}{W_{\mathrm{ridge}}} + \frac{1-\beta^2}{2M_1^2c^4}\,W^2\right)[1-g(W)]\,\Theta(W_{\mathrm{ridge}} - W), \tag{15}$$

$$\frac{\mathrm{d}\sigma_k^{\mathrm{dl}}}{\mathrm{d}W} = \mathcal{B}\,\frac{1}{W}\left(\int_{Q_-}^{Q_c}\frac{2m_{\mathrm{e}}c^2}{Q(Q+2m_{\mathrm{e}}c^2)}\,g(Q)\,\mathrm{d}Q\right)\delta(W-W_k)\,\Theta(Q_c - Q_-), \tag{16}$$

and

$$\frac{\mathrm{d}\sigma_k^{\mathrm{dt}}}{\mathrm{d}W} = \mathcal{B}\,\frac{1}{W}\left[\ln\left(\frac{1}{1-\beta^2}\right) - \beta^2 - \delta_{\mathrm{F}}\right]\delta(W-W_k)\,\Theta(Q_c - Q_-). \tag{17}$$

Let us evaluate the quantity

$$\begin{aligned}
G &\equiv \int_{Q_-}^{Q_c}\frac{2m_{\mathrm{e}}c^2}{Q(Q+2m_{\mathrm{e}}c^2)}\,g(Q)\,\mathrm{d}Q \\
&= \int_{Q_-}^{Q_c}\frac{2m_{\mathrm{e}}c^2}{Q(Q+2m_{\mathrm{e}}c^2)}\,\mathrm{d}Q - \int_{\max(Q_-,U_k)}^{Q_c}\frac{2m_{\mathrm{e}}c^2}{Q(Q+2m_{\mathrm{e}}c^2)}\,\frac{Q^2-U_k^2}{b^2W_k^2}\,\mathrm{d}Q \\
&= \left[\ln\left(\frac{Q}{Q+2m_{\mathrm{e}}c^2}\right)\right]_{Q_-}^{Q_c} \\
&\quad - \frac{2m_{\mathrm{e}}c^2}{b^2W_k^2}\left[Q - 2m_{\mathrm{e}}c^2\,\ln(Q+2m_{\mathrm{e}}c^2) - \frac{U_k^2}{2m_{\mathrm{e}}c^2}\,\ln\left(\frac{Q}{Q+2m_{\mathrm{e}}c^2}\right)\right]_{\max(Q_-,U_k)}^{Q_c} \\
&= \ln\left(\frac{Q_c}{Q_-}\,\frac{Q_-+2m_{\mathrm{e}}c^2}{Q_c+2m_{\mathrm{e}}c^2}\right) - \frac{2m_{\mathrm{e}}c^2}{b^2W_k^2}\left[Q_c - Q_1 - 2m_{\mathrm{e}}c^2\,\ln\left(\frac{Q_c+2m_{\mathrm{e}}c^2}{Q_1+2m_{\mathrm{e}}c^2}\right)\right] \\
&\quad + \frac{U_k^2}{b^2W_k^2}\,\ln\left(\frac{Q_c}{Q_1}\,\frac{Q_1+2m_{\mathrm{e}}c^2}{Q_c+2m_{\mathrm{e}}c^2}\right)
\end{aligned} \tag{18}$$

with $Q_1 = \max(Q_-, U_k)$.

The energy-loss DCS for close collisions with $W > Q_c$ is

$$\frac{\mathrm{d}\sigma_k^{\mathrm{ch}}}{\mathrm{d}W} = \mathcal{B}\,\frac{1}{W^2}\left(1 - \beta^2\,\frac{W}{W_{\mathrm{ridge}}} + \frac{1-\beta^2}{2M_1^2c^4}\,W^2\right)\Theta(W_{\mathrm{ridge}} - Q_c), \tag{19}$$

and for $U_k \le W \le Q_c$,

$$\begin{aligned}
\frac{\mathrm{d}\sigma_k^{\mathrm{cl}}}{\mathrm{d}W} &\simeq \frac{\mathcal{B}}{b^2W_k^2}\left(1 - \beta^2\,\frac{W}{W_{\mathrm{ridge}}}\right)\frac{W^2-U_k^2}{W^2}\,\Theta(W_{\mathrm{ridge}} - U_k)\,\Theta(Q_c - W_{\mathrm{ridge}}) \\
&= \frac{\mathcal{B}}{b^2W_k^2}\left(1 - \frac{\beta^2}{W_{\mathrm{ridge}}}\,W - \frac{U_k^2}{W^2} + \frac{\beta^2U_k^2}{W_{\mathrm{ridge}}W}\right)\,\Theta(W_{\mathrm{ridge}} - U_k)\,\Theta(Q_c - W_{\mathrm{ridge}}),
\end{aligned} \tag{20}$$

where we have used that $Q_c \ll M_1c^2$. Notice that in the case of the conduction band ($U_{\rm cb}=0$) all the terms proportional to U_k^2 have to be removed.

The integrated one-electron cross sections,

$$\sigma_k^{(n)} \equiv \int W^n \frac{{\rm d}\sigma_k}{{\rm d}W}\,{\rm d}W = [\sigma_k^{\rm c}]^{(n)} + \left[\sigma_k^{\rm dl}\right]^{(n)} + \left[\sigma_k^{\rm dt}\right]^{(n)}, \tag{21}$$

can be evaluated analytically. The partial contributions from close collisions are

$$\begin{aligned}[\sigma_k^{\rm c}]^{(0)} &= \frac{\mathcal{B}}{b^2W_k^2}\left[W - \frac{\beta^2}{W_{\rm ridge}}\,\frac{1}{2}\,W^2 + U_k^2\,\frac{1}{W} + \frac{\beta^2U_k^2}{W_{\rm ridge}}\,\ln W\right]_{U_k}^{\min(Q_c,W_{\rm ridge})}\Theta(W_{\rm ridge}-U_k)\\ &\quad + \mathcal{B}\left[-\frac{1}{W} - \frac{\beta^2}{W_{\rm ridge}}\,\ln W + \frac{1-\beta^2}{2M_1^2c^4}\,W\right]_{Q_c}^{W_{\rm ridge}}\Theta(W_{\rm ridge}-Q_c),\end{aligned} \tag{22}$$

$$\begin{aligned}[\sigma_k^{\rm c}]^{(1)} &= \frac{\mathcal{B}}{b^2W_k^2}\left[\frac{1}{2}\,W^2 - \frac{\beta^2}{W_{\rm ridge}}\,\frac{1}{3}\,W^3 - U_k^2\,\ln W + \frac{\beta^2U_k^2}{W_{\rm ridge}}\,W\right]_{U_k}^{\min(Q_c,W_{\rm ridge})}\Theta(W_{\rm ridge}-U_k)\\ &\quad + \mathcal{B}\left[\ln W - \frac{\beta^2}{W_{\rm ridge}}\,W + \frac{1-\beta^2}{2M_1^2c^4}\,\frac{1}{2}\,W^2\right]_{Q_c}^{W_{\rm ridge}}\Theta(W_{\rm ridge}-Q_c),\end{aligned} \tag{23}$$

and

$$\begin{aligned}[\sigma_k^{\rm c}]^{(2)} &= \frac{\mathcal{B}}{b^2W_k^2}\left[\frac{1}{3}\,W^3 - \frac{\beta^2}{W_{\rm ridge}}\,\frac{1}{4}\,W^4 - U_k^2\,W + \frac{\beta^2U_k^2}{W_{\rm ridge}}\,\frac{1}{2}W^2\right]_{U_k}^{\min(Q_c,W_{\rm ridge})}\Theta(W_{\rm ridge}-U_k)\\ &\quad + \mathcal{B}\left[W - \frac{\beta^2}{W_{\rm ridge}}\,\frac{1}{2}\,W^2 + \frac{1-\beta^2}{2M_1^2c^4}\,\frac{1}{3}\,W^3\right]_{Q_c}^{W_{\rm ridge}}\Theta(W_{\rm ridge}-Q_c).\end{aligned} \tag{24}$$

The contributions from distant interactions are

$$\begin{aligned}\left[\sigma_k^{\rm dl}\right]^{(0)} &= \frac{\mathcal{B}}{W_k}\,G\,\Theta[Q_c-Q_-(W_k)]\\ &= \frac{\mathcal{B}}{W_k}\left[\ln\left(\frac{Q_c}{Q_-}\frac{Q_-+2m_{\rm e}c^2}{Q_c+2m_{\rm e}c^2}\right) - \frac{2m_{\rm e}c^2}{b^2W_k^2}\left\{Q_c - Q_1 - 2m_{\rm e}c^2\,\ln\left(\frac{Q_c+2m_{\rm e}c^2}{Q_1+2m_{\rm e}c^2}\right)\right.\right.\\ &\quad \left.\left. - \frac{U_k^2}{2m_{\rm e}c^2}\,\ln\left(\frac{Q_c}{Q_1}\frac{Q_1+2m_{\rm e}c^2}{Q_c+2m_{\rm e}c^2}\right)\right\}\right]\Theta[Q_c-Q_-(W_k)],\end{aligned} \tag{25}$$

$$\left[\sigma_k^{\rm dt}\right]^{(0)} = \frac{\mathcal{B}}{W_k}\left[\ln\left(\frac{1}{1-\beta^2}\right) - \beta^2 - \delta_{\rm F}\right]\Theta[Q_c-Q_-(W_k)], \tag{26}$$

and

$$\begin{aligned}\left[\sigma_k^{\rm dl}\right]^{(1)} &= W_k\left[\sigma_k^{\rm dl}\right]^{(0)}, &\qquad \left[\sigma_k^{\rm dl}\right]^{(2)} &= W_k^2\left[\sigma_k^{\rm dl}\right]^{(0)},\\ \left[\sigma_k^{\rm dt}\right]^{(1)} &= W_k\left[\sigma_k^{\rm dt}\right]^{(0)}, &\qquad \left[\sigma_k^{\rm dt}\right]^{(2)} &= W_k^2\left[\sigma_k^{\rm dt}\right]^{(0)}.\end{aligned} \tag{27}$$

2.1 Integrated angular cross sections

Inelastic collisions cause small deflections of the projectile and contribute to the directional spreading of particle beams when they penetrate matter. For simulation purposes, it is convenient to describe angular deflections by means of the variable

$$\mu \equiv \sin^2(\theta/2) = \frac{1-\cos\theta}{2} \tag{a.39}$$

instead of the polar scattering angle θ. The recoil energy Q can then be expressed as

$$\begin{aligned} Q(Q+2m_\mathrm{e}c^2) &= (cp)^2 + (cp')^2 - 2\,cp\,cp'\,(1-2\mu) \\ &= (cp-cp')^2 + 4\,cp\,cp'\,\mu. \end{aligned}$$

It follows that

$$\mu(Q,W) = \frac{Q(Q+2m_\mathrm{e}c^2) - (cp-cp')^2}{4\,cp\,cp'}\,. \tag{28}$$

In distant interactions with the k-th oscillator, $W = W_k$ and the magnitude p_k' of the linear momentum of the projectile after the collision,

$$(cp_k')^2 = (E-W_k)(E-W_k+2m_\mathrm{e}c^2), \tag{29}$$

is fixed, which implies that μ is a function of Q only. In close collisions $Q = W$ and

$$\mu(W,W) = \frac{W(W+2m_\mathrm{e}c^2) - \left(cp - \sqrt{(E-W)(E-W+2M_1c^2)}\right)^2}{4\,cp\,\sqrt{(E-W)(E-W+2M_1c^2)}}\,. \tag{30}$$

The total angular cross section, the first transport cross section, and the second transport cross section for inelastic collisions with the k-th oscillator are defined, respectively, as

$$[\sigma_k^\mathrm{ang}]^{(0)} = \int \frac{\mathrm{d}\sigma_\mathrm{in}}{\mathrm{d}\mu}\,\mathrm{d}\mu\,, \tag{31}$$

$$[\sigma_k^\mathrm{ang}]^{(1)} = \int 2\mu\,\frac{\mathrm{d}\sigma_\mathrm{in}}{\mathrm{d}\mu}\,\mathrm{d}\mu\,, \tag{32}$$

and

$$[\sigma_k^\mathrm{ang}]^{(2)} = \int 6(\mu-\mu^2)\frac{\mathrm{d}\sigma_\mathrm{in}^{(\mathrm{s})}}{\mathrm{d}\mu}\,\mathrm{d}\mu\,, \tag{33}$$

where $\mathrm{d}\sigma_\mathrm{in}/\mathrm{d}\mu$ is the DCS, differential in the deflection μ. Naturally, both the differential and the integrated angular cross sections per molecule are the sums of contributions from the various oscillators,

$$[\sigma^\mathrm{ang}]^{(n)} = \left[\sigma_\mathrm{cb}^{(\mathrm{ang})}\right]^{(n)} + \sum_k f_k \left[\sigma_k^{(\mathrm{ang})}\right]^{(n)}. \tag{34}$$

The contribution of close collisions with the k-th oscillator to the integrated angular cross sections can be calculated in terms of the energy-loss DCS, while that of distant longitudinal interactions is conveniently calculated in terms of the DCS differential in the recoil energy,

$$\frac{\mathrm{d}\sigma_k^{\mathrm{dl}}}{\mathrm{d}Q} = \int \frac{\mathrm{d}^2\sigma_k^{\mathrm{dl}}}{\mathrm{d}Q\,\mathrm{d}W}\,\mathrm{d}W = \mathcal{B}\,\frac{1}{W_k}\,\frac{2m_{\mathrm{e}}c^2}{Q(Q+2m_{\mathrm{e}}c^2)}\,g(Q)\,\Theta(Q_c-Q)\,\Theta[Q-Q_-(W_k)]\,. \tag{35}$$

We have

$$\left[\sigma_k^{(\mathrm{ang})}\right]^{(0)} = \left[\sigma_k^{\mathrm{dt}}\right]^{(0)} + \int_{Q_-(W_k)}^{Q_c} \frac{\mathrm{d}\sigma_k^{\mathrm{dl}}}{\mathrm{d}Q}\,\mathrm{d}Q + \int_{U_k}^{W_{\mathrm{ridge}}} \frac{\mathrm{d}\sigma_k^{\mathrm{c}}}{\mathrm{d}W}\,\mathrm{d}W = \sigma_k^{(0)}\,, \tag{36a}$$

$$\left[\sigma_k^{(\mathrm{ang})}\right]^{(1)} = 2\int_{Q_-(W_k)}^{Q_c} \mu(Q,W_k)\,\frac{\mathrm{d}\sigma_k^{\mathrm{dl}}}{\mathrm{d}Q}\,\mathrm{d}Q + 2\int_{U_k}^{W_{\mathrm{ridge}}} \mu(W,W)\,\frac{\mathrm{d}\sigma_k^{\mathrm{c}}}{\mathrm{d}W}\,\mathrm{d}W\,, \tag{36b}$$

and

$$\begin{aligned}\left[\sigma_k^{(\mathrm{ang})}\right]^{(2)} &= 6\int_{Q_-(W_k)}^{Q_c} \left[\mu(Q,W_k)-\mu^2(Q,W_k)\right]\frac{\mathrm{d}\sigma_k^{\mathrm{dl}}}{\mathrm{d}Q}\,\mathrm{d}Q \\ &\quad + 6\int_{U_k}^{W_{\mathrm{ridge}}} \left[\mu(W,W)-\mu^2(W,W)\right]\frac{\mathrm{d}\sigma_k^{\mathrm{c}}}{\mathrm{d}W}\,\mathrm{d}W\,. \end{aligned} \tag{36c}$$

Since in distant transverse interactions the projectile is not deflected, those interactions do not contribute to the transport cross sections. The integrals in Eqs. (36) are required only for class-II simulations, where they are restricted to outer-shell oscillators and to energy transfer less than a certain cutoff value W_{cc}. In our simulation code the restricted angular integrals are evaluated numerically by building a table of the integrand, which is subsequently integrated by using linear log-log interpolation.

2.2 Simulation of inelastic collisions

Individual inelastic collisions with the k-th oscillator are simulated from the DDCS given by Eqs. (a.93-95) and (a98) using the exact algorithm described below. A presentation of elementary sampling methods is given in the PENELOPE manual (Salvat, 2019). Notice that the probability distribution functions (pdf's) considered here are not normalized; normalization is automatically satisfied when each call to a sampling routine delivers one value of the relevant random variable.

• Distant interactions

Distant interactions have a resonant character with a fixed energy loss $W = W_k$ or W_k', Eq. (a.116). In distant transverse interactions, $Q = Q_-$ so that $\cos\theta = 1$, *i.e.*, the projectile is not deflected. Distant longitudinal interactions involve a continuum of recoil energies with the pdf

$$p(Q) = \frac{2m_{\mathrm{e}}c^2}{Q(Q+2m_{\mathrm{e}}c^2)}\,g(Q), \qquad \text{if } Q_- < Q < Q_c\,, \tag{37}$$

where

$$g(Q) = 1 - \frac{Q^2-U_k^2}{b^2W_k^2}\,\Theta(Q-U_k). \tag{38}$$

Random values of Q from this distribution are sampled by means of the following rejection algorithm.

1) Tentative values of Q are generated from the pdf

$$p_1(Q) = \frac{2m_\mathrm{e}c^2}{Q(Q+2m_\mathrm{e}c^2)} \tag{39}$$

by using the inverse transform method, which gives the sampling formula

$$Q = Q_- \, 2m_\mathrm{e}c^2 \left[\left(\frac{Q_-}{Q_c} \, \frac{Q_c + 2m_\mathrm{e}c^2}{Q_- + 2m_\mathrm{e}c^2} \right)^{\xi} (Q_- + 2m_\mathrm{e}c^2) - Q_- \right]^{-1}, \tag{40}$$

where ξ is a random number uniformly distributed in the interval (0,1).

2) These values are subject to a rejection process; they are accepted with probability

$$R_1(Q) = \frac{g(Q)}{g(U_k)} = \begin{cases} 1 & \text{if } Q < U_k, \\ 1 - (Q^2 - U_k^2)/(bW_k)^2 & \text{if } Q \geq U_k. \end{cases} \tag{41}$$

That is, the Q value is accepted if a new random number ξ satisfies the condition $\xi < R_1(Q)$; otherwise the value is rejected and we repeat the sampling from $p_1(Q)$.

Once the recoil energy Q has been determined, the polar scattering angle θ of the projectile is obtained as

$$\cos\theta = \frac{E(E+2M_1c^2) + (E-W_k)(E-W_k+2M_1c^2) - Q(Q+2m_\mathrm{e}c^2)}{2\sqrt{E(E+2M_1c^2)\,(E-W_k)(E-W_k+2M_1c^2)}}. \tag{42}$$

The interaction causes the release of a secondary electron with kinetic energy $E_\mathrm{s} = W_k - U_k$ in the direction of the momentum transfer, defined by the polar angle θ_r given by

$$\cos\theta_\mathrm{r} = \frac{W_k/\beta}{\sqrt{Q(Q+2m_\mathrm{e}c^2)}} \left(1 + \frac{Q(Q+2m_\mathrm{e}c^2) - W_k^2}{2W_k(E+M_1c^2)} \right). \tag{43}$$

As indicated in the parent article, in the case of distant excitations of an inner subshell, the energy loss W is sampled from the triangular pdf, Eq. (a.115), which serves to spread the discrete resonances predicted by our GOS model into a continuum distribution keeping their average value $\langle W \rangle = W_k'$.

• Close collisions

In close interactions $Q = W$, and the energy loss W is sampled from the pdf determined by the corresponding energy-loss DCS.

The pdf for low-W collisions is

$$p(W) = \left(1 - \beta^2 \frac{W}{W_\mathrm{ridge}} \right) \frac{W^2 - U_k^2}{W^2} \qquad \text{if } U_k < W < Q_c\,. \tag{44}$$

The sampling from this distribution is performed by means of the following rejection algorithm.

1) Tentative values of W are generated from the distribution

$$p_2(W) = 1 - \frac{U_k^2}{W^2} \tag{45}$$

by the inverse transform method, which gives the sampling formula

$$W = A + \sqrt{A^2 - U_k^2} \qquad \text{with} \qquad A = \frac{\xi}{2}\left(Q_c + \frac{U_k^2}{Q_c}\right) + (1-\xi)\, U_k\,. \tag{46}$$

2) The generated W values are accepted with probability

$$R_2(W) = \frac{1 - \beta^2\, W/W_{\rm ridge}}{1 - \beta^2\, U_k/W_{\rm ridge}}\,. \tag{47}$$

The pdf of the energy loss in high-W close collisions is

$$p(W) = \frac{1}{W^2}\left(1 - \beta^2\,\frac{W}{W_{\rm ridge}} + \frac{1-\beta^2}{2M_1^2c^4}\,W^2\right) \qquad \text{if } \; Q_c < W < W_{\rm ridge}\,. \tag{48}$$

Again, the sampling from this pdf may be performed by the rejection method:

1) Sample trial values of W from the distribution

$$p_3(W) = \frac{1}{W^2} \tag{49}$$

by the inverse-transform formula

$$W = \frac{W_{\rm ridge}\, Q_c}{W_{\rm ridge} - \xi(W_{\rm ridge} - Q_c)}\,. \tag{50}$$

2) Accept these values with probability

$$R_3(W) = \left[1 - \beta^2\,\frac{W}{W_{\rm ridge}} + \frac{1-\beta^2}{2M_1^2c^4}\,W^2\right]\left[1 - \beta^2\,\frac{Q_c}{W_{\rm ridge}} + \frac{1-\beta^2}{2M_1^2c^4}\,Q_c^2\right]^{-1}. \tag{51}$$

Recalling that $Q = W$ in close collisions, the polar scattering angle θ of the projectile and the emission angle $\theta_{\rm r}$ of the secondary electron can be expressed as

$$\cos\theta = \frac{E(E + 2M_1c^2) - W(E + M_1c^2 + m_{\rm e}c^2)}{\sqrt{E(E+2M_1c^2)\,(E-W)(E-W+2M_1c^2)}} \tag{52}$$

and

$$\cos\theta_{\rm r} = \sqrt{\frac{W}{\beta^2(W + 2m_{\rm e}c^2)}}\left(1 + \frac{m_{\rm e}c^2}{(E + M_1c^2)}\right), \tag{53}$$

respectively.

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