Recent developments toward improving Geant4 capability of modelling low energy(< 1.0 GeV) electron/positron multiple scattering

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Abstract

A review of models for simulating low energy electron/positron multiple scattering effects in Geant4 has been started recently. The current report is a short summary of recent improvements and further plans.

Note, that the model is under development in Geant4 and therefore this document will be regularly updated when the development goes further.

1 Introduction

Elastic interaction of electrons(positrons) with free atoms are well understood and the corresponding differential cross sections (DCS) can be computed based on first principles. The electron transport problem in matter, including the effects of elastic scattering, can be solved exactly by using these DCSs (with corrections to account solid state effects) in a traditional event-by-event Monte Carlo simulation. However, event-by-event simulation is feasible only if the mean number of interactions per particle track is below few hundred. This limits the applicability of the detailed simulation model only for electrons with relatively low kinetic energies (up to $E_{kin} \sim 100$ keV) or thin targets. A fast ($E_{kin} > 100$ keV) electron undergoes a high number of elastic collisions in the course of its slowing down in tick targets. Since detailed simulation becomes very inefficient, high energy particle transport simulation codes employ condensed history (or Class I.) simulation model. Each particle track is simulated by allowing to make individual steps that are much higher than the average step length between two successive elastic interactions. The net effects of these high number of elastic interactions such as angular deflection and spacial displacement is accounted at each individual condensed history step by using multiple scattering theories. The accuracy of modelling the cumulative effects of many elastic scattering in one step strongly depends on the capability of the employed multiple scattering theory to describe the angular distribution of electrons after travelling a given path length.

2 Angular distribution in multiple scattering

The accuracy of modelling the cumulative effects of many elastic scattering in one step strongly depends on the capability of the employed multiple scattering theory to describe the angular distribution of electrons after travelling a given path length. Goudsmit and Saunderson [1] derived an expression for this angular distribution in the form of an expansion in Legendre polynomials (neglecting energy loss along the step). One of the biggest advantage of the Goudsmit-Saunderson distribution is its formal independence of the form of the single scattering DCS. Therefore, any DCS can be combined with the GS angular distribution. First the GS distribution will be derived in this section. Then the screened Rutherford cross section will be combined ...

2.1 Goudsmit-Saunderson angular distribution

The Goudsmit-Saunderson angular distribution will be derived in this section by following the notations in [2]. Assuming that the particle was initially moving into the $\hat{\hat{z}}$ direction the probability density $F(s;\theta)$ of finding the particle moving into a direction falling into the solid angle element $\mathrm{d}\Omega$ around the direction defined by the polar angle θ after having travelled a path length s is

$$F(s;\theta) = \sum_{n=0}^{\infty} f_n(\theta)\mathcal{W}_n(s) \tag{1}$$

$f_n(\theta)$ is the angular distribution after n elastic interactions and $\mathcal{W}_n(s)$ is the probability of having n elastic interactions while travelling a path length s.

The single scattering angular distribution $f_{n=1}(\theta)$ is given by

$$f_1(\theta) = \frac{1}{\sigma}\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}(\theta) \tag{2}$$

where $\mathrm{d}\sigma/\mathrm{d}\Omega$ is the DCS for elastic scattering and $\sigma = 2\pi\int_0^{\pi} \mathrm{d}\sigma/\mathrm{d}\Omega \sin(\theta)\mathrm{d}\theta$ is the corresponding elastic scattering cross section (assuming spherical symmetry). It can be seen (with the variable change $\theta \to \cos(\theta)$) that

$$2\pi f_1(\cos(\theta)) = 2\pi\frac{1}{\sigma}\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}(\cos(\theta)) = p(\cos(\theta)) \tag{3}$$

i.e. the probability density of having a direction in single elastic event that corresponds to $\cos(\theta)$. The single scattering distribution can be expressed in terms of Legendre polynomials (see Appendix A.1 for more details)

$$f_1(\cos(\theta)) = \sum_{\ell=0}^{\infty}\frac{2\ell+1}{4\pi}F_\ell P_\ell(\cos(\theta)) \tag{4}$$

where

$$F_\ell = 2\pi \int_{-1}^{1} f_1(\cos(\theta)) P_\ell(\cos(\theta)) \mathrm{d}(\cos(\theta)) = \langle P_\ell(\cos(\theta)) \rangle \tag{5}$$

and $P_\ell(x)$ is the ℓ-th Legendre polynomial. The quantity

$$G_\ell \equiv 1 - F_\ell = 1 - \langle P_\ell(\cos(\theta)) \rangle \tag{6}$$

is the transport coefficient and the ℓ-th inverse transport mean free path is defined by

$$\lambda_\ell^{-1} \equiv \frac{G_\ell}{\lambda} = \frac{1 - F_\ell}{\lambda} = \frac{1 - \langle P_\ell(\cos(\theta)) \rangle}{\lambda} \tag{7}$$

where

$$\lambda \equiv \frac{1}{\mathcal{N}\sigma} \tag{8}$$

is the elastic mean free path ($\mathcal{N}$ is the number of atoms per unit volume). Notice that λ^{-1} is the probability of elastic interaction per unit path length. Furthermore, $F_0 = 1$, $G_0 = 0$ and the value of F_ℓ decreases with ℓ due to the faster oscillation of $P_\ell(\cos(\theta))$ [2]. Therefore, G_ℓ goes to unity and hence λ_ℓ tends to λ when ℓ goes to infinity.

The angular distribution of particles after n elastic interactions can be written as (see Appendix A.1 for more details)

$$f_n(\cos(\theta)) = \sum_{\ell=0}^{\infty} \frac{2\ell + 1}{4\pi} (F_\ell)^n P_\ell(\cos(\theta)) \tag{9}$$

The number of elastic interactions along a path length s travelled by the particle follows Poisson distribution with parameter s/λ (mean number of elastic interactions along s)

$$\mathcal{W}_n(s) = \exp(-s/\lambda) \frac{(s/\lambda)^n}{n!} \tag{10}$$

Integrating Eq.(1) over ϕ (that gives a 2π factor due to cylindrical symmetry), changing the variable θ to $\cos(\theta)$ and inserting Eqs.(9, 10)

$$\begin{aligned}
F(\cos(\theta);s) =& 2\pi \sum_{n=0}^{\infty} f_n(\cos(\theta))\mathcal{W}_n(s) = \sum_{n=0}^{\infty}\sum_{\ell=0}^{\infty} \frac{2\ell+1}{2}(F_\ell)^n P_\ell(\cos(\theta))\exp(-s/\lambda)\frac{(s/\lambda)^n}{n!} \\
=& \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2}\exp(-s/\lambda)\left[\sum_{n=0}^{\infty}\frac{(s/\lambda)^n}{n!}(F_\ell)^n\right] P_\ell(\cos(\theta)) \\
=& \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2}\exp(-s/\lambda)\underbrace{\left[\sum_{n=0}^{\infty}\frac{(s/\lambda)^n}{n!}\langle P_\ell(\cos(\theta)\rangle^n\right]}_{\exp(s/\lambda\langle P_\ell(\cos(\theta))\rangle)=\exp(s/\lambda(1-\lambda/\lambda_\ell))} P_\ell(\cos(\theta)) \\
=& \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2}\exp(-s/\lambda)\exp(s/\lambda(1-\lambda/\lambda_\ell))P_\ell(\cos(\theta)) \\
=& \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2}\exp(-s/\lambda_\ell)P_\ell(\cos(\theta))
\end{aligned} \tag{11}$$

that is the p.d.f. of having a final direction that corresponds to $\cos(\theta)$ after travelling a path s derived by Goudsmit and Saunderson [1].

In order to compute the angular distribution for a given path length s based on a given single scattering elastic DCS one needs to compute the transport mean free paths λ_ℓ that practically means the computation of the transport coefficients G_ℓ given by Eq.(6) that involves the computation of the integral Eq.(5). This integral needs to be computed numerically when the single scattering DCS is given in numerical form that can be challenging in case of large ℓ values due to the strong oscillation of the corresponding Legendre polynomials. The convergence of the Goudsmit-Saunderson series given by Eq.(11) is determined by the exponential factor $\exp(-s/\lambda_\ell) = \exp(-sG_\ell/\lambda)$. The number of terms needed to reach convergence of the series increases by decreasing path lengths and for short s path lengths a large number of terms are needed to be computed. The convergence can be improved by separating the contribution of unscattered ($n = 0$) and single-scattered ($n = 1$) electrons in the series as it was suggested by Berger and Wang [3] and applied e.g. in [4]. This from of the Goudsmit-Saunderson angular distribution was used by Bielajew [5] to construct his hybrid simulation model that will be discussed in the next section.

2.2 Hybrid simulation model

According to Eq.(10) the probability of having no ($n = 0$), single ($n = 1$) or at least two ($n \geq 2$) elastic scattering along a path length s travelled by the particle are

$$\begin{aligned}\mathcal{W}_{n=0}(s) &= \exp(-s/\lambda)\\ \mathcal{W}_{n=1}(s) &= \exp(-s/\lambda)(s/\lambda)\\ \mathcal{W}_{n\geq 2}(s) &= 1 - \exp(-s/\lambda) - \exp(-s/\lambda)(s/\lambda)\end{aligned} \tag{12}$$

Separating these three terms in Eq.(11) gives

$$\begin{aligned}F(\mu;s) =& 2\pi\sum_{n=0}^{\infty} f_n(\mu)\mathcal{W}_n(s) = 2\pi f_{n=0}(\mu)\mathcal{W}_{n=0} + 2\pi f_{n=1}(\mu)\mathcal{W}_{n=1} + 2\pi\sum_{n=2}^{\infty} f_n(\mu)\mathcal{W}_n(s)\\ =& \underbrace{\exp(-s/\lambda)\delta(1-\mu) + \exp(-s/\lambda)(s/\lambda)2\pi f_{n=1}(\mu)}_{\chi}\\ &+ \sum_{n=2}^{\infty}\sum_{\ell=0}^{\infty}\frac{2\ell+1}{2}(F_\ell)^n P_\ell(\mu)\exp(-s/\lambda)\frac{(s/\lambda)^n}{n!}\\ =& \chi + \sum_{\ell=0}^{\infty}\frac{2\ell+1}{2}P_\ell(\mu)\exp(-s/\lambda)\underbrace{\sum_{n=2}^{\infty}(F_\ell)^n\frac{(s/\lambda)^n}{n!}}_{\sum_{n=0}^{\infty}x^n/n!-1-x,\; x=F_\ell(s/\lambda)}\\ =& \chi + \sum_{\ell=0}^{\infty}\frac{2\ell+1}{2}P_\ell(\mu)\exp(-s/\lambda)\left[\exp(F_\ell(s/\lambda)) - 1 - F_\ell(s/\lambda)\right]\\ =& \chi + \sum_{\ell=0}^{\infty}\frac{2\ell+1}{2}P_\ell(\mu)\mathrm{e}^{-s/\lambda}\left[\mathrm{e}^{(1-G_\ell)(s/\lambda)} - 1 - (1-G_\ell)(s/\lambda)\right]\\ =& \chi + \sum_{\ell=0}^{\infty}\frac{2\ell+1}{2}P_\ell(\mu)\mathrm{e}^{-s/\lambda}\left[\mathrm{e}^{s/\lambda}\mathrm{e}^{-(s/\lambda)G_\ell} - 1 - (1-G_\ell)(s/\lambda)\right]\\ =& \mathrm{e}^{-s/\lambda}\delta(1-\mu) + (s/\lambda)\mathrm{e}^{-s/\lambda}2\pi f_{n=1}(\mu) +\\ &\sum_{\ell=0}^{\infty}\frac{2\ell+1}{2}P_\ell(\mu)\left\{\mathrm{e}^{-(s/\lambda)G_\ell} - \mathrm{e}^{-(s/\lambda)}\left[1 + (s/\lambda)(1-G_\ell)\right]\right\}\end{aligned} \tag{13}$$

with $\mu = \cos(\theta)$. This is the same probability density function as Eq.(11) in the form of suggested by Berger and Wang [3] and used by Bielajew [5] to construct his hybrid simulation model. Notice that the first term is the probability of having no elastic scattering along the path s ($\mathrm{e}^{-s/\lambda}$) multiplied by the corresponding angular distribution (a delta function; $\int_{-1}^{+1}\delta(1-\mu)\mathrm{d}\mu = 1$). The second term is the probability of having exactly one elastic scattering along the path s ($(s/\lambda)\mathrm{e}^{-s/\lambda}$) multiplied by the corresponding single scattering angular distribution ($2\pi f_{n=1}(\mu) = p(\mu)$ i.e. p.d.f. of μ in single scattering; $\int_{-1}^{+1} 2\pi f_{n=1}(\mu)\mathrm{d}\mu = 1$). Since $F(\mu; s)$ is the p.d.f. of μ for a given path length s it is normalised to unity i.e. $\int_{-1}^{+1} F(\mu; s)\mathrm{d}\mu = 1$. Therefore, integrating the last term(s) over μ gives $1 - \mathrm{e}^{-s/\lambda} - (s/\lambda)\mathrm{e}^{-s/\lambda}$ i.e. the probability of having at least two elastic scattering along the path length s. In order to have this last term in the same form as the first and second (i.e. probability of event multiplied by the corresponding normalised distribution) one needs to normalise this term i.e.

$$F(\mu; s) = \mathrm{e}^{-s/\lambda}\delta(1-\mu) + (s/\lambda)\mathrm{e}^{-s/\lambda}2\pi f_{n=1}(\mu) + (1 - \mathrm{e}^{-s/\lambda} - (s/\lambda)\mathrm{e}^{-s/\lambda})F(\mu; s)^{2+} \quad (14)$$

[5, 6] where $F(\mu; s)^{2+}$ is the probability density function of having a direction given by $\mu = \cos(\theta)$ after at least two elastic interactions along the path s [5, 6]

$$F(\mu; s)^{2+} \equiv \sum_{\ell=0}^{\infty}(\ell + 0.5)P_\ell(\mu)\frac{\mathrm{e}^{-(s/\lambda)G_\ell} - \mathrm{e}^{-(s/\lambda)}\left[1 + (s/\lambda)(1 - G_\ell)\right]}{1 - \mathrm{e}^{-s/\lambda} - (s/\lambda)\mathrm{e}^{-s/\lambda}} \quad (15)$$

When a model based on Eq.(14) is used to describe the angular distribution of the particles after travelling a given path, the single and multiple scattering cases are combined into one model that suggests the adverb *hybrid*. In case of short path lengths (when $s \sim \lambda$)Eq.(14) is almost entirely contributed by the second, single scattering term. In case of longer path lengths ($s \gg \lambda$) the multiple scattering part will be dominated. Geometry adaptive particle transport algorithms, that limits the allowed path length near the boundary, can exploit this property: by limiting the path length near the boundary the the condensed history algorithm transforms to single scattering algorithm. Such a combination of single and multiple scattering algorithm into one model results in a *hybrid* model for elastic scattering that can exploit both the computational efficiency of multiple scattering theories and the accuracy of single scattering approach [5, 6] when needed.

Kawrakow and Bielajew [6] developed an any-angle multiple scattering model based on the Goudsmit-Saunderson angular distribution and the screened Rutherford elastic scattering cross section. Using the screened Rutherford elastic DCS in the Goudsmit-Saunderson series results in a compact numerical representation of the corresponding angular distributions that makes possible on-the-fly sampling of the angular deflections including any angles for any condensed history steps. [6, 7, 8]. This model will be discussed in the next section.

2.3 Using the screen Rutherford DCS for elastic scattering of electrons in the Goudsmit-Saunderson model

2.3.1 The screened Rutherford DCS and some derived expressions

The screened Rutherford DCS can be obtained by solving the scattering equation under the first Born approximation and using a simple exponentially screened Coulomb potential as scattering potential (see Appendix A.2 for more details)

$$V(r) = \frac{ZZ'e^2}{r} e^{-r/R} \tag{16}$$

with a screening radius R (target atomic number of Z and projectile charge $Z'e$) that leads to the screened Rutherford DCS for elastic scattering

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}^{(SR)} = \left(\frac{ZZ'e^2}{pc\beta}\right)^2 \frac{1}{(1-\cos(\theta)+2A)^2} \tag{17}$$

where p is the momentum, β is the velocity of the particle in units of speed of light c and A is the screening parameter

$$A \equiv \frac{1}{4}\left(\frac{\hbar}{p}\right)^2 R^{-2} \tag{18}$$

The corresponding total elastic scattering cross section

$$\sigma^{(SR)} = \left(\frac{ZZ'e^2}{pc\beta}\right)^2 \frac{\pi}{A(1+A)} \tag{19}$$

and the single elastic scattering angular distribution

$$f_1(\theta)^{(SR)} = \frac{1}{\pi}\frac{A(1+A)}{(1-\cos(\theta)+2A)^2} \tag{20}$$

The corresponding ℓ-th transport coefficient G_ℓ [2]

$$G_\ell^{(SR)}(A) = 1 - \ell[Q_{\ell-1}(1+2A) - (1+2A)Q_\ell(1+2A)] \tag{21}$$

where $Q_\ell(x)$ are Legendre functions of the second kind. Substituting $\ell = 1$ and the corresponding forms of the Legendre functions of the second kind $Q_0(x) = 0.5\ln((x+1)/(x-1))$ and $Q_1(x) = 0.5x\ln((x+1)/(x-1)) - 1$, the first transport coefficient

$$G_{\ell=1}^{(SR)}(A) = 2A\left[\ln\left(\frac{1+A}{A}\right)(A+1) - 1\right] \tag{22}$$

and the corresponding first transport mean free path

$$\lambda_{\ell=1}^{-1(SR)} = \frac{G_{\ell=1}^{(SR)}(A)}{\lambda^{(SR)}} \tag{23}$$

by using Eq.(7)

2.3.2 Single scattering angular distribution

According to Eqs.(3,20) the PDF of $\mu = \cos(\theta)$ in single scattering can be written as

$$2\pi f_{n=1}(\mu) = 2\pi \frac{1}{\pi} \frac{A(A+1)}{[1-\mu+2A]^2} = \frac{2A(A+1)}{[1-\mu+2A]^2} \tag{24}$$

when the screened Rutherford DCS is used to describe elastic scattering. The corresponding cumulative density function (CDF) $\mathcal{P}(\mu; A)$ is

$$\begin{aligned} \mathcal{P}(\mu = \cos(\theta); A) &= \int_0^\theta \frac{2A(A+1)}{[1-\cos(\theta)+2A]^2} \sin(\theta)\mathrm{d}\theta = \int_\mu^{+1} \frac{2A(A+1)}{[1-\mu+2A]^2} \mathrm{d}\mu \\ &= \left[\frac{2A(A+1)}{1-\mu+2A}\right]_\mu^{+1} = (A+1)\left[1 - \frac{2A}{1-\mu+2A}\right] = \frac{(A+1)(1-\mu)}{1-\mu+2A} \end{aligned} \tag{25}$$

Having $\eta \in \mathcal{U}(0,1)$ random variable one can derive the inverse function $\mathcal{P}^{-1}(\eta; A)$ by solving $\eta = \mathcal{P}(\mu; A) = (A+1)(1-\mu)/(1-\mu+2A)$ for μ which results in

$$\mu = \mathcal{P}^{-1}(\eta; A) = 1 - \frac{2A\eta}{1-\eta+A} \tag{26}$$

Therefore, given the screening parameter A and a random number $\eta \in \mathcal{U}(0,1)$, deflection μ in single elastic scattering can be sampled analytically by using this expression.

2.3.3 More than one scattering case

$F(\mu; s)^{2+}$ as given by Eq.(15) is the conditional PDF of the angular deflection μ along the path length s with the condition that at leat two elastic interaction happen along this path. The shape of this PDF shows high variation as a function of possible parameter values and can easily span sever order of magnitudes that makes the numerical treatment (sampling, interpolation, etc.) of these PDF delicate. In order to avoid numerical problems one either needs to store a high amount of these precomputed PDF or come up with a proper variable transformation that makes these PDF as flat as possible. A special variable transformation for screened Rutherford DCS was suggested in [9, 5], generalised in [6].

Let the transformation function f and the transformed variable u

$$u = f(a_1, ..., a_n; \mu) \tag{27}$$

where $u \in \mathcal{U}(0,1)$ and $a_1, ..., a_n$ are parameters of the transformation that control the shape of the result of the transformation. We want the transformed PDF of $q^{2+}(u)$ to satisfy

$$q^{2+}(s; u)\mathrm{d}u = F(s; \mu)^{2+}_{GS}\mathrm{d}\mu \tag{28}$$

i.e. the probability of having u falling into the du interval around u according to the transformed PDF $q^{2+}(u)$ is equal to the probability of having μ falling into the du interval around μ according to the original PDF $F(s;\mu)^{2+}_{GS}$. From this [6]

$$q^{2+}(s;u) = F(s;\mu)^{2+}_{GS}\frac{\mathrm{d}\mu}{\mathrm{d}u} \tag{29}$$

where

$$\frac{\mathrm{d}\mu}{\mathrm{d}u} = \left(\frac{\mathrm{d}u}{\mathrm{d}\mu}\right)^{-1} = \left(\frac{\partial f(a_1,...,a_n;\mu)}{\partial\mu}\right)^{-1} \tag{30}$$

The values of $a_1,...,a_n$ parameters (that gives a transformation that results in a "as flat as possible" transformed distribution) can be determined by minimizing

$$\int_0^1 \left[q^{2+}(s;u) - 1\right]^2 \mathrm{d}u \tag{31}$$

with respect to $a_1,...,a_n$ (i.e. try to find $a_1,...,a_n$ that results in a transformation $f(a_1,...,a_n;\mu)$ that makes the transformed PDF $q^{2+}(s;u)$ as close to the uniform distribution on $[0,1]$ as possible). The optimal values of $a_1,...,a_n$ can be found by solving the set of equations [6]

$$\begin{aligned}
0 &= \frac{\partial}{\partial a_i}\left[\int_0^1 \left[q^{2+}(s;u)-1\right]^2 \mathrm{d}u\right] \\
&= \frac{\partial}{\partial a_i}\left\{\int_{-1}^{+1}\left[F(s;\mu)^{2+}_{GS}\left(\frac{\partial f(a_1,...,a_n;\mu)}{\partial\mu}\right)^{-1}\right]^2\left(\frac{\partial f(a_1,...,a_n;\mu)}{\partial\mu}\right)\mathrm{d}\mu\right\} \\
&- \frac{\partial}{\partial a_i}\left\{\int_{-1}^{+1}\left[2F(s;\mu)^{2+}_{GS}\left(\frac{\partial f(a_1,...,a_n;\mu)}{\partial\mu}\right)^{-1}\right]\left(\frac{\partial f(a_1,...,a_n;\mu)}{\partial\mu}\right)\mathrm{d}\mu\right\} \\
&= \int_{-1}^{+1}\frac{\partial}{\partial a_i}\left\{\left[F(s;\mu)^{2+}_{GS}\right]^2\left(\frac{\partial f(a_1,...,a_n;\mu)}{\partial\mu}\right)^{-1}\right\}\mathrm{d}\mu \\
&- 2\int_{-1}^{+1}\underbrace{\frac{\partial}{\partial a_i}2F(s;\mu)^{2+}_{GS}}_{0}\mathrm{d}\mu \\
&= \int_{-1}^{+1}\left[F(s;\mu)^{2+}_{GS}\left(\frac{\partial f(a_1,...,a_n;\mu)}{\partial\mu}\right)^{-1}\right]^2\left[\frac{\partial^2 f(a_1,...,a_n;\mu)}{\partial\mu\partial a_i}\right]\mathrm{d}\mu, \quad i=1,...,n
\end{aligned} \tag{32}$$

Notice that this formalism is independent of the form of the adopted DCS.

When the single elastic scattering is described by the screened Rutherford DCS (i.e. DCS for electric scattering computed under the first Born approximation by using a simple exponentially screened Coulomb potential; see Appendix A.2) one can take [6]

$$u = f(\mu;a) = \frac{(a+1)(1-\mu)}{1-\mu+2a} \tag{33}$$

that is the single scattering CDF corresponding to the screened Rutherford DCS with a scaled screening parameter $a = w^2 A$ (see Eq.(25)) where the scaling factor w is arbitrary at the moment. Choosing this form of transformation function is motivated by the fact, that according to Eq.(29) the transformed distribution becomes $q^{2+}(s;u) \equiv \mathcal{U}[0,1]$ i.e. the uniform distribution on the $[0,1]$ interval when the transformation function is chosen to be the CDF. The corresponding inverse transformation can be derived by solving $u = f(a;\mu)$ for μ that gives

$$\mu = 1 - \frac{2au}{1-u+a} \tag{34}$$

Taking the partial derivatives

$$\frac{\partial f(a;\mu)}{\partial \mu} = -\frac{2a(1+a)}{[1-\mu+2a]^2} \tag{35}$$

$$\frac{\partial^2 f(a;\mu)}{\partial \mu \partial a} = -2\frac{1-\mu(1+2a)}{[1-\mu+2a]^3} \tag{36}$$

plugging them into Eq.(32) and solving for a gives the optimal value of the parameter a of the chosen transformation function given by Eq.(33) (where optimality means that the corresponding transformed $q^{2+}(s;u)$ PDF is as close to the uniform distribution as possible) [6] (see Appendix A.3)

$$a = \frac{\alpha}{4\beta} + \sqrt{\left(\frac{\alpha}{4\beta}\right)^2 + \frac{\alpha}{4\beta}} \tag{37}$$

where

$$\begin{aligned} \alpha = \sum_{\ell=0}^{\infty} \xi_\ell(s,\lambda,A) \Bigg\{ &\left(1.5\ell + \frac{0.065}{\ell+1.5} + \frac{0.065}{\ell-0.5} + 0.75\right) \xi_\ell(s,\lambda,A) \\ &-2(\ell+1)\xi_{\ell+1}(s,\lambda,A) + \frac{(\ell+1)(\ell+2)}{(2\ell+3)} \xi_{\ell+2}(s,\lambda,A) \Bigg\} \end{aligned} \tag{38}$$

$$\beta = \sum_{\ell=0}^{\infty} (\ell+1)\xi_\ell(s,\lambda,A)\xi_{\ell+1}(s,\lambda,A) \tag{39}$$

with

$$\xi_i(s,\lambda,A) = \frac{\mathrm{e}^{-(s/\lambda)G_i(A)} - \mathrm{e}^{-(s/\lambda)}\left[1 + (s/\lambda)(1-G_i(A))\right]}{1 - \mathrm{e}^{-s/\lambda} - (s/\lambda)\mathrm{e}^{-s/\lambda}} \tag{40}$$

i.e. the last part of $F(s;\mu)^{2+}_{GS}$ given by Eq.(15).

When the screened Rutherford DCS is adopted with the transformation given by Eq.(33), the transformed PDF can be given by using Eq.(29), substituting Eq.(15), Eq.(35)

according to Eq.(30) and using Eq.(34) to replace μ in the Legendre polynomials that yield

$$q^{2+}(s,\lambda,a,A;u) = \frac{2a(1-a)}{[1-u+a]^2}\sum_{\ell}^{\infty}(\ell+0.5)P_\ell\left[1-\frac{2au}{1-u+a}\right]\xi_\ell(s,\lambda,A) \tag{41}$$

In order to computed this transformed PDF as a function of the transformed variable $u \in [-1,1]$ the parameters s,λ,a,A need to be given.

The computation involves Eq.(40) which means that one needs to be able to compute $G_\ell(A)$ transport coefficients up to a high enough value of ℓ in order to achieve convergence even in the case of short path lengths (i.e. small number of elastic interactions along the given s pathlength). When the screened Rutherford DCS is adopted these $G_\ell(A)$ transport coefficients can be computed by using Eq.(A.34) that involves the computation of Legendre functions of the second kind $Q_\ell(x)$ with $x = 1+2A > 1$. Special care needs to be taken to evaluate the Legendre functions of second kind $Q_\ell(x)$ based on their recurrence relation in order to avoid numerical inaccuracies. One solution is given in Appendix A. of [2] that ensures numerical stability of the computed $Q_\ell(x)$ up to high values of ℓ even in the case of $x > 1$. The other possibility is to use the approximate expression for $G_\ell(A)$ given in [6]

$$G_\ell(A) = 1 - y_\ell(A)K_1(y_\ell(A))\left\{1+0.5y_\ell^2(A)[\Phi(\ell)-0.5\ln(\ell(\ell+1))-\gamma]\right\} \tag{42}$$

where $y_\ell(A) = 2\sqrt{\ell(\ell+1)A}$, $K_1(x)$ is the modified Bessel function of the second kind, $\Phi(\ell) = \sum_{m=1}^{\ell} 1/m$ is the ℓ-th harmonic number and γ is the Euler constant. In the present work the $G_\ell(A)$ transport coefficients were computed up to $\ell_{max} = 10000$ by using Eq.(42) that ensures convergence in Eq.(41) even for small number of elastic interactions and/or small value of A.

The second point regarding the transformed PDF Eq.(41) is the computation of the parameter a (i.e. parameter of the variable transformation Eq.(33)). Computation of the optimal value of a by Eq.(37) is a numerically intensive task that not an issue regarding the precomputation phase. However, one needs to compute the proper values of a during the simulation after each sampling of u from $q^{2+}(s,\lambda,a,A;u)$ in order to be able to apply the proper inverse transformation Eq.(34) that delivers the corresponding sampled $\mu = \cos(\theta)$ according to $F(s;\mu)_{GS}^{2+}$ given by Eq.(15). One can replace the computation of the optimal a (Eq.(37)) by an approximation of the corresponding w^2 values in the $A \to 0$ case [7]

$$\frac{\tilde{w}^2}{0.5(s/\lambda)+2} = \begin{cases} 1.347 + t(0.209364 - t(0.45525 - t(0.50142 - t0.081234))) & \text{if } \lambda < 10 \\ -2.77164 + t(2.94874 - t(0.1535754 - t0.00552888)) & \text{otherwise} \end{cases} \tag{43}$$

where $t = \ln(s/\lambda)$. Then corresponding approximate value of a can be computed by $\tilde{a} = \tilde{w}^2 A$ both for the pre-computation of $q^{2+}(s,\lambda,\tilde{a},A;u)$ and run time. The parameter $\tilde{a}$ won't be as optimal as the one obtained by the exact computation but will be very close to that especially in case of small values of A i.e. at high energies when the non-transformed distributions $F(s;\mu)^{2+}_{GS}$ strongly peaked to the forward direction.

The optimal value of the parameter a of the variable transformation Eq.(33) computed by Eq.(37) is shown together with the corresponding approximate values $\tilde{a}$ for some selected s/λ (mean number of elastic events) and $G_1 s/\lambda$ values in Table 1-4. The corresponding optimal $q^{2+}(s,\lambda,a,A;u)$ and approximately optimal $q^{2+}(s,\lambda,\tilde{a},A;u)$ transformed PDFs are shown in Fig. 1. Note, that when the screened Rutherford DCS is used and both s/λ and $G_1 s/\lambda$ are given, the corresponding screening parameter A is determined by Eq.(22) and can be obtained through the numerical solution of Eq.(22) for the given value of G_1. Therefore, one can determine A if s/λ and $G_1 s/\lambda$ are given then either a or $\tilde{a} = \tilde{w}^2 A$ can be computed by using Eq.(37) or Eq.(43) respectively. Then the corresponding optimal $q^{2+}(s,\lambda,a,A;u)$ or approximately optimal $q^{2+}(s,\lambda,\tilde{a},A;u)$ transformed PDF can be calculated by means of Eq.(41).

2.3.4 Screening parameter

When elastic scattering is described by the screened Rutherford DCS, the screening parameter A given by Eq.(18) plays an essential role. The screening radius R can be estimated from the Thomas-Fermi model of atom that gives

$$R = C_{TF}\frac{a_0}{Z^{1/3}} \tag{44}$$

where a_0 is the Bohr radius

$$a_0 = \hbar/(m_e c\alpha) \tag{45}$$

with $\hbar$, m_e, c, α reduced Planck constant, electron rest mass, speed of light and fine structure constant and C_{TF} is the Thomas-Fermi constant

$$C_{TF} \equiv \frac{(3\pi)^{\frac{2}{3}}}{2^{\frac{7}{3}}} \approx 0.88534 \tag{46}$$

Substituting Eq.(44) into Eq.(18) and using the above expression for the Bohr radius yields

$$A^{(TF)} = \frac{m_e^2 c^2 \alpha^2 Z^{2/3}}{4pC_{TF}^2} = \frac{(m_e c^2)^2 \alpha^2 Z^{2/3}}{4(pc)^2 C_{TF}^2} \tag{47}$$

Moliere derived the DCS for elastic scattering based on a Thomas-Fermi potential and applying WKB-expansion to the radial equation without making use of the Born approximation [10]. Then he derived a correction to $A^{(TF)}$ by fitting the average scattering angle squared computed from the screened Rutherford DCS to that resulted from his DCS and he finally obtained

$$A^{(M)} = A^{(TF)}\left[1.13 + 3.76\left(\frac{\alpha Z}{\beta}\right)^2\right] \tag{48}$$

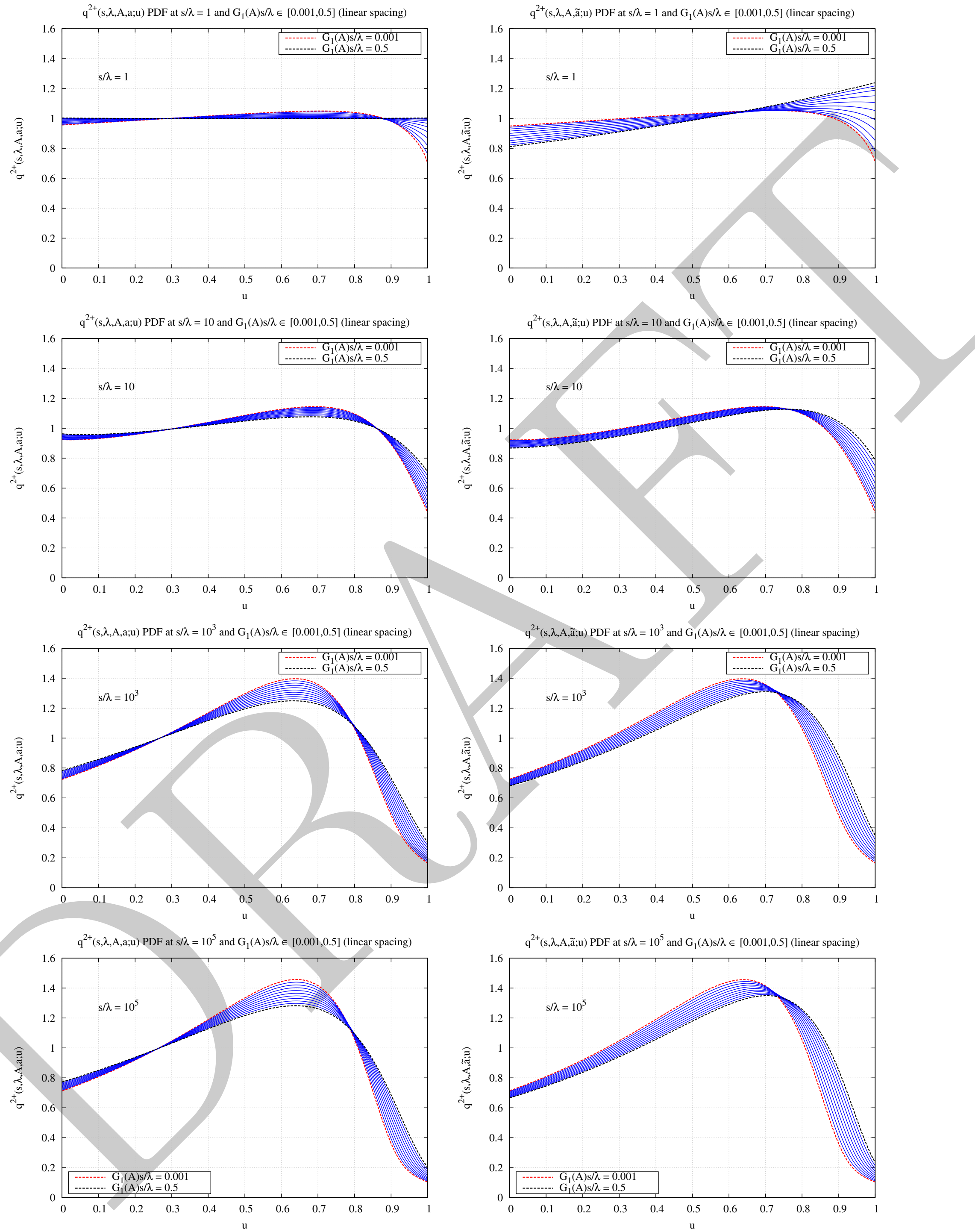

Figure 1: $q^{2+}(s, \lambda, a, A; u)$ (left) and $q^{2+}(s, \lambda, \tilde{a}, A; u)$ transformed PDFs that correspond to the parameter values shown in Table 1-4.

The corresponding inverse elastic mean free path for electron or positron incident can be given by Eq.(8) using Eq.(19) with $A = A^{(M)}$ that results in

$$\lambda^{-1} = \mathcal{N}\sigma^{(SR)} = \mathcal{N}\left(\frac{Ze^2}{pc\beta}\right)^2 \frac{\pi}{A^{(M)}(1+A^{(M)})} = \mathcal{N}\frac{Z^2 r_0^2 (m_e c^2)^2 \pi}{(pc)^2\beta^2 A^{(M)}(1+A^{(M)})} \tag{49}$$

where $\mathcal{N} = \rho\mathcal{N}_{\mathcal{A}}/M = \rho/(uA_M)$ is the number of atoms per unit volume (ρ is the density of the material, $\mathcal{N}_{\mathcal{A}}$ is the Avogadro number, M is the molar mass, $u = M_u/\mathcal{N}_{\mathcal{A}}$ is the atomic mass unit, $M_u = 1$ [g/mol] is the molar mass constant and A_M is the relative atomic mass) and $e^2 = r_0 m_e c^2$ was used with r_0 being the classical electron radius. Replacing Z^2 by $Z(Z+1)$ in order to take into account scattering by atomic electrons [11] one can write

$$\lambda^{-1}(1+A^{(M)}) = \frac{\rho Z(Z+1) r_0^2 (m_e c^2)^2 \pi}{(pc)^2\beta^2 u A_M A^{(M)}} = \frac{1}{\beta^2}\frac{4\pi r_0^2 C_{TF}^2}{\alpha^2 u 1.13}\frac{\rho}{A_M}\frac{Z^{1/3}(Z+1)}{1+3.33\left(\frac{\alpha Z}{\beta}\right)^2} \approx \frac{b_c^*}{\beta^2} \tag{50}$$

where the material dependent parameter

$$b_c^* = \frac{4\pi r_0^2 C_{TF}^2}{\alpha^2 u 1.13}\frac{\rho}{A_M}\frac{Z^{1/3}(Z+1)}{1+3.33(\alpha Z)^2} = 7827.68\left[\frac{\mathrm{cm}^2}{\mathrm{g}}\right]\frac{\rho}{A_M}\frac{Z^{1/3}(Z+1)}{1+3.33(\alpha Z)^2} \tag{51}$$

with $1/\alpha = 137.0356$, $r_0 = 2.81794\times10^{-13}$ [cm], $u = 1.660538\times10^{-24}$ [g] and C_{TF} as given by Eq.(46) was used and β^2 was neglected. According to Eq.(48), $A^{(M)}$ can be expressed by using this material dependent b_c^* parameter as

$$A^{(M)} = \frac{1}{4(pc)^2}\frac{1}{b_c^*}\chi_{cc}^{*2} \tag{52}$$

where

$$\chi_{cc}^{*2} = \frac{4\pi r_0^2 (m_e c^2)^2}{u}\frac{\rho}{A_M}Z(Z+1) = 0.156914\left[\frac{\mathrm{cm}^2\mathrm{MeV}^2}{\mathrm{g}}\right]\frac{\rho}{A_M}Z(Z+1) \tag{53}$$

is also a material dependent parameter ($m_e c^2 = 0.510998$ [MeV]).

Moliere's screening angle χ_α [10] for mixtures was derived in [12] based on the corresponding expression given by Scott [13]. Moliere's screening parameter for mixtures that consist of N_e elements with having n_i the proportion by number of element Z_i can be written as [12]

Our starting point is Eq. (2.14.43) from [12]

$$\ln\chi_\alpha^2 = \frac{\sum_i^{N_e} n_i Z_i (Z_i+\xi_e)\ln\chi_{\alpha_i}^2}{\sum_i^{N_e} n_i Z_i(Z_i+\xi_e)} \tag{54}$$

where χ_α is Moliere's screening angle (the screening parameter is $A^{(M)} = \chi_\alpha^2/4$) of the compound that builds up from N_e elements, χ_{α_i} are the screening angles characterising the $i-th$ components with corresponding atomic number Z_i and n_i is the proportion by number of the $i-th$ atom ($n_i = \rho\mathcal{N}_{\mathcal{A}}/M_i = \rho/(uA_{M_i})$ (Note, that Z^2 is replaced by $Z(Z+\xi_e)$ with $\xi_e \in [0,1]$ to account scattering from sub-threshold inelastic events). The individual Moliere's screening angles are expressed in terms of the corresponding Thomas-Fermi screening angle χ_{0_i} as

$$\ln \chi^2_{\alpha_i} = \ln \chi^2_{0_i} + \ln \left[1.13 + 3.76(\alpha Z_i)^2\right] \tag{55}$$

(where the $1/\beta^2$ part was dropped from the last term similarly to Eq.(51)). The Thomas-Fermi screening angle for the $i-th$ components with atomic number Z_i is

$$\ln \chi^2_{0_i} = \ln \left[\frac{(m_e c^2)^2 \alpha^2}{(pc)^2 C^2_{TF} Z_i^{-2/3}}\right] = \ln \left[\frac{(m_e c^2)^2 \alpha^2}{(pc)^2 C^2_{TF}}\right] - \ln Z_i^{-2/3} \tag{56}$$

and the second term can be written as

$$\ln \left[1.13 + 3.76(\alpha Z_i)^2\right] = \ln 1.13 \left[1 + 3.34(\alpha Z_i)^2\right] = \ln 1.13 + \ln \left[1 + 3.34(\alpha Z_i)^2\right] \tag{57}$$

Substituting these two equations back into Eq.(55) one can get

$$\ln \chi^2_{\alpha_i} = \ln \left[\frac{(m_e c^2)^2 \alpha^2}{(pc)^2 C^2_{TF}}\right] - \ln Z_i^{-2/3} + \ln 1.13 + \ln \left[1 + 3.34(\alpha Z_i)^2\right] = \ln \left[\frac{(m_e c^2)^2 \alpha^2 1.13}{(pc)^2 C^2_{TF}}\right] - \ln Z_i^{-2/3} + \ln \left[1 + 3.34(\alpha Z_i)^2\right] \tag{58}$$

Inserting this expression to the component wise screening angles into Eq.(54) one can get

$$\begin{aligned}
\ln \chi^2_{\alpha} &= \frac{\sum_i^{N_e} n_i Z_i (Z_i+\xi_e) \left\{\ln \left[\frac{(m_e c^2)^2 \alpha^2 1.13}{(pc)^2 C^2_{TF}}\right] - \ln Z_i^{-2/3} + \ln \left[1 + 3.34(\alpha Z_i)^2\right]\right\}}{\sum_i^{N_e} n_i Z_i (Z_i+\xi_e)} \\
&= \ln \left[\frac{(m_e c^2)^2 \alpha^2 1.13}{(pc)^2 C^2_{TF}}\right] + \frac{\sum_i^{N_e} n_i Z_i (Z_i+\xi_e) \left\{- \ln Z_i^{-2/3} + \ln \left[1 + 3.34(\alpha Z_i)^2\right]\right\}}{\sum_i^{N_e} n_i Z_i (Z_i+\xi_e)} \\
&= \ln \left[\frac{(m_e c^2)^2 \alpha^2 1.13}{(pc)^2 C^2_{TF}}\right] + \frac{\sum_i^{N_e} n_i Z_i (Z_i+\xi_e) \ln \left[1 + 3.34(\alpha Z_i)^2\right]}{\sum_i^{N_e} n_i Z_i (Z_i+\xi_e)} - \frac{\sum_i^{N_e} n_i Z_i (Z_i+\xi_e) \ln Z_i^{-2/3}}{\sum_i^{N_e} n_i Z_i (Z_i+\xi_e)}
\end{aligned} \tag{59}$$

Then using the relation $A^{(M)} = \chi^2_\alpha/4$ between the screening parameter and screening angle, Moliere's screening parameter for compounds can be written as

$$\begin{aligned}
A^{(M)} =& \frac{\chi^2_\alpha}{4} \\
=& \left[\frac{(m_e c^2)^2 \alpha^2 1.13}{4(pc)^2 C^2_{TF}}\right] \exp \left[\frac{\sum_i^{N_e} n_i Z_i (Z_i+\xi_e) \left\{- \ln Z_i^{-2/3} + \ln \left[1 + 3.34(\alpha Z_i)^2\right]\right\}}{\sum_i^{N_e} n_i Z_i (Z_i+\xi_e)}\right] \\
=& \left[\frac{(m_e c^2)^2 \alpha^2 1.13}{4(pc)^2 C^2_{TF}}\right] \frac{\exp \left[\frac{\sum_i^{N_e} n_i Z_i (Z_i+\xi_e) \ln \left[1+3.34(\alpha Z_i)^2\right]}{\sum_i^{N_e} n_i Z_i (Z_i+\xi_e)}\right]}{\exp \left[\frac{\sum_i^{N_e} n_i Z_i (Z_i+\xi_e) \ln Z_i^{-2/3}}{\sum_i^{N_e} n_i Z_i (Z_i+\xi_e)}\right]} \\
=& \left[\frac{(m_e c^2)^2 \alpha^2 1.13}{4(pc)^2 C^2_{TF}}\right] \frac{\exp \left[\frac{Z_X}{Z_S}\right]}{\exp \left[\frac{Z_E}{Z_S}\right]}
\end{aligned} \tag{60}$$

by using the notations given in Eqs.(63)

$$A^{(M)} = \frac{\chi_\alpha^2}{4} = \left[\frac{(m_ec^2)^2\alpha^2 1.13}{4(pc)^2 C_{TF}^2}\right] \exp\left[\frac{\sum_i^{N_e} n_i Z_i(Z_i+\xi_e)\left\{-\ln Z_i^{-2/3} + \ln\left[1+3.34(\alpha Z_i)^2\right]\right\}}{\sum_i^{N_e} n_i Z_i(Z_i+\xi_e)}\right] \tag{61}$$

according to the $A^{(M)} = \chi_\alpha^2/4$ relation between the screening parameter and the corresponding Moliere's screening angle. Notice that the $1/\beta^2$ in Eq.(48) is also neglected in Eq.(61). Furthermore, $Z(Z+1)$ has been changed to $Z(Z+\xi_e)$ where $\xi_e \in [0,1]$. Note, that Z^2 was previously change to $Z(Z+1)$ in order to take into account scattering from atomic electrons. However, in a usual simulation deflections due to scattering from atomic electrons that results in discrete delta ray are already taken into account. Therefore, keeping $\xi_e = 1$ would lead to double counting of the deflections due these above-production cut discrete secondary electron generations. ξ_e should be chosen such that only the sub-production cut angular deflections are included in the multiple scattering part thus ξ_e depends on the production cut. On the other hand, ξ_e should be zero if angular defections due sub-production cut interactions. See more a detailed discussion in [14].

Eq.(61) can be written in the more compact form

$$A^{(M)} = \frac{\chi_\alpha^2}{4} = \frac{(m_ec^2)^2\alpha^2 1.13}{4(pc)^2 C_{TF}^2}\frac{\exp(Z_X/Z_S)}{\exp(Z_E/Z_S)} \tag{62}$$

by introducing [12]

$$\begin{aligned}
Z_S &= \sum_{i=1}^{N_e} n_i Z_i(Z_i+\xi_e) \\
Z_E &= \sum_{i=1}^{N_e} n_i Z_i(Z_i+\xi_e)\ln Z_i^{-2/3} \\
Z_X &= \sum_{i=1}^{N_e} n_i Z_i(Z_i+\xi_e)\ln\left[1+3.33\alpha^2 Z_i^2)\right] \\
A &= \sum_{i=1}^{N_e} n_i A_i
\end{aligned} \tag{63}$$

where n_i is the fraction of the $i-th$ atom in the compound by number n_i = number-of-atoms-per-unit-volume$_i$ per total number of atoms per volume. (Note, that only the ratios are important since a possible constant term will be cancelled later: (i) Z_X/Z_S and Z_E/Z_S will appear in Z-s; (ii) b_c, χ_{cc}^2 will contain a Z_S/A term where $A = \sum_i n_i A_i$ relative molecular mass with A_i being the molar mass of the $i-th$ atom).

NOTE: If we have an element wise correction parameter κ_i to Moliere's screening parameters $A_i^{(M)}$ such that $A_i^{(M_{corr})} = \kappa_i A_i^{(M)}$then one can use Eq.(54) to obtain the corrected screening parameter for a compound

$$A^{(M_{corr})} = \frac{(m_e c^2)^2 \alpha^2}{4(pc)^2 C_{TF}^2} \exp\left[\frac{\sum_i^{N_e} n_i Z_i (Z_i + \xi_e) \ln[\kappa_i Z_i^{2/3}(1.13 + 3.76(\alpha Z_i)^2)]}{\sum_i^{N_e} n_i Z_i (Z_i + \xi_e)}\right] \tag{64}$$

Similarly to Eq.(50), in case of mixtures

$$\lambda^{-1}(1 + A^{(M)}) \approx \frac{b_c}{\beta^2} \tag{65}$$

where the material dependent parameter now

$$b_c = 7827.68 \left[\frac{\mathrm{cm}^2}{\mathrm{g}}\right] \frac{\rho Z_S}{A} \frac{\exp(Z_E/Z_S)}{\exp(Z_X/Z_S)} \tag{66}$$

According to Eq.(62), $A^{(M)}$ for mixtures can be expressed by using this material dependent b_c parameter as

$$A^{(M)} = \frac{1}{4(pc)^2} \frac{1}{b_c} \chi_{cc}^2 \tag{67}$$

where now

$$\chi_{cc}^2 = 0.156914 \left[\frac{\mathrm{cm}^2 \mathrm{MeV}^2}{\mathrm{g}}\right] \frac{\rho Z_S}{A} \tag{68}$$

. Meg ξ_e rol szolni kell Egy szo arrol, ha mass fraction-nal van megadva a material aztan mit hasznalunk es hogyan. Aztan PWA.

3 some

In theory, the most accurate multiple scattering distribution can be obtained by using the most accurate single scattering DCSs derived from partial wave analysis in the Goudsmit-Saunderson angular distribution. However, in order to be able to obtain the necessary angular distributions on-the-fly one should store a high number (high order to get proper convergence even for short steps) of transport mean free path as a function of the energy and one should sum up the Legendre series at each steps. This would lead to an unaffordable numerical effort at each step.

step. One of the biggest advantage of the GS distribution is that Particle transport Monte Carlo simulation codes that applies multiple scattering theory to model elastic scattering of electrons in the course of their transport in complex geometry systems need to .... The employed multiple scattering theory needs to provide accurate description of the angular distribution of electrons as a function of the travelled path length.

Appendix A Angular distribution

A.1 Goudsmit-Saunderson series

First the single scattering distribution, given by Eq.(2), will be expressed in terms of Legendre polynomials. Legendre polynomials form a *complete orthogonal system* on $\{-1,+1\}$ where orthogonality is

$$\int_{-1}^{1} P_\ell(x)P_k(x)\mathrm{d}x = \begin{cases} C_\ell = \frac{2}{2\ell+1} & \text{if } \ell = k \\ 0 & \text{if } \ell \neq k \end{cases} \tag{A.1}$$

and completeness means that for any $f(x)$ continuous functions on $\{-1,+1\}$

$$\lim_{\ell\to\infty} E_\ell(a_0,\cdots,a_\ell) \equiv \lim_{\ell\to\infty} ||f(x) - \sum_\ell a_\ell P_\ell(x)||^2 = 0 \tag{A.2}$$

i.e. the least square error E_ℓ converges to zero. So any $f(x)$ function on $\{-1,+1\}$ can be written as

$$f(x) = \sum_{\ell=0}^{\infty} a_\ell P_\ell(x) \tag{A.3}$$

where the a_ℓ coefficients can be derived by multiplying both side by $P_k(x)$, integrating both side over x while using the orthogonality property of the Legendre polynomials that yields

$$a_\ell = \frac{2\ell+1}{2}\int_{-1}^{+1} P_\ell(x)f(x)\mathrm{d}x \tag{A.4}$$

Therefore, the single scattering distribution $f_1(\theta)$ can be written as

$$f_1(\cos(\theta)) = \sum_{\ell=0}^{\infty} a_\ell P_\ell(\cos(\theta)) \tag{A.5}$$

where the coefficients are

$$\begin{aligned} a_\ell =& \frac{2\ell+1}{2}\int_{-1}^{1} f_1(\cos(\theta))P_\ell(\cos(\theta))\mathrm{d}\cos(\theta) = \frac{2\ell+1}{4\pi}\overbrace{\int_{-1}^{1} \underbrace{2\pi f_1(\cos(\theta))}_{p(\cos(\theta))\leftarrow Eq.(3)} P_\ell(\cos(\theta))\mathrm{d}\cos(\theta)}^{\langle P_\ell(\cos(\theta))\rangle = F_\ell} \\ =& \frac{2\ell+1}{4\pi}F_\ell = \frac{2\ell+1}{4\pi}\langle P_\ell(\cos(\theta))\rangle \end{aligned} \tag{A.6}$$

and using them

$$f_1(\cos(\theta)) = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{4\pi} F_\ell P_\ell(\cos(\theta)) \tag{A.7}$$

The second step is to obtain the expression for $f_{n>1}(\cos(\theta))$ i.e. angular distribution of particles after $n > 1$ elastic interactions. The angular distribution after $n = 2$ elastic interaction will be derived first. Suppose that the particle was originally moving into the $\hat{\vec{z}}$ direction and the first interaction resulted θ_1, ϕ_1 with corresponding direction of $\hat{\vec{d}}_1$ while the second θ_2, ϕ_2. In order to get a direction $\hat{\vec{d}}$ defined by θ, ϕ after the second interaction

$$
\begin{aligned}
\cos(\theta_2) =& \hat{\vec{d}}_1^{\,T} \hat{\vec{d}} \\
=& [\sin(\theta_1)\cos(\phi_1), \sin(\theta_1)\sin(\phi_1), \cos(\theta_1)] \begin{bmatrix} \sin(\theta)\cos(\phi) \\ \sin(\theta)\sin(\phi) \\ \cos(\theta) \end{bmatrix} \\
=& \cos(\theta)\cos(\theta_1) + \sin(\theta)\sin(\theta_1) \underbrace{[\cos(\phi_1)\cos(\phi) + \sin(\phi_1)\sin(\phi)]}_{\cos(\phi_1-\phi)} \\
=& \cos(\theta)\cos(\theta_1) + \sin(\theta)\sin(\theta_1)\cos(\phi_1 - \phi)
\end{aligned} \tag{A.8}
$$

must be fulfilled. The probability of finding the particle after two interactions moving into the solid angle element $\mathrm{d}\omega$ around the direction $\hat{\vec{d}}$ defined by θ ϕ

$$
f_{n=2}(\theta)\mathrm{d}\omega = \int_0^{\pi}\int_0^{2\pi} f_1(\theta_1) f_1(\theta_2)\sin(\theta_1)\mathrm{d}\phi_1\mathrm{d}\theta_1 \underbrace{\sin(\theta)\mathrm{d}\theta\mathrm{d}\phi}_{\mathrm{d}\omega} \tag{A.9}
$$

and

$$
\begin{aligned}
f_{n=2}(\cos(\theta)) &= \int_{-1}^{+1}\int_0^{2\pi} f_1(\cos(\theta_1)) f_1(\cos(\theta_2))\mathrm{d}\phi_1\mathrm{d}(\cos(\theta_1)) \\
&= \int_{-1}^{+1}\int_0^{2\pi} \left[\sum_{\ell=0}^{\infty} \frac{2\ell+1}{4\pi} F_\ell P_\ell(\cos(\theta_1))\right]\left[\sum_{\ell'=0}^{\infty} \frac{2\ell'+1}{4\pi} F_{\ell'} P_{\ell'}(\cos(\theta_2))\right]\mathrm{d}\phi_1\mathrm{d}(\cos(\theta_1))
\end{aligned} \tag{A.10}
$$

(note that F_k is $\langle P_k(\cos(\chi))\rangle$ in a single interaction). To make the next step one need to use the requirement for $\cos(\theta_2)$ given by Eq.(A.8) and the corresponding result from the addition theorem for spherical harmonics i.e.

$$
P_\ell(\cos(\theta_2)) = P_\ell(\cos(\theta))P_\ell(\cos(\theta_1)) + 2\sum_{m=1}^{\ell} \frac{(\ell-m)!}{(\ell+m)!} P_\ell^m(\theta,\phi) P_\ell^m(\theta_1,\phi_1)\cos[m(\phi-\phi_1)] \tag{A.11}
$$

The addition theorem of spherical harmonics says that if

$$
\cos(\theta_2) \equiv \cos(\theta)\cos(\theta_1) + \sin(\theta)\sin(\theta_1)\cos(\phi_1 - \phi) \tag{A.12}
$$

then

$$P_\ell(\cos(\theta_2)) = \frac{4\pi}{2\ell+1}\sum_{m=-\ell}^{\ell} Y_\ell^m(\theta,\phi){Y_\ell^*}^m(\theta_1,\phi_1) \tag{A.13}$$

One can use:
the associated Legendre polynomials:

$$P_\ell^{-m}(x) = (-1)^m \frac{(\ell-m)!}{(\ell+m)!}P_\ell^m(x) \tag{A.14}$$

the spherical harmonics

$$Y_\ell^m(\theta,\phi) = \sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}P_\ell^m(\cos(\theta))\exp(im\phi) \tag{A.15}$$

and the complex conjugate of the spherical harmonics

$$\begin{aligned}{Y_\ell^*}^m(\theta,\phi) =&(-1)^m Y_\ell^{-m}(\theta,\phi) = (-1)^m\sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell+m)!}{(\ell-m)!}}P_\ell^{-m}(\cos(\theta))\exp(-im\phi)\\ =&(-1)^m\sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell+m)!}{(\ell-m)!}}(-1)^m\frac{(\ell-m)!}{(\ell+m)!}P_\ell^m(\cos(\theta))\exp(-im\phi)\end{aligned} \tag{A.16}$$

to plug in these into Eq.(A.13)

$$\begin{aligned}P_\ell(\cos(\theta_2)) =&\frac{4\pi}{2\ell+1}\sum_{m=-\ell}^{\ell} Y_\ell^m(\theta,\phi){Y_\ell^*}^m(\theta_1,\phi_1) = \frac{4\pi}{2\ell+1}\sum_{m=-\ell}^{\ell}\left\{\sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}P_\ell^m(\cos(\theta))\exp(im\phi)\right.\\ &\left.(-1)^{2m}\sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell+m)!}{(\ell-m)!}}\frac{(\ell-m)!}{(\ell+m)!}P_\ell^m(\cos(\theta_1))\exp(-im\phi_1)\right\}\\ =&\sum_{m=-\ell}^{\ell}\frac{(\ell-m)!}{(\ell+m)!}P_\ell^m(\cos(\theta))P_\ell^m(\cos(\theta_1))\exp(im(\phi-\phi_1))\\ =&\underbrace{P_\ell(\cos(\theta))P_\ell(\cos(\theta_1))}_{m=0\text{ case}} + \sum_{m=-\ell}^{-1}\frac{(\ell-m)!}{(\ell+m)!}P_\ell^m(\cos(\theta))P_\ell^m(\cos(\theta_1))\exp(im(\phi-\phi_1))\\ &+\sum_{m=1}^{\ell}\frac{(\ell-m)!}{(\ell+m)!}P_\ell^m(\cos(\theta))P_\ell^m(\cos(\theta_1))\exp(im(\phi-\phi_1))\\ =&P_\ell(\cos(\theta))P_\ell(\cos(\theta_1)) + \sum_{m=1}^{\ell}\frac{(\ell+m)!}{(\ell-m)!}P_\ell^{-m}(\cos(\theta))P_\ell^{-m}(\cos(\theta_1))\exp(-im(\phi-\phi_1))\\ &+\sum_{m=1}^{\ell}\frac{(\ell-m)!}{(\ell+m)!}P_\ell^m(\cos(\theta))P_\ell^m(\cos(\theta_1))\exp(im(\phi-\phi_1))\\ =&P_\ell(\cos(\theta))P_\ell(\cos(\theta_1)) + \sum_{m=1}^{\ell}\frac{(\ell+m)!}{(\ell-m)!}\underbrace{(-1)^m\frac{(\ell-m)!}{(\ell+m)!}P_\ell^m(\cos(\theta))}_{P_\ell^{-m}(\cos(\theta))}\\ &\underbrace{(-1)^m\frac{(\ell-m)!}{(\ell+m)!}P_\ell^m(\cos(\theta_1))}_{P_\ell^{-m}(\cos(\theta_1))}\exp(-im(\phi-\phi_1))\end{aligned} \tag{A.17}$$

$$
\begin{aligned}
&+\sum_{m=1}^{\ell}\frac{(\ell-m)!}{(\ell+m)!}P_\ell^m(\cos(\theta))P_\ell^m(\cos(\theta_1))\exp(im(\phi-\phi_1))\\
=&P_\ell(\cos(\theta))P_\ell(\cos(\theta_1))+\sum_{m=1}^{\ell}\frac{(\ell-m)!}{(\ell+m)!}P_\ell^m(\cos(\theta))P_\ell^m(\cos(\theta_1))\exp(-im(\phi-\phi_1))\\
&+\sum_{m=1}^{\ell}\frac{(\ell-m)!}{(\ell+m)!}P_\ell^m(\cos(\theta))P_\ell^m(\cos(\theta_1))\exp(im(\phi-\phi_1))\\
=&P_\ell(\cos(\theta))P_\ell(\cos(\theta_1))+\sum_{m=1}^{\ell}\frac{(\ell-m)!}{(\ell+m)!}P_\ell^m(\cos(\theta))P_\ell^m(\cos(\theta_1))\left\{\underbrace{\exp[-im(\phi-\phi_1)]+\exp[im(\phi-\phi_1)]}_{2\cos[m(\phi-\phi_1)]}\right\}\\
=&P_\ell(\cos(\theta))P_\ell(\cos(\theta_1))+2\sum_{m=1}^{\ell}\frac{(\ell-m)!}{(\ell+m)!}P_\ell^m(\cos(\theta))P_\ell^m(\cos(\theta_1))\cos[m(\phi-\phi_1)]
\end{aligned}
$$

Substituting Eq.(A.11) into Eq.(A.10) yields one can get

$$
\begin{aligned}
f_{n=2}(\cos(\theta)) = \int_{-1}^{+1}\int_{0}^{2\pi}&\left[\sum_{\ell=0}^{\infty}\frac{2\ell+1}{4\pi}F_\ell P_\ell(\cos(\theta_1))\right]\left[\sum_{\ell'=0}^{\infty}\frac{2\ell'+1}{4\pi}F_{\ell'}P_{\ell'}(\cos(\theta))P_{\ell'}(\cos(\theta_1))\right.\\
&\left.+2\sum_{m=1}^{\ell'}\frac{(\ell'-m)!}{(\ell'+m)!}P_{\ell'}^m(\cos(\theta))P_{\ell'}^m(\cos(\theta_1))\cos[m(\phi-\phi_1)]\right]\mathrm{d}\phi_1\mathrm{d}(\cos(\theta_1))
\end{aligned}
\tag{A.18}
$$

Carrying out the integration over ϕ_1 all the contributions coming from the last term will disappear. What remains is

$$
f_{n=2}(\cos(\theta)) = 2\pi\int_{-1}^{+1}\left[\sum_{\ell=0}^{\infty}\frac{2\ell+1}{4\pi}F_\ell P_\ell(\cos(\theta_1))\right]\left[\sum_{\ell'=0}^{\infty}\frac{2\ell'+1}{4\pi}F_{\ell'}P_{\ell'}(\cos(\theta))P_{\ell'}(\cos(\theta_1))\right]\mathrm{d}(\cos(\theta_1))
\tag{A.19}
$$

Using the orthogonality of the Legendre polynomials on the $\{-1,+1\}$ interval (i.e. only the terms $\ell=\ell'$ will give non-zero contribution to the sum of integrals)

$$
\begin{aligned}
f_{n=2}(\cos(\theta)) =& 2\pi\sum_{\ell=0}^{\infty}\left(\frac{2\ell+1}{4\pi}\right)^2(F_\ell)^2P_\ell(\cos(\theta))\underbrace{\int_{-1}^{1}P_\ell(\cos(\theta_1))P_\ell(\cos(\theta_1))\mathrm{d}\cos(\theta_1)}_{2/(2\ell+1)}\\
=&\sum_{\ell=0}^{\infty}\frac{2\ell+1}{4\pi}(F_\ell)^2P_\ell(\cos(\theta))
\end{aligned}
\tag{A.20}
$$

and in general after n elastic interactions the angular distribution

$$
f_n(\cos(\theta)) = \sum_{\ell=0}^{\infty}\frac{2\ell+1}{4\pi}(F_\ell)^n P_\ell(\cos(\theta))
\tag{A.21}
$$

A.2 The screened Rutherford DCS

The screened Rutherford DCS for elastic scattering and the corresponding expressions for elastic scattering cross section, single scattering distribution, transport coefficients will be derived in this section. The screened Rutherford DCS can be obtained by solving the scattering equation under the first Born approximation using a simple exponentially screened Coulomb potential as scattering potential.

The differential elastic scattering cross section $\mathrm{d}\sigma/\mathrm{d}\Omega$ can be expressed by the scattering amplitude $f(\theta,\phi)$ as

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = |f|^2 \quad \sigma = \int \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\mathrm{d}\Omega \tag{A.22}$$

The scattering amplitude in the first Born approximation can be written as

$$f_{B1}(\theta,\phi) = -\frac{2m}{4\pi\hbar^2}\int e^{i(\bar{k}_f-\bar{k}_i)\bar{r}'}V(\bar{r}')\mathrm{d}^3r' \tag{A.23}$$

where $\bar{k}_i$ is the wave vector of the incident plane wave, $\bar{k}_f$ is the wave vector of the outgoing (scattered) spherical wave. Note that in elastic scattering $k_i = k_f \equiv k$. Furthermore, $\hbar\bar{q} = \hbar(\bar{k}_f - \bar{k}_i)$ is the momentum transfer and $q^2 = |\bar{k}_f - \bar{k}_i|^2 = 2k^2(1-\cos(\theta)) = 2k^2(2\sin^2(\theta/2))$ where $\theta = \angle(\bar{k}_i, \bar{k}_f)$ is the scattering angle. Let assume $V(\bar{r}) \equiv V(r)$ i.e. spherically symmetric scattering potential and substitute $\bar{q} = \bar{k}_f - \bar{k}_i$ by choosing the coordinate system for the integration such that $\bar{q} = q\hat{\bar{z}}$

$$\begin{aligned}
f_{B1}(\theta) &= -\frac{2m}{4\pi\hbar^2}\int_0^\infty\int_0^\pi\int_0^{2\pi} e^{iqr'\cos(\theta')}V(r')\mathrm{d}\phi'\sin(\theta')\mathrm{d}\theta' r'^2\mathrm{d}r \\
&= -\frac{2m}{4\pi\hbar^2}2\pi\int_0^\infty\int_0^\pi e^{iqr'\cos(\theta')}V(r')\sin(\theta')\mathrm{d}\theta' r'^2\mathrm{d}r' \\
&= -\frac{2m}{4\pi\hbar^2}2\pi\int_0^\infty\left[-\frac{e^{iqr'\cos(\theta')}}{iqr'}\right]_0^\pi V(r')r'^2\mathrm{d}r' \\
&= -\frac{2m}{4\pi\hbar^2}2\pi\int_0^\infty\frac{2\sin(qr')}{qr'}V(r')r'^2\mathrm{d}r' \\
&= -\frac{2m}{q\hbar^2}\int_0^\infty\sin(qr')r'V(r')\mathrm{d}r'
\end{aligned} \tag{A.24}$$

where $(\exp(ix) - \exp(-ix))/2i = \sin(x)$ was used to get $2\sin(qr')/qr'$. Using a simple exponentially screened Coulomb potential as a scattering potential

$$V(r) = \frac{ZZ'e^2}{r}e^{-r/R} \tag{A.25}$$

with a screening radius R (target atomic number of Z and projectile charge $Z'e$)

$$\begin{aligned}
f_{B1}(\theta) &= -\frac{2m}{q\hbar^2} ZZ'e^2 \int_0^\infty \sin(qr')e^{-r'/R}\mathrm{d}r' \\
&= -\frac{2m}{q\hbar^2} ZZ'e^2 \left[\frac{-Re^{-r'/R}[qr'\cos(qr') + \sin(qr')]}{q^2R^2+1}\right]_0^\infty \\
&= -\frac{2m}{q\hbar^2} ZZ'e^2 \left[\frac{R^2 q}{q^2R^2+1}\right] = -\frac{2m}{\hbar^2} ZZ'e^2 \left[\frac{1}{q^2+R^{-2}}\right] \\
&= -\frac{2m}{\hbar^2} ZZ'e^2 \left[\frac{1}{2k^2[1-\cos(\theta)+R^{-2}/(2k^2)]}\right]
\end{aligned} \tag{A.26}$$

where $q^2 = 2k^2(1-\cos(\theta))$ was used to obtain the last equation. The corresponding elastic DCS

$$\begin{aligned}
\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} &= |f_{B1}(\theta)|^2 = (ZZ'e^2)^2 \frac{4m^2}{\hbar^4 4k^4} \frac{1}{(1-\cos(\theta)+R^{-2}/(2k^2))^2} \\
&= \left(\frac{ZZ'e^2}{pc\beta}\right)^2 \frac{1}{(1-\cos(\theta)+R^{-2}/(2k^2))^2}
\end{aligned} \tag{A.27}$$

where $\hbar k = p$ and

$$\frac{4m^2}{\hbar^4 4k^4} = \left(\frac{2m}{\hbar^2 2k^2}\right)^2 = \left(\frac{2m}{\hbar^2 2p^2/\hbar^2}\right)^2 = \left(\frac{m}{p^2}\right)^2 = \left(\frac{mc^2}{p^2c^2}\right)^2 = \left(\frac{E_t}{p^2c^2}\right)^2 = \left(\frac{1}{pc\beta}\right)^2 \tag{A.28}$$

was used to obtain the last equation. One can introduce a *screening parameter* A such that

$$A \equiv \frac{1}{4}\left(\frac{\hbar}{p}\right)^2 R^{-2} \tag{A.29}$$

and since

$$\frac{1}{2k^2R^2} = \frac{1}{2(p/\hbar)^2R^2} = \frac{1}{2R^2}\left(\frac{\hbar}{p}\right)^2 = \frac{1}{2}\left(\frac{\hbar}{p}\right)^2 R^{-2} = 2A \tag{A.30}$$

the elastic DCS then can be written as

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \left(\frac{ZZ'e^2}{pc\beta}\right)^2 \frac{1}{(1-\cos(\theta)+2A)^2} \tag{A.31}$$

The total cross section then becomes

$$
\begin{aligned}
\sigma = \int \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\mathrm{d}\Omega &= \int_0^{\pi}\int_0^{2\pi}\left(\frac{ZZ'e^2}{pc\beta}\right)^2 \frac{1}{(1-\cos(\theta)+2A)^2}\mathrm{d}\phi\sin(\theta)\mathrm{d}\theta \\
&= \left(\frac{ZZ'e^2}{pc\beta}\right)^2 2\pi \int_0^{\pi} \frac{1}{(1-\cos(\theta)+2A)^2}\sin(\theta)\mathrm{d}\theta \\
&= \left(\frac{ZZ'e^2}{pc\beta}\right)^2 2\pi \left[\frac{1}{(\cos(\theta)-1-2A)}\right]_0^{\pi} \\
&= \left(\frac{ZZ'e^2}{pc\beta}\right)^2 2\pi \left[\frac{1}{2A}-\frac{1}{2+2A}\right] \\
&= \left(\frac{ZZ'e^2}{pc\beta}\right)^2 \frac{\pi}{A(1+A)}
\end{aligned}
\tag{A.32}
$$

and the single elastic scattering angular distribution

$$
\begin{aligned}
f_1(\theta) = \frac{1}{\sigma}\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} &= \left(\frac{pc\beta}{ZZ'e^2}\right)^2 \frac{A(1+A)}{\pi}\left(\frac{ZZ'e^2}{pc\beta}\right)^2 \frac{1}{(1-\cos(\theta)+2A)^2} \\
&= \frac{1}{\pi}\frac{A(1+A)}{(1-\cos(\theta)+2A)^2}
\end{aligned}
\tag{A.33}
$$

The corresponding ℓ-th transport coefficient G_ℓ [2]

$$
\begin{aligned}
G_\ell = 1 - F_\ell &= 1 - 2\pi\int_{-1}^{+1} f_1(\theta)P_\ell(\cos(\theta))\mathrm{d}(\cos(\theta)) \\
&= 1 - 2\pi\frac{1}{\pi}A(1+A)\int_{-1}^{+1}\frac{P_\ell(\cos(\theta))}{(1-\cos(\theta)+2A)^2}\mathrm{d}(\cos(\theta)) \\
&= 1 - \ell[Q_{\ell-1}(1+2A) - (1+2A)Q_\ell(1+2A)]
\end{aligned}
\tag{A.34}
$$

where $Q_\ell(x)$ are Legendre functions of the second kind.

The ℓ-th transport mean free path λ_ℓ with the ℓ-th transport coefficient G_ℓ is given by Eq.(7) and the elastic mean free path λ is by Eq.(8) that yields

$$
\lambda_\ell^{-1} = \frac{G_\ell}{\lambda} = \mathcal{N}\sigma G_\ell \tag{A.35}
$$

Substituting the total elastic cross section Eq.(A.32) into this expression

$$
\lambda_\ell^{-1(SR)} = \mathcal{N}G_\ell\left(\frac{ZZ'e^2}{pc\beta}\right)^2\frac{\pi}{A(1+A)} \tag{A.36}
$$

where the superscript SR indicates that the expression was derived by using a screened Rutherford DCS. In order to get the expression for the first transport mean free path, first one needs to derive the expression for the $G_{\ell=1}$ based on the screened Rutherford DCS of Eq.(A.34) at $\ell = 1$.

$$\begin{aligned} G_{\ell=1}^{(SR)} =& 1 - [Q_0(1+2A) - (1+2A)Q_1(1+2A)] \\ =& 2A\left[\ln\left(\frac{1+A}{A}\right)(A+1) - 1\right] \end{aligned} \tag{A.37}$$

by using the forms of the Legendre functions of the second kind $Q_0(x) = 0.5\ln((x+1)/(x-1))$ and $Q_1(x) = 0.5x\ln((x+1)/(x-1)) - 1$. Substituting this into the above expression for the first transport mean free path, one can get

$$\begin{aligned} \lambda_1^{-1(SR)} =& \mathcal{N}\left(\frac{ZZ'e^2}{pc\beta}\right)^2 \frac{\pi}{A(1+A)} 2A\left[\ln\left(\frac{1+A}{A}\right)(A+1) - 1\right] \\ =& \mathcal{N}\left(\frac{ZZ'e^2}{pc\beta}\right)^2 2\pi\left[\ln\left(\frac{1+A}{A}\right) - \frac{1}{1+A}\right] \end{aligned} \tag{A.38}$$

Then one can use this expression to determine the screening parameter A such that $\lambda_1^{(W)} = \lambda_1$ where λ_1 is the accurate first transport mean free path computed from PWA-DCS. Then using the Wentzel model with this screening parameter (that provides accurate $\lambda_1^{(W)} = \lambda_1$) in the Goudsmit-Saunderson series will give an angular distribution that mean is equal to that computed from accurate PWA-DCS (note that $\langle(\cos(\theta))\rangle_{GS} = \exp(-s/\lambda_1)$ i.e. depends only on the first transport mean free path). However, higher order moments (affected by the second transport mean free path as well) might be in error.

A.3 Optimal parameter of the variable transformation

The optimal value of the parameter a of the transformation Eq.(33) can be determined by plugging Eqs.(35,36) into Eq.(32) and soling for a:

$$
\begin{aligned}
0 =& \int_{-1}^{+1} \left[F(s;\mu)^{2+}_{GS}\left(-\frac{[1-\mu+2a]^2}{2a(1+a)}\right)\right]^2 \left[-2\frac{1-\mu(1+2a)}{[1-\mu+2a]^3}\right] \mathrm{d}\mu \\
=& \int_{-1}^{+1} \left[F(s;\mu)^{2+}_{GS}\right]^2 \left[\left(-\frac{[1-\mu+2a]}{4a^2(1+a)^2}\right)(-2(1-\mu(1+2a))\right] \mathrm{d}\mu \\
=& \sum_{\ell=0}^{\infty}(\ell+0.5)\xi_\ell(s,\lambda,A)\sum_{k=0}^{\infty}(k+0.5)\xi_k(s,\lambda,A)\int_{-1}^{+1}\left[-\frac{(1+2a)(1-\mu)^2}{2a^2(1+a)^2}+\frac{2\mu}{(1+a)^2}\right]\mathrm{d}\mu \\
=& -\frac{(1+2a)}{2a^2(1+a)^2}\underbrace{\left[\sum_{\ell=0}^{\infty}(\ell+0.5)\xi_\ell(s,\lambda,A)\sum_{k=0}^{\infty}(k+0.5)\xi_k(s,\lambda,A)\int_{-1}^{+1}P_\ell(\mu)P_k(\mu)(1-\mu)^2\mathrm{d}\mu\right]}_{\alpha} \\
&+\frac{2}{(1+a)^2}\underbrace{\left[\sum_{\ell=0}^{\infty}(\ell+0.5)\xi_\ell(s,\lambda,A)\sum_{k=0}^{\infty}(k+0.5)\xi_k(s,\lambda,A)\int_{-1}^{+1}P_\ell(\mu)P_k(\mu)\mu\mathrm{d}\mu\right]}_{\beta} \\
=& 4\beta a^2-2\alpha a-\alpha
\end{aligned}
\tag{A.39}
$$

where

$$
\xi_i(s,\lambda,A)=\frac{\mathrm{e}^{-(s/\lambda)G_i(A)}-\mathrm{e}^{-(s/\lambda)}\left[1+(s/\lambda)(1-G_i(A))\right]}{1-\mathrm{e}^{-s/\lambda}-(s/\lambda)\mathrm{e}^{-s/\lambda}} \tag{A.40}
$$

i.e. the last part of $F(s;\mu)^{2+}_{GS}$ given by Eq.(15) and the solution is

$$
a=\frac{\alpha}{4\beta}+\sqrt{\left(\frac{\alpha}{4\beta}\right)^2+\frac{\alpha}{4\beta}} \tag{A.41}
$$

One can use the normality properties of Legendre polynomials with weight functions of $g(x)=1, g(x)=x, g(x)=x^2$ i.e.

$$
\int_{-1}^{+1}P_\ell(x)P_k(x)\mathrm{d}x=\frac{2}{2\ell+1}\delta_{\ell k} \tag{A.42}
$$

$$
\int_{-1}^{+1}P_\ell(x)P_k(x)x\mathrm{d}x=\begin{cases}\frac{2(\ell+1)}{(2\ell+1)(2\ell+3)} & \text{if } k=\ell+1\\[2ex] \frac{2\ell}{(2\ell-1)(2\ell+1)} & \text{if } k=\ell-1\end{cases} \tag{A.43}
$$

$$\int_{-1}^{+1} P_\ell(x)P_k(x)x^2\mathrm{d}x = \begin{cases} \frac{2(\ell+1)(\ell+2)}{(2\ell+1)(2\ell+3)(2\ell+5)} & \text{if } k=\ell+2 \\ \frac{2(2\ell^2+2\ell-1)}{(2\ell-1)(2\ell+1)(2\ell+3)} & \text{if } k=\ell \\ \frac{2\ell(\ell-1)}{(2\ell-3)(2\ell-1)(2\ell+1)} & \text{if } k=\ell-2 \end{cases} \tag{A.44}$$

to compute the integrals necessary to get the expressions for α and β. Using the first property

$$\begin{aligned} &\sum_{\ell=0}^{\infty}(\ell+0.5)\xi_\ell(s,\lambda,A)\sum_{k=0}^{\infty}(k+0.5)\xi_k(s,\lambda,A)\int_{-1}^{+1}P_\ell(\mu)P_k(\mu)\mathrm{d}\mu \\ &=\sum_{\ell=0}^{\infty}(\ell+0.5)[\xi_\ell(s,\lambda,A)]^2 \end{aligned} \tag{A.45}$$

using the second property

$$\begin{aligned} &\sum_{\ell=0}^{\infty}(\ell+0.5)\xi_\ell(s,\lambda,A)\sum_{k=0}^{\infty}(k+0.5)\xi_k(s,\lambda,A)\int_{-1}^{+1}P_\ell(\mu)P_k(\mu)\mu\mathrm{d}\mu \\ &=\sum_{\ell=0}^{\infty}(\ell+0.5)\xi_\ell(s,\lambda,A)\left\{(\ell-1+0.5)\frac{2\ell}{(2\ell-1)(2\ell+1)}\xi_{\ell-1}(s,\lambda,A)\right. \\ &\left.+(\ell+1+0.5)\frac{2(\ell+1)}{(2\ell+1)(2\ell+3)}\xi_{\ell+1}(s,\lambda,A)\right\}=\sum_{\ell=0}^{\infty}\xi_\ell(s,\lambda,A)\left\{\frac{\ell}{2}\xi_{\ell-1}(s,\lambda,A)\right. \\ &\left.+\frac{\ell+1}{2}\xi_{\ell+1}(s,\lambda,A)\right\}=\sum_{\ell=0}^{\infty}(\ell+1)\xi_\ell(s,\lambda,A)\xi_{\ell+1}(s,\lambda,A) \end{aligned} \tag{A.46}$$

and the third

$$
\begin{aligned}
&\sum_{\ell=0}^{\infty}(\ell+0.5)\xi_\ell(s,\lambda,A)\sum_{k=0}^{\infty}(k+0.5)\xi_k(s,\lambda,A)\int_{-1}^{+1}P_\ell(\mu)P_k(\mu)\mu^2\mathrm{d}\mu \\
&=\sum_{\ell=0}^{\infty}(\ell+0.5)\xi_\ell(s,\lambda,A)\left\{\frac{(\ell-2+0.5)2\ell(\ell-1)}{(2\ell-3)(2\ell-1)(2\ell+1)}\xi_{\ell-2}(s,\lambda,A)\right. \\
&\left.+\frac{(\ell+0.5)2(2\ell^2+2\ell-1)}{(2\ell-1)(2\ell+1)(2\ell+3)}\xi_\ell(s,\lambda,A)+\frac{(\ell+2+0.5)2(\ell+1)(\ell+2)}{(2\ell+1)(2\ell+3)(2\ell+5)}\xi_{\ell+2}(s,\lambda,A)\right\} \\
&=\sum_{\ell=0}^{\infty}\xi_\ell(s,\lambda,A)\left\{\frac{\ell(\ell-1)}{2(2\ell-1)}\xi_{\ell-2}(s,\lambda,A)+\frac{(\ell+0.5)(2\ell^2+2\ell-1)}{(2\ell-1)(2\ell+3)}\xi_\ell(s,\lambda,A)\right. \\
&\left.+\frac{(\ell+1)(\ell+2)}{(2(2\ell+3)}\xi_{\ell+2}(s,\lambda,A)\right\}=\sum_{\ell=0}^{\infty}\frac{(\ell+0.5)(2\ell^2+2\ell-1)}{(2\ell-1)(2\ell+3)}[\xi_\ell(s,\lambda,A)]^2 \\
&+\sum_{\ell=0}^{\infty}\xi_\ell(s,\lambda,A)\left\{\frac{\ell(\ell-1)}{2(2\ell-1)}\xi_{\ell-2}(s,\lambda,A)+\frac{(\ell+1)(\ell+2)}{(2(2\ell+3)}\xi_{\ell+2}(s,\lambda,A)\right\} \\
&=\sum_{\ell=0}^{\infty}\frac{(\ell+0.5)(2\ell^2+2\ell-1)}{(2\ell-1)(2\ell+3)}[\xi_\ell(s,\lambda,A)]^2+\sum_{\ell=0}^{\infty}\frac{(\ell+1)(\ell+2)}{(2\ell+3)}\xi_\ell(s,\lambda,A)\xi_{\ell+2}(s,\lambda,A)
\end{aligned}
\tag{A.47}
$$

Substituting these three equations into α and β results in

$$
\begin{aligned}
\alpha=\sum_{\ell=0}^{\infty}\xi_\ell(s,\lambda,A)&\left\{\left(1.5\ell+\frac{0.065}{\ell+1.5}+\frac{0.065}{\ell-0.5}+0.75\right)\xi_\ell(s,\lambda,A)\right. \\
&\left.-2(\ell+1)\xi_{\ell+1}(s,\lambda,A)+\frac{(\ell+1)(\ell+2)}{(2\ell+3)}\xi_{\ell+2}(s,\lambda,A)\right\}
\end{aligned}
\tag{A.48}
$$

$$
\beta=\sum_{\ell=0}^{\infty}(\ell+1)\xi_\ell(s,\lambda,A)\xi_{\ell+1}(s,\lambda,A) \tag{A.49}
$$

that can be used in Eq.(A.41) to compute the optimal value of the parameter a of the transformation given by Eq.(33)

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List of Tables

Table 1: $s/\lambda = 1$ and $\tilde{w}^2 = 3.3675$
Screening parameter A and the corresponding optimal value of parameter a of the transformation $f(a;\mu)$ with the corresponding w^2 values at $s/\lambda = 1$ as a function of $G_1 s/\lambda$. The approximate value $\tilde{w}^2$ value computed by Eq.(43) and the corresponding $\tilde{a}$ values are also shown.

$G_1 s/\lambda$	A	a	$w^2 = a/A$	$\tilde{a} = \tilde{w}^2 A$
1.000e-03	5.699162e-05	1.933615e-04	3.392806e+00	1.919193e-04
5.090e-02	6.168356e-03	2.120923e-02	3.438393e+00	2.077194e-02
1.008e-01	1.553012e-02	5.448068e-02	3.508066e+00	5.229768e-02
1.507e-01	2.779892e-02	1.000408e-01	3.598728e+00	9.361288e-02
2.006e-01	4.319982e-02	1.603297e-01	3.711352e+00	1.454754e-01
2.505e-01	6.216947e-02	2.392574e-01	3.848470e+00	2.093557e-01
3.004e-01	8.533942e-02	3.425741e-01	4.014254e+00	2.873805e-01
3.503e-01	1.135762e-01	4.787333e-01	4.215084e+00	3.824679e-01
4.002e-01	1.480622e-01	6.604428e-01	4.460576e+00	4.985995e-01
4.501e-01	1.904288e-01	9.074555e-01	4.765328e+00	6.412689e-01
5.000e-01	2.429743e-01	1.251795e+00	5.151963e+00	8.182161e-01

Table 2: $s/\lambda = 10$ and $\tilde{w}^2 = 2.289938e+01$
Same as Table1

$G_1 s/\lambda$	A	a	$w^2 = a/A$	$\tilde{a} = \tilde{w}^2 A$
1.000e-03	4.412635e-06	1.011501e-04	2.292283e+01	1.010466e-04
5.090e-02	3.683146e-04	8.502289e-03	2.308431e+01	8.434178e-03
1.008e-01	8.253681e-04	1.922263e-02	2.328976e+01	1.890042e-02
1.507e-01	1.339376e-03	3.150770e-02	2.352415e+01	3.067090e-02
2.006e-01	1.899663e-03	4.518052e-02	2.378344e+01	4.350111e-02
2.505e-01	2.500655e-03	6.018001e-02	2.406570e+01	5.726345e-02
3.004e-01	3.138897e-03	7.649451e-02	2.436987e+01	7.187882e-02
3.503e-01	3.812052e-03	9.413963e-02	2.469526e+01	8.729364e-02
4.002e-01	4.518446e-03	1.131484e-01	2.504145e+01	1.034696e-01
4.501e-01	5.256847e-03	1.335664e-01	2.540809e+01	1.203785e-01
5.000e-01	6.026322e-03	1.554486e-01	2.579493e+01	1.379991e-01

Table 3: $s/\lambda = 10^3$ and $\tilde{w}^2 = 6.070075e + 03$
Same as Table1

$G_1 s/\lambda$	A	a	$w^2 = a/A$	$\tilde{a} = \tilde{w}^2 A$
1.000e-03	3.067520e-08	1.859172e-04	6.060830e+03	1.862008e-04
5.090e-02	2.108620e-06	1.294233e-02	6.137819e+03	1.279948e-02
1.008e-01	4.451370e-06	2.771704e-02	6.226632e+03	2.702015e-02
1.507e-01	6.925284e-06	4.378737e-02	6.322827e+03	4.203699e-02
2.006e-01	9.493600e-06	6.100034e-02	6.425417e+03	5.762686e-02
2.505e-01	1.213737e-05	7.930613e-02	6.534047e+03	7.367473e-02
3.004e-01	1.484477e-05	9.869717e-02	6.648617e+03	9.010885e-02
3.503e-01	1.760764e-05	1.191890e-01	6.769165e+03	1.068797e-01
4.002e-01	2.041995e-05	1.408122e-01	6.895816e+03	1.239506e-01
4.501e-01	2.327707e-05	1.636088e-01	7.028755e+03	1.412935e-01
5.000e-01	2.617528e-05	1.876300e-01	7.168216e+03	1.588859e-01

Table 4: $s/\lambda = 10^5$ and $\tilde{w}^2 = 9.629423e + 05$
Same as Table1

$G_1 s/\lambda$	A	a	$w^2 = a/A$	$\tilde{a} = \tilde{w}^2 A$
1.000e-03	2.362253e-10	2.269574e-04	9.607668e+05	2.274713e-04
5.090e-02	1.495453e-08	1.457531e-02	9.746419e+05	1.440035e-02
1.008e-01	3.093671e-08	3.063026e-02	9.900942e+05	2.979027e-02
1.507e-01	4.750198e-08	4.781334e-02	1.006554e+06	4.574167e-02
2.006e-01	6.447247e-08	6.601397e-02	1.023909e+06	6.208327e-02
2.505e-01	8.175856e-08	8.520270e-02	1.042126e+06	7.872878e-02
3.004e-01	9.930534e-08	1.053831e-01	1.061203e+06	9.562531e-02
3.503e-01	1.170754e-07	1.265770e-01	1.081158e+06	1.127368e-01
4.002e-01	1.350413e-07	1.488185e-01	1.102022e+06	1.300370e-01
4.501e-01	1.531824e-07	1.721514e-01	1.123833e+06	1.475058e-01
5.000e-01	1.714820e-07	1.966278e-01	1.146638e+06	1.651273e-01