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A model for the accurate computation of the lateral scattering of protons in water

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Abstract

A pencil beam model for the calculation of the lateral scattering in water of protons for any therapeutic energy and depth is presented. It is based on the full Molière theory, taking into account the energy loss and the effects of mixtures and compounds. Concerning the electromagnetic part, the model has no free parameters and is in very good agreement with the FLUKA Monte Carlo (MC) code. The effects of the nuclear interactions are parametrized with a two-parameter tail function, adjusted on MC data calculated with FLUKA. The model, after the convolution with the beam and the detector response, is in agreement with recent proton data in water from HIT. The model gives results with the same accuracy of the MC codes based on Molière theory, with a much shorter computing time.

Keywords: proton therapy, multiple scattering theory, lateral dose distribution

(Some figures may appear in colour only in the online journal)
1. Introduction

In intensity modulated proton therapy a fast and accurate dose computation is essential. The best accuracy in this kind of calculations is obtained by Monte Carlo Methods like FLUKA (Böhlen et al 2014, Ferrari et al 2005), GEANT4 (GEANT4 Collaboration 2004), MCNP (Los Alamos National Laboratory 2002), but at the expense of a long computing time.

Alternatively, models can be used that calculate the total dose as the sum of the dose delivered by an ensemble of pencil beams corresponding to the structure of the real beam delivered by the accelerator.

The purpose of this paper is to present, in section 2, a flexible model for the calculation of the lateral deflection of a pencil proton beam. The model relies on the full Molière theory of Coulomb multiple scattering rather than on standard approaches based on double Gaussian or other parametrizations (Soukup et al 2005, Pedroni et al 2005, Bellinzona et al 2015) or on the Fermi–Eyges approximation (Eyges 1948).

The model distinguishes explicitly the electromagnetic and the nuclear contributions. For the electromagnetic interaction the use of the original equations of the theory removes the need for any free parameter, at the expense of a reasonable increase in the computing time: in addition to the traditional angular distribution, the linear lateral displacement is also provided. For the treatment of the nuclear interactions the model relies only on two parameters that are determined as a function of energy and depth by best fits to FLUKA MC simulations.

The model agrees very well with the MC code predictions and with experimental data for protons in water, which were acquired at the Heidelberg Ion Beam Therapy Center (HIT) at clinically relevant energies and depths. It shows the same accuracy of MC codes with much faster computational time, and, when compared to the other currently available parametrizations, has a better accuracy with a comparable evaluation time (see Bellinzona et al (2015) and section 3.2).

Although the comparison has been considered in water, the treatment presented here can be extended to any element, molecule or mixture.

2. Methods and materials

In this note we review and collect the most relevant results to describe the multiple Coulomb scattering of heavy charged particles in media, focusing on protons in water. This study results in a theoretical model that is implemented as a standalone C++ code that can be used in the context of treatment planning for hadrontherapy.

The model is developed here for a pencil beam and is extended in section 3.3 to more realistic cases to reproduce mathematically the lateral beam scan of a given region. In addition to the Molière theory, summarized in the appendix, we have also considered the energy loss of protons in water with the aim of calculating the lateral displacement at any depth.

2.1. Energy loss

Since we will consider very long paths of protons in water, we have to modify the basic equations of the appendix to take into account the energy loss process. Since the parameters \( \chi_c \) and \( \chi_\alpha \) of the Molière theory depend on \( p\beta \), the energy loss problem can be solved if one finds the dependence of these quantities on the water thickness \( x \) traversed. If we indicate as \( p(x) \) and \( \beta(x) \) the current values at the depth \( x \) in the target, from equation (A.19) we have:
At this point we use the formula reported by Gottschalk (2010) for protons; the current $p(x)\beta(x)$ value of a charged particle of incident momentum $p\beta$, after traversing a slab of thickness $x$, is given by:

$$p(x)\beta(x)^2 = p^2\beta^2\left(1 - \frac{x}{R}\right)^k,$$  

(2)

where $R$ is the range for that particle of incident momentum $p$. This formula is fairly accurate for many materials of density $\rho$ (g cm$^{-3}$) and radiation length $X_0$ (cm) if $k$ is chosen with the formula (Schneider et al. 2001):

$$k = 1.0753 + 0.12\exp(-0.09\rho X_0).$$  

(3)

We verified that, with $k = 1.07$, this equation is accurate for water within 2% both for protons and carbon ions, up to distances of about 0.995$R$.

The range $R$ in the previous formula can be easily calculated. For an incident proton of kinetic energy $E_k$(MeV), a very accurate formula for a medium of density $\rho$ (g cm$^{-3}$) is that of Ulmer and Schaffner (2011):

$$R(cm) = \frac{1}{\rho} \sum_{n=1}^{N} \frac{A_n Z_n}{Z_M} \ln \frac{10^{1.1569 - 6.202 X_n}}{1 - (1 - \frac{x}{R})^{1-k}},$$  

(4)

where $E_i$ is the mean ionization potential of the medium (in eV) and $Z_M$ and $A_M$ are from equation (A.18). For water, we use $E_i = 77.0$ eV (Parodi et al. 2012). For water and protons of incident kinetic energy $E_k < 300$ MeV, a sum with $N = 4$ gives results accurate to a more than 0.5% (Ulmer and Schaffner 2011). The coefficients $\alpha_i$ and $p_i$ are reported in Table 1.

With energy loss by equation (2), equation (1) becomes:

$$\chi^2_c = \chi^2_w \int_0^x \frac{1}{p(t)^2 \beta(t)^2} dt.$$  

(5)

$$\chi^2_c = \chi^2_w \frac{R[(1 - x/R)^{1-k} - 1]}{(k - 1) \cdot p^2 \beta^2}.$$  

(6)

The calculation of $\chi_0$ is more complicated and cannot be obtained in closed form. From equations (2), (A.19)–(A.22) we obtain:

$$\ln \chi^2_0 = \frac{1}{\chi^2_c} A_M \sum_{i} \frac{n_i Z_i^2}{p_i^2 \beta_i^2} \int_0^x \ln \frac{\ln \left[\frac{\chi^2_0}{\chi^2_c} \right] - \ln \frac{\chi^2_0}{\chi^2_c} \cdot \frac{d_i}{Z_{i}}}{\left(1 - \frac{x}{R}\right)^k} dt,$$  

(7)
where $A_M$ is from equation (A.18), $\mu_i$ is a function of $\beta(x)$ and $\chi_0$ is a function of $p(x)$. They can be calculated from equations (A.4) and (A.5) with $Z_i = Z_i, Z_0$ and $\chi_i$ from equation (6). Equation (7) can be evaluated with good precision with the Simpson numerical integration rule because of the smooth behavior of the integrand. In water, integration steps of 0.5 cm are enough to provide good accuracy. Since $\mu_i$ and $\chi_0$ depend on $p$ and $\beta$ separately, we have to calculate them from the current product $p(x)\beta(x)$ resulting during the numerical integration.

2.2. The lateral displacement

With the inclusion of the energy loss effects, we can derive a general formula, that permits the passage from angular (Molière theory) to spatial displacements.

The $\chi^2$ of the transverse displacement on a measuring plane at $x$ due to a layer $d$ at the depth $t$ is given by $(x-t)\theta_{LR}$, where the angle is given by equation (A.16). The angular squared rms is a product of $\chi^2 c$, which is a quantity that depends on the thickness $x$ and that can be combined in quadrature and of the parameter $B$, which depends on the thickness in a logarithmic way. This fact is unavoidable and is present in many formulae that calculate the angular rms, such as the one used by Highland (1975). The physical meaning is that two successive layers act in a dependent manner, since the second layer receives trajectories deflected by the first one. By following the usual procedure (Gottschalk et al. 1993), we combine in quadrature the $\chi^2 c$ contributions and multiply for an average value the $B$ ones.

With the replacement $x \to \int dt$, taking into account the energy loss, from equations (1)–(5), (A.16) and (A.19), by adding in quadrature all the $\chi^2 c$ contributions, for a thickness $x$ and a detector plane placed at a distance $D \geq x$, we obtain (see also figure 1):

$$y_M = \frac{\chi_c \sqrt{B}}{\sqrt{2p/\beta}} \left[ \int_0^x \frac{(D-t)^2}{(1 - \frac{t}{R})^2} \, dt \right]^{1/2}$$

(8)

The $B$ contribution is calculated from equation (A.15) with the final values of $\chi^2 c$ and $\chi^2 \alpha$ from equations (5) and (7). From equation (A.17), this corresponds to the use of the mean number of collisions, taking into account all the relevant processes.

One can also find the displacement at the plane corresponding to the distance $x$ (the usual case) by replacing the term $D - t$ in the integrand with $x - t$.

When $D = x$, Microsoft Mathematics (Microsoft Corporation 2014) gives a rather simple analytical solution for the integral in equation (8):

$$y_M = \frac{R^2 [2R(1 - x/R)^3 - k] - 2R^2 + 6x - 2R]}{(k - 1)(k - 2)(k - 3)} = \frac{R^2}{k - 1}, \quad k > 1.$$  

(9)

Other more complicated analytical expressions can be found when $x < D \leq R$ and $D > R$.

The $\chi^2$ from equation (8) corresponds to the projection on the measuring plane of the $\chi^2$ of the Gaussian core of the angular distribution. Therefore, the factor

$$\delta = \frac{y_M}{\theta_{LR}} = \frac{y_M \sqrt{2}}{\chi_c \sqrt{B}}$$

(10)

represents the scale factor that allows the passage from the angular to the spatial distribution observed after the passage of a thickness $x$. The change of variable therefore is
\[ \delta = \frac{y}{\theta_i} \quad \Rightarrow \quad \theta_i = \frac{y}{\delta}, \quad (11) \]

and equation (A.11) becomes:

\[ f_M(y) = \frac{1}{\pi\chi_c\delta} \int_0^\Gamma \cos\left(\frac{y\eta}{\chi_c\delta}\right) \exp\left[-\frac{\eta^2}{4} \left( b - \ln \frac{\eta^2}{4} \right)\right] \eta d\eta. \quad (12) \]

2.3. MC codes

Up to now we have assembled all the Molière basic formulae in a complete model without free parameters. As such the key equations (8)–(12) allow the passage from angular to the lateral spatial distribution in a general way. Therefore, our results will be directly compared in section 3.1 with the same distributions predicted by some MC codes of current use (FLUKA 2011.2c and MCNP6) with all nuclear effects switched off.

FLUKA Böhlen et al (2014) and Ferrari et al (2005) uses a special transport algorithm, based on Molière’s theory of multiple Coulomb scattering improved by Bethe (Ferrari et al 1992), and takes into account correlations between path length corrections and scattering angle, and also between the lateral deflection and the scattering angle. Benchmarks of its capabilities related to multiple Coulomb scattering can be found in Ferrari et al (1992) and Fassó et al (1995). MCNP6 instead is based on the full Goudsmit-Saunderson model of multiple scattering as described in Goorley et al (2013).

2.4. Nuclear effects

In the appendix the pure electromagnetic part of the multiple scattering process has been completely described in terms without free parameters. However, particularly when large thicknesses are involved, nuclear interactions play an important role, with an additional term to the deposited dose that can be estimated as about 1% per cm of depth.

This term describes the interaction of non-primary particles that affects the tails to the distribution and must be added to the Molière distribution in the proper way, i.e. accounting for the primary protons fluence decrease.
However at therapeutic energies ($E < 300$ MeV), a minor contribution arises also from nuclear reactions that result in the production of secondary particles and heavy recoils. Ulmer (2007) provides a formula for the determination of the percentage $W_p$ of protons that have only had electromagnetic interactions, i.e. no nuclear interactions, as a function of the traversed thickness, for protons of incident kinetic energy $E_k$ and range $R$ in water, at a certain water thickness $x$:

$$W_p = \frac{1}{2} \left[ 1 - \left( \frac{E_k - E_{th}}{m} \right) \frac{x}{R} \right] \left[ 1 + \text{erf} \left( \frac{R - x}{\tau} \right) \right],$$

where erf is the error function, $f = 1.032$, $m$ is the proton mass in MeV, $E_{th} = 7$ MeV is the $^{16}O$ threshold energy for the $(p,p')$ reaction.

The parameter $\tau$ takes into account the range variation due to the straggling along the beam path and can be parametrized as (Ulmer and Schaffner 2011):

$$\tau = 0.0179651452 R^t,$$

where $t = \begin{cases} 0.9352 & \text{if } R \geq 1 \text{ cm} \\ 1.1763 & \text{if } R < 1 \text{ cm} \end{cases}$

Once the weight of the nuclear interactions has been parametrized, we should describe the influence of the secondary reaction products on the lateral distribution. Following a suggestion of Soukup et al (2005) and Li et al (2012), we use a modified Cauchy–Lorentz distribution for the nuclear tail contribution to be added to the electromagnetic core:

$$t(y) = \frac{1 - A \exp \left[ -\frac{y^2}{2b^2\sigma^2} \right]}{\pi b \left( \frac{y^2}{b^2} + 1 \right)}$$

where the three free parameters are the amplitude $A$, the Half Width Half Maximum (HWHM) $b$ and the variance $\sigma^2$.

The total normalized final distribution for the lateral displacement, is then given by:

$$f(y) = W_f f_M(y) + (1 - W_p) \frac{t(y)}{\int_{\infty}^{\infty} t(y) \, dy},$$

where $f_M(y)$ is the distribution of equation (12) and $W_p$ is the weight from equation (13). Both $f_M(y)$ and $t(y)$ are normalized to unit area.

The free parameters $A, b$ and $\sigma^2$, contained in equations (15) and (16), have been determined by fitting the FLUKA MC lateral displacement distributions with the nuclear interactions switched on (Fassò et al 2001). The difference, with respect to the pure electromagnetic case, is evident on the tails of the curve, for the larger deviations. During the fit procedure we found that good results were obtained with the variance fixed at the value $\sigma^2 = 1$.

The behaviour of the remaining two free parameters $A$ and $b$ as a function of normalized depth is analyzed for two energies. We found that a simple parametrization with Chebyshev polynomials well describes the parameters $A$ and $b$ with third and eighth degree respectively and makes the model useable in water.

In case of a different material, the nuclear parametrization has to be recalculated, again by fitting a MC simulation, and the parameters have to be stored in a different database.

In conclusion, the FLUKA MC code fully describes the nuclear processes, while our model uses a phenomenological approach with two free parameters, $A$ and $b$ in equation (15), with $\sigma^2 = 1$. 


To compare model and data, we have to take into account the beam divergence that is mainly determined by the beam optics, but also by the multiple scattering before the phantom, since the protons cover a distance in air (for instance 1.12 m at HIT) between the nozzle and the isocenter. To this aim, FLUKA simulations were started from dedicated phase-space files, containing the initial beam information (position, energy, cosine directors) sampled at about 1.12 m upstream distance from the isocenter. These phase-spaces (see figure 2(left)) were obtained from separate FLUKA simulations carried out at HIT, including the detailed modeling of the large area ionization chambers and multiwire proportional chambers of the BAMS according to the manufacturer (Parodi et al 2013). The beam scanning process of the line was simulated with a dedicated source routine, similar to the one described in Parodi et al (2010).

A FLUKA calculation is performed by simulating the particles transport in a geometry in which water is replaced with vacuum, to take into account only the beam divergence. The output is scanned at every geometrical depth of interest to obtain the fit of the lateral profiles with the following function:

\[
b(y) = \frac{a}{s} \exp\left[\frac{-y^2}{2s^2}\right] + \frac{b \cdot c}{(y^2 + c)^2}\]

where \(a\) and \(s\) are amplitude and sigma of the Gaussian respectively and \(b\) and \(c\) are amplitude and parameter of the hyperbolic (à la Rutherford) term (Bellinzona et al 2015). The use of the fit is shown in figure 2 (right). The observed lateral profile is then given by the convolution between the distribution of equation (17) and that of equation (16) for water:

\[
F(y) = f * b \equiv \int f(t)b(y - t)dt.
\]

Another effect that should be considered, in the comparison between theory and data, is that due to the detector size. For the data that we analyze, this effect can be taken into account through the parabolic normalized resolution function (Schwaab et al 2011):

\[
S(x) = \frac{2}{\pi R^2} \sqrt{R^2 - x^2} \text{ when } x < R, \ 0 \text{ otherwise},
\]

\[
(19)
\]
where $x$ is the lateral position and $R$ is the effective detector radius, quoted as $R = 0.145$ cm. To correct for these effects, we convolute this function with our final distributions of equation (18), resulting after the convolution with the beam. The results of this second convolution, as already noted by Schwaab et al (2011), have a very small effect for all the cases considered here.

2.6. The model

In conclusion, the model here developed consists of the following steps:

1. the kinetic energy in GeV and the water thickness $x$ are assigned. The momentum $p$ and $\beta$ are calculated with the standard formulae.
2. The parameter $\chi_c$ is calculated through equations (5) and (A.20).
3. The parameter $\chi_c = \sqrt{\exp[\ln \chi_c^2]}$ is calculated from equation (7).
4. The parameters $b$ and $B$ are calculated from equations (A.9) and (A.15).
5. The displacement $y_M$ is calculated from equation (8) and then the scale factor $\delta$ is evaluated from equation (10).
6. The Molière Coulomb multiple scattering distribution $f_{M}(y)$ for the lateral displacement is calculated with equation (12).
7. The final distribution, including the nuclear effects, is given by equation (16), where the Cauchy–Lorentz distribution of equation (15), depending on two free parameters determined from the fit of the FLUKA simulated data, is added to the Molière one. These are the only empirical parameters of the model.
8. In the comparison between model and data in water, we have considered the convolution with a beam and detector response.

2.7. Experimental data

In order to compare the predictions of the model to a realistic situation of proton beam broadening in water, including both the effects of multiple Coulomb scattering and nuclear processes, we used experimental data acquired at the HIT Heidelberg Ion Beam Therapy Center (Schwaab et al 2011).

These dosimetric measurements were performed in a water phantom with entrance window at the treatment isocenter, using a special arrangement of 24 PinPoint ionization chambers (PTW Freiburg, type 31 015, 0.030 cm$^3$ active volume) with six rows of four chambers aligned in lateral offset patterns (in beam-eye view) not to shadow each other, and controlled by a step motor. Lateral profiles were sampled at different depths in water by repeated acquisitions at horizontally shifted positions of the detector block for irradiation of a vertically scanned line pattern of 10 cm length and 1 mm scanning step size. Therapeutically relevant doses of 1–2 Gy were delivered as an acceptable compromise between irradiation time and signal noise, especially in the low dose region. More details of the experimental setup can be found in Schwaab et al (2011).

The comparisons reported in this work refer to initial beam energies of 81.49 MeV and 158.58 MeV and to beam sizes of 17.55 and 10.7 mm FWHM in air at the isocenter, respectively (figures 4 and 5). The beam divergence is considered negligible in the geometrical configuration of this study.

The errors on the data range from 2% to 15%, going from the high dose points to the lowest dose regions (Schwaab et al 2011).
3. Results

3.1. Comparison of electromagnetic core with MC codes

The comparisons of the electromagnetic contribution have shown that the prediction of our model is fully in agreement with those of FLUKA and in good agreement with MCNP6. A typical result is shown in figure 3.

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**Figure 3.** Comparison between the model (red line), FLUKA (blue histogram), and MCNP6 (green histogram, slightly below the line on the log scale) in water for 200 MeV protons at a depth of 18 cm in log (left) and decimal (right) scale. All the nuclear effects (target fragmentation) are excluded.

**Figure 4.** Comparison between model, FLUKA simulation and experimental data for 81.49 MeV in water for a thickness of: \( z = 1.57 \) cm in logarithmic (left) and linear (right) scales. The curves are normalized to the maximum of the FLUKA histogram, obtained by fitting the highest dose channels with a smooth curve. In the normalization zone the error of the data points is 2% (see section 2.7).
Therefore, we can say that, concerning the electromagnetic interaction, our model has the same predictive power as the Monte Carlo codes based on the Molière theory, as FLUKA. For this reason, FLUKA will be assumed as the MC code of reference in the following.

3.2. Comparison with data and discussion

In figures 4–5 the data are compared with the prediction of FLUKA and of the model of section 2.6.

The detector response of equation (19) has been taken into account. However, its inclusion does not significantly modify the agreement with data. We have found that in any case FLUKA and the calculations agree very well, and that the agreement with the measurement data is good.

The behaviour of the two free parameters $A$ and $b$ that describe the nuclear effects as a function of the normalized depth is reported in figure 6 for two energies. We also report the values of the coefficients of the best fit Chebyshev polynomials of third and eighth order at the same energies. A database of these parameters at different energies and depths can be easily constructed with our model and is currently in preparation. Therefore for the evaluation of the nuclear parameters, we propose two different approaches: the fit of the lateral distribution tails (which requires a set of pre-calculated MC distribution) or the use of a pre-compiled external database. The latter solution does not ask in advance for a full MC simulation and reproduces the same results. The two approaches are equivalent both in accuracy and in calculation time.

To quantify the level of agreement we have performed a Kolmogorov Smirnov test (Kolmogorov et al 1933) between our calculation the FLUKA distribution. The model pass the test with a good $p$-value and we use the maximum distance $D$ returned by the test to estimate the different fits quality in a relative manner as a function of depth: the maximum value of $D$ obtained in our study is $7 \times 10^{-3}$ indicating a very good agreement. In case of binned data this is an accepted practice taking into account that $D$ is a parameter that does not have a universal statistical meaning.

The comparison with the analogous MC calculation in case of a mono-energetic pencil beam shows a good agreement and our calculation is much faster than the simulation. The calculation time of the code for the evaluation of the projected distribution is mainly...
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4. Conclusions

In this paper we have shown that a pencil beam model based on Molière theory, when all the physical effects are included and equation (10) is used to pass from the deflected angle to the

determined by the evaluation of the integral of equation (12): this integral in our code is computed only once for each depth and stored in a database that can be read and interpolated at any subsequent call. In this way the calculation time is reduced in average by a factor 2.

3.3. Beam scan

As a further test we reproduce a typical beam scan to compare our model with MC simulations in the context of hadrontherapy. The single beam profile can be shifted in the transverse direction to mimic a lateral scan with a given step (figure 7): in case of homogeneous materials the calculation can be performed only once and the profile can be simply moved by adding the single contributions to the dose. For the MC this is achieved by modifying accordingly the source routine and for the model by laterally shifting the single distribution.

In these conditions, on a DELL XPS computer with an INTEL core i7 (8 cores), with 3.6 GHz CPU, 16 Gbyte RAM and a 64 bit configuration, we have estimated that the computing time of the full lateral profile, using the aforementioned database for the Molière integrals, is about 3 s for each depth: hence for example the time required for 100 depths is about 5 min, to be compared with 90 min taken by the full MC simulation with a statistics of $10^7$ primaries.

Figure 6. Behaviour of the free parameters $A$ and $b$ as a function of normalized depth for 81.49 MeV (upper) and for 158.58 MeV (lower).
Spatial displacement on a detecting plane, is able to reproduce the lateral deflection in water predicted by the current MC codes. The model avoids any free parameter for the electromagnetic interaction. This allowed us to use only two parameters to include the nuclear effects in the tail of the lateral displacement.

A systematic study has been presented for protons in water, showing that the results of the model obtained in this way are practically identical to those of the FLUKA code, for any therapeutic energy and water depth. The comparison with data, at two different energies, shows very good agreement between data, model and FLUKA.

We foresee the application of this model also to other materials and beam particles of interest in hadrontherapy and we are currently investigating its possible implementation in a treatment planning system. The optimal solution in this field would be a Monte Carlo TPS (Mairani et al 2013), but it is still prohibitive due to the high demand in computational time in a clinical context. In the near future great expectations are now placed in GPU computing (Jia et al 2012) which could reduce the run time both for MC, fast MC and analytical calculations. Since the model is much faster and in homogeneous volumes has the same accuracy of MC codes, in principle it could be inserted in the computing engines for the dose calculation in treatment planning once the energy deposit, the effects of different materials and the geometry of the problem are properly taken into account.

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Appendix

A.1. Molière theory

Mathematically, the Molière theory (Molière 1948) is based on the standard transport equation, the Bessel transforms and the small angle approximation (\( \sin \theta \approx \theta \)). Physically, the theory only accounts for electromagnetic interactions and assumes the Rutherford form for the single scattering cross section:

\[
\rho \sigma(\theta) = 2 \chi_c^2 \frac{1}{(\theta^2 + \chi_c^2)^2},
\]  

(A.1)

where \( \rho \) is the number of atoms/cm\(^2\), the axial integration is performed and \( \chi_c, \chi_\alpha \) are the two crucial parameters of the model.

The first one is connected to the rms scattering angle (see below):

\[
\chi_c^2 = 0.1569 \cdot 10^{-6} Z^2 x^2 \frac{1}{A p^2 \beta^2},
\]  

(A.2)

where \( z \) is the atomic number of the incident particle, \( Z \) and \( A \) the atomic number and the mass number of the target, \( x \) is the thickness of the target (g cm\(^{-2}\)), \( p \) is the momentum in GeV c\(^{-1}\) and \( \beta = v/c \), where \( v \) is the velocity of the projectile.

The second one is the parameter connected to the electron screening of the Coulomb potential:

\[
\chi_\alpha^2 = \mu^2 \chi_0^2
\]  

(A.3)

\[
\mu^2 = \left( 1.13 + 3.76 \frac{Z^2}{137^2 \beta^2} \right)
\]  

(A.4)

\[
\chi_0^2 = \left( \frac{\hbar}{p} \frac{0.468 \cdot 10^{-8} \text{(cm)}}{0.1569 \cdot 10^{-6} Z^2 x^2} \right)^2.
\]  

(A.5)

When \( \mu = 0 \) equation (A.1) is the Rutherford cross section of a point charge. This expression of the \( \mu \) parameter has been obtained by Molière by parametrizing the screened Coulomb potential by the sum of three exponentials and using the Wentzel–Kramers–Brillouin method.

Since \( hc = 197.327 \) MeV fm, the parameter \( \chi_0 \) can be written as:

\[
\chi_0 = 4.216 \cdot 10^{-6} \frac{Z^{1/3}}{p},
\]  

(A.6)

where the momentum \( p \) is in GeV c\(^{-1}\).

The total number of multiple scattering events, from equation (A.1), is given by:

\[
\rho \int_0^\infty \sigma(\theta) d\theta = \int_0^\infty 2 \chi_c^2 \frac{\theta}{(\theta^2 + \chi_c^2)^2} d\theta = \frac{\chi_c^2}{\chi_\alpha^2} \equiv \Omega_0.
\]  

(A.7)

Sometimes a factor 1.16 is reported in the denominator of \( \Omega_0 \) (Gottschalk et al 1993).

The standard form for the Molière distribution is given by Scott (1963):
\[ f(\theta) d\theta \frac{\theta d\theta}{\chi_c} = \int_0^\Gamma J_0 \left( \frac{\theta \eta}{\chi_c} \right) \exp \left[ -\frac{\eta^2}{4} \left( b - \ln \frac{\eta^2}{4} \right) \right] \eta d\eta \]  

(A.8)

where \( J_0 \) is the Bessel function,

\[ b = \ln \frac{\chi_c^2}{\chi_0^2} - 0.154432 = \ln \Omega_0 - 0.154432, \]  

(A.9)

and \( \Gamma \) has to be chosen at the minimum of the exponent in the integrand (Bethe 1953), that is

\[ \Gamma = 2 \exp((b - 1)/2). \]  

(A.10)

The projected angle \( \theta_x \) follows the distribution (Scott 1963, p. 271):

\[ f(\theta_x) d\theta_x = \frac{d\theta_x}{\pi \chi_c} \int_0^\Gamma \cos \left( \frac{\theta_x \eta}{\chi_c} \right) \exp \left[ -\frac{\eta^2}{4} \left( b - \ln \frac{\eta^2}{4} \right) \right] \eta d\eta \]  

(A.11)

In the small angle approximation, the connection between the two projected angles in the transverse plane and the spatial angle is a matter of elementary geometry:

\[ \theta = \sqrt{\theta_x^2 + \theta_y^2}. \]  

(A.12)

Since \( \theta_x \) and \( \theta_y \) have the same distribution, the connection between the mean square angles is:

\[ \langle \theta^2 \rangle = 2 \langle \theta_x^2 \rangle. \]  

(A.13)

The distributions (A.8) and (A.11) are the sum of a Gaussian core and of some corrective terms that describe the tails. The rms of the Gaussian core of the spatial distribution is given by Bethe (1953):

\[ \theta_c \equiv B \chi_c \sqrt{\langle \theta^2 \rangle}, \]  

(A.14)

where \( B \) is the solution of the equation:

\[ B - \ln B = b. \]  

(A.15)

Therefore, from equation (A.13), the connection between the rms of the space and projected angles is, with obvious notation:

\[ \theta_{cr} = \frac{\theta_c}{\sqrt{2}} = \frac{\chi_c \sqrt{B}}{\sqrt{2}}. \]  

(A.16)

The \( B \) parameter of equation (A.15) can be approximated, within 2–3%, with the following formula, due to Scott (1963), that uses the total number of collisions of equation (A.7):

\[ B \simeq 1.153 + 1.122 \ln \Omega_t. \]  

(A.17)

A.2. Mixtures and compounds

Now we have to modify the calculation of \( \chi_c \) and \( \chi_\alpha \) to the case of mixtures and compounds, specifically the water molecule. In this case the basic formulae must be substituted by a proper summation over the constituents.

In the following the sum over atomic numbers \( Z_i \) and atomic weights \( A_i \) of the molecule or mixture of \( n_i \) components will be used frequently:
\[ Z_M = \sum_i n_i Z_i \quad A_M = \sum_i n_i A_i. \] (A.18)

For water, \( Z_M = 10 \) and \( A_M = 18 \).

Equation (A.2) for the calculation of \( \chi_c \) must be modified as follows:

\[ \chi_c^2 = \sum_i \chi_{ci}^2 = \chi_W^2 \frac{x}{p^2 \beta^2}, \quad (A.19) \]

where \( \chi_W^2 \) represents the energy loss independent part. For water, it is given by:

\[ \chi_W^2 = 0.1569 \cdot 10^{-6} \sum (Z_H^2 + Z_O^2) \frac{\chi_{ci}^2}{A_M}. \] (A.20)

where \( Z_H = 1 \) and \( Z_O = 8 \).

The generalization of \( \chi_\alpha \) to a molecule is more complicated. Since the logarithm of the Bessel transform of the cross section, that gives the effective number of events, depends on \( \chi_\alpha^2 \), the equation is (Scott 1963, Gottschalk et al 1993):

\[ \ln \chi_\alpha^2 = \frac{1}{\chi_c^2} \sum_i \chi_{ci}^2 \ln \chi_{ci}^2 \] (A.21)

where \( \chi_c^2 \) and \( \chi_{ci}^2 \) are defined in equation (A.19), whereas \( \chi_{ci}^2 \) are calculated from equations (A.3)–(A.5) with the substitution \( Z = Z_i, i = H, O, Z_H = 1, Z_O = 8 \). To complete the theory for the water molecule, one has to take into account the fact that the incident particle is scattered by atomic electrons as well as by the screened Coulomb field of the nucleus. We use the recipe described by Gottschalk et al (1993), which requires the modification of equation (A.21) as follows:

\[ \ln \chi_\alpha^2 = \frac{1}{\chi_c^2} \sum_i \chi_{ci}^2 \left( \ln \chi_{ci}^2 - \frac{D_i}{Z_i} \right), \] (A.22)

where \( D_i \) is the Fano correction (Fano 1954, Scott 1963):

\[ D_i = \ln \left( \frac{1130}{Z_{ci}^{4/3} \left( \frac{1}{Z_i} - 1 \right)} \right) + u_i - \frac{\beta^2}{2}, \] (A.23)

where \( u_H = 3.6 \) and \( u_O = 5.0 \) (Fano 1954).

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