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USE MULTSCAT-PDF with PDFlatex Multiple Coulomb scattering, equilibrium emittances, the PDG expression and all that

1 Introduction

It has been observed [1] that the equilibrium emittances of low Z materials in MICE predicted by both ICOOL and G4MICE simulations are significantly smaller than those estimated from the muon cooling formula. The rms angles of muons scattered in the absorbers are also significantly smaller than those estimated from the PDG expression for multiple scattering. In both cases the discrepancy increases with decreasing atomic number, Z.

The heating term in the cooling formula is based on the PDG expression[2] for the (2D) projected rms angle of multiple scattering in a thickness x of material:

$$\theta_0 = \frac{1}{\sqrt{2}}\theta^{\rm rms}_{\rm space} = \frac{13.6{\rm MeV}}{\beta cp} z\sqrt{x/X_0}[1+0.038\ln{(x/X_0)}]\,. \tag{1}$$

The symbols have their conventional meaning; X_0 is the radiation length of the material and (somehow) describes the properties of the material. The heating term is derived using

$$\frac{d\theta_0^2}{dx} = \left(\frac{13.6{\rm MeV}}{\beta cp}\right)^2 \frac{1}{X_0}\,. \tag{2}$$

It is instructive to understand the origin of this expression. Firstly a brief discussion of the physics of multiple scattering (and energy loss) is in order.

2 The physical processes

When a fast charged particle passes through a medium it interacts electromagnetically with the atoms and it will both lose energy and be scattered. Conventionally energy loss is considered to result from the interaction of the particle with electrons, both as excitation of the atomic energy levels or ‘hard’ collisions with quasi-free electrons. Similarly, scattering is considered to arise from the interaction of the particle with the Coulomb field of the nuclei[1].

Scattering and energy-loss are usually considered to be independent processes. The cross-section for scattering by the nucleus scattering is proportional to Z^2 because the Z charges of the nucleus act coherently; the large nuclear mass means that the incident particle will lose little kinetic energy in an elastic collision. Conversely the Z electrons of an atom are quasi-independent and their relatively small mass means that the incident particle can lose a substantial amount of energy (by a factor $\approx M_N/m_e \geq 2000$) in a collision with a single electron. The distinction between energy loss and scattering is not strictly true and there will be some correlation between energy loss and scattering. The scattering by electrons will be important in low Z materials, especially hydrogen. In

[1] It was, of course, the study of scattering which led to the discovery of the nucleus by Rutherford 101 years ago.

the following discussions the contribution of the electrons to scattering will be considered although the correlation between energy loss and scattering will be ignored.

The basic, and simplest, expression for the probability that a unit-charged particle is scattered into an element of solid angle $d\omega = 2\pi\theta d\theta$ by the Coulomb fields of the nuclei after traversing an infinitesimal thickness dx gm cm^{-2} of material of atomic number Z and atomic mass A is given by the Rutherford scattering formula [3]:

$$P(\theta)d\omega dx = 4N\frac{Z^2}{A}r_e^2\left(\frac{m_e c}{\beta p}\right)^2\frac{d\omega}{\theta^4}dx \tag{3}$$

where N is Avogadro's number, $r_e = e^2/m_e c^2 = 2.818 \times 10^{-13}$ cm is the classical radius of the electron and m_e is the electron mass. A similar expression with the replacement of Z^2 by Z will describe the scattering from the electrons (although this is the subject of discussion later). Equation 3 for Rutherford scattering can be derived classically. The expression 'multiple scattering' refers to the deflection received by a particle after a succession of many single scatters.

A number of caveats are associated with Equation 3. As written, it assumes small angle scatters (which is reasonable for our purposes). Relativistic effects, which depend on the spin of the projectile are ignored but are important only at large momentum transfers (i.e. at large scattering angles). The main difficulty is that $P(\theta)d\omega$ becomes infinite as θ goes to zero, which is quite unphysical. In reality the nuclear Coulomb field is screened by the electrons in the atoms and $P(\theta)d\omega$ must go to zero as θ goes to zero. There is a similar problem at large angles where a cut-off angle corresponding to the finite size of the nucleus must be introduced[2].

3 The origin of the PDG expression

The PDG expression for the rms multiple scattering angle, Equation 1, originates the 1941 review paper by Rossi and Griesen[4]. The same derivation is given in Section 2.16 of Rossi's book [3]. Following Rossi, the rate of increase of mean square angle of scattering in dx is

$$\frac{d\langle\theta^2\rangle}{dx} = \int_{\theta_1}^{\theta_2}\theta^2 P(\theta)d\omega \tag{4}$$

where $P(\theta)$ is the Rutherford expression given by Equation 3 and $d\omega = 2\pi\theta d\theta$ The lower cutoff angle, θ_1, is related (essentially by the uncertainty principle) to the size of the atom, r_a. Assuming the Fermi-Thomas model of the atom, $r_a = r_e Z^{-1/3}/\alpha^2$ and

$$\theta_1 = \frac{Z^{\frac{1}{3}}}{137}\frac{m_e c}{p}\,. \tag{5}$$

Similarly, the upper cutoff angle, θ_2, is related to the nuclear size and is given by

$$\theta_2 = 280A^{-\frac{1}{3}}\frac{m_e c}{p}\,. \tag{6}$$

[2]Classically there is a direct inverse correspondence between impact parameter, b, and scattering angle: $\theta = 2Ze^2/b\beta cp$. Quantum mechanically, the transverse momentum transfer, p_t and 'size' of the scattering object, Δx, are related by the uncertainty principle: $\Delta p = p_t = p\theta = \hbar/\Delta x$ so $\theta \geq \hbar/p\Delta x$ in order to resolve structures smaller than Δx .

Upon integration

$$\begin{aligned}\frac{d\langle\theta^2\rangle}{dx} &= 8\pi N\frac{Z^2}{A}r_e^2\left(\frac{m_e c}{\beta p}\right)^2 \ln\left(\frac{\theta_2}{\theta_1}\right) \\ &= 16\pi N\frac{Z^2}{A}r_e^2\left(\frac{m_e c}{\beta p}\right)^2 \ln\left[196 Z^{-\frac{1}{3}}\left(\frac{Z}{A}\right)^{\frac{1}{6}}\right] . \end{aligned} \tag{7}$$

At this point it is observed by Rossi and Greisen that the terms appearing in Equation 7 are very similar to those appearing in the expression for the radiation length of the material as given in their review article:

$$\frac{1}{X_0} = 4\alpha\frac{N}{A}Z^2 r_e^2 \ln(183 Z^{-\frac{1}{3}}) \tag{8}$$

and furthermore that the arguments of both the logarithmic terms are only approximate[3]. With the use of Equation 8 and assuming that the logarithmic terms cancel, Equation 7 can be written as

$$\begin{aligned}\frac{d\langle\theta^2\rangle}{dx} &= \frac{1}{X_0}\frac{4\pi}{\alpha}(m_e c^2)^2\frac{1}{\beta^2 c^2 p^2} \\ &= \frac{E_c^2}{\beta^2 c^2 p^2}\frac{1}{X_0} . \\ &= \frac{(21.2\ \text{MeV})^2}{\beta^2 c^2 p^2}\frac{1}{X_0} . \end{aligned} \tag{9}$$

The cancellation between the logarithmic terms in Equations 7 and 8 is excellent, with the ratio varying from unity for $Z = 1$ to 1.017 for $Z = 29$ (copper) and 1.023 for $Z = 82$ (lead). Recalling that the rms projected angle is $\theta_0 = \theta^{\text{rms}}_{\text{space}}/\sqrt{2}$ and assuming negligible energy loss in a thickness x of material, Equation 9 immediately gives the original Rossi and Griesen expression:

$$\theta_0 = \frac{E_c}{\sqrt{2}}\frac{1}{\beta pc}\sqrt{\frac{x}{X_0}} = \frac{15\,\text{MeV}}{\beta pc}\sqrt{\frac{x}{X_0}} . \tag{10}$$

Note that, as is well known, the distribution of scattering angles is not Gaussian and θ_0 as given by Equation 10 should not be interpreted too literally as the 'Gaussian' width of the distribution. Nevertheless, Equation 4 is a perfectly good formal definition of $d\langle\theta^2\rangle/dx$.

Equation 10 was modified by Highland [5] and subsequently Lynch and Dahl [6] to give the current PDG formula. Highland re-evaluated E_c based on the $1/e$ angle from Molière theory and found that E_c falls for $Z < 20$. He also introduced the logarithmic term to account for a thickness dependence. Lynch and Dahl made fits to GEANT simulations of a modified form of the Molière distribution and modified the coefficient $E_c/\sqrt{2}$ to 13.6 MeV, and also the coefficient of Highland's logarithmic term, to obtain Equation 1. The most important modifications made by Lynch and Dahl to the GEANT GMOLS routine was to use $Z(Z+1)$ instead of Z to include the scattering by atomic electrons. They do not say what momentum particles were simulated but simply that $\beta = 1$. They comment that fractional radiation length is a poor measure of scattering and suggest a rather different formula for θ_0 (Equations 7, 8 and 9 of [6]) motivated by the angular distribution of screened Rutherford scattering, although the physics underlying their expression is not immediately transparent.

[3]It is not clear why the terms should not be identical since it is the acceleration of the incident particle as it scatters from the nucleus which gives rise to its radiative energy loss, i.e. radiation and scattering are two facets of the same process.

Figure 1: Radiation lengths

4 The radiation length, atomic electrons and the Rossi and Greisen formula

The derivations of Equations 7 and 8 both ignore atomic electrons, i.e. they assume that scattering by nuclei is the only contribution, and that electrons do not contribute to radiative processes. In his book [3] Rossi says that the contribution of atomic electrons to radiative processes can be taken into account by replacing Z^2 by $Z(Z+1)$ in the expression (Equation 8) for the radiation length:

$$\frac{1}{X_0^e} = 4\alpha \frac{N}{A} Z(Z+1) r_e^2 \ln(183 Z^{-\frac{1}{3}}) \tag{11}$$

where the superscript e indicates that the atomic electrons are included in the definition of radiation length. Use of X_0^e in expression 1 or 10 for θ_0 will therefore implicitly include a contribution to scattering from the atomic electrons and increase the calculated value of θ_0

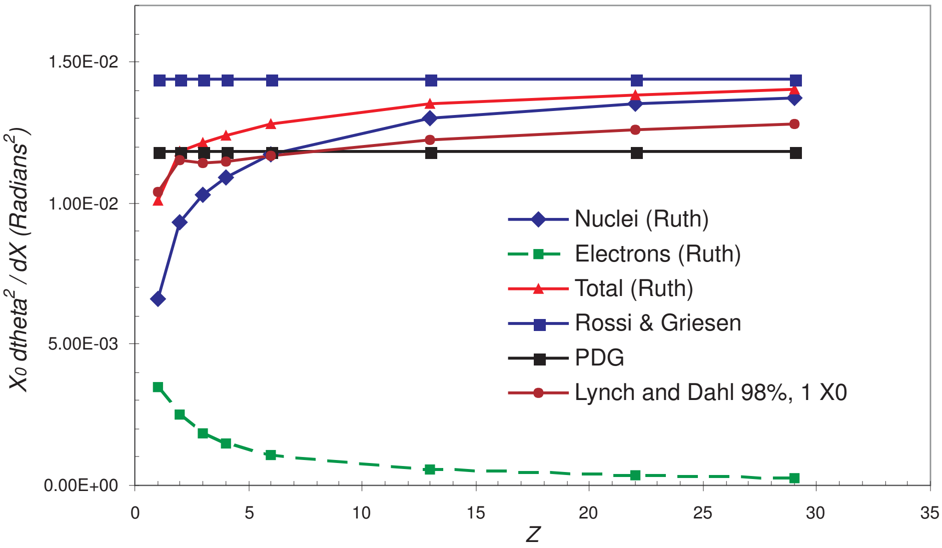

Figure 2: Mean square angle of scattering per PDG radiation length. Rutherford formula with hard cutoffs.

by a factor of $\sqrt{Z(Z+1)/Z}$ over that from the nuclei alone. In his book (page 69), Rossi also comments that the derivation of Equation 7 does not include scattering by atomic electrons and 'Presumably one can take this effect into consideration ... by replacing Z^2 with $Z(Z+1)$ ...' and that Equation 9 is therefore still valid if the radiation length including electrons (i.e. X_0^e, Equation 11) is used.

The radiation lengths given by the PDG [2] (*q.v.*) explicitly include the atomic electrons and, as shown in Figure 1, are very similar to X_0^e as given by Rossi's expression (Equation 11). In other words, the use of the PDG radiation length effectively multiplies Equation 7 for $d\langle\theta^2\rangle/dx$ by $Z(Z+1)/Z$. As will be discussed shortly this modification, which is less than ten percent for all elements above Lithium but amounts to a factor of two for hydrogen, is incorrect, at least for muons with momenta of $\mathcal{O}(200)$ MeV/c.

5 Including the atomic electrons

It has been pointed out by a number of authors, including Bethe [7] and Fano [8] that the scattering by electrons should be included. Fano and Tollestrup [9] (at least) have also pointed out that there is a kinematic limit to the maximum scattering angle of a heavy particle by an electron. This maximum angle is about 4.8 milliradians for a 200 MeV/c muon to be compared with θ_2 (Equation 6) of ≈ 0.7 radians for Hydrogen and ≈ 0.38 radians for Lithium. A better expression for $d\langle\theta^2\rangle/dx$, which takes into account the different maximum angles of scattering by the nuclei and the electrons can be (almost trivially) obtained by repeating the steps leading to Equation 7 with different limits of integration for the nuclear and electronic contributions. This gives

$$\frac{d\langle\theta^2\rangle}{dx} = 8\pi N\frac{Z^2}{A}r_e^2\left(\frac{m_e c}{\beta p}\right)^2\left[\ln\left(\frac{\theta_2}{\theta_1}\right)+\frac{1}{Z}\ln\left(\frac{\theta_2^e}{\theta_1^e}\right)\right] \tag{12}$$

where θ_1^e and θ_2^e are the lower and upper limits of integration over $d\omega$ for the electrons. It can be argued that $\theta_1^e \approx \theta_1$; θ_2^e is the maximum kinematically allowed scattering angle for muons by electrons. (**We need an algebraic expression for this...know how to do it.**)

Figure 2 shows a comparison of $d\langle\theta^2\rangle/dx$ computed from Equation 12 multiplied by X_0 for 200 MeV/c muons for six elements between hydrogen and copper, assuming $\theta_1^e = \theta_1$ as given by Equation 5, θ_2 as given by Equation 6 and $\theta_2^e = 0.0048$ radians. The PDG value of X_0 has been used. As well as the total, the contributions from the nuclei and the electrons are shown separately. Also shown are the Rossi and Griesen expression (Equation 10), and the PDG and the Lynch and Dahl expressions computed for $x = 1X_0$.

The PDG and Rossi and Griesen expressions (obviously) predict that $X_0 d\langle\theta^2\rangle/dx$ is independent of Z; there is some Z dependence in the Lynch and Dahl formula. The Rossi and Griesen expression (Equation 7) modified to take into the upper kinematic limit for scattering by electrons (Equation 12) shows a strong Z dependence at low Z. The asymptotic value of $X_0 d\langle\theta^2\rangle/dx$ is higher than the PDG value at high Z and about twenty percent lower than the PDG value at $Z = 1$. Scattering by the electrons accounts for about thirty percent of the total at $Z = 1$ whereas an application of $Z^2 \to Z(Z+1)$ would give equal contributions from the electrons and nuclei for hydrogen.

To summarise, the Rossi and Griesen and the PDG expressions for $d\langle\theta^2\rangle/dx$, although they were originally derived for scattering by nuclei, both include scattering by atomic electrons since the radiation length also includes the effect of electrons. Neither formulation takes account of the relatively small maximum kinematically allowed scattering angle for a heavy particle by an electron. A simple modification of Rossi and Griesens' original expression (not expressed in terms of radiation length) which explicitly allows for the upper limit on the scattering angle by electrons predicts a Z dependence of $X_0 d\langle\theta^2\rangle/dx$ which is similar to that seen in the simulations.

6 Allowance for screening

Equation 12 was derived from the Rutherford scattering expression with hard cutoffs. No allowance was made for the screening of the nuclear charge by the atomic electrons. The first derivation of scattering by a screened nucleus was made using the Born approximation by Wentzel in 1927 [10] who assumed scattering by a potential of the form $V \propto r^{-1}e^{-r/R}$. The result was a differential scattering cross-section of the form (in the small angle limit)

$$\frac{d\sigma}{d\omega} \propto \frac{1}{(\theta^2 + \theta_1^2)^2} \tag{13}$$

where θ_1 is a screening angle. Molière's derivation [11] was more involved and included corrections to the Born approximation. For multiple scattering he proposed essentially the same cross-section with

$$\theta_1 = \frac{Z^{1/3}}{137}\frac{m_e}{p}\sqrt{1.13 + 3.76a^2} \tag{14}$$

where $a = zZ/137\beta$ (ze is the charge of the scattered particle). The form of the cross-section given by Equation 13 is an improvement on the Rutherford cross-section since $P(\theta)d\omega$ remains finite as θ goes to zero. If the Wentzl-Molière cross-section is used

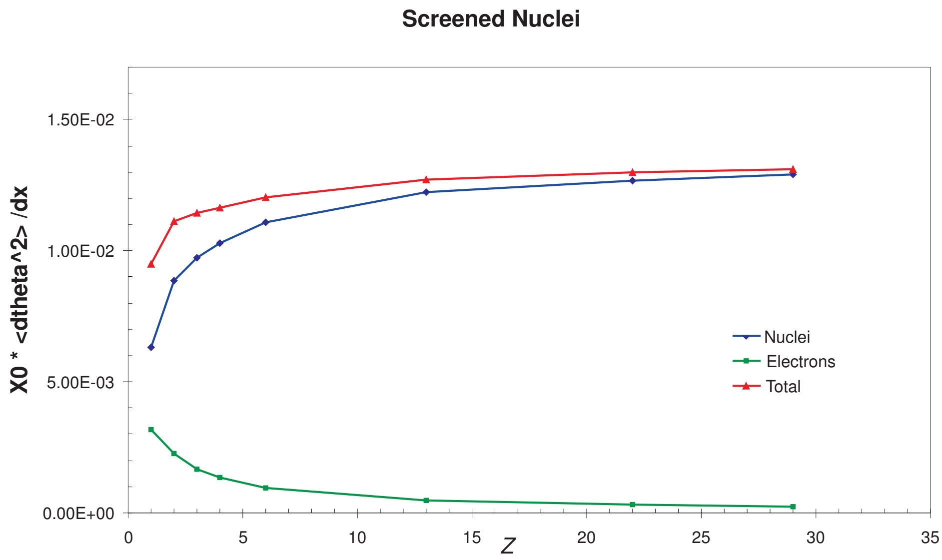

Figure 3: Mean square angle of scattering per PDG radiation length. G and S formula.

in place of the Rutherford cross-section, the differential scattering probability (compare Equation 3) becomes

$$P(\theta)d\omega dx = 4N\frac{Z^2}{A}r_e^2\left(\frac{m_e c}{\beta p}\right)^2 \frac{d\omega}{(\theta_1^2+\theta^2)^2}\,dx\,. \tag{15}$$

(Rossi attributes this expression to Goudsmit and Saunderson [12] although they cite Wentzl.) Using this expression for the scattering probability, and including the electrons in the same way as for the Equation 12 but integrating over θ from zero, then

$$\begin{aligned}\frac{d\langle\theta^2\rangle}{dx} &= 4\pi N\frac{Z^2}{A}r_e^2\left(\frac{m_e c}{\beta p}\right)^2\left\{\ln\left[\left(\frac{\theta_2}{\theta_1}\right)^2+1\right]-1\right.\\ &+ \left.\frac{1}{Z}\left(\ln\left[\left(\frac{\theta_2^e}{\theta_1^e}\right)^2+1\right]-1\right)\right\}\,. \end{aligned} \tag{16}$$

Figure 3 shows $X_0 d\langle\theta^2\rangle/dx$ computed from Equation 16 with $\theta_1^e = \theta_1$ (from Eq. 5 – haven't used Molière expression), θ_2s as before. *Should put hard cutoff Rutherford line on this for comparison !!*

Should

1) repeat with G&S cross-section both for N and e - will give something $5 - 10\%$ smaller

1.5) Compare with Muscat

2) Put in better value for θ_2^e (do the kinematics)

3) Waffle about θ_2 – what is appropriate for cooling??

5) Figure out some equilibrium emittances and compare

6) Need to do the Monte-carlo..

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