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Approximations to multiple Coulomb scattering

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The width of the angular distribution of the multiple Coulomb scattering of relativistic heavy particles can be described by simple formulas. The familiar one, which uses the number of radiation lengths, is accurate to 34% for all Z and can be accurate to 11% if a logarithmic path length correction is included. A fairly simple representation that does not use the radiation length agrees with the predictions of Molière scattering to 2%.

1. Introduction

Physicists often have a need for a simple representation of the effects of multiple Coulomb scattering. Although the angular distribution of multiple Coulomb scattering has much larger tails than does a Gaussian distribution, we may want to get the "best" Gaussian representation of the angular distribution. There are many contexts in which such a Gaussian representation is called for. In some cases we use such a representation to get an answer more quickly than we could from a more accurate representation. When we combine the Coulomb scattering error with other errors and then propagate the combined error in subsequent error analyses, a Gaussian approximation is needed.

The angular distribution from multiple Coulomb scattering has been worked out in detail by Molière [1] and Molière's work has been subsequently expanded and clarified by Bethe [2] and by Scott [3]. In this paper we assume that the Molière theory is correct and we investigate various simple approximations to the scattering distribution to see how well they agree with Molière. This extends the work that was done by Highland [4].

2. The treatment of scattering from atomic electrons

It is not enough to say that we use Molière scattering, because different authors have calculated Molière scattering in different ways, often without realizing or acknowledging that their methods differed from those used by others. The Molière scattering formulas are expressed in terms of two angles – the characteristic angle χ_c and the screening angle χ_α, which are defined as follows:

$$\chi_c^2 = 0.157[Z(Z+1)X/A][z/(p\beta)]^2, \quad \text{and} \tag{1}$$

$$\chi_\alpha^2 = 2.007\times 10^{-5} Z^{2/3}\left[1+3.34(Z z\alpha/\beta)^2\right]/p^2, \tag{2}$$

where p is the momentum in MeV/c, X is the path length in gm/cm^2, Z and A are the charge and atomic weight of the scattering material, z is the charge of the projectile, β is the particle velocity, and $\alpha = 1/137$.

The original work of Molière considered only Coulomb scattering from the nucleus and defined χ_c^2 with Z^2 rather than $Z(Z+1)$. Many people who have used Molière's formulas have used this original Molière form. In 1953 Bethe [2] stated that one needs to use $Z(Z+1)$ to account for the scattering of heavy particles off of the atomic electrons, crediting Kulchitsky and Latyshev [5] for recognizing that this was needed. In 1954 Fano [6] looked into this question of the contribution of the atomic electrons to multiple Coulomb scattering and concluded that the $Z(Z+1)$ that Bethe advocated provides only an order of magnitude correction to account for the scattering from atomic electrons. Fano [6] derived a more complicated correction to account for the scattering from atomic electrons. His change, which, for heavy particles, was a correction to χ_α^2 rather than χ_c^2, always produces a correction that is greater than the $Z(Z+1)$ correction.

Fortunately there are good experimental data to resolve the problem of which of these three treatments of scattering from atomic electrons is correct. In 1979 Shen et al. [7] published measurements of multiple Coulomb scattering in a number of elements for a number of beam particles in the momentum range of 50 to 200 GeV/c. They found that in all cases their data

agreed with the Bethe prescription of Molière scattering. Their measured value for the width of the multiple scattering distribution after about 0.05 radiations lengths of hydrogen, which has an accuracy of 0.8%, disagrees with the original Molière form by 40 standard deviations and disagrees with the Fano form by more than 16 standard deviations! It is interesting to note that Shen et al. do not say that they used $Z(Z+1)$ rather than Z^2 but their clear presentation of their calculations leaves no doubt that $Z(Z+1)$ is what they used.

It may be fortuitous that the theory with $Z(Z+1)$ agrees with experiments as well as it does, especially at low Z, where the Thomas–Fermi model of the atom that is used by Molière is not very accurate. Nevertheless, it seems that the original Molière form and also the Fano form give incorrect answers and that the Bethe form [eq. (1)] is very nearly correct. This means that many Coulomb scattering calculations that have been made in the past have been wrong. For example the papers of Highland [4] and of Mayes et al. [8] used Z^2 rather than $Z(Z+1)$, as does the GEANT [9] Monte Carlo program when Molière scattering of heavy particles is called for. Traditionally the multiple Coulomb scattering of incident electrons has been calculated using $Z(Z+1)$. Thus the formulas that give answers that agree with experiment for the scattering of heavy particles are the ones that have often been used for electrons, but not for other particles. We are unaware of good experimental data that can allow us to check the accuracy of the calculations of the scattering of electrons.

3. Calculation of the Coulomb scattering distribution

To calculate the projected multiple Coulomb scattering distribution we used the subroutine GMOLS that is in the GEANT [9] Monte Carlo program to generate 10^6 scatters of singly charged heavy particles for 14 different elements and 7 different thicknesses ranging from 10^{-4} radiation lengths to 100 radiation lengths. We modified GMOLS in four ways to make it give a more faithful generation of Coulomb scattering. One change was to use $Z(Z+1)$ rather than Z^2 in eq. (1). The other three changes, which had little effect on our results for $\beta = 1$ particles, improved the interpolation procedure, corrected the β dependence of the formulas, and modified the program to use plural scattering when the number of scatters is too small for the Molière scattering formulas to be reliable.

In order to get a Gaussian representation of the Coulomb scattering angular distribution we made maximum likelihood fits to the Coulomb scattering distribution projected onto a plane. In every fit we cut out some of the large angle tail – doing fits to a central fraction F of the distribution. It is necessary to truncate the distribution in this way because in the small angle approximation the RMS width of the scattering distribution is infinite. Fits were done with $F = 0.7$, 0.9, 0.95, 0.98, 0.99, 0.995, and 0.997. The figures in this article are from the fits with $F = 0.98$. In most cases the statistical accuracy of the calculated widths was better than 0.2 percent. One point that we present, the one for 10^{-4} radiation lengths of uranium, is less accurate – about 1%. For this case, in which the mean number of scatters is about 3 and Molière theory is not expected to be reliable, we checked the calculation by generating the distribution with individual scatters (plural scattering).

4. Approximations that are in use

A simple form for the width of the projected multiple Coulomb scattering distribution of singly charged particles that is widely used is

$$\sigma = S_1 \frac{\sqrt{X/X_0}}{p\beta}, \tag{3}$$

with $S_1 = 15$ MeV. X is the thickness of the scatterer and X_0 is the radiation length. We have used the radiation lengths as calculated by Tsai [10]. This handy form was advanced by Rossi and Greisen [11] and was quoted by the Particle Data Group (PDG) from 1957 to 1974. It is a crude approximation to the scattering. Figs. 1a and 1b show how inaccurate this formula is. It is a plot of the ratio of the σ from the Gaussian fit to the Molière scattering distribution to the value obtained by using the Rossi–Greisen form [eq. (3)]. We see that this approximation is sometimes in error by more than thirty percent. It ignores considerable dependency on path length and Z.

In 1974 Highland [4] showed that the length dependence can be fairly well taken into account by a correction term that is proportional to the logarithm of the number of radiation lengths. Since 1982 the Reviews of Particle Properties (RPP) [12] of the PDG has quoted his formula in the form

$$\sigma = S_2 \frac{\sqrt{X/X_0}}{p\beta}\left[1 + \epsilon \log_{10}(X/X_0)\right], \tag{4}$$

with $S_2 = 14.1$ MeV and $\epsilon = 1/9$. It was based on a representation of the $1/e$ point on the Molière distribution of the square of the total scattering angle for $Z = 47$ (silver) and $\beta = 1$. Figs. 1c and 1d illustrate the accuracy of this form at $\beta = 1$. Although this expression takes out much of the length dependence, it is still poor at low Z.

The numbers that were quoted by Highland were different than the ones that are in eq. (4). His coefficient of the log term was $1/8$ rather than $1/9$. This is not a real difference, but merely a consequence of his choosing to quote S_2 at 0.1 radiation lengths rather than

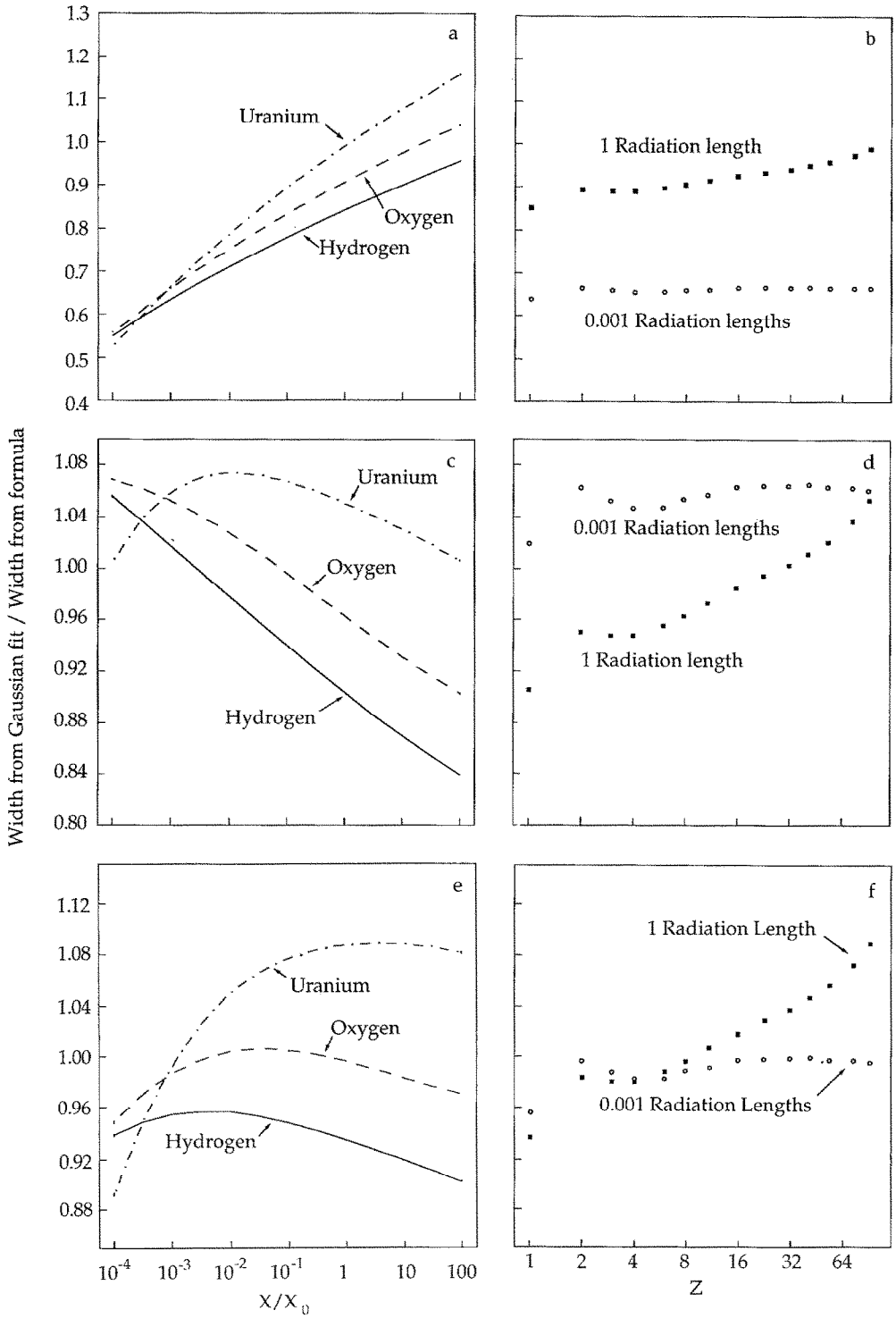

Fig. 1. The ratio of the σ for Gaussian fits to the central 98% of the projected multiple Coulomb scattering distribution of heavy particles with $\beta = 1$ to the values predicted by eqs. (3) and (4), plotted against the logarithm of the number of radiation lengths and against the logarithm of Z. (a) and (b) are for the Rossi-Greisen form [eq. (3)]; (1c) and (1d) are for the Highland form [eq. (4)] with the original Highland constants of $S_2 = 14.1$ MeV and $\epsilon = 1/9$; (1e) and (1f) represent the Highland form with $S_2 = 13.6$ MeV and $\epsilon = 0.088$.

one radiation length. His value of 17.5 for S_2 was for the space angle rather than our projected angle. Corresponding to this 17.5 our S_2 should be $S_2 = 17.5 \times (9/8)/\sqrt{2} = 13.9$. We do not know why the formula in the RPP has 14.1 rather than 13.9.

5. Variations on the Highland form

Highland pointed out in this paper that he would have obtained 17.0 rather than 17.5 if he had not made a correction to Molière. The correction that Highland made was to modify the interpolation formula (the $1 + 3.34(Zz\alpha/\beta)^2$ term) that Molière used in calculating the screening angle. This correction was based on the work of Mayes et al. [8], who arrived at the correction from a comparison of Molière theory with experimental data. However, Mayes et al. also made another correction to Molière having to do with a center-of-mass transformation that had been used by Hungerford et al. [13]. This modification was recognized to be incorrect by Highland in an erratum that was published in 1979. Furthermore Mayes et al. used Z^2 instead of $Z(Z+1)$ in their calculation of χ_c. We have not used this modified form of χ_α that was advocated by Mayes et al. and used by Highland, not only because it seems to be based on an incorrect analysis, but also because it disagrees with the measurement of Shen et al. [7] for all Z. When we use the original Molière interpolation formula to calculate χ_α and we use $Z(Z+1)$ to calculate χ_c (in other words, use eqs. (1) and (2)), we find $S_2 = 13.5$ for the fit to the 1/e point for $\beta = 1$ in silver rather than the 13.9 that one obtains from Highland's paper or the 14.1 that is quoted in the RPP. When we determine the constants in the Highland equation [eq. (4)] using a Gaussian fit with $F = 98\%$ we get $S_2 = 14.2$ and $\epsilon = 0.096$ when we use only $Z = 47$, and get $S_2 = 13.6$ and $\epsilon = 0.088$ when we fit to all Z. Figs. 1e and 1f show how well this parameterization represents multiple Coulomb scattering. This last parameterization is considerably better than the original Highland parameterization at low Z, at the expense of making the large Z representation worse. We consider it the best parameterization of the Highland form. For this value of F (98%) the maximum deviation from the fit for all Z and for $10^{-3} < X/X_0 < 100$ is less than 11%. When one uses different values of F, the values of this parameterization change. A fairly good approximation to this change is to keep ϵ at 0.088 and use

$$S_2 = 12.1 - 0.4 \ln(1 - F). \tag{5}$$

For values of F in the range of $0.7 < F < 0.997$ we found a maximum deviation of less than 14% when we used eq. (5), and a maximum deviation of 20% when we held S_2 fixed at 14.2.

6. Attempts to improve the Highland form

The radiation length has a logarithmic dependence on Z, and the coefficient of this log term happens to be close to ϵ. This suggests a form in which the $\log_{10}(X/X_0)$ in eq. (4) becomes $\log_{10}(ZX/X_0)$. For path lengths greater than 0.1 radiation length this form is accurate for $\beta = 1$ particles to an accuracy better than 4% for $F = 98\%$, but a small thicknesses, it is worse than the form without the Z in the log term.

So far we have only considered singly charged $\beta = 1$ particles. For multiply charged particles z comes into Coulomb scattering in the form z/β and, in the lowest order, β comes into Coulomb scattering in the form X/β^2. Therefore a better expression for the scattering is

$$\sigma = \frac{S_2 z}{p\beta}\sqrt{\frac{X}{X_0}}\left[1 + \epsilon \log_{10}\left(\frac{Xz^2}{X_0\beta^2}\right)\right]. \tag{6}$$

This form takes into account the β and z dependence quite well at small Z, but for large Z and small X the β-dependence is not taken into account very well. For example, for 10^{-3} radiation lengths of lead and $\beta = 0.1$, it overestimates Molière scattering angle by 25% for singly charged particles.

7. A much better approximation without using the radiation length

Much of the difficulty in approximating multiple Coulomb scattering in terms of the radiation length is that the number of radiation lengths is a poor measure of the scattering. We can get a much better simple expression for the scattering if we do not use the radiation length. An expression that does much better than the previous ones is

$$\sigma = \frac{\chi_c^2}{1 + F^2}\left[\frac{1+\upsilon}{\upsilon}\ln(1+\upsilon) - 1\right], \tag{7}$$

where

$$\upsilon = 0.5\Omega/(1 - F), \tag{8}$$

F is (as defined in section 3) the fraction of the tracks that is in the sample, and

$$\Omega = \chi_c^2/\chi_\alpha^2 \tag{9}$$

is the mean number of scatters.

This form, which is not exact, was motivated from a calculation of the RMS angle of the screened Rutherford cross section, for which the distribution in the scattering angle θ is $2\chi_\alpha^2/(\chi_\alpha^2 + \theta^2)^2$. The constant 0.5 in eq. (8) was determined empirically. For F anywhere in the range of 90% to 99.5% this expression represents Molière scattering to better than 2% for Ω between 10 and 10^8, which includes singly charged particles with $\beta = 1$ for all Z and for X/X_0 between 10^{-3} and 100.

Thus this formula is much better than the Rossi–Greisen and Highland formulas for representing multiple Coulomb scattering.

8. Application of these approximations to complex scatters

Whereas the preceding formulas are for scattering in a single material, the usual problem involves the multiple scattering of a particle that traverses many different pieces and pieces that are mixtures of elements. One must take care in applying these formulas in such cases. The wrong way to use them is to calculate a σ for each piece and then add these separate values of σ together in quadrature. The result of such a procedure will get smaller and more incorrect the more pieces that the scatterer is divided into. A much better way to use these approximate formulas is to sum over the pieces before doing the calculation of σ. For example, the generalized version of eq. (6) is written in the following way as a sum over n pieces.

$$\sigma = S_2 z \sqrt{\sum_{i=1}^{n} \frac{X}{X_0 p^2 \beta^2}} \left[1 + \epsilon \log_{10} \left(\sum_{i=1}^{n} \frac{X z^2}{X_0 \beta^2} \right) \right] \tag{10}$$

where all of the quantities within the sums may change from one piece to another. For eq. (7) the effective χ_c^2 is the sum of the individual values of χ_c^2. To a fair approximation the effective Ω is the sum of the individual values of Ω. A more accurate effective Ω is given by using an effective χ_α of the form

$$\ln(\chi_{\alpha\text{-effective}}) = \sum_{i=1}^{n} \frac{XZ(Z+1)}{A} \ln(\chi_\alpha) \Big/ \sum_{i=1}^{n} \frac{XZ(Z+1)}{A} \tag{11}$$

9. Conclusions

We have considered a number of approximations for the RMS projected multiple Coulomb scattering angle for heavy particles. For singly charged particles with $\beta = 1$ the Rossi–Greisen formula [eq. (3)] can be in error by as much as 34%. The Highland modification of this form [eq. (4)] takes out much of the path length dependence and is good to better than 17%. Although this form does not take into account much of the Z dependence, it does a better job at low Z than had been realized by Highland and others because many people have calculated the Z dependence of multiple Coulomb scattering incorrectly in the past. When we determine the constants in Highland's formula to fit to all Z rather than just $Z = 47$ we get the formula [an explicit form of eq. (4)].

$$\sigma = 13.6 \frac{\sqrt{X/X_0}}{p\beta} [1 + 0.088 \log_{10}(X/X_0)], \tag{12}$$

which is good to better than 11% everywhere.

We also present a much better approximation [eq. (7)] that is straightforward to calculate, though not as easy to remember as the formulas of Rossi–Greisen and Highland. It agrees with the predictions of Molière scattering to 2% for all Z.

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