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Suitability of Moliere scattering theory for ionization cooling simulations

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The Moliere theory is currently being used in the Monte Carlo programs ICOOL and DPGEANT to model multiple scattering of muons in various ionization cooling schemes. Paul LeBrun recently raised the question of how well the model describes our scattering. We continue that discussion in this paper. We begin by describing the essential features of the Moliere theory. We examine the theoretical and experimental justification for using the model. Experimental data indicate that the theory may underestimate the strength of large angle scattering in low Z materials.

1 Moliere scattering theory

We present here the essential results of Moliere scattering theory[1,2]. The characteristic scattering parameter is

$$\begin{aligned} \chi_C^2 &= 4\pi N_A r_e^2 (m_e c^2)^2 \frac{\rho t}{A} \frac{Z(Z+1)}{(p\beta c)^2} \\ &= 0.157 \frac{\rho t}{A} \frac{Z(Z+1)}{(p\beta c)^2} \end{aligned} \tag{1}$$

where the units are [gm, cm, MeV]. The theory gives unit probability of obtaining a single scatter through an angle greater than χ_C. The original theory of Moliere was modified with the Z(Z+1) factor to account for scattering off atomic electrons[3]. The de Broglie wavelength of the incident particle is

$$\begin{aligned} \lambda' &= \frac{h'}{p} \\ &= \frac{1.97 \, x \, 10^{-11}}{p \, [MeV/c]} \; [cm] \end{aligned} \tag{2}$$

The theory uses the Thomas-Fermi model of the atom, where the atomic radius is

$$a_{TF} = \frac{0.468 \, x \, 10^{-8}}{Z^{\frac{1}{3}}} \; [cm] \tag{3}$$

The angle χ_o sets the scale at which electron screening effects in the atom are important.

$$\begin{aligned} \chi_o &= \frac{\lambda'}{a_{TF}} \\ &= \frac{4.21 \, x \, 10^{-3} \, Z^{\frac{1}{3}}}{p \, [MeV/c]} \end{aligned} \tag{4}$$

Using the parameter

$$\alpha_B = \frac{Z}{137\beta} \tag{5}$$

the atomic screening parameter is

$$\chi_\alpha^2 = \chi_o^2 \, (1.13 + 3.76 \, \alpha_B^2) \tag{6}$$

The effective number of scatters in the absorber is

$$\Omega = \frac{\chi_c^2}{\chi_\alpha^2} \tag{7}$$

Validity of the theory requires that $\Omega \geq 20$. From this one determines a parameter[2]

$$\begin{aligned} B &= \ln B - 0.1544 + \ln\Omega \\ &\approx 1.153 + 1.122 \ln\Omega \end{aligned} \tag{8}$$

The angle at which the intensity drops to 1/e of its value at 0° is then given by

$$\begin{aligned} w &= \chi_c \sqrt{B-1.2} \quad (space) \\ &= \chi_c \sqrt{B-0.7} \quad (projected) \end{aligned} \tag{9}$$

Using these parameters and a series of expansion functions, the theory can be used to predict the probability of scattering at any angle. The quantity $\chi_C\sqrt{B}$ represents a characteristic scattering angle in the theory. If actual scattering angles are expressed in units of this characteristic angle,

$$s = \frac{\theta}{\chi_c \sqrt{B}} \tag{10}$$

then the space angle distribution is

$$f(\theta)\,\theta\,d\theta = s\,ds\left[2\,e^{-s^2} + B^{-1}F_1(s) + B^{-2}F_2(s) + \ldots\right] \tag{11}$$

where F_1 and F_2 are known functions, which can be found for example in tabular form in the paper by Bethe[3]. The first term in $f(\theta)$ is the gaussian, which dominates for small scattering angles. The F_1 term approaches the single scattering distribution in the large angle limit.

2 Multiple scattering in the alternating solenoid cooling system

We present here the predicted multiple scattering distributions from the main scattering sources in the alternating solenoid transverse cooling system. The major source of scattering is the liquid hydrogen that provides the dE/dx required for cooling. The differential cross section for space angle scattering in each of these 64 cm long cells is shown in Fig. 1. At the 10^{-4} level the tail extends to angles of 150 mr. The actual observed distribution of angles at the end of a cell will of course be modified from this due to the finite emittance of the incident beam and the presence of the solenoidal field.

The other main source of scattering is the beryllium windows on the *rf* cavities. The differential cross section for space angle scattering in each of these 5 mil windows is shown in Fig. 2. At the 10^{-4} level the tail extends to angles of 10 mr. We assume that scattering in the thin windows of the liquid hydrogen container will be similar to this.

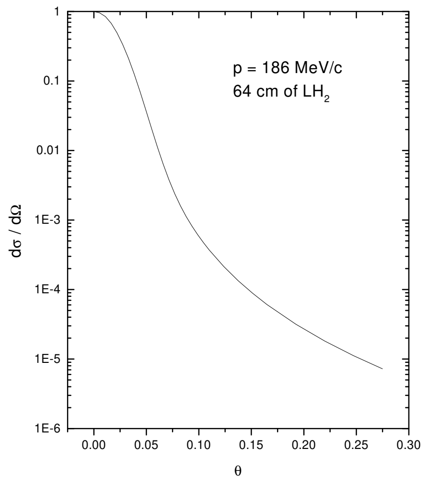

Fig. 1 Multiple scattering distribution for liquid hydrogen absorbers.

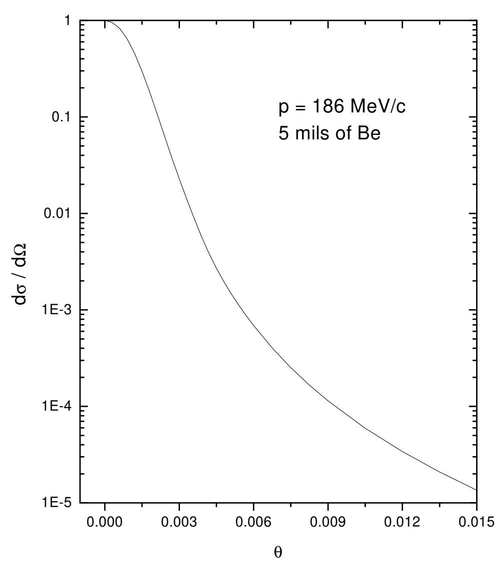

Fig. 2 Multiple scattering distribution for beryllium *rf* windows.

3 Survey of experimental data

Obviously the best test of the applicability of the Moliere theory would be a direct comparison with experimental measurements. However, we have been unable to find any specifically relevant scattering data, i.e. for 100-300 MeV/c muons in liquid hydrogen, LiH, Li and Be. Therefore in this section we review the data that we have found that is closest to what we want.

3.1 Muon

Whittemore and Shutt[4] reported on scattering of 0.3 - 3.1 GeV/c cosmic ray muons in 5 cm of lead. The data for the entire momentum range is summed together and distributions of the projected value of the variable $p\theta$ is given for positive and negative muons. The gaussian part of the curves agree well with the theory of Scott-Snyder (which is very similar to Moliere theory). For negative muons data in the tail regions extend to probabilities of ~3 10^{-4} of the 0^{o} value. The experimental error bars are large, but agree with the theory to within 1 standard deviation. For positive muons data in the tail regions extend to probabilities of ~2 10^{-3} of the 0^{o} value. The data agree with the theory to within 1 standard deviation. The good agreement for the large angle tail may be accidental since nuclear form factors should modify the theoretical results in this case.

Akimenko et al[5] measured scattering of high energy muons on a 1 radiation length thick copper target. The data at 7.3 GeV/c agreed with Moliere theory up to ~4 $\chi_C \sqrt{B}$. From 4-10 $\chi_C \sqrt{B}$ the measured tail was smaller than theory. The theory could be brought into agreement with the measurements by introducing a nuclear form factor. For 11.7 GeV/c muons the data agreed with Moliere theory up to ~8 $\chi_C \sqrt{B}$.

3.2 Electron

Electron data with energies comparable or larger than the critical energy will be complicated by angle changes due to bremsstrahlung emission in the material.

Kulchitsky and Latyshev[6] measured the multiple scattering of 2.25 MeV electrons in thin foils of a number of elements {Al, Fe, Cu, Mo, Ag, Sn, Ta, Au, Pb}. This experiment preceded Moliere's work , so obviously there is no comparison given with his theory. However, Hanson et al (below) did compare the 1/e widths from this data with Moliere theory and found good agreement. This paper shows the angular distributions for each sample in graphical form with data out to ~40^{o}. In a subsequent paper Andievsky et al[7] continued these measurements in low Z materials{Li, Be, C}. These measurements are discussed in more detail in section 4.

Hanson et al[8] showed that scattering of 15.7 MeV electrons in two gold foils agree very well with Moliere theory in the gaussian and in the tail regions. The 1/e widths agreed with theory to ~3%. The claimed experimental uncertainty was 2-3%. The data extended out to ~27 χ_C. The accuracy was slightly worse in the intermediate plural scattering region. Some comments on the validity of this discrepancy and a plot of the Hanson et al gold data in finer detail have been given by Spencer and Blanchard[9]. The measured 1/e widths for beryllium foils were narrower than predicted by the theory (see discussion in Sec. 4 below). Unfortunately, no angular distribution was shown for Be. The authors combined their data for 1/e widths with the earlier electron data from Kulchitsky et al[6,7]. In general the agreement shown with Moliere theory is quite good. The maximum deviation of any measurement from theory is ~7%. For the low Z elements, the measured width of carbon is larger than theory by ~4%, the average value for the Be measurements is narrower than theory by ~4%, and the measured Li width agreed with theory to less than 1%.

3.3 Hadron

Unfortunately, hadron beam data has the complications of (1) angle changes due to nuclear interactions and (2) target recoil effects for light Z absorbers.

Bichsel[10] presented multiple scattering data for protons with energy between 0.7 and 4.8 MeV off foils of Al, Ni, Ag, and Au. Data for the mean width agreed with theory for all samples at all energies to within the ±5% experimental uncertainty, except possibly for Al below 1 MeV, where the measured width was ~10% narrower than theory. Actual data is shown for one Al sample. The tail data extends to values ~1% of the central value.

Dixon et al[11] have measured multiple scattering of 3-5 MeV protons on thick Al, Ni, Mo, and Ta foils. Data is presented for the 1/e widths, as well as the angles where the distributions fall to 10% and 1% of the central value. The angular distribution for 4 MeV protons on Mo is given. The data extend to the plural scattering region. No comparison is given with Moliere theory. Widths are also given for deuteron beams.

Vincour and Bem[12] studied multiple scattering of 6.6 MeV protons in silicon targets. The angular distribution data, which extended to probabilities ~0.005 of the central value, agreed with Moliere theory to within several per cent for the 50 and 93 μm samples. The data was greater than the theory for the 264 μm sample by ~15%, but energy loss in the sample was not taken into account for the theory. Distributions were also given for deuteron and alpha particle beams.

Mayes et al[13] measured the small angle multiple scattering of positive and negative pions in the energy range 139-220 MeV for C, Al, Cu and Pb targets. The theory was modified to account for target recoil effects. They did not use a factor Z(Z+1) for pion-electron scattering in the targets. The measured rms angles were 5-15% larger than the modified theory predicted for all samples. The discrepancy was largest for small Z. There were no significant deviations in the tails starting at 3-4 times the rms angle, contrary to the group's observations[14] in the proton data.

Hungerford et al[14] measured the multiple scattering of 600 MeV protons on C, Al, Cu, Cd, and Pb targets. Before comparing with measurements the theory had to be modified, since target recoil effects were significant with the high energy proton projectile. They did not use a factor Z(Z+1) for proton-electron scattering in the targets. The measured rms angles agreed with the modified theory to within a few per cent. The measured data in the tails of the distributions starting at 3-4 times the rms angle differed significantly from the modified theory. In C the data exceeded theory in the tail. The deviation fell with increasing Z and finally changed sign for the Pb target. This deviation was thought to be due to nuclear scattering and the finite size of the nuclear charge distribution.

Shen et al[15] measured the 1/e angles for positive and negative π, K, and p beams at 50-200 GeV/c on H, Be, C, Al, Cu, Sn, and Pb targets. There was no significant difference of the measured 1/e widths with theory for different projectile types. Data from different projectiles was then combined. The Moliere prediction was in excellent agreement with the measured widths. The largest measured deviation from theory was ~1.5 standard deviations. This was also true for the hydrogen and beryllium targets, where the screening model in Moliere theory is suspect.

4 Discussion

4.1 Single scattering law

The Moliere theory is not dependent on the particular form of the single scattering differential cross section, so long as it goes over into the same limit as the Rutherford cross section at large angles[3]. The Rutherford cross section is given by

$$\frac{d\sigma}{d\Omega_R} = \frac{Z^2}{4} r_e^2 \left(\frac{mc^2}{p\beta c} \right)^2 \frac{1}{\sin^4 \frac{\theta}{2}} \qquad \textbf{(12)}$$

The small angle approximation is assumed and an electron screening model is used to prevent the divergence at $\theta = 0$. The small angle approximation ($\sin\theta = \theta$) is accurate to 3% up to an angle of 25^o.

The Rutherford cross section was derived for a spin 0 particle in a Coulomb potential. The corresponding cross section for a spin ½ particle like the muon is that due to Mott, which is given by[16]

$$\frac{d\sigma}{d\Omega_M} = \frac{d\sigma}{d\Omega_R} \left(1 - \beta^2 \sin^2 \frac{\theta}{2} \right) \qquad \textbf{(13)}$$

In the worst case ($\beta = 1$) the correction term differs from the assumed Rutherford scattering by 3% for angles greater than 20^o. This condition could be used to set an upper limit on allowed step sizes in ICOOL.

4.2 Multiple scattering from atomic electrons

The original Moliere theory[1] used a factor Z^2 to account for scattering off the nucleus. Bethe[3] used the same charge dependence for the contribution of the scattering off the Z atomic electrons, thus replacing the factor Z^2 by Z(Z+1). This prescription was criticized by several authors and alternative methods were proposed, as discussed by Lynch and Dahl[17]. However, the high accuracy experiment of Shen et al showed that the Z(Z+1) factor gave excellent agreement with measurements, while the proposed improvements did not. This was even true for light elements, such as hydrogen. For that reason the Z(Z+1) factor is used in both GEANT 3.2.1 and in ICOOL.

4.3 Atomic screening model

The electrons in the atom screen a portion of the nuclear charge for small scattering angles. The Moliere theory uses a screening correction that is derived from the Thomas-Fermi model of the atom. The screening is parameterized by a multiplicative factor[2]

$$q(\chi) = \frac{\chi^4}{(\chi^2 + \chi_\alpha^2)^2} \tag{14}$$

This factor has the value 0.98 when $\chi = 10\,\chi_\alpha$ and decreases towards smaller angles. It has the value 0.25 when $\chi = \chi_\alpha$. Screening form factors based on the Thomas-Fermi model are accurate[18] for all elements with Z > 4. Unfortunately, this means the screening is inaccurate to some extent for H, He, Li, and Be, the very elements that give the best cooling performance.

From Eqs. 7 and 8 we see that the screening parameter χ_α also occurs in the determination of the mean number of collisions and in the expansion parameter B in the theory. Thus an erroneous screening model can also have an effect on the spectrum at angles beyond the region where the q(x) correction is important.

4.4 Nuclear form factors

We expect the scattering angle distribution to be modified when the de Broglie wavelength of the incident particle becomes comparable with or smaller than the radius of the nucleus in the scattering medium [19]. The de Broglie wavelength is 1.1×10^{-13} cm for 186 MeV/c muons. The nuclear radius is given by

$$R_N \approx 1.4 \times 10^{-13} A^{\frac{1}{3}} \quad [cm] \tag{15}$$

where A is the atomic mass number. Thus nuclear size effects should be important for 186 MeV/c muons at some large angle for any material. This effect could be parameterized by multiplying the point nucleus cross section in the theory by a form factor $F_N(\theta)$. For example[2,20]

$$F_N = \frac{1}{\left[1 + \left(\frac{\theta}{\theta_N}\right)^2\right]^4} \tag{16}$$

where θ_N is a characteristic angle for the effect. This function has the value 1 at 0°, 0.96 at $\theta = 0.1\,\theta_N$, and 0.06 at $\theta = \theta_N$. The characteristic angle is given by

$$\theta_N = \frac{\lambda'}{R_N} = \frac{140.7}{p[MeV/c]\ A^{\frac{1}{3}}} \quad \textbf{(17)}$$

This angle for 186 MeV/c muons is 0.76 radians in H and 0.48 radians in Be. This will modify the predicted angular distributions given in Figs. 1 and 2. However, at the angle corresponding to a 10^{-4} probability level, the effect of using the form factor above is only 14% for hydrogen and 16% in beryllium. In addition, since the nuclear form factors act to decrease the probability of large angle scattering from the predicted values, the current version of ICOOL (without the form factor effect included) gives a conservative estimate of the actual scattering.

4.5 What can we learn from the experimental data?

We concentrate here on the electron and muon data since their interpretation is clearer.

We compare in Figs. 3-5 the measured electron scattering data of Andrievsky et al for Al, Be, and Li with our computations of the Moliere theoretical predictions. Fig. 3 shows that the experiment and theory agree well for aluminum, including the tail region out to 0.5 radians. This confirms that the theory works for elements with Z>4, where the Thomas-Fermi model should be adequate. The de Broglie wavelength for the 2.7 MeV/c electrons is $7.3\text{x}10^{-12}$ cm, while the nuclear radius for aluminum is $4.2\text{x}10^{-13}$ cm, so nuclear form factor effects should not modify the spectrum for this data. The comparison for Be in Fig. 4 shows that the measured probability in the tail exceeds the theoretical prediction by ~10% at large angles. However, the data in the large angle tail for Li, shown in Fig. 5, exceed the theoretical prediction by almost a factor of 2 at large angles. The worrisome aspect is the trend and its implication for hydrogen since the discrepancy is growing as Z is decreasing. The most likely explanation for the discrepancy is that the Thomas-Fermi model is giving a poor prediction for χ_α for low Z materials and this is generating an erroneous spectrum, as discussed above.

We show in Table 1 the measured 1/e widths of electrons in Be by Hanson et al. We show for comparison three calculations of the width using Moliere theory. The predictions in the last column were done by me. Nuclear form factor effects should not be important for this data. The measured 1/e width is narrower than the calculations. This would imply that the measured tail would be smaller than the predicted tail, contrary to the results of Fig. 4, but unfortunately no experimental spectrum was presented. In any case the discrepancy for Be was not large. It is possible that impurities in the Be samples could play some role.

The only other low Z measurements are in the high energy hadron beam experiment of Shen et al who found good agreement of the 1/e widths of H and Be with theory. This is the only measurement we have for H.

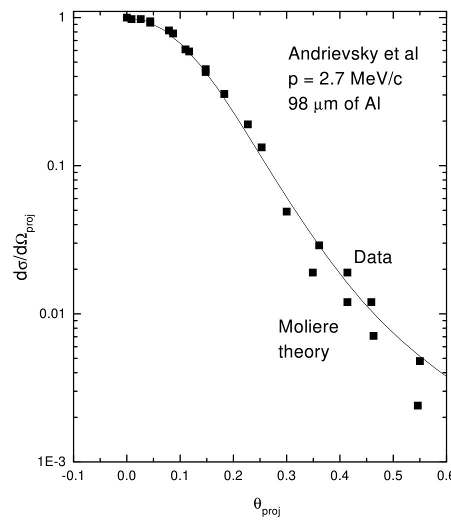

Fig. 3 Comparison of Moliere theory with aluminum data of Andrievsky et al.

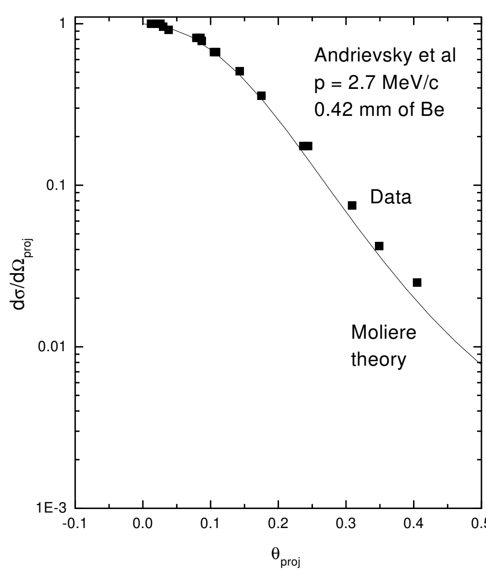

Fig. 4 Comparison of Moliere theory with beryllium data of Andrievsky et al.

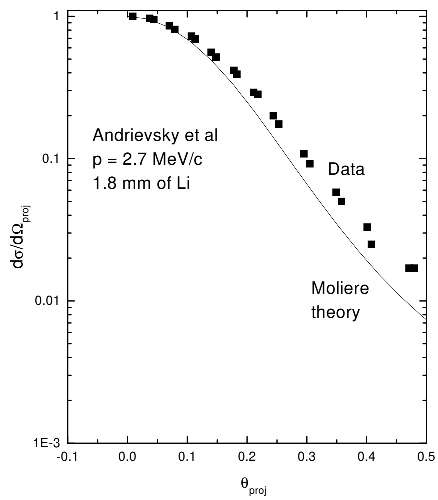

Fig. 5 Comparison of Moliere theory with lithium data of Andrievsky et al.

Table 1 1/e angles [degrees] for beryllium				
thickness [mm]	Hanson et al	Moliere[8]	Moliere[2]	Moliere
1.39	3.06	3.13	3.10	3.19
2.66	4.25	4.57	4.53	4.66

5 Conclusions

The disagreement of the Moliere theory with the Li scattering data of Andievsky et al is particularly worrisome. If the tails of the distribution in hydrogen are also being underestimated by a factor of ~2, we could be overestimating the amount of cooling we expect in the proposed alternating solenoid cooling scheme.

The previous discussions suggest at least three possible improvements to the simulation codes.

(1) We could attempt to develop individual scattering models for hydrogen and the other low Z elements that we plan to use. The easiest implementation would probably be to use specific atomic models to recompute the scattering parameter χ_α , but otherwise use the Moliere formalism, as is[3]. These models could then be used for low Z materials in ICOOL in place of the Moliere model.

(2) For 186 Mev/c muons nuclear form factors should decrease the predicted scattering at large angles by ~15%. This is a sufficiently large effect that we should probably include some form factor correction in ICOOL.

(3) We should also look into modifying ICOOL to set an upper limit on the step size, so that there is negligible probability of violating the small angle approximation used in the theory.

We should also consider including multiple scattering measurements of critical materials as part of the program for the MUCOOL experiment.

Notes and references

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