Modified Moliere's screening parameter and its impact on multiple coulomb scattering

Sergei Striganov
Fermi National Accelerator Laboratory, US

Abstract

The Moliere approximation of elastic Coulomb scattering cross-sections plays an important role in accurate description of multiple scattering, non-ionisation energy, DPA radiation damage etc. The cross-section depends only on a single parameter that describes the atomic screening. Moliere calculated the screening angle for the Tomas-Fermi distribution of electrons in atoms. In this paper, the screening parameter was recalculated using a more accurate atomic form-factor obtained from the self-consistent Dirac-Hartree-Fock-Slater computations. For relativistic particles, the new screening angle can differ from the Moliere approximation by up to 50%. At the same time, it is rather close to other independent calculations. At low energies, the new screening angle is different for positrons and electrons. The positron screening parameter is much larger than the electron one for heavy nuclei at energies of ~Z keV. The impact of the screening angle on particle transport and calculated quantities is discussed.

Introduction

The Moliere's approximation of the elastic Coulomb scattering cross-section plays an important role in an accurate description of the multiple scattering. The cross-section depends only on a single parameter that describes the atomic screening. Moliere [1] calculated the screening angle using Tomas-Fermi model. Since the Tomas-Fermi model is statistical, for light element it cannot provide a high accuracy of calculation. More precise results can be obtained within the Hartree-Fock approach. It takes into account individual properties of atoms – in particular, their shell structure. Salvat et al. [2] proposed a simple analytical approximation for the atomic screening functions depending on five parameters which are determined from the results of Dirac-Hartree-Fock-Slater calculations. In this study we recalculate Moliere screening angle using this approximation. The impact of new values of screening parameters on Moliere's theory prediction is considered.

Moliere screening angle

Using Salvat et al. approximation [2], the atomic form factor can be written as:

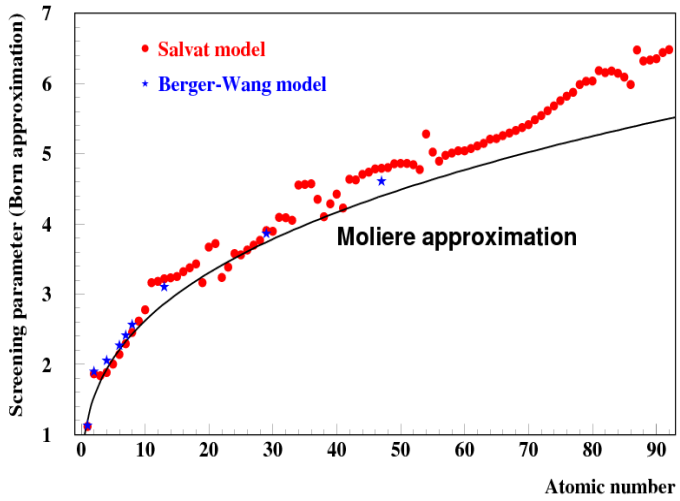
$$F_a(q) = \sum_{i=1}^{3} A_i \alpha_i^2 / (\alpha_i^2 + q^2), \qquad (1)$$

where $\boldsymbol{q}$ - momentum transfer. After tedious algebra, one finds that in the Born approximation the Moliere "screening angle" reads:

$$\chi_{HF}^{B} = m_e \alpha \chi_0 / p$$
$$\ln \chi_0 = \sum_{i=1}^{3} A_i (\ln \alpha_i - 0.5) + 2A_1A_2(\alpha_2^2 \ln \alpha_2 - \alpha_1^2 \ln \alpha_1)/(\alpha_2^2 - \alpha_1^2) + \quad (2)$$
$$2A_1A_3(\alpha_3^2 \ln \alpha_3 - \alpha_1^2 \ln \alpha_1)/(\alpha_3^2 - \alpha_1^2) + 2A_2A_3(\alpha_3^2 \ln \alpha_3 - \alpha_2^2 \ln \alpha_2)/(\alpha_3^2 - \alpha_2^2) - 0.5$$

where $\boldsymbol{p}$ – projectile momentum, α – fine structure constant, $\boldsymbol{m_e}$ – electron mass. Figure 1 presents the screening parameter χ_o calculated using Equation (2) and parameters obtained in [2].

Figure 1. Screening parameter χ_o in Born approximation



For the determination of the screening angle, Moliere [1] uses his own calculation of the single scattering by a Tomas-Fermi potential. Berger and Wang [3] calculated the correction to Moliere's approximate formula using a modern version of Moliere's method and Hartree-Fock potential. In Figure 1, we compare the screening parameter calculated using different atomic form factors in Born approximation. One can see that the models based on Hartree-Fock form factors are in good agreement. HF screening parameter is larger than Moliere's one, but the difference exceeds 20% for helium only.

The Coulomb correction is the difference between the values of parameters calculated in the eikonal approximation and in Born approximation. An exact formula for the differential cross-section in terms of an integral is given in Moliere's paper [1], but his final evaluation of integral is numerical and only approximate. Recently, Kuraev et al. [4] have found an exact solution in the ultra-relativistic limit. Their result reveals significant deviation from Moliere's approximation for sufficiently heavy elements.

Fernandez-Varea et al. [5] proposed an accurate formula for elastic Coulomb scattering based on the Hartree-Fock atomic form factor for electrons/positrons with energies larger Z keV. This cross-section is used in the popular PENELOPE code [6] for simulation of the multiple Coulomb scattering. To improve an agreement with precise partial wave calculation they introduced a correcting factor $t(\beta,Z)$ which can be considered as estimate of Coulomb correction. Note that the above mentioned correction factor depends on particle charge. It can be shown that in the small angle approximation the screening angle reads

$$\chi_{HF} = \chi_{HF}^{B} \cdot t(\beta, z) \quad (3)$$

In the ultra-relativistic limit difference between positive and negative particle is not large. As shown in Figure 2, the "Coulomb correction" calculated according to Equation (3) is close to results of Dubna group [4], but at large Z is lower than Moliere Coulomb correction by about 10%.

Figure 2. Coulomb correction in ultra-relativistic limit

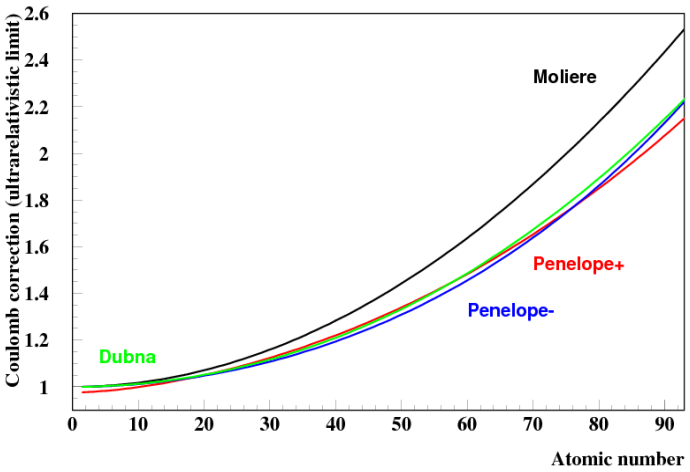


Figure 3 presents a comparison of the screening parameters calculated by different approaches for ultra-relativistic particles. The most prominent difference is seen for low-Z nuclei. HF screening angle squared is larger than Moliere one for heavy nuclei by ~20%.

Seltzer [7] has compared the transport cross-section obtained using Moliere approach and exact phase shift calculations. He found that agreement can be generally improved by making a strictly empirical adjustment to Moliere's screening angle. Seltzer's correction significantly decreases the screening angles for electrons at low energies as approach proposed by Fernandez-Varea et al. [5].

Figure 3. X^2_{HF}/X^2_M in ultra-relativistic limit

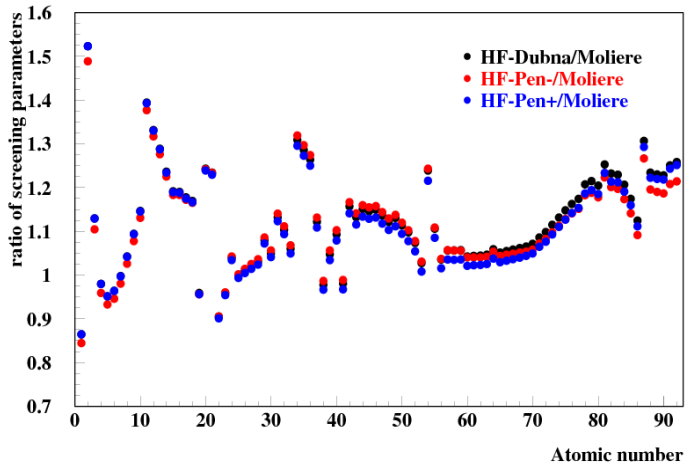
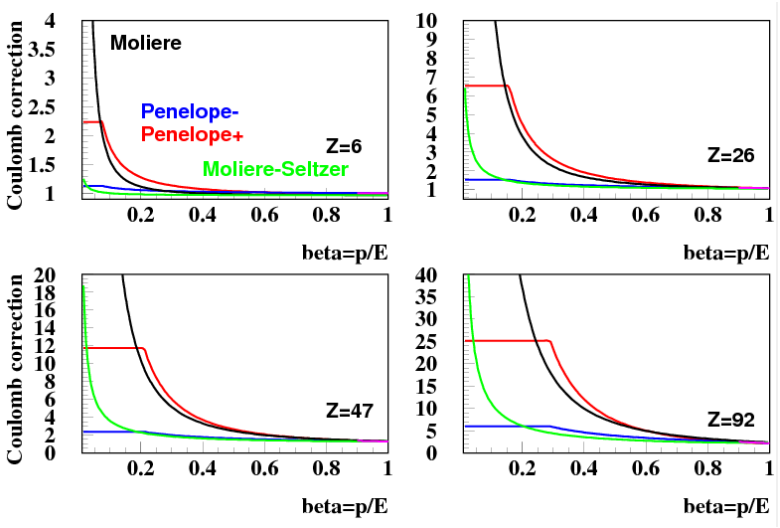


Figure 4 shows the energy dependence of the screening angle calculated by the different approaches. It is seen that Seltzer model [7] is close to Penelope correction [5] for electrons. For positive particles Moliere and Penelope results are rather similar also. Note that at low energies, Coulomb correction for positive particles is much larger than for negative.

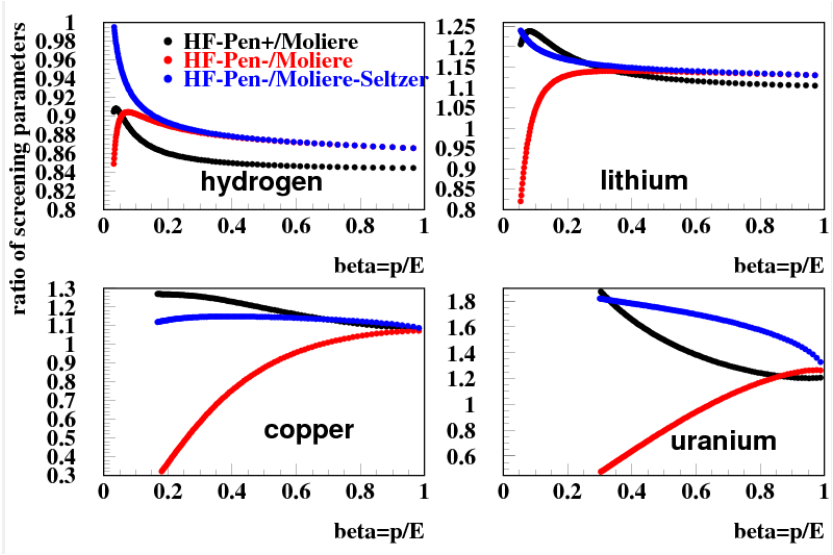
Figure 4. Energy dependence of Coulomb corrections



For energies less than Z keV, the accuracy of Penelope correction factor [5] progressively deteriorates. However, the Penelope approximation still yields reasonable results for electron/positron second transport cross-section if the correction factor $t(\beta,Z)$ is evaluated using the value of velocity β corresponding to a kinetic energy E_c=0.25Z when $E<E_c$ [5].

The energy dependence of the screening angle is shown in Figure 5. It is seen that the new screening parameter (3) is very different from Moliere's one for slow particles especially for heavy nucleus.

Figure 5. Energy dependence of X^2_{HF}/X^2_M



Sensitivity of the angular distribution width to screening angle

In Moliere theory the angular distribution depends only on a single parameter B. It is defined by transcendental equation:

$$B = \ln B - 0.1544 + \ln \Omega; \quad \Omega = \frac{\chi_c^2}{\chi_M^2} \tag{4}$$

Ω is mean number of scattering events that occur in thickness z. An approximative interpolation solution of Equation (4) reads [8]:

$$B = 1.153 + 2.583 \log_{10} \Omega \tag{5}$$

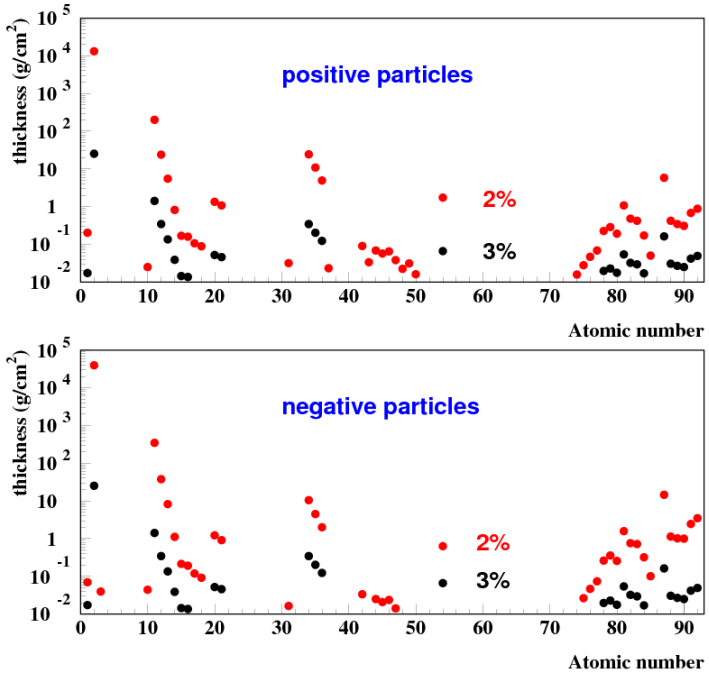
Now, we can estimate sensitivity of parameter B to value of screening angle:

$$\frac{B_{HF}}{B_M} = 1 + \frac{\ln(\chi_{HF}^2 / \chi_M^2)}{1.027 + \ln \Omega} \tag{6}$$

For large thickness even a large error in the definition of the screening parameter does not change prediction of Moliere theory. It should be noted that Moliere theory can be applied for foil thickness corresponding to large number of scatterings only, Ω>100.

Using Equation (4) we can predict the ratio of the angular distribution width calculated by Moliere prescription and more precise Hartree-Fock screening angle (3). Figure 6 shows the thicknesses where the ratio reaches 2% and 3% for relativistic particles. If one needs to know the angular distribution parameters with precision about 3%, new screening angle (3) should be used for rather low thicknesses, usually less than 1 g/cm2. If the better accuracy is needed, the newly defined values of the screening parameter can improve the quality of calculation at the larger thickness also.

Figure 6. Three percent and two percent thicknesses for positive and negative projectiles



Conclusion

Moliere's screening angle was recalculated using a precise approximation of the partial wave differential cross-section [5]. Our results are in close agreement with other estimates [3,4,7]. The deviation from Moliere approximation [1] could reach factor 2 at lower energies. The new screening angle depends on the particle charge. Positron screening angle is about 5 times larger than electron's one in large Z material and low momentum. Because of the generally logarithmic dependence of the angular distribution width on the screening parameter the ultimate effect of using more precise screening model is small. The accuracy of experiment to date (a few percent) is not enough to resolve difference between Moliere's and our approaches. But the angular distribution after very thin foils (see Figure 6) is predicted more accurately with newly defined screening parameter (3).

Acknowledgements

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References

[1] G. Moliere (1948), "Theorie der Streuung schneller geladener Teilchen II. Mehrfach- und Vielfachstreuung", *Z. Naturforsch.*, 3a, pp. 78-97.

[2] F. Salvat, J.D. Martinez, R. Moyol, J. Parellada (1987), "Analytical Dirac-Hartree-Fock-Slater screening function for atoms (Z=1-92)", *Phys. Rev.*, A36, pp. 467-474.

[3] M.J. Berger, R. Wang (1988), "Multiple-Scattering Angular Deflections and Energy-Loss Stragling", *Monte Carlo transport of Electrons and Photons, eds. T.M. Jenkins, W.R.Nelson, A. Rindi (Plenum Press, New York)*.

[4] A. Tarasov, O. Voskresenskaya (2012), "An Improvement of the Moliere-Fano multiple scattering theory", *arXiv:1107.5018 [hep-ph]*.

[5] J.M. Fernandez-Varea, R. Moyol and F. Salvat (1993), "Cross sections for elastic scattering of fast electrons and positrons by atoms", *Nucl. Meth.*, B82, pp. 39-45.

[6] F. Salvat, J.M. Fernandez-Varea, J. Sempau (2011), "PENELOPE-2011: A Code System for Monte Carlo Simulation of Electron and Photon Transport", *OECD NEA Data Bank/NSC DOC(2011)/5*.

[7] S.M. Seltzer (1988), "An Overview of ETRAN Monte Carlo Methods", *Monte Carlo transport of Electrons and Photons, eds. T.M. Jenkins, W.R.Nelson, A. Rindi (Plenum Press, New York)*.

[8] W.T. Scott (1963), "The Theory of Small-Angle Multiple Scattering of Fast Charged Particles", *Rev. Mod. Phys.*, 35, pp. 231-313.