Modified Moliere's Screening Parameter and its Impact on Multiple Coulomb Scattering

SATIF-12

S.I.Striganov, ***Fermilab, Batavia, IL 60510, U.S.A***

Introduction

The Moliere's approximation of elastic Coulomb scattering cross section plays an important role in accurate description of multiple scattering, non-ionization energy loss, radiation damage. The cross section depends only on a single parameter that describes the atomic screening. Moliere 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 propose a simple analytical approximation for atomic screening function 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.

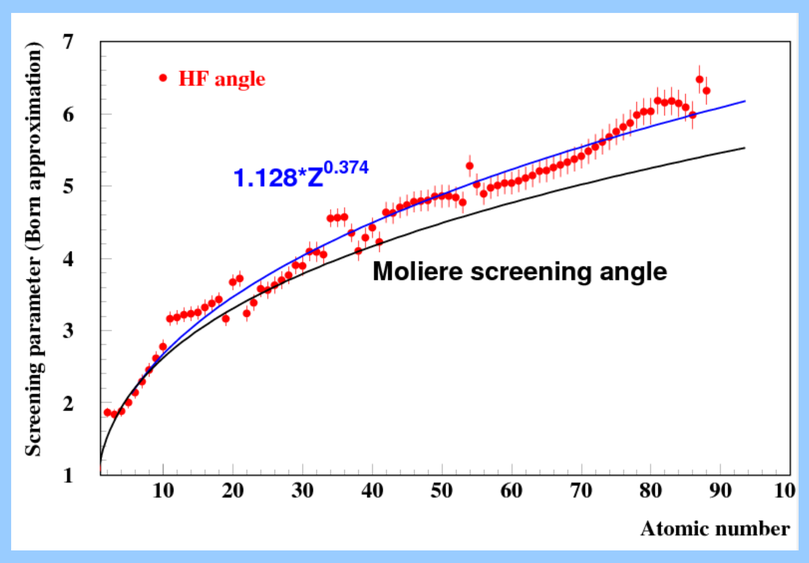
Moliere "screening angle"

Using Salvat et al approximation, atomic form factor can be written as

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

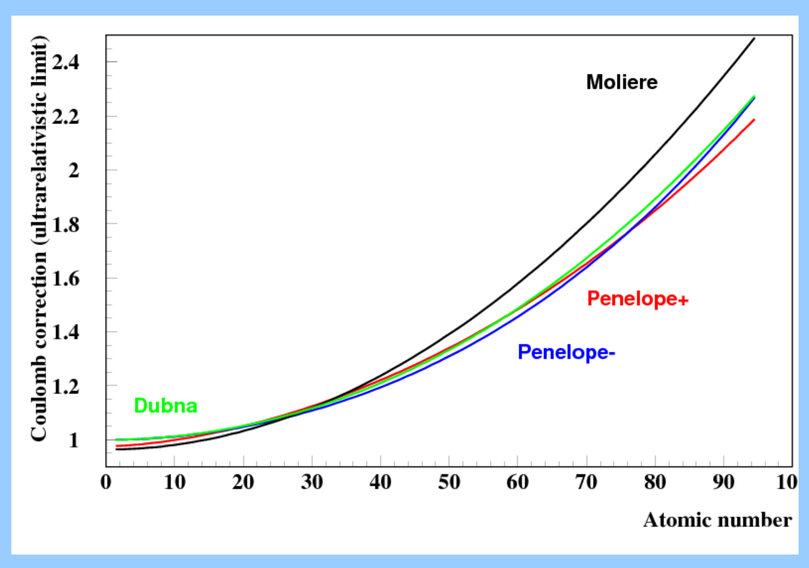
In the Born approximation the Moliere "screening angle" reads

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



It is difficult to approximate the Hartree-Fock (HF) screening angle by a simple expression with accuracy better than 5%.

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, but his final evaluation of integral is numerical and only approximate. Recently, Kuraev et al have found exact solution in the ultrarelativistic limit. Their result reveals significant deviation from Moliere's approximation for sufficiently heavy elements.



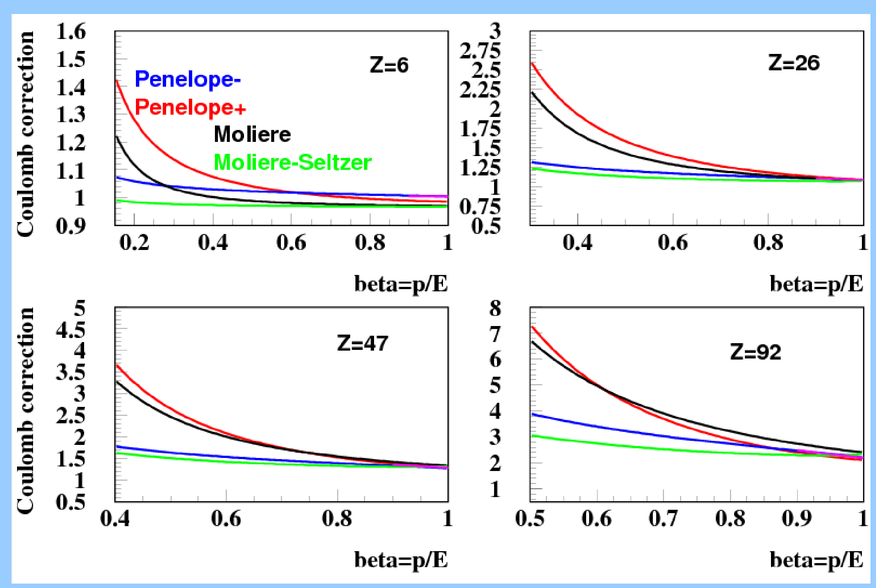
Fernandez-Varea et al proposed a precise form for elastic Coulomb scattering based on Hartree-Fock atomic formfactor for electrons/positrons with energy > Z keV

$$\frac{d\sigma}{d\Omega} = \frac{d\sigma_R}{d\Omega} R(\theta)(1 - F_a(t^{-1}q))^2 F_n^2(q) \qquad (3)$$

First factor is the relativistic Rutherford differential cross section, which describes the scattering of a spinless particle in the Coulomb potential of a bare point nucleus. Second factor is Mott spin correction. Third factor accounts for the screening of the nuclear field by atomic electrons. Last factor is nuclear formfactor. The parameter *t* is introduced to improve agreement with precise partial wave calculation. This cross section is used in popular PENELOPE code for simulation of multiple Coulomb scattering

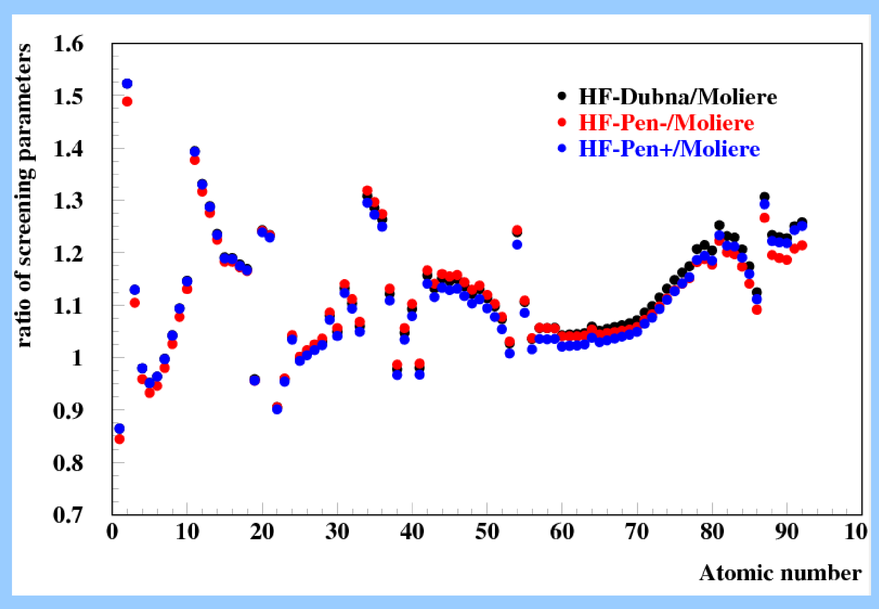
Moliere "screening angle" obtained from the cross section (3) is similar to formula (2) except for additional *ln(t)* term. Note, that parameter *t* depends on particle charge. In the ultrarelativistic limit difference between positive and negative particle is not large. "Coulomb correction" is closed to results of Dubna group (Kuraev et al).

Seltzer compared the transport cross section obtained using Moliere approach and exact phase shift calculations. He found that agreement can be generally appoved by making a strictly empirical adjustment to Moliere's screening angle



It is seen that Seltzer model is close to Penelopa correction for electrons. For positive particles Moliere and Penelopa results are rather similar. Note that at low energies, screening parameter for positive particles is about 2 times larger than for negative.

Let's compare screening angle calculated by different methods for ultrarelativistic particles.



As we expected, the most prominent difference is seen for low Z nuclei. HF screening parameter larger about 30% than Moliere one for heavy nuclei also.

Next plot presents the ratio of screening parameters obtained by different methods. It is seen, that difference between HF and Moliere screening angles rises at low energies. Moliere-Seltzer

Sensitivity of 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

$$B = \ln B - 0.1544 + \ln \Omega$$
$$\Omega = \chi_c^2 / \chi_a^2 \qquad (4)$$

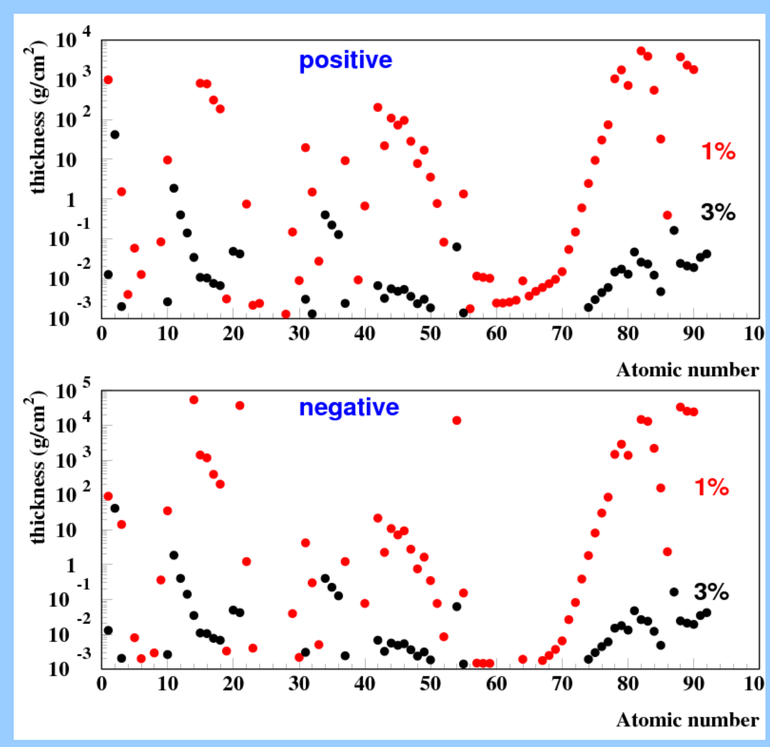
Ω - the mean number of scattering that occur in thickness z a solution of equation (4) reads

$$B = 1.153 + 2.583 \log_{10} \Omega \qquad (5)$$

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

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

So, for large thickness even large error in definition of screening parameter does not change prediction of Moliere theory. Using equation (6) we can calculate thickness where width of angular distribution calculated using Moliere prescription agree better than 1,3% with width calculated with more precise Hartree-Fock screening parameter. Next figures shows above thicknesses for relativistic particles.



If one needs to know the angular distribution parameters with precision about 3%, new precise "screening" angle could be useful for small thickness lower than 1 g/cm2. But if precision about 1% is needed the newly defined values of a screening parameter can improve quality of calculation at large thickness also.