Molière’s multiple scattering theory revisited

O. Voskresenskaya* and A. Tarasov

Joint Institute for Nuclear Research, 141980 Dubna, Russia

Abstract

A part of Molière’s multiple scattering theory concerning the determination of the screening angular parameter is revised. An universal form of the Coulomb corrections to the screening angle, the exponential part of the distribution function, and the angular distribution is discussed within the small-angle approximation of this theory. The accuracy of the Molière theory in determining the screening angle is estimated.

1 Introduction

The theory of multiple scattering of fast charged particles by atoms is of importance in analysis of experimental results for many high-energy experiments, such as [1] etc. Precise measurements of multiple scattering effect in these experiments requires adequate accuracies in their theoretical description.

Multiple scattering of charged particles in the Coulomb field of nuclei is described by a number of theoretical treatments [2–6]. The various theories differ mainly in their treatment of the single scattering law. The Molière method is independent of the exact form of the single scattering law, but contains a model-dependent parameter representing the atomic screening, the so-called ‘screening angular parameter’ $\chi_a$, which enters into other important quantities of the Molière theory.

Molière calculated his screening parameter by using the Thomas–Fermi potential and the WKB method. He obtained an approximate expression for this parameter

$$\chi_a \approx \chi_B \sqrt{1 + 3.34 \left( \frac{Z\alpha}{\beta} \right)^2},$$

valid to second order in $a = Z\alpha/\beta$, where only first term is determined quite accurately, while the coefficient in the second term is found numerically and approximately.

In the present work, we have obtained for $\chi_a$ and some other quantities of the Molière theory rigorous results valid in all orders of the parameter $a$. In other words, we have found analytical expressions for the so-called ‘Coulomb corrections’ to the Born results. Also, we have evaluated numerically these Coulomb corrections and studied their $Z$-dependence. In addition, we have estimated the accuracy of the Molière theory in determining the screening angle $\chi_a$.

The outline of the paper is as follows. In Sections 2–4, we review some basic results of [3], i.e., solving the transport equation (Sec. 2), Molière’s expansion method (Sec. 3), and determining the screening parameters by Molière (Sec. 4). The results of the present work are given in Sections 5–6. In Sec. 5, we consider another determination of the screening parameters allowing to obtain rigorous relations between their exact and Born values. In Sec. 6, we evaluate the numerical values of the obtained Coulomb corrections in the range $Z = 4$ to $Z = 82$. Also, we estimate the accuracy of the Molière theory in determining the screening angle. Finally, in Sec. 7, we summarize the main results of this work. In Appendix, we present an alternative way of obtaining the approximate solution of the transport equation for the thick targets.

*On leave of absence from Siberian Physical Technical Institute. Electronic address: voskr@jinr.ru
2 The transport equation and its solution

The basis for studies of multiple scattering effects in a nearly-isotropic and quasi-homogeneous medium by the transport equation method is the Boltzmann transport equation often used in statistical physics of systems with a large number of degrees of freedom. It can be used as well in the relativistic Molière scattering problem \[4, 5\] within the semiclassical approach to particle transport in matter.

Let all scattering angles are small \( \theta \ll 1 \) so that \( \sin \theta \sim \theta \), and \( \sigma(\chi) \) be the elastic differential cross section for the single scattering into the angular interval \( \vec{\chi} = \vec{\theta} - \vec{\theta}' \). Define now \( W_M(\theta,t) \) as the number of scattered particles in the interval \( d\theta \) after traversing a thin homogeneous foil of thickness \( t \). Then can be used the standard transport equation \[4\]:

\[
\frac{\partial W_M(\theta, t)}{\partial t} = -n_0 W_M(\theta, t) \int \sigma(\chi) d^2 \chi + n_0 \int W_M(\vec{\theta} - \vec{\chi}, t) \sigma(\chi) d^2 \chi,
\]

(2)

where \( n_0 = (N_A \rho)/M \) (cm\(^{-3}\)) is the number density with the Avogadro number \( N_A = 6.02 \times 10^{23} \) mol\(^{-1}\), the mass density of the target matter \( \rho \) measured in units g/cm\(^3\), and the molar mass of target atoms \( M \) (g/mole). The quantity \( n_0 \) is the number of the target atoms per cm\(^3\).

Following Molière, we introduce the Fourier–Bessel transformation of distribution and get to the distribution function \( W_M(\theta, t) \) a general expression

\[
W_M(\theta, t) = \int_0^\infty J_0(\theta \eta) g(\eta, t) \eta d\eta,
\]

(3)

in which

\[
g(\eta, t) = \exp[N(\eta, t) - N_0(0, t)],
\]

(4)

\( \theta \) is the polar angle between the track of a scattered particle and the initial direction \( z \), \( \eta \) is the Fourier transform variable corresponding to \( \theta \), and the Bessel function \( J_0 \) is an approximate form for the Legendre polynomial appropriate to small scattering angles \[3, 4\].

In the notation of Molière,

\[
N(\eta, t) = 2\pi n_0 t \int_0^\infty \sigma(\chi) J_0(\chi \eta) \chi d\chi,
\]

(5)

and \( N_0 \) is the value of (5) for \( \eta = 0 \), i.e., the total number of collisions

\[
N_0(0, t) = 2\pi n_0 t \int_0^\infty \sigma(\chi) \chi d\chi.
\]

(6)

The magnitude of \( N_0 - N \) is much smaller than \( N_0 \) for values \( \eta \), which are important. It can be called ‘the effective number of collisions’.

Inserting (4)–(6) back into (3), we have

\[
W_M(\theta, t) = \int_0^\infty \eta d\eta J_0(\theta \eta) \exp\left[-2\pi n_0 t \int_0^\infty \sigma(\chi) \chi d\chi [1 - J_0(\chi \eta)]\right].
\]

(7)

This equation is exact for any scattering law, provided only the angles are small compared with a radian, and is equivalent to Lewis’ result \[2\].

For \( g(\eta, 0) = 1 \) and all \( \eta \), the expressions (3)–(6) can be rewritten as follows:

\[
W_M(\theta, t) = \int_0^\infty J_0(\theta \eta) e^{-n_0 t Q(\eta)} \eta d\eta,
\]

(8)
\[ Q(\eta) = 2\pi \int_0^\infty \sigma(\chi)[1 - J_0(\chi\eta)]\chi d\chi. \] (9)

This result is mathematically identical to the result of Snyder and Scott for the distribution of projected angles \[3\].

3 Molière’s expansion method

One of the most important results of the Molière theory is that the scattering is described by a single parameter, the so-called ‘screening angle’ \(\chi_a\) or \(\chi'_a\):

\[ \chi'_a = \sqrt{1.167}\chi_a = [\exp (C_e - 0.5)]\chi_a \approx 1.080\chi_a, \] (10)

where \(C_e = 0.57721\) is the Euler constant.

More precisely, the angular distribution \(W_M(\theta)\theta d\theta\) depends only on the logarithmic ratio of the ‘characteristic angle’ \(\chi_c\) describing the foil thickness to the ‘screening angle’, which describes the scattering atom:

\[ b = \ln \left(\frac{\chi_c}{\chi_a}\right)^2 \equiv \ln \left(\frac{\chi_c}{\chi_a}\right)^2 + 1 - 2C_e \sim \ln N_0. \] (11)

The screening angle \(\chi_a\) can be determined approximately by the relation

\[ \chi_a^2 \approx \chi_0^2 \left(1.13 + 3.76 a^2\right) = (\chi_a^0)^2 \left(1 + 3.34 a^2\right) \] (12)

with the so-called ‘Born parameter’ \(a = Z\alpha/\beta\). The second term in (12) represents the deviation from the Born approximation. If the value of this term equal to zero, the screening angle becomes \(\chi_a = \chi_a^0 = \chi_0\sqrt{1.13}\).

The angle \(\chi_0\) is defined by

\[ \chi_0 = 1.13 \frac{Z^{1/3} m}{137; p} = \frac{Z^{1/3} m\alpha}{0.885 p}, \] (13)

where \(p = mv\) is the incident particle momentum, and \(v\) is the particle velocity in the laboratory frame.

The characteristic angle is defined as

\[ \chi_c^2 = 4\pi\alpha a k \left(\frac{Z\alpha}{\beta p}\right)^2. \] (14)

Its physical meaning is that the total probability of single scattering through an angle greater than \(\chi_c\) is exactly one.

Putting \(\chi_c\eta = y\) and setting \(\theta/\chi_c = u\), we get Molière’s transformed equation

\[ W_M(\theta)\theta d\theta = u du \int_0^\infty y dy J_0(uy) e^{-y^2/4} \left\{ b - \ln \left(\frac{y^2}{4}\right)\right\}, \] (15)

for the most important values of \(\eta\) of order of \(1/\chi_c\). This equation is much simpler than (14).

In order to obtain a result valid for large all angles, Molière defines a new parameter \(B\) by the transcendental equation

\[ B - \ln B = b. \] (16)
The angular distribution function can then be written as

\[ W_M(\theta, B) = \frac{1}{\bar{\theta}^2} \int_0^\infty y dy J_0(\theta y) e^{-y^2/4} \exp \left[ \frac{y^2}{4B} \ln \left( \frac{y^2}{4} \right) \right]. \]  

(17)

The Molière expansion method is to consider the term \( y^2 \ln(y^2/4)/4B \) as a small parameter. This allows expansion of the angular distribution function \( W_M \) in a power series in \( 1/B \):

\[ W_M(\theta, t) = \sum_{n=0}^{\infty} \frac{1}{B^n} W_n(\theta, t) \]  

(18)

with

\[ W_n(\theta, t) = \frac{1}{\bar{\theta}^2} \int_0^\infty y dy J_0(\theta y) e^{-y^2/4} \left[ \frac{y^2}{4} \ln \left( \frac{y^2}{4} \right) \right]^n, \]  

(19)

\[ \bar{\theta}^2 = \chi^2 c_B = 4\pi n_0 \left( \frac{Z\alpha}{pv} \right)^2 B(t). \]

This method is valid for \( B \geq 4.5 \) and \( \bar{\theta}^2 < 1 \). The first function \( W_0(\theta, t) \) has a simple analytical form:

\[ W_0(\theta, t) = \frac{2}{\bar{\theta}^2} \exp \left( -\frac{\bar{\theta}^2}{\theta^2} \right), \]  

(20)

\[ \bar{\theta}^2 \sim t \to \infty t \ln t. \]  

(21)

For small angles, i.e., \( \theta/\bar{\theta} = \theta/(\chi \sqrt{B}) \) less than about 2, the Gaussian (20) is the dominant term. In this region, \( W_1(\theta, t) \) is in general less than \( W_0(\theta, t) \), so that the corrections to the Gaussian is of order of \( 1/B \), i.e., of order of 10%. An alternative way of obtaining the approximate solution (20) of (7) for a thick target is given in Appendix.

A good approximate representation of the distribution for any angle is \( W_0(\theta, t) + B^{-1}W_1(\theta, t) \), where

\[ W_1(\theta, t) = \frac{2}{\bar{\theta}^2} \exp \left( -\frac{\bar{\theta}^2}{\theta^2} \right) \left\{ \left[ \frac{\bar{\theta}^2}{\theta^2} - 1 \right] \left[ Ei \left( \frac{\bar{\theta}^2}{\theta^2} \right) - \ln \left( \frac{\bar{\theta}^2}{\theta^2} \right) \right] + 1 \right\} - 2, \]  

(22)

\[ Ei(\Theta) = Ei(\Theta) + \pi i \]  

(23)

with the exponential integral [7]

\[ Ei(\Theta) = - \int_{-\Theta}^{\infty} e^{-t} \frac{dt}{t}. \]  

(24)

4 Molière’s determination of the screening parameters

On the one hand, Molière writes the elastic Born cross section for the fast charged particle scattering in the atomic field as follows:

\[ \sigma^a(\chi) = \sigma^a(\chi) \left( 1 - \frac{F_1(p\chi)}{Z} \right)^2 = \sigma^a(\chi) q^a(\chi). \]  

(25)
For angles \( \chi \) small compared with a radian, the exact Rutherford formula has a simple approximation:

\[
\sigma^n(\chi) = \frac{\theta^2}{4\pi n_0(1 - \cos \chi)^2} q^n(\chi) \tag{26}
\]

\[
\approx \frac{\theta^2}{\pi n_0} q^n(\chi). \tag{27}
\]

Here, \( F_A \) is the atomic form factor and \( q^n(\chi) \) is the ratio of actual to the Rutherford scattering cross sections in the Born approximation.

Then the screening angle \( \chi^a_{\alpha} \) in the Born approximation one can represent via \( F_A \) or \( q^n(\chi) \) by the equations

\[
- \ln (\chi^a_{\alpha}) = \lim_{\varsigma \to \infty} \left[ \int_0^\varsigma \left( 1 - \frac{F_A(p\chi)}{Z} \right)^2 \frac{d\chi}{\chi} + \frac{1}{2} - \ln \varsigma \right] \tag{28}
\]

\[
= \lim_{\varsigma \to \infty} \left[ \int_0^\varsigma \frac{q^n(\chi)d\chi}{\chi} + \frac{1}{2} - \ln \varsigma \right] \tag{29}
\]

with an angle \( \varsigma \) such as

\[
\chi_0 \ll \varsigma \ll 1/\eta \sim \chi_c. \tag{30}
\]

Molière’s approximation for the Thomas–Fermi form factor \( F_T - F(q) \) with momentum transfer \( \vec{q} \) can be written as

\[
F_T - F(q) = \sum_{i=1}^{3} \frac{c_i \lambda^2_i}{q^2 + \lambda^2_i}, \tag{31}
\]

in which

\[
c_1 = 0.35, \quad c_2 = 0.55, \quad c_3 = 0.10,
\]

\[
\lambda_1 = 0.30\lambda, \quad \lambda_2 = 4\lambda_1, \quad \lambda_3 = 5\lambda_2.
\]

When the Born parameter becomes zero, the equation (28) for the screening angle can be evaluated directly, using the facts that \( q(0) = 0 \) and \( \lim_{\varsigma \to \infty} q^{\alpha}(\varsigma) = 1 \). Then with use of (25) and (31), can also be obtained the following approximation for \( (\chi^a_{\alpha})^n \) [3, 5]:

\[
(\chi^a_{\alpha})^n = \left[ \exp(C_E - 0.5) \right] \frac{\lambda}{\rho} A = \sqrt{1.174} \chi_0 A, \tag{32}
\]

where \( \lambda = m_e\alpha Z^{1/3}/0.885 \). Note that a misprint is admitted in [3, 4], i.e. the factor \( A = 1.0825 \) in [32] should be replaced by \( A = 1.065 = \sqrt{1.15} \).

On the other hand, Molière writes the nonrelativistic Born cross section in the form

\[
\sigma^n(\chi) = k^2 \int_0^\infty \rho d\rho J_0 \left( 2k\rho \sin \frac{\chi}{2} \right) \Phi^n_\alpha(\rho)^2 \tag{33}
\]

where the Born phase shift is given in units of \( \hbar = c = 1 \) by

\[
\Phi^n_\alpha(\rho) = -\frac{2}{\sqrt{\rho^2}} \int_0^\infty \frac{U_\alpha(r)dr}{\sqrt{r^2 - \rho^2}} = -\frac{1}{v} \int_{-\infty}^\infty U_\alpha \left( r = \sqrt{\rho^2 + z^2} \right) dz. \tag{34}
\]
Here, \( k \) is the wave number of the incident particle, the variable \( \rho \) corresponds to the impact parameter of the collision, and \( U_\lambda(r) \) is the screened Coulomb potential of the target atom

\[
U_\lambda(r) = \pm Z \frac{\Lambda(\lambda r)}{r}
\]

with Molière’s fit to the Thomas–Fermi screening function \( \Lambda(\lambda r) \)

\[
\Lambda(\lambda r) \simeq 0.1e^{-0.3\lambda r} + 0.55e^{-1.2\lambda r} + 0.35e^{-0.1\lambda r}.
\]

In order to obtain a result valid for large \( a \) and also for large angles \( \chi \), Molière uses the WKB technique in his calculations of the screening angle.

Exact formulas for the WKB differential cross section \( \sigma(\chi) \) and the corresponding \( q(\chi) \) are given in Molière’s paper [3] as follows:

\[
\sigma(\chi) = k^2 \left| \int_0^\infty \rho \, dp \, J_0(k \rho) \left\{ 1 - \exp \left[ i \Phi_M(\vec{\rho}) \right] \right\} \right|^2,
\]

\[
q(\chi) = \frac{(k\chi)^2}{4a^2} \left[ \int_0^\infty \rho \, dp \, J_0(k \rho) \left\{ 1 - \exp \left[ i \Phi_M(\vec{\rho}) \right] \right\} \right]^2
\]

with the phase shift given by

\[
\Phi_M(\vec{\rho}) = \int_{-\infty}^{\infty} \left[ k_\rho(r) - k \right] dz,
\]

where \( k_\rho(r) \) is the relativistic wave number for the particle at a distance \( r \) from the nucleus, and the quantity \( \rho \) is seen to be impact parameter of the trajectory or ‘ray’. As before, \( k \) is the initial or asymptotic value of the wave number.

When \( k_\rho(r) \) is expanded as a series of powers of \( U_\lambda(r)/k \), the first-degree term yields the same expression for \( \Phi_M(\vec{\rho}) \) as (31). The Born approximation for (37) is obtained by expanding the exponential in (38) to first order in the Born parameter \( a \).

The relations (27) and (29) between the quantities \( \sigma^a(\chi) \), \( q^a(\chi) \), and \( \chi^a \) remain valid for the quantities \( \sigma(\chi) \), \( q(\chi) \), and \( \chi \).

Despite the fact that the formulas (37) and (38) are exact, evaluation of these quantities was carried out by Molière only approximately. To estimate (38), Molière used the first-order Born shift (44) with (35) and (36), what is good only to terms of first order in \( a \), and he found

\[
q(\chi) \approx 1 - \frac{4ia(1-ia)}{(\chi/\chi_0)^2} \left\{ -0.81 + 2.21 \left[ -\Re[\psi(ia)] - \frac{1}{1-ia} + \frac{1}{2ia} + \log \frac{\chi}{2\chi_0} \right] \right\}^2.
\]

Here, \( \psi \) is the so-called ‘digamma function’, i.e., the logarithmic derivative of the \( \Gamma \)-function \( \psi(x) = d\ln \Gamma(x)/dx \).

He has fitted a simple formula to the function \( \Re[\psi(ia)] \) from (40):

\[
\Re[\psi(ia)] \simeq \frac{1}{4} \log \left( a^4 + \frac{a^2}{3} + 0.13 \right).
\]

Inserting (41) into (40) and neglecting terms of orders higher than \( a^2 \), he got

\[
q(\chi) \approx 1 - \frac{8.85}{(\chi/\chi_0)^2} \left[ 1 + 2.303 a^2 \log \frac{7.2 \cdot 10^{-4}(\chi/\chi_0)^4}{(a^2 + a^2/3 + 0.13)} \right].
\]
Molière has calculated $q(\chi)$ for different $a$ values. As a result, he has devised an interpolation scheme based on a linear relation between $(\chi/\chi_0)^2$ and $a^2$ for fixed $q$:

$$(\chi/\chi_0)^2 \approx A_q + a^2 B_q.$$  

(43)

Calculating the screening angle defined by

$$-\ln (\chi_a) = \frac{1}{2} + \lim_{\varsigma \to \infty} \left[ \frac{1}{\varsigma} \int_0^\frac{\varsigma}{\chi} \frac{q(\chi) d\chi}{\chi} - \ln \varsigma \right] = \frac{1}{2} - \ln \chi_0 - \int_0^1 d\zeta \ln \left( \frac{\chi}{\chi_0} \right)$$  

(44)

and assuming a linear relation between $\chi_a^2$ and $a^2$, Molière writes finally the following interpolating formula for the screening angle:

$$\chi_a \approx \chi_0 \sqrt{1.13 + 3.76 a^2}.$$  

(45)

Critical remarks to his derivation of this result are given in [5, 6].

5 Alternative determining the screening parameters

To obtain an exact correction to the first-order Born screening angle $(\chi'_a)^n$, we will carry out our analytical calculation in terms of the function $Q(\eta)$:

$$Q(\eta) = 2\pi \int_0^\infty \sigma(\chi)[1 - J_0(\chi\eta)] d\chi \equiv \int d^2 \rho \left[ 1 - \cos[\Delta \Phi(\vec{\rho}, \vec{\eta})] \right]$$  

(46)

where the phase shift can be determined by the equation

$$\Delta \Phi(\vec{\rho}, \vec{\eta}) = \Phi(\rho_+) - \Phi(\rho_-), \quad \vec{\rho}_\pm = \vec{\rho} \pm \vec{\eta}/2.$$  

(47)

Substituting the expression for the cross section

$$\sigma(\chi) = \frac{\chi^2}{\pi n_0 t \chi^4} q(\chi)$$  

(48)

into (46), we rewrite it in the form:

$$n_0 t Q(\eta) = 2\chi_c^2 \int_0^\infty [1 - J_0(\chi\eta)] q(\chi) \chi^{-3} d\chi.$$  

(49)

For the important values of $\eta$ of order of $1/\chi_c$ or less, it is possible to split the last integral into two integrals at the angle $\varsigma$ [50]:

$$I(\eta) = \int_0^\infty [1 - J_0(\chi\eta)] q(\chi) \chi^{-3} d\chi$$

$$= \int_0^\varsigma [1 - J_0(\chi\eta)] q(\chi) \chi^{-3} d\chi + \int_\varsigma^\infty [1 - J_0(\chi\eta)] q(\chi) \chi^{-3} d\chi$$

$$= I_1(\varsigma \eta) + I_2(\varsigma \eta).$$  

(50)

For the part from 0 to $\varsigma$, we can write $1 - J_0(\chi\eta) = \chi^2 \eta^2/4$, and the integral $I_1$ reduces to a universal one, independently on $\eta$:  

7
Using (38) and (47), we get for the last integral
\[ I_1(\varsigma) = \frac{\eta^2}{4} \int_0^\varsigma q(\chi) \, d\chi. \]  
(51)

For the part from \( \varsigma \) to infinity, the quantity \( q(\chi) \) can be replaced by unity, and the integral \( I_2 \) can be integrated by parts. This leads to the following result for \( I_2 \):
\[ I_2(\varsigma) = \frac{\eta^2}{4} \left[ 1 - \ln(\varsigma\eta) + \ln 2 - C_\varphi + O(\varsigma) \right]. \]  
(52)

Integrating (51) with the use of (44), substituting obtained solutions back into (49), and using the definition
\[ \ln \left( \chi_c/\chi_a \right)^2 + 1 - 2C_\varphi = \ln \left( \chi_c/\chi_a' \right)^2, \]
we arrive at a result for \( Q(\eta) \):
\[ Q(\eta) = -\frac{(\chi_c \eta)^2}{2n_\sigma} \left[ \ln \left( \frac{\eta^2}{\chi_c^2} \right) - \ln \left( \frac{\chi_c}{\chi_a'} \right)^2 \right] = -\frac{(\chi_c \eta)^2}{2n_\sigma} \ln \left( \frac{\eta^2}{\chi_a'^2} \right). \]  
(53)

Finally, considering the definition of \( \theta_c \), we can represent \( Q(\eta) \) by the following expression:
\[ Q(\eta) = -2\pi \left( \frac{Z\alpha}{\beta p} \right)^2 \eta^2 \ln \left( \frac{\eta^2 (\chi_a')^2}{4} \right). \]  
(54)

Then the screening angle \( \chi_a' \) can be determined via \( Q(\eta) \) by a linear equation:
\[ -\ln \left( \chi_a' \right)^2 = \ln \left( \frac{\eta^2}{4} \right) + \left[ 2\pi \eta^2 \left( \frac{Z\alpha}{\beta p} \right) \right]^{-1} Q(\eta). \]  
(55)

Let us present the quantity \( Q_c(\eta) \) in the form:
\[ Q(\eta) = Q^a(\eta) - \Delta_{cc}[Q(\eta)]. \]  
(56)

Making use of (54), the difference \( \Delta_{cc}[Q_c(\eta)] < 0 \) between the Born approximate \( Q^a(\eta) \) and exact in the Born parameter results for the quantity \( Q_c(\eta) \) can be reduced to a difference between the quantities \( \ln \left( \chi_a' \right)^2 \) and \( \ln \left( \chi_a \right)^2 \):
\[ \Delta_{cc}[Q(\eta)] = Q^a(\eta) - Q(\eta) \]
\[ = 4\pi \eta^2 \left( \frac{Z\alpha}{\beta p} \right)^2 \left[ \ln \left( \chi_a' \right)^2 - \ln \left( \chi_a \right)^2 \right] \equiv 4\pi \eta^2 \left( \frac{Z\alpha}{\beta p} \right)^2 \Delta_{cc}[\ln \left( \chi_a' \right)]. \]

On the other hand, this difference can be reduced to a difference \( \Delta q(\chi) = q^a(\chi) - q(\chi) \):
\[ \Delta_{cc}[Q(\eta)] = 2\pi \int_0^\infty \chi \, d\chi \Delta q(\chi) [1 - J_0(\chi\eta)] = \frac{2\chi^2}{n_\sigma} \int_0^\infty \frac{d\chi}{\chi^2} \Delta q(\chi) [1 - J_0(\chi\eta)]. \]  
(57)

Using (66) and (17), we get for the last integral
\[ \Delta_{cc}[Q(\eta)] \underset{\eta \to 0}{=} 4\pi \eta^2 \left( \frac{Z\alpha}{\beta p} \right)^2 \left[ \frac{1}{2} \psi \left( i \frac{Z\alpha}{\beta} \right) + \frac{1}{2} \psi \left( -i \frac{Z\alpha}{\beta} \right) - \psi(1) \right] \]
\[ = 4\pi \eta^2 \left( \frac{Z\alpha}{\beta p} \right)^2 \left\{ \Re \left[ \psi \left( 1 + i \frac{Z\alpha}{\beta} \right) \right] + C_\varphi \right\}, \]  
(58)
(59)
where

\[ \Re [\psi (1 + ia)] = \Re [\psi (1 - ia)] = \Re [i\alpha (ia)] = \Re \psi (-ia) \]

\[ = -C_E + a^2 \sum_{n=1}^{\infty} \frac{1}{n(n^2 + a^2)} = -C_E + f(a), \quad (60) \]

\[ -\infty < a < \infty, \]

\[ \psi(1) = -C_E, \text{ and } f(a) = a^2 \sum_{n=1}^{\infty} [n(n^2 + a^2)]^{-1} \text{ is 'an universal function of } a = Z\alpha/\beta'. \]

Finally, we get the following rigorous relations between the quantities \( \ln (\chi'_{\alpha}) \) and \( \ln (\chi'_{\alpha}) \):

\[ \ln (\chi'_{\alpha}) - \ln (\chi'_{\alpha})^{(\eta)} = \Re [\psi(1 + ia) - \psi(1)], \quad (61) \]

\[ \Delta_{cc}[\ln (\chi'_{\alpha})] = a^2 \sum_{n=1}^{\infty} [n(n^2 + a^2)]^{-1}. \quad (62) \]

We point out that the relations (59), (61), and (62) are independent on the form of electron distribution in atom and are valid for any atomic model.

From (59) also follows an expression for the correction to the exponent of (7). Since \( \ln [g(\eta)] = -n_0 t Q \), we have:

\[ \Delta_{cc}[\ln g(\eta)] = \ln [g(\eta)] - \ln [g^{(\eta)}(\eta)] \]

\[ = 4\pi \eta^2 n_0 t \left( \frac{Z\alpha}{\beta \rho} \right)^2 f(a). \quad (63) \]

For the specified value of \( \eta^2 = 1/\chi^2_c \), we can evaluate this correction using the definition of \( \chi_c \):

\[ \Delta_{cc}[\ln g(\chi_c)] = \frac{4\pi n_0 t}{\chi^2_c} \frac{\chi^2_c}{4\pi n_0 t} f(a) = f(a). \quad (64) \]

The formulas for the so-called ‘Coulomb corrections’ (CC), defined as a difference between the exact and the Born approximate results, are known as the Bethe–Bloch formulas for the ionization losses [9] and the formulas for the Bethe–Heitler cross section of bremsstrahlung [10].

The similar expression was found for the total cross section of the Coulomb interaction of compact hadronic atoms with ordinary target atoms [8]. Also, Coulomb corrections were obtained to the cross sections of the elastic and quasielastic electron scattering, the coherent electroproduction of vector mesons [12], the pair production in nuclear collisions [13], as well as to the solutions of the Dirac and Klein–Gordon equations [14].

Specificity of the expressions obtained in the present work is that they define the Coulomb corrections to the screening angle \( \left( \chi'_{\alpha} \right)^{(\eta)} \), the exponential part \( g(\eta, t) \) of the distribution function \( W(\theta) \), and the angular distribution. A characteristic feature of these corrections is their positive value, in contrast to a negative value of the Coulomb corrections to the cross sections and the energy spectrum in the high energy region.

6 Relative Coulomb corrections to the Born approximation

Let us write (62) as follows:

\[ (\chi'_{\alpha}) = \left( \chi'_{\alpha} \right)^{(\eta)} \exp \left[ f(a) \right]. \quad (65) \]

\[ ^1\text{This result can also be obtained in other ways, with use of the technique developed in [8].} \]

\[ ^2\text{The more complicate formal expression for CC was derived by I. Øverbø in [11].} \]
Then relative Coulomb correction to the Born screening angle \( (\chi'_a)^n \) can be represented as

\[
\delta_{cc}(\chi'_a) = \chi'_a - (\chi'_a)^n = \frac{\Delta(\chi'_a)}{(\chi'_a)^n} = \delta_{cc}(\chi_a) = \exp[f(a)] - 1. \tag{66}
\]

As follows from (64), the relative CC to the exponent \( g^n(\eta) \) at \( \eta^2 = 1/\chi'^2 \) can also be determined by this quantity: \( \delta_{cc}(\chi_a) = \delta_{cc}[g(\chi_a)] \). Moreover, because

\[
\Delta_{cc}[W'(\chi_c, t)] = W_{M}\tilde{\chi}_M = \int_0^\infty J_0(\theta\eta)\Delta g(\chi_c)\eta d\eta, \tag{67}
\]

accounting for \( \int_0^\infty d\eta J_0(\theta\eta) = 0 \), we get

\[
\delta_{cc}[W_M(\chi_c, t)] = \frac{\Delta_{cc}[W'(\chi_c, t)]}{W_M(\chi_c, t)} = \frac{\Delta_{cc}[g(\chi_c)]}{g(\chi_c)} = \exp[f(a)] - 1. \tag{68}
\]

Thus,

\[
\delta_{cc} \equiv \delta_{cc}(\chi_a) = \delta_{cc}[g(\chi_a)] = \delta_{cc}[W_M(\chi_c, t)] = \exp[f(a)] - 1. \tag{69}
\]

The numerical values of this correction are presented in Table 1. Figure 1 illustrates their \( Z \) dependence.

Let us notice that the following equivalent to (40) equation

\[
q(\chi) \approx 1 - \frac{8.85}{(\chi/\lambda)^2} \left( 1 + 4a^2 \left[ \ln \left( \frac{\chi}{2\lambda} \right) - f(a) - 0.543 \right] \right), \tag{70}
\]

yields an approximate expression for the relative correction \( \delta(\sigma) = (\sigma - \sigma^R)/\sigma^R \) to the Rutherford cross section:

\[
\delta(\sigma) \approx \frac{8.85}{(\chi/\lambda)^2} \left( 1 + 4a^2 \left[ \ln \left( \frac{\chi}{2\lambda} \right) - f(a) - 0.543 \right] \right). \tag{71}
\]

The inner part of this expression is close in the form to the inside of the formulas’ of Bethe–Bloch [9], Bethe–Maximon [10], and the formula’s for the total cross section obtained in [8].

In order to estimate the accuracy of the Molière theory in determining the Coulomb correction to the screening angle \( \chi_a \), we define the difference and relative difference between the values of \( \delta_M(\chi_a) \) and \( \delta_{cc}(\chi_a) \) by the relation

\[
\delta_{ccM}(\delta_{cc}) = \frac{\Delta_{ccM}(\delta_{cc})}{\delta_M(\chi_a)} = \frac{\delta_{cc}(\chi_a) - \delta_M(\chi_a)}{\delta_M(\chi_a)} = 1 - \frac{\delta_{cc}(\chi_a)}{\delta_M(\chi_a)}, \tag{72}
\]

where

\[
\delta_M(\chi_a) = \frac{\chi_a - \chi'_a}{\chi'_a} = \sqrt{1 + 3.34} - 1. \tag{73}
\]

To estimate the accuracy of the Molière theory in determining the screening angle itself by the following relative difference between the approximate \( \chi_a^M \) and exact \( \chi_a \) results

\[
\delta_{ccM}(\chi_a) \equiv \frac{\chi_a - \chi'_a}{\chi'_a} = \frac{\chi_a}{\chi'_a} - 1, \tag{74}
\]

we rewrite (66) and (73) as \( \delta_{cc}(\chi_a) + 1 = \chi_a/\chi'_a \) and \( \delta_M(\chi_a) + 1 = \chi_a^M/\chi'_a \). As a result, we obtain the expression

\[
\delta_{ccM}(\chi_a) = \frac{\Delta_{ccM}(\delta_{cc})}{\delta_M(\chi_a) + 1}. \tag{75}
\]

In order to obtain the numerical results for the above Coulomb corrections \( \Delta_{cc} \left[ \ln(\chi_a') \right] = \Delta_{cc} \left[ \ln g(\chi_a) \right] = f(a) > 0, \delta_{cc} \equiv \delta_{cc}(\chi_a) = \delta_{cc}[g(\chi_a)] = \delta_{cc}[W_M(\chi_c, t)] > 0, \) and \( \delta_{ccM}[\chi_a] \), according to (62), (66), and (75), we must first calculate the values of the function \( f(a) = \Re[\psi(1+ia)] + C_R \).
Table 1. The $Z$ dependence of the corrections and the differences defined by (66), (72), (73), (75), (79), and (80).

| $M$ | $Z$ | $\delta_{CC}(\chi_a)$ | $\sum_{n=1}^{\infty} f(Z\alpha)$ | $\delta_{M}(\chi_a)$ | $\Delta_{CCM}(\delta_{CC})$ | $\delta_{CCM}(\delta_{CC})$ | $\delta_{CCM}(\chi_a)$ |
|-----|-----|-------------------------|-------------------------------|-------------------|------------------------|------------------------|---------------------|
| Be  | 4   | 0.0010                  | 1.2012                        | 0.0010            | 0.0004                 | 0.2989                 | 0.0004              |
| Al  | 13  | 0.0108                  | 1.1928                        | 0.0107            | 0.0041                 | 0.2764                 | 0.0040              |
| Ti  | 22  | 0.0308                  | 1.1758                        | 0.0303            | 0.0114                 | 0.2701                 | 0.0109              |
| Ni  | 28  | 0.0499                  | 1.1602                        | 0.0487            | 0.0179                 | 0.2646                 | 0.0168              |
| Mo  | 42  | 0.1103                  | 1.1127                        | 0.1046            | 0.0360                 | 0.2459                 | 0.0314              |
| Sn  | 50  | 0.1544                  | 1.0799                        | 0.1436            | 0.0473                 | 0.2345                 | 0.0396              |
| Ta  | 73  | 0.3175                  | 0.9710                        | 0.2758            | 0.0784                 | 0.1981                 | 0.0562              |
| Pt  | 78  | 0.3590                  | 0.9467                        | 0.3067            | 0.0840                 | 0.1895                 | 0.0582              |
| Au  | 79  | 0.3670                  | 0.9414                        | 0.3125            | 0.0850                 | 0.1880                 | 0.0585              |
| Pb  | 82  | 0.3930                  | 0.9262                        | 0.3316            | 0.0890                 | 0.1846                 | 0.0600              |
| U   | 92  | 0.4845                  | 0.8761                        | 0.3951            | 0.0985                 | 0.1689                 | 0.0622              |

From the digamma series [7]

$$\psi(1 + a) = 1 - C_E - \frac{1}{1 + a} + \sum_{n=2}^{\infty} (-1)^n \left( \zeta(n - 1) \right) a^{n-1}, \quad |a| < 1,$$

(76)

where $\zeta$ is the Riemann zeta function, leads the corresponding power series for $\Re[\psi(1 + ia)] = \Re[\psi(ia)]$

$$\Re[\psi(ia)] = 1 - C_E - \frac{1}{1 + a^2} + \sum_{n=1}^{\infty} (-1)^{n+1} \left( \zeta(2n + 1) \right) a^{2n}, \quad |a| < 2,$$

(77)

and the function

$$f(a) = a^2 \sum_{n=1}^{\infty} \frac{1}{n(n^2 + a^2)}$$

(78)

can be represented as follows [15]:

$$f(a) = 1 - \frac{1}{1 + a^2} + \sum_{n=1}^{\infty} (-1)^{n+1} \left( \zeta(2n + 1) \right) a^{2n}, \quad |a| < 2,$$

$$= 1 - \frac{1}{1 + a^2} + 0.2021 a^2 - 0.0369 a^4 + 0.0083 a^6 - \ldots$$

(79)

An equivalent way to estimate $f(a)$ to four decimal figures is to present the sum from (78) in the following form [10]:

$$\sum_{n=1}^{\infty} [n(n^2 + a^2)]^{-1} = (1 + a^2)^{-1} + \sum_{n=1}^{\infty} (-a^2)^{n-1} \left( \zeta(2n + 1) - 1 \right),$$

$$= (1 + a^2)^{-1} + 0.20206 - 0.0369 a^2 + 0.0083 a^4 - 0.002 a^6.$$ 

(80)

Eq. (80) is sufficient to evaluate this sum up to $a < 2/3 = 0.667$.

The calculation results for the sum (80), the function $f(a)$ (79), the relative Coulomb correction $\delta_{CC}$ (60), its difference with the Molière correction $\delta_M$, and the relative difference in determining the screening angle $\delta_{CCM}(\chi_a)$ are given in Table 1. Some results from Table 1 are presented by Figure 1.
The Table 1 shows that the $f(Z\alpha)$ values, obtained on the basis of (79) and (80), coincide up to four decimal digits and show good agreement with the corresponding values of this function from paper [16]. So $f(Z\alpha) = 0.3129$ [16] and $f(Z\alpha) = 0.3125$ (Table 1) for $Z = 79$; $f(Z\alpha) = 0.3318$ [16] and $f(Z\alpha) = 0.3316$ (Table 1) for $Z = 82$. The maximum value of the relative Coulomb correction $\delta_{CC}$ amounts approximately to 50% for $Z = 92$.

In [6] it was found that the deviation of the screening angle from the first Born approximation is much smaller than this effect determined by Molière’s expression for this quantity. Our results confirm this conclusion (Figure 1).

From Table 1 and Figure 1 it is obvious that the absolute inaccuracy $\Delta_{CCM}(\delta_{CC})$ of the Molière theory in determining the relative Coulomb correction to the screening angle increases up to 10% with the rise of $Z$, and the corresponding relative inaccuracy $\delta_{CCM}(\delta_{CC})$ varies between 17 and 30% over the range $4 \leq Z \leq 92$; the $\delta_{CCM}(\chi_a)$ value reaches about 6% for high $Z$ targets.

Thus, we can conclude that the such large Coulomb corrections as $\Delta_{cc} \equiv \Delta_{CCM} \left[ \ln (\chi'_a) \right] = \Delta_{CC} \left[ \ln g(\chi_c) \right] = f(a)$ and $\delta_{cc} \equiv \delta_{CC} (\chi_a) = \delta_{CC} [g(\chi_c)] = \delta_{CC} [W_M(\chi_c, t)] = \exp [f(a)] - 1$ should be taken into account in describing the high-energy experiments with nuclear targets. The accuracy of the Molière theory in determining the Coulomb correction to the screening angle and the screening angle itself must also be taken into consideration.
7 Summary and Conclusions

1. We obtained the rigorous relations between Born and the exact values of the quantities $Q(\eta)$, $\ln[g(\eta)]$, and $\chi''_a$, which do not depend on the shape of the electron density distribution in the atom and are valid for any atomic model. The main limitation of the presented exact results consists in their applicability for small scattering angles.

2. Also, we evaluated numerically the Coulomb corrections $\Delta_{CC} \equiv \Delta_{CC}[\ln(g(\chi_c))] = \exp[f(a)] - 1$ for nuclear charge ranged from $Z = 4$ to $Z = 92$.

3. We found that these Coulomb corrections have a large value for high $Z$ targets. For instance, the magnitude of $\delta_{CC}(\chi_a)$ is about $40 \div 50\%$ for $Z \sim 80 \div 90$. The contribution of such corrections is larger than experimental errors in the most high energy experiments whose measurement accuracy has an order of a few percent, and these corrections should be appropriately considered in experimental data processing.

4. We estimated numerically the difference and relative differences between our results and those of Molière over the range $4 \leq Z \leq 92$, and we found that while the values of $\delta_{CCM}(\chi_a)$ and $\Delta_{CCM}(\delta_{CC})$ increase with $Z$ up to 6% and 10%, respectively, the relative difference $\delta_{CCM}(\delta_{CC})$ varies between 17 and 30% over the range $4 \leq Z \leq 92$. Thus, we can conclude that these corrections to the approximate Molière result must also be taken into account for a rather accurate description of high energy experiments with nuclear targets.

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Appendix: Approximate solution for the thick targets

We can obtain the approximate solution (20) of (7) for a thick target in the following simple way. When the total number of collisions is

$$N_0 = 2\pi n_0 \int_0^\infty \sigma(\chi) \chi d\chi \gg 1,$$

we can write

$$1 - J_0(\chi \eta) \approx \frac{\chi^2 \eta^2}{4},$$

for small angles like $\chi \eta \ll 1$. This allows one to reduce the integral (7) to a much simpler one:

$$W_M(\theta, t) = \int_0^\infty \eta d\eta J_0(\eta \theta) \exp[-2\pi n_0 \frac{\eta^2}{4} \int_0^\infty \sigma(\chi) \chi^3 d\chi].$$

Since

$$\lim_{\chi \to \infty} \sigma(\chi) \chi^3 \to 0,$$

the corresponding integrand from (83) is a convergent integral

$$\int_0^\infty \sigma(\chi) \chi^3 d\chi < \infty.$$
Taking into account
\[ \int_0^\infty d\eta \, J_0(\theta \eta) = 2c^{-2} \frac{\Gamma(1)}{\Gamma(0)} = 0 \]  
with the Gamma function \( \Gamma(x) = (x - 1)! \), we get a final result for (83):
\[ W_M(\theta, t) \approx 2 \theta^2 \exp\left(-\frac{\theta^2}{\theta_0^2}\right), \]  
where
\[ \theta_0^2 = 2\pi n_0 t \int \sigma(\chi) \chi^3 d\chi. \]  
For the Rutherford law
\[ \sigma_R(\chi) = \left(\frac{2Z\alpha}{\beta p}\right)^2 \frac{1}{\chi^4}, \]  
when \( \sigma_R(\chi) \gg \theta_0 = \chi_0 \), the quantity \( \theta_0^2 \) takes a value
\[ \theta_0^2 = 2\pi n_0 t \int \sigma(\chi) \chi^3 d\chi = \infty, \]  
and the approximate solution (87) is not applicable.

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