Abstract  Nonperturbative (Coulomb) correction to the Molière screening angle in the multiple Coulomb scattering theory is evaluated taking into account the inelastic contribution. Treating the atom as an assembly of pointlike electrons and the nucleus, and summing the scattering probability over all the final states of the atom, it is shown that besides the Coulomb correction due to close encounters of the incident charged particle with atomic nuclei, there are similar corrections due to close encounters with atomic electrons, being the counterpart of Bloch correction in ionization energy loss. For low \( Z \neq 1 \) the latter contribution can reach \( \sim 25\% \).

1 Introduction

Interaction of nonrelativistic and/or highly charged fast ions with atoms often requires nonperturbative treatment. For certain important observables, relative deviation from their first Born approximation appears to depend solely on the Coulomb parameter—the product of nuclear charges of the colliding particles and their reciprocal collision velocity, but not on the target atom structure. The corresponding contribution is thus generally termed “Coulomb correction.” In the 1930s to 1950s, corrections of that kind were discovered independently for ionization energy loss [1], multiple Coulomb scattering [2–4], electron–atom bremsstrahlung [5, 6], and electron–positron pair production [7]. For different processes, different formalisms were adopted, such as Coulomb wave functions in parabolic coordinates [1,5,7,8], eikonal approximation [2–9], and partial wave expansion [13,14], so final results were sometimes presented in different forms.

In pioneering work [1], a correction

\[
\Delta L_{\text{Bloch}} = -f \left( \frac{Z_1 e^2}{hv} \right),
\]

(1)

to the stopping number \( L \) entering the Bethe–Bloch formula

\[
\frac{dE}{dx} = \frac{4\pi n_a Z}{m_e} \left( \frac{Z_1 e^2}{v} \right)^2 L
\]

(2)

for a particle of high velocity \( v \) losing energy \( dE \) per unit path \( dx \) in a uniform medium of atomic density \( n_a \) was expressed in terms of the function

\[
f(s) = \Re \psi (1 + is) - \psi(1), \quad f(-s) = f(s),
\]

(3)

where \( \psi(s) = \Gamma'(s)/\Gamma(s) \) is the digamma function, \( Z_1 \) and \( Z \) are the incident particle and the target atom nucleus charges in units of the proton charge \( e \), \( e^2/h = c/137 \), and \( m_e \) is the electron mass.

In [5], evaluating spectra of bremsstrahlung from an ultrarelativistic electron in a bare Coulomb field, and of \( e^+e^- \) pair production in such a field, a nonperturbative correction to the large logarithm was obtained in terms of function (3) with argument \( \frac{Z e^2}{hv} \), where \( Ze \) is the charge of the target nucleus.

In [2,3], where a theory of multiple scattering on screened Coulomb potentials of atoms in matter was developed (as briefly recalled here in Appendix A), the universal dependence of the screening angle \( \chi_a \) on the Coulomb parameter \( \frac{Z_1 e^2}{hv} \) was expressed in the form of an algebraic interpolation

\[
\frac{\chi_a \left( \frac{Z_1 e^2}{hv} \right)}{\chi_a(0)} = \sqrt{1 + \frac{3.76}{1.13} \left( \frac{Z_1 e^2}{hv} \right)^2}.
\]

(4)

In the decades that followed, it was realized that all those corrections are essentially of the same physical origin [15]. In [12], it was argued (see also [11,16]) that (4) should more precisely be presented in terms of the function (3) in exponentiated form:

\[
\frac{\chi_a \left( \frac{Z_1 e^2}{hv} \right)}{\chi_a(0)} = e^{f \left( \frac{Z_1 e^2}{hv} \right)}.
\]

(5)

The old algebraic form (4), however, is still often used in applications [17,18].
The physical origin of corrections described by the function (3), however, proved to be intricate and sparked discussions. In application to the Bloch correction [Eqs. (1)–(3)], a paradox was stated in [13]: Since, as implied by formula (1), the correction does not depend on atomic electron binding, it is likely to stem from close collisions; but the close-collision contribution to the differential cross section is described by the Rutherford formula, which coincides with its first Born approximation, so the nonperturbative correction then should be absent at all. To resolve this paradox, [14] looked into the dependence of the ionization energy loss on the angle of deflection of the incident ion, and discovered the Bloch correction to actually correspond to small rather than large deflection angles. Taking into account the reciprocity relationship between the momentum transfer and the impact parameter, that should in turn correspond to large impact parameters. But then the absence of dependence on the screening function appears puzzling. It is also noteworthy that no analog of the Coulomb correction arises in straggling (including an additional weighting factor proportional to the deflection angle squared as compared to mean \(\frac{dE}{dx}\)) [13], in spite that close collisions normally yield large fluctuations, as in Landau theory for example [19].

A similar discussion was held for \(e^+e^-\) pair production in collisions of bare heavy ions [11,20].

For Coulomb corrections related to angular deflections rather than ionization energy loss in atomic scattering, as in Molière’s theory of multiple scattering in amorphous matter, or in nonperturbative theories of bremsstrahlung and \(e^+e^-\) pair production on atoms, the situation is largely the same, but the question is about accuracy with which the Coulomb correction is independent of the Coulomb field screening. For simplicity of evaluation of multiple integrals in analytic calculations, presuming the dominant contribution to stem from small impact parameters, the screening is usually merely neglected from the outset. The discussion quoted above may cast doubt upon the legitimacy of such a procedure, but for any specific choice of the scattering function, the difference between (5), (3), and the prediction of the eikonal approximation (see Sect. 2.2) for scattering in a screened potential can be numerically checked to be compatible with zero. Therefore, the result (5) actually seems to be exact, although a rigorous general proof of that statement is lacking.

For atomic scattering, there is an additional complication that, besides the elastic contribution (for which the atom remains intact), dominant for high-\(Z\) target atoms, there always exists an inelastic contribution, which becomes commensurate with elastic at low \(Z\). A modification of the screening angle due to scattering on electrons was offered in [21], but only at the Born approximation level. Collisions with electrons, however, can be nonperturbative as well, because although the electron charge is lower than that of the nucleus (for \(Z > 1\)), the Coulomb parameter of its collision with an incident ion involves a \(Z_1/v\) factor, which can be large. To describe inelastic processes, atomic electrons must be treated as separate pointlike quantum particles rather than an averaged static charge distribution.

Some insight can be gained by noting that nonperturbative treatment of inelastic deflections must be directly related to the Bloch correction in energy loss (2), (1). Since the latter differs from the elastic scattering contribution (5) by the absence of the factor \(Z\) in the argument of \(f\), the aggregate Coulomb correction should depend on two rather than on one argument.

To take on such a nontrivial problem as nonperturbative inelastic scattering, we need a formalism which is able to treat quantum scattering in few-center fields created by atomic electrons “frozen” at definite coordinates during the fast projectile passage, and is able to resolve the controversy between small- and large-distance contributions. A suitable tool for that is the eikonal approximation, in which the momentum transfer at high energy is approximated by a transverse vector, and the scattering amplitude by a pure Fourier integral over the impact parameter plane. After integration over all the momentum transfers, it yields an integral identity ensuring the absence of nonperturbative corrections to the transport cross section in a nonsingular potential (Sect. 2). When applied to a potential with a Coulomb singularity, this integral identity holds only partly—for a “soft” part of the integral whereas for the “hard” part, the cancellation of nonperturbative effects is incomplete, giving rise to the Coulomb correction (Sect. 3).

Granted that the mentioned integral identity holds irrespective of the central symmetry, our calculation can be extended to inelastic scattering on an atom as a few-body system, including pointlike atomic electrons (Sect. 4). Evaluation of the corresponding eikonal scattering amplitude, summation of its square over all the final states, and averaging over the initial quantum state leads to a Coulomb correction comprised of contributions described by the function (3), but with two different (\(Z\)-dependent) weighting factors and arguments. One contribution corresponds to multiple scattering on atomic nuclei, and another to scattering on individual atomic electrons. The dependence on the initial state wave function eventually drops out, like for multiple scattering in an ideal plasma. Estimates for experimental verification of the predicted two-argument Coulomb correction are made in Sect. 5. Our results are summarized in Sect. 6.

2 Preliminary considerations

It will be expedient to precede evaluation of the Coulomb correction for multiple scattering on few-electron atoms with a discussion of its physical origin for a prescribed scattering potential. Different interpretations of the origin of the corre-
sponding correction will be shown to be equally admissible. Their reconciliation is based on a certain integral identity.

Coulomb corrections of the sort discussed here arise for quantities related to the transport cross section or, equivalently, the mean square momentum transfer

$$\langle q^2 \rangle \propto \int d^2 q q^2 \frac{d\sigma}{d^2 q}.$$  \hspace{1cm} (6)

Here, $d\sigma/d^2 q$ is the differential cross section of fast particle small-angle deflection with momentum transfer $q = p - p'$. The latter is typically nearly transverse with respect to the initial momentum, because longitudinal momentum transfer $q_z = q \cdot p/p \approx q^2/2p$ is small, being determined by the reciprocal large momentum of the incident particle. In our treatment within the leading order of high-energy expansion, such terms will be neglected throughout. The integration over the sphere of deflection angles is thus replaced in (6) by that over the tangential transverse momentum plane. Due to the weighting factor $q^2 = q_z^2$, the relative role of large momentum transfers, i.e., small transverse distances, is enhanced, whereas the dependence on the screening function diminishes, but a priori needs not disappear entirely.

To proceed, we need to evaluate $d\sigma/d^2 q$, which generally requires quantum mechanical treatment. Fortunately, at high energy, even a quantal scattering problem is straightforward to solve.

2.1 Conditions of eikonal approximation

In the simplest case of scattering of a particle with charge $Z_1e$ and velocity $v$ by a prescribed electrostatic potential $\psi(r)$, in the leading order of the high-energy expansion (relativistic or nonrelativistic), the differential scattering cross section

$$\frac{d\sigma}{d^2 q} = |a|^2$$  \hspace{1cm} (7)

is expressed in terms of the eikonal scattering amplitude [2, 16, 22–24]

$$a(q) = \frac{1}{2\pi i \hbar} \int d^2 b e^{i q \cdot b} \left[ 1 - e^{i \chi_0(b)} \right].$$  \hspace{1cm} (8)

Here,

$$\chi_0(b) = -\frac{Z_1e}{v} \int_{-\infty}^{\infty} dz \psi(z, b)$$  \hspace{1cm} (9)

is the eikonal phase depending on the impact parameter $b$—the transverse component of $r$. The integral over longitudinal coordinate $z$ in (9) physically corresponds to that over the particle trajectory, which at high energy is nearly straight within the scattering field region. Beyond this region, the distorted wave function disperses into a superposition of plane waves corresponding to deflected particles. Thereby, contributions from different trajectories interfere, as in the Huygens principle for Fraunhofer diffraction on a transparent refracting body. That is taken into account in (8) by the integral over all the impact parameters. When $\chi_0/\hbar \gg 1$, a stationary phase approximation in the impact parameter plane applies, and for a certain $q$, only a small vicinity of a certain $b$ contributes [2, 16, 22, 24]. That leads to a classical picture [see Eq. (25) below].

Due to the approximation of straight-line passage through the entire field action domain, the particle charge sign dependence in the eikonal differential cross section drops out. The same is also the salient feature of Coulomb corrections, described by the charge-even function (3). Thus, for their description, the eikonal approximation seems to be adequate. For the charge-odd Barkas correction, manifesting itself at lower energies, higher-order corrections to the eikonal approximation may be necessary, but they are beyond the scope of the present paper.

The conditions of validity of the eikonal approximation [22, 24] may be stated as

$$pv \gg Z_1ev \psi,$$  \hspace{1cm} (10)

$$\lambda = \hbar/p \ll r_{scr},$$  \hspace{1cm} (11)

where $r_{scr}$ is a typical spatial scale on which $\psi(r)$ varies significantly. They are better fulfilled the higher the particle momentum $p$. Note that if the incident particle is an ion, while potential $\psi$ is atomic, condition (11) is weaker than (10), because it implies that the incident particle wavelength is short locally (semiclassical and straight-line passage), whereas (10) demands that energy is high globally (semiclassical and straight-line passage). This difference is made specific by the use of the virial theorem $e\psi \sim m_ee\psi_0$, where $v_0$ is the typical velocity of bound electrons in the atom, and $\hbar/r_{scr} \sim m_ee\psi_0$. The conditions (10) and (11) are thus recast correspondingly as

$$v \gg \frac{Z_1m_e}{m_1\gamma} v_0$$  \hspace{1cm} (12)

and

$$v \gg \frac{Z_1m_e}{m_1\gamma} v_0,$$  \hspace{1cm} (13)

where $m_1 = A m_p$ is the ion mass, being $A$ times the proton mass $m_p$, and $\gamma$ is the ion Lorentz factor. The right-hand sides of both (12) and (13) contain small factors, but the square root factor in (12) is greater. It should be noted, however, that those are only the conditions for high-energy scattering in a static (mean atomic) potential, created primarily by the atomic nucleus. To be able to treat atomic electrons as static, a more stringent condition $v \gg v_0$ is also needed. The account of electron orbital motion (wave functions), however, will be postponed until Sect. 4.
2.2 An integral identity: absence of Coulomb correction for \( q^2 \) in potentials without Coulomb singularity

An expedient transformation of the integrand in (6) is

\[
q^2 \frac{d\sigma}{d^2q} = \left|qa\right|^2. \tag{14}
\]

Carrying factor \( q \) under the \( b \)-integral sign, transforming it into a gradient acting on the plane wave as

\[
q e^{i q \cdot b} = \hbar \frac{\partial}{\partial b} e^{i q \cdot b}.
\]

and switching the gradient action onto the eikonal phase factor by partial integration allows one to eliminate \( q \) everywhere except the plane wave factor:

\[
q a = \frac{1}{2\pi} \int d^2b e^{i q \cdot b} \frac{\partial}{\partial b} \left[ 1 - e^{i \chi_0(b)} \right]. \tag{15}
\]

The integral is thereby brought to an ordinary Fourier form. The benefit is that if in Eq. (6) with (14), (15) the integral is finite when extended over the entire \( q \) plane, it is promptly evaluated using the familiar formula

\[
\int d^2q e^{i q \cdot (b - b')} = (2\pi\hbar)^2 \delta(b - b') \tag{16}
\]

of Fourier inversion, that is,

\[
\int d^2q q^2 \frac{d\sigma}{d^2q} = \int d^2b \left| \frac{\partial}{\partial b} e^{i \chi_0(b)} \right|^2 \int d^2q q^2 \frac{d\sigma}{d^2q}.
\]

Here, \( d\sigma_1/d^2q \) is the first Born approximation for \( d\sigma/d^2q \), obtained by putting \( e^{i \chi_0} \rightarrow 1 + \frac{i \hbar \chi_0}{\hbar} \).

The non-perturbative result for \( (q^2) \) in the eikonal approximation thus appears to be equal to that in the first Born approximation [as well as to the classical result, since \( \partial / \partial b \chi_0(b) \) is the classical momentum transfer (25)] [25]. There would be neither Coulomb correction nor Lindhard–Sørensen paradox in that case.

When a Coulomb singularity is present in the \( \varphi \) potential, the integral identity (17) does not strictly apply. Violation of (10) in a narrow vicinity of the nucleus does not invalidate the general applicability of the eikonal approximation (7), (8), provided typical small deflection angles are considered rather than Rutherford wide-angle scattering (e.g., backscattering) [2]. But since the differential cross section at \( q \) higher than typical has the Rutherford asymptotics

\[
\frac{d\sigma}{d^2q} \approx \int \frac{d\sigma}{d^2q} \propto q^{-4}, \tag{18}
\]

upon insertion of such a differential cross section into the integral (6), it logarithmically diverges at large \( q \). The relation (17) with both its sides infinite then becomes meaningless. Furthermore, even the difference

\[
\int d^2q q^2 \left( \frac{d\sigma}{d^2q} - \frac{d\sigma_1}{d^2q} \right), \tag{19}
\]

which is finite due to mutual cancellation of the Rutherford “tails” in the integrand, may be nonzero, as we demonstrate below.

2.3 Large-\( q \) regularization for Coulomb scattering: Molière’s screening angle

Self-consistent theories should operate with finite quantities. If a divergence arises in some approximation, a more accurate approximation is needed which is divergence-free. Herein we will be concerned with the problem of multiple Coulomb scattering in amorphous matter. The corresponding finite theory due to Molière [2–4, 16, 26] (see also Appendix A) describes the procedure for separation of soft and hard contributions to scattering. For characterization of the soft scattering part alone, the entire dependence on the atom structure is encapsulated into the quantity

\[
\ln q_o(Z_1/v) = \lim_{q_R \to \infty} \left( \ln q_R - \int_0^{q_R} \frac{dq}{q} \frac{d\sigma}{d\sigma_R} \right) - \frac{1}{2}, \tag{20}
\]

where the single-differential Rutherford cross section for scattering on a bare nucleus of charge \( Z_e \) equals

\[
\frac{d\sigma}{dq} = \frac{2\pi}{q^3} \left( \frac{2Z_e Z \ell e^2}{v} \right)^2. \tag{21}
\]

Since \( d\sigma_R/dq \propto q^{-3} \), the integrand in (20) is proportional to that in (6), but the integral is cut off on the upper limit, and the leading asymptotic dependence on the cutoff \( q_R \) is subsequently subtracted, while the nontrivial part is the next-to-leading logarithmic contribution. The notation \( q_o \) is introduced here so that rescaling

\[
\chi_o = q_o / \ell
\]

by the large longitudinal (nearly conserved) momentum \( \ell \) yields Molière’s screening angle \( \chi_o \) [2–4]. It will be preferable for us to work with \( q_o \) rather than \( \chi_o \), since \( q_o \) depends only on the target atom. But then we have to deal with logarithms of dimensional quantities in (20) and hereinafter.

The conventional term 1/2 in the right-hand side of (20) is introduced so that for a purely exponentially screened Coulomb potential \( \varphi(r) = \frac{Ze}{r} e^{-r/r_{scr}} \), \( q_o(0) \) exactly equals \( h / r_{scr} \).

It should be emphasized that \( q_R \) has to be large only compared with \( h / r_{scr} \), not with \( p \), so the presence of the formal limit \( q_R \to \infty \) (physically implying \( q_R \gg q_o \) in (20)) does not contradict the physical applicability of the small-angle approximation for the evaluation of \( q_o \).
It is also noteworthy that if Eq. (20) is recast as
\[ \ln q_a + \frac{1}{2} = \lim_{q_R \to \infty} \left( \ln q_R - \int_0^{q_R} \frac{dq}{q} \frac{d\sigma}{d\sigma_R} \right) + \int_0^{q_R} \frac{dq}{q} \frac{d\sigma_1}{d\sigma_R}, \]  
(23)
identification of the limit in the right-hand side with \( \frac{1}{2} + \ln q_a(0) \) leads to a relationship
\[ \ln \frac{q_a(Z_1/v)}{q_a(0)} = \int_0^{\infty} \frac{dq}{q} \frac{d\sigma_1}{d\sigma_R}. \]  
(24)
Since \( d\sigma_R \propto dq/q^3 \), the right-hand side of (24) is proportional to (19). If it were zero, that would imply \( q_a(Z_1/v) \equiv q_a(0) \). But the numerical calculation based on Eqs. (20) and (7)–(9) gives a positive function rising indefinitely with the increase of \( Z_1/v \), which confirms the existence of the Coulomb correction.

2.4 Classical limit: Coulomb correction as a manifestation of \( q \) proportionality to \( Z_1/v \)

The simplest interpretation of the Coulomb correction is possible in high-energy classical mechanics. In that case, \( q \) (again, a predominantly transverse vector) is fully determined by the particle impact parameter \( b \) via
\[ q(b) = \frac{\partial}{\partial b} x_0, \]  
(25)
where \( x_0(b) \) is defined by Eq. (9). Assuming the atomic field to be characterized by a singularity \( \varphi(r) \sim \frac{Ze}{r} \), with the nucleus charge \( Ze \), and spherically symmetrical screening outwards from the nucleus, it is convenient to express the scattering indicatrix \( q(b) \) dependence as
\[ q(b) = \frac{2Z_1Ze^2}{vb} S_1(b). \]  
(26)
According to Eqs. (25) and (9), the factor \( S_1 \) depends only on the target atom, and not on the incident particle charge to velocity ratio \( Z_1/v \). (For brevity, we will not explicate the \( Z \) dependence of \( S_1 \).) Since the screening function decreases monotonically with \( r \), the function \( S_1(b) \) decreases monotonically with \( b \) and assumes limiting values
\[ S_1(0) = 1, \]  
(27)
\[ S_1(\infty) = 0. \]  
(28)
The inverse function \( b(q) \) is then single-valued, and the classical differential cross section derives from it by differentiation:
\[ \frac{d\sigma_{cl}}{dq} = 2\pi b \left| \frac{db}{dq} \right|. \]  
(29)
As a check, the pure Rutherford scattering differential cross section (21) can be retrieved by putting in (26) \( S_1 \equiv 1 \), solving for \( b(q) \), and inserting to (29). But we are interested in complete screening functions obeying the condition (28). Instead of \( d\sigma/dq \), it is often more convenient to work with the dimensionless ratio \( d\sigma/d\sigma_R \). In our problem, Eq. (20) involves \( \frac{dq}{q} \frac{d\sigma_{cl}}{d\sigma_R} \), which is expressible through \( S_1^2(b) \) and a power factor singular at \( b \to 0 \):
\[ \frac{dq}{q} \frac{d\sigma_{cl}}{d\sigma_R} = \frac{1}{2\pi} \left( \frac{vq}{Z_1Ze^2} \right)^2 \frac{d\sigma_{cl}}{d\sigma_R} = \frac{S_1^2(b)}{2\pi b^2}. \]  

[In the first equality, we substituted \( d\sigma_R/dq \) from Eq. (21), and in the second, \( q \) from Eq. (26).] Changing in (20) from integration over \( q \) to integration over \( b \), i.e., writing \( d\sigma_{cl} = 2\pi bdb \), we get
\[ \ln q_a(Z_1/v) + \frac{1}{2} = \lim_{q_R \to \infty} \left[ \ln q_R - \int_0^{2\pi Z_1Ze^2/vq} \frac{db}{b} S_1^2(b) \right]. \]  
(30)
Next, introducing
\[ b_R = \frac{2Z_1Ze^2}{vq}, \]  
(31)
and transforming limit \( q_R \to \infty \) to \( b_R \to 0 \), we equivalently present \( \ln q_a + 1/2 \) as a sum of two terms:
\[ \ln q_a(Z_1/v) + \frac{1}{2} = \ln \frac{2Z_1Ze^2}{v} \]  
\[ + \lim_{b_R \to 0} \left[ \ln \frac{1}{b_R} - \int_{b_R}^{\infty} \frac{db}{b} S_1^2(b) \right]. \]  
(32)
The second line in (32) depends only on screening, i.e., on \( Z \), implicit in \( S_1 \), but not on \( Z_1/v \). Therefore, the dependence of \( q_a \) on \( Z_1/v \) is a pure proportionality,
\[ q_a(Z_1/v) \propto \frac{Z_1}{v}. \]  
(33)
That is merely the classical impulse approximation scaling property,\(^1\) where the imparted momentum is proportional to the strength of the force acting on the particle, i.e., to its charge, and to the action time reciprocal to \( v \).

Incidentally, comparing Eq. (32) with Eq. (5), which by putting
\[ f(s) \approx \ln s + \gamma_E \]  
(34)
\(^1\) Drawing a parallel with the ionization energy loss, where a Coulomb correction was historically first discovered (see Introduction), one can see that in definition (20), the right-hand side is an analog of the stopping number \( L \) (large log) in Eq. (2). Since the left-hand side of (32) also contains \( \ln q_a \), whereas the right-hand side contains a logarithm of the large Coulomb parameter, the latter is the counterpart of Bohr’s classical logarithm [27].
in the classical limit simplifies to
\[ q_a(Z_1/v) \simeq \frac{Z_1Ze^2}{\hbar v} e^{\gamma_E} q_a(0), \] (35)
one infers
\[ \ln \frac{q_a(0)}{2\hbar} + \frac{1}{2} + \gamma_E = \lim_{b_R \to 0} \left[ \ln \frac{1}{b_R} - \int_{b_R}^{\infty} \frac{db}{b} S_1^2(b) \right]. \] (36)

While the factor \( Z_1/v \) in (35) complies with Eq. (33), the presence of Euler's constant \( \gamma_E = -\psi(1) = 0.577 \) here looks nontrivial. We will directly prove formula (36) along with (35) in Sect. 3, and see that term \( \gamma_E \) is not of classical origin.

2.5 Reconciliation of small-\( q \) and large-\( q \) interpretations

Now one observes a superficial paradox, similar to that mentioned in the Introduction. From Eq. (30), where cutoff (31) at a fixed \( q_R \) depends on \( Z_1/v \), whereas the integrand \( S_1^2(b)/b \) does not, it may be concluded that the Coulomb correction stems from asymptotically small \( b \), while moderate \( b \) always give the same contribution.

In the momentum transfer representation, however, the situation is ostensibly different. If, as is customarily done [2, 14, 17, 29], \( d\sigma/d\sigma_R \) is plotted vs. \( q \) (see Fig. 1), the area under such a curve is related to \( \ln q_a \) by Eq. (20). The area between two such curves corresponding to different Coulomb parameters (e.g., the dot-dashed and the solid curves in Fig. 1) then equals the increment of the Coulomb correction. This area is independent of the cutoff \( q_R \), provided \( q_R \) is large enough (the vertical dotted line in Fig. 1), and, evidently, is always concentrated at moderate \( q \). But moderate \( q \) cannot physically, in the sense of classical reciprocal relationship (26), correspond to asymptotically small \( b \).

That paradox for the classical case is simple enough to resolve. In fact, \( q_a \) is an integral which receives commensurate contributions from both large and small \( q \). Comparing two such integrals at different Coulomb parameters, one can isolate regions whose contributions are equal. The rest then may be regarded as responsible for the Coulomb correction. But isolation of equal contributions needs not be unique. In our case, the distribution \( d\sigma/d\sigma_R \) is observed to level off at large \( q \), while with the increase in the Coulomb parameter, it just shifts to the right as a whole (cf. dot-dashed and solid curves in Fig. 1), like a paste squeezed out from the tube. The cutoff position (the "tube end") at that remains fixed. Thus, two possibilities may be distinguished for identification of equal contributions.

One possibility is to refer to the fact that at large \( q \), the ratio \( d\sigma/d\sigma_R \to 1 \) is independent of the Coulomb parameter. The Coulomb correction is then attributed to the difference between functions \( d\sigma/d\sigma_R(q) \) at different values of the parameter \( Z_1Ze^2/hv \).

Another way is to note that functions \( d\sigma/d\sigma_R(q) \) at different values of parameter \( Z_1Ze^2/hv \) have the same shape and differ only by a shift in \( \log q \). But if the integral is evaluated taking into account the shift, the cutoff will move accordingly (depending on \( Z_1Ze^2/hv \)) and differ for the two integrals.

The latter viewpoint is formalized by passing from the integration variable \( q \) to
\[ Q(b) = \frac{v}{2Z_1Ze^2} q(b) = \frac{1}{b} S_1(b), \] (37)
whose advantage is that it is a function of \( b \) alone, and not of the Coulomb parameter. We then observe that the ratio
\[ \frac{d\sigma_{\text{cl}}}{d\sigma_R} = Q^4 \frac{d\sigma_{\text{cl}}}{d^2Q} = \frac{db^2}{dQ^2} = R(Q) \] (39)
depends only on \( Q \) (and on \( Z \), which in the meantime we presume to be fixed), but not on \( Z_1/v \), and assumes limiting values
\[ R(0) = 0, \quad R(\infty) = 1. \]

Therefore, (20) rewrites...
\[ \ln q_R(1/v) + \frac{1}{2} = \lim_{q_R \to \infty} \left[ \ln q_R - \int_0^{q_R} \frac{dQ}{Q} \mathcal{R}(Q) \right] \]

\[ = \ln \frac{2Z_1Z e^2}{v} + \lim_{Q_R \to \infty} \left[ \ln Q_R - \int_0^{Q_R} \frac{dQ}{Q} \mathcal{R}(Q) \right]. \]

(40)

with

\[ Q_R = \frac{v q_R}{2Z_1Z e^2}. \]

(41)

That is equivalent to employing the \( b \) representation, since \( b \) is unambiguously related to \( Q \), and similarly, in the integrand of (32), the distribution \( \frac{1}{\pi} S_1^2(b) \) involving all the dependence on the screening function is independent of the Coulomb parameter. The Coulomb parameter dependence instead enters the \( b \) cutoff [see Eq. (30)].

Such are the two alternative approaches to evaluation and interpretation of the Coulomb correction. Physically, it is consistent to attribute its origin to moderate \( q \), i.e., moderate \( b \). It is there where nonperturbative effects in the differential cross section develop dynamically. But then the term “Coulomb correction” may sound mysterious.

A more shortcut approach giving the same results is the low-\( b \) one, when the \( b \) distribution is regarded as fixed, while the cutoff [in Eq. (30)] or the subtraction term \( \ln 2Z_1Z e^2 \) [in Eq. (32)] is regarded as moving. Not only does it make the term “Coulomb correction” intuitive, but it also opens prospects for generalization onto multi-center scatterers. For scattering in overlapping fields of several scattering centers, each screened in a complicated way, all that matters is the absence of overlap of impact parameter projections of small vicinities of their Coulomb singularities, where the screening can be neglected. That makes it plausible that the Coulomb correction will be independent of screening in that case as well.

Since in the impact parameter representation one may be tempted to render \( b_R \) as low as possible, a proviso is that the applicability of the theory of multiple scattering itself sets a lower limit to \( b_R \). The physical condition (84) implies

\[ b_R \gg \frac{2Z_1Z e^2}{pv\chi_c} \approx \frac{Z_1}{\sqrt{\pi n_a l}}. \]

(42)

At that, for the Rutherford “tail” to manifest itself in multiple Coulomb scattering, the right-hand side of (42) must be much greater than the nuclear radius, which amounts to a few femtometers. With typical solid matter density values \( n_a \approx 0.06 \text{ Å}^{-3} \), that will be fulfilled if the target thickness \( l \ll 1 \text{ m} \). For nonrelativistic incident particles, their slowing down by ionization energy loss becomes significant at much smaller thicknesses.

The demonstration of equivalence of small-\( b \)-moderate-\( q \) points of view given above is gratifyingly simple, but is based on scaling in the classical impulse approximation, and is thus valid only in the classical scattering regime. In the quantum regime \( \frac{Z_1Ze^2}{\hbar \alpha} < 1 \), the ratio \( d\sigma/d\sigma_R \) depends on \( \log q \) and \( \frac{Z_1Ze^2}{\hbar \alpha} \) independently, rather than through their sum only. Thus the Coulomb parameter dependence of the distribution does not reduce to a pure translation in \( \log q \) (cf. dashed and dot-dashed curves in Fig. 1). In that case, to justify a possibility of the small-\( b \) point of view, we will need to use more flexible mathematical techniques like the integral identity of Sect. 2.2. That will be done in the next section.

### 3 Quantal treatment for static screening

Let us now proceed to the problem of quantum scattering in a screened Coulomb potential. Our treatment, again, will be based on the eikonal approximation (see Sect. 2.1). In its framework, in fact, the assumption of central symmetry of the screening function can be lifted. Such a generalization will be needed for application to inelastic scattering in the next section.

We start with casting the eikonal phase in form

\[ \chi_0(b) = 2\alpha S_0(b), \]

(43)

where the dependence on Coulomb parameter

\[ \alpha = \frac{Z_1Ze^2}{\hbar v} \]

is isolated similarly to Eq. (26). The absence of screening for \( b \ll r_{\text{sc}} \) is expressed as

\[ S_0(b) \approx \ln \frac{b}{b_0}. \]

(44)

[Insertion thereof to Eq. (25) and differentiation over \( b \) checks to lead to Eq. (26) with \( S_1(b \ll r_{\text{sc}}) \approx S_1(0) = 1 \).] The actual knowledge of the constant \( b_0 \approx r_{\text{sc}} \) with \( S_0(b) \) will not be needed for us in what follows.

It will be expedient first to show how the pure Coulomb scattering amplitude and differential cross section are obtained. Inserting (44) to (8), we get [2,24]

\[ \sigma_R = b_0^{-2\alpha} \frac{i}{2\pi \hbar} \int d^2b e^{ibq} b^{2\alpha} \]

\[ = b_0^{-2\alpha} \frac{i}{\hbar} \int_0^{\infty} db b^{1+2\alpha} f_0(q b / \hbar) \]

\[ = \frac{2\alpha}{q^{2\alpha}} \left( \frac{2\hbar}{q b_0} \right)^{2\alpha} \Gamma(1+\alpha) \Gamma(1-i\alpha). \]

(45a)

\[ = \frac{2\alpha}{q^{2\alpha}} \left( \frac{2\hbar}{q b_0} \right)^{2\alpha} \Gamma(1+\alpha) \Gamma(1-i\alpha). \]

(45b)

Here, all the \( b_0 \) and nonlinear \( \alpha \) dependencies are contained in a pure phase factor \( \left( \frac{2\hbar}{q b_0} \right)^{2\alpha} \Gamma(1+\alpha) \Gamma(1-i\alpha) \). In the differential cross section (7), it squares to unity:

\[ \frac{d\sigma_R}{dq} = \frac{8\pi \hbar^2 a^2}{q^3}. \]

(46)
Our next task is to evaluate the limit (20), where \( d\sigma_R/dq \) is given by Eq. (46), and \( d\sigma \) by the eikonal approximation (7), (8), (43). Similarly to Eq. (14), we transform the encountered integral to the form

\[
\int_0^{q_{cr}} dq \frac{d\sigma}{d\sigma_R} = \frac{1}{2\pi} \int_{q_{cr}} d^2q \left| \frac{q a}{2i\alpha} \right|^2. \tag{47}
\]

Now, to perform the integration over the \( q \) plane restricted by the condition \( q < q_{cr} \), it will be expedient to isolate the Coulomb singularity contribution by breaking \( \int d^2b \) in (15) into two parts: one over a small disk centered at the origin, \( b < b_R \), and another one over its exterior \( b > b_R \). In contrast to the previous section, the boundary \( b_R \) is not assumed to be strictly related to \( q_{cr} \), and is just chosen so small \( (b_R \ll r_{sc}) \) that at \( b < b_R \) the screening is entirely negligible, i.e., small-\( b \) asymptotics (44) holds. A caveat is that since the primary definition (20) implies \( q_{cr} \to \infty \), we must subject \( b_R \), in spite of its smallness, to condition

\[
q_{cr} b_R / \hbar \gg 1. \tag{48}
\]

Inserting amplitude (8) to Eqs. (15), (20), (47), we get the logarithm of the Molière screening momentum

\[
\ln q_{cr}(\alpha) + \frac{1}{2} = \lim_{\hbar \to 0} \left[ \ln q_{cr} - \frac{1}{(2\pi)^3} \hbar^2 \right. \times \int_{q < q_{cr}} d^2q \left. \left| \int_{b < b_R} d^2b e^{i\frac{qa}{b}} \left( \frac{b}{b_0} \right)^{2i\alpha} + \int_{b > b_R} d^2b e^{i\frac{qa}{b}} e^{2i\alpha S_0(b)} \frac{\partial}{\partial b} S_0 \right|^2 \right], \tag{49}
\]

where in the \( b < b_R \) integral the derivative of the eikonal phase factor was evaluated as

\[
\frac{\partial}{\partial b} e^{2ia \ln \frac{b}{b_0}} = 2ia \frac{b}{b_0} \left( \frac{b}{b_0} \right)^{2i\alpha}. \]

When the square of the sum encountered in Eq. (49) is expanded, in the square of the second term (free from the small-\( b \) singularity) and in the cross term, by virtue of condition (48), it is legitimate to simply put \( q_{cr} \to \infty \). Thereupon \( \int d^2q \) gives a delta function (16). The cross term then vanishes completely, since the delta function for it always has a nonzero argument \( \{b \text{ and } b' \} \) belong to nonoverlapping spatial domains, and thus cannot coincide. That leads to a representation

\[
\ln q_{cr}(\alpha) + \frac{1}{2} = \ln H(\alpha) - \ln b_d, \tag{50}
\]

where

\[
\ln H(\alpha) = \lim_{q_{cr} b_R \to \infty} \left[ \ln q_{cr} b_R - \frac{1}{(2\pi)^3} \hbar^2 \right. \times \int_{q < q_{cr}} d^2q \left. \left| \int_{b < b_R} d^2b e^{i\frac{qa}{b}} \left( \frac{b}{b_0} \right)^{2i\alpha} \right|^2 \right] \tag{51}
\]

\[
(\text{the constant phase factor } b_0^{-2i\alpha} \text{ has dropped out after squaring), and}
\]

\[
\ln b_d = \lim_{b_R \to 0} \left[ \ln b_R + \frac{1}{(2\pi)^3} \hbar^2 \times \int d^2q \int_{b > b_R} d^2b e^{i\frac{qa}{b}} e^{2i\alpha S_0(b)} \frac{\partial}{\partial b} S_0 \right]^2 \right]. \tag{52}
\]

Integrating in (52) over the full \( q \) plane similarly to Eq. (17), one gets:

\[
\ln b_d = \lim_{b_R \to 0} \left[ \ln b_R + \frac{1}{2\pi} \int_{b > b_R} d^2b \left| e^{2i\alpha S_0(b)} \frac{\partial}{\partial b} S_0 \right|^2 \right] \equiv \lim_{b_R \to 0} \left[ \ln b_R + \frac{1}{2\pi} \int_{b > b_R} d^2b \left| \frac{\partial}{\partial b} S_0 \right|^2 \right]. \tag{53}
\]

Crucial here is that the eikonal phase factor \( e^{2i\alpha S_0(b)} \) has canceled, as in (17). That offers the possibility in the impact parameter representation to regard the moderate-\( b \) contribution to the Coulomb correction to \( q_{cr} \) as absent. If the potential is spherically symmetric, Eq. (53) reduces to the form

\[
\ln b_d = \lim_{b_R \to 0} \left[ \ln b_R + \int_{b > b_R} \frac{db}{b} S_1^2(b) \right]. \tag{54}
\]

Turning to \( \ln H(\alpha) \) defined by Eq. (51), due to the presence of the small-\( b \) singularity, it cannot be simplified by application of the identity (16). But a simplification comes from the absence of screening. Integrating in (51) over the azimuth of \( b \), and passing from \( b \) to a rescaled variable \( \phi = qb/\hbar \), one observes that due to the scale invariance of the integrand, a reciprocal \( q \) factor carries out of the integral:

\[
\left| \int_{b < b_R} d^2b e^{i\frac{qa}{b}} \left( \frac{b}{b_0} \right)^{2i\alpha} \right|^2 = \left( \frac{2\pi \hbar}{q} \right)^2 G_d(q b_R / \hbar). \tag{55}
\]

with

\[
G_d(s) = \left| \int_0^s d\phi \phi^{2i\alpha} J_1(\phi) \right|^2. \tag{56}
\]

Insertion of (55) to the \( q \) integral in (51) brings the latter to a form depending on \( q_{cr} \) and \( b_R \) only through their product:

\[
\ln H(\alpha) = \lim_{q_{cr} b_R \to \infty} \left[ \ln q_{cr} b_R - \int_0^{q_{cr} b_R / \hbar} \frac{ds}{s} G_d(s) \right]. \tag{57}
\]

with

\[
s = \frac{q b_R}{\hbar}. \]

Before we proceed, let us examine the structure of the function \( G_d(s) \) in the integrand.

In the definition (56) of \( G_d \), the \( \phi \) integral at \( s \to \infty \) tends to a constant

\[
\int_0^\infty d\phi \phi^{2i\alpha} J_1(\phi) = 2^{2i\alpha} \frac{\Gamma(1 + i\alpha)}{\Gamma(1 - i\alpha)}. \tag{58}
\]
It equals the familiar phase factor encountered above in the pure Coulomb scattering amplitude \((45b)\). On the contrary, at finite \(s\), due to the finite upper limit of the integral in \((53)\), the absolute value of \(G_\alpha(s)\) differs from unity. Moreover, it tends to zero at \(s \to 0\), describing diffraction on an “almost empty” disk \(b < b_R\). Therefore, \(\int_0^{b_R b_R/h} \frac{dk}{k} G_\alpha(s)\) converges at the lower limit, and logarithmically diverges when the upper limit \(q_R b_R/h\) tends to infinity. Thus, \(G_\alpha(s)\) may be regarded as a square of the incomplete Coulomb phase factor, which is responsible for the Coulomb correction.

A general \(s\) dependence of \(G_\alpha(s)\) is illustrated in Fig. 2. For small \(\alpha\), it exhibits strong oscillations. They might be partly mitigated if we took into account the neglected interference part, but that will not concern us for the present purposes. In the classical limiting case \(\alpha \to \infty\), \(G_\alpha(s)\) tends to a unit step function\(^2\)

\[
G_\alpha(s) \to \Theta(s - 2\alpha) \quad (60)
\]

to a unit step function, furnishing a sharp cutoff at \(q = 2h\alpha/b_R\) related to the moving \(Q_R(\alpha)\) given by Eq. \((41)\).

In spite of the fact that the function \(G_\alpha(s)\) is rather complicated, the integral \((57)\) containing it can be evaluated in to a fairly simple form, as is demonstrated in Appendix B. The result reads

\[
\ln H(\alpha) = \ln H(0) + f(\alpha), \quad (61)
\]

with \(f(\alpha)\) given by Eq. \((3)\), and

\[
\ln H(0) = \ln 2h - \gamma_E. \quad (62)
\]

Combining \((62)\) with \((54)\) in Eq. \((50)\), one retrieves the formula \((36)\). Substitution of \((61)\) to \((50)\) leads to the formula \((5)\) quoted in the Introduction.

Thus, even in the presence of a Coulomb singularity, it is possible to cancel eikonal phases in the entire screening region, provided a vicinity of the singularity is isolated and treated carefully. The exact value \(b_R\) of the cutoff is unimportant, but its very existence and constancy for all \(q\) makes the structure of the isolated hard part different from that of the soft part. The impact parameter integral with the finite upper limit does not equal a pure phase factor \((58)\), and can go down to zero. The shape of the crossover function \(G_\alpha(s)\) in the quantum case differs from the unit step function \((60)\) characteristic for the classical case. Compared with Sect. 2.5, one can say that the “paste squeezed out of a tube” becomes quantal and oscillates. What is important, however, is not the shape of the crossover, but the location of its main rise, which is monotonically dependent on \(\alpha\). That leads to a monotonic \(\alpha\)-dependence of the Coulomb correction \(f(\alpha)\).

With these clarifications about cancellation of the eikonal phases, we do not need to presume applicability of the perturbation theory in the partly screened region ad hoc. That is vital, because the physical conditions of applicability of the Born approximation \(\chi_0/h \sim \alpha \ll 1\) break down in the partly screened region, if they do so in the unscreened one.

Having rectified physical and mathematical issues about the Coulomb correction in our problem, we are now in a position to extend its treatment regarding atomic electrons as pointlike charged particles as well.

### 4 Account of inelastic scattering

At low \(Z\), the approximation of scattering in a mean static potential (the field of the nucleus screened by the mean electron charge distribution in the initial state) is generally inadequate. Rigorously, the atom must be treated as a few-body system, containing a finite number of electrons. But the high-energy approximation (eikonal formula) still works, albeit under somewhat more stringent conditions.

Specifically, during a fast collision of the incident high-energy particle with an atom, i.e., under condition \([26]\)

\[
v \gg v_a, \quad (63)
\]
the motion of all the atomic electrons may be neglected. When the incident particle is an ion, this condition appears to be stronger than (12), (13), since there is no small factor in the right-hand side \( Z_1 m_e/m_1 \sim m_e/m_p \ll 1 \). Nonetheless, it is also easy to fulfill if \( v \geq 0.1c \), since \( v_0 \sim e^2/\hbar = c/137 \).

Therefore, during their interaction with a sufficiently fast projectile, atomic electrons are effectively static (“frozen” in definite positions). Subsequently they transform to final states, but on much longer, atomic times, on which the electrons evolve quantum mechanically. The only technical difference from the previous section is that an averaging over the initial atomic electron distribution has to be performed after evaluation of the eikonal amplitude. Since for the present problem we are not concerned with the final electron distribution, summation (integration) over probabilities of all possible outcomes is due. In such an inclusive approach, by virtue of the eikonal phase cancellation along with the closure relation for the final states, the actual knowledge of the atomic dynamics will not be needed.

For simplicity, we still assume the incident particle to be structureless. It can experience close collisions with the atomic nucleus and atomic electrons. Compared with the perturbative case, when hard collisions with electrons are equivalent to inelastic, in a nonperturbative close collision with the nucleus, a possibility of atom ionization by additional soft interactions with atomic electrons is not precluded. But the description of multiple Coulomb scattering involves only the inclusive differential cross section and its Rutherford asymptotics, rather than the separation into elastic and inelastic channels.

4.1 Molière angle for inclusive scattering

Taking into account the remarks above, we start with the evaluation of the scattering amplitude kernel, assuming atomic electrons to have arbitrary fixed positions \( r_1, \ldots, r_Z \), and the nucleus to be located at the origin. They create a classical electrostatic field, which is not spherically symmetric. The eikonal amplitude of scattering of the projectile in such a field is similar to (8):

\[
a(r_1, \ldots, r_Z; q) = \frac{1}{2\pi i \hbar} \int d^3b e^{i\langle b|q - b\rangle/\hbar} \times \left\{ 1 - e^\frac{i}{\hbar} \chi_0(b_1, \ldots, b_Z; b) \right\}.
\]

(64)

Eikonal phase \( \chi_0(b_1, \ldots, b_Z; b) \) for an assembly of pointlike charged scatterers can be evaluated explicitly:

\[
\chi_0(b_1, \ldots, b_Z; b) = -\frac{Z_1 e^2}{v} \int_{-\infty}^{\infty} dz \sum_{k=1}^{Z} \frac{1}{r_k - \sum_{k'=1}^{Z} r_{k'}} = \frac{Z_1 e^2}{v} \ln b - \frac{Z_1 e^2}{v} \sum_{k=1}^{Z} \ln |b - b_k|.
\]

(65)

To obtain from (64) the amplitude of scattering with excitation or ionization of the atom from the initial (normally, ground) state \( \psi_0 \) to an arbitrary (discrete or continuum) state \( |n\rangle \), we must convolve (64) with wave functions \( \psi_0, \psi_n \) of those states [22]:

\[
\langle n|a|0\rangle = \sum_{s_1, \ldots, s_Z, q} \int d^3r_1 \ldots d^3r_Z \psi^*_n(r_1, s_1, \ldots, r_Z, s_Z) \\
\times a(r_1, \ldots, r_Z; q) \psi_0(r_1, s_1, \ldots, r_Z, s_Z).
\]

(66)

(\( s_1, \ldots, s_Z \) are electron spin quantum numbers.)

Next, the amplitude (66) is squared to yield the generic partial differential cross section, and summed over all \( n \) to give the inclusive differential cross section (see Fig. 3).

Employing the closure relation \( \sum_{n=0}^{\infty} |n\rangle \langle n| = 1 \), we get

\[
\frac{d\sigma_{0\rightarrow X}}{d^2q} = \int_{0}^{\infty} d|n\rangle \langle n| = \langle 0|a^*a|0\rangle
\]

\[
= \int d^3r_1 \ldots d^3r_Z \rho_0(r_1, \ldots, r_Z) |a(r_1, \ldots, r_Z; q)|^2.
\]

(67)

Here,

\[
\rho_0(r_1, \ldots, r_Z) = \sum_{s_1, \ldots, s_Z} |\psi_0(r_1, s_1, \ldots, r_Z, s_Z)|^2
\]

(68)

is the initial-state electron coordinate probability distribution, normalized by condition

\[
\int d^3r_1 \ldots d^3r_Z \rho_0(r_1, \ldots, r_Z) = 1.
\]

The subscript 0 at \( d\sigma \) and \( \rho \) indicates that the initial state was \( |0\rangle \).

Fig. 3 Schematic illustration of inclusive scattering of a fast charged particle on an atom in initial state \( |0\rangle \). Due to the large Coulomb parameter, the particle–atom interaction is nonperturbative, i.e., multiple photon exchanges can contribute significantly. After the scattering, the fast particle is imparted a momentum \(-q\), while its energy changes relatively slightly. The excited atom goes to an arbitrary state with total momentum \( q \). Such states are collectively designated as \( X \). The process differential cross section is summed over all of them.
Thereupon, (67) is inserted into the definition of \( q_{at} \) similar to (20):
\[
\ln q_{at} + \frac{1}{2} = \lim_{q_R \to \infty} \left( \ln q_R - \frac{1}{2} \int_{0}^{q_R} \frac{dq}{q} \frac{d\sigma_{0-x}}{d\sigma_R} \right),
\]
(69)
where \( d\sigma_R \) is now the high-\( q \) asymptotics of \( d\sigma_{0-x} \), such that
\[
\frac{d\sigma_R}{dq} = \frac{2\pi Z(Z+1)}{q^3} \left( \frac{2Z_1e^2}{v} \right)^2.
\]
(70)
The factor \( Z(Z+1) \) takes into account hard scattering on electrons. The subscript \( at \) in (69) distinguishes it from \( q_{at} \) in Eq. (20), which is reserved for the elastic cross section [21, 30].

4.2 Isolation of the Coulomb correction

Computation of the corresponding averaged differential cross section (67) is somewhat more involved than that for scattering in the averaged atomic potential, but the principle of isolation of the Coulomb correction remains the same. The integration over the electron coordinates and summation over the final states can be deferred to the last calculation stage. Employing Eq. (15), we write
\[
\ln q_{at} + \frac{1}{2} = \lim_{q_R \to \infty} \left[ \ln q_R - \frac{1}{2} \int_{q < q_R} \frac{d^2q}{2Z^3} 2q^2 |a|^2 \right] \ln v
\]
\[
= \lim_{q_R \to \infty} \left[ \ln q_R - \frac{1}{(2\pi)^3 Z(Z+1)} \left( \frac{u}{2Z_1e^2} \right)^2 \right] \times \langle 0 | d^2q d^2q_{bat} \left| \frac{d}{db} \ln \frac{Z_1e^2}{hv} \right|^2 \rangle | 0 \rangle, \tag{71}
\]
where \( \chi_0 \) is now given by Eq. (65). The last line in (71) involves a multiple integral, which can be evaluated similarly to what was done in Sect. 3, provided we isolate all the Coulomb singularities in the \( b \) plane (Fig. 4):
\[
\int d^2b = \int_{b < b_R} d^2b + \sum_{k=1}^{Z} \int_{|b - b_k| < b_R} d^2b + \sum_{k=Z+1}^{Z} \int_{|b - b_k| > b_R} d^2b.
\]

Once the square of this sum of \( b \)-integrals is expanded, and the limit \( q_R \to \infty \) is taken, in close similarity to what was done in Sect. 3, the interference between the partial \( b \)-integrals vanishes:
\[
\ln q_{at} + \frac{1}{2} = \lim_{q_R \to \infty} \left[ \ln q_R - \frac{1}{2} \int_{q < q_R} \frac{d^2q}{2Z^3} 2q^2 |a|^2 \right] \ln v
\]
\[
= \frac{Z}{Z+1} \ln \left( \frac{Z_1e^2}{hv} \right) + \frac{1}{Z+1} \ln \left( \frac{Z_1e^2}{hv} \right) - \ln b_{at}.
\]

Here, the hard part
\[
\langle 0 | \ln \left( \frac{Z_1e^2}{hv} \right) | 0 \rangle = \ln \left( \frac{Z_1e^2}{hv} \right)
\]
is given by Eq. (57) (since we neglect overlaps of the regions contributing to the Coulomb correction, they are completely independent of the electron distribution), and
\[
\ln b_{at} = \ln b_R + \frac{1}{(2\pi)^3 Z(Z+1)} \left( \frac{v}{2Z_1e^2} \right)^2 \times \langle 0 | d^2q d^2q_{bat} \left| \frac{d}{db} \ln \frac{Z_1e^2}{hv} \right|^2 \rangle | 0 \rangle. \tag{73a}
\]
\[
= \ln b_R + \frac{1}{2\pi Z(Z+1)} \left( \frac{v}{2Z_1e^2} \right)^2 \times \langle 0 | d^2q d^2q_{bat} \left| \frac{d}{db} \chi_0(b) \right|^2 \rangle | 0 \rangle. \tag{73b}
\]
In Eq. (73a) we have set \( q_R = \infty \) (no divergence occurs), whereas in (73b) we employed identity (16).

Since after cancelation of eikonal phases \( b_{at} \) becomes independent of the Coulomb parameter, as in Eq. (36), we can relate it to \( q_{at}(0) \):
\[
\ln b_{at} = \ln \left( \frac{Z_1e^2}{hv} \right) - \ln q_{at}(0) - \frac{1}{2}. \tag{74}
\]
Equation (72) then can be written as
\[
\ln q_{at} = \ln q_{at}(0) + \frac{Z}{Z+1} \ln \left( \frac{Z_1e^2}{hv} \right) \ln H(0)
\]
\[
+ \frac{1}{Z+1} \ln \left( \frac{Z_1e^2}{hv} \right) \frac{H(0)}{H(0)}. \tag{75}
\]
Employing Eq. (96), it is brought to the final form

\[ \frac{q_{at}}{q_{at}(0)} = e^{-\frac{q_{at}}{2\pi f}} f(Z Z_1 e^2/hv) + \frac{1}{2\pi f} f(Z_i e^2/hv). \]  

(76)

It can also be straightforwardly generalized to scatterers consisting of arbitrary charges \( Z_k e \) (electrons and nuclei of atoms of different sorts):

\[ \frac{q_{at}}{q_{at}(0)} = \exp \left[ \sum_k Z_k^2 f \left( Z_k Z_1 e^2/hv \right) / \sum_k Z_k^2 \right]. \]  

(77)

This formula has the same structure as for multiple Coulomb scattering in a composite substance [3, 16].

Equation (76), which is the main result of the present article, has a clear meaning. Since the Coulomb correction is independent of screening, the contributions to it from atomic electrons and nuclei may be calculated independently, as if they stemmed from scattering on bare particles in an ideal plasma. It must be realized yet that, generally, the electronic contribution \( \frac{1}{2\pi f} f \left( Z_1 e^2/hv \right) \) is neither purely inelastic nor elastic. Only at the Born level it holds that

\[ q_{at}(0) = q_{at} \frac{q_{at}}{q_{at}(0)} q_{at}(0). \]  

(78)

In the Fano theory [21], the term containing \( f \left( Z_1 e^2/hv \right) \) [essentially the Bloch correction, cf. Eq. (1)] is absent, whereas \( f \left( Z Z_1 e^2/hv \right) \), approximated as in (4) and neglecting the \( \frac{1}{2\pi f} \) factor, is attributed to the elastic channel. Thus, [21] takes into account the inelastic contribution to \( q_{at}(0) \), but not to its Coulomb correction. As we pointed out at the beginning of Sect. 4,

\[ q_{a} \neq e^{-\frac{q_{at}}{2\pi f}} f \left( Z Z_1 e^2/hv \right) q_{at}(0), \]

\[ q_{in} \neq e^{-\frac{1}{2\pi f}} f \left( Z_i e^2/hv \right) q_{in}(0), \]

because nonperturbative evolution of \( q_{a} \) and \( q_{in} \) is not independent (they intermix). Nonetheless, in the inclusive calculation, any process (elastic or inelastic) occurring before and after the particle approaches to the Coulomb singularity is inconsequential, and the “strength” (partial contribution) of each singularity in the eikonal phase is determined only by the charge of the corresponding particle, exactly resembling the situation in a composite substance.

5 Practical remarks

Let us now analyze the obtained result quantitatively.

5.1 Analysis of the two-variable dependence

Unlike the formula (5) for multiple scattering in a mean static atomic potential, the obtained expression (76) for inclusive scattering with the account of pointlike electrons depends on two variables. Only for \( Z \gg 1 \) or \( Z = 1 \) (as long as for a hydrogen atom high-energy Rutherford scattering at its nucleus and electron has the same strength) does its exponent reduce to \( f \left( Z Z_1 e^2/hv \right) \), leading back to Eq. (5). To illustrate the deviation of Eq. (76) from (5), let its two independent variables be \( Z \) and \( Z Z_1 e^2/hv \). Fig. 5 shows that, for any \( Z \), the ratio (76) increases monotonically (in the classical regime, linearly) with \( Z Z_1 e^2/hv \), while its slope is \( Z \)-dependent. To give an idea of the latter dependence, it may suffice to consider two extreme but nearly overlapping cases.

At \( Z Z_1 e^2/hv < 1 \) (e.g., for relativistic incident electrons or protons, when \( |Z_1| e^2/hv \sim 10^{-2} \), while \( Z < 10^2 \) for all substances), arguments of both functions \( f \) in (76) are small. This function may then be expanded in a Taylor series to the leading, quadratic order:

\[ f(s) \approx \sum_{s=0}^{\infty} \zeta(s)s^2, \]

where \( \zeta(3) = -\psi''(1)/2 = \sum_{n=1}^{\infty} n^{-3} = 1.202. \) For \n\[ \ln \frac{q_{at}}{q_{at}(0)} \] 
\[ \ln \frac{q_{at}}{q_{at}(0)} = \zeta(3) \left( \frac{Z}{Z + 1} + \frac{1}{Z + 1} \right) \left( \frac{Z Z_1 e^2}{hv} \right)^2 \]
\[ \equiv (1 - Z^{-1} + Z^{-2}) \zeta(3) \left( \frac{Z Z_1 e^2}{hv} \right)^2. \]  

(79)

Here, the pure coherent scattering result \( \zeta(3) \left( \frac{Z Z_1 e^2}{hv} \right)^2 \) corresponding to Eq. (5) is multiplied by a modulating factor \( 1 - Z^{-1} + Z^{-2} \). The latter has a minimum at \( Z = 2 \), where it equals 3/4, whereas at \( Z = 1 \) and \( Z \to \infty \) it turns to unity (see Fig. 6, dashed curve). The variation of this factor in the entire range is thus moderate, but appreciable.

In the opposite case \( Z Z_1 e^2/hv > 1 \) (e.g., for \( \alpha \)-particles with energies \( T < 500 \) keV), the arguments of both functions \( f \) in (76) are large. Then for those functions one can employ

\[ q_{at}/q_{at}(0) \]

Fig. 5 Ratio (76) of the Molière screening angle to its Born value at \( Z Z_1 e^2/hv \to 0 \) \( [q_{at}/q_{at}(0) = q_{at}/q_{at}(0)] \). Black solid curve, for \( Z = 1 \), also virtually the same for \( Z > 50 \). Dashed, \( Z = 2 \) (helium). Dot-dashed, \( Z = 4 \) (beryllium). Dotted, \( Z = 14 \) (silicon). Red solid (the uppermost) curve, Molière’s algebraic interpolation (4).
the large-argument asymptotics (34) to get
\[ \frac{q_{at}}{q_{at}(0)} \simeq Z^{-1/4} \frac{Z_{1} Z e^{2}}{\hbar v} e^{\chi_{a}}. \]  
(80)

The last two factors here may be identified with the coherent scattering contribution [cf. Eq. (35)]. The first factor \( Z^{-1/4} \) furnishes a modulation. At \( Z = 1 \) and \( Z \to \infty \) it turns to unity (see Fig. 6, solid curve), while in between it has a minimum at \( Z = 3.6 \), where it equals 0.756. Hence, at \( ZZ_{1} e^{2}/\hbar v \gtrsim 1 \) and low \( Z \neq 1 \), the (negative) difference of \( q_{at}/q_{at}(0) \) from its coherent counterpart (5) or (35) is \( \sim 25 \%), remaining sizable also at medium \( Z \) (see the dotted curve for silicon in Fig. 5). The modulation in the semiclassical case is somewhat stronger than in the quantum case considered above, but is of the same order.

5.2 Experimental evidence

We conclude that the electronic contribution to the Coulomb correction becomes substantial at low \( Z \). It can be much greater, for example, than the inaccuracy of the Molière parametrization (4) for the purely coherent contribution (the difference between the two solid curves in Fig. 5) pointed out in [31]. But the Molière–Fano theory was tested against a broad variety of target materials, projectile types, and energies, so could deviations from it have already been seen before?

In this regard, it should be realized first of all that in the Molière theory, \( \chi_{a} \) enters only as a constant correction to a large logarithm \( \ln \frac{Z_{a}^{2}}{Z} \), where \( \chi_{a}^{2} \) grows in proportion to the target thickness (see [3,16] and Appendix A). The angular distribution is nowhere exceptionally sensitive to \( \chi_{a} \) [32], so, for determination of the latter parameter, there is no better way than to measure the distribution width, for which the statistics is the highest. The applicability of Molière’s multiple scattering theory demands that \( \frac{Z_{a}^{2}}{Z} > 10^{2} \) [16,30], corresponding to \( \ln \frac{Z_{a}^{2}}{Z} > 5 \). Moreover, as we found at the end of Sect. 4, the deviation from Molière’s prediction for the screening angle \( \chi_{a} \) does not exceed 25\%. Hence, relative effects in the distribution width stemming from the electronic contribution to \( q_{a} \) numerically do not exceed \( \frac{\Delta q_{at}}{q_{at}} \lesssim 0.25/5 = 0.05 \). Such minute corrections might elude attention for years, but should ultimately become discernible in high-statistics experiments.

Given that the sensitivity to \( \chi_{a} \) is modest (see also [33]), let us assess optimal target and beam parameters. To ensure that incident charged particles are pointlike (fully stripped ions only), in practice it is simplest to use proton beams (\( Z_{1} = 1 \)). To ensure that \( q_{at}/q_{at}(0) \) differs substantially from unity, the Coulomb parameter needs to be made sizable, but velocities that are too low are undesirable, because energy losses then become commensurate with the initial particle energy. Relative deviations close to the maximal value \( \Delta q_{at}/q_{at}(0) \sim 0.25 \) can be reached already at
\[ Z_{1} Z e^{2}/\hbar v = Ze^{2}/\hbar v \sim 2 \]  
(81)

(see Fig. 5). That is still compatible with the condition (63) for the impulse approximation. Condition (81) at \( Z = 6 \) (carbon, being one of the most popular low-\( Z \) targets)\(^3\) corresponds to velocities \( v/c \sim Z e^{2}/2 \cdot 10^{-2} \), i.e., to proton energies \( T = m_{p} v^{2}/2 \sim 200 \) keV.

Experiments on multiple scattering of sub-MeV protons on carbon foils have been carried out since the 1960s [34,35]. Notably, the experiment [35] aimed to measure effective screening radii for \( T = 60–270 \) keV protons scattered by carbon and germanium foils, and reported an excess of the measured screening radii over the theoretical predictions (obtained in a \( Z_{1} \)-modified Thomas–Fermi approximation [36]) by 20\% for carbon and by 10\% for germanium. That may be viewed as a candidate signal in favor of our prediction for the screening angle \( \chi_{a} \) does not exceed 25\%. Hence, relative effects in the distribution width stemming from the electronic contribution to \( q_{a} \) numerically do not exceed \( \frac{\Delta q_{at}}{q_{at}} \lesssim 0.25/5 = 0.05 \). Such minute corrections might elude attention for years, but should ultimately become discernible in high-statistics experiments.

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\(^3\) The need to account for nuclear form factors then does not arise.

\(^4\) At that, longitudinal momentum \( p = \sqrt{2m_{p} T} \sim 20 \) MeV/c is much larger than transverse momentum transfers in Fig. 1, ensuring the validity of the small-angle approximation.
complications due to poor fulfillment of condition (63) or beam slowdown due to its energy loss in the target.

6 Summary and outlook

An expression for the nonperturbative correction to Molière’s screening angle applicable to few-electron atoms has been derived here. The refined formula (76) differs from formula (5) for scattering in the mean static screened potential by an extra term expressed through function (3) with an argument lacking the factor Z. This term bridges the gap between Fano’s result, where the contribution of atomic electrons to multiple scattering on atoms is taken into account only perturbatively, and Bloch’s result, in which energy loss of the projectile at its interaction with atomic electrons is evaluated nonperturbatively, but its relationship with the ion multiple-scattering deflection angle is not brought out. The nonperturbative inelastic contribution is sizable for low-Z projectiles. Quantitatively, this was discussed in Sect. 5. An account of such a nonperturbative correction may also be desirable for a unified theory of multiple scattering and ionization energy loss extended to particles heavier than electrons.

Finally, it may be worth emphasizing that among various processes involving Coulomb corrections, multiple Coulomb scattering is the simplest. For our derivation, which was aided by the use of the eikonal approximation, it was essential that the weighting factor in the integral defining Molière’s screening angle was exactly an integer power of q, convertible into derivatives under the Fourier integral sign. In other problems featuring Coulomb corrections, where the weighting factor is proportional to q^2 only asymptotically (as is the case, e.g., for ionization energy loss), additional complications can arise.

Acknowledgements The author wishes to thank X. Artru and V. G. Serbo for reading the manuscript and useful comments. This work was supported in part by the National Academy of Sciences of Ukraine (program “Support for the Development of Priority Areas of Scientific Research” 6541230 and project C-2/56-2022).

Data Availability Statement This manuscript has no associated data or the data will not be deposited. [Authors’ comment: This is a theoretical paper; all the data used can be found in the cited literature.]

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Funded by SCOAP^3. SCOAP^3 supports the goals of the International Year of Basic Sciences for Sustainable Development.

Appendix A: Molière’s theory of multiple Coulomb scattering

The present appendix briefly reminds the reader of the procedure behind the multiple scattering approximation in the solution of the transport equation for Coulomb scattering in atomic matter. This procedure leads to definition (20) of qa, which is the object of study in the present paper. For more detail, see reviews and monographs [16–18,26].

The probability distribution f(θ,l) of fast particles deflected to a small angle θ after a path length l in an amorphous medium of atomic density na is described by the transport equation

\[
\frac{df}{dl} = na \int d\sigma(\chi) [f(\theta - \chi, l) - f(\theta, l)].
\]  (82)

Here, d\σ(\chi) = d^2\chi \frac{d\sigma}{d\chi} is the differential cross section of the fast particle scattering on one atom through a typical small angle \(\chi = q/p\).

The solution of Eq. (82) for a perfectly collimated initial beam

\[f(\theta, 0) = \delta(\theta)\]

can be expressed in an integral form [38,39]

\[f(\theta, l) = \frac{1}{2\pi} \int_0^\infty d\rho \rho J_0(\rho\theta) e^{-na l} \int d\sigma(\chi) [1 - J_0(\rho\chi)] .\]  (83)

For most of the macroscopic solid targets, there are many atoms encountered along the particle path (the coefficient naσl in the exponent is large), so the scattering process may be regarded as multiple. Under such conditions, the detailed knowledge of d\σ(\chi) is unnecessary, because the integral in (83) can be simplified by expanding the exponent of the sharply peaking exponential around its maximum at \(\rho = 0\). With the account of the Coulomb character of atomic scattering, the expansion begins with terms scaling as \(\rho^2(\ln \rho + \text{constant})\).

To evaluate the latter constant characterizing the atom, the standard procedure [4] is to break the χ semiaxis, over which the integration in the exponent of (83) is performed, by an intermediate value \(\chi_R\) such that

\[\chi_a \ll \chi_R \ll \chi_c.\]  (84)
For the hard part $\chi > \chi_R$, using the Rutherford asymptotics (21) for $d\sigma(\chi)$ throughout, and combining all the prefactors into$^5$

$$\chi_c^2 = 4\pi n_a \left( \frac{Z_1 Z e^2}{p \nu} \right)^2,$$  \hspace{1cm} (85)

we get

$$n_a l \int_{\chi_R}^{\infty} d\sigma(\chi) [1 - J_0(\rho \chi)] \simeq 2 \chi_c^2 \int_{\chi_R}^{\infty} \frac{d\chi}{\chi^3} [1 - J_0(\rho \chi)].$$

This integral is further simplified under the multiple scattering condition $\rho \sim \chi_c^{-1} < \chi_R^{-1}$ making the lower integration limit effectively small:

$$n_a l \int_{\chi_R}^{\infty} d\sigma(\chi) [1 - J_0(\rho \chi)] \simeq \frac{\chi_c^2 \rho^2}{2 \rho \chi_R} \int_{\rho \chi_R}^{\infty} \frac{ds}{s^3} [1 - J_0(s)] \simeq \frac{\chi_c^2 \rho^2}{2} \left( \ln \frac{2}{\rho \chi_R} + 1 - \gamma_E \right).$$  \hspace{1cm} (86)

On the other hand, the soft part $\chi < \chi_R$, with the use of the approximation $1 - J_0(\rho \chi) \simeq \frac{1}{4} \rho^2 \chi^2$ throughout, becomes

$$n_a l \int_0^{\chi_R} d\sigma(\chi) [1 - J_0(\rho \chi)] \simeq \frac{\rho^2}{4} n_a l \int_0^{\chi_R} d\sigma(\chi) \chi^2.$$  \hspace{1cm} (87)

Due to the Rutherford asymptotics of $d\sigma(\chi)$ at $\chi \gg \chi_a$, the latter integral scales logarithmically with $\chi_R$. The atom-specific (due to $\chi \sim \chi_a$ contributions) constant next to $\ln \chi_R$ is conventionally written in the form

$$\int_0^{\chi_R} \frac{d\chi}{\chi} \frac{d\sigma}{d\sigma_R \chi} \simeq \ln \frac{\chi_R}{\chi_a} - \frac{1}{2}. $$  \hspace{1cm} (88)

[The convenience of such a definition including the term $-1/2$ is that for Born scattering in a purely exponentially screened weak Coulomb potential, i.e., if $d\sigma/d\sigma_R = (1 + \chi_a^{-2}/\chi^2)^{-2}$, the parameters $\chi_a$ in the left- and right-hand sides of (88) are equal]. Therefore,

$$n_a l \int_0^{\chi_R} d\sigma(\chi) [1 - J_0(\rho \chi)] \simeq \frac{\chi_c^2 \rho^2}{2} \left( \ln \frac{\chi_R}{\chi_a} - \frac{1}{2} \right).$$  \hspace{1cm} (89)

Adding (86) and (89), we obtain the limiting form for the exponent

$$n_a l \int_0^{\infty} d\sigma(\chi) [1 - J_0(\rho \chi)] \simeq \frac{\chi_c^2 \rho^2}{2} \left( \frac{\ln 2}{\rho \chi_a} + 1 - \gamma_E \right) \equiv \frac{\chi_c^2 \rho^2}{2} \left( \frac{\ln 2}{\rho \chi_a} + 1 - \gamma_E \right).$$  \hspace{1cm} (90)

where the modified screening angle $\chi_a' = \chi_a e^{\gamma_E - 1/2}$ enters the integral representation of the distribution function [4]

$$f(\theta, t) = \frac{1}{2\pi} \int_0^{\infty} d\rho \rho J_0(\rho \theta) e^{-\frac{\chi_c^2 \rho^2}{2} \ln \frac{2}{\rho \chi_a} + \frac{\ln 2}{\rho \chi_a} + 1 - \gamma_E}. $$  \hspace{1cm} (91)

The $\theta$-dependence of this distribution has been studied by many authors (see [16,32] and refs. therein). The object of our present study will be $\chi_a$ itself, or the screening momentum $q_a = \rho \chi_a$, which is $\rho$-independent, and characterizes only the target atom. Definition (88) for $\chi_a$ is equivalent to definition (20) for $q_a$.

**Appendix B: Evaluation of integral (57) expressing the Coulomb correction**

Our goal here is to analytically evaluate the integral (57) involving the function (56), which in turn is a square of a certain integral. The first simplification can be gained if we note that the integral entering (56) depends on $s$ only through its upper limit. Integration in (57) over $s$ by parts brings $\ln H(\alpha)$ to the form of a double integral

$$\ln H(\alpha) = \int_0^\infty ds \ln s \frac{d}{ds} G_a(s) = 2 \Re \int_0^\infty ds s^{-2\alpha} \ln s J_1(s) \int_0^s d\phi \phi^{2\alpha} J_1(\phi). $$  \hspace{1cm} (92)

This can be further simplified by rescaling once again the integration variable, $\phi = sy$, which eliminates one of the $\alpha$-dependent factors in the integrand:

$$\ln H(\alpha) = 2 \Re \int_0^\infty ds s \ln s J_1(s) \int_0^1 dy y^{2\alpha} J_1(1) J_1(y). $$  \hspace{1cm} (93)

The integral in (93) is evaluated straightforwardly if $\alpha = 0$. In that case

$$\ln H(0) = 2 \int_0^\infty ds \ln s J_1(s) \int_0^1 dy J_1(y) = 2 \int_0^\infty ds \ln s J_1(s) [1 - J_0(s)] = \ln 2 - \gamma_E.$$

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We are thereby led to Eq. (62).

For \( \alpha \neq 0 \), evaluation of the double integral (93) is hampered by the fact that \( \int_0^1 dy y^{2\alpha} J_1(sy) \) is a complicated function of both \( s \) and \( \alpha \). That difficulty can be circumvented by changing the integration order and utilizing a relatively simple integral

\[
\int_0^\infty ds s \ln s J_1(s) J_1(sy) = -\frac{y}{1 - y^2} \quad (|y| < 1).
\]

(95)

But such a procedure needs caution, since the convergence of the \( s \)-integral is neither absolute nor uniform, so the change in the integration order is generally not permissible. Indeed, the right-hand side of (95) diverges at \( y \to 1 \), causing in turn a divergence of the \( y \)-integral

\[
\int_0^1 dy \frac{y^{1+2\alpha}}{1 - y^2}
\]

on the upper limit, whereas physically the result must obviously be finite.

In fact, the \( s \)-integral in (93), (95) converges as \( s \to \infty \) only due to the oscillatory behavior of Bessel functions in the integrand. As in the Fourier integral theory, rigorously, a factor \( e^{-\epsilon \alpha} \) with \( \epsilon > 0 \) must be introduced in the integrand, and after evaluation of the \( s \) integrals, the limit \( \epsilon \to +0 \) be taken. Such a regularization already makes the integral converge absolutely and uniformly, permitting the change of the integration order. In this procedure, the right-hand side of (95) gets regularized by \( \epsilon \) at \( y \to 1 \), and the regularized integral must be inserted to the \( y \)-integral. Of course, that would make the procedure technically more complicated.

Fortunately, there is a possibility to circumvent such technical complications altogether. It suffices to form a difference \( \ln H(\alpha) - \ln H(0) \) needed for the ratio \( q_\alpha/q_\alpha(0) \) [cf. Eq. (24)]. It is insensitive to \( \epsilon \) regularization at \( y \to 1 \) due to the factor \( 1 - y^{2\alpha} \) vanishing in this limit. Therefore, it may safely be evaluated by changing the integration order with the aid of (95) as if the regularization was applied, yielding:

\[
\ln H(\alpha) - \ln H(0) = 2\pi \epsilon \int_0^\infty ds s \ln s J_1(s) \int_0^1 dy (y^{2\alpha} - 1) J_1(sy)
\]

\[
= 2\pi \epsilon \int_0^1 dy y \frac{1 - y^{2\alpha}}{1 - y^2} = 2\pi \epsilon \psi(1 + i\alpha) + \gamma_E.
\]

(96)

[The latter integral, by presenting \( \frac{dy}{1 - y^2} = -d \ln(1 - y^2) \) and integrating by parts, reduces to a derivative of Euler’s beta function.] That leads to a finite result (61) with \( f(\alpha) \) defined by Eq. (3).

Subtracting Eq. (93) from (50) and employing Eq. (96), we recover equation (5), while with the aid of Eqs. (94) and (54), \( q_\alpha(0) \) checks to satisfy equation (36).

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