Alternative treatment for the energy-transfer and transport cross section in dressed electron-ion binary collisions

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A formula for determining the electronic stopping power and the transport cross section in electron-ion binary collisions is derived from the induced density for spherically symmetric potentials using the partial-wave expansion. This approach is the scattering potential \( V(r) \), from which the phase shifts can be calculated. Since the general form for the self-consistent electron-scattering potential \( V(r) \) is still an issue, numerous publications simply use a screened Coulomb (Debye-Hückel or Yukawa) potential

\[
V(r) = -Z \frac{e^{-\alpha r}}{r},
\]

where \( Z \) is the atomic number of the ion and \( \alpha^{-1} \) is a velocity-dependent screening length. At high velocities, the use of the Yukawa potential with \( \alpha = \omega_p/v \) [16], where \( \omega_p \) is the plasmon frequency, given by \( \omega_p^2 = 4\pi n_0 \), is consistent with the spherical average of the scattering potential calculated by perturbation theory. However, the weakest part of using the Yukawa potential is the asymptotic high-velocity limit given by Eqs. (1) and (2): It does not give the well-established Bethe formula

\[
\frac{dE}{dz} = Z^2 \frac{\omega_p^2}{v^2} \ln \left( \frac{2v^2}{\omega_p} \right),
\]

but instead results in

\[
\frac{dE}{dz} = Z^2 \frac{\omega_p^2}{v^2} \left[ \ln \left( \frac{2v^2}{\omega_p} \right) - \frac{1}{2} \right].
\]

This shortcoming is attributed to the actual scattering potential, which has cylindrical symmetry around the ion-velocity vector. Therefore, it is noncentral, in contradiction to the basis of Eq. (2). However, the origin of this shortcoming has not really been understood so far and many works have circumvented this issue by introducing an ad hoc energy-loss mechanism as in the binary theory of stopping power [15] used in Ref. [17], by rescaling the screening length of the interaction [12], or by simply calculating relative quantities [11,18,19].

In this work I demonstrate that a central potential [such as the Yukawa potential from Eq. (3)] and the corresponding partial-wave analysis can still be used by replacing Eq. (2) with

\[
\sigma_{tr}(v') = \frac{4\pi}{v'^2} \sum_{\ell=0}^{\infty} (\ell + 1) \sin^2(\delta_\ell - \delta_{\ell+1}).
\]
a different one [see Eq. (19)], which is not derived from the
definition of the transport cross section (from the momentum-
transfer cross section) but rather from the retardating force acting
on the ion due to the induced charge density. The resulting
retarding force gives the correct Bethe limit according to Eq. (4)
and, in addition, is consistent with the full nonperturbative
Bloch formula [20].

In what follows we first consider a degenerate electron
gas. In particular, the energy loss to valence electrons from
a solid or lesser-bound molecules in molecules has been
successfully modeled by a degenerate electron gas system
[9,10,12,14,16,21–25]. Most of the nonperturbative stopping-
power calculations in an electron gas system have been
performed by evaluating the transport cross section \( \sigma_r \)
from Eq. (2) and integrating over all states inside the Fermi sphere.
Thus, Eq. (1) becomes [10,14]

\[
\frac{dE}{dz} = \frac{1}{16\pi^2v^2} \int_{|v-\nu_f|}^{v+\nu_f} dk^2 \sigma_r(k)[k^2 - (v - \nu_f)^2] 
\times[(v + \nu_f)^2 - k^2],
\tag{6}
\]

where \( \nu_f \) is the Fermi velocity of the electron gas determined
from \( n_0 = \nu_f^3/3\pi^2 \). For \( v \ll \nu_f \) and \( v \gg \nu_f \), Eq. (6) gives the
well-known expressions [10] for the stopping power

\[
\frac{dE}{dz} = \begin{cases} 
(n_0^2v^2 \sigma_r(\nu_f)) & \text{for } v \ll \nu_f \\
(n_0^2v^2 \sigma_r(v)) & \text{for } v \gg \nu_f.
\end{cases}
\tag{7}
\]

II. THEORETICAL PROCEDURE

In the following, the electronic stopping power is calculated
from the retarding force due to the induced asymmetric
charge density acting on the projectile. This principle is well
known, but so far has been treated mostly for the perturbative
regime [9,10]. For an electron gas system, this method should
be equivalent to the one in Eq. (1), as long as the actual self-consistent scattering potential is used. For approximate scattering potentials, both methods may differ, as will be shown.

A central potential \( V(r) \) is used to generate a noncentral
induced density \( n_{\text{ind}}(\vec{r}) \) from the partial-wave expansion of the stationary wave function for the electron-ion collision [26],

\[
\psi_{\ell}(\vec{r}) = 4\pi \sum_{\ell,m} i^\ell e^{i\ell\vec{k} \cdot \vec{r}} Y_{\ell,m}(\hat{\vec{r}}) f_{\ell,m}(\vec{k}),
\tag{8}
\]
in the rest frame of the ion. Then \( \vec{k} \) corresponds to the incident electron momentum and \( R_{\ell,k}(r) \) is the corresponding radial wave function with angular momentum quantum number \( \ell \). The spherical harmonics \( Y_{\ell,m} \) from Eq. (8) are functions of \( \vec{k} \) and \( \ell \), the directions of \( \vec{k} \) and \( \hat{k} \), respectively, and depend on the azimuthal quantum number \( m \) (|m| \( \leq \ell \)). This wave function
is used to calculate the induced electron density according to

\[
n_{\text{ind}}(\vec{r}) = \frac{2}{(2\pi)^3} \int_{\text{DFS}} (|\psi_{\ell}|^2 - 1) d^3k,
\tag{9}
\]
where the \( \vec{k} \) integration is performed over the displaced Fermi sphere (DFS) [16,25,27,28], the target Fermi sphere in the ion
reference frame. The induced force \( \vec{F}_{\text{ind}} \) at the ion \( (\vec{r} = 0) \) or the
potential \( V_{\text{ind}}(\vec{r}) \) is obtained from the induced electron-density
\( n_{\text{ind}}(\vec{r}) \) and is related to the stopping force by [29]

\[
\frac{dE}{dz} = -\frac{1}{v} \vec{F}_{\text{ind}} \cdot \vec{v} = Z \left[ \frac{\partial V_{\text{ind}}}{\partial z} \right]_{\vec{r}=0}
= -Z \left[ \int_{\text{DFS}} \frac{\partial}{\partial z} n_{\text{ind}}(\vec{r}) d^3r \right]_{\vec{r}=0}
\tag{10}
\]
for a bare ion with charge \( Z \).

A. High-energy limit \( v \gg \nu_f \)

Let us consider the limit \( v \gg \nu_f \), where the Fermi sphere is
fully displaced and the incident electron momentum \( \vec{k} \) is given
asymptotically by \( \vec{k} = -\vec{v} \), where \( \vec{v} \) is the ion velocity. In this
case, the induced density is simply given by

\[
n_{\text{ind}}(\vec{r}) = n_0(|\psi_{\ell}|^2 - 1).
\tag{11}
\]
Then the stopping force from Eq. (10) yields

\[
\frac{dE}{dz} = -Z \frac{\alpha_p^2}{2v} \int d^3r' \frac{|\psi_{\ell}|^2 - 1}{v_f^3}.
\tag{12}
\]
The last term vanishes after the integration. Inserting the partial-wave expansion from Eq. (8) into Eq. (12) and using
the mathematical properties depicted in the Appendix, a straightforward but cumbersome calculation gives the fol-
lowing surprisingly simple expression for electronic stopping power as a function of the phase shifts \( \delta_\ell \) at energies \( \epsilon = v_f^2/2 \):

\[
\frac{dE}{dz} = \frac{Z\alpha_p^2}{2v} \sum_{\ell=0}^\infty \sin[2(\delta_\ell - \delta_{\ell+1})],
\tag{13}
\]
which is notably different from the transport cross-section
approach given by Eq. (2).

Using the Born approximation for the Yukawa potential,
the phase shifts can be calculated analytically and then
the stopping power from Eq. (13) will become (see the Appendix
for further details) the Bethe formula as in Eq. (4). Moreover,
for the case of \( v \gg \nu_f \) but \( Z/v > 1 \), the Born approximation cannot be used anymore. However, Eq. (13) reproduces, as shown in the Appendix, the correct nonperturbative Bloch
formula [20]

\[
\frac{dE}{dz} = \frac{\alpha_p^2}{2v} Z^2 \left[ \ln\left( \frac{2v^2}{\omega_p} \right) + \Psi(1) - \Re \Psi(1 + iz/Z) \right],
\tag{14}
\]
where \( \Psi(x) \) denotes the digamma function [9].

B. General case

Now we consider the case where the integration over \( \vec{k} \)

is performed exactly in the DFS zone. The general expression is
obtained by combining Eq. (8) with Eq. (9) in Eq. (10) and is
expressed as
\[
\frac{dE}{dz} = Z \left[ \frac{2}{(2\pi)^2} \int_{|v_f|} \frac{d^3k}{|k|} \right] \times \sum_{\ell \ell'} \sum_{m, m'} i'(-i') e^{i(k' - k)} Y_{\ell, m}(k) Y_{\ell', m'}(k) \\
\times \int d\Omega' \cos \theta Y_{\ell, m}(\hat{r}') Y_{\ell', m'}(\hat{r}') \\
\times \int dr' \frac{1}{r'^2} [r'^2 R_{k, \ell}(r')] [r'/R_{k, \ell}(r')].
\]
\hspace{1cm} (15)

Using the properties from the Appendix, the spherical harmonics addition theorem, and the relation between the spherical harmonics and Legendre polynomials, a straightforward calculation leads to
\[
\frac{dE}{dz} = \frac{Z}{8\pi v_f^2} \int_{|v_f|} dk \times \left[ 2k^2 (v_f^2 + v^2) - k^4 - (v_f^2 - v^2)^3 \right] \\
\times \sum_{\ell = 0}^\infty \sin(2[\delta_\ell(k) - \delta_{\ell+1}(k)]),
\]
\hspace{1cm} (16)
whose limit as \(v \to 0\) is
\[
\frac{dE}{dz} = \frac{Z v_f^2}{2 v_f^2} \sum_{\ell = 0}^\infty \sin(2[\delta_\ell(v_f) - \delta_{\ell+1}(v_f)]),
\]
\hspace{1cm} (17)
which is similar to Eq. (7). As expected, for \(v \gg v_f\), Eq. (16) gives the special case from Eq. (13). Finally, the present formalism can be generalized to a nondegenerate electron gas and is thus useful for the description of ion beams interacting with plasmas by using
\[
\frac{dE}{dz} = \frac{Z v_f^2}{v} \sum_{\ell = 0}^\infty \sin(2[\delta_\ell(v_f) - \delta_{\ell+1}(v_f)]),
\]
\hspace{1cm} (18)
which is identical to Eq. (1) with the effective transport cross section
\[
\sigma_{tr}(v') = \frac{2\pi Z}{v_f^3} \sum_{\ell = 0}^\infty \sin(2[\delta_\ell(v') - \delta_{\ell+1}(v')]).
\]
\hspace{1cm} (19)

III. DISCUSSION

Figure 1 shows an example of the use of the stopping-force formula based on the well-established transport cross-section concept from Eq. (6) in comparison with the present formula based on the induced density from Eq. (16) for H\(^+\) ions impinging on an electron gas with the same density as the Al valence electrons (for further details see the figure caption). The phase shifts were calculated for the Yukawa potential from Eq. (3) with \(\sigma = \omega_p / v\) by numerically solving the radial Schrödinger equation. As can be observed from this figure, the stopping formula based on the transport cross section from Eq. (2) converges to the Bethe formula very slowly as predicted by Eq. (5), whereas the present one does converge to the Bethe formula for the energy range where it is established \((2v_f^2 / \omega_p \gtrsim 20)\).\(^9\) In fact, the present formulation is superior because the induced density is noncentral, although the scattering potential is central.

The effect of higher-order terms for high-energy projectiles is enhanced for Ne\(^{10+}\) projectiles, as displayed in Fig. 2. The present formulation converges to the Bloch formula, which contains for all \(n\) even \(Z^n\) higher-order terms. The difference between the present calculations and the Bloch formula at high velocities is due to the Barkas effect\(^9\). The formulation based on the standard transport cross section does not converge to the Bloch formula for the displayed energy range. In fact, as mentioned above, previous works have circumvented this issue by using different methods and now it is clear that this is a consequence of nonspherical symmetry of the electron-ion scattering potential.

The stopping power results from Eq. (16) are compared with experimental data in Fig. 3 for H\(^+\) ions in Al and H\(_2\)O targets.
FIG. 3. Electronic stopping cross section for \( H^+ \) ions in Al (polycrystalline) and H\(_2\)O (ice, liquid, and vapor) as a function of the projectile energy. The value for the electron radius \( r_s \) that describes the three (eight) valence electrons of Al (H\(_2\)O) is 2.07 (1.12). The contribution of the inner shells is shown by the red dashed lines. The experimental results are taken from Ref. [30]. The blue dashed lines correspond to calculations using the standard definition of the transport cross section.

(see the thick solid lines). Al is a free-electron metal with an electron density corresponding to \( r_s = 2.07 \). In the case of H\(_2\)O, a material of crucial importance for hadron therapy, the value of \( r_s = 1.12 \) is obtained from the mean ionization energy of 39 eV for the valence electrons of water. The contributions of the inner shells were added, as calculated by the CASP program [31,32] and no energy loss to charge-changing processes has been considered. Owing to the use of \( \alpha = \omega_p/v \), good agreement is expected only at high projectile energies. In both cases, the agreement is remarkable for \( E > 100 \) keV. Particularly for Al, the good agreement for lower energies has to be considered accidental, as the Yukawa scattering potential with \( \alpha = \omega_p/v \) does not satisfy charge neutrality (the Friedel sum rule) [16]. As expected, the calculations from the standard transport cross-section approach (blue dashed lines) underestimate the stopping at high energies.

Finally, in order to test the present formula in the nonperturbative regime, a comparison is also provided for multiple charged Ne ions. Here the experimental data for pure charge states \( q \) are used to avoid additional complications from charge-changing processes. In Fig. 4, the experimental stopping data [33] are displayed as a function of \( q^2 \) for 2-MeV/nucleon Ne ions in carbon foils. The extension of Eq. (16) to dressed ions is straightforward and is shown in the Appendix. Results from the Bloch model realized by the CASP program [31,32] (using the unitary convolution approximation (UCA) mode without the Barkas effect) are also shown. As can be observed from this figure, the deficiencies of the standard formula manifest in the nonperturbative limit and the positive Barkas effect (the difference between the thick solid and dashed lines) is well described by the present formulation.

IV. CONCLUSION

In summary, an improved formula for the electronic stopping power and an alternative formula for the transport cross section (19) is derived in terms of the phase shifts from the scattering of electrons at the ion. The effective transport cross section is superior to the well-established textbook formula from Eq. (2) when the ion is much faster than the electrons. This formula offers perspectives to reanalyze the role of higher-order effects found in numerous publications so far and solves an old problem in the stopping power area.

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APPENDIX

1. Mathematical details

The stopping formula at high projectile energies (13) was derived using the property

\[
\int_0^\infty dr \mathcal{R}_{k,\ell}(r) \mathcal{R}_{k,\ell}(r) = \frac{1}{k} \frac{\sin[\delta_\ell - \delta_\ell - (\ell' - \ell)\pi/2]}{\ell(\ell + 1) - \ell'(\ell' + 1)},
\]

which can be obtained from elementary properties of the radial wave function \( \mathcal{R}_{k,\ell} \). In addition, the angular integration can be
determined from the Wigner 3- j symbols \[34\] and reads

\[
\int d\Omega \cos \theta Y_{\ell m}^*(\theta') Y_{\ell' m'}(\theta') = \sqrt{\frac{(\ell' + m' + 1)(\ell' - m' + 1)}{(2\ell' + 1)(2\ell' + 3)}} \delta_{\ell,\ell'} \delta_{m,m'} \quad (A2)
\]

2. Born approximation

In the Born approximation, the phase shifts are given by \[34\]

\[
\delta_\ell = -2k \int_0^\infty dr r^2 V(r) j_\ell^2(kr), \quad (A3)
\]

where \(j_\ell(x)\) is the spherical Bessel function as defined in Ref. \[34\]. For the Yukawa potential \(V(r) = -Ze^{-\alpha r}/r\), we have

\[
\delta_\ell = -2k \int_0^\infty dr r^2 \left(-\frac{Ze^{-\alpha r}}{r}\right) j_\ell^2(kr). \quad (A4)
\]

In addition, we use

\[
\sin[2(\delta_\ell - \delta_{\ell+1})] \equiv 2(\delta_\ell - \delta_{\ell+1}). \quad (A5)
\]

Therefore,

\[
\frac{dE}{dz} = \frac{2\pi n_0}{k} \delta_0, \quad (A6)
\]

where

\[
\delta_0 = \frac{2kZ}{k^2} \int_0^\infty dr e^{-\alpha r} \left(\frac{\sin^2 kr}{r}\right) = \frac{2k}{k^2} \frac{1}{4} \ln \left(\frac{\alpha^2 + (2k^2)}{\alpha^2}\right). \quad (A7)
\]

Finally, we have

\[
\frac{dE}{dz} = Z^2 \frac{4\pi n_0}{v^2} \ln \left(\frac{2v}{\alpha}\right) = \frac{2\pi n_0}{v^2} \ln \left(\frac{2v^2}{\omega_p}\right). \quad (A8)
\]

Using \(k = v, \alpha = \omega_p/v, \) and \(2v \gg \alpha,\) we obtain

\[
\frac{dE}{dz} = Z^2 \frac{4\pi n_0}{v^2} \ln \left(\frac{2v}{\alpha}\right) = Z^2 \frac{4\pi n_0}{v^2} \ln \left(\frac{2v^2}{\omega_p}\right). \quad (A9)
\]

the Bethe formula in atomic units, where \(v\) is the ion velocity and \(\omega_p\) the plasmon frequency.

The kinematic range for which the Bethe formula is established can be obtained from Ref. \[9\] and reads (including the electron mass and \(h\) explicitly)

\[
\frac{2m_e v^2}{\hbar \omega_p} \gtrsim 20. \quad (A10)
\]

Figure 5 shows this region and the asymptotic limit given by the standard transport cross-section approach. The difference between both curves is much less visible at very high energies, however, the effect on the ion range is quite remarkable. For instance, the range of 200-MeV protons in water using both procedures differs by about 2 cm, which is crucial in the case of proton therapy.

![Bethe formula divided by 4\pi Z^2/\omega_p as a function of 2v^2/\omega_p](image)

**FIG. 5.** Bethe formula divided by \(4\pi Z^2/\omega_p\) as a function of \(2v^2/\omega_p\). For \(2v^2/\omega_p > 20\) the Bethe formula is established, but the stopping force from the standard transport cross-section approach still underestimates the Bethe formula.

3. Bloch formula

The Bloch formula \[20\] can be deduced at high velocities using the Coulomb phase shifts \[34\]

\[
\delta_\ell = \arg \Gamma(\ell + 1 + i\chi) = \delta_0 + \sum_{s=1}^l \arctan \left(\frac{\chi}{s}\right), \quad (A11)
\]

where \(\chi = \frac{Ze^2}{\hbar v}\). Therefore,

\[
\delta_{\ell+1} - \delta_\ell = \arctan \left(\frac{\chi}{\ell + 1}\right) \quad (A12)
\]

or

\[
\sin(\delta_{\ell+1} - \delta_\ell) = \frac{\chi}{\sqrt{\chi^2 + (\ell + 1)^2}}. \quad (A13)
\]

and

\[
\cos(\delta_{\ell+1} - \delta_\ell) = \frac{l + 1}{\sqrt{\chi^2 + (\ell + 1)^2}}. \quad (A14)
\]

The formula (13) can be rewritten as

\[
\frac{dE}{dz} = \frac{Ze^2}{v^2} \sum_{\ell} \sin(\delta_{\ell+1} - \delta_\ell) \cos(\delta_{\ell+1} - \delta_\ell)
\]

\[
- \frac{Ze^2}{v} \sum_{\ell} \sin(\delta_{\ell+1}^B - \delta_\ell^B) \cos(\delta_{\ell+1}^B - \delta_\ell^B)
\]

\[
+ Z^2 \frac{\omega_p^2}{v^2} \ln \left(\frac{2v^2}{\omega_p}\right), \quad (A15)
\]

where \(\delta_\ell^B\) are the phase shifts in the Bethe limit \(\chi \to 0\). Finally, using Eqs. (A13) and (A14), we have

\[
\frac{dE}{dz} = \frac{Ze^2}{v} \sum_{\ell} \left(\frac{\ell + 1}{\chi^2 + (\ell + 1)^2} - \frac{1}{\ell + 1}\right)
\]

\[
= \frac{Ze^2}{v} \left[\ln \left(\frac{2v^2}{\omega_p}\right) + \Psi(1) - \text{Re}\Psi(1 + iZ/v)\right], \quad (A16)
\]
where $\Psi(x)$ denotes the digamma function as defined in Ref. [35].

4. Semiclassical approximation

The classical limit for the stopping formula (13) can be obtained by replacing $\ell$ by the impact parameter $b = h\ell/m_e\nu$ and the phase shifts $\delta_{\ell+1} - \delta_{\ell}$ by the scattering angle $\theta = 2(\delta_{\ell+1} - \delta_{\ell})$ as in Ref. [36]. In atomic units we have

$$\frac{dE}{dz} = -\frac{Z\omega_p^2}{2} \int_0^\infty db \sin(\theta). \quad (A17)$$

As in Ref. [9], the collisions can be divided into close and distant collisions, where the scattering angle $\theta$ can be determined as a function of the impact parameter $b$ for the Yukawa potential according to

$$\tan \left( \frac{\theta_{\text{close}}}{2} \right) = -\frac{Z}{b\nu^2}, \quad (A18)$$

$$\theta_{\text{distant}} = -\frac{2Z\omega_p^2}{v^3} K_1 \left( \frac{\omega_pb}{v} \right), \quad (A19)$$

where $K_1(x)$ is the modified Bessel function of the second kind [35]. Let $b_0$ be an impact parameter that divides the integration in Eq. (A17) into two parts: close [using Eq. (A18)] and distant [using Eq. (A19)] collisions. Thus, the stopping force can be written as

$$\frac{dE}{dz} = -\frac{Z\omega_p^2}{2} \left( \int_0^{b_0} db \sin(\theta_{\text{close}}) + \int_{b_0}^\infty db \sin(\theta_{\text{distant}}) \right) \approx \frac{Z^2\omega_p^2}{v^2} \ln \left( \frac{1.1229v^3}{\omega_p|z|} \right), \quad (A20)$$

which is the Bohr formula [9] after assuming $\sin(\theta_{\text{distant}}) \approx \theta_{\text{distant}}$ and $|z|/v^2 \ll b_0 \approx \omega_p/v$. For this case, the result does not depend on $b_0$. The semiclassical approximation from Eq. (A17) also agrees with the binary theory of the stopping power [9] as long as $(\frac{2\hbar}{m_e}) K_1(\frac{2\hbar}{m_e}) \approx 1.$

5. Dressed projectiles

The stopping formula (13) is valid only for point charges and can be straightforwardly generalized to dressed ions carrying $n_e$ bound electrons with charge state $q = Z - n_e$, according to

$$\frac{dE}{dz} = \frac{\omega_p^2}{v} \int_0^\infty \sin(\delta_{\ell} - \delta_{\ell+1}) [q \cos(\delta_{\ell} - \delta_{\ell+1}) + n_e \Delta_{\ell}] \left( \int_0^\infty dz \right). \quad (A21)$$

with

$$\Delta_{\ell} = 2k(\ell + 1) \int_0^\infty \frac{r^2}{\omega_p} \Phi'(r) R_{k,\ell}(r) R_{k,\ell+1}(r), \quad (A22)$$

where $\Phi'(r)$ is the derivative of the screening function from the bound electrons.


