

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. In contrast to the previous one found in many textbooks, the present formula converges to the Bethe and Bloch stopping-power formulas at high ion velocities and agrees rather well with experimental stopping-power data, as shown here for Al, C, and H₂O targets. It can be employed in plasma physics and particularly in any application that requires electronic stopping-power values of quasifree electrons with high accuracy.

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I. INTRODUCTION

The energy transfer between electrons and ions in plasmas and the corresponding momentum-transfer rate have been investigated using the concept of the transport cross section σ_{tr} . It is a fundamental quantity used in different fields (e.g., atomic and plasma physics) and in particular it is directly related to the electronic stopping power of charged particles, which is important for a wide range of applications stretching including ion-beam analysis [1], materials modifications [2], and ion-driven fast ignition in plasmas [3]. Moreover, its most appealing application is dosimetry for cancer treatment using ions [4], because of the increasing worldwide use of protons and heavier ions in radiation therapy. Here an alternative formula for the transport cross section used for stopping-power calculations and energy-transfer rates in electron-ion binary collisions is reported for spherically symmetric electron-ion potentials.

The energy transfer between electrons and ions in binary collisions has been studied for more than 100 years [5] and was a subject of interest for many prominent scientists, such as Bohr [6], Landau [7], and Lindhard [8], who first established the underlying physics. The stopping power or force dE/dz is connected to the transport cross section [9] by

$$\frac{dE}{dz} = n_0 m_e \left\langle \frac{|\vec{v}_e - \vec{v}|}{v} \vec{v} \cdot (\vec{v} - \vec{v}_e) \sigma_{tr}(|\vec{v}_e - \vec{v}|) \right\rangle_{\vec{v}_e}, \quad (1)$$

where m_e is the electron mass, $\langle \dots \rangle$ stands for the average over the electron velocities \vec{v}_e , \vec{v} is the ion velocity, and n_0 is the undisturbed electron density. Atomic units (a.u.) and nonrelativistic expressions will be used throughout, unless stated otherwise.

Usually, calculations of the transport cross section σ_{tr} assume a central potential for the electron scattering at the ion and therefore make use of the partial-wave expansion. Thus, $\sigma_{tr}(k)$ can be expressed by phase shifts δ_ℓ at the relative speed v' , according to [9]

$$\sigma_{tr}(v') = \frac{4\pi}{v'^2} \sum_{\ell=0}^{\infty} (\ell + 1) \sin^2(\delta_\ell - \delta_{\ell+1}). \quad (2)$$

Stopping-power calculations and energy-transfer rates based on Eq. (2) have been employed in a large number of papers (see, for example, a list of them in Refs. [9,10]) in order to investigate, for instance, higher-order effects [11,12] and relaxation time in dense plasmas [13]. The central aspect of this approach is the scattering potential $V(\vec{r})$, from which the phase shifts can be calculated.

Since the general form for the self-consistent electron-ion scattering potential $V(\vec{r})$ is still an issue, numerous publications simply use a screened Coulomb (Debye-Hückel or Yukawa) potential

$$V(r) = -Z \frac{e^{-\alpha r}}{r}, \quad (3)$$

where Z is the atomic number of the ion and α^{-1} is a velocity-dependent screening length [10,12,14,15]. At high ion velocities v , the use of the Yukawa potential with $\alpha = \omega_p/v$ [16], where ω_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

$$\frac{dE}{dz} = Z^2 \frac{\omega_p^2}{v^2} \ln \left(\frac{2v^2}{\omega_p} \right), \quad (4)$$

but instead results in

$$\frac{dE}{dz} = Z^2 \frac{\omega_p^2}{v^2} \left[\ln \left(\frac{2v^2}{\omega_p} \right) - \frac{1}{2} \right]. \quad (5)$$

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

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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 retarding force acting on the ion due to the induced charge density. The resulting stopping 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 electrons 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 σ_{tr} from Eq. (2) and integrating over all states inside the Fermi sphere. Thus, Eq. (1) becomes [10,14]

$$\frac{dE}{dz} = \frac{1}{16\pi^2 v^2} \int_{|v-v_f|}^{v+v_f} dk k^2 \sigma_{tr}(k) [k^2 - (v - v_f)^2] \times [(v + v_f)^2 - k^2], \quad (6)$$

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

$$\frac{dE}{dz} = \begin{cases} n_0 v_f v \sigma_{tr}(v_f) & \text{for } v \ll v_f \\ n_0 v^2 \sigma_{tr}(v) & \text{for } v \gg v_f. \end{cases} \quad (7)$$

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],

$$\psi_{\vec{k}}(\vec{r}) = 4\pi \sum_{\ell, m} i^\ell e^{i\delta_\ell} \mathcal{R}_{k, \ell}(r) Y_{\ell, m}(\hat{r}) Y_{\ell, m}^*(\hat{k}), \quad (8)$$

in the rest frame of the ion. Then \vec{k} corresponds to the incident electron momentum and $\mathcal{R}_{k, \ell}(r)$ is the corresponding radial wave function with angular momentum quantum number ℓ . The spherical harmonics $Y_{\ell, m}$ from Eq. (8) are functions of \hat{r} and \hat{k} , the directions of \vec{r} and \vec{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

$$n_{\text{ind}}(\vec{r}) = \frac{2}{(2\pi)^3} \int_{\text{DFS}} (|\psi_{\vec{k}}|^2 - 1) d^3k, \quad (9)$$

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}_{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]

$$\begin{aligned} \frac{dE}{dz} &= -\frac{1}{v} \vec{F}_{\text{ind}} \cdot \vec{v} = Z \left[\frac{\partial V_{\text{ind}}}{\partial z} \right]_{\vec{r}=0} \\ &= -Z \left[\int \frac{\partial}{\partial z} \frac{n_{\text{ind}}(\vec{r}')}{|\vec{r} - \vec{r}'|} d^3r' \right]_{\vec{r}=0} \end{aligned} \quad (10)$$

for a bare ion with charge Z .

A. High-energy limit $v \gg v_f$

Let us consider the limit $v \gg v_f$, 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

$$n_{\text{ind}}(\vec{r}) = n_0 (|\psi_{\vec{k}}|^2 - 1). \quad (11)$$

Then the stopping force from Eq. (10) yields

$$\frac{dE}{dz} = -Z \frac{\omega_p^2}{4\pi} \int d^3r' \frac{z' (|\psi_{\vec{k}}|^2 - 1)}{r'^3}. \quad (12)$$

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 following surprisingly simple expression for electronic stopping power as a function of the phase shifts δ_ℓ at energies $\epsilon = v^2/2$:

$$\frac{dE}{dz} = \frac{Z\omega_p^2}{2v} \sum_{\ell=0}^{\infty} \sin[2(\delta_\ell - \delta_{\ell+1})], \quad (13)$$

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 $v \gg v_f$ 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]

$$\frac{dE}{dz} = \frac{\omega_p^2}{v^2} Z^2 \left[\ln \left(\frac{2v^2}{\omega_p} \right) + \Psi(1) - \text{Re} \Psi(1 + iZ/v) \right], \quad (14)$$

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

$$\begin{aligned} \frac{dE}{dz} &= Z \frac{2}{(2\pi)^3} \int_{\text{DFS}} d^3k (4\pi)^2 \\ &\times \sum_{\ell\ell'} \sum_{m,m'} i^{\ell} (-i^{\ell'}) e^{i(\delta_{\ell} - \delta_{\ell'})} Y_{\ell,m}(\hat{k}) Y_{\ell',m'}^*(\hat{k}) \\ &\times \int d\Omega' \cos\theta Y_{\ell,m}^*(\hat{r}') Y_{\ell',m'}(\hat{r}') \\ &\times \int dr' \frac{1}{r'^2} [r' \mathcal{R}_{k,\ell}(r')] [r' \mathcal{R}_{k,\ell'}(r')]. \end{aligned} \quad (15)$$

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

$$\begin{aligned} \frac{dE}{dz} &= \frac{Z}{8\pi v^2} \int_{|v_f-v|}^{v_f+v} \frac{dk}{k} \\ &\times [2k^2(v_f^2 + v^2) - k^4 - (v_f^2 - v^2)^2] \\ &\times \sum_{\ell=0}^{\infty} \sin(2[\delta_{\ell}(k) - \delta_{\ell+1}(k)]), \end{aligned} \quad (16)$$

whose limit as $v \rightarrow 0$ is

$$\frac{dE}{dz} = \frac{Z v \omega_p^2}{2v_f^2} \sum_{\ell=0}^{\infty} \sin(2[\delta_{\ell}(v_f) - \delta_{\ell+1}(v_f)]), \quad (17)$$

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

$$\frac{dE}{dz} = n_0 m_e \left\langle \frac{|\vec{v}_e - \vec{v}|}{v} \vec{v} \cdot (\vec{v} - \vec{v}_e) \sigma_{tr}^{\text{eff}}(|\vec{v}_e - \vec{v}|) \right\rangle_{\vec{v}_e}, \quad (18)$$

which is identical to Eq. (1) with the effective transport cross section

$$\sigma_{tr}^{\text{eff}}(v') = \frac{2\pi Z}{v'^3} \sum_{\ell=0}^{\infty} \sin(2[\delta_{\ell}(v') - \delta_{\ell+1}(v')]). \quad (19)$$

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 $\alpha = \omega_p/v$ 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 ($2v^2/\omega_p \gtrsim 20$) [9]. In fact, the present formulation is superior because the induced density is noncentral, although the scattering potential is central.

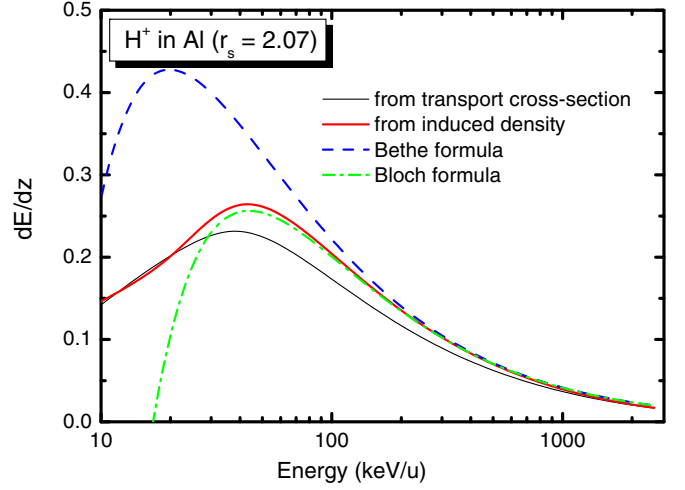


FIG. 1. Stopping force dE/dz as a function of energy for H^+ ions in an electron gas with electron radius $r_s = 2.07$, which corresponds to the Al valence-electron density of $1.81 \times 10^{23} \text{ cm}^{-3}$. The thin black solid line corresponds to calculations using the standard transport cross section from Eq. (6). The thick red solid line corresponds to the formula (16). For comparison, the Bethe [Eq. (4)] and Bloch [Eq. (14)] formulas are also shown with dashed and dot-dashed lines, respectively.

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_2O targets

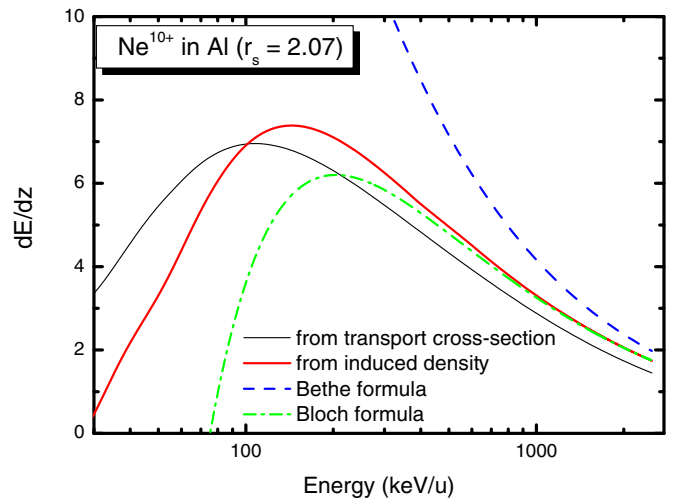


FIG. 2. Same as in Fig. 1 for Ne^{10+} projectiles.

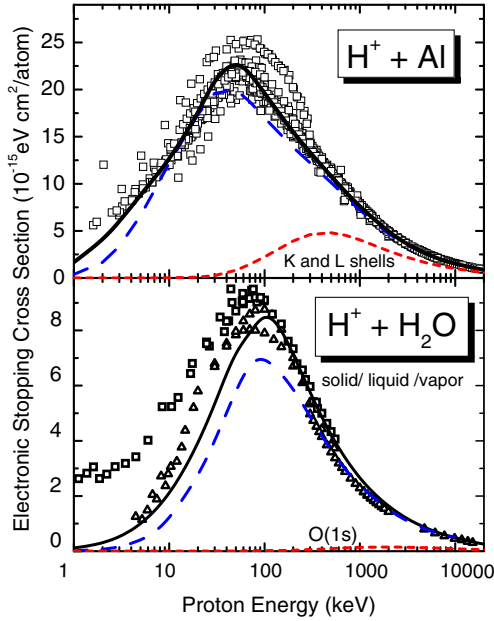


FIG. 3. Electronic stopping cross section for H^+ ions in Al (polycrystalline) and H_2O (ice, liquid, and vapor) as a function of the projectile energy. The value for the electron radius r_s that describes the three (eight) valence electrons of Al (H_2O) is 2.07 (1.12). The contribution of the inner 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_2O , 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

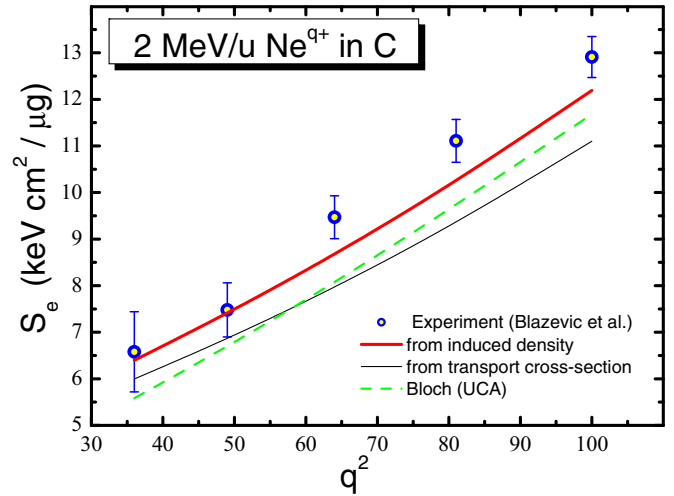


FIG. 4. Pre-equilibrium stopping for pure charge states q for 2 MeV/nucleon Ne in carbon. The $2s$ and $2p$ shells are modeled by an electron gas with $r_s = 1.56$ using the present (from induced density) and standard (from the transport cross section) stopping formulas. The contribution of the C $1s$ shell is taken from the CASP program.

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

$$\int_0^\infty dr \mathcal{R}_{k,\ell}(r)\mathcal{R}_{k,\ell'}(r) = \frac{1}{k} \frac{\sin[\delta_{\ell'} - \delta_\ell - (\ell' - \ell)\pi/2]}{\ell(\ell + 1) - \ell'(\ell' + 1)}, \quad (A1)$$

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

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

2. Born approximation

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

$$\delta_\ell = -2k \int_0^\infty dr r^2 V(r) J_\ell^2(kr), \quad (\text{A3})$$

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

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

In addition, we use

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

Therefore,

$$\frac{dE}{dz} = Z \frac{4\pi n_0}{k} \delta_0, \quad (\text{A6})$$

where

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

Finally, we have

$$-\frac{dE}{dz} = Z^2 \frac{4\pi n_0}{k^2} \frac{1}{2} \ln \left(\frac{\alpha^2 + (2k^2)}{\alpha^2} \right). \quad (\text{A8})$$

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

$$-\frac{dE}{dz} = Z^2 \frac{4\pi n_0}{v^2} \ln \left(\frac{2v}{\alpha} \right) = Z^2 \frac{4\pi n_0}{v^2} \ln \left(\frac{2v^2}{\omega_p} \right), \quad (\text{A9})$$

the Bethe formula in atomic units, where v is the ion velocity and ω_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 \hbar explicitly)

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

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.

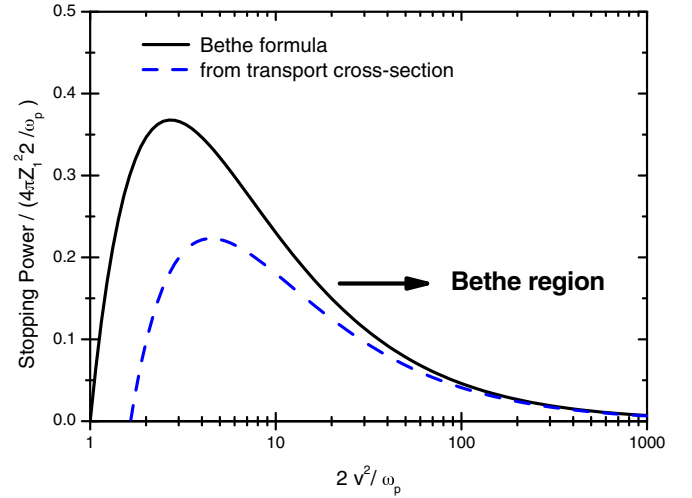


FIG. 5. Bethe formula divided by $4\pi Z^2/\omega_p$ as a function of $2v^2/\omega_p$. For $2v^2/\omega_p > 20$ the Bethe formula is established, but the stopping force from the standard transport cross-section approach still underestimates the Bethe formula.

3. Bloch formula

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

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

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

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

or

$$\sin(\delta_{\ell+1} - \delta_\ell) = \frac{\chi}{\sqrt{\chi^2 + (\ell + 1)^2}} \quad (\text{A13})$$

and

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

The formula (13) can be rewritten as

$$\begin{aligned} \frac{dE}{dz} &= \frac{Z\omega_p^2}{v} \sum_{\ell} \sin(\delta_{\ell+1} - \delta_\ell) \cos(\delta_{\ell+1} - \delta_\ell) \\ &\quad - \frac{Z\omega_p^2}{v} \sum_{\ell} \sin(\delta_{\ell+1}^B - \delta_\ell^B) \cos(\delta_{\ell+1}^B - \delta_\ell^B) \\ &\quad + Z^2 \frac{\omega_p^2}{v^2} \ln \left(\frac{2v^2}{\omega_p} \right), \end{aligned} \quad (\text{A15})$$

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

$$\begin{aligned} \frac{dE}{dz} &= \frac{Z\omega_p^2}{v} \sum_{\ell} \left(\frac{\ell + 1}{\chi^2 + (\ell + 1)^2} - \frac{1}{\ell + 1} \right) \\ &= \frac{Z\omega_p^2}{v} \left[\ln \left(\frac{2v^2}{\omega_p} \right) + \Psi(1) - \text{Re}\Psi(1 + iZ/v) \right], \end{aligned} \quad (\text{A16})$$

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 ℓ by the impact parameter $b = \hbar\ell/m_e v$ 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

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

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

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

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

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

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

which is the Bohr formula [9] after assuming $\sin(\theta_{\text{distant}}) \approx \theta_{\text{distant}}$ and $|Z|/v^2 \ll b_0 \ll v/\omega_p$. 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 $(\frac{\omega_p b_0}{v}) K_1(\frac{\omega_p b_0}{v}) \approx 1$.

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

$$\frac{dE}{dz} = \frac{\omega_p^2}{v} \sum_{\ell=0}^\infty \sin(\delta_\ell - \delta_{\ell+1}) [q \cos(\delta_\ell - \delta_{\ell+1}) + n_e \Delta_\ell], \quad (\text{A21})$$

with

$$\Delta_\ell = 2k(\ell + 1) \int_0^\infty dr r^2 \Phi'(r) \mathcal{R}_{k,\ell}(r) \mathcal{R}_{k,\ell+1}(r), \quad (\text{A22})$$

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

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