Bohr's stopping-power formula derived for a classical free-electron gas

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Bohr's centenary stopping-power formula is rederived for a free electron gas (FEG) system within the framework of nonrelativistic classical mechanics. A simple and more concise expression for the stopping power of charged particles in FEG is demonstrated on classical grounds. Using semiclassical arguments and the Euler-Maclaurin well-known mathematical formula, Bloch's correction that links Bethe's quantum theory to Bohr's classical model is also recovered. The proposed semiclassical stopping-power formula contains the main physical ingredients for a general stopping formula applicable for different systems and energies and facilitates computational calculations.

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I. INTRODUCTION

The energy loss of energetic charged particles in matter is a key quantity in many areas of knowledge and has been investigated for more than a century by many prominent scientists such as Bohr [1,2], Bethe [3], and Bloch [4]. Its foundations are described in a wide literature including different textbooks [5–7]. The seminal work by Niels Bohr [1] "On the Theory of the Decrease of Velocity of Moving Electrified Particles on Passing Through Matter" provided the first reliable formula for the stopping power of charged ions in matter more than 100 years ago. It gives the energy loss of a point charge (Z_1e) interacting with a harmonically bound electron (resonance frequency ω) as

$$\left(\frac{dE}{dx}\right)_{\text{Bohr}} = \frac{4\pi n Z_1^2 e^4}{mv^2} \ln \frac{1.1229mv^3}{|Z_1|e^2\omega},$$
 (1)

where v is the ion speed, e is the elementary charge, m is the electron mass, and n is the density of oscillators with frequency ω . This formula is demonstrated in textbooks (see, e.g., Ref. [6]) and is valid for high velocities as otherwise it can give negative stopping values. It has been extended to low projectile energies many years ago [8] and more recently [9,10]. Here this formula is derived in an alternative way for a classical free electron gas (FEG) with density n and corresponding plasmon frequency ω_p . The present derivation of Bohr's formula only follows from the dressed ion-electron interaction for a FEG. It is much simpler and does not use any ad hoc adiabatic cutoff distance or classical oscillators. In the original derivation of Bohr's formula, the frequency associated with adiabatic cutoff distance is not determined apriori and instead is chosen to emulate quantum-mechanical dipole transitions. Bloch [4] could show that the Bohr formula is consistent with a (partial or restricted) nonlinear solution of the Schrödinger equation for strong perturbations. This explains the success of Bohr's formula.

Many calculations of the stopping power of ions in a FEG system have been proposed in the literature as, e.g., the linear-response theory [11], first and second-order perturbation schemes [12–14], DFT [15], TDDFT [16–18] and transport cross-section and semiclassical approaches [19,20]. Here the focus is on classical and semiclassical calculations. Besides the rederivation of Bohr's stopping formula, a straightforward formula for the classical stopping power of charged ions in a FEG is demonstrated and connected with the standard stopping models by Bethe [3] and Bloch [4]. Nonrelativistic expressions will be used throughout this work.

II. DERIVATION OF THE CLASSICAL FREE-ELECTRON GAS STOPPING-POWER FORMULA

Let us first consider the slowing down of a point charge (Z_1) in a classical FEG with density *n* where the electrons are at rest (static FEG). In the reference frame where the projectile is at rest, there is a beam of electrons of density *n* and velocity \vec{v} that is scattered by the fixed point charge or ion (see Fig. 1). This scattering is described by a screened potential $V(\vec{r})$, where \vec{r} is the electron position and the ion is at the origin. The classical trajectories are denoted by $\vec{r}_{cl}(t, \vec{b})$ for electrons coming from the left to the right with initial velocity \vec{v} and impact parameter \vec{b} . The stationary density of electrons with initial density *n* is then given by

$$\rho(\vec{r}) = nv \int dt \int d^2 b \delta^{(3)}(\vec{r} - \vec{r}_{\rm cl}(t, \vec{b})).$$
(2)

The induced density $n_{ind}(\vec{r}) = \rho(\vec{r}) - n$ will be then responsible for a force acting on the projectile \vec{F}_{ind} . This retarding force is the stopping force or simply stopping power defined as [11]

$$\frac{dE}{dx} = \frac{1}{v}\vec{F}_{\text{ind}} \cdot \vec{v} = Z_1 e^2 \left[\int \frac{\partial}{\partial x} \frac{n_{\text{ind}}(\vec{r'})}{|\vec{r} - \vec{r'}|} d^3 r' \right]_{\vec{r}=0}.$$
 (3)

The determination of the stopping power by the induced force [21] or by the wakefield generated in the medium is equivalent to the traditional method of calculating the energy

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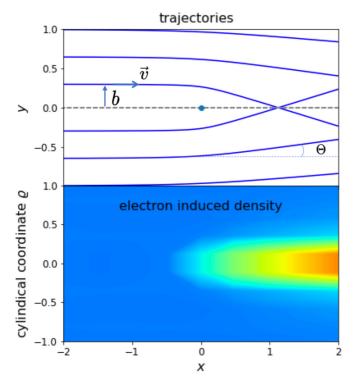


FIG. 1. Illustration of the electron trajectories (top) and induced density (below) for an ion at (x = 0, y = 0, z = 0). Electrons come from the left to right with velocity \vec{v} and impact parameter *b*. *x* is the direction of the motion, and Θ the scattering angle. Simulations were performed for a proton in the laboratory system with v = 5 and electron Wigner-Seitz radius $r_s = 2.07$ in atomic units.

transfers from the ion to the medium as used originally by Bohr.

Using the electron density $\rho(\vec{r})$ from Eq. (2) we get

$$\frac{dE}{dx} = nv \int dt \int d^2b \frac{Z_1 e^2 \cos(\theta_{\rm cl})}{r_{\rm cl}(t, \vec{b})^2},\tag{4}$$

where $\theta_{cl}(t, \vec{b})$ is the angle of the electron related to its initial velocity. After changing the order of time and impactparameter integrals, the time integration can replaced by an integral over $\theta = \theta_{cl}(t, \vec{b})$ as

$$\frac{dE}{dx} = nv \int d^2b \int_{\pi}^{\Theta(\bar{b})} d\theta \frac{1}{\dot{\theta}} \frac{Z_1 e^2 \cos(\theta)}{r_{\rm cl}(t(\theta, \bar{b}), \bar{b})^2}, \qquad (5)$$

with $\Theta(\vec{b})$ being the electron-scattering angle. For a central potential the angular momentum, namely,

$$\mathcal{L} = m r_{\rm cl}^2 \dot{\theta}_{\rm cl},\tag{6}$$

is conserved and given in terms of the impact parameter as $\mathcal{L} = -mvb$. Therefore Eq. (5) will read

$$\frac{dE}{dx} = -2\pi n Z_1 e^2 \int_0^\infty db \int_\pi^{\Theta(b)} d\theta \cos(\theta)$$
$$= -2\pi n Z_1 e^2 \int_0^\infty db \sin \Theta(b), \tag{7}$$

and finally using the relation between the plasmon frequency and electron density $\omega_p^2 = 4\pi n e^2/m$ [7] we obtain the stopping formula,

$$\frac{dE}{dx} = -\frac{Z_1 m \omega_p^2}{2} \int_0^\infty db \sin \Theta(b), \qquad (8)$$

which differs from the traditional one

$$\left(\frac{dE}{dx}\right)_{\text{binary}} = mnv^2 \int_0^\infty d^2 b [1 - \cos\Theta(b)] = mnv^2 \sigma_{tr},$$
(9)

based on the transport or momentum transfer cross section σ_{tr} in binary collisions [7]. Equation (8) was recently obtained in Ref. [22] by means of a semiclassical approximation for the phase shifts in electron-ion scattering. As shown in Refs. [22,23], the use of the momentum transfer approach is more suitable at low projectile energies. In contrast, the stopping based on induced force solves a critical convergence problem at high projectile energies.

At high projectile velocities, the collisions can be divided into close and distant collisions [8,9,24], where the scattering angle Θ can be determined as a function of the impact parameter *b* for the Coulomb potential at close collisions and the Yukawa potential with screening length v/ω_p (obtained here self-consistently, see Appendix A) at distant collisions according to [24]

$$\tan\left(\frac{\Theta_{\text{close}}}{2}\right) = -\frac{Z_1 e^2}{bmv^2},\tag{10}$$

$$\Theta_{\text{distant}} = -\frac{2Z_1 e^2 \omega_p}{m v^3} K_1 \left(\frac{\omega_p b}{v}\right), \tag{11}$$

where K_n is the modified Bessel function of the second kind [25]. As in Ref. [9] let b_0 be an impact parameter that divides the integration in Eq. (8) in two parts: close [using Eq. (10)] and distant [using Eq. (11)] collisions. Moreover, at high projectile velocities these two regions are well separated and merge to each to other at b_0 as long as $|Z_1|e^2/mv^2 \ll$ $b_0 \ll v/\omega_p$. For these conditions and $\sin \Theta_{\text{distant}} \approx \Theta_{\text{distant}}$ the stopping force reads

$$\frac{dE}{dx} = \left(\frac{dE}{dx}\right)_{\text{close}} + \left(\frac{dE}{dx}\right)_{\text{distant}}$$
$$= -\frac{Z_1 m \omega_p^2}{2} \left(\int_0^{b_0} db \sin \Theta_{\text{close}} + \int_{b_0}^{\infty} db \Theta_{\text{distant}}\right).$$
(12)

These two integrals are analytical and read

$$\left(\frac{dE}{dx}\right)_{\text{close}} = \frac{Z_1^2 e^2 \omega_p^2}{2v^2} \ln(1 + (b_0 m v^2 / Z_1 e^2)^2), \quad (13)$$

$$\left(\frac{dE}{dx}\right)_{\text{distant}} = \frac{Z_1^2 e^2 \omega_p^2}{v^2} K_0\left(\frac{\omega_p b_0}{v}\right). \tag{14}$$

The close-collision part is identical to the standard expression based on binary collisions for a Coulomb interaction. The distant-collision part is equal to the one from Ref. [9] at high projectile velocities, where $\frac{\omega_p b_0}{v} K_1(\frac{\omega_p b_0}{v}) \approx 1$. Both expressions in the limit $|Z_1|e^2/mv^2 \ll b_0 \ll v/\omega_p$ are [25]

$$\left(\frac{dE}{dx}\right)_{\text{close}} = \frac{Z_1^2 e^2 \omega_p^2}{v^2} \ln(b_0 m v^2 / |Z_1| e^2), \quad (15)$$

$$\left(\frac{dE}{dx}\right)_{\text{distant}} = \frac{Z_1^2 e^2 \omega_p^2}{v^2} \ln\left(\frac{2e^{-\gamma} v}{\omega_p b_0}\right),\tag{16}$$

where $\gamma = 0.57721$ is Euler's constant and $2e^{-\gamma} = 1.1229$. The sum of the above terms gives Bohr's stopping formula Eq. (1) for $\omega = \omega_p$. Note that b_0 cancels out and therefore its exact value is immaterial under the present conditions. Bohr's stopping formula is valid only for high projectile velocities and different schemes have been proposed to extend its validity down to lower projectile energies [8–10,26,27]. It is pointed out that the dynamic screening is the critical point to understand this rederivation of Bohr's stopping formula for a FEG. The present model goes beyond binary collisions since the electron-ion interaction is obtained self-consistently, as demonstrated in Appendix A.

III. SEMICLASSICAL APPROXIMATION

The classical stopping power from Eq. (8) can be written in terms of the angular momentum $\hbar \ell = mvb$ and the integral over the impact parameters can be replaced by a sum over ℓ according to the following semiclassical approximation (see Appendix B):

$$\left(\frac{dE}{dx}\right)_{\rm sc} = -\frac{Z_1 \omega_p^2}{2v} \hbar \sum_{\ell=0}^{\infty} \sin \Theta(\hbar \ell/mv).$$
(17)

This expression is more general and recovers the Bloch and Bethe stopping formulas, as demonstrated in what follows. It is also quite suitable for numerical calculations since there are different and efficient methods to calculate the scattering angle $\Theta(b)$ in two-body problems.

Using the well-known Euler-Maclaurin formula [25] to convert the sum in Eq. (17) to an integral, the stopping expressions (8) and (17) can be easily connected to each other as

$$\left(\frac{dE}{dx}\right)_{\rm sc} = -\frac{Z_1\omega_p^2}{2v}\hbar\sum_{\ell=0}^{\infty}\sin\Theta(\hbar\ell/mv)$$
(18)
$$Z_\ell m\omega^2 \ \ell^{\infty}$$

$$= -\frac{Z_{1}m\omega_{p}}{2} \int_{0}^{\infty} db \sin \Theta(b) + \frac{Z_{1}\omega_{p}^{2}}{2v} \hbar \sum_{k=1}^{\infty} \Delta^{2k-1} \frac{B_{2k}}{(2k)!} F^{(2k-1)}(0), \quad (19)$$

where $F(b) = \sin \Theta(b)$, for which $F(0) = F(\infty) = 0$, B_n are the Bernoulli coefficients, and $\Delta = \hbar/mv$. The *n*th derivative of F(b) at b = 0 is denoted by $F^{(n)}(0)$. For such a vanishing impact parameter, Coulomb scattering prevails $[F(b) = -\frac{2Z_1e^2}{v}\frac{bmv}{(Z_1e^2/v)^2 + (bmv)^2}]$, and therefore

$$F^{(n)}(0) = -\frac{2Z_1 e^2}{v} (-1)^{\frac{n-1}{2}} \frac{(mv)^n n!}{\left(\frac{Z_1 e^2}{v}\right)^{n+1}},$$
 (20)

for *n* odd. Putting the above coefficients into expression (19) we have

$$\left(\frac{dE}{dx}\right)_{sc} = -\frac{Z_1 m \omega_p^2}{2} \int_0^\infty db \sin \Theta(b) - \frac{Z_1^2 e^2 \omega_p^2}{v^2} \sum_{k=1}^\infty (-1)^{k-1} \frac{1}{2k} B_{2k} \frac{1}{\chi^{2k}}$$
(21)
$$= -\frac{Z_1 m \omega_p^2}{2} \int_0^\infty db \sin \Theta(b) + \frac{Z_1^2 e^2 \omega_p^2}{v^2} [\ln(\chi) - \operatorname{Re}\Psi(1+i\chi)],$$
(22)

where $\chi = Z_1 e^2 / \hbar v$ and $\Psi(x)$ is the digamma function, whose expansion in terms of the Bernoulli coefficients is found in Ref. [25]. The first term corresponds to the Bohr formula in the high-velocity limit as demonstrated above. The second term corresponds to the inverse Bloch correction $L_{invBloch} =$ $\ln(\chi) - \text{Re}\Psi(1 + i\chi)$ [24,28]. The so-called Bloch correction is an expression originally derived by Bloch [4] that bridges the Bethe and Bohr formulas. It was also derived by Lindhard and Sørensen for a FEG [29]. It is an additive correction on the Bethe formula, which includes higher-order terms from close collisions approaching the Bohr formula in the limit of very strong perturbations $\chi \gg 1$. The second term of Eq. (22) does the opposite. It corrects classical results to account for quantum effects in close collisions. In the limit of small perturbations at high speeds $(\chi \to 0)$, the semiclassical stopping approaches the Bethe formula $\frac{Z_1^2 e^4 \omega_p^2}{m v^2} \ln(\frac{2mv^2}{\hbar \omega_p})$. The correction's origin is only due to the conversion of the sum by the integral over the orbital angular momentum. Therefore, the physical origin of the Bloch correction is evident in the current approach. It comes from close collisions for which quantum effects of the quasi-Coulomb scattering are important. Another feature of the derivation is that the inverse Bloch correction is tightly connected with the logarithm term as recently demonstrated in Ref. [28]. The inverse-Bloch correction is used in the binary theory of the stopping power (realized by the PASS code) [26]. It was shown recently that proper account of the Bloch correction and the ion charge form the key to a quantitative description of the electronic stopping of heavy ions [28].

The results of the classical and semiclassical stopping formulas for H, He, and C in a FEG system corresponding to the Al valence electrons are shown in Fig. 2. The classical results converge to Bohr's classical theory from ion velocities somewhat after the maximum of the classical stopping. For increasing Z_1 , classical and semiclassical formulas give nearly the same results for v > 1. In addition, for a FEG system, the high-velocity limit is given exactly by the Lindhard dielectric formalism [11]. The present semiclassical results converge to the dielectric formalism for protons at high projectile velocities (v > 2). Note that dynamical exchange and correlation effects are of minor importance at high projectile energies [23].

The semiclassical expression for the stopping power (17) is quite general. It must be corrected at low projectile velocities by the effect that electrons are not, in fact, at rest. The usual

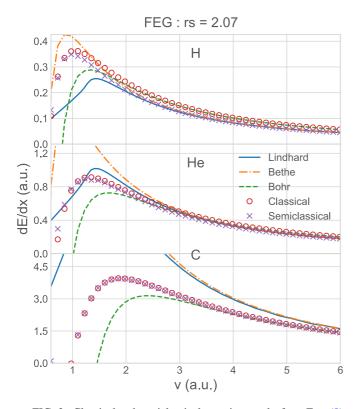


FIG. 2. Classical and semiclassical stopping results from Eqs. (8) and (17), respectively, for H, He, and C in FEG with electron radius $r_s = 2.07$ as a function of the ion velocity v. The Yukawa potential was used with $\alpha = \omega_p/v$. For comparison, the Bohr [1], Bethe [3], and Lindhard [11] models are also present. All results are in atomic units (a.u.).

way [24,30] to account for this effect is the application of the following kinematic transformation on the semiclassical stopping (17):

$$\left(\frac{dE}{dx}\right)_{\rm sc, corr} = \int d^3 v' f(v') \frac{\boldsymbol{v} \cdot (\boldsymbol{v} - \boldsymbol{v}')}{v|\boldsymbol{v} - \boldsymbol{v}'|} \left(\frac{dE}{dx}\right)_{\rm sc} (v, |\boldsymbol{v} - \boldsymbol{v}'|),$$
(23)

where f(v) is the velocity distribution of the electrons in an undisturbed target. Therefore, nondegenerate FEG and thus effects of temperature can be taken into account in Eq. (23) by using, for instance, a Maxwell -Boltzmann distribution for f(v).

Note that the correction above to the semiclassical approach fails at very low projectile velocities since full quantum-mechanical effects dominate the electron-ion scattering as the de Broglie wavelength increases. Therefore, it will not reproduce the so-called Z_1 oscillations of the stopping power [31] at very low projectile velocities. Moreover, for these low energy projectiles, dynamic exchange and correlation effects must be included in the calculations [17,18].

IV. CONCLUSIONS

In summary, we derive a formula for the stopping power [Eq. (8)] of charged particles in a classical system of electrons at rest with initial-state density *n* (classical static FEG),

assuming a central potential for the ion-electron interaction. It gives the same results as Bohr's classical theory in its range of validity. The suggested semiclassical generalization encompasses Bloch's stopping theory, which links Bethe's perturbative quantum theory of stopping power of charged particles in matter and Bohr's classic theory. The current treatment indicates that the Bloch correction can also be understood as a consequence of the semiclassical approximation and conversion of the sum over angular momenta, as realized by the Euler-Maclaurin formula. It affects mostly small impact parameters and thus close collisions.

The stopping formula Eq. (17) captures the basic stopping processes regarding target ionization and excitation and can be applied to real systems after considering different target densities, shell corrections, screening, and charge states of the projectile.

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APPENDIX A: CHARGE NEUTRALIZATION CONDITION

The classical expression for the density $\rho(\vec{r})$ [Eq. (2)] can be used to derive a rule for the neutralization condition

$$\int d^3 r[\rho(\vec{r}\,) - n] = Z_1. \tag{A1}$$

Using Eq. (2) in Eq. (A1), we have, after some algebra,

$$2n\int d^2b \int_{r_0}^{R} \frac{dr}{\sqrt{1 - \frac{2V(r)}{mv^2} - (b/r)^2}} - \frac{4\pi}{3}R^3n = Z_1 \quad (A2)$$

for $R \to \infty$. r_0 is the distance of closest approach. Using the expression for the semiclassical phase shifts δ_{ℓ} [32] we get the following expression:

$$2n\pi\hbar^{3}\frac{1}{m^{3}v^{2}}\sum_{\ell}(2\ell+1)\frac{d\delta_{\ell}(v)}{dv} = Z_{1}, \qquad (A3)$$

which agrees with the expression from Arista and Lifschitz [33] derived from quantum mechanics. Indeed, the classical expression for the density $\rho(\vec{r})$ from Eq. (2) describes the density of electrons coming from one direction with a single asymptotic speed. Equation (2) can be generalized to allow for electrons coming from any direction and different asymptotic speeds. By averaging the electron velocity in Eq. (A3) over the static Fermi sphere, with v_f as the maximum speed, we retrieve the Friedel sum rule in the usual form [33,34] for a static impurity,

$$Z_1 = \frac{2}{\pi} \sum_{\ell} (2\ell + 1)\delta_{\ell}(v_f).$$
 (A4)

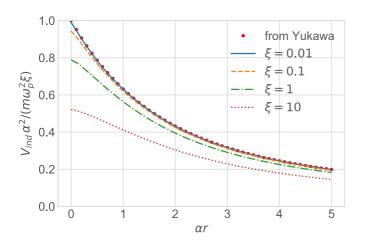


FIG. 3. Numerical calculations for the spherical averaged induced potential $V_{\text{ind}} = e^2 \int d^3 r' n_{\text{ind}}(\vec{r}\,')/|\vec{r}-\vec{r}\,'|$ in reduced units for different $\xi = 2Z_1 e^2 \alpha/mv^2$ values. The closed circles correspond to the induced potential determined from the Yukawa potential as $-\frac{Z_1 e^2}{r} e^{-\alpha r} + \frac{Z_1 e^2}{r}$.

The classical expression (A2) for charge neutralization in the limit of high velocities is

$$2n \int d^2 b \frac{1}{b^2 v^2} \int_b^\infty \frac{dr}{m\sqrt{1 - b^2/r^2}} \frac{d}{dr} [r^3 V(r)] = Z_1 \quad (A5)$$

according to the procedure of Lehmann and Leibfried [see Eq. (A117) in Ref. [7]]. For the Yukawa potential $[V(r) = -\frac{Z_1 e^2}{r} e^{-\alpha r}]$ we have

$$Z_{1} = -\frac{2nZ_{1}e^{2}}{mv^{2}} \int d^{2}b \frac{1}{b^{2}} \int_{b}^{\infty} \frac{dr}{\sqrt{1 - b^{2}/r^{2}}} (2r - r^{2}\alpha)e^{-\alpha r},$$

$$Z_{1} = \frac{\omega_{p}^{2}Z_{1}}{v^{2}} \int_{0}^{\infty} bdb \frac{1}{b^{2}} \frac{1}{4}b^{2}[-4K_{0}(\alpha b) + 3\alpha bK_{1}(\alpha b) - 4K_{2}(\alpha b) + \alpha bK_{3}(\alpha b)],$$

$$Z_{1} = \frac{\omega_{p}^{2}Z_{1}}{v^{2}} \frac{1}{\alpha^{2}},$$
(A6)

which means $\alpha = \frac{\omega_p}{v}$. Therefore, for $\xi = 2Z_1 e^2 \alpha / mv^2 \ll 1$, where the above expansion holds true, the screening parameter $\alpha = \frac{\omega_p}{v}$ used in Eq. (11) is obtained from the neutralization condition. Moreover, numerical calculations for the spherical averaged induced potential (see Fig. 3) show the self-consistence of the Yukawa potential at high projectile velocities ($\xi \ll 1$). Dipolar effects of the induced potential are expected to be of minor importance at high-projectile velocities [35] since the Coulomb potential dominates the scattering

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at close collisions. At distant collisions, the dipole contribution vanishes according to the impulse approximation.

APPENDIX B: SEMICLASSICAL APPROXIMATION

The semiclassical approximation used to derive Eq. (17) matches full quantum mechanics calculations of stopping power for a FEG in the high-energy limit $v \gg v_f$, where v_f is the Fermi velocity. It reads [22]

$$\frac{dE}{dx} = \frac{Z\omega_p^2}{2v}\hbar \sum_{\ell=0}^{\infty} \sin[2(\delta_\ell - \delta_{\ell+1})],$$
 (B1)

where δ_{ℓ} are the phase shifts at the velocity v for a scattering described by a central potential. The semiclassical formula (17) is obtained by relating the phase shifts to the scattering angle as $2(\delta_{\ell+1} - \delta_{\ell}) \rightarrow \Theta$ [5].

A different semiclassical approach has been proposed [6] and used in several works. It relies on an ad hoc introduction of a minimal impact parameter determined from the de Broglie wavelength in the perturbative limit. Although it provides stopping results similar to the sum over the angular momentum in Eq. (17), this procedure is misleading. A minimum impact parameter for a two-body problem gives the false impression that the cross section for large energy transfers is strongly affected. For large energy transfers, there is not such a large difference between quantum and classical calculations.

APPENDIX C: NEUTRAL PROJECTILE

Let us now consider a neutral projectile interacting with a classical static FEG system. The difference now is the electron-point-charge force in Eq. (4), Z_1e^2/r_{cl}^2 , which is replaced by $V'(r_{cl})$, where $V(r_{cl})$ is the potential that describes the interaction between the electron from the FEG and the neutral projectile. Thus, the stopping force will now read

$$\frac{dE}{dx} = -nv \int dt \int d^2b \cos(\theta_{\rm cl}) V'(r_{\rm cl}(t,\vec{b})), \qquad (C1)$$

or, in terms of the force along the x direction $F_x = -\cos(\theta_{cl})V'(r_{cl}(t, \vec{b})),$

$$\frac{dE}{dx} = -nv \int d^2b \int dt F_x = -nv \int d^2b \Delta P_x$$
$$= nv \int d^2bmv[1 - \cos(\Theta)] = mnv^2\sigma_{tr}, \quad (C2)$$

which is the standard stopping formula in terms of the transport cross section σ_{tr} [7].

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