Stopping power of electrons in a semiconductor channel for swift point charges

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The nonperturbative kinetic framework for the stopping power of a charged-particle system for swift point projectiles is implemented. The pair-interaction potential energy required in this framework to two-body elastic scattering is based on the screened interaction energy between system particles. In such an energetically optimized modeling the swift bare projectile interacts with independent screened constituents of a fixed-density interacting many-body target. The first-order Born momentum-transfer (transport) cross section is calculated and thus a comparison with stopping data obtained [Phys. Rev. B 26, 2335 (1982)] by swift ions, $Z_i \in [9, 17]$ and $(v/v_0) \approx 11$, under channeling condition in Si is made. A quantitative agreement between the elastic scattering-based theoretical stopping and the experimentally observed reduced magnitude is found. Conventionally, such a reduced magnitude for the observable is interpreted, applying an equipartition rule, as inelastic energy loss mediated by a collective classical plasma-mode without momentum transfer to the valence-part. Beyond the leading, i.e., first-order Born-Bethe term ($Z_i^2$), the Barkas ($Z_i^3$) and Bloch ($Z_i^4$) terms are discussed, following the arguments of Lindhard for screened interaction. An extension to the case of stopping of warm dense plasma for swift charges is outlined as well.

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I. THE STATUS OF THE PROBLEM

In this short theoretical note we start with dedicated experiment [1] for the stopping of swift ions, $Z_i \in [9, 17]$ and $(v/v_0) \approx 11$, at channeling conditions in Si target. It was found that the measured data are only about half of the result based on the conventional (linearized self-consistent field) dielectric [2] result for the stopping power in an electron gas

$$\frac{dE}{dx} = \frac{4\pi n_0 Z_i^2 e^4}{mv^2} \ln \frac{2mv^2}{\hbar \Omega_{pl}}, \quad (1)$$

where $\Omega_{pl}^2 \equiv 4\pi n_0 e^2/m$ is the classical plasma frequency in terms of the number-density $n_0$, electron charge $e$, and mass $m$. This classical (independent of $\hbar$) quantity represent a collective mode because the restoring force on the displaced charged particles arises from the self-consistent classical electric field generated by the local excess charges [4].

In the consideration of a charge-compensated degenerate electron gas, the prototype model of free-electron metals, the classical collective mode appears in the equation of motion for the operator of charge density fluctuation $n_q = \sum_j \exp(iq \cdot r_j)$ at small wavelenght

$$\ddot{n}_q = -\Omega_{pl}^2 n_q$$

The underlying field-theoretic (second-quantized) method rests on the Heisenberg equation of motion for $n_q$ and application of the random-phase approximation introduced in the pioneering normal-mode treatment of an interacting electron gas [5, 6]. According to that pioneering treatment [5], the number of collective modes ($n'$) appears as subsidiary condition on which the ground-state energy of the system depends. The variational constraint on that energy result in $(n'/n_0) << 1$ in terms of the number density $n_0$ of electrons.

For a recent comprehensive discussion of Eq.(1) in plasma physics, we refer to [7]. Besides, in an earlier detailed Lecture Notes [8] which includes the classical (i.e., the induced electric field) interpretation of the retarding force, an equipartition in the total stopping power was emphasized. Namely, in a single-pole approach for the response function of the model of a charged electron-gas-at-rest (bosonic) system, there are equal contributions to the stopping power, $dE/dx$, from "free" and "resonant" collisions.

In the self-consistent-field approach [8], the system
Fourier variables for energy- and momentum-change to inelastic processes \((\hbar \omega = q \cdot v)\) are reinterpreted \((\hbar \omega = q \cdot v)\) in terms of an externally fixed variable \((v)\) of a heavy ion. On the role of the (undamped) classical collective mode in an inelastic process, like the external-electron-charged-medium interaction, we refer to a particularly clear discussion in \[8\]. Briefly, in such an inelastic process the momentum transfer and the (positive) energy loss may be varied independently. An isolated resonant peak in the dynamical structure function of the system have been observed in the transmission \[9\] of electrons through certain thin metallic films.

The above-mentioned equipartition in Eq. (1) is based \[8\] on re-writing it into the form

\[
\frac{dE}{dx} = \frac{4\pi n_0 Z^2 e^4}{mv^2} \ln \left( \frac{q_{\max}}{q_{\min}} \right) \\
= \frac{4\pi n_0 Z^2 e^4}{mv^2} \left[ \ln \frac{q_{\max}}{q_0} + \ln \frac{q_0}{q_{\min}} \right]
\]

To such a momentum-transfer-based representation of the logarithm-argument in Eq. (1) the maximum and minimum are determined by the two real solutions of a Bogoliubov-type \[4\] (now, for Coulomb forces) energetic constraint \[8, 10\] within the single-pole approximation

\[
\frac{(\hbar q_0)^2}{2m} + (h\Omega_{pl})^2 = (hqv)^2.
\]

The two solutions result in the following mathematical identification of a \(q_0\) value

\[
\frac{\hbar^2}{2m} (q_{\max} \cdot q_{\min}) = h\Omega_{pl} = \frac{(hq_0)^2}{2m},
\]

independently of \(v\). In the large velocity limit one gets \(\ln(q_{\max}/q_{\min}) = 2 \ln(q_{\max}/q_0)\). Thus, an equipartition rule in stopping is demonstrated in this manner. Such a rule is applied in a textbook \[11\] to experimental (reduced) ion-stopping at channeling condition by supposing the dominating role of the collective polarization response and excluding binary events. We notice here, however, that one may interpret the logarithm-argument in Eq. (1) as the ratio of energy losses in elastic binary \(2mv^2\) and collective inelastic \(h\Omega_{pl}\) excitations.

The motivating experiment \[1\] on Si, as we mentioned, yields about half of the value based on the conventional form. Besides, a detailed analysis of the higher-order (with opposite-sign) terms was given by pointing out their efficient cancellation. This leaves the first-order Born scaling \((\propto Z^2)\) as the proper one at the experimental conditions with positive ions. Notice, that an about \((1/v^2)\)-scaling for the sign-dependent \((\propto Z^2)\) term was predicted in CERN-experiment \[12\] using swift protons and antiprotons and a Si detector-target.

This paper is devoted to the problem outlined above. We will use the kinetic theory for the stopping power in which the swift heavy intruder interacts with system constituent via elastic scattering transferring momentum and energy in independent binary processes. The applied theory is well-established \[8, 13\]. However, its implementation needs a reasonable two-particle interaction energy in which a large part of physics is encoded \[10\]. In particular, this interaction energy should respect the interaction-time aspect of the binary process and the many-body aspect of the charged system without the external swift projectile \[17\].

II. MODELING, RESULTS, AND DISCUSSION

In the kinetic theory \[8, 13\] one has for the observable, i.e., for the stopping power

\[
\frac{dE}{dx} = n_0 \sigma_{tr}(k),
\]

at high ion-velocities. The momentum-transfer \((tr)\) cross section is thus calculated at relative wave-number \(k = mv/h\) in quantum mechanics. For swift heavy \((M > > m)\) projectiles we can neglect an averaged recoil term \([\propto (m/M)]\) of elastic binary collisions \[13, 14\]. Notice that, in quantum mechanics, the kinematically transparent Eq. (2) contains statistical and quantum mechanical averaging. The former appears as a cumulative factor \((\propto n_0)\) at high velocities, the latter by calculating the expectation value of the force operator \[15, 16\] over the set of scattering eigen-states with \(l \rightarrow (l + 1)\) selection in matrix elements.

The quantum-mechanical transport cross section \(\sigma_{tr}\) for elastic electron scattering in the center-of-mass system with a spherical interaction potential is defined as follows

\[
\sigma_{tr}(k) = 2\pi \int_0^\pi d\theta \sin \theta (1 - \cos \theta)|f(k, \theta)|^2,
\]

in terms of the (complex) scattering amplitude. Its partial-wave representation

\[
f(k, \theta) = \frac{1}{k} \sum_{l=0}^\infty (2l + 1) e^{i\delta_l(k)} \sin[\delta_l(k)] P_l(\cos \theta),
\]

in the defining expression to an averaged momentum transfer in Eq. (3) results in

\[
\sigma_{tr}(k) = \frac{4\pi}{k^2} \sum_{l=0}^\infty (l + 1) \sin^2[\delta_l(k) - \delta_{l+1}(k)],
\]

where \(\delta_l(k)\) are Bessel phase shifts determined by the scattering Schrödinger equation.

Considering the experimental conditions, \((v/v_0) = 11\), we apply the first-order Born (B) approximation where, instead of solving the radial wave equations, one uses unperturbed plane waves (eigenfunctions of the momentum operator) for incoming and outgoing states. Since
in our case the phase shifts are small, \([\delta_l(k) - \delta_{l+1}(k)] \propto \left[{1/(k)/(l+1)}\right]\), we can write

\[
    f^{(B)}(k, \theta) = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) \delta_l^{(B)}(k) P_l(\cos \theta)
\]

\[
    = \frac{2m}{\hbar^2} \int_0^\infty V(r) \frac{\sin(Kr)}{Kr} r^2 dr
\]

\[
    = f^{(B)}(K)
\]

where \(K = 2k \sin(\theta/2)\), and thus \(\sin(\theta d\theta) = (K/k^2) dK\) and \((1 - \cos \theta) = K^2/2k^2\) to Eq.(3). The above correspondence is based on the definition of the first-order Born phase shifts, in terms of \(V(r)\) and Bessel functions \([j_l(x)]\) of the first kind, and application of an identity

\[
    \frac{\sin(Kr)}{Kr} = \sum_{l=0}^{\infty} (2l+1) j_l^2(kr) P_l(\cos \theta).
\]

Now, we arrived at the basic task in our modeling. According to the short discussion in the previous Section and in [17], we suppose that the swift bare projectile interact with screened independent constituents of the many-body system via \(V(r) = -Z_1 v(r)\) in elastic scattering. In other words, to justify a Sommerfeld-like (free-particle) picture we employ a simplified version of the heuristic quasiparticle-description of Landau, which is in fact a canonical approximation procedure. Thus the residual interaction between system particles (without external intruder) is characterized by \(v(r)\). It is a residual interaction when all averaging, correlating, and screening effects in the system have been taken into account [18].

Next, we turn to a physics-based design of the interparticle \(v(K)\), and refer to a canonical, Bogoliubov-type form [4] for the square of the normal mode excitation (\(E_{ex}\)) energy

\[
    (E_{ex})^2 = \left[\frac{(\hbar K)^2}{2m^*}\right]^2 + 2v(K) \eta_0 \frac{(\hbar K)^2}{2m^*}
\]

which might allow a renormalization (field-theoretical) procedure via the effective mass. Clearly, in order to keep a Sommerfeld-like free-particle picture we get \(v(K \rightarrow 0) \propto K^2\). In the opposite limit, i.e., at large \(K\), which corresponds to the short-range in real space, one should recover the well-known Coulomb form \(v(K \rightarrow \infty) \propto 1/K^2\).

The small \(K\) limit for \(v(K)\), as Eq.(6) shows, is related to a Friedel-like [19] sum of phase shifts since at the forward limit \((\theta = 0)\) one has \(k = 0\) and \(P_l(1) = 1\) for the Legendre polynomials. Such a sum determines, via the Fumi theorem [10], the kinetic-energy-change in the many-body system. At first-order in interparticle \(v(r)\) the variational consistency on the ground state requires its minimization. And, in harmony with this energetic constraint, the Friedel sum must be zero since we do not consider an excess charge in the charged host.

Based on the above physics-details, and restricting ourselves to the simplest (i.e., one-parametric) form with mathematical (limit) consistency, we write a bosonic form

\[
    V(K) = -Z_1 v(K) = -Z_1 e^2 \frac{4\pi K^2}{K^4 + 4\Lambda^4},
\]

where, in the equal-mass case [22], \(\Lambda^4 = (2\pi n_0)/\hbar^2\) and \((1/\hbar^2) = me^2/\hbar^2\). Thus we get

\[
    v(r) = \frac{e^2}{r} e^{-\Lambda r} \cos(\Lambda r).
\]

Notice, that a Poisson-equation-based classics would give for an "induced" hole-density \(\Delta n(r) = (\Lambda^2/2\pi)(1/r)e^{-\Lambda r} \sin(\Lambda r)\) . This is finite at \(r = 0\), as expected.

At this point we return to the experimentally motivated [1] basic-problem in stopping power of valence electrons of a semiconductor (Si) channel, for swift ions. The kinetic formalism for elastic binary scattering, implemented by our potential energy, results in

\[
    \frac{dE}{dx} = n_0 \frac{mv^2}{\hbar^2} \sigma_{tr}(k
\]

\[
    \simeq n_0 \frac{4\pi Z_1^2 e^4}{mv^2} \frac{1}{2} \left( \ln \frac{1 + 4k^4}{\Lambda^4} - \frac{1}{2} \right)
\]

after a quite straightforward quadrature. Here the Bohr unit \((1/\hbar) = me^2/\hbar^2\) to \(\Lambda^4\) is re-introduced in order to arrive at the final expression, formally in terms of a quantized collective mode of a polarizable extended charged medium. Thus we found an explanation, without uncontrolled mixing, to the experimental fact with a half-value for the observable. Our work may contribute to earlier efforts performed by using quantum mechanical convolution approximation [2], and classics-based approximation [24] using Bohr modeling. Of course, a trajectory-based classical attempt, i.e., an attempt without angular-momentum quantization in electron scattering, is not able to reproduce the perturbative Born-Bethe limit. Classics may be quantitative at large enough \(Z_1/(a_0k)\) values for coupling in stopping. We note at this qualitative statement that the semi-classical WKB approach becomes mathematically quantitative [25] for Coulomb phases \([\sigma_l(Z_1, l, k)]\) at about \(Z_1/(a_0k) \gtrsim 2\). The situation in experiments [1] was not very far from that range, but from below.

At the end of this Section, we make an other (independent) control of our formalism. Following the lead of Lindhard [26], and a strongly related analysis [27], on the charge-sign \((Z_1^2)\) effect in stopping we discuss this effect observed [12] in Si detector-target by using charge-conjugated swift \((v > 5v_0)\) particles, protons and antiprotons \(Z_1 = \pm 1\). In particular, we address the origin (classical or quantal) of the effect based on the ingredients of the leading-order expression. First we observe,
following the lead of [26], that the transport cross section scales as $k^{-4} \sim E^{-2}$, i.e., inversely as the square of the large kinetic energy of the scattering particle. Next, the series expansion of $V(r)$ for small distances results in a shift of this kinetic energy giving for it an effective value $E_{eff} \simeq E(1 - Z_1 e^2 \Lambda/E)$ both to classical and quantum treatments [26]. Using the such-modified energy to Eq.(10), we get

$$\frac{dE}{dx} \simeq \frac{4\pi n_0 Z_1^2 e^4}{mv^2} \left[ \frac{1}{2} \ln \frac{2mv^2}{\hbar \Omega_{pl}} \right] + Z_1 \frac{e^2}{mv^2} (2\Lambda) \ln \left( \frac{2mv^2}{\hbar \Omega_{pl}} \right),$$

and the second term will be denoted as $Z_1 L_1$, according to tradition [12 17 26].

It is important to compare Eq.(11) with the result based on the higher-order response function approach [28, 29] for a polarizable medium to characterize the induced (retarding) electric field at the swift-projectile position. There, at the RPA level, one obtains

$$\frac{dE}{dx} \simeq \frac{4\pi n_0 Z_1^2 e^4}{mv^2} \left[ \ln \frac{2mv^2}{\hbar \Omega_{pl}} + \frac{Z_1 e^2}{mv^2} \left( \frac{3\pi \Omega_{pl}}{2v} \right) \ln \left( \frac{2mv^2}{2.13\hbar \Omega_{pl}} \right) \right],$$

(12)

Figure 1 contains the experimental data denoted by open circles and open triangles with error bars. They are taken from Fig. 4 of [12], where the two corresponding thickness for Si detector-target were also indicated. The solid curve is based on Eq.(11), the dashed one on Eq.(12). To implement these theoretical expressions, an $r_s = 2a_0$ for the system Wigner-Seitz radius, i.e., density parameter, is employed. At that value $\Lambda \simeq 0.66/a_0$ in our modeling, thus $(\Lambda)^{-1} < r_s$. A mathematical equivalence of the two forms for the sign-coefficient would result in $\Lambda(v) = (3\pi/4)(\Omega_{pl}/v) << (r_s)^{-1}$. One might regard such a deduced form as conveying information on the dynamical response of the medium in a stationary (Poisson-equation-based) self-consistent field approximation for swift-ion screening. This adiabatic parametrization in the first term of Eq.(10) would results in its numerical doubling in contradiction with channeling data. And a large volume, $V \propto [\Lambda(v)]^{-3}$ with interacting system particles, is excluded from local binary elastic scattering. Mathematical tuning of $\Lambda$ results in a re-balancing [17] of the two leading terms in the perturbative stopping power.

Our form for the $L_1$ sign-dependent term is in reasonable harmony with data. Especially, its experimentally emphasized $(1/v^3)$-dependence is gratifying. The dielectric modeling gives a quite different, $(1/v^3)$-scaling. It underestimates the data by taking the same density for the homogeneous host system. The common argument [28, 29], to cure this underestimation, rests on normalized-weighting over an inhomogeneous atomistic charge density $n(R)$ by defining a local $r_s(R)$ from it. However, while such an empirical averaging could result in a very reasonable (due to a sum rule) effective excitation energy in the denominator of the Born-Bethe logarithm, an essential part of excitation-physics behind a sign-dependent term is improperly treated. For close impact ($R$ is small) the negative swift projectile moves inside atomic orbits. There, the consideration of shift in discrete electron-binding results in a sign-effect opposite [30, 31] to the above-discussed one. Thus, the cancellation of opposite-sign trajectory-dependent terms may strongly influence the formal enhancement based on an empirical weighting of homogeneous results, considering random collisional conditions. Moreover, due to the mean spacing between lattice-ions in solids, applications of large-distance dipole fields to projectile-atomic-electron excitation have a limited validity.

Close impact, i.e., an energy- and impact parameter-dependent [31] small closest approach in nuclear collision, indeed plays a decisive role in stopping of negative projectiles according to the insightful analysis [32] of Fermi and Teller which was motivated by the slowing down of negative mesotrons (i.e., muons) in matter (metal, insulator, and gas). Recent ab initio work for proton and antiproton stopping in LiF target also signals [33] the possibility of an opposite sign-effect, by quantifying the dominant role of small close impact via antiproton-made destabilization of a $p$-type anion orbit in $F^-$. The unified treatment of interrelated nuclear collision and electronic excitation is highly desirable, as [31 34] indicate.

In the light of the above discussion on the sign-dependent term in stopping power, finally we return oncemore to the motivating experimental work in [1]. There, besides stating the half-like magnitude of the observable, it was pointed out that there could be an efficient cancellation between the sign-dependent $Z_1 L_1$ term and the next-order negative $(Z_1^2 L_2)$ so-called Bloch term
for swift positive projectiles used in experiment. This term is about
\[ Z_1^2 L_2 \simeq -\left( \frac{Z_1 v_0}{v} \right)^2 = -\left( \frac{Z_1}{a_0 k} \right)^2 \]
by considering the dominating \([l = 0 \rightarrow (l = 1)]\) angular-momentum selection with a bare Coulomb force. The dominance of such a contribution in a mathematically convergent series [actually, a sum for Riemann \(\zeta(3)\)] is compatible with the physical form of interaction at short range. Obviously, due to the \((1/v^2)\)-dependence of \(L_1\) in our Eq. (11), we arrive at a simple, kinematical [17], explanation to terms-cancellation in the positive-ion case.

III. SUMMARY AND OUTLOOK

The nonperturbative kinetic framework for the stopping power of an homogeneous electron gas for swift projectiles is implemented. The pair-interaction potential energy required in this framework to two-body elastic scattering is based on the screened interaction energy between system particles. In such an energetically optimized modeling the swift bare projectile interacts with independent screened constituents of a fixed-density interacting many-body target. We contrasted the such-obtained theoretical results with independent experimental data obtained for Si target by using swift ions. We found harmony with the reduced value of the stopping power under channeling condition. Similarly, the magnitude of the charge-sign effect and its velocity-scaling are in accord with measurements for the observable. The origin of cancellation between higher-order terms for positive projectiles is discussed as well. Based on these above, a coherent modeling to further efforts is found.

Recently, in the very promising field of warm dense plasma [33], measurement of stopping of energetic \([v/v_0] \simeq 25\) protons, produced via fusion reaction with \(D^3He\) fuel, signals that Eq. (1) would need an essentially larger denominator in the logarithmic factor then the conventional estimation with \(\Omega_{pl}\) of valence electrons. The target \((t)\) is a heated solid berillium metal for which \(Z_t = 4\) and it has two valence electrons. In addition, at an estimated electron temperature, \(k_B T \simeq 32\ eV\), enhancement in stopping was observed in comparison with data obtained for cold target. At that, still moderately high, temperature and for \(v/v_0 = 25\) for protons, the conventional temperature-independent [3] form in Eq. (1) is supposed to be correct for a homogeneous system. However, as was pointed out in a single-parametric \((I)\) Bethe-style [33] analysis of random stopping data based on
\[ \frac{dE}{dx} = \frac{4\pi n_0 Z_t^2 e^4}{mv^2} \ln \left( \frac{2mv^2}{\langle I \rangle} \right), \]
with an effective \((\langle I \rangle)\) target characteristics, the \(\langle I \rangle = h\Omega_{pl}\) identification is not a proper choice to interpret enhancement in stopping data as a function of the temperature.

We speculate that a temperature-dependent extension of our approach might contribute to a deeper understanding of experimental predictions. Namely, superimposing the random thermalized motion of target electrons \((e)\) in Eq. (8) via a new [22] statistical term in
\[ V(K, T) = -Z_1 v(K, T) = -Z_1 e^2 \frac{4\pi (K^2 + \langle k_s^2 \rangle)}{K^4 + K^2 \langle k_s^2 \rangle + 4\Lambda^4}, \]
with a thermal-excess, \((\langle k_s^2 \rangle \propto (k_B T m/\hbar^2)\), could increase \((dE/dx)_{T=0}\). At small temperature we expect a \(T\)-linear enhancement in our Born expression by growing temperature since
\[ \frac{dE}{dx}_T \simeq n_0 \frac{4\pi Z_t^2 e^4}{mv^2} \left( \frac{1}{2} \ln \frac{2k^2}{\Lambda^2} + \frac{1}{8} \frac{k_s^2}{\Lambda^2} \arctan \frac{2k^2}{\Lambda^2} \right), \]
perturbatively. At the experimental conditions (see, above) the second term is roughly 1/5 of the first one. This is not in contradiction with subtracted data [33]. A more quantitative analysis is left to a dedicated paper. For a berillium target \((Z_t = 4,\) with two valence and two 1s-type electrons in cold metals), the number-density \([n_0(T)]\) of effective electrons at fixed volume seems to be a Saha-ionization-based parameter. Thus it could be, for berillium, \(n_0(T) = 2n_0\) already at moderate temperatures due to such [33, 37] ionization.

More generally, and according to [33, 38], an accurate theory of charged-particle stopping in electron plasmas is a fundamental challenge. It has an impact on our understanding of energy-deposition processes and thus on a reasonable estimation for the ignition threshold in fusion research. However, at high temperatures the target ionic component, not considered in the above outlook, may also contribute to the ion-stopping [38] via nuclear collisions.

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