The Brandt–Kitagawa Heavy Ion Model:
Embedding in the Homogeneous Electron Gas

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Abstract

The ion model by Brandt and Kitagawa [Phys. Rev. B 25 (1982) 5631] has played a major role in the development of the effective charge theory for the electronic stopping of heavy ions in solids. Embedding it into the electron gas of the target leads to an enhanced screening of its bound electrons, modification of its size parameter and eventually of its effective charge. A basic, earlier calculation [T. Kaneko, Phys. Rev. A 41 (1990) 4889] overestimates the effect, but can be improved by confining the influence of the target dielectric to the region of the outermost bound electrons of the ion.

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1 The BK ion model and Coulomb energies

The wide-spread use of the Brandt–Kitagawa (BK) ion model [1] in the theory of the electronic energy loss of heavy ions is based on its simplicity, which leads to some general, closed form expressions for the electronic energy loss in the dielectric formulation. The electronic stopping power as calculated in the program by Ziegler, Biersack and Littmark (ZBL) is based on it [2], and it is implicitly used in programs founded on the ZBL formulation [3]. Abdesselam et al. [4,5] and Niemann et al. [6] compared experiments with the original theory. A model hybridized with results by the density functional theory (DFT) was proposed [7], and results including local-field effects of the dielectric function and dielectric functions at finite temperatures have been calculated [8]. This article focuses on a classified problem that arises when initially separated ion

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and dielectric target models are fused. Neither a review of heavy ion energy losses in general nor of effective charge theories in particular is intended; the dominant differences to the scattering theory approach are summarized in App. A.

The treatment calculates

\[
-\frac{dE}{dt} = \int d^3r \rho_m(\vec{r}, t) \vec{v} \vec{E}_{\text{ind}}(\vec{r}, t),
\]

(1)

where \( \vec{E}_{\text{ind}} = -\nabla \Phi_{\text{ind}} \) is the electric field of the induced charges, \( \vec{v} \) the ion velocity, and \( \rho_m \vec{v} \) its electric current density. The ion charge density comprises the point charge of the nucleus with ion atomic number \( Z_1 \), and the bound electrons with number density \( n_e \),

\[
\rho_m = \rho_n + \rho_e = Z_1 e \delta(\vec{r}) - e n_e(\vec{r}),
\]

(in the ion rest frame). The Fourier transform is

\[
\rho_m(\vec{k}, \omega) \equiv \int d^3r d t e^{-i(\vec{k} \cdot \vec{r} - \omega t)} \rho_m(\vec{r}, t) = 2\pi \delta(\omega - \vec{k} \cdot \vec{v}) \rho_m(\vec{k}).
\]

(2)

The BK form is obtained with the ansatz

\[
n_e(\vec{r}) = \frac{N}{4\pi \Lambda^2} \exp\left(-\frac{r}{\Lambda}\right),
\]

(3)

normalized to contain \( N = \int n_e \, d^3r \) bound electrons, kept roughly within a distance \( \Lambda \), a variational parameter, from the nucleus. (For brevity, “bound” means “bound to the ion” hereafter and never refers to features of the induced charges or charges that are represented by the dielectric function \( \epsilon(\vec{k}, \omega) \) of the target.) BK decomposed the energy of the isolated ion by a Hartree-type energy for the electron-electron repulsion, the electron-nucleus Coulomb energy, and a local density approximation for the kinetic energy (SI units throughout)

\[
E_{\text{BK}} = E_{ee} + E_{ne} + E_{\text{kin}}
\]

\[
= \lambda \frac{1}{2} \int d^3r \, d^3r' \frac{\rho_e(\vec{r}) \rho_e(\vec{r}')}{4\pi \epsilon_0 |\vec{r} - \vec{r}'|} + \int d^3r \frac{Z_1 e \rho_e(\vec{r})}{4\pi \epsilon_0 R} + \frac{3}{10} \frac{\hbar^2}{m} \int d^3r n_e(\vec{r}) k_F^2(n_e)
\]

\[
= \lambda \frac{e^2}{4\pi \epsilon_0} \frac{N^2}{4\Lambda} - \frac{\epsilon^2}{4\pi \epsilon_0} \frac{Z_1 N}{\Lambda} + \frac{\hbar^2}{m} a^5 N^{5/3}/\Lambda^2
\]

(4)

with \( a \approx 0.24 \) a numerical constant, \( e \) the elementary charge unit, \( m \) the free electron rest mass, \( \epsilon_0 \) the permittivity of vacuum, and \( \hbar \) the reduced Planck
constant. They fixed the coupling parameter \( \lambda \), introduced as a correction for missing exchange and correlation contributions to the electron-electron interaction, by demanding a vanishing chemical potential for the neutral atom,

\[
\frac{\partial E_{BK}(Z_1, N, \Lambda, \lambda)}{\partial N} \bigg|_{N=Z_1} = 0. 
\]

(5)

\( \Lambda(N) \) was fixed for each \( N \) by energy minimization

\[
\frac{\partial E_{BK}(Z_1, N, \Lambda, \lambda)}{\partial \Lambda} = 0 
\Rightarrow \quad \Lambda = \frac{2a(1 - q)^{2/3}}{Z_1^{1/3} \left[ 1 - \lambda(1 - q)/4 \right]} a_0.
\]

(6)

(7)

\( a_0 \) denotes the Bohr radius and \( q \equiv 1 - N/Z_1 \) the ionization degree.

If the total charge of the ion in the sea of target electrons is decomposed into the three parts \( \rho_n \), \( \rho_e \) and the induced electron charge density \( \rho_{\text{ind}} \) obeying

\[
\Phi_{\text{ind}}(\vec{r}) = \frac{1}{4\pi \epsilon_0} \int \frac{\rho_{\text{ind}}(\vec{r}')}{|\vec{r} - \vec{r}'|} d^3r'.
\]

(8)

the classical Coulomb energy of the Maxwell field partitions in turn into six terms, each an integral over a product of two of these charge components. Two of them are already represented by \( E_{ee} \) and \( E_{ne} \) in \( E_{BK} \); three of them do not depend on \( \rho_e \) and will not be discussed here because they cannot influence the ion parameterization. The remaining term

\[
\frac{1}{4\pi \epsilon_0} \int \frac{\rho_e(\vec{r})\rho_{\text{ind}}(\vec{r})}{|\vec{r} - \vec{r}'|} d^3r d^3r' = \int \rho_e(\vec{r}) \Phi_{\text{ind}}(\vec{r}) d^3r
\]

(9)

describes a Stark-effect [9,10]. Section 2 describes the components of this energy that must be added to the BK energy (4) to consider the influence of the target electrons on the size parameter \( \Lambda \). Section 3 demonstrates that this generalized ion energy is equivalent to an effective screening of all potential energies in (4) by the dielectric function \( \epsilon \), but much too elementary. Without need to change the underlying concepts, section 4 argues that a correction of the spatial distribution of the induced charges, i.e., an inhomogeneous dielectric function, removes the major discrepancies.
The key ingredient of effective charge theory is the partial penetration of the induced charges into regions also occupied by bound electrons. A step towards a self-consistent description is the determination of the ion parameters not for the ion in free space as in section 1, but for the ion in touch with the dielectric environment. We obtain a realization by inclusion of the energy (9) into (4), in so far as the field \( \Phi_{\text{ind}} \) of the induced charges is “external” to the bound electrons in the same way as the field of the ion nucleus. This refinement of the BK model calculates the net force of \( E_{\text{ind}} \) on the ion via (1) and allows the bound electrons to find a new minimum of energy (in the rest frame of the ion) by adjustment of their distribution \( n_e(\vec{r}) \) to this additional field. The quotation-marks around “external” above indicate that (1) and (9) describe classical (Hartree-only) interactions between \( \rho_e \) and \( \rho_{\text{ind}} \), which allows for a unique partitioning of charges and (with care) of fields into “internal” and “external” parts. [A fully quantum-mechanical treatment of indistinguishable electrons would minimize an energy functional of all electrons, but therefore leave the scope of the familiar dielectric theory of electronic stopping, which encapsulates the target response in a given, linear or nonlinear, \( \epsilon(\vec{k}, \omega) \).]

The Fourier transform of the Poisson equation for the induced charges, using (2), has the form

\[
\Phi_{\text{ind}}(\vec{k}, \omega) = 2\pi \delta(\omega - \vec{k}\vec{v}) \left( \rho_n(\vec{k}) + \rho_e(\vec{k}) \right) \left[ \frac{1}{\epsilon(\vec{k}, \omega)} - 1 \right] \frac{1}{\epsilon_0 k^2}. \tag{10}
\]

The sum of the spatial Fourier transforms of the bound electrons and the ion nucleus for the BK ion model reads

\[
\rho_n(\vec{k}) + \rho_e(\vec{k}) = Z_1 e - \frac{N e}{1 + (k\Lambda)^2}. \tag{11}
\]

This superposition splits the energy (9) into two terms that describe the interaction of the bound electrons with electrons induced (i) by the ion nucleus and (ii) by the bound electrons themselves. The first defines the energy

\[
E_n \equiv \int d^3r \rho_e(r) \int \frac{d^3k \, d\omega}{(2\pi)^3} e^{i(k\vec{r} - \omega t)} \delta(\omega - \vec{k}\vec{v}) Z_1 e \frac{1}{\epsilon_0 k^2} \left[ \frac{1}{\epsilon(\vec{k}, \omega)} - 1 \right] \]

\[
= -\frac{Z_1 Ne^2}{2\pi^2\epsilon_0 v} \int_0^\infty \frac{dk}{k} \frac{1}{1 + (k\Lambda)^2} \int_0^{kv} \text{Re} \left[ \frac{1}{\epsilon(\vec{k}, \omega)} - 1 \right] d\omega, \tag{12}
\]

while the second gives the energy...
\[ E_e \equiv \frac{\tilde{\lambda}}{2} \int d^3r \rho_e(r) \int \frac{d^3k \, d\omega}{(2\pi)^3} e^{i(k_\perp r - \omega t)} \delta(\omega - \vec{k} \cdot \vec{v}) \frac{-Ne}{1 + (k\Lambda)^2} \frac{1}{\epsilon_{k(\omega)}} \left[ \frac{1}{\epsilon_{k(\omega)}} - 1 \right] \]

\[ = \frac{\lambda}{2} \frac{N^2 \epsilon^2}{2\pi^2 \epsilon_0 v} \int_0^\infty \frac{dk}{k} \frac{1}{1 + (k\Lambda)^2} \int_0^{kv} \text{Re} \left[ \frac{1}{\epsilon(k, \omega)} - 1 \right] d\omega. \] (13)

Note that \( E_e \) is not a direct insertion of (10) into (9): (i) An additional division by 2 anticipates that we wish to define the energy of the bound electrons, so that half of the original energy term must be attributed to the induced electrons. As the induced charges change synchronized with \( \rho_e \) (like mirror charges), the work stored in the part \( \rho_e \) is half of the final field energy [10]. (ii) The additional factor \( \tilde{\lambda} \) is meant to take an opportunity to correct this electron-electron interaction in the same fashion as with \( \lambda \) for \( E_{ee} \) in (4).

Examples of these energies for \( ^{15}\text{P} \) and \( ^{38}\text{Sr} \) ions and the Lindhard dielectric function [11] with density parameter \( r_s \equiv 3\sqrt{9\pi/4}/(k_F a_0) \) (\( k_F \) the Fermi wave number) are shown in Figs. 1 and 2 as functions of the ionization degree \( q \). The approximate proportionalities \( E_n \propto 1 - q \) and \( E_e \propto (1 - q)^2 \) are apparent from the prefactors \( N \) in (12) and \( N^2 \) in (13), as the additional dependence \( \Lambda(N) \) inside the integrals hardly turns up. The sum \( E_n + E_e \) is dominated by \( E_n \) and therefore is approximately \( \propto N \) [12].

3 Complete screening: Underbinding

The definition of the energy of the electronic subsystem of the bound electrons, generalizing (4) for ions in touch with the target polarization, is

\[ E_M \equiv E_{BK} + E_n + E_e = E_{\text{kin}} + E_{ne} + E_n + E_{ee} + E_e. \] (14)

Let us assume for the present that \( \tilde{\lambda} = \lambda \). For this choice a short calculation proves that the addition of \( E_n \) to \( E_{ne} \) effectively substitutes the bare \( \rho_e - \rho_n \) Coulomb interaction \( \propto 1/(\epsilon_0 k^2) \) in the internal ion energy by a screened propagator \( \propto 1/[\epsilon_0 \epsilon(\vec{k}, \omega) k^2] \). The addition of \( E_e \) to \( E_{ee} \) modifies the \( \rho_e - \rho_e \) interaction in exactly the same way. The multiplication of \( 1/(\epsilon_0 k^2) \) with \( 1/(\epsilon - 1) \) in (12) and (13) demonstrates this exchange of propagators, and shows the independence on the ion model and the dielectric function. This screening by the dielectric background induces a change in the size parameter \( \Lambda \) which may be determined by the analogue of (6),

\[ \frac{\partial E_M(Z_1, q, \Lambda, \lambda)}{\partial \Lambda} \bigg|_{N=Z_1} = 0. \] (15)
The same result ensues from enforcing the validity of the virial theorem in the combined potential of the nucleus and the bound and induced charges. The new \( \Lambda \) is only 1–2\% larger than the BK value, but special emphasis must be put on the energies \( E_M \) as a function of the ionization degree in Fig. 3. We see that the energy minima are shifted from ionization degrees \( q = 0 \) (in the vacuum) to very large \( q \), predicting a spontaneous loss of a large number of electrons even for ions at rest. (This pathology is \textit{not} cured, if — more accurately — we localize the equilibrium point not where the slope is zero, but where it is commensurate with the chemical potential of the target electron gas. This fact becomes clear when looking at the huge slopes for neutral atoms, as tabulated in the figure.) At the same time, the energy rises much more than about 1\%, the more realistic order of magnitude in these cases [13].

The model fails because screening of \textit{all} Coulomb interactions with the target dielectric function weakens the binding of electrons considerably. There is no appreciable compensation by changes of the kinetic energy \( E_{\text{kin}} \), because the relative change of \( E_{\text{kin}} \) is only about two times the relative change of \( \Lambda \) according to (4). If we approximate \( \epsilon(\vec{k}, \omega) \) furthermore by the Thomas-Fermi static screening, valid for small \( v \) (App. B), we end up with the model proposed by Kaneko [14] and used later by Yang [15]:

\[
\frac{E_M}{E_0} \approx 2a \frac{N^{5/3}}{(\Lambda/a_0)^2} + \frac{N}{\Lambda(1 + \beta \chi)/a_0} \left[ \frac{\lambda}{2} \frac{N}{1 + \beta \chi} - 2Z_1 \right], \tag{16}
\]

with \( \beta \equiv 2k_F \Lambda = 2\Lambda/(\pi \chi^2 a_0) \) and \( E_0 \) meaning 1 Rydberg.

To here, the BK coupling constant \( \lambda = 4/7 \) has been used throughout. In accordance with the spirit of the model, Kaneko [14] intended to redetermine \( \lambda \) via the generalization of (5), which would enforce and guarantee a zero slope at \( q = 0 \) in Fig. 3. Unfortunately, an unrestricted numerical solution of the two resulting coupled algebraic equations for the two unknowns \( \lambda \) and \( \Lambda \), which bypasses his additional approximations, leads to \( \Lambda \) \textit{smaller} than the BK value for \textit{all} cases listed in [14, Tab. 1], and to negative values of \( \lambda \), for example, in the regions \( Z_1 \leq 10 \) for \( r_s = 1.5 \) and \( r_s = 2 \). Trying to enforce a zero chemical potential of this model therefore would mean that the effective electron-electron interaction must in some cases even become artificially attractive and the effective electron-nucleus interaction artificially repulsive to prevent the ion from emitting its electrons in the host. In short, employing \( \lambda \) as a degree of freedom leads to severe artifacts and does \textit{not} improve the model.

A first approach to change this basic model would notice that identical correction factors \( \lambda \) (for the interaction between bound electrons) and \( \tilde{\lambda} \) (between bound electrons and charges induced by bound electrons) do not treat electron-electron interactions equally. (i) The energy \( E_n \) in (12) is also a Coulomb
energy of electron-electron interactions and should be treated on the same footing as $E_e$, i.e., should include $\tilde{\lambda}$. (ii) The energy loss (1) does not include such a factor to compute the force of $\rho_{\text{ind}}$ on $\rho_e$. The presumably most consistent treatment would go back to (14), (12) and (13), which reads in the TF approximation

$$
\frac{E_M}{E_0} \approx 2a \frac{N^{5/3}}{(\Lambda/a_0)^2} + \frac{N^2}{2\Lambda/a_0} (\lambda - \tilde{\lambda}) + \frac{N}{\Lambda(1 + \beta\chi)/a_0} \left[ \frac{\tilde{\lambda}}{2} \frac{N}{1 + \beta\chi} - 2Z_1 \right],
$$

and becomes (16) for $\tilde{\lambda} = \lambda$. It would then set $\tilde{\lambda} = 1$, i.e., establish a purely classical interaction between all “internal” (to the ion, $\rho_n$, $\rho_e$) and “external” ($\rho_{\text{ind}}$) charges in the system. This choice is supported by the fact that the common dielectric functions represent the response of the target to “external” potentials that have to be, by definition, free of exchange-correlation admixtures to the mutual interaction. Numerical results of (17), however, show that $\tilde{\lambda} = 1$ only leads to a significant improvement of the location of the minimum of $E_M(q)$, caused by a stronger cancellation between $E_n$ and $E_e$, but no reduction of the strong rise of this energy on immersion into the target dielectric.

4 Space restricted polarization charges

The remaining inconsistency can be removed by restricting the shielding by the target dielectric function to the outermost regions of the ion charge cloud $\rho_m(r)$. The reasoning is exactly the same that we gave in [16]. For simplicity, let us use the same model of a “dead sphere”

$$
\Phi_{\text{ind}}(\vec{r}) = \frac{1}{4\pi \epsilon_0} \int \frac{\rho_{\text{ind}}(\vec{r}')}{|\vec{r} - \vec{r}'|} \, d^3r',
$$

which sets the induced charge density to zero inside a sphere of radius $r_c$ around the ion nucleus, and leads back to (8) for $r_c \to 0$. $r_c$ represents the size of the heavy ion core which is impenetrable to target electrons. The function corrects the simplifying representation of the ion as an external electromagnetic field, which would not impose phase-space restrictions on excited electron-hole pairs, whereas in reality the bound electrons introduce phase-space blocking by the Pauli exclusion principle [17]. The assumption of spherical symmetry of this correction is consistent with the spherical symmetry of the charge cloud $\rho_e$ of bound electrons in the model, has been used at non-zero velocities before [18], and serves to calculate some intermediate integrals in closed form [16]; it does not imply or cause sphericity of the induced charges.
or the wake field. Qualitatively, the electronic energy loss and the coupling energies (Figs. 1–2) measure the deviation from sphericity to be expected in models of polarizable ions. Both are decreasing at high velocities, and, though the shapes of $\rho_{\text{ind}}(\mathbf{r})$ and $\Phi_{\text{ind}}(\mathbf{r})$ become conical, $r_c$ simultaneously becomes small as the stripping degree increases.

First, fig. 4 extends the previous set of ion-target combinations [16] to underline the general improvement of the calculated energy loss cross section $S \propto dE/dt$ by applying (18). The upper lines show the scaled stopping cross sections obtained with the ZBL parameterization of $\Lambda$ and $q$, and Kaneko’s dielectric functions [19], i.e., the standard treatment with $r_c = 0$. (The homogeneous electron gas is hereby augmented by dielectric functions of the target core states, which is essential to extend results to higher velocities prior to comparison with experimental data.) The lower lines with the choice $r_c = 1.1A$ yield obviously better results.

Second, fig. 5 shows that the contribution of the energy terms $E_n + E_e$ to $E_M$ is indeed reduced with increasing $r_c$; this reduction is important, if $r_c$ has about the magnitude of the radii of the outermost electrons, defined with some arbitrariness in Tab. 1. Realistic values of $r_c$ are expected to depend dominantly on the ion size, and hence implicitly on $q(v)$, but also on $k_F$. If we are reluctant to import the ZBL ion sizes or information obtained from more sophisticated ion models like, for example, in Tab. 1, $r_c$ might be determined by comparison of the electron density $n_e$ in (3) with the target electron density $k_F^3/(3\pi^2)$.

A more satisfactory theory would be based on building a joint dielectric function of the target and the bound electrons, extending the work by Guinea et al. [20] to the case of heavy ions.

5 Summary

The relaxation of the cloud of bound electrons after insertion into the electron gas of the target may be formulated as the replacement of the internal Coulomb interaction by screened interactions. A complete pervasion of the ion by the dielectric function of the target host overestimates the effect. The increases of electronic energy losses of heavy ions derived in previous publications are in fact upper bounds. They may for example be concealed by $Z_1$-oscillations, which cannot be an ingredient of the Brandt–Kitagawa statistical ion model, by nonlinearities of the dielectric function, and by deficiencies of the random phase approximation to the dielectric function. A model of an inhomogeneous dielectric function in the target, which removes the polarization from a region very close to the heavy ion, works well to diminish the energy terms that couple
the bound electrons and the target electrons. This theory of the electronic energy loss consistently inserts the same (inhomogeneous) dielectric function in (i) these energy terms to calibrate the ion parameters and (ii) their time derivatives which yield the stopping power.

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A Approaches to Heavy Ion Stopping

Advantages of computing the energy loss in the homogeneous electron gas via the scattering theory applied to potentials obtained from the DFT have already been described [21]. This theory includes (i) the non-linear target response \( O(Z^3) \) terms in \( dE/dx \) and the shell-structure of ions, (ii) the interaction between the bound and the target electrons beyond the Hartree-approximation, and (iii) self-consistent values of the ionization degree. The obvious limitation of the known DFT results is: They are strictly valid only at \( v = 0 \), because they are based on (i) the familiar DFT, not the (time-dependent) current functional theory [22], and (ii) scattering theory in the limit of spherical potentials. Fortunately, the energy loss function \( \text{Im}1/\epsilon(k, \omega) \) is \( \propto \omega \) (single-particle excitations are dominant) for small \( \omega \) in the jellium model, which extends the approximate validity to higher velocities.

The “dielectric” theories [1,19,23] employ fully dynamical dielectric functions and are one way to handle ions of any velocity. Their rigour for proton stopping has been extended by the inclusion of the non-linear response and local-field corrections [24] — \( Z_1 \)-oscillations [25] are still treated by empirical variation of the size parameter [2,26], but would as well result from enforcement of the Friedel sum rule in the spirit of Ref. [27]. They seem to be much less pronounced for trajectories in “random” than in channeling directions. The introduction of an all-electron dielectric function [16,19] has in essence overcome the earlier effective charge theory which had to make use of the heavy-ion scaling rule to include the inner-shell target excitations.

The Firsov theory of the energy loss in binary atomic collisions does not know the homogeneous electron gas, but points at ion-target binding effects that might dominate the energy loss at small velocities [28].
B Energy Terms at Small Velocities

Analytical approximations of the Lindhard function \[ \epsilon \equiv 1 + \chi^2(f_1 + i f_2)/z^2 \] for small angular frequencies \( \omega \) and hence for small \( v \) as functions of the parameters \( m v_F = \hbar k_F, z \equiv k/(2k_F), u \equiv \omega/(v_F k) \) and \( \chi^2 \equiv 1/(\pi k_F a_0) \) are

\[
\lim_{u \to 0} f_2(z, u) = 0;
\]
\[
\lim_{u \to 0} f_1(z, u) = \frac{1}{2} + \frac{1}{4z} (1 - z^2) \log \frac{|z + 1|}{|z - 1|} \approx 1 - \frac{1}{3} z^2 - \frac{1}{15} z^4 + O(z^6).
\]

\[
\Rightarrow \lim_{v \to 0} \frac{1}{v/v_F} \int_0^{v/v_F} du \frac{1}{\epsilon(z, u)} = \lim_{u \to 0} \frac{1}{\epsilon(z, u)} \approx \frac{z^2}{\chi^2 + (1 - \chi^2/3) z^2 + O(z^4)}.
\]

If we use this small-\( z \) Taylor expansion on the whole \( z \)-axis, a technique used also by Moneta \[29\], and define \( \beta \equiv 2k_F \Lambda \), we obtain

\[
\lim_{v \to 0} \frac{1}{v/v_F} \int_0^{v/v_F} du \frac{1}{\epsilon(z, u)} \approx \pi \frac{2(1 - \beta^2 \chi^2 - \chi^2/3)}{\beta} \left[ \frac{1}{\beta} - \frac{\sqrt{\chi^2 - 1 - \chi^2/3}}{1 - \chi^2/3} \right],
\]

\[
\lim_{v \to 0} \frac{1}{v/v_F} \int_0^{v/v_F} du \frac{1}{\epsilon(z, u)} \approx \pi \frac{2(1 - \beta^2 \chi^2 - \chi^2/3)}{\beta} \left\{ \frac{1 - \chi^2/3}{\beta} - \chi \sqrt{1 - \chi^2/3} \right\} - \frac{1}{2 \beta},
\]

with \( \beta z = k \Lambda \) and \( \beta \chi = 2\Lambda/(\pi \chi a_0) \). These approximations are the analogue to the Lindhard–Winther formulas for the energy loss at small \( v \) \[23\]. The Thomas-Fermi (TF) approximation is defined by the slightly different replacement

\[
\frac{1}{\epsilon(z, u)} \approx \frac{z^2}{\chi^2 + z^2} = \frac{k^2}{k_{TF}^2 + k^2}, \quad (B.1)
\]
and $k_{\text{TF}} \equiv 2/(\pi a_0 \chi)$ the TF screening wave number. It is equivalent to substituting all occurrences (seven) of $\chi^2/3$ in the formulas above with zero. The BK limit of the isolated ion is generally restored when $r_s, \chi \to \infty$ and $\beta \chi \to 0$.

C Energies with the “dead sphere”

The generalization of the energy (12) for nonzero $r_c$ in (18) reads

$$E_n = \int d^3 r \rho_e(\vec{r}) \frac{Z_1 e}{4\pi \epsilon_0} \int d^3 r' \frac{1}{|\vec{r} - \vec{r}'|} \times \int \frac{d^3 k d\omega}{(2\pi)^3} e^{i(\vec{k}' - \vec{v})t} \left[ \frac{1}{\epsilon(k, \omega)} - 1 \right] \delta(\omega - \vec{k} \vec{v}).$$

A calculation similar to [16, App. A] results, for isotropic $\epsilon(k, \omega)$ and spherically symmetric $\rho_e(k)$, in

$$E_n = \frac{Z_1 e}{\epsilon_0 \pi^3 v} \int_0^\infty \frac{dk'}{k'} \rho_e^*(k') \int_0^\infty \frac{dr}{r_c} \sin(k'r) \int_0^\infty \frac{dk}{k} \int_0^\infty d\omega Re \left[ \frac{1}{\epsilon(k, \omega)} - 1 \right].$$

Within the BK model for $\rho_e$ two of these integrals can be solved analytically. If the TF approximation (B.1) is used also, this further simplifies to

$$\frac{E_n}{E_0} = \frac{4Z_1 N}{\pi \chi} e^{-\chi r_c/\Lambda} \left[ 1 - \frac{\beta \chi e^{-r_c/\Lambda}}{1 + \beta \chi} \right]. \quad \text{(C.1)}$$

The corresponding generalization of (13) may be written as

$$E_e = \frac{\tilde{\lambda}}{8\pi \epsilon_0} \int d^3 r \rho_e(\vec{r}) \int d^3 r' \frac{1}{|\vec{r} - \vec{r}'|} \times \int \frac{d^3 k d\omega}{(2\pi)^3} e^{i(\vec{k}' - \vec{v})t} \rho_e(\vec{k}) \left[ \frac{1}{\epsilon(k, \omega)} - 1 \right] \delta(\omega - \vec{k} \vec{v})$$

$$= \frac{\tilde{\lambda}}{2\epsilon_0 \pi^3 v} \int_0^\infty \frac{dk'}{k'} \rho_e^*(k') \int_0^\infty \frac{dr}{r_c} \sin(k'r) \int_0^\infty \frac{dk}{k} \int d\omega Re \left[ \frac{1}{\epsilon(k, \omega)} - 1 \right],$$

giving
\[
\frac{E_c}{E_0} = -\frac{\tilde{\lambda}N}{\pi \chi} \left[ \frac{1}{1 - \beta \chi} - \frac{1}{1 + \beta \chi} \right] \\
\times \left[ e^{-\beta \chi r_c / \Lambda} \left( \frac{1}{\beta \chi} - e^{-r_c / \Lambda} \right) + e^{-r_c / \Lambda} \left( \frac{e^{-r_c / \Lambda}}{2} - 1 \right) \right]
\]  
(C.2)

in the special case of the BK model within the TF approximation. The Kaneko model [14] corresponds to \( \tilde{\lambda} = \lambda \) and \( r_c = 0 \).

References


Within an energy criterion of the heavy ion stripping degree [26], these contributions are virtually indistinguishable from the term $\mu N$, where $\mu$ is the chemical potential of the target material. They would be integrated into the term $\frac{1}{2}mv^2N$, the kinetic energy of the bound electrons in the target rest frame, by defining a relative velocity.


Even the most sophisticated calculations of the jellium model overestimate the electron density nearby the ion core, because the positive homogeneous background attracts more electrons than the isolated point charge $Z_1e$ alone. A nonzero $r_c$ removes some of this bias of the jellium model, too.


Fig. 1. The energy $E_{ne}$ (lowest curve) according to (4) and $E_n$ (six upper curves a–f for different $\nu$) according to (12) as a function of the ionization degree with $\tilde{\lambda} = \lambda = 4/7$ and (7) for $\Lambda$. $E_0$ denotes 1 Rydberg. The values follow from a numerical integration of the Lindhard dielectric function at $r_s = 2$. Results are very close to each other in the cases a–c where velocities are too low to excite plasmons. For faster ions, the oscillatory behaviour of the wake field causes cancellations in the spatial integrals [30], and diminishes the energies $E_n$ and $E_e$.

Fig. 2. The energy $E_{ee}$ (upper curve) and $E_e$ (six lower curves a–f) for the parameters as in Fig. 1.
Fig. 3. The ion energy $E_M$ for two different atomic numbers and two densities of the target electron gas with $\tilde{\lambda} = \lambda = 4/7$ (curves a–d). The original BK energy is the limit of “embedding” into the vacuum (lowest curve, $r_s = \infty$). Also shown is $\mu \equiv \partial E_M(Z_1, N)/\partial N$ at $q = 0$. The readjustment of $\Lambda$ via (15) is included here but not in Figs. 1–2.
Fig. 4. Scaled stopping cross sections for seven combinations of ions and elemental solid targets. Broken lines refer to the theory with the homogeneous dielectric \( (r_c = 0) \), solid lines to the theory with the “dead sphere” correction and the “gap” correction of \([16, \text{Sec. III}]\). Kinks in the curves are created by those in ZBL’s \( \Lambda \). Experimental values: ■ Ref. [5,31], □ Ref. [32], ○ Ref. [33], and △ Ref. [34].
Fig. 5. The energies $E_n > 0$ according to (C.1) and $E_e < 0$ according to (C.2) for the neutral atom ($N = Z_1, q = 0$) as a function of the dead sphere radius $r_c$, inserting $\tilde{\lambda} = 1, \lambda = 4/7$ and (7). Because the TF approximation is implied here, the values at $r_c = 0$ differ by a few percent from the $q \to 0$-limit of the curves a–c in Fig. 1.
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Table 1
Sub-shell radii of some atoms in units of $a_0$, defined by the maxima of $4\pi r^2|\psi(r)|^2$, computed from the wave functions $\varphi(r)$ of the Clementi–Roetti [35] tables with the extended basis sets with the assumption that the occupancies of all sub-shells but the one in the first column are zero.