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Dielectric Theory of the Electronic Energy Loss of Heavy Ions in Solids

by

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Dielectric Theory of the Electronic Energy Loss of Heavy Ions in Solids

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The present work deals with the effective charge theory of the electronic energy loss in homogeneous solids from the point of view of target and ion models:

- Chapter 1 is an introduction and contains a review of the Lindhard-Winther-Theory.

- Chapter 2 deals with the stopping of ions in the homogeneous electron gas. A calculation of the linear susceptibility of interacting target electrons is presented in the lowest order, i.e., the next order beyond the Random Phase Approximation. Complementary to a calculation known from the literature, more compact notations of integrals are given for the real part, which allow to bypass a Kramers-Kronig analysis.

  When applied to the energy loss of punctiform ions, the noticeable increase of the stopping power compared with the Random Phase Approximation at low velocities that is known from density functional calculations is confirmed. At high velocities, which are treated by time-independent density functional calculations solely via extrapolations, a correction of the opposite sign is found, which can be understood on the basis of a sum rule of the polarization.

- Chapter 3 first recalls the Brandt-Kitagawa-Theory of the electronic energy loss of heavy ions and the description by Ziegler et al. that builds on it. It is pointed out, in how far the true
charges which they derived from effective charges (as defined by the electronic energy loss) are uncertain due to model assumptions and approximations.

An energy-stability criterion of the ionization degree as a function of the ion velocity — the most essential ion parameter — is introduced, which is known, but has hitherto been regarded as inferior. A couple of reasons are discussed that demonstrate the superiority of its way of explaining ionization degrees relative to the competing velocity criterion that has been used up to know. A generalization in terms of an adaptation of the electro-chemical potential of the electrons bound to the ion to the potential of the electrons in the solid is given.

• Chapter 4 commences a discussion on the influence of target features on the electronic stopping. Using the Kaneko theory, which composes targets by atomic shells of individual electrical susceptibilities, we first elucidate why the older effective charge theories are able to describe the effective charge of ions approximately correctly, though their target is the homogeneous electron gas: at low ion velocities, just the free target electrons are excited indeed, and in the limit of high velocities the binary encounter approximation becomes valid, where the free target electrons deliver *pars pro toto* a good description after scaling with the heuristic “heavy ion scaling rule.”

• This application of the Kaneko theory uncovers limits of its validity for heavy ions and is the motivation to present the following improvements in the final chapter 5: (i) the inclusion of excitation gaps to the polarization of target core electrons, (ii) the removal of the target polarization in close vicinity to the ion core, which is strongly suppressed in reality. An argument is given that introduces a different representation of the $p$ and $d$ sub-shells, but the impact on the stopping power stays low. Finally, as an obvious improvement, the replacement of a sum over target shells by a sum over susceptibilities is presented. It massively changes results in the case of transition metals, but meets its limitations by a too crude representation of $d$ electrons in these solids.
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Chapter 1

Introduction

1.1 Thematic Classification

The electronic, “inelastic” energy loss of the stopping of ions dominates the better understood nuclear, “elastic” contribution at middle and high energies. The electronic energy loss (EL) not just primarily determines the range in detectors, of dopants in semiconductor devices etc., but contributes indirectly to additional displacements, annealing and so on as the electron energy is transferred via phononic coupling to target atoms [70, 117, 199, 208, 252].

Nowadays, the theory of the EL of heavy ions virtually divides into the dielectric or effective charge theory on one hand and the scattering phase method on the other. Publications based on the competing Bethe-Theory, the kinetic theory or the harmonic oscillator model, which would fundamentally contribute to the basics for spatially extended ions, i.e., do not use ad-hoc measures like a substitution of charges by effective charges, are not known. In [225], for example, only energy loss ratios are quoted for ions up to and including $6\text{C}$. One may assume that this is not caused by an inherently different physical description of the target electrons, but by the considerably more compact target description by the effective charge theory in terms of the dielectric functions, facing a self-contained ion form factor. In this respect the restriction of this dissertation to the dielectric theory does not signify an assessment. Corrections and dependences within the model of completely separated ion and target features are created by screening of the outer electrons of the ion by target
electrons for example, or the model of the “dead sphere” that will be proposed here for the first time.

The current work looks exclusively at target models with a spatially homogeneous ground state. The energy loss in the case of channeling and its impact parameter dependence in BCA-type calculations are — with the exception of the comment in Chapt. 5.3 — not treated. For spatially extended ions the conceptionally little rigorous ansatz of the local plasma approximation [15, 46, 99, 136, 184, 185, 181, 249, 251, 261, 264] exists to that, and more fundamental calculations [116, 121, 155, 171, 220] from perturbational and therefore developable approaches in the semi-classical approximation for highly stripped ions, where isolated atoms are the target. String models attempt a reduction of the problem to a two-dimensional plane perpendicular to channeling directions [4, 141, 147, 196]. Some other models cannot be classified there or are hybrids [18, 67, 171, 172, 186, 187, 221]. The Firsov model [54, 56, 57] has lost importance. Parameterizations have been found through fits within Monte-Carlo codes or to experimental range distributions [191, 206, 207]. The proper generalization of the dielectric theory, however, is given by the extension to lattice periodic dielectric function [34, 42, 53, 79, 146, 151, 176, 241, 253]; the implementation of the dielectric matrix establishes a hurdle, though, and may present a disproportionate expenditure to describe sufficiently localized electrons of low-lying bands of solids. A general unification of the point of view of ion-atom collisions and the “macroscopic” dielectric theory comparable with the thoughts on harmonic oscillators in [25] could present a doable compromise in the future.

Due to the magnitude of typical Fermi energies relative to optical gaps, the FEG model may often be used for valence and conduction bands. Also for the lower lying “atomic” shells of targets — the résumé of the Kaneko theory — no systematic deviation between the homogenized description and the experiments with “random” targets remains. That means, after integration over all collision (impact) parameters in the experiment, the EL is generally compatible with a homogeneous spatial smearing of the individual target shells. Contributing to this finding is that (i) heavy ions take a quasi-average over an interval of impact parameters with their diameter, (ii) the Coulomb field of an ions penetrates the target atoms as a long range external potential, and (iii) for the dominant ionization processes the transition probability of a target electron is
determined by the matrix element between the extended initial atomic state and the extended final
plane-wave state.

The sequence of the material presented in this work follows the historical development of
the theory, and also proceeds from the special and fundamental to the superior and more realistic.
At the beginning we have the Lindhard-Winter theory of punctiform charges in the free electron
gas (FEG). Contributions to the effective charge theory with the ion form factor the additional
degree of freedom follow, built upon the FEG model at the beginning of the eighties by Brandt et
al. The Kaneko theory of the late eighties, which describes also the inner shells of target atoms by
a dielectric function, is the ending. The FEG is contained therein as a prospective component of
solid state targets.

Chapter 2 applies previously reported results of many-particle solid-state physics to the
EL theory. The present work includes the linear susceptibility of the FEG in the order of one
interaction in the polarization diagram (the order following the RPA) in the EL calculation. From
the outside this calculation aims to make actual use of the advantage that the dielectric theory
hitherto has compared with density-functional results, the prediction covering all frequencies of
the dielectric response, hence the complete interval of ion velocities. The non-linear susceptibility
of the FEG may be considered to be known, following the work by Sung, Pitarke et al. [59, 110,
201, 202, 203, 239], and has also been often treated in the literature beside electron gas models
[68, 78, 166, 165, 174, 225, 228, 232]. From the point of view of scattering of target electrons off
the ion potential it is classified as higher order Born terms [65], and is established by expansion of
the self-consistent equations of the scattering problem in orders of the ion atomic number (App.
I). Nothing will be added to these results here. The literature also knows dielectric functions that
have been progressed from static local field corrections. The present work fills some gap in this
part of the theory.

The contents of chapter 3 deals with the central, but hitherto neglected parameter of ef-
fective charge theory, the ionization degree as a function of ion atomic number and velocity. The
characteristic ansatz of effective charge theory interprets the ion charge that is measured in the
stopping process as an average over the ion radius, i.e. the screening of the nuclear charge, and the
excitation spectrum of the target. The transition from the true, but experimentally not directly accessible ion charge to its effective charge therefore calls for the full knowledge of the stopping mechanism. From the point of view of the theory, the rule of thumb which obtains the EL of heavy ions by substitution of the charge by the effective charge is not helpful, because it hides a number of interdependences; it merely works as a definition of the effective charge. At the end of the seventies, a criterion based on relative velocities held the field versus the energy criterion to determine ionization degrees as a function of ion velocities and ion species. The object of the dissertation is to correct the impression that energies are the worse or less suitable parameters. The remarkably simple intermediate result is: because the ion increases the ionization degree by one more step, if a target electron can muster the ionization energy in form of its kinetic energy, simple calculation of roots of the ionization energies reproduces the fit of the ionization degree by Ziegler, Biersack and Littmark.

The chapter is rather voluminous (i) to work off a number of places in the literature in a careful manner, and (ii) to demonstrate that energies exist as a counterpart to the energy loss, which we have to direct our attention to in the framework of an energy criterion.

Chapter 4 first presents the dielectric description of all atomic shells of the target by the Kaneko theory. It helps to understand in a retrospective view how the predecessor theories transplanted the effective ionization degrees of FEG targets into real solids via a scaling with experimental proton energy losses. The Kaneko theory introduces a way to calculate heavy ion energy losses directly, without detour via the Heavy Ion Scaling Rule. After that, the “effective charge” theory would just be called “dielectric” theory, as the key importance of the effective charges is restrained.

The application of the Kaneko theory to the EL of slow heavy ions as demonstrated in chapter 4 generally over-estimates the energy loss. In chapter 5 some clear arguments lead to the construction of corrections that upgrade the theory, the systematics of these discrepancies always kept in mind. In principle, the flaws may be ion models which screen too inefficiently, or too strong excitations of the target. The most impressive result is typical of the way the EL is calculated here: not the isolated view on the ion or target model, but regard of the volume that the ion takes
up in the dielectric function, and leaving the model of a homogeneous target offer a systematic explanation.

### 1.2 The Basic Equation of the Dielectric Theory

The dielectric theory describes the ion as a classical charge cloud that moves with velocity $v$ through the target. It consists of a punctiform nucleus $\rho_n(r) = Z_1 e\delta(r)$ with atomic number $Z_1$ and a charge cloud $\rho_e$ of electrons bound to it:

$$\rho_m(r) = \rho_n(r) + \rho_e(r).$$

The target is assumed to be homogeneous and is described exclusively via its dielectric function. Standard electrodynamics deduces the induced polarization charge

$$\rho_p(k, \omega) = \rho_m(k, \omega) \left[ \frac{1}{\epsilon(k, \omega)} - 1 \right],$$

(1.1)

where

$$\rho_m(k, \omega) = 2\pi \rho_m(k) \delta(\omega - kv)$$

(1.2)

denotes the Fourier transform of $\rho_m(r, t)$ and $\rho_m(k) \equiv \int d^3 r \exp(ikr)\rho_m(r)$ the ion form factor. The total charge $\rho$ is composed of the charge $\rho_m$ of the moving ion and the induced charge $\rho_p$ in the target material:

$$\rho = \rho_m + \rho_p.$$  

(1.3)

In parallel to this formula, the total electric potential $\Phi$, the potential $\Phi_0$ of the ion charge and the potential $\Phi_{\text{ind}}$ of the induced charges obey

$$\Phi = \Phi_0 + \Phi_{\text{ind}}.$$  

Pictures of this wake-like induced field in real space have been drawn often [19, 44, 71, 86, 213]. The potentials may be computed from the charges via Poisson’s law (the Gauss law of integrals), and read in Fourier space

$$\Phi_0 = \frac{\rho_m(k, \omega)}{\epsilon_0 k^2} ; \quad \Phi_{\text{ind}} = \frac{\rho_m(k, \omega)}{\epsilon_0 k^2} \left[ \frac{1}{\epsilon(k, \omega)} - 1 \right].$$
The energy that is transferred between the field $E_{\text{ind}}$ and the ion determines the electronic energy loss. The Coulomb force, which is exerted by the induced charges on the ion, and the energy transfer are each equivalent to the stopping power \[78, 89\]

\[
\frac{dE}{dx} = \frac{1}{v} \frac{dE}{dt}; \quad \frac{dE}{dt} = \int j_m E_{\text{ind}} d^3r < 0; \quad (1.4)
\]

\[
j_m = \rho_m v; \quad E_{\text{ind}} = -\nabla \Phi_{\text{ind}}. \quad (1.5)
\]

Under the assumption of a homogeneous target and a spherically symmetric ion $\rho_m(r)$, the integrations over the polar and azimuthal angles of $k$ relative to $v$ may be carried out, and the EL becomes just a double integral over the absolute value $k$ of the wave number and the angular frequency $\omega$ \[36, 81, 149, 150\]

\[
\frac{dE}{dx} = \frac{1}{2\pi^2 \epsilon_0 v^2} \int_0^\infty \frac{dk}{k} \left| \rho_m(k) \right|^2 \int_0^{\infty \omega} d\omega \omega \text{Im} \left[ \frac{1}{\epsilon(k,\omega) - 1} \right]. \quad (1.6)
\]

A generalized and therefore rather long-winded derivation is presented in section 5.4.1 and App. H.1 later on.

As the energy transfer between the ion and target electrons is represented by the exchange of electromagnetic waves with momentum $\hbar k$ and energy $\hbar \omega$, the ion mass does not appear in this equation. This ansatz does not endorse the philosophy of a balance of the ion kinetic energy prior and after collisions with target electrons that are seen as individual events \[195\]. Rather the ion velocity is assumed to be constant in (1.2). The energy transfer to the target electrons computed above is compensated by an additional virtual force in this model. The construction resembles the insertion of virtual forces in replacement of constraints in the D’Alembert principle. The ion mass does actually not show up, because this is equivalent to target electrons knocking against a rigid wall. The energy-momentum conservation on the target side during the creation (annihilation) of an electron-hole pair by the electromagnetic field is implicitly contained in $\epsilon(k,\omega)$.

Within this steady-state description of a time-independent ion charge $\rho_m$, the so-called projectile-inelastic contributions to the EL are missing, which are also treated under the keyword of dynamical screening of the ion by the electrons it carries along \[121, 171\]. The contributions play a role only for small atomic numbers \[11, 13, 193\], because the excitation of the ion is hindered
for large $Z_1$ due to the larger binding energies of its electrons, and the relative difference between the two excited states $\rho_m$ of the ion becomes smaller. This does not prevent the application of the theory to $^1$H projectiles, which are an important reference within effective charge theory, because these are bare protons over a wide velocity interval, are described as such by $\rho_m$, and cannot be excited further. The theory handles the ion and the target asymmetrically with regard to two things. (i) The excitation spectrum of the target is written down for all $k$ and $\omega$, but the ion charge is constant in time (though not necessarily in the ground state [132]). (ii) The target is translationally invariant whereas the ion charge exists just once at one point in space [229].

The velocity will always be chosen as the natural parameter to scale the axes in the way it enters in (1.6), not the ion energy. Therefore the wording “heavy” ion is a somewhat misleading classification in this scheme, because it will more or less exclusively refer to the electric features hidden in $\rho_m$ in the subsequent text, and to the ion size in a chemical way of thinking within effective charge theory. No delicacies of the interpretation emerge from this.

The non-linear susceptibilities of the target create effects of the order $L \propto \rho^3_m$ and higher. These “Barkas” and “Bloch” effects are also often called effects of the order $Z^3_1$ and higher. In the context of heavy ions this may be sloppy, because effective charge theory is generally non-linear in the ion models. Therefore even in the case of a linear response of the target, $dE/dx$ may already contain terms of $O(Z^3_1)$ [19].

The electronic straggling will not be discussed further [17, 29, 126, 253, 259]. The frequency spectrum transferred to the ion reaches from 0 to $kv$ according to (1.6). Because the energy loss function $\text{Im}(1/\epsilon)$ is not sharp in general, but offers absorption bands, (1.6) is to be interpreted as an averaging over the energy exchange $\hbar\omega$. The straggling, the expectation values of the higher moments of the energy transfer, may therefore be computed via insertion of an additional $\hbar\omega$ in the integrand. Fluctuations of the charge state $\rho_m$ are another, simple to understand source of electronic straggling [24]. Both cases establish an energy uncertainty in a homogeneous target. The straggling of the nuclear energy loss, on the contrary, transforms the geometrical uncertainty of the statistics of impact parameters into an energy straggling via the kinematics of the scattering process.
1.3 The Lindhard-Winther Model

If we (i) simplify further to the case of punctiform ions with charge $Z_1 e$, i.e., $\rho_m(k) = Z_1 e$, and (ii) assume the target is a homogeneous electron gas of density $n$, the dimensionless Lindhard stopping number $L$ can be split off:\ref{1.6} \cite{1.78, 1.45} \cite{1.39, 1.114, 1.148, 1.149, 1.150}:

$$\frac{dE}{dx} = \frac{Z_1^2 e^4}{4\pi \epsilon_0^2 m v^2 n L}$$

$$L \equiv \frac{-1}{\pi \omega_0^2} \int_0^\infty dq \int_{-qv}^{qv} q_0 dq_0 \text{Im} \left[ \frac{1}{\epsilon(q)} - 1 \right].$$ \hfill (1.7)

The squared plasmon frequency is defined via $\omega_0^2 \equiv (e^2 n) / (\epsilon_0 m)$. $q_0$ denotes the circular frequency, $q$ the absolute value of the wave number $q$, and subsequently often the “4-momentum” $(q_0, q)$ in an argument.

1.3.1 The Zeroth Order Polarization, Lindhard Function

If especially the penetrated medium is a free, isotropic electron gas at temperature 0 K above a positive homogeneous background, one parameter remains, either the Fermi wavenumber $k_F$, or the average electron density $n$, or the density parameter $\chi^2$, or the Fermi velocity $v_F$, or the one-electron radius $r_s$

$$\hbar k_F = m v_F \quad ; \quad \chi^2 \equiv \frac{1}{\sqrt{3} \pi^3 n} a_0 = \frac{v_0}{\pi v_F} \quad ; \quad r_s \equiv \sqrt{\frac{9\pi}{4}} \frac{v_0}{v_F}$$ \hfill (1.8)

$a_0$, $v_0$…Bohr radius and velocity

$h$ …reduced Plank constant

The dielectric function is acquired from the Dyson-Equation for the screened effective Coulomb potential $U$,

$$U(q) = U_0(q) + U_0(q) \Pi^*(q) U(q)$$ \hfill (1.9)

and

$$U(q) = U_0(q) / \epsilon(q)$$ \hfill (1.10)

$$\epsilon(q) \equiv 1 - U_0(q) \Pi^*(q)$$ \hfill (1.11)
by insertion of the unscreened, bare Coulomb potential

\[ U_0(q) = \frac{e^2}{\epsilon_0 q^2} \]

and of the contributions of the connected polarization diagrams \( \Pi^*(q) \). In this context the starlet at \( \Pi^* \) does not mean complex-conjugation, but always the subset of connected graphs.

The so-called random phase approximation (approximation of the non-interacting electron gas) means the restriction to the zeroth order of the polarization

\[ \Pi^* \approx \Pi^{*(0)} = -\frac{2i}{\hbar} \int \frac{d^4k}{(2\pi)^4} G^0(k)G^0(k+q), \quad (1.12) \]

where

\[ G^0(k) = \frac{\Theta(k - k_F)}{k_0 - \omega_k + i\eta} + \frac{\Theta(k_F - k)}{k_0 - \omega_k - i\eta} \quad (1.13) \]

denotes the time-ordered Green function with wave number \( k \) and frequency \( k_0 \), and the notation

\[ \omega_k \equiv \hbar k^2/(2m) \]

is used. The Feynman diagram is shown in Fig. 1.1.

---

Figure 1.1: Polarization in zeroth order (RPA)

---

The orders are named according to the number of internal electron-electron interaction lines. The calculation of these functions yields [28][82, chapt. 12][149]

\[ -U_0\Pi^{*(0)} = \frac{\chi^2}{z^2}(f_1 + if_2), \quad \epsilon \equiv 1 + \frac{\chi^2}{z^2}(f_1 + if_2) \quad (1.14) \]

and, if all momenta are measured in units of the Fermi momentum and a scaled dimensionless
frequency $\nu$ and the Lindhard variables $z$ and $u$ are defined [114, 82],

$$z \equiv q/2$$

(1.15)

$$\nu \equiv \frac{m}{\hbar k_F^2}$$

(1.16)

$$u \equiv \nu/q$$

(1.17)

$$a \equiv q/2 - \nu/q$$

(1.18)

$$f_1(z,u) \equiv \frac{1}{2} + \frac{1}{8z} [1 - (z - u)^2] \ln \left| \frac{z - u + 1}{z - u - 1} \right| + \frac{1}{8z} [1 - (z + u)^2] \ln \left| \frac{z + u + 1}{z + u - 1} \right|$$

(1.19)

$$f_2(z,u) \equiv \begin{cases} \frac{1}{2} \pi u, & 2u + a < 1 \\ \frac{\pi(1-a^2)}{8z}, & |a| < 1 < u + z \\ 0, & |a| > 1 \end{cases}$$

(1.20)

$$L = \frac{6}{\pi \lambda^2} \int_0^{v/v_F} \int_{-u}^1 udu \int_{-(u+a)^{3/2}}^{(u+a)^{3/2}} \left[ \frac{\chi^2 f_2(u,a)da}{[(u+a)^2 + \chi^2 f_1(u,a)]^2 + [\chi^2 f_2(u,a)]^2} \right]$$

(1.21)

### 1.3.2 RPA Plasmon Dispersion and Electronic Energy Loss

Fig. 1.2 shows some electronic energy losses, i.e., the equivalent $L/(v/v_F)^2$ for different Fermi and target velocities, and Fig. 1.3 the stopping number $L$ according to (1.21).

This reference shape of the EL as a function of the ion velocity is interpreted in the framework of the basic equation (1.6) as follows: The real part of the polarization characterizes the field strength of the induced (dipolar) field, but the stopping is determined in essence also by the imaginary part of the polarization. In a medium with “unstable,” rapidly decaying polarization, the polarization field can follow the spherically symmetric field of the ion instantaneously. From the point of view (in the coordinate system) of the moving ion the polarization field therefore looks nearly spherical, which lets the sum of the forces and the stopping vanish. — The study in terms of the Joule heat demands in an equivalent manner that the net dot product, integrated over the ion volume, between the ion current and the electrical field must exist to result in stopping.

On the other hand a medium with more stable, inert, slowly decaying polarization field cannot adapt its state fast enough to the Coulomb field of a swift ion. The total field seen by the ion attains larger components parallel to the flight direction, the stopping power becomes
Figure 1.2: The electronic energy loss in RPA for different Fermi and projectile velocities; $L$ is the stopping number. The numbers at the curves are $v_F/v_0$.

Figure 1.3: The stopping number $L$ for varying Fermi and projectile velocities. The curves are labeled with the values of $v_F/v_0$.

larger. For very large ion velocities the ion escapes the induced field nearly completely, and sees an unperturbed, non-polarized environment. In this velocity regime the stopping becomes smaller
again.

This view does not depend on the assumption of a non-retarded potential $U_0(q)$ down the line for the propagation of the electromagnetic field. It is actually based on the definition $P(q) = \epsilon_0 \chi^R(q) E(q)$ of the retarded susceptibility $\chi^R$ in frequency space. Its imaginary part describes — a fundamental feature of the Fourier transform — the part that is odd as a function of time, i.e., the retarded share. Mediated by its velocity the ion experiences this retardation as a distance in space; eventually the polarization charges seem to be displaced in the ion coordinate frame and can exert a net force.

The zero of the dielectric function (1.14), given by

$$\begin{align*}
(u + a)^2 + \chi^2 f_1(u, a) &= 0, \\
f_2(u, a) &= 0
\end{align*}$$

(1.22)

(1.23)

describes the plasmon dispersion, which reads in our scaled units

$$\nu(q) = \nu_0 \left(1 + \frac{9q^2}{40\chi^2} + O(q^4)\right) = \nu_0 + \frac{3}{10} \frac{q^2}{\nu_0} + O(q^4)$$

(1.24)

$$\nu_0 \equiv \frac{\omega_0 m}{\hbar k_F} = 2 \chi/\sqrt{3}.$$ 

(1.25)

It “ends” in the continuum of single-particle excitations $f_2 \neq 0$ (Fig. 1.4).

The onset of the plasmon excitation becomes most visible at low Fermi velocities: the region of linear dependence between stopping and velocity gets a kink left of the maximum in Fig. 1.2 [3, 81]. This is a manifestation of the “equi-partition rule” [150, §4], which states among others that at this point the right-side derivative of the curve is twice as large as the left-side derivative. The intersection of the dispersion curve with the region $f_2 \neq 0$ is obtained from (1.22) through insertion of $a = -1$, which means

$$u \ln \frac{u}{u - 1} = \frac{2}{\chi^2} (u - 1)^2 + 1.$$ 

Insertion of an expansion for large $u$

$$u \ln \frac{u}{u - 1} \approx \frac{u}{u - 1} + \left(\frac{1}{2} - 1\right) \frac{1}{u} + \left(\frac{1}{3} - 1\right) \frac{1}{u^2} \cdots$$

and restriction to the first two terms delivers the approximation

$$u \approx \sqrt{\chi^2/4 + 1},$$
which under-estimates this intersection by a relative error between 0 and 5% for all $\chi^2$: The plasmon excitation does not contribute within the RPA below $v/v_F = \sqrt{\chi^2/4 + 1}$. A similar, more rough estimate is presented in [28, (9)].

Some plasmon dispersions in RPA with the “natural” axis choice frequency $\nu$ versus wavenumber $q$, and the equivalent curves for the parameters $a$ and $u$ are displayed in Fig. 1.5.

The plasmon pole at small wave numbers $q$ is not of much interest to calculate the stopping, because the integration is confined to the interval $u = \nu/q < v/v_F$. This is the dominant difference compared with optical excitations that interrogate (if phonon support is neglected) the target excitation spectrum at $q \approx 0$.

By the excitation spectrum of the FEG one may construct a simple semiconductor model by setting $\text{Im} \epsilon$ to zero below an energy $E_g$. With Fig. 1.4 and (1.6) the EL vanishes if $v \lesssim E_g/(2\hbar k_F)$.

In a detailed example with values of $^{14}$Si, $v_F = 0.97v_0$ and $E_g = 1.1$ eV, we get an “ionic” transparency analog to the optical transparency for $v \lesssim 0.02v_0$, which means below 10 eV/u. If $2k_F$ is replaced by the radius $\pi/5.43\AA$ of the Brillouin zone, i.e., umklapp processes are excluded, this limit becomes $0.13v_0$ or 440 eV/u. These velocities and the corresponding reduction of the
Figure 1.5: Dispersion of the plasmon pole in RPA as a function of the scaled wavenumber $q$ and the scaled frequency $\nu$ (left) and for an axis choice $u$ and $a$ that is more suitable to integrate the dielectric function [114]. The numbers at the curves represent the Fermi velocity in units of the Bohr velocity.

electronic energy loss are so small that they will be neglected here as common in the literature. The range of applicability of the FEG model to the EL therefore comprises considerably more targets than just the metals, so far as the Fermi energies and plasmon energies in real semiconductors often are substantially larger than the band gaps. The larger $E_g$ of low-lying bands, however, will be explicitly taken into account in Sect. 5.3.
Chapter 2

The First-Order Polarization of the Free Electron Gas

2.1 Motivation

We ask for the reliability of the approximation of non-interacting electrons in the medium (random phase approximation, RPA) within the first Born approximation (linear susceptibility), and test it by inclusion of the next higher order in an internal perturbation series. This is the perturbation series along orders of the field which is produced by the electrons in the medium themselves. For an atomic target this is discussed for example in [175]. Calculations of these local field corrections in the FEG are known in the long-range limit $q \to 0$ [69 92], but do not provide the information covering all wave numbers needed to calculate the integral (1.7). The static limit $\omega \to 0$ has also been reported [35 91 153 179], but its range of validity and hence the interval where the EL stays proportional to the velocity is unknown \textit{a priori}. Interpolation formulas have been proposed [60], which come without an estimate of their accuracy. The main preparatory work to what is presented here has already been published by Holas \textit{et al.} [109]. New are mainly a further reaching analytical representation of the real part of the first order polarization, and the insertion and application of the first order polarization (in)to the formula of the dielectric energy loss.
2.2 The Feynman Diagrams

The Feynman diagrams of the first order (which follows on the RPA) are in Fig. 2.1.

Diagrams a) and e) do not contribute to the polarization, because $U_0(q = 0) = 0$ holds for the electron gas with positive homogeneous background. The first-order diagrams are of $O(\chi^4)$: The expansion along orders of the polarization may be regarded as an expansion along orders of $\chi^2$. The RPA is the $O(\chi^2)$ and ought to become exact at high electron densities. But the Lindhard function of Sect. 1.3 actually under-estimates the stopping power, as the polarization has been calculated with a non-relativistic dispersion of the electrons, whereas at large electron densities (that is large Fermi energies) the electrons close to the Fermi surface become relativistic. Subsequently the electron densities and Fermi wave numbers are always sufficiently small not to
turn to a relativistic description of the electron propagator. For $v_F \lesssim 7v_0$, this correction of the
electronic energy loss is $\lesssim 0.2\% \ [180]$, hence only of interest for calculations based on the LPDA.
Another relativistic correction at large relative velocities between ion and target is known as the
Fermi density effect [222].

The screened interaction $U(q)$ of (1.9) can be written as

$$U(q) = U_0(q) + U_0(q)\Pi^*(q)U_0(q) + U_0(q)\Pi^*(q)U_0(q)\Pi^*(q)U_0(q) + \cdots$$

It contains all diagrams of the effective electron-electron interaction that can be build by coupling
diagrams of Fig. 1.1 and 2.1 by their ends, mixed orders included, but not those that are constructed
by insertion of sub-graphs into others.

Application of the Feynman rules to diagram b) produces a factor 2 after execution of the
sum over spins and then

$$\Pi^{(1)}_b(q) = (-2)(\frac{i}{\hbar})^2 \int \frac{d^4k d^4l}{(2\pi)^8} G^0(k)G^0(k-l)G^0(k+q-l)G^0(k+q)U_0(l).$$

Application of the Feynman rules to diagrams c) (upper sign) and d) (lower sign) gives

$$\Pi^{(1)}_{c,d} = (-2)(\frac{i}{\hbar})^2 \int \frac{d^4k d^4l}{(2\pi)^8} G^0(k)G^0(k-l)G^0(k)G^0(k \pm q)U_0(l).$$

The calculation of these multiple integrals is of purely mathematical nature and is possible
as presented in App. A.1 and A.2. The intermediate result while calculating the energy loss function
is the first-order polarization in App. A.3.

2.3 Results

2.3.1 The Modified Plasmon Dispersion

The plasmon dispersion of the improved polarization

$$\Pi^* \approx \Pi^{* (0)} + \Pi^{* (1)}$$

is calculated by extension of (1.19) and insertion into (1.23) [109, (3.16)]

$$f_1 \rightarrow f_1 - \text{Re} \Pi^{* (1)}/(4\frac{mk_F}{\hbar^2}).$$
Examples are shown in Fig. 2.2

As \( \Pi^{(1)} \) is of \( O(\chi^2) \), but the original \( f_1 \) of \( O(1) \), the modified plasmon curve approaches the RPA results in the limit of large Fermi velocities (large electron densities). The onset of plasmon excitation in the energy loss curve \( S(v) \propto L/v^2 \) on the velocity axis is not modified much compared with the RPA, because the two approximation of the plasmon dispersions intersect. The errors of the curves can be tracked down to uncertainties of the numerical calculation of the double integral of \( \text{Re}\Pi^{(1)}_b \). The numerics generally suffers under strong mutual cancellation of the individual contributions \( \text{Re}\Pi^{(1)}_{c+d} \) and \( \text{Re}\Pi^{(1)}_b \). The approximation

\[
\nu(q) \approx \nu_0 + \frac{3}{10\nu_0} \left( 1 - \frac{1}{4\nu_0^2} \right) q^2 + O(q^4)
\]

(2.2)

to the modified plasmon dispersions in [109 (3.19)] is verified by the numerical results. The curves in Fig. 2.2 that include the first order approach \( \nu_0 \) and reveal a more shallow, “softer” dispersion in the limit \( q \to 0 \), because the factor in front of \( q^2 \) in (2.2) is a bit smaller than the one of the RPA [1.24].
2.3.2 The Modified Electronic Energy Loss

First of all fig. 2.3 summarizes the result of the energy loss.

![Figure 2.3: Electronic energy loss for various Fermi velocities and projectile velocities; \( L \ldots \) stopping number. Thin: RPA as in Fig. 1.2. Bold: including the first-order polarization [157]. Numbers at curves denote \( v_F/v_0 \). The integration over the parameters \( u \) and \( a \) acc. to (1.21) was done by setting up a table of values with mesh widths \( \Delta a = \Delta u = 0.01 \) and linear interpolation therein.]

The energy loss by excitation of target electrons is increased in the region of linear dependence on the particle velocity, if the first-order polarization is added to the familiar results of the zeroth order. The Feynman expansion shows positive and negative values of \( \text{Im} \Pi^* \), which means regions with energy loss and gain. This artifact is hidden by the integration over \( u \) and \( a \) that calculates the stopping power. It is known that the patches with energy gain are eliminated by adding terms of even higher orders than presented here [8, 92, 109].

Above the onset of the plasmon excitation, the energy loss now is smaller than predicted by the RPA, which in essence can be attributed to the sign change of \( \text{Im} \Pi^{* (1)} \) for \( u > 1 \). This sign change quasi is enforced by fulfillment of the sum rule (A.11), and compensates the influence of diagrams c) and d) to some extent.

The influence of the additional polarization diagrams fits into the general interpretation of the relationship between the polarization life-time and the EL of Sect. 1.3.2 as follows: The
Feynman diagrams of type b) on one hand and of types c) and d) on the other hand gain different influence on the behavior of the polarization field by the different signs of the imaginary parts of the polarizations. Diagrams c) and d) prevent the electron-hole recombination during the time when the electron or hole carries momentum $\mathbf{k} - \mathbf{l}$ instead of $\mathbf{k}$. This reduces the flexibility of the polarization field, hence increases its life-time. The influence of diagram b) is opposite: the increase of the phase space by opening a new decay channel — the electron and hole may be annihilated with momenta that differ from those they had at the time of their creation — reduces the life-time of the excitation as implied by the golden rule.

This balance is correct as long as no plasmons are excited. (Otherwise the stopping power would be larger than the prediction by the RPA at all velocities.)

The net influence of the first-order diagrams on the correlation energy of the FEG is an increase (de-stabilization) through diagram b), as taught by \[82\] (30.83) and \[194\] (3.32). This statement, however, relates to the polarization which is integrated over frequencies and momenta. Therefore it does not fit into a comparison here, because the moving ion merely “tests” the polarization in the energy interval $\nu/q < \nu/\nu_F$ to the lower-right of the straight line in Fig. 1.4.

The noticeable increase of the stopping power by about 30% for realistic Fermi velocities in the low velocity range corresponds to the results of DFT calculations \[72\], \[73\], \[110\]. A direct comparison is not possible, because

- the DFT calculations inherently contain the non-linear susceptibilities. The differences caused by $Z^3_1$ effects could be estimated by inclusion of the calculations by Pitarke \textit{et al.} \[201\], \[202\], \[203\], \[239\]. Because these calculations internally use the RPA to model the linear susceptibility, a deconvolution of the linear and nonlinear susceptibilities is not straight forward.

- the polarization of a given order does not represent a certain order of the self energy and vice versa. Both physical quantities are related to each other like geometric series if converted. Therefore one order of the polarization or local field corrections yields a subset of terms of all orders of the respective other quantity \[75\], \[153\], \[179\], \[244\].
Chapter 3

Stripping Criteria: On the Velocity and the Energy Criterion

3.1 Overview

Sect. 3.2 offers a tutorial to the ansatz of the effective charge theory of ion stopping in homogeneous media. The effective charge theory by Brandt and Kitagawa (BK) and by Ziegler, Biersack and Littmark (ZBL) is presented. The aim is to stress that the ion charges they determined were deduced from experimental effective ion charges, hence depend on approximations and assumptions of this step of the calculation.

This overview finishes in Sect. 3.3 with the comment that — in contrast to the transformation of the ion charge into an effective charge — the fundamental ionization degree, the input to effective charge theory, has only been explained in a cursory way. This motivates the establishment and extension of the energy criterion, which had fallen into oblivion, in the subsequent main chapters.

Sect. 3.4 summarizes the velocity stripping criterion, which has been favored during the establishment of effective charge theory, and resumes a discussion of the forties that dealt with an energy criterion. Sect. 3.5.1 develops simple analytical predictions by the energy criterion and statistical ion models and analyses a bunch of comparing assessments given in the literature. Sect. 3.5.2 deals with wishful refinements by improved ion models and offers a explanation of the
ionization-excitation gap at low velocities in conclusion.

Whereas Sect. 3.5 focuses on the kinetic energies introduced a long time ago, Sect. 3.6 installs to another improvement under the umbrella of the energy criterion by inclusion of the interaction between the electrons bound to the ion and the target electrons — without equivalent by the velocity criterion. A simple substitution of potentials inside the ion by screened potentials is developed in a known form first, then recognized as insufficient, and finally restricted in a model to the outermost electrons of the ion. These terms are not needed to assess the quality of the energy criterion, if EL and ionization degree are treated on equal footing.

Sect. 3.7 establishes the recognition of non-zero Fermi velocities in the energy criterion very similar to the (improved) effective charge theory. Sect. 3.8 looks at the kinematic boundary conditions and means a new rating of the simplest kinetic energy term, which becomes necessary to explain the velocity dependence of the ionization degrees above approximately $\frac{1}{2}$ to satisfaction.

Part of the chapter has been published in [159].

3.2 Known Aspects of Effective Charge Theory

3.2.1 The Brandt-Kitagawa Model

The Lindhard-Winther description of the electronic energy loss assumes that the ion is a point charge that moves with constant velocity through a FEG [149, 150]. With the same target model Brandt et al., hereafter BK, generalized to ions with an extended charge cloud of bound electrons [36, 38, 140, 154, 224]; the LW theory is reproduced in the limit of completely stripped ions, when the charge number $Q = qZ_1$ becomes equal to the atomic number $Z_1$, the ionization degree $q = Q/Z_1$ equals one, and the number $N = Z_1 - Q$ of bound electrons equals zero.

The Ion Model and Its Internal Energy

The BK model assumes the following class of functions of the radial density distributions of the bound electrons

$$n_e = \frac{N}{4\pi \Lambda^2} \frac{e^{-r/\Lambda}}{r} ; \quad \int n_e d^3r = N,$$

(3.1)
where $\Lambda$ represents the size parameter (the screening length). The Fourier transform (the form factor) of the total ion charge in the rest frame of the ion then reads

$$
\rho_m(k) \equiv \rho_e(k) + \rho_n(k) = Z_1 e \frac{q + (k\Lambda)^2}{1 + (k\Lambda)^2} \quad ; \quad \rho_e(k) = -Ne \frac{1}{1 + (k\Lambda)^2}.
$$

The total internal energy of the bound electrons is subject to a simple density functional \[36\]

$$
E_{BK} \equiv E_{ee} + E_{ne} + E_{kin}
$$

$$
= \lambda \frac{1}{2} \int d^3r d^3r' \frac{\rho_e(r)\rho_e(r')}{4\pi\epsilon_0 |r - r'|} + \int d^3r \frac{\rho_e(r)Z_1 e}{4\pi\epsilon_0 r} + \frac{3}{10} m \int d^3r n(r) k_F^2(n)
$$

$$
= \lambda \frac{e^2}{4\pi\epsilon_0} \frac{N^2}{4\Lambda} - \frac{Z_1 N}{\Lambda} \frac{e^2}{4\pi\epsilon_0} + \frac{h^2}{m} \frac{N^{5/3}}{\Lambda^{2}}
$$

(3.3)

$$
\text{with } \phi \equiv \frac{1}{2} \left( \frac{3}{4\pi} \right)^{2/3} \left( \frac{3}{5} \right)^{7/3} \Gamma \left( \frac{4}{3} \right) \approx 0.24005.
$$

(3.4)

$E_{BK}$ comprises the electron-electron-interaction $E_{ee}$, the interaction energy $E_{ne}$ between the electrons and the nucleus, and a LSDA of the kinetic energy of the electrons (in the ion rest frame), $E_{kin}$. The Hartree approximation to the electron-electron interaction has already been multiplied with a coupling parameter $\lambda$, which will be fitted, and is tasked with the correction of the missing exchange and correlation terms \[36\] — in contrast to the TF ion model. The size parameter is fixed via minimization of this energy

$$
\frac{\partial E_{BK}(Z_1, N, \Lambda, \lambda)}{\partial \Lambda} = 0
$$

$$
\Rightarrow \quad \Lambda = \frac{2\phi (1 - q)^{2/3}}{Z_1^{1/3} \left[ 1 - \frac{\lambda}{4} (1 - q) \right]} a_0.
$$

(3.7)

(3.8)

The same result could also be derived by enforcement of the virial theorem as demonstrated in a generalized context in Sect. 3.6.2. The electron-electron coupling constant $\lambda$ is fixed by demanding that the chemical potential of the neutral atom be zero,

$$
\left. \frac{\partial E_{BK}(Z_1, N, \Lambda, \lambda)}{\partial N} \right|_{N = Z_1} = 0 \quad \Rightarrow \quad \lambda \equiv 4/7.
$$

(3.9)

$\Lambda$ and $\lambda$ inserted in $E_{BK}$ yield the internal energy of the BK ion model \[36\]

$$
\frac{E_{BK}}{E_0} = -\frac{Z_1^{7/3}}{2\phi} (1 - q)^{1/3} \left[ 1 - \frac{\lambda}{4} (1 - q) \right]^2 < 0,
$$

(3.10)
given here in units of $E_0 \equiv \frac{1}{2}mv_0^2 = 1$ Rydberg. It may be expanded in a Taylor series around the state with $N$ electrons

$$E_{BK|N-1} \approx E_{BK|N} - \frac{dE_{BK}}{dN} \big|_N + \frac{1}{2} \frac{d^2E_{BK}}{dN^2} - \frac{1}{6} \frac{d^3E_{BK}}{dN^3},$$

(3.11)

$$\frac{d(E_{BK}/E_0)}{dN} = -\frac{Z_1^{1/3}}{6\phi(1-q)^{2/3}} \left[ 1 - \frac{7}{4} \lambda (1 - q) \right] \left[ 1 - \frac{\lambda}{4} (1 - q) \right] < 0,$$

(3.12)

$$\frac{d^2(E_{BK}/E_0)}{dN^2} = \frac{Z_1^{1/3}}{18\phi(1-q)^{5/3}} \left[ 2 + 2\lambda (1 - q) - \frac{7}{4} \lambda^2 (1 - q)^2 \right] > 0,$$

which provides the first ionization energy to lowest order

$$I_1 \equiv E_{BK|Z_1-1} - E_{BK|Z_1} \approx \frac{E_0}{2} \frac{d^2(E_{BK}/E_0)}{dN^2} \big|_{Z_1} = \frac{Z_1^{1/3}}{36\phi} \left[ 2 + 2\lambda - \frac{7}{4} \lambda^2 \right] E_0$$

(3.13)

as a special case. These are realistic orders of magnitude, but the shell structure, i.e., the variation along a column in the PSE, is missing.

The advantage of the BK ion model compared with the TF model [198, 235](→ App. D) are some closed formulas for the radial charge distribution, the internal energy etc.

**Effective Charges**

For bare ions with $\rho_m(k) = Z_1 e$ the stopping power scales like $dE/dx \propto Z_1^2$ in arbitrary targets according to (1.6), if $\epsilon$ itself does not depend on $Z_1$, i.e., if we restrict to the linear susceptibility of the target [203, 239, 260]. Partially stripped ions are characterized by $Q_e < \rho_m(k) < Z_1 e$, where $Q_e = \int \rho_m(r)d^3r$ denotes the total ion charge. A deviation from the $Z_1^2$ scaling results, and assumes concrete forms by definition of the effective charge $\gamma Z_1$ and the effective charge fraction $\gamma$:

$$S(Z_1, v, q) \equiv (\gamma Z_1)^2 S(Z_1 = 1, v, q = 1).$$

(3.14)

The energy loss is proportional to the cross section $S$ of the single target atom and to the atomic density $\rho_{at}$ of the target,

$$|dE/dx| = S \rho_{at}.$$

(3.15)

The cross section $S$ is a suitable description in the case of independent target atoms, and is not used, of course, in the theory of the FEG, where $\rho_{at}$ is not defined.
The calculations of heavy ion energy losses within the present theory did not use (3.14) as a definition, but on the contrary interpreted it as the “heavy ion scaling rule” \[36, 261, 262\]. They first theoretically estimated the dependence $\gamma(q, Z_2, v)$ with a FEG target model. Then $\gamma$ was inserted with experimental proton data $S(Z_1 = 1, v, q = 1)$ on the right hand side of the scaling rule to compute the stopping of the heavy ions. This scaling step is essential to gather the full information on the target excitation that is missing in the estimation of $\gamma$. The experimental proton energy loss data deliver the contributions of the inner electron shells of target atoms. The theme of Chaps. 4 and 5 is how these can also be calculated. Fig. 3.1 just demonstrates which wealth of experimental data is incorporated into the calculations with this procedure.

The effective charge theory determines the EL in two inherent steps. First a description of the ion, in essence the charge distribution of the bound electrons, is put up. For all ion models the major free parameter is the ionization degree $q$ as a function of the ion velocity. Second, the energy loss function and its integral, the stopping number, are calculated via a model of the dielectric function. The third step within the BK theory and the ZBL realization, which is shortly discussed later on in Sect. 3.2.2 is to extract effective charges in a FEG target, to forget the theoretical proton and heavy ion stopping data of the FEG, and to insert the experimental proton data into the heavy ion scaling rule. However, this step is not inherent, because it ought to become superfluous when the model of the energy loss function is improved (Chapt. 5).

An upper bound of the EL is obtained in this framework by the approximation $\rho_m(k) \approx Z_1 e$ of a naked ion nucleus inserted into the generalization of (1.7)

$$L \equiv -\frac{1}{\pi \omega_0^2} \int_0^\infty \frac{dk}{k} \left| \frac{\rho_m(k)}{Z_1 e} \right|^2 \int_{-k\nu}^{k\nu} \omega d\omega \text{Im} \left[ \frac{1}{\epsilon(k, \omega)} - 1 \right].$$

(3.16)

A lower bound emerges by the approximation of the ion by a point charge $Q_e$, $\rho_m(k) \approx qZ_1 e$. The name giving “effective charge fraction” for $\gamma$ points to this connection with the ionization degree $q \approx \gamma$. Because $\rho_e(r)$ does now switch signs, the Fourier transform yields $Q_e \leq \rho_m(k) \leq Z_1 e$, and because the energy loss function also has one unique sign, $q \leq \gamma \leq 1$ for all ion models in this linear theory.

An analytical approximation of the Lindhard number yields for the BK ion charge distribu-
\[ \gamma = q + C(k_F)(1 - q) \ln \left[ 1 + (2k_F\Lambda)^2 \right] \]

with \( C(k_F) \equiv \frac{\pi k_F}{1 + \pi k_F} I(\pi k_F) - \frac{2}{\pi k_F} \) and \( I(z) \equiv \ln(1 + z) - \frac{z}{1 + z} \).

The error caused by this approximation relative to

\[ \gamma = \sqrt{\frac{dE}{dx}(q, Z_1)} \sqrt{L(q, Z_1)} \]

of a full numerical integration is displayed in Fig. 3.2.
Figure 3.2: Effective ionization degrees $\gamma$ of frozen charge states derived from the approximate formula at small $v$ (3.17) (horizontal) versus values of numerically integrated Lindhard numbers (3.16) and (3.18) (ascending lines). $v_F = v_0$ has been chosen; consequently plasmon excitation (in RPA) contributes to the stopping above $v/v_F \geq 1.36$. The estimates $\gamma^2 = \frac{1}{2} + \frac{1}{2}q^2$, which have been given for large $v$ [36], lie above the upper frames of the graphs.

The approximation (3.17) works well below the plasmon excitation, but under-estimates the exact results the higher the velocity and the smaller the ionization degree are. Among others it also implies $\partial \gamma(v_F, q, \Lambda) / \partial v_F > 0$. (This is either found numerically, or seen by inspection of [36, Fig 4].) This means that the effective ionization degree grows with the target electron density if the ion parameters are fixed, which may be understood by illustration: target electrons with large impact parameter see only the total charge $Qe$, those with small impact parameter more the charge of the nucleus $Z_1 e$. The effective charge is an average and in between. The integral of the stopping number puts this into numbers in momentum space: the ion form factor $\rho_m(k)/(Z_1 e)$ is about $q$ for small momentum transfers $k$ (soft, distant collisions) and about 1 for large momentum transfers (hart, close collisions). In the integral (3.16)

$$L = -\frac{6}{\pi^2} \int_0^\infty dz \, z \, \left( q + (2z k_F \Lambda)^2 \right) \, \left( 1 + (2z k_F \Lambda)^2 \right)^2 \, \int_0^{v/v_F} u \, \text{Im} \frac{1}{\epsilon(z, u)} \, du$$

27
\( \rho_m(z) \) is a weight function. If \( k_F \) grows, the transition from the weighting with small \( k \) to the weighting with large \( k \) moves towards smaller \( z \), i.e., close collisions become relatively more important. Because the \( u \)-integral does only shift little as a function of \( z \), \( \gamma \) increases. In physical terms: the product \( k \Lambda \) in the ion form factor compares the ion size \( \Lambda \) with the average distance between target electrons \( r_s \sim 1/k_F \). If the target electrons are packed denser, more come closer to the ion nucleus, and \( \gamma \) grows.

3.2.2 The Realization by Ziegler, Biersack and Littmark

A further fit of the BK theory to a large set of experimental data was done by Ziegler, Biersack and Littmark (ZBL) \[261, 262\]. The actual result is reported in App. \[C.2\]. Only a few differences to the BK theory are indicated here.

**Effective Ion Velocity**

The concept of an effective ion velocity with an inclusion of the target Fermi velocity \( v_F \) was adopted from the work by Kreussler et al. \[140\]. It became clear that the parameterization of the EL may be unified better, if \( v \) and the scaled variable \( y \equiv v/(v_0Z_1^{2/3}) \) are replaced by the scaled effective variables \( \tilde{v}_r \) and \( y_r \equiv v_r/(v_0Z_1^{2/3}) \) with

\[
\tilde{v}_r \equiv \begin{cases} 
 v \left(1 + \frac{1}{5(v/v_F)^2}\right) & ; 
 (v \geq v_F) \\
 \frac{3}{4}v_F \left(1 + \frac{2}{5} \left(\frac{v}{v_F}\right)^2 - \frac{1}{15} \left(\frac{v}{v_F}\right)^4\right) & ; 
 (v \leq v_F) 
\end{cases}
\]

(3.19)

\[
\leftrightarrow v = \begin{cases} 
 v_F \sqrt{5 - 2 \sqrt{10 - 5 \frac{v_r}{v_F}}} & ; 
 (\tilde{v}_r \leq \frac{6}{5}v_F) \\
 \frac{v_r}{2} + \sqrt{\frac{v_r^2}{4} - \frac{v_F^2}{v}} & ; 
 (\tilde{v}_r \geq \frac{6}{5}v_F) 
\end{cases}
\]

(3.20)

The formulas had been derived within the velocity criterion of the ionization degree (Sect. 3.4). \( \tilde{v}_r \) is an average relative velocity between the ion and the target electrons, which are found in the target rest frame at velocities between 0 and \( v_F \). The equations (3.19)-(3.20) represent the actual
values \( y_r \) that determine the ionization \( q(y_r) \) only roughly. Additional limits (lines 32–34 in App. C.1) modified the effective velocity that was used \textit{de facto} to read
\[
v_r \equiv \max\{v_0, \bar{v}_r, 0.13v_0Z_1^{2/3}\}, \quad (3.21)
\]
the horizontal lines in Fig. 3.3.

---

**Figure 3.3:** The effective velocities \( v_r \) in units of \( v_F \) as a function of the ion velocity \( v \) by ZBL. The dotted lines are the original theory, \((3.19)\). The target elements form groups acc. to \( v_F \).

---

**Ion Size and Ionization Degree**

The universal ion size \( \Lambda \) of Eq. \((3.8)\) is modified essentially. \( \tilde{\Lambda} \) gets a correction factor that is tabulated as a function of \( Z_1 \) and models that the ion is composed of atomic shells which causes the associated \( Z_1 \) oscillations of the electronic energy loss. The completion of [261, Fig. (3-24)] yields the stepped curves of Fig. 3.4 shown together with the value of the BK energy that is modified implicitly. The plateaus, however, are not compatible with the remark of [261, p. 103] that the “bump” reflects the enlargement of the K shell, because they move to the left (not to the right) with increasing \( Z_1 \).

A fit formula for the ionization degree as a function of the effective velocity [261] was developed,
\[
q = 1 - \exp \left[ 0.803y_r^{0.3} - 1.3167y_r^{0.6} - 0.38157y_r - 0.00893y_r^2 \right]. \quad (3.22)
\]
Figure 3.4: Bold lines: the BK electron energy $E_{\text{BK}}(\Lambda, q, Z_1)$ in units of $E_0 Z_1^{7/3}$ acc. to (3.5), and the BK size parameter $\Lambda$ in units of $a_0/ Z_1^{1/3}$ acc. to (3.5) and (3.8). Others: the corresponding values using $\bar{\Lambda}$ (l of line 52 in App. C.1), but again (3.5). The values are independent of $Z_2$ for practical purposes. The non-scaled value of $\Lambda$ is in general smaller for larger $Z_1$.

It comes close to the values that were tabulated by BK and developed in [260], as Fig. 3.5 demonstrates. Differences for $y_r \lesssim 0.2$ are not important, since the comparison with experimental data by Brandt and Kitagawa did not cover this range [224]. $Z_1$ shell effects of the ionization degree like those reported in [227] for the average ionization degree after passage through carbon foils or in [107] for the ionization degree after scattering off surfaces, are unfamiliar to this universal formula. Because they are not very pronounced, one may assume (if one reduces the problem to a correct description of the EL) that ZBL stored this dependence in the ion size. The combined action of ionization degree and ion size that construct an effective charge fraction is the only relevant result. Prospective hindrances to relate the ionization degrees that were measured outside the solid (and plotted in Fig. 3.5 for comparison) to the conditions inside the solid will not be discussed here [96].
Effective Ionization Degree

(3.17) was reformulated as

$$\gamma = q + \frac{1}{2(v_F/v_0)^2} (1 - q) \ln \left[ 1 + (4\alpha\tilde{\Lambda}_k)^2 \right].$$

(3.23)

After multiplication by a factor to incorporate $Z_1^3$ effects, this formula was used for all velocities with the exception of the very small $\rightarrow$ lines 55–64 in App. C.1 which yield the values shown here instead of (3.23). This effective ionization degree is smaller for larger $v_F$, if the ion parameters $q$ and $\Lambda$ are kept fixed. This artifact shows up simply either after a change of Fermi velocities in the data file, or by the expansion $\ln(1 + x) \approx x - \frac{1}{2} x^2$ of the logarithm that creates a negative coefficient in front of the $O(v_F^2)$. This negative slope of $\gamma(v_F)$ hence contradicts the BK formula (3.17) and the remarks at the end of Sect. 3.2.1. It is small, however, and is hidden by the dominant $Z_2$ dependence of the proton cross sections and of the $q$ values when heavy ions are calculated. This indicates that (3.23) should not be regarded as an isolated formula.

The construction of effective ionization degrees from ionization degrees and ion sizes is summarized in Fig. 3.6. It is remarkable that the $Z_1$ oscillations are clearly assumed to be weaker than what results from DFT calculations in the jellium model and has been documented for stopping
data of channelled ions (→[19, 40, 46, 54, 73], App. 1 and 30 for the nuclear energy loss). This difference to the conditions inside the homogeneous electron gas may indicate that the filling of open shells of the ion by $Q$ target electrons in scattering states — the physical mechanism creating $Z_1$ oscillations — is disturbed by the neighborhood of target atoms in the case of large ions of arbitrary flight direction in solids.

Figure 3.6: Examples of the $Z_1$ dependence of ZBL variables: ion size $\tilde{\Lambda}$, ion charge $Q = qZ_1$ and effective charge $\gamma Z_1$. The velocities correspond to 4 keV/u, 25 keV/u, 100 keV/u and 400 keV/u.
The strong variations of stopping powers as a function of $Z_2$ seen in Fig. 3.1 is nearly eliminated looking at $\gamma$. They are strongly correlated with the shell structure of the target atoms. Though the theory is completely build on the energy loss in the FEG, no further $Z_2$ dependence (up to a weak $v_F$ dependence in (3.17)) remains thanks to the scaling with $^1$H and $^2$He data. Setting Fig. 3.7 against 3.8 aims at illustrating this.

Figure 3.7: Examples of the $Z_2$ dependence of the squared effective charge fractions $\gamma^2$ acc. to ZBL (lines 64 and 67 of App. C). Differences to (3.23) arise from the inclusion of $Z_3^1$ effects (lines 54–55) and at low energies (lines 57–64).

Figure 3.8: Fermi velocities in units of the Bohr velocity taken from the ZBL data file (→ 263 Fig. 3).
3.2.3 How Reliable are the Known Ionization Degrees?

Effective charge fractions are data accessible by experiment. Ionization degrees that are deduced from them depend on model assumptions, the ion model, the dielectric function, but also on approximations made in calculations, which is emphasized next. Fig. 3.2 shows that the approximation of low velocities under-estimates $\gamma$ systematically. Frozen charge states are shown there, which complicates the estimate of the corresponding error, because $q$ actually grows with $v$. This is detailed below by showing which function $q(y_r)$ results, if (i) the experimental $\gamma(v)$ of ZBL results are accepted, but (ii) the full-numerical stoppig numbers and the BK ion model (replacing (3.23)) are inserted in (3.18). Fig. 3.9 shows the results of this new deduction of $q$ that exactly stays within the model.

Figure 3.9: Ionization degrees $q$ by (3.22) for all ion-target combinations (Bold Line), and by (3.18) for 12 individual ion-target combinations (thin lines) with mutually equal effective charges. The vertical lines appear because (3.21) maps various $v$ onto the same $y_r$, whereas the $q(v)$ that are fitted to $\gamma$ continue to change.

The general under-estimation of the effectivity of the stoppig power of BK ions by the low-velocity formula obviously is compensated by ZBL through (i) increase of $q$ with the help of the fit formula (3.22) and (ii) a general enlargement of the ion (Fig. 3.4). Because (3.22) is valid at low velocities, however, the increase of $\Lambda$ is enticed through a decrease of $q$. The summary is: If we return to the basics, the BK ion model and the FEG target, consistent ionization degrees of
medium and heavy ions need to be set below the ZBL values.

A re-determination of the ionization degree on the basis of the BK model including the exchange energy of App. B.1 just needs the substitution \( \Lambda \rightarrow \Lambda_x \) in (3.2). Because these ions of different size stop somewhat weaker, the deduced values of \( q \) are higher. These deviations are so small that no separate illustration is given here.

Effective charge theory also permits — with more expense — the inclusion of more precise ion models of RHF calculations in \( \rho_m \). On the basis of Clementi-Roetti wavefunctions [50] for example, the radial electron densities and the energy losses of frozen charge states of Fig. 3.10 follow. The axes have been chosen to enable comparisons with HF calculations for solids in [26].

The calculation first averages the radial wavefunctions over all directions of \( \hat{r} \), and sub-shells with nonzero angular momentum quantum number are also represented by spherically symmetric charge distributions. The Fourier transform of these charge distributions \( \rho_e(\mathbf{r}) \) has to be calculated to obtain the form factor \( \rho_m(k) \) in (3.16). One does not need a numerical Fourier transform, because the radial charge distribution, the sum of the squares of the wavefunctions, may also be written as a sum of STO’s,

\[
n_e(r) = \sum_{sh=1s,2s,2p,...} N_{sh} \left( C_{i\lambda_p} N_{\lambda_p} r^{n_{\lambda_p}-1} e^{-\zeta_{\lambda_p} r} + \ldots \right) \frac{1}{4\pi} 2^{n_{\lambda_p}-1} \pi^{\frac{n_{\lambda_p}}{2}} \\
= \frac{1}{4\pi} \sum_{sh=1s,2s,2p,...} N_{sh} \sum_{(\lambda_1p_1)(\lambda_2p_2)} C_{i\lambda_1p_1} C_{i\lambda_2p_2} N_{\lambda_1p_1} N_{\lambda_2p_2} r^{n_{\lambda_1p_1}+n_{\lambda_2p_2}-2} e^{-(\zeta_{\lambda_1p_1}+\zeta_{\lambda_2p_2})r},
\]

if we define a new “principal quantum number” \( n \equiv n_{\lambda_1p_1} + n_{\lambda_2p_2} - 1 \), the new exponents \( \zeta \equiv \zeta_{\lambda_1p_1} + \zeta_{\lambda_2p_2} \) and the new expansion coefficients \( C \equiv C_{i\lambda_1p_1} C_{i\lambda_2p_2} \). The Fourier transform of this class of functions is known [26]:

\[
\int e^{ikr} r^{n-1} e^{-\zeta r} Y_l^m(\hat{r}) d^3r = 2^{n+2}\pi(n-l)! (ik)^l \zeta^{n-l} Y_l^m(\hat{k}) \sum_{j=0}^{[n-l]} \frac{\omega_{jl}^n}{(k^2 + \zeta^2)^{n+1-j}}, \quad (3.24)
\]

with \( \omega_{jl}^n \equiv (-1/[4\zeta^2])^j(n-j)!/[j!(n-l-2j)!] \). Fig. 3.10 reveals that the low-charged ions of the CR tables are stopped massively stronger than the ions of the BK model, which is caused by the rather large radii of the outside electrons. Following the standard interpretation of effective charge theory this lets fly target electrons in this range of impact parameters through less screened
Figure 3.10: CR radial electron densities with scaling \( 4\pi r^2 n_e \) and electronic energy losses compared with the BK ion model in the FEG, with the RPA of the dielectric function and at \( v_F = v_0 \). (3.16) has been integrated numerically. The curves are labeled with the number of bound electrons \( N \). The upper 4 figures represent \( ^{27}\text{Co} \), the lower 3 \( ^{15}\text{P} \). For comparison, the two shallow parabolas in the graphs of the density show the spatially homogeneous density \( n \) with (1.8) connecting to \( v_F \).
nuclear potentials and enhances the stopping. Looking at one isolated of these ions does not suggest shell effects. Neither are the $dE/dx$ of the frozen charge states bundled as closed shells of bound electrons, nor does $\rho_m(k)$ reveal more structure than the BK ion model. This is easily understood, as $v_F = v_0$, i.e., a one-electron radius of 1.0 Å has been chosen for the curves as shown, which is too large to enable target electrons to resolve the internal structure of the ions. (Probably thanks to this circumstance, the BK ion model is applicable in the EL theory despite of its infinite charge density at the nucleus site (→ App. B.2).)

Even if the wave-functions of free ions at large radii become unsuitable at the latest when the electron density approaches the target electron density, the increase of the stopping power relative to the BK model supports the conclusion that the ZBL ionization degrees have to be lowered on the basis of what has been said up to here. A straightforward re-compilation of ionization degrees similar to Fig. 3.9 of BK ions is no longer simple for CR ions that are only defined over a set of discrete $Q$-values. Especially because an important correction of the basic equation is presented under the headline “dead sphere” in Sect. 5.4.1, it does not make much sense to present these results for heavy ions here.

By the way, the introduction of heavy ion charge densities with atomic structure permits a closer look at prospective $Z_1$ oscillations with a plot that is “orthogonal” to the one in Fig. 3.10 and uses $Z_1$ instead of $v$ as the principal parameter. These calculations are summarized in Fig. 3.11 for CR ions again and show a weak replica of the period $^3\text{Li}…^\text{Ne}$, no replica of the period $^\text{11}\text{Na}…^\text{18}\text{Ar}$ and somewhat stronger a grouping of the 3d elements $^\text{21}\text{Sc}…^\text{30}\text{Zn}$. Note that they are part of the linear susceptibility of the FEG in the RPA and are created when the ion imprints its shell structure on the target electrons in form of a polarization and interacts with this polarization in a retarded or spatially shifted manner. This is a manifest refutation of the impression that nonlinear susceptibilities or, from the point of view of scattering of target electrons off the ion potential, the higher Born orders are an inevitable prerequisite to $Z_1$ oscillations of the effective charge.

Two features of $Z_1$ oscillations are reproduced: First, the periods of the PSE are more pronounced if the Fermi velocities are smaller, and second, they vanish for velocities above the
threshold of plasmon excitation.

Counterintuitive to physical insight, Fig. 3.11 shows smaller effective charges at some points and hence less stopping for simple positive ions than for the neutral atoms. The reason is the somewhat arbitrary selections of electronic configurations from the CR tables, and the remaining degrees of freedom in the model become apparent. The stopping of the 4s\(^0\)3d\(^4\) (\(^5\)D) configuration of \(^{23}\)V\(^{1+}\), for example, is smaller than the value of the 4s\(^2\)3d\(^3\) (\(^4\)F) configuration of \(^{23}\)V\(^0\). The stopping force of the alternative 4s\(^1\)3d\(^3\) (\(^5\)F) configuration of \(^{23}\)V\(^{1+}\) is within the line thickness equal to the force acting on the neutral atom.

### 3.3 The Open Question of a General Computation of the Ionization Degree

Effective charge theory aims at bypassing the *ab-initio*, self-consistent computation of all electrons starting with the ion nucleus as external potential, and borrow results of the atomic theory to describe the ion with \(N\) electrons bound to it. The philosophy — especially for heavy ions — is simply that the electron distribution close to the ion is primarily determined by the nuclear charge...
of the ion and only secondarily by the electron distribution of the target background. Caused by this kind of cross-entry instead of an *ab-initio* theory the ionization degree becomes an open parameter that has to be regulated in addition.

In the early history of the energy loss theory up to the later development of effective charge theory, mainly two classes of criteria have been discussed to calculate and explain the ionization degree in its central role among the ion parameters. The velocity criterion lets ions shed off its electrons that are too slow, the energy criterion those with too small binding energy. Up to the publication by Yarlagadda *et al.* [260], both had been discussed as of equal rank, but later the energy criterion was no longer mentioned [36], or both had been replaced by the formula that is to be considered merely as a fit (3.22).

The subsequent chapters are an outspoken plead for the more clear and more general energy criterion which also offers better prospects. Despite its eminent importance as an initial parameter of heavy ion stopping the ionization degree must be declared the least developed area within effective charge theory. The review argues that the energy criterion has to be accepted at least as an equal-ranked starting point to explain ionization degrees in the future. One may foresee that the calculation of explicit stripping criteria by parameterization of the energy will generally become superfluous once the time-dependent HF method or the time-dependent DFT will be applied, as they already are in the region $v \approx 0$ (→ App. I).

### 3.4 The Velocity Criterion

The oldest general stripping criterion is the Bohr criterion of orbital velocities: the share of electrons with orbital velocity $v_e$ below the ion velocity will be considered stripped [32]. Two realizations on the basis of the TF ion model [260] have been quoted in the literature in connection with effective charge theory:

1. The TF equation is solved for an ion with radius $r_c$ (App. I). Assuming that the most outside electron with orbital radius $r_c$ has a velocity $v_e$ reflecting its potential energy, $\frac{1}{2}mv_e^2 =
$qZ_1e^2/(4\pi\epsilon_0rc)$, the velocity criterion has been given the explicit form \[260\] (4.2)]

\[
v_e = v \quad \Rightarrow \quad y^2 = \frac{2^{10/3}}{(3\pi)^{2/3}} \frac{q}{x_c(q)}.
\]

(3.25)

This procedure establishes one of the ionization degrees of Fig. 3.12.

**Figure 3.12:** Ionization degrees $q$ as a function of effective velocity $y$ by the velocity criterion and the TF ion model acc. to (3.25) (thin line), by the equivalent calculation with the BK model acc. to (3.29) for $\tilde{b} = 1$ or 0.77 (dashed), and according to the ZBL formula (3.22) (bold).

2. The alternative implementation used by BK \[36\] is reproduced as follows \[37\] \[38\] \[140\] \[154\] \[173\] \[200\] \[260\]: the electrons of a neutral TF atom are stripped off if they are outside a stripping radius $r_s$. If $n_e(r)$ and $\tilde{\varphi}(x)$ denote the solution of the TF equations of the neutral atom, the ion charge becomes

\[
Q = \int_{r<r_s} n_e(r) \: d^3r = \frac{1}{8\pi a_0} \int_{r<r_s} \Delta \left( \frac{e(\varphi - \mu)}{E_0} \right) \: d^3r = -\left( \frac{r_s}{a_0} \right)^2 \left| \text{grad}_{\varphi_0} \frac{e(\varphi - \mu)}{2E_0} \right|
\]

\[
= -Z_1x_s \frac{d\tilde{\varphi}}{dx}|_{x_s} + Z_1\tilde{\varphi}(x_s) \quad \Rightarrow \quad q = \tilde{\varphi} - x \frac{d\tilde{\varphi}}{dx}.
\]

(3.26)

by applying the Gauss law of integrals. The velocity criterion was formulated with an additional *ad hoc* stripping parameter $b$

\[
v = bv_e(r_s).
\]

(3.27)
The orbital velocity was associated with the electron density via the standard formula of the LSDA, \( v_e(r)/v_0 = \sqrt[3]{3\pi^2 n_e(r)a_0} \), which lets (3.27) become

\[
y \equiv \frac{v}{v_0 Z_1^{2/3}} = b\sqrt{\frac{32}{3\pi}} \sqrt{\frac{\varphi}{x}}.
\]

(3.28)

Altogether with (3.26) this is the implicit representation of the BK ionization degree, which has already been inserted in Fig. 3.5 using \( b = 1.33 \) that has been considered as the best fitting choice.

We may replace the TF atom model in this calculation by the BK model (3.1) and (3.8). Let us insert the analog charge distribution for \( q = 0 \) into (3.8) and determine via \( N = (Z_1/\Lambda^2) \int_0^{r_s} \exp(-r/\Lambda)/rdr \) a new ionization degree \( q = \exp(-r_s/\Lambda)(1 + r_s/\Lambda) \) by removal of the electrons outside of the radius \( r_s \). If \( v \overset{!}{=} \tilde{b} v_e(r_s) \) is again the ansatz of the velocity criterion with the LSDA for the orbital velocity, the parameter representation

\[
y = \tilde{b}^{1 - \frac{\lambda}{2\phi}} \sqrt{\frac{3\pi}{4}} \frac{e^{-z}}{z} \quad \text{und} \quad q = e^{-z}(1 + z)
\]

(3.29)

follows directly, with \( z \equiv r_c/\Lambda \) a parameter. For \( \tilde{b} = 1 \) or 0.775 the result is contained in Fig. 3.12. This calculation does not appear in the literature, which may be attributed to a basic conceptional shortcoming of this ansatz. If we let relax the ions, which have been created here under item 2 by a sharp clip of atomic charge clouds, into “self-consistent” charge densities, new exponential fringes of the density distribution are created that would have to be clipped again according to the velocity criterion. An uncompromising recursive application of this principle would always result in nonsensical, completely bare ions.

The fitting factor \( b \) become necessary within the Brandt theory to obtain realistic ion charges by the velocity criterion, but due to its 30-percent correction of \( v \) it discloses the criterion to be heuristics. A very simple interpretation is offered by computing an average over the electrons that circle the ion with individual velocities \( v_e \), relative to the target electrons. [The idea is the straight analogue to replacing \( v \) by \( v_r \) as in Sect. 3.2.2 based on the velocity distribution of target electrons.]

In contrast, the statistics here scans only the isotropic probability distribution of the directions of the velocity \( \mathbf{v}_e = (v_e \cos \varphi \sin \theta, v_e \sin \varphi \sin \theta, v_e \cos \theta) \) of the electrons which are candidates of being
stripped, not in addition the absolute values. The average over the velocity distribution of the electron that may be stripped then is relative to the target \[261\] (3-19)]

\[
\bar{v}_l \equiv \left\langle \begin{pmatrix} v_e \cos\varphi \sin\theta \\ v_e \sin\varphi \sin\theta \\ v_e \cos\theta + v \end{pmatrix} \right\rangle = \frac{1}{4\pi} \int_0^\pi d\cos\theta \int_0^{2\pi} d\varphi \left\langle \begin{pmatrix} v_e \cos\varphi \sin\theta \\ v_e \sin\varphi \sin\theta \\ v_e \cos\theta + v \end{pmatrix} \right\rangle = \frac{(v_e + v)^3 - |v_e - v|^3}{6v_e v},
\]

\[\text{ergo } 1.33v \text{ for } v_e = v.\] The average velocity of the bound electron increases, which hinders it from being stripped within the philosophy of the velocity criterion, increases the required ion velocity, and is expressed as \(b > 1\).

A puzzle nevertheless remains: these two reasons to increase the relative velocity of electrons, (i) a nonzero velocity of target electrons relative to the lattice, and (ii) a statistical distribution of velocity directions of the marginally bound electrons are interpreted by the criterion in opposing ways, once weakening and once stabilizing the binding.

This contradiction is elucidated, if we look at the velocities \(v_e\) — the virial theorem \[76, 137, 143, \S 10, 168, 198, 214\] providing the bridge — as mere representatives of energies that carry additional signs. The orbital velocities represent the energy eigenvalues in a quantized ion model and the density of states in a statistical ion model, i.e., the binding energy. In the approximation of a \(1/r\) potential for an electron the binding energy and the kinetic energy have equal absolute value and different sign. The velocity criterion is converted into an energy criterion in this approximation, which simply states: electrons are stripped if the sum of their binding energy with the ion and the additional kinetic energy measured in the target system is larger than zero. In the case of more general potentials the equivalence is not exact, because the kinetic energy of an electron in a screened potential is

\[
\langle T \rangle = \frac{1}{2} \langle r \frac{\partial \varphi}{\partial r} \rangle.
\]

Then \(\langle T \rangle = -\langle \varphi \rangle/2\) only holds with respect to the total electron energy (because the electron-electron interaction and the electron-nucleus interaction are of the \(1/r\) type \[137\]).

Therefore the remark on p. 11 of \[261\], “A definitive clarification was made by Northcliffe, who reduced a wide variety of experimental data by dividing . . . at the same velocity” is wrong, because in \[188\] only light ions \(\text{\textit{5B . . . 10Ne}}\) are investigated at energies where only K-shell electrons
stay bound (→ Fig. 3.16), 5B at $\xi > 1.27$, $y_r > 2.17$, 6C at $\xi > 1.06$, $y_r > 1.93$ etc., where $\xi$ denotes the ion velocity divided by the orbital velocity of the first K electron. Because the nuclear potential is not screened for K electrons for practical purposes, both criteria are identical in this limit as mediated by the virial theorem. Eq. (1-7) that immediately follows in [261] (and probably aims to stress the issue) and (3-15) likewise are quoted from [188] in a falsifying manner, because the velocity of the first K electron in the hydrogen problem $v_0 Z_1$ is not $\propto Z_1^{2/3}$ like in “statistical” ion models. Consequently, the work by Sols and Flores [233], which treats ions with $N = 0 \ldots 1$, uses the variable $v/(Z_1 v_0)$ for scaling, and [242] the “adiabaticity parameter”, the ratio of $\frac{1}{2}mv^2$ over the binding energy of the K shell.

### 3.5 Fundamentals of the Energy Criterion: Kinetic Energies

The basic energy criterion has already been proposed a long time ago by Lamb [142] on the basis of the TF ion model and states: The ion becomes unstable with respect to dropping another electron, when the total energy of binding energy and kinetic energy relative to the target system

$$E \equiv E_i + E_{cm}, \quad E_{cm} \equiv \frac{1}{2}mv^2 N$$

may be lowered. Therefore the number $N$ of bound electrons is realized, where the reduction of the kinetic energy by $\frac{1}{2}mv^2$ (via release of another electron) is insufficient to deliver the corresponding increase of the (negative) internal energy, and where at the same time the capture of another electron with additional kinetic energy $\frac{1}{2}mv^2$ would not be accompanied by an even greater reduction of the internal energy. This energy balance and stability argument is equivalent with a minimization of the total energy $E$ as a function of $N$. The principle of energy minimization for stationary processes is more fundamental and general than the previously discussed velocity criterion.

The energy criterion could be judged more thoroughly if the ZBL calculations would not just tabulate ionization degrees but also make consistent statements about the internal energy in the spirit of a complete ion model. The aim of Fig. 3.4 is to show that one cannot allege that the BK energy functional is also valid for the ZBL ion, for example, because the energy minima would be shifted to much too high ionization degrees. Because $q(y)$ is a fitting function for ZBL,
effective charge theory does not offer incentives to be furthermore concerned with their internal energy, because the EL then is solely determined by the ion form factor. In conjunction with the energy criterion this is the formal reason to examine ion models once again.

### 3.5.1 Results with Statistical Ion Models

Results in closed form are most easily obtained by this criterion on the basis of the BK ion model, i.e., insertion of $E_{BK}$ of (3.5) into $E_i$. By this procedure, the total kinetic energy of the bound electrons is explicitly partitioned into a center-of-mass part $E_{cm}$ and the part $E_{kin}$ measured in the ion rest frame. This is also valid in a quantum mechanical treatment as demonstrated in a tutorial in App. E in conjunction with [163, Ch. 9.3.3].

The total energy $E$ is the most simple generalization of the internal energy $E_{BK}$ of bound electrons in the case of non-zero ion velocity. As for the free ion (Sect. 3.2.1) the most stable state ought to have the minimum energy. If the neutral atom is assigned the chemical potential zero at rest, $\lambda = 4/7$ follows as in (3.9), and equivalently by

$$\frac{\partial E(Z_1, N, \Lambda, v)}{\partial \Lambda} = 0$$

(3.31)

again (3.8), because $E_{cm}$ does not depend on $\Lambda$. Within the statistical BK ion model, $N$ is a continuous variable, and the energy criterion may be written down in the differential form of a derivative

$$\frac{\partial E(Z_1, N, \Lambda, v)}{\partial N} = 0 \quad \Rightarrow \quad -\frac{2Z_1}{\Lambda/a_0} + \lambda \frac{N}{\Lambda/a_0} + \frac{10}{3} \frac{N^{2/3}}{(\Lambda/a_0)^2} + \left(\frac{v}{v_0}\right)^2 = 0.$$  

(3.32)

This becomes after insertion of (3.8)

$$6\#(1 - q)^2/3 \left(\frac{v}{v_0 Z_1^{2/3}}\right)^2 = \left[1 - \frac{\lambda}{4}(1 - q)\right] \left[1 - \frac{7}{4}\lambda(1 - q)\right],$$

(3.33)

and is plotted in Fig. 3.13. Again more expensive (due to the necessity to solve the TF equation) is this procedure if $E_i$ is the energy of the TF ion as in [260 (4.2)], which is also plotted. A final variant to be mentioned is the internal energy of the BK model including an exchange term (App.
The faster rise of \( q(y) \) for the TF ion model is caused by the more gentle slope of \( E(q) \) at low ionization degrees, which may be deduced from Fig. 3.14.

The energy minimization compares the slope of the internal energy \( E_{BK} \) (Fig. 3.14) with the additional kinetic energy of a captured electron, measured in the target rest frame. Due to \( E_{BK} \sim Z_1^{7/3}, \) \( dE_{BK}/dN \sim Z_1^{4/3} \) and \( E_{cm} \sim v^2 \) the natural scaling variable for the BK and also for the TF ion \( y \sim v/Z_1^{2/3} \) or rather \( y^2 \) using this criterion. On first glance this kind of scaling proposes a velocity criterion, because the internal kinetic energy is \( E_{kin}(Z_1,q)/N \sim Z_1^{4/3} \) and the mean velocity of the bound electrons therefore \( \sim Z_1^{2/3} \). This paragraph has shown in a simple way that this scaling behavior does not at all exclude the energy criterion, because the ionization energies are also in general \( \sim Z_1^{4/3} \) acc. to (3.12). The affirmation supporting the velocity criterion
which we may read in [261, p. 94] “The \( Z_{1}^{2/3} \) \ldots comes from the Thomas-Fermi atom \ldots for the velocities of electrons in heavy ions” is therefore void.

The energy criterion explains in simple terms, why \( q(y) \), in contrast to the thin continuous curve in Fig. 3.12 for example, does not follow a linear trend close to the origin, but is “suppressed,” and adapts to the gap at \( y_{r} \lesssim 0.18 \) of the ZBL fit. As the first ionization energy — in contrast to the higher ionization energies — is \( I_{1} \sim Z_{1}^{1/3} \) acc. to (3.13), the curve becomes \( q \sim y^{2} \) at low velocities, which we may derive from a Taylor expansion of (3.33). A general consequence of the energy criterion is that the ionization degree (a scalar quantity) is an even function of the velocity \( v \), a function of the energy (another scalar quantity) with no dependence on odd powers of \( v \). This relates to the isotropy of the problem, because the ionization degree should not depend on the direction of the ion velocity vector. An order \( q \propto v \) like in Fig. 3.12 for example would mean that stopping of the ion down to \( v = 0 \) and acceleration into the counter direction — a gedanken experiment that is allowed with \( v \) as a parameter — creates a discontinuous step in the ion reload current \( \dot{q}(v = 0) \). In case of the TF model with a very flat dependence \( E_{i}(q) \) the quadratic behavior
is limited to an interval very close to the origin.

A series of prospective objections against the energy criterion has to be discussed now:

1. Knipp and Teller [137] obtained values of \( q(y) \) that are very close to those of the energy criterion with the BK ion (Fig. 3.13), but emphasize that they use a velocity criterion. Looked at more closely, they calculate the number of bound electrons \( \Delta N \) in an infinitesimal interval \( \Delta \mu \) of the chemical potential of a TF ion, which is

\[
\Delta N = \int \Delta n d^3r \quad ; \quad \Delta n = -\Delta \mu \frac{1}{2\pi^2} \left( \frac{e(\varphi - \mu)}{E_0} \right)^{1/2}
\]

because of (D.2). They define “the mean square velocity of the electrons in the range” via multiplication of the integrand by \( 2e(\varphi - \mu)/m \) [since \( e(\varphi - \mu) = \frac{1}{2}mv^2 \)] and division through \( \Delta N \). This calculation, however, may also be derived from the energy criterion, if we write \( dE/dN = (dE/d\mu)/(dN/d\mu) \), include a sign change with the help of the virial theorem of the total energy [235] to obtain the kinetic energy, and eventually replace the total derivatives by partial derivatives at fixed \( \varphi \). The later corresponds to a non-self-consistent description, because the ion parameters do not move up as the number of electrons changes. In summary, they define the “velocity of the most loosely bound electron” via the energy of the next “infinitesimal” electron; it is a matter of an energy criterion in my classification with a slightly misleading wording “mean square velocity.” The aspect of including the target electron velocities, which Knipp and Teller see as an essential support of the velocity criterion, i.e., the substitution \( v \to v_r \), is integrated into the energy criterion in Sect. 3.7. Their work does also not serve as a reference to the superiority of the velocity criterion.

2. Using the kinetic energy of the bound electrons measured in the target rest frame treats this frame with some arbitrary distinction. A spectator in a system that moves with velocity \( v_G \) in the target rest frame may measure any positive value \( \frac{1}{2}m(v - v_G)^2N \); there is no absolute zero for the kinetic energy as well as for the potential energy. At first we can meet this objection by noticing that only the energy difference between the kinetic energies is the physically relevant quantity, which is the same in all reference frames. The energy criterion compares two states: (i) an ion with velocity \( v - v_G \) and mass \( M \), (ii) the stripped electron
with mass $m$ and velocity $-v_G$ (again in the target rest frame), plus the ion with remaining mass $M - m$ and velocity $v' - v_G$. The electron loss must conserve momentum

$$M(v - v_G) = -mv_G + (M - m)(v' - v_G) \quad \Rightarrow v' = \frac{M}{M - m}v.$$  

The difference between the kinetic energies of both states is

$$\frac{1}{2}mv_G^2 + \frac{1}{2}(M - m)(v' - v_G)^2 - \frac{1}{2}M(v - v_G)^2 = \frac{1}{2}mv^2 \frac{M}{M - m} \approx \frac{1}{2}mv^2 \quad \text{(since } M \gg m),$$

independent of the spectator system $v_G$, and equal to the term accepted in the energy criterion. (Energy is conserved as this energy is added to the internal energy of the ion.) Upon a closer look at this calculation a more relevant objection persists: the term $\frac{1}{2}mv^2$ is determined in essence by the assumption that the stripped electron is at rest in the target rest system after the event, which still accentuates the target system. Up to now we did not refer to any particular ion-target interaction mechanism; this missing piece of information causes this arbitrariness in Lamb’s basic form of the energy in the energy criterion. We may re-formulate the objection as follows: without the reference system of the target, i.e., in the vacuum, the ion would not loose electrons “spontaneously” as long as $E_i$ is smaller than zero. Considering the physics of the stripping event leads to a modification of this writing of the energy criterion in section 3.8.

3. An obvious disadvantage of the criterion is the over-estimation of ionization degrees for $q \gtrsim 0.5$. This tendency would be further enhanced in the case of ion models with flatter $E(q)$ dependency and smaller ionization energies as for example in App. B.2. The relation with the previous criticism is also elucidated in section 3.8.

4. One objection might be that the term $\frac{1}{2}mv^2$ means the energy needed to accelerate the $N$ bound electrons of the target system to the ion velocity, but that de facto $N$ itself depends on $v$. (In a formal manner one could re-write this in terms of a $v$-dependent total mass $mN$ of the bound electrons similar to relativistic mechanics.) Such an average of the energy over all velocities from 0 up to $v$, however, would be equivalent to building also an average of $q(v)$. This contradicts the insight that the ionization is a function, not a functional of $v$. 

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The ion actually adjust its ionization degree without “remembrance” of previous velocities. We may assume that the ionization degree is not synchronized after retardation, because the characteristic time interval to change the average ion charge by one electron is about 150–300 fs over a wide interval of \( Z_1, v \) and \( q \), whereas the equilibrium value adjusts about 2–3 orders of magnitude faster \[13\] \[113\].

3.5.2 Quantized Ion Models, Clementi-Roetti Ions

The energy criterion ought, more accurately than assumed in the previous section, compare energies of states with ion charge numbers \( Q \) and \( Q \pm 1 \), because electrons can only be caught or lost in integer numbers. The differential form ought to be replaced by the quantized stability criterion

\[
\text{MIN}\{N\} : \quad I_{Q+1} \equiv E_i(N-1) - E_i(N) \geq \frac{1}{2} m v^2.
\]

Accordingly the ionization from \( N \) to \( N - 1 \) bound electrons occurs, if the kinetic energy \( \frac{1}{2} m v^2 \) of the stripped electron surpasses the \( Q + 1 \)st ionization energy \( I_{Q+1} \).

The differential form of the “statistical” ion models of the previous section tends to underestimate the ionization energies, as the \( E_i(q) \) are convex functions \( (d^2 E_i/dq^2 > 0) \). The electrons are slightly tighter bound than the tangent approximation to \( E_i(q) \) predicts. One might correct this by using more orders of the Taylor expansion (with the aid of \[3.11\] for example) to approximate the difference in \[3.35\]. Instead and without additional expense, the following variant makes direct use of the more realistic ionization energies of tabulated RHF calculations \[50\].

With these Clementi-Roetti energies \( E_{CR} \), which already have been part of Fig. \[3.14\] the observation is confirmed that depended on the quality of the ionization energies in the previous section: The first ionization energy takes care that \( q(y_{(r)}) \) does not cross the origin — attempts at interpretations like in \[261\] p. 90 are not necessary. The gap that opens is estimated as \( y \approx 0.13 \) by \[3.22\] and \( y \approx 0.07 \) by \[261\] \[3-38\], respectively. (The fit by Klein et al. \[136\] or by Shima et al. \[227\] Fig. VI] ignores it.) The energy criterion \[3.35\] delivers

\[
q = 0 \quad \text{for} \quad \frac{1}{2} m v_r^2 \leq I_1; \quad q \geq \frac{1}{Z_1} \quad \text{for} \quad \frac{1}{2} m v_r^2 \geq I_1
\]

(3.36)
and proposes that $q \neq 0$ can only occur at $y_r \geq \sqrt{I_1/E_0/Z_1^{2/3}}$. Fig. 3.15 displays these points $(y = \sqrt{I_1/E_0/Z_1^{2/3}}, q = 1/Z_1)$ together with the ionization energies on which they are based. If no element of the period $37^{\text{Rb}}$ up to $54^{\text{Xe}}$ is incorporated, a gap opens left from $y \approx 0.07$, indeed.

Figure 3.15: Left: lower bounds for scaled velocities $y$ caused by the finite first ionization energies $I_1$ acc. to (3.36). The points are labeled with the chemical symbols of $Z_1 = 3, \ldots, 54$ and placed at $q = 1/Z_1$. The line represents the ZBL fit (3.22). Right: the first ionization energies $I_1$ that the left part is based on as a function of atomic number, taken from [50] by subtraction of the total energies of single ionized and neutral atoms.

The ionization energies are obviously dominated by the shell structure and not by a power of $Z_1$ [72, 73]. Bohr [32] already noticed that the ion ought to be single ionized at the velocity corresponding to $I_1$, and hence referred to an energy criterion. If we replace $I_1(Z)$ by a constant, the trend deduced from the energy criterion reads $q \sim y_r^{3/2}$. The statistical BK ion model, however, yields $I_1 \sim Z_1^{1/3}$ (3.13) and switches to $E/N \sim Z_1^{4/3}$ at middle ionization degrees. For highly stripped ions $I_{Z_1} \sim Z_1^2$, the result of the hydrogen problem, should be valid, as already Northcliffe [188] expressed by choosing $v_k$ as the “velocity of the first k electron” in a fit $\gamma^2(v/v_k)$. To summarize, a general feature of the statistical models is the failure at both ends of the $q$ interval, and a universal dependence $q(v)$ is no longer to be expected in these regions. A larger spread of the
experimental values at these abscissa values is possible.

Fig. 3.16 shows the steps at \( q = 1 - N/Z_1 \) \((N = 0, 1, 2, \ldots Z_1)\) over a larger velocity interval as predicted by the energy criterion (3.35). The over-estimation of the ionization degree already known from the statistical ion models persists for \( y_r \gtrsim 1 \), but may now be identified to relate to ions of half-filled \( 2p \)-shells.

![Graph showing ionization degrees as a function of the scaled velocity](image)

Figure 3.16: Thin lines: ionization degrees \( q \) as a function of the scaled velocity \( y_r \) by the energy criterion (3.35) using the CR energy levels [50] for light (left) and heavy ions (right). Fig. 3.15 shows a section of the left corners of the steps. Bold lines: ZBL fit (3.22). Adding even heavier ions is avoided here, because ZBL did not report on heavier ions than shown here over the entire energy region.

### 3.6 Energy Criterion: Coupling to the Induced Field

The kinetic center-of-mass energy of Sect. 3.5 is the dominant contribution to the energy criterion. A first extension and generalization of the formulation (3.30) is presented via inclusion of another energy term, which has not yet been discussed in the literature in conjunction with the energy criterion.
3.6.1 Energies of the Maxwell Fields

Addition energy forms result from the electric interaction (IA) between the electrons bound to the ion and the induced field. The corresponding effect on the EL has already been introduced by Kaneko in a static approximation for the IA of the target electrons \[126\] and was used later on by Yang \[259\].

The total energy of the Maxwell field of all charges is \[33\]

\[
E_{\rho\rho} \equiv \frac{1}{2} \int \frac{1}{4\pi \epsilon_0} \left| \frac{\rho(r)\rho(r')}{|r - r'|} \right| d^3rd^3r'.
\] (3.37)

After insertion of the three charges \[1.3\] \(E_{\rho\rho}\) decouples into six charge-charge interaction energies. The three terms \(\int \rho_n \rho_n\), \(\int \rho_p \rho_p\) and \(\int \rho_n \rho_p\) do not depend on \(\rho_e\) and are ignored from now on, because they do not contribute to the energy of the bound electrons. The two terms \(\int \rho_n \rho_e\) and \(\int \rho_p \rho_e\) are already listed as \(E_{ne}\) and \(E_{ee}\) in the internal energy of the ion \[3.5\]. This decomposition of a Hamiltonian is known from \[167\], where a level-shift of electrons bound to the ion caused by the Stark field \(E_{\text{ind}}\) is calculated. We use the term in the limit of strong fields \(\Phi_{\text{ind}}\), in the sense of field ionization and of the Franz-Keldysh effect. The only missing part is the (un-screened) interaction of the bound electrons with the induced field

\[
\frac{1}{4\pi \epsilon_0} \int \frac{\rho_e(r)\rho_p(r')}{|r - r'|} d^3rd^3r' = \int \rho_e(r)\Phi_{\text{ind}}(r)d^3r.
\] (3.38)

One may put it into a familiar form if one defines the polarization \(P = \epsilon_0 \text{grad} \Phi_{\text{ind}}\), the field that is created by \(\rho_e\) via \(\epsilon_0 \Delta \Phi_e \equiv -\rho_e\), and uses the first Green Lemma \[62\] S. 2.8.4:

\[
\cdots = -\epsilon_0 \int \Delta \Phi_e \Phi_{\text{ind}} d^3r = \epsilon_0 \int \text{grad} \Phi_e \text{grad} \Phi_{\text{ind}} d^3r = \int \text{grad} \Phi_e P d^3r = -\int E_e P d^3r.
\]

The term \[3.38\] is decomposed further into a sum, since the induced field is created by contributions by the nuclear charge \(\rho_n\) and by the bound electrons \(\rho_e\).

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

In the special case of the charge distribution of the BK ion \[167\],

\[
\rho_e(k) + \rho_n(k) = -N e \frac{1}{1 + (k\Lambda)^2} + Z_1 e,
\] (3.39)
the first energy becomes (3.38)

\[
E_\Phi = \int d^3r \rho_e(r) \int \frac{d^3k\omega}{(2\pi)^4} e^{i(kr-\omega t)} 2\pi \delta(\omega - kv) \frac{Z_1e}{\epsilon_0 k^2} \left[ \frac{1}{\epsilon(k,\omega)} - 1 \right]
\]

(3.40)

\[
\begin{align*}
E_\Phi &= -\frac{Z_1N e^2}{\epsilon_0 v} \frac{2}{(2\pi)^2} \int_0^\infty \frac{dk}{k} \frac{1}{1 + (k\Lambda)^2} \int_0^{kv} d\omega \Re \left[ \frac{1}{\epsilon(k,\omega)} - 1 \right] \\
&= -\frac{Z_1N e^2}{\epsilon_0 v} \frac{2}{(2\pi)^2} \int_0^\infty \frac{dk}{k} \frac{1}{1 + (k\Lambda)^2} \int_0^{kv} d\omega \left[ -1 \right]
\end{align*}
\]

(3.41)

The real part shows up after integration over negative \( \omega \). The difference to the calculation of the stopping power, the imaginary part there, is the power of \( \omega \). It reflects one missing time derivative, the difference of the charge contributing to the energy and the current contributing to the energy loss, which is expressed in the Fourier transform by one missing factor of \( \omega \). If the plasmon pole is passed, the integral is interpreted as the principal value.

\( E_\Phi \) generalizes and completes \( E_{ne} \) in presence of an external polarizable medium. Adding \( E_\Phi \) is just a substitution of the \( 1/r \) potential of the nucleus by a screened \( 1/(\epsilon r) \) potential. Generally the factor \( \Re[1/\epsilon - 1] \) first removes the bare Coulomb interaction, \( 1/k^2 \) in Fourier representation, and replaces it by \( 1/(\epsilon(k,\omega)k^2) \), the dynamically screened interaction. In detail, the last term in (3.41) cancels \( E_{ne} \):

\[
\begin{align*}
&-\frac{Z_1N e^2}{\epsilon_0 v} \frac{2}{(2\pi)^2} \int_0^\infty \frac{dk}{k} \frac{1}{1 + (k\Lambda)^2} \int_0^{kv} d\omega \left[ -1 \right] = 2E_0 \frac{Z_1N}{\Lambda/a_0} = -E_{ne}.
\end{align*}
\]

Fig. 3.17 shows that the reduction of \( E_{ne} \) due to the additional \( E_\Phi \) is more or less independent of \( v \) for \( v \lesssim v_F \), and becomes swiftly smaller as the velocity increases.

The second term created by (3.38) is the interaction of the bound electrons with the charges induced by themselves.

\[
E_\rho = \frac{\lambda}{2} \int d^3r \rho_e(r) \int \frac{d^3k\omega}{(2\pi)^4} e^{i(kr-\omega t)} 2\pi \delta(\omega - kv) -\frac{Ne}{1 + (k\Lambda)^2} \epsilon_0 k^2 \left[ \frac{1}{\epsilon(k,\omega)} - 1 \right]
\]

(3.42)

\[
\begin{align*}
E_\rho &= \frac{\lambda N^2 e^2}{2} \frac{2}{(2\pi)^2} \int_0^\infty \frac{dk}{k} \frac{1}{1 + (k\Lambda)^2} \int_0^{kv} d\omega \Re \left[ \frac{1}{\epsilon(k,\omega)} - 1 \right]
\end{align*}
\]

This definition of \( E_\rho \) implies:

1. Only half of the contribution released by \( E_{\rho \rho} \) has been taken over, because the energy of the induced electrons in the field of the bound electrons must not be added to their energy, if their energy is to be minimized, and this is half of the \( E_{\rho \rho} \) part. This decomposition of the
Figure 3.17: The energies $E_{ne}$ (lower bold lines) and $E_{\Phi}$ (higher thin) as a function of the ionization degree $q$ for $Z_1 = 15$ and 38 and density parameter $r_s = 2$ with (3.41), (3.5), (3.8) and the Lindhard function (Sect. 1.3.1). The ion velocities increase from line a to f.

The proportionality $E_{\Phi} \propto 1 - q$ is understood by the factor $N$ in (3.41) if $k\Lambda \ll 1$.

2. The factor $\lambda$ has been added similar to the ansatz for the BK energy $E_{ee}$, because (3.37) again is just a Hartree approximation to the electron-electron interaction. $E_\rho$ is thus treated on equal footing with the electron-electron interaction $E_{ee}$.

As in the case $E_{ne} + E_{\Phi}$, $E_{ee} + E_\rho$ replaces the Coulomb potential between the bound electrons by a dynamically screened interaction as provided in the dielectric function of the target. The last
term in (3.42) cancels $E_{ee}$:

$$
\frac{\lambda N^2 e^2}{2} \frac{2}{\varepsilon_0 v} \frac{1}{(2\pi)^2} \int_0^\infty dk \frac{1}{k} \left[ 1 + (k\Lambda)^2 \right] \int_0^{kv} d\omega \Re \left[ -1 \right] = \frac{\lambda N^2}{2 \Lambda/a_0} E_0 = -E_{ee}.
$$

The comparison of magnitudes of $E_{ee}$ and $E_\rho$ follows in the examples of Fig. 3.18.

Figure 3.18: The energies $E_{ee}$ (upper bold lines) and $E_\rho$ (lower thin) in units of $E_0 Z_1^{7/3}$ as a function of the ionization degree $q$ for $Z_1 = 15$ and 38 and one-electron radius $r_s = 2$ acc. to (3.42), (3.5), (3.8) and the Lindhard function as in Fig. 3.17 $E_\rho \propto (1-q)^2$ is caused by the factor $N^4$ in (3.42).

The total energy of the BK ion in a medium with dielectric function $\epsilon(k, \omega)$ contains (3.42), (3.41) and (3.5),

$$
E_M \equiv E_{BK} + E_\rho + E_\Phi
$$

(3.43)

$$
\frac{E_M}{E_0} = 2\Phi \frac{N^{5/3}}{(\Lambda/a_0)^2} + \frac{8}{(\pi \chi)^2} \frac{Z_1 N}{v \nu_F} \int_0^\infty dz \left[ \frac{1 - q}{2 1 + (2k_F z\Lambda)^2} - 1 \right] \frac{1}{1 + (2k_F z\Lambda)^2} \int_0^{v/\nu_F} \Re \frac{du}{\epsilon(z, u)}
$$

(3.44)

if the Lindhard variables (1.15)–(1.18) are utilized. App. E develops approximations of the integral for small $v$. We should remark that $E_\Phi$ causes a larger change in the energy than $E_\rho$. Because $E_\Phi$ essentially follows $\propto N$, the sum of both energies behaves similar to the contribution $E_{cm} = \frac{1}{2} mv^2 N$
if inserted into the energy criterion. Acc. to Fig. 3.17, they act like a velocity-independent increase
of the energy of each electron bound to the ion, as long as \( v \ll v_F \). They may be absorbed by \( v \) by
the definition of a relative velocity, like it has already been found advantageous within the velocity
criterion which absorbs the constant \( v_F \).

### 3.6.2 Modified Ion Size and Electron-Electron Coupling

The insertion of the non-modified size parameter \( \Lambda \) of the BK theory would violate the virial
theorem, if the potential between the ion nucleus and bound electrons was just extended by the
potential of section [3.6.1]. It is re-installed by a re-determination of \( \Lambda \) with the minimization
condition

\[
\frac{\partial E_M|_{Z_l,q,\lambda}}{\partial \Lambda} = 0 \quad (3.45)
\]

in the form

\[
E_{ee} + E_{ne} - \left< \frac{r}{d\Phi} \right> - \left< \frac{r}{d\Phi_p} \right> + 2E_{\text{kin}} = 0. \quad (3.46)
\]

The definition of the nuclear potential \( \Phi \), which is screened by the target electrons and the
potential of the bound electrons that are likewise screened are near at hand,

\[
\Phi_\Phi(k,\omega) \equiv \rho_n(k,\omega) \left[ \frac{1}{\epsilon(k,\omega)} - 1 \right] ; \quad \Phi_\rho(k,\omega) \equiv \frac{\lambda\rho_e(k,\omega)}{\epsilon_0 k^2} \left[ \frac{1}{\epsilon(k,\omega)} - 1 \right]. \quad (3.47)
\]

[The validity of the virial theorem is proven by interchange of the derivative in (3.44), which emerges
through (3.45), and the integration, which computes values of (3.46) in Fourier space, i.e.,

\[
\left< \frac{r}{d\Phi} \right> \equiv \int d^3r \rho_e(r) \frac{d\Phi}{dr} = \frac{i}{\epsilon_0} \int d^3r \rho_e(r) \int \frac{d^3k d\omega}{(2\pi)^4} k^2 \rho_n(k,\omega) \frac{1}{\epsilon(k,\omega)} \left[ \frac{1}{\epsilon(k,\omega)} - 1 \right] e^{ikr}
\]

and after insertion of (3.39) by the result

\[
\int d^3r \rho_e(r) r k e^{ikr} = -iNe \frac{2(k\Lambda)^2}{[1 + (k\Lambda)^2]^2}. \quad (3.48)
\]

The re-determination increases \( \Lambda \) by about 1–2%. The change is rather unimportant because the
virial energies in (3.46), i.e., the factor \( k\Lambda \) in (3.48), are small. Fig. 3.19 displays some of these
energies \( E_M \) that include this re-determination of \( \Lambda \).
These energies lead to an unrealistic, giant ionization, which is defined by the minimum of the curves in the plot, even at the tiny velocity chosen. They also imply that the chemical potential of the neutral atom is about one order of magnitude larger than the potential of the surrounding host material. These non-physical results are understood looking at the assumptions of the model: the interaction between the bound electrons and the nucleus and among themselves has been replaced everywhere by a screened interaction, the screening length of which is defined by the target electron density. This reduction of the potential — with no massive change of the kinetic energy, the small change of Λ notwithstanding — supports the emission of the electrons. The dominant error is the screening of all Coulomb interactions, even at points close to the nucleus where target electrons do not exist but where the contributions of the Coulomb potentials are large due to large electron densities.

In the spirit of this model one could think of improving these predictions by modification of the coupling parameter λ to arrange for a more realistic chemical potential µ of the ion in matter at rest. The potential has been assumed to be zero in [126], just as in the case of the free atom, (3.9). To reduce the numerical expense we might use an approximation of the TF type, the static, zero-velocity limit of the dielectric function, (E.2) and (E.4), inserted in the energy (3.44).
close bundling of the curves a, b and c in Figs. 3.17 and 3.18 indicates a validity approximately up to the plasmon excitation.

\[
\frac{E_M}{E_0} \approx 2\phi \frac{N^{5/3}}{(\Lambda/a_0)^2} + \frac{N}{a_0} \left( \frac{\lambda}{2(1 + \beta \chi)} \left[ \frac{N}{1 + \beta \chi} - 2Z_1 \right] \right) ; \quad \beta \equiv 2k_F \Lambda = \frac{2}{\pi \chi^2 a_0}
\]

The steps to compute the free parameters \( \lambda \) and the size parameter \( \Lambda \) follow the case of the free atom \((\rightarrow (3.31),(3.32),(B.2),(B.3) and [126])\). The original BK variables are retained in the limits \( \chi \to \infty, \beta \chi \to 0, r_s \to \infty, \lambda \to 0.571 \) and \( \Lambda \Gamma_1^{1/3}/a_0 \to 0.560 \).

\[
\frac{\partial E_M(\lambda, N, Z_1)}{\partial N} \bigg|_{N=Z_1} = \mu
\]

\[
\Rightarrow \frac{10}{3} \frac{\phi}{(\Lambda \Gamma_1^{1/3}/a_0)^2} + \frac{1}{(1 + \beta \chi) \Lambda \Gamma_1^{1/3}/a_0} \left[ \frac{\lambda}{1 + \beta \chi} - 2 \right] - \frac{\mu}{Z_1^{4/3}E_0} = 0. \quad (3.49)
\]

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

\[
\Rightarrow \frac{2\phi}{(\Lambda \Gamma_1^{1/3}/a_0)^2} + \frac{1}{\pi \chi \Gamma_1^{1/3}(1 + \beta \chi)} \left\{ \frac{\lambda}{2(1 + \beta \chi)} \left[ \frac{1}{\beta \chi} + \frac{2}{1 + \beta \chi} \right] - \frac{2}{\beta \chi} - \frac{2}{1 + \beta \chi} \right\} = 0. \quad (3.50)
\]

These two equations (3.49) and (3.50) for the unknowns \( \lambda \) and \( \Lambda \) are easily solved numerically and establish the values of Tab. 3.1. They differ drastically from the results published in [126] and are obviously useless: the electron-electron interaction becomes attractive in some cases (via a change in the sign of \( \lambda \)), and \( \Lambda \) is always smaller than the value of the free atom. The values by a fully numerical integration of (3.44) are only slightly better. The results indicate that the “spontaneous” emission of electrons that was calculated for \( \lambda = 4/7 \) may be prevented under the assumption of a weaker or even attractive electron-electron interaction, which causes the ion to reduce its size and to contract.

The criticism means that the description of the ion that is not influenced by the solid (as in Figs. 3.10 and 3.11) cannot be replaced by the opposite extremum, the complete penetration by a background dielectric constant. The argument is recalled in Sect. 5.4.1 to remove explicitly the contributions (there: to the stopping power) inside a “dead sphere.” Let us just indicate here that a consistent application of this model reduces also the energy terms drastically. The required generalization of (3.41) is calculated in App. H.2 and simplified to an approximation by the static
Table 3.1: The electron-electron coupling parameter $\lambda$, the size parameter $\Lambda$ and the total internal energy $E_M$ of the BK atom in a model of the screening of all Coulomb potentials under influence of the target electrons in the static TF approximation, i.e., the solution of the system of equations (3.49) and (3.50) using $\mu = 0$, $\chi^2$ acc. to (1.8) and $N = Z_1$. The parameter set has been chosen for comparison with [126].

TF screening. As Fig. 3.20 shows, the assumption of a dead sphere, with a size comparable with the atomic radius (comparable with those listed in Tab. 3.2), leads to the indispensable decrease of this energy.

Figure 3.20: The energy $E_\Phi$ acc. to [H.5] of the electrons bound to the ion in the field of the polarization charges which are created by the nucleus, for “dead” spheres of different radii $r_c$ around the ion nucleus, inside which the polarization charges have been set to zero. Because [H.5] is computed within the TF approximation for $\epsilon(k, \omega)$, the values shown here for $N = Z_1$ differ slightly at $r_c = 0$ from the curves a–c at $q = 0$ in Fig. 3.17.
Table 3.2: Radii of sub-shells in units of $a_0$, defined by the maxima of $4\pi r^2|\varphi_1(r)|^2$, where the CR wave-functions of the extended basis sets are inserted into $\varphi_1(r)$, and the occupancies of all other shells are set each time to zero.

<table>
<thead>
<tr>
<th>shell</th>
<th>$^{15}$P</th>
<th>$^{33}$As</th>
<th>$^{36}$Kr</th>
</tr>
</thead>
<tbody>
<tr>
<td>3s</td>
<td>1.586</td>
<td>0.530</td>
<td>0.475</td>
</tr>
<tr>
<td>3p</td>
<td>1.844</td>
<td>0.526</td>
<td>0.468</td>
</tr>
<tr>
<td>3d</td>
<td>0.481</td>
<td>0.414</td>
<td></td>
</tr>
<tr>
<td>4s</td>
<td>1.673</td>
<td>1.378</td>
<td></td>
</tr>
<tr>
<td>4p</td>
<td>2.010</td>
<td>1.568</td>
<td></td>
</tr>
</tbody>
</table>

### 3.6.3 Summarizing Assessment of This Contribution to the Energy

The influence of the target electrons that diminishes the binding of the electrons bound to the ion may be integrated in terms of an external potential into the terms of the internal energy.

An implementation proposed by Kaneko replaces all Coulomb interactions of the free ion by interactions that are screened with the dielectric function of the target electrons, and leads, after thorough study, to unrealistic and much too strong influences on the ion size and ion energy. The only result is that the energy derived from the stopping region that is proportional to $v$ is an upper limit for changes at higher velocities. A model may be constructed that restricts the action of the dielectric function of the target to a region outside a minimum distance from the ion nucleus, and reduces the Coulomb energy of the bound electrons in the field of the polarization charges.

Another quantitative theory that would describe the change of the outer electron shells of the ion due to the presence of the target electrons at all $v$ is hitherto missing in the literature. The construction of a combined, joint dielectric function of the target in consideration of the ion, as presented by Guinea et al. [100] for $^1$H and $^2$He projectiles, could serve as a guideline.

There is one reason of conceptional nature why this energy term is not included in the stripping criterion here. The energy leads, as described, to a relaxation of the charge distribution of the electrons bound to the ion when the size parameter is re-determined. Because this change of the ion form factor has not been included in any of the calculations of the electronic energy loss, especially not in Sect. 3.2.3, the stopping and the stripping would be described by different ion models otherwise. Along these lines the energy of Sect. 3.6 here is eventually not used in a comparative assessment of the energy criterion.
3.7 Energy Criterion: Fermi Velocity of the Target

An open item of the discussion is the inclusion of the Fermi velocity \( v_F \) of the target material into the ion velocity which has been introduced in Sect. 3.2.2 in the case of the velocity criterion. Up to here we have tacitly used \( y_r \) synonymous to \( y \), as if the modification of the kinetic energy \( E_{cm} = mv^2N/2 \) would have already been worked out in a modified formula. The following paragraphs supply a proof of a comparable improvement of equal standard within the energy criterion.

3.7.1 The Chemical Potential of the Target

The extension of the energy concept in a surrounding medium is given by thermodynamics — again a more fundamental and general starting point than the velocity criterion —. In generalization of (3.31), the chemical potential of the ion must become equal to the external potential of the host material,

\[
\frac{\partial E(\lambda, N, Z_1, \Lambda)}{\partial N} \bigg|_{N=Z_1} = \mu.
\]

We assume that the total energy (3.30) is given by the internal energy of the BK ion model \( E_i = E_{BK} \), i.e., (3.5), and again use its minimization to determine the size parameter \( \Lambda \). The coupling parameter \( \lambda \) and its Taylor expansion become

\[
\lambda = 4 \left( 1 - \sqrt{\frac{9}{49} - \frac{6\phi}{7Z_1^{4/3}E_0}} \right) = \frac{1}{7} + \frac{\phi\mu}{Z_1^{4/3}E_0} + O(\mu^2).
\]

Equations (3.5), (3.31), (3.10) and (3.8) remain valid, if the modified coupling parameter is inserted. The BK energy obtains a Taylor expansion around \( \mu = 0 \):

\[
\frac{E_{BK}}{E_0Z_1^{4/3}} = \left[ \frac{E_{BK}}{E_0Z_1^{4/3}} \right]_{\mu=0} + (1 - q)^{1/3} \left[ 1 - \frac{1 - q}{7} \right] \frac{\mu}{E_0Z_1^{4/3}} + O(\mu^2).
\]

The impact on the energy \( E_{BK}(q) \) is demonstrated in Fig. 3.21 for realistic chemical potentials \( \mu \), which have been coupled to the one-electron radius \( r_s \) via the simple “Hartree” kinetic energy as

\[
\mu = \frac{1}{2}mv_F^2, \quad \mu = \frac{E_0}{(\alpha r_s)^2}.
\]

(3.52) leads to an energy increase by \( \frac{6}{7}\mu Z_1 \) at \( q = 0 \) by immersion in an environment with chemical potential \( \mu \). Though the model is simple, the results are comparable with the immersion
energies of DFT calculations by Puska et al., as Tab. 3.3 demonstrates. The BK ion model does not possess oscillations as a function of the filling degree of shells, of course.

The energy minimum over all $N$ for $v = 0$ is found in this generalization at $q = 1 - 4/[7\lambda(\mu)]$, which is the root of (3.33) or (3.12). The ionization degrees of the ion at rest in the medium become comparable with those by ZBL. (Some values are plotted in Fig. 3.22, though the TRIM85 data are not meant to be quantitatively reliable if they are looked at in this isolated manner.)

3.7.2 Transformation into an Effective Velocity

Solely for comparison with the velocity criterion this increase of the ionization degree by the chemical potential of the medium can be translated into an effective velocity. If we insert the Taylor

<table>
<thead>
<tr>
<th>Element</th>
<th>He</th>
<th>Li</th>
<th>Be</th>
<th>B</th>
<th>C</th>
<th>N</th>
<th>O</th>
<th>F</th>
<th>Ne</th>
<th>Na</th>
<th>Mg</th>
<th>Al</th>
<th>Si</th>
<th>Cl</th>
<th>Ar</th>
</tr>
</thead>
<tbody>
<tr>
<td>Imm</td>
<td>8.53</td>
<td>11.3</td>
<td>12.4</td>
<td>10.6</td>
<td>9.3</td>
<td>9.9</td>
<td>9.2</td>
<td>13.4</td>
<td>26.0</td>
<td>30.0</td>
<td>34.2</td>
<td>35.4</td>
<td>35.7</td>
<td>43.7</td>
<td>52.9</td>
</tr>
<tr>
<td></td>
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<td>8.7</td>
<td>10.8</td>
<td>13.0</td>
<td>15.2</td>
<td>17.4</td>
<td>19.5</td>
<td>21.7</td>
<td>23.9</td>
<td>26.0</td>
<td>28.2</td>
<td>30.4</td>
<td>36.9</td>
<td>39.0</td>
</tr>
</tbody>
</table>
Figure 3.22: Stars: Number of elementary charges $Q = qZ_1$ by ZBL for velocity $v = 0$, $r_s > 1.5$ and $Z_1 = 3, \ldots, 53$ (line 40 in App. C.1). Lines: ion charges by the minimum of $E_{BR}(N)$ at $r_s = 2$ or $r_s = 3$ and $v = 0$ assuming (3.53) of the non-interacting electron gas.

series (3.51) into the energy criterion (3.33), we get

$$6\phi(1-q)^{2/3}\left(\frac{v}{v_0Z_1^{2/3}}\right)^2 + \frac{6\phi\mu}{E_0Z_1^{4/3}}(1-q)(1+\frac{q}{3}) + O(\mu^2) = \left[1 - \frac{\lambda}{4}(1-q)\right]|_{\mu=0} \left[1 - \frac{7}{4}\lambda(1-q)\right]|_{\mu=0}. $$

The left side implies after division through the factor in front of $v^2$ that the relative velocity should be defined as

$$\left(\frac{v_r}{v_0}\right)^2 = \left(\frac{v}{v_0}\right)^2 + \frac{\mu}{E_0}(1-q)^{1/3}\left(1 + \frac{q}{3}\right) + O(\mu^2)$$

$$\Rightarrow \quad v_r \approx \sqrt{v^2 + v_F^2} \quad (\text{as } q \approx 0)$$

if the chemical potential is derived acc. to (3.53) from the “Hartree” kinetic energy. We also may insert the HF approximation of an interacting electron gas [101, (55)],

$$\frac{\mu}{E_0} = \frac{1}{(\alpha r_s)^2} - 2\frac{1}{\pi \alpha r_s} = \left(\frac{v_F}{v_0}\right)^2 - 2\frac{v_F}{\pi v_0}$$

(3.55)

and $v_r$ becomes smaller. Slightly more precise results are obtained by a numerical determination of $q(v, \mu)$ with the energy criterion (3.33), plus a definition of $v_r$ as the velocity which leads to the same ionization degree as with $\mu = 0$ and $\lambda = 4/7$. This results in the curves of Fig. 3.23.

Following the “Hartree” approximation of the chemical potential we are close to the ZBL values of Fig. 3.3. For diluted electron gases $\mu$ may become negative in the HF approximation.
and sometimes, as in the case of the lowest of the curves, no velocity of the BK ion may be found that provides the negative $q$ required. Including the correlation energy \cite{82} (12.62) would overcome this artifact.

In conclusion, the equivalence of the energy criterion has also been demonstrated in conjunction with the implementation of an effective ion velocity $v_r$, based on equivalent qualities of the assumptions, i.e., the PRA to the electronic energy loss, purely kinetic argumentation by the velocity criterion and the most simple approximation to the chemical potential. The previous showing of the ZBL ionization degrees together with the results of the energy criterion is herewith justified.

The two influences of the target electrons, which have been treated in Sect. \ref{3.6} and \ref{3.7} as external electrical and chemical potential, may be combined from the thermodynamical point of view to an adaptation of the electro-chemical potential of the ion to the electro-chemical potential of the target electrons, which form the “bath.” The minimization of the energy of the isolated ion has implicitly explicitly been transformed into the minimization of the corresponding thermodynamic potentials. No new insights follow from this unification.
3.8 The Available Kinetic Energy, Kinematics

The most important weakness left on part of the energy criterion up to here is the over-estimation of the ion charge at \( q \gtrsim 0.5 \), the diagnosis in Fig. 3.16, because the previously discussed electrochemical energies modify the ionization at small velocities only. The reason is in essence that the Lamb energy term, \( \frac{1}{2}mv^2 \) for each of the \( N \) bound electrons, is too large. The basic formulation of the kinetic energy term ought to be re-interpreted as follows: the ionization by the target electrons that move relative to the ion with velocity \( v \) cannot dispose of the full kinetic energy \( \frac{1}{2}mv^2 \), because (i) both, the ionizing and the lost electron, need to have some minimum kinetic energy after the event (process) to be considered stripped, and (ii) energy may be diverted in form of a “projectile inelastic” energy to excite the ion. The term of the kinetic energy has thus been re-interpreted: it no longer represents the kinetic energy of a bound electron measured in the target system, but the energy transferred from a target electron to the ion. As for item (ii) one may hope that it does not perturb the energy balance, because the ions are excited basically before and after the electron capture or loss, which lets this addition internal energy show up at all ionization degrees and partially cancel in the energy review. Taking it into consideration might lead to inconsistencies between the EL’s computed here, because we do not incorporate “hollow” atoms as in [132] with increased radii and therefore increased energy loss.

Item (i) may be put into numbers. If a target electron hits \( \tilde{N} \) bound electrons with relative velocity \( v \), the total energy available to knock electrons out of the ion potential is with observance of momentum conservation the total kinetic energy of the joint center of mass, \( \frac{1}{2}mv^2 \tilde{N}/(1 + \tilde{N}) \). The ion would implicitly be divided into interior “rigid” shells plus a soft, decoupled hull of \( \tilde{N} \) electrons, where only the latter absorbs energy and momentum.

The target reference frame of the Lamb energy term, which was found to be arbitrary in Sect. 3.5.1, is implicitly substituted by the only one that is outstanding energetically, the center-of-mass system of two colliding partners that minimizes the total kinetic energy. At the same time this implements the consideration of the target electrons in the energy term of the stripping criterion which was asked for above. If \( \tilde{N} \) is large, \( \frac{1}{2}mv^2 \) are available to remove a bound electron, but for \( \tilde{N} = 1 \) only \( \frac{1}{4}mv^2 \). A stripping parameter comparable to the one within the velocity criterion
would lie between 1 ($\tilde{N} \to \infty$) and $\sqrt{2}$ ($\tilde{N} = 1$). If we assume furthermore that $\tilde{N}$ is the number of bound electrons remaining in the outermost sub-shell and that the more interior closed shells are mere spectators, Fig. 3.16 is replaced by Fig. 3.24. A related result is the inelastic scattering

Figure 3.24: Thin lines: ionization degree as a function of the scaled velocity obtained from the energy criterion and the CR energy levels [50] for different heavy ions. Unlike Fig. 3.16, $\frac{1}{2}mv^2$ has been replaced by the energy transfer $\frac{1}{2}mv^2 \tilde{N}/(1 + \tilde{N})$. In (a) and (b) $\tilde{N}$ is the number of electrons in the outermost partially or completely occupied ion sub-shell, i.e., 1–2 for s shells, 1–6 for p shells and 1–10 for d shells, in (c) the number of electrons in the outermost partially or completely occupied principal shell, i.e., $N$ for $N \leq 2$, $N - 2$ for $3 \leq N \leq 10$, $N - 10$ for $11 \leq N \leq 18$, $N - 18$ for $19 \leq N \leq 36$. $N \equiv Z_1 - Q$. Bold lines: ZBL fit (3.22).
cross section of many-electron atoms. In the lowest Born order for the ground state it becomes approximately proportional to $Z$ by a summation over space coordinates of electrons in multiply occupied shells \[156]. (This lowest perturbative order is by nature most inaccurate at the ionization threshold.)

The switch-over from steep inclinations to broader steps in the $q(y)$ plot becomes smoother. In the region of large ionization degrees the comparison with ZBL is more satisfactory, in the region of low ionization degrees the values move below the ZBL values as demanded in Sect. 3.2.3. This model of the energy that can be transferred to the ion may create the artifact that the $1s^22s^22p^1$ configuration is guessed to be more stable than the more ionized $1s^22s^2$ configuration. In Fig. 3.24 the loops that run backs show these cases. The vertical line of the transition $2s^22p^1 \rightarrow 2s^2$ is placed to the right of the vertical line of the ionization $2s^2 \rightarrow 2s^1$.

A more thorough discussion of the excitation of the ion by the target electrons is not intended here. There are principal similarities to the excitation of target atoms by the ion, as discussed later on in this work within the Kaneko theory, but exchange effects for indistinguishable scattering electrons and the non-applicability of a classical straight-line approximation to the trajectory of a scattered electron are essential differences. The aim was to emphasize that the kinematic constraints and matrix transition elements, which are commonly parameterized by generalized oscillator strengths \[116, 155, 226\], play an important role as we go beyond the Lamb energy criterion. Energies cannot describe dynamic mixing and statistics of charge states \[12, 27, 31, 43, 58, 102, 105, 169, 177, 188, 227, 233\], the influence of virtual transitions etc., but presume stationary states.

### 3.9 Summary

After discussion of some arguments that are defeated easily in some cases, the velocity criterion of the general determination of the ionization degree unfolds as heuristically successful but hardly substantiated. The energy criterion is more fundamental, explains on simple grounds the gap of the ionization observed at low velocities, permits the use of quantum-mechanical as opposed to statistical ion models, and integrates the influence of the electro-chemical potential of target
electrons in a natural manner. A systematic contradiction in the handling of the electric potential in a work by Kaneko is explained by a first hint at a polarization-free zone surrounding the ion.

The ansatz to the basic contribution to the energy has been given in the forties and is the kinetic energy of the electrons bound to the ion measured in the target system. To apply the criterion successfully, it must be re-interpreted as the energy that can be transferred by a target electron to allow ionization. The consideration of kinematic constraints leads to a reduction of the theoretical ionization degrees. The virial theorem on one hand and this impact of momentum conservation on the other hand may be considered the bridging elements between the velocity and the energy criterion.
Chapter 4

Effective Charges: Do the Free Electrons Represent the Target?

4.1 Motivation

In this chapter the Kaneko theory and its generalized description of the target electrons in the ground state are used to answer the retrospective question, why the previous theories could in general provide realistic results on the basis of the homogeneous electron gas.

The ZBL approximation took the Lindhard function at low frequencies, from the point of view of the EL at small projectile velocities, to transform the ion charge into an effective charge. The target has been a free electron gas. The Fermi velocity remains the only dependence of the effective ionization degree $\gamma(q, Z_2)$ on the target; more complicated dependences on $Z_2$ were excluded. This approximation lets arise the question: Why and how far can the more complicated target electron density that is build of atomic shells be parameterized by the Fermi velocity to describe the effective charge? Any superior theory which provides separate numbers for the contribution of shells can be appointed to assess this assumption. This theory will be the Kaneko theory of individual target shells of free and bound electrons in the following, a natural generalization of the Lindhard theory. Other target models with this option of looking at shells will not be used here. The results introduced here have been published in.
4.2 Introduction to the Kaneko Theory

The Kaneko theory computes the cross section per target atom via the independent superposition of the cross sections of 1s, 2s, 2p, \ldots shells, and, if appropriate, a “shell” of free electrons,

\[ S = \sum_{sh=bnd,free} S_{sh}. \]  \hspace{1cm} (4.1)

The free electrons are handled exactly as in the LW theory (Sect. 1.3) and are parameterized by the one-electron radius \( r_s \). The susceptibility \( \chi^R \) of each inner target shell is computed in a similar way within the lowest order of perturbation theory (RPA). The ground state of the electrons of these shells was approximated by a Gaussian distribution in momentum space with a characteristic width \( \bar{q} \).

\[ w(p) = \exp \left\{ -\left( \frac{p}{\bar{q}} \right)^2 \right\}. \]  \hspace{1cm} (4.2)

This momentum distribution is obtained for example starting from a wave-function with Gaussian shape in real space \([45]\). Because the Kaneko theory ignores the localization of the wave-function in real space after that and uses the momentum distribution merely as a probability in a homogeneous real space, the description resembles the description of an electron plasma with molten Fermi surface at high temperature \([250]\). In many regards the wave number \( \bar{q} \) of the inner shells takes the role of \( k_F \) of the free electrons.

This wave packet model plus the dispersion of free plane waves in the denominator already provide a complete input to compute the susceptibility in the RPA,

\[ \text{Im} \chi^R(k, \omega) = -\frac{e^2}{4\pi^2\hbar k^2\epsilon_0} \int d^3p \left( w(p + k) - w(p) \right) \delta \left( \omega - \frac{\hbar(p + k)^2}{2m} + \frac{\hbar p^2}{2m} \right). \]  \hspace{1cm} (4.3)

As before, \( \chi^R \) denotes the susceptibilities and \( \chi^2 \equiv 1/(\pi\bar{q}a_0) \) the (squared) density parameter. The Kramers–Kronig (KK) analysis for example may be used to obtain \( \text{Re} \chi^R \) and produces mainly Confluent Hypergeometric Functions. The explicit representations of the original theory are covered by the case \( l = 0 \) in App. H.3. Shell by shell the individual dielectric functions \( \epsilon_{sh} = 1 + \chi^R \) are
inserted into the stopping cross sections of the shells:

\[ s_{\text{bnd}} = -\frac{2}{\sqrt{\pi} \varepsilon^2} \frac{1}{q^3} N_{\text{bnd}} \int_0^\infty \frac{dk}{k} |\rho_m(k)|^2 \int_0^{kv} \omega \text{Im} \left[ \frac{1}{\epsilon_{\text{bnd}}(k, \omega)} - 1 \right] d\omega \] \tag{4.4}

\[ = \frac{Z_1^2 e^4}{4\pi^2 \varepsilon_0 m v^2} N_{\text{bnd}} L_{\text{bnd}}. \] \tag{4.5}

The number of electrons in the shells are integer numbers and fixed by the atomic theory, up to 2 for \( s \) shells, 6 for \( p \) shells etc.

\[
\sum_{\text{sh=\text{bnd,free}}} N_{\text{sh}} = Z_2.
\]

Similar to (1.7) a Kaneko stopping number

\[
L_{\text{bnd}} \equiv -\frac{8}{\pi^{3/2} \chi^2} \int_0^\infty dzz \left| \frac{\rho_m(z)}{Z_1 e} \right|^2 \int_0^{v/\bar{v}} u \text{Im} \left[ \frac{1}{\epsilon_{\text{bnd}}(z, u)} - 1 \right] du
\] \tag{4.6}

and a characteristic electron velocity

\[
\bar{v} \equiv \hbar \bar{q}/m
\]

of each inner shell are defined. The dimensionless “Kaneko variables” \( z \equiv k/(2\bar{q}) \) and \( u \equiv m\omega/(\hbar \bar{q}k) \) of inner shells are likewise defined as analog to the Lindhard theory (1.15)–(1.18).

The characteristic wave numbers \( \bar{q} \) representing wave packets with \( N_{\text{sh}} \) electrons were derived from the one-electron orbitals \( \varphi_1 \) of RHF wave-functions \([41, 50, 138, 161]\) as follows:

\[
\bar{q} = N_{\text{bnd}}^{1/3} \tilde{q}_1 \quad \tilde{q}_1 = 2\sqrt{\pi} \left| \int d^3r \varphi_1(r) \right|^{-2/3}. \tag{4.7}
\]

The wave packet occupied by only one electron had also to be approximated first by the Gauß form

\[
w_1(p) \propto \exp\left\{ -(p/\tilde{q}_1)^2 \right\}. \tag{4.8}
\]

The quality of this approximation may be directly judged by comparison with the Fourier transform of atomic wave-functions \( \varphi_1(p) \), where Fig. 4.1 offers one example.

In (4.7) the characteristic width \( \tilde{q}_1 \) of the momentum distribution was derived from the value \( \varphi_1(p = 0) \). This is made possible by the normalization of the wave-function of the orbitals, which lets each increase of \( \tilde{q}_1 \) be directly associated with a decrease of \( \varphi_1(p = 0) \). The extension to the
The Kaneko Gaussian fit Clementi-Roetti tables

Figure 4.1: The approximation $(2\sqrt{\pi}/q_1)^3 \exp\left\{-\frac{(p/q_1)^2}{2}\right\}$ for the Si 2s shell with $q_1 a_0 = 1.89$ in comparison to the values $|\varphi_1(q)|^2$ of CR wave-functions [50] of the extended basis set. Both are shown in atomic units, i.e., $a_0^3$, and normalized as $\int d^3 p = (2\pi)^3$.

distribution $w(p)$ with $N_{sh}$ electrons in a shell is an application of statistical physics; the additional electrons are not packed like $w(p) = N_{sh}w_1(p)$ with linearly increasing density into momentum space, but, due to the fixed number of available states in phase space, at higher momenta by increase of the characteristic wave number. This leans upon the homogeneous electron gas, where new electrons are only added at $k_F$, resulting in $k_F \propto n^{1/3}$. It is less comparable to atomic compositions, where electrons are primarily put into orbitals that are degenerate with respect to the magnetic quantum number according to Hund’s rule.

The integrand to calculate the stopping cross section then looks like in Fig. 4.2. The excitation branch that ends at large momentum and energy transfers, i.e., large $z$ and $u$, correlates to the Bethe ridge of atomic one-particle excitations. In the limit of quasi-free target electrons, when the binding energy and kinetic energy of the initial state are small compared to $\hbar \omega$, it runs along $\hbar \omega / E_0 = (k a_0)^2$, in our units $u = z$ [116 Sect. 3.2]. This just reflects the demands of momentum and energy conservation, which force the individual target electron to stay on the dispersion curve after the excitation.

The Kaneko theory defines a plasmon energy $\hbar \omega_p$ of each shell [124]

$$\hbar \omega_p = \frac{2E_0}{(\pi^{7/4}\chi^3)} \quad (4.9)$$
and a plasmon dispersion

\[ u^2 \approx \sqrt{\pi} \chi^2/(4z^2) + 3/2 + z^2. \] (4.10)

Due to the finite life time of the plasmons of the inner shells it appears as another ridge like in the upper left corner of Fig. 4.2a. In contrast to the free electron gas at 0 K, no undamped plasmons obeying \( \varepsilon_{sh}(z, u) = 0 \) develop for the inner shells. There is no clear separation of the two branches of the excitation in \((k, \omega)\) or \((u, z)\) parameter space and therefore not precise equipartition rule. The rough features, however, are similar: at constant \( u \) the integrand contributes only up to \( k \approx 2.5\bar{q} \) \((z \approx 1.2)\). The inner shells also yield \( L_{sh} \propto v^3 \) and hence stopping cross sections proportional to velocity \( [123] \) at small velocities. This is valid within the original theory for each individual shell and eventually for the sum, and is taken up again in Sect. 5.3.

The original publications contain a series of results, \( Z_1 \) oscillations and the straggling in a

---

Figure 4.2: Left image: contour lines of the integrand \(-z \text{Im}(1/\varepsilon_{bnd}(z, u))\) of the Kaneko stopping number in case of the example \( \chi^2 = 1/(\pi\bar{q}a_0) = 0.1 \). (This value of \( \chi^2 \) has been chosen to simplify direct comparison with [150 Fig. 1].) Right image: cross sections for constant \( u = 0.1 \) and varying density parameter \( \chi^2 \).
Figure 4.3: Thin lines: shell-by-shell contributions to the total stopping of protons by the Kaneko theory for solid state targets of $^{12}$Mg, $^{14}$Si, $^{28}$Ni and $^{32}$Ge in units of $Z^2\epsilon$ eV cm$^2/10^{15}$ atoms as a function of $v/v_0$. Parentheses contain the occupancies of target sub-shells per atom. Bold lines: corresponding ZBL stopping cross sections by lines 1–17 of App. [C.1].

The application of the Kaneko theory to the EL in composite materials, especially application to the Bragg rule [45, 95, 190, 205, 211, 212, 240, 246, 263] may be developed rather easily on
the basis of the theory. If the elemental materials or the composite contain electrons that are considered to be free in the solid, and if the target shells are superimposed independently, deviations from the simple rule of a weighting according to the percental concentration are to be expected. The related problem of the EL of a target material in different states of aggregation (gas-solid effect) \[21, 22, 23, 106\] has been tackled through the introduction of autonomous parameter sets in the theory. (An additional dependence of the ionization degree on the state of aggregation is not yet taken into account by such a step.)

The typical features of the inner target shells are discussed in the next chapter within an application of the theory, and in Chapt. 5 the theory itself and improvements are in the limelight. Some positive characteristics in practical operation may be listed already here:

1. fit-free parameterization of all shells of all elements with parameters derived from atom theory
2. generally good agreement of the total stopping cross sections with experimental curves in the case of light ions,
3. analytical expressions for the susceptibilities of the individual shells as a function of momentum and energy.

4.3 Effective Charges as Function of the Target Atomic Number

The Kaneko theory provides stopping cross sections for protons and for heavy ions, and therefore effective ionization degrees \( \gamma^2 = S(q(v), Z_2)/[S(q = 1, Z_2)Z_2^2] \). Especially the parameterization of the shells lets results depend on \( Z_2 \). We employ this to assess the ansatz of a mere dependence on \( v_F \) by the aforementioned BK and ZBL calculations, and ask the question: How good can a representation of all shells by the Fermi velocity (ie, by the “shell” of free electrons) be, which was presumed in the heavy-ion scaling rule (3.14) by using the ansatz (3.17) or (3.23)?

To unbundle these \( Z_2 \) oscillations and examine the reduction to a \( v_F \)-dependence, the ion parameters \((q, \Lambda, v)\) are first kept fixed. Fig. 4.4 shows \( \gamma^2 \) as the ratios of heavy ion and proton stopping data, which follow by insertion of the BK ion model, (3.2) and (3.8), at frozen charge states into the Kaneko model. The integrals over \( z \) and \( u \) in (4.6) have been evaluated with the
help of the subroutines d01amf and c05ajf of the NAG library [178]. Similar curves are shown in [129] for $^2$He projectiles with the form factor of the hydrogen atom with one electron.

We see

Figure 4.4: Squared effective charge degrees of the Kaneko Model with the parameters of the solids and the BK form factor for ions in frozen charge states. Upper pictures: $Z_1 = 5$, lower: $Z_1 = 15$. Right pictures: examples of correlations with the Fermi velocities of TRIM85 for one curve of the left side respectively. The chemical symbols represent targets.
From a simple heuristic point of view the effective ionization degrees are positively correlated with the Fermi velocities of the targets (Fig. 3.8). For this conclusion one ought to ignore in the right pictures the points of $Z_2 = 7 \ldots 10, 18, 36$, i.e., the solid state targets of elements with melting points below $-157^\circ C$, and $Z_2 = 43$, Techneticum. In principle this provides support to characterize targets only by $v_F$. The dependence of the ionization degrees on the Fermi velocities (Sect. 3.7) that was discussed in the previous sections is not yet contained in these results with frozen charge states. But as $q$ ought also be positively correlated with $v_F$, the correlation between $\gamma$ and $v_F$ would nothing but enhance and the observation be further supported.

The spread of the $\gamma$ values as a function of $Z_2$ is considerably larger than the spread of the ZBL values in Fig. 3.7. This difference does not find an explanation by the building blocks of the model presented up to here. The ZBL treatment generally and automatically contains effects of higher orders of $Z_1$ and exchange-correlations effects beyond RPA via the proton data, which are not included in the Kaneko model. The improvements of the Kaneko theory that are detailed in Sections 5.3 and 5.4.1 produce figures with very similar results and do not offer explanations. In anticipation and as a documentation of this observation, Fig. 4.5 is inserted here.

We also observe that the variation of $\gamma^2$ through the PSE could be reduced considerably by omission of the $3d$ and $4d$ elements. It comes in via the proton energy loss data ($\rightarrow$ Fig. 4.7), which strongly depend on the division of target electrons into $N_{\text{free}}$ and $N_{3d/4d}$ around their maximum, and on the parameterization of the $d$ electrons. We may just state that a general change of the description of $d$ electrons in the Kaneko theory could remove this discrepancy with the ZBL values.

At high energies the Kaneko theory also predicts a small ascent of $\gamma(Z_2)$. The explanation is sound: in the Bethe-Bloch regime all target electrons, conduction and valence band, and inner shell electrons are excited equally on the basis of binary collisions. This is discussed below on the background of switching on deeper and deeper shells as the velocity increases.
If we define a quasi-Fermi-velocity $\tilde{v}_F$ by a homogeneous distribution of all target electrons,

$$\frac{\tilde{v}_F}{v_0} = \sqrt{\frac{3\pi^2 L Z_2}{V_{\text{mol}}}} a_0$$

($L \ldots$ Avogadro number; $V_{\text{mol}} \ldots$ molar volume), we also obtain a rising line with the structure of the PSE superimposed (Fig. 4.6). Because the effective ionization degree measures the ratio of the ion radius over the average distance between target electrons, the ion looks less point-like for larger $\tilde{v}_F$, i.e., for larger $Z_2$, if $q$ is kept constant.

The experimental data of effective ionization degrees at high energies as a function of $Z_2$ have been summarized in [111] as “Effective charge parameters are higher in light stopping media than in the heavy ones,” which seems to contradict the calculations here. After a closer look at the targets used there ($^{14}$Si, $^{28}$Ni, $^{29}$Cu, $^{46}$Pd, $^{47}$Ag) and at the Fig. 1 given one realizes that this subset of values would stimulate the same (and on the basis of a complete set wrong) conclusion within the Kaneko theory. This discrepancy is not actually present.
These results are based on intermediate results that are shown in Fig. 4.7 for some examples.

The theory sets up strong contributions of the inner target shells to the heavy ion stopping even at small velocities (upper Fig. 4.7), whereas the proton stopping is built up more by the free electrons there (lower Fig. 4.7). First this does not seem to agree with the correlation of the effective ionization degree with the target Fermi energy. One would not expect an influence of $v_F$ on the ratio $\gamma^2 \sim S(q)/S(q = 1)$, if $S(q)$ is strongly affected by the inner shells. The resolution of this puzzle is: the stronger influence of the free electrons on the proton stopping (on the bare ion with $q = 1$) than on the ion with small $q$ is produced by the factor $\rho^2_m(k)$ in the integrand of the stopping number (4.6). For $q = 1$ all shells are compiled by the $z$-integral in an equal manner. If $q$ is small, the factor suppresses the contributions at small $z$, i.e., small wave numbers, and therefore the target shells with large $\chi^2$, small $\bar{q}$ and $k_F$. This influence of the density parameter on the momentum spectrum that is “offered” by the target is shown in Fig. 4.2b. The cross section per electron is smaller at larger densities (!) in the case of free electrons and hence in the case of targets with a stopping cross section that is dominated by free electrons. Proton stopping cross sections for $Z_2 = 11 \ldots 14$, $3d$ and $4d$ metals in the PSE are anti-correlated to $v_F$. Finally, the EL $dE/dx$ in
the FEG is positively correlated with $v_F$, because it follows by the multiplication with the electron density (a factor $\propto v_F^2$).
To summarize, the calculation of the effective ionization degree by the ratio of the total heavy ion and proton stopping cross sections is a division of a functions which is rather independent of \( v_F \) through a function which is anti-correlated to \( v_F \), and therefore correlated with \( v_F \). This is the origin of the positive correlation between \( \gamma^2 \) and \( v_F \) in this BK-Kaneko theory.

### 4.4 Effective Charges as a Function of Ion Velocity

Up to here it was only discussed whether a formal relation between the effective charge fraction and \( v_F \) exists which can be extracted from \( Z_2 \) dependences. Below it is shown that the substitution of the target by merely the part of the free electrons leads even to quantitative agreement with the results by all shells at high velocities. If the free target electrons contribute the same percentage to the total stopping power felt by protons as to the one felt by heavy ions, programs — like TRIM85 — may calculate reliable heavy ion energy losses through scaling of effective charge degrees with proton data. This is also true, if the share of the free electrons is very small or depends on velocity. This effect is first demonstrated with the help of the Kaneko theory. In the BK ion model the ionization degrees \( q \) of heavy ions are individually varied at each velocity for each ion-target pair until the Kaneko theory provides the effective charge degree of the ZBL results. (It is a consistent re-determination of \( q \) starting from known values of \( \gamma \) as in Chapt. 3.) This implicitly fixes within the Kaneko theory not only \( S \) but also the contributions \( S_{\text{free}} \) for heavy ions, using \( q = 1 \) for protons. The results are shown in the left plots of Fig. 4.8.

The right plots in Fig. 4.8 demonstrate on the basis of the same data that the replacement

\[
\gamma^2 = \frac{S(Z_1, q, v)}{S(Z_1 = 1, q = 1, v)Z_1^2} \approx \frac{S_{\text{free}}(Z_1, q, v)}{S_{\text{free}}(Z_1 = 1, q = 1, v)Z_1^2}
\]

is more and more accurate as the ion velocity increases. The few free electrons then represent (in the sense of the effective charge fraction) all target electrons, though their share \( S_{\text{free}} \) in \( S \) sometimes is only a few 10%. The physical explanation is: at high velocities the atomic variables like binding energies and characteristic wave numbers of the target electrons become increasingly unimportant and may be approximated by a binary collision approximation of the ion-target interaction. The stopping cross section \( S_{\text{sh}} \) of a shell becomes equal to the occupation number \( N_{\text{sh}} \) multiplied by the
Figure 4.8: Left: the total and partial stopping cross sections for $^{15}\text{P} \Rightarrow ^{14}\text{Si}$ and $^{15}\text{P}$, $^5\text{B} \Rightarrow ^{28}\text{Ni}$ with fitted $q$-values that set the ratio of total cross sections for ions and protons in the Kaneko theory equal to the ZBL effective charges. Right: bold lines are the squared effective ionization degrees that are enforced by this calculation $S(Z_1, q, v) / [Z_1^2S(1, 1, v)]$; thin lines show the values by dividing the share of free target electrons, $S_{\text{free}}(Z_1, q, v) / [Z_1^2S_{\text{free}}(1, 1, v)]$. The complementary $^1\text{H}$ data are given in Fig. 4.3. Dashed lines are the values of $q$. 
cross section of one electron, and the transition from the left side of Eq. (4.12) to the right side is just a reduction of these occupation numbers that are the same for heavy ions and protons. The right parts of Fig. 4.8 show that the representation (4.12) may work, though the values of $S_{sh}$ are not yet proportional to $N_{sh}$ in the left parts, indicating that binding features are not yet negligible. The preceding explanation is based on the approximate equality of the Kaneko numbers $L_{sh}$ of all target electrons, but may be moderated and generalized by watching $S_{sh}$, i.e., using the shells as basic units: the share of the free electrons to the stopping cross sections does not need to be $N_{\text{free}}/\sum_{sh} N_{sh}$. It is sufficient if it does not dependent on the ion atomic number. Remembering Chapt. 3.1 this merely means that the ion must be sufficiently small compared with the average spacing between target electrons. This limit is already reached at rather low velocities, or if $Z_1$ is small (here $5B$ versus $15P$) earlier because the ionization degree is larger.

Aside these explanations at high $v$, the free target electrons themselves represent the major contribution to the total stopping cross section at very small velocity, because the inner shells are hardly excited. Then (4.12) should become valid directly. In this limit, however, the theoretical model breaks down, which reveals itself as no more values of $q$ can be found that reproduce the requested effective charges. The curves of Fig. 4.8 end at this point at small velocity. (Some of the $q$ had already to be chosen with negative, unphysical values as the dashed lines document.) This region of small $v$ that is not accessible via a fit of $q$ becomes larger as $Z_1$ becomes larger. Obviously the model over-estimates the energy loss of heavy ions at small velocities. This provides the motivation to improve the original model in Chapt. 5.

In addition, the approximation (4.12) is improved if the free electrons represent a larger percentage of all target electrons. One may understand, why the calculation for the semiconductor $^{14}\text{Si}$ with 4 out of 14 electrons considered to be free works better in the approximation by free electrons than the calculation for the metal $^{28}\text{Ni}$ with 2 out of 28.

Post Scriptum: the two investigations presented in this chapter that deal with the use of the FEG model to determine effective ionization degrees vary one of the two parameters of $S(Z_2, v)$ at a time in an “orthogonal” manner. When investigating the correlation, the FEG has been parameterized by $v_F$ as found in the ZBL tables, later by $N_{\text{free}}$ and $\rho_{at}$ as provided by the Kaneko
theory. Both ways are not strictly equivalent: to verify the assumption (3.23), the correlation has been consistently tested with the values of $v_F$ (which is $1.2v_0$ for $^{28}$Ni, meaning 4.3 free electrons per atom, and $0.974v_0$ for $^{14}$Si, meaning 4.23 free electrons per atom), without stiffening the test. Hence at least two of the Ni 3d electrons contribute to the Fermi velocity, not just the two electrons that are treated as free by the Kaneko theory. For Si on the other hand, the 4.23 ZBL electrons are close to the 4 electrons of the Kaneko theory. (The rather small size of the $1s^22s^22p^6$ ion cores in the Si crystal contributes to this. The density of states of the valence band [61, 248] has about three maxima. One may derive a plasmon energy rather close to the experimental value by shuffling the density of states until it shows the root dependence of the FEG. If the band dispersion is unfolded into the second and third Brillouin zone, its shape becomes also well parabolic.) The ZBL method to incorporate Fermi velocities derived from experimental plasmon energies (these often from electron energy loss experiments) thus reaches far beyond the simple division into an integer number of bound and free electrons of the Kaneko theory, and implicitly uses information on the dynamical response beyond linear susceptibility and RPA. One might guess that the somewhat poorer representation by free electrons in the case of $^{28}$Ni in Fig. 4.8 stems from a poorer division of the $N_{sh}$. But the same calculation for $^{15}$P $\Rightarrow$ $^{26}$Fe within the Kaneko theory does not provide a better agreement in (4.8), though the Kaneko value $r_s = 2.118 \rightarrow v_F = 0.906v_0$ is close to the ZBL value $v_F = 0.92705v_0$. This argumentation is not decisive. The open problem of the Kaneko theory rather seems to be the adequate representation of $d$ bands in transition metals. The division into two classes of free electrons and of electrons with Gaussian momentum distribution within this theory is a too rough model in particular for proton energy losses. (It typically predicts two maxima in the curve.) This aspect is touched again shortly in Sects. 5.5, 5.6.

4.5 Summary

The Kaneko theory is based on a more fundamental representation of the target energy loss function than the preceding BK and ZBL descriptions. It brings out the reasons for the success of a description as a FEG: In the low as well as in the high velocity region an effective charge fraction which is exclusively calculated from the free target electrons yields representative values that would
also be derived from the set of all target electrons. Though the heavy ion energy losses that are implicitly calculated in the BK theory are much too small at middle and high velocities, because they neglect the excitation of inner shells, the subsequent use of the theoretical effective ionization degrees only and insertion into the heavy ion scaling rule yields useful results. The experimental proton data that are added contain the indispensable information on the polarizability of all target shells and play a key role within the BK and ZBL theory.

Through this carefully directed mobilization of a set of experimental proton data that is easy to survey, ZBL’s method of calculation of heavy ions becomes fast and universal. In this respect the subsequent treatise on the Kaneko theory does not aim at finding a rivaling method for applications in Monte-Carlo programs, but wishes to throw light on hitherto concealed effects of the ion-solid interaction.

The Kaneko theory offers the advantages that are known from the Lindhard theory over calculations which are in essence derived from the Bethe theory [118]. Without further assumptions the EL is calculated over the entire velocity interval consistently via the dielectric function. Questions concerning “close” and “distant” collisions do not arise. In the shell-by-shell formulation, target shells are “activated” and “de-activated” smoothly as a function of velocity, based on parameters known from atomic theory. Notions like “shell corrections” and “effective ionization potentials” that slip in if one emanates from the Bethe theory [5, 231], become extraneous and superfluous. They may at best gain in significance if one is interested in efficient, fast implementations that are based on parameters that might be extracted from the Kaneko theory.
Chapter 5

Extensions and Corrections to the Kaneko Theory

5.1 Motivation

The application of the Kaneko theory demonstrated above shows that the theory calculates heavy ion stopping powers by direct use of (1.6) and therefore from a more ab initio point of view than the BK and ZBL methods. The determination of the ion form factor and the energy loss function that were part of the three steps of the BK and ZBL calculations remain. The third step, the computation of the effective charge and use of the heavy ion scaling rule, is dropped. The heavy ion energy losses are decoupled from the proton calculations; a positive side effect is an improved insensitiveness against terms of higher order in $Z_1$, which play an increasingly minor role as ions become heavier.

The driving force of the subsequent chapter of this thesis is the deterioration of the results with increasing $Z_1$, which was testified in the previous sections. Implicitly there is the question, why the theory was presented in the literature often only for light ions, for heavy ions with bad quantitative results only once [127], in high-charge states [131], or with an additional scaling of its effective charges [256, 257]. (The contents of this investigation will be published in [158, 160].)
5.2 Adaptation of Characteristic Wave Numbers

The characteristic wave numbers $\bar{q}_1$ of the shells are not free parameters. Some freedom is brought in as the “double zeta” functions on one hand or the extended bases of the Clementi-Roetti (CR) tables on the other may be used in (4.7). (The name “double zeta” indicates that each orbital with a principal quantum number is represented by two functions with screening wave number “zeta”.) Examples are listed in table 5.1.

<table>
<thead>
<tr>
<th>shell</th>
<th>Mg $^1$S</th>
<th>Si $^3$P</th>
<th>Fe $^5$D</th>
<th>Fe $^3$F</th>
<th>Co $^4$F</th>
<th>Ni $^3$F</th>
<th>Cu $^2$S</th>
<th>Cu $^2$D</th>
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<tr>
<td>$2s$</td>
<td>1.518</td>
<td>1.496</td>
<td>4.089</td>
<td>4.166</td>
<td>4.172</td>
<td>4.250</td>
<td>4.429</td>
<td>4.625</td>
</tr>
<tr>
<td>$3s$</td>
<td>1.3337</td>
<td>1.3344</td>
<td>1.406</td>
<td>1.410</td>
<td>1.413</td>
<td>1.473</td>
<td>1.532</td>
<td>1.584</td>
</tr>
<tr>
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<td>.3365</td>
<td>.3354</td>
<td>.3365</td>
<td>.3422</td>
<td>.3493</td>
<td>.3125</td>
<td>.3151</td>
<td>.3640</td>
</tr>
<tr>
<td>$2p$</td>
<td>1.421</td>
<td>1.378</td>
<td>1.839</td>
<td>1.797</td>
<td>4.228</td>
<td>4.429</td>
<td>4.617</td>
<td>4.856</td>
</tr>
<tr>
<td>$3p$</td>
<td>.3932</td>
<td>.3833</td>
<td>1.266</td>
<td>1.262</td>
<td>1.265</td>
<td>1.328</td>
<td>1.390</td>
<td>1.436</td>
</tr>
<tr>
<td>$3d$</td>
<td></td>
<td></td>
<td>.9629</td>
<td>.8447</td>
<td>.8229</td>
<td>.8837</td>
<td>.9272</td>
<td>1.035</td>
</tr>
</tbody>
</table>

Table 5.1: Values of characteristic wave numbers $\bar{q}_1 a_0$ by the “double zeta” functions (column ‘d’) and the functions with the extended basis sets (column ‘e’) of the CR tables [50] as by insertion into (4.7). The publication [130] quotes “double zeta” values for Mg, Fe and Cu and values with the extended basis for Si. Cu $^2$S is a $3d^{10}$ $4s^1$ and Cu $^2$D a $3d^9$ $4s^2$ configuration. The values in parentheses do not come into play for solid targets, because the corresponding shells are replaced by the LW model.

Even rougher and faster estimates are obtained, if $\varphi_1$ is represented by a single orbital

$$\varphi_1(r) = (2\zeta)^{n+1/2}r^{n-1}e^{-\zeta r}Y_0^0(\hat{r})/\sqrt{(2n)!}$$

with principal quantum number $n$. The coefficient $\zeta$ could be taken from the “single zeta” values of the CR tables [50] related to the expansion coefficient which is closest to ±1. Using (3.24) in (4.7) with the “single zeta” approximation yields $\bar{q}_1 = \frac{1}{2}\pi^{1/6}\zeta$ if $n = 1$, $\bar{q}_1 = \frac{1}{2}\pi^{1/6}\zeta$ if $n = 2$, and $\bar{q}_1 = 2^{-8/3}\pi^{1/6}\zeta$ if $n = 3$ as the width of the momentum distribution. The proportionality to the size parameter of the shell is a realization of the uncertainty relation.

Alternatively one could obtain $\bar{q}_1$ by setting the quotient $\int p^t w(p) d^3p / \int w(p) d^3p$ of the ansatz (4.2) equal to moments of the momentum expectation value $\langle p^t \rangle$ derived from more exact atomic calculations. $\bar{q}_1$ would have to be $\sqrt{\pi\langle p^t \rangle}/2$, $\sqrt{2\langle p^2 \rangle}/3$, $2/(\sqrt{\pi\langle p^{-1} \rangle})$ and $\sqrt{2/(p^{-2})}$. With $\langle p^t \rangle$ again from RHF calculations [87], the conspicuous results are:
The difference of these alternative values to the Kaneko values is largest for \( p \) and \( d \) sub-shells. This is explained and discussed in Sect. 5.5.

The alternative values are for example 25–30% higher than the Kaneko values for the 1\( s \) shells, \( Z_2 = 3, \ldots, 28 \) and \( t = 1 \), 32–57% higher in the same group of 2\( s \) shells, but approach them if they are derived from the moments \( t = -1 \) and \( -2 \). This results from the fact that the Kaneko values are derived from wave-functions at \( p = 0 \), whereas the moments characterize the global shape of the occupancy everywhere in momentum space. The smaller and negative moments put more weight on the occupancies close to \( p = 0 \) and hence come closer to the Kaneko values. Looking at Fig. 4.1 the curve of the RHF data is lying to the left of the values of the Gaussian approximation, which seems to propose a slightly smaller first moment. At first glance this seems to contradict that the values extracted from RHF moments are larger, because the actual estimates for the Si 2\( s \) shell with the preceding equations are [87]:

<table>
<thead>
<tr>
<th>( t )</th>
<th>-2</th>
<th>-1</th>
<th>1</th>
<th>2</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \bar{q}_1 a_0 )</td>
<td>1.952</td>
<td>2.052</td>
<td>2.906</td>
<td>4.205</td>
</tr>
</tbody>
</table>

The first note is that the visual estimate of the moment of the radial part in Fig. 4.1 has to be compared with the moment \( t = -1 \) of the table (since the Jacobi determinant adds a factor \( p^2 \)). Nevertheless, the value is larger than the value \( \bar{q}_1 a_0 = 1.89 \) of Fig. 4.1 and is solely caused by the contributions in the region \( p a_0 > 4 \), as a numerical integration demonstrates. The contradiction is only spurious, but leaves open the question, which moment and which \( \bar{q}_1 \) provides the best parameterization of the excitation spectra.

The values derived with these “global” estimates generally tend to increase the characteristic wave numbers. As a rough estimate, the maximum of the stopping cross section \( S_{\text{bnd}}(v) \) shifts proportional to \( \bar{q}_1 \). In conclusion, the contributions of the s-type sub-shells would move to higher velocities if the characteristic wave numbers would be derived from moments of the momentum distribution.
5.3 Excitation Energy Gaps of Inner Target Shells

Proton data derived with the original Kaneko theory generally compare well with experimental data (Fig. 4.3 and 5.1).

Figure 5.1: Proton stopping cross sections $S$ and $S_{sh}$ in targets of $^{12}$Mg or $^{14}$Si. Dotted lines: original Kaneko theory. Bold lines: ZBL [261]. Thin lines: results under the influence of the additional energy gaps of Tab. 5.2. The occupation numbers $N_{sh}$ are given in parentheses.

In the region of high velocities they over-estimate the stopping power by about 5 to 10%. $Z_1^3$ effects would increase it by additional 3% for velocities above [16]. One may assume that the over-estimation is caused by a too large energy loss function, because the integral (4.3) permits the scattering of an electron without constraints to the momentum or energy transfer. However, excitations with energy transfer $h\omega$ smaller than the binding energy $E_g$, i.e., that scatter into band gaps or into fully occupied states cannot contribute to the polarization. In principle, $E_g$ should represent the smallest energy difference between the shell level and the next higher empty or partially filled band. It was approximated in the subsequent application by the energy difference between the shell and the highest occupied state of the free target atom [50] (Fig. 5.2). Band widths and band dispersions of the solids have been neglected and replaced by simple atomic models so
Figure 5.2: Scheme of the estimate of excitation gaps for the example $^{14}\text{Si}$. On the left the ladder of atomic levels. On the right the extracted excitation gaps for the ten electrons in the three inner shells, which are not ascribed to the “shell” with four free electrons.

<table>
<thead>
<tr>
<th>shell</th>
<th>Mg $^{1}\text{S}$</th>
<th>Si $^{3}\text{P}$</th>
<th>Fe $^{5}\text{D}$</th>
<th>Cu $^{2}\text{S}$</th>
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<td>261.1</td>
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<tr>
<td>$2s$</td>
<td>3.515</td>
<td>5.859</td>
<td>31.68</td>
<td>40.58</td>
</tr>
<tr>
<td>$3s$</td>
<td>3.911</td>
<td>4.773</td>
<td>27.16</td>
<td>35.38</td>
</tr>
<tr>
<td>$2p$</td>
<td>2.029</td>
<td>3.959</td>
<td>27.16</td>
<td>35.38</td>
</tr>
<tr>
<td>$3p$</td>
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<td>3.086</td>
<td></td>
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</tr>
<tr>
<td>$3d$</td>
<td>0.3887</td>
<td>0.2528</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 5.2: The energies $E_g$ that have been used here to limit/cut the Kaneko susceptibility in (5.1), in atomic units. For $^{12}\text{Mg}$ they are the energy differences to the $3s$ shell, for $^{14}\text{Si}$ to the $3p$ shell and for $^{26}\text{Fe}$ and $^{29}\text{Cu}$ those to the $4s$ shell of the free atoms $[50]$.

In addition a simple manual correction was used, and $\text{Im}\chi_R$ of the Kaneko theory changed via the replacement

$$\text{Im}\chi_R(k,\omega) = 0, \quad \text{falls } |\hbar\omega| < E_g.$$  \hspace{1cm} (5.1)

This is likewise found in $[10]$, where the susceptibility of a FEG was the starting point to model energetically low shells. It is not equivalent to a shell-dependent cut in the ion velocity that was presented in $[243]$ (22) to confine the Bethe theory, because they would cut “diagonally” in $(k,\omega)$-space, but we “horizontally” (Fig. 1.4). Eq. (5.1) reads in terms of Kaneko variables

$$\text{Im}\chi^R(u, z) = 0, \quad \text{if } uz < \frac{1}{2} \left(\pi\chi^2\right)^2 \frac{E_g}{2E_0}.$$  \hspace{1cm} (5.2)

The values for $|\hbar\omega| > E_g$ or the “shells” of free electrons are simply taken over as they are.
This intervention in $\text{Im}\chi^R$ ought to be accompanied by a re-determination of $\text{Re}\chi^R$ via (H.6), but no closed formula was found to represent these values. Because the only alternative is a time-consuming numerical integration during the evaluation of (4.6), the data of Figs. 5.1 to 5.8 have been calculated by use of the original values of $\text{Re}\chi^R$ in $\epsilon_{\text{sh}} = 1 + \chi^R$ and (4.6). To test the error that is linked to this violation of the KK relation, the values of $\text{Im}(1/\epsilon_{\text{sh}})$ are compared in one example in Fig. 5.3 for the cases that uses the re-determined (exact) and the case of the original $\text{Re}\chi^R$.

Figure 5.3: (a) Contour lines of $-z\text{Im}[1/\epsilon_{\text{sh}}(z,u)]$ and (b) of $-\text{Im}[1/\epsilon_{\text{sh}}(k,\omega)]$. Parameters represent the Si 2$p$ shell: $q_1a_0 = 1.797$, $E_g = 3.959$ a.u., $N_{\text{sh}} = 6$ and $l = 0$ in the spirit of the original theory, similar to Fig. 4.2. The bold hyperbola and the bold horizontal line divide the area acc. to (5.1)–(5.2). The energy-cut sets the values below and left to it to zero. Continuous lines use the energy-cut (5.2) including the re-determined $\text{Re}\chi^R$ that complies with the KK formula, the dashed lines simply use the approximate, original values.

It shows that the differences are small and restricted to small areas close to $\hbar\omega \approx E_g$, the bold curves. Inclusion of the KK analysis would lead to a smaller reduction of the integrand in the vicinity of the plasmon ridge and another decrease of the stopping.

The plasmon pole defined by (4.10), which appears in the upper left corner of Fig. 5.3,
Figure 5.4: Contour lines of $\text{Re}\chi^R(k, \omega)$ (left) and $\text{Im}\chi^R(k, \omega)$ (right) with the parameters and meanings as in Fig. 5.3. The bold line of the energy cut $\hbar \omega = E_g$ is horizontal for this choice of axes. On the left we see that in this case the plasmon pole (characterized by $\text{Re}\chi^R = -1$ and $\text{Im}\chi^R \approx 0$) run above $E_g$, and survives (without KK analysis) if the energy-cut is made. In the right picture the simple ansatz (5.1) means that the dashed and continuous lines are identical. The combination of these curves yields Fig. 5.3.

is within the region that is left intact by the energy-cut. The simple criterion $E_g > \hbar \omega_p$ would mean that the energy-cut removes the plasmon excitation of all $s$ shells, of $2p$ shells of the target elements heavier than ("beyond") $^{14}\text{Si}$, of $3p$ shells beyond $^{25}\text{Mn}$, of $4p$ shells beyond $^{42}\text{Mo}$, of $5p$ shells beyond $^{56}\text{Ba}$ and of $3d$ shells beyond $^{43}\text{Tc}$.

The effect of this energy-cut is established in Fig. 5.1. The high-energy tail of the theory is improved and now fits convincingly to the proton data collected by Ziegler, Biersack and Littmark (ZBL). Another difference is that the stopping cross sections of shells with an energy-cut are no longer $\propto v$ at small velocities but grow with a higher power of $v$ [63, 83, 245]. At small velocities the total stopping cross sections become worse than the original theory, because the contributions of the inner shells decrease. This residual under-estimation, however, is a known feature of the RPA, as shown among others in Chapt. 2.2 and also an effect of the neglect of non-linear susceptibilities.

92
of the FEG \[153, 183, 201, 217].

A more fundamental alternative consideration of band gaps may be found by insertion of
the energy difference into the Schrödinger equation and therefore into the propagators. For the
free electron gas one would add an energy difference \( E_g \) for particles inside and outside the Fermi
sphere, replacing (1.13),

\[
G_0^0(k) = \frac{\Theta(k - k_F)}{k_0 + E_g/\hbar - \omega_k + i\eta} + \frac{\Theta(k_F - k)}{k_0 - \omega_k - i\eta}.
\]

(The same results of the susceptibility follows if \( E_g \) is transferred with the opposite sign into the
denominator of the second term.) After integration over the frequency in (1.12) and switching
to the retarded polarization one obtains a form that looks similar to [71, (15)], where a \( E_g^2 \) is
inserted into the resonance denominator of a classical approximation to the susceptibility. After
the \( \Theta \) function is replaced by (4.2), the result for the linear susceptibility within the RPA may be
summarized as follows: In the formulas of App. [1.3] \( u - z \) must be replaced by \( u + z + u_g \) and \( u + z \)
by \( u + z - u_g \), with \( u_g \equiv (\pi \chi^2)E_g/(4E_0z) \). In this formulation the KK analysis yields (using the
formulas already known) closed expressions for \( \text{Re}\chi^R \). In contrast to the method proposed above,
we do not get genuine gaps in \( \text{Im}\chi^R(\omega) \), but only a strong suppression of the energy loss function.
Because the reduction of the stopping cross sections in the high-velocity region is much stronger
and more unrealistic than with the simple cut [5.1], this ansatz is not pursued in detail here.

### 5.4 The Model of the Dead Sphere for Expanded Ions

#### 5.4.1 Suppression of the Target-Polarizability at the Ion Site

The preceding chapter dealt with protons as projectiles to study the dielectric features of the target,
because they are the probes with the most accurately known form factor \( \rho_m(k) \). We turn towards
partially stripped, heavy ions. Let the reference model of the ions be the BK ion model (3.1)–(3.2),
which was used in Chaps. 4.3 and 4.4, to describe the ion with \( N \equiv Z_1 - Q \) bound electrons and
size parameter \( \Lambda \), and let us refer to the ionization degree \( q \) and \( \tilde{\Lambda} \) of the ZBL program [261]. By
these means the shell structure of the ion (Fig. 3.4) and the related \( Z_1 \) oscillations can be taken
into consideration and included.
Because $q$ and $\Lambda$ have been fixed by a joint fit to experimental data \[261\] we may hope that prospective artifacts of one of both parameters is moderated by using both together. The disadvantage might be that the pair of parameters was bound to the correctness of the fit formula \[3.23\], which we replace explicitly by using \[4.5\]–\[4.6\] for protons and for heavy ions.

The broken lines compared with the bold lines in Fig. 5.5 illustrate that the stopping cross sections of the known theory become worse and worse as $Z_1$ increases. This is most evident in the region of the maxima of $S(v)$ \[127\].

The discrepancy is explained and removed subsequently. This is done independent of the actual target model, insofar no feature of the dielectric function is utilized. The key idea is that the polarization charge $\rho_p$ \[1.1\] vanishes inside a sphere of radius $r_c$ around the ion nucleus,

$$\Phi_{\text{ind}}(r, t) = \frac{1}{4\pi \epsilon_0} \int_{|r' - vt| > r_c} \frac{\rho_p(r', t)}{|r - r'|} d^3r'. \tag{5.3}$$

This sphere is baptized “dead sphere” in free association with the dead-layer model of the vanishing exciton polarization close to a semiconductor surface \[236\]. The excitation of target electrons in close neighborhood to the ion nucleus, where the available space is already occupied by the electrons bound to it, ought not to be permitted (in contrast to the previous calculations) and therefore not contribute to the polarization. Inside this region the electron density ought to be defined by the atomic model of the ion and be adequate there. The jellium model of an infinitely extended, homogeneous positive background \[254\] should be replaced inside the sphere by the local atomic theory which provides the better “external” potential for these electrons. The model we have in mind eliminates the contributions of two processes under the assumption that they are heavily suppressed in reality, the processes where (i) a target electron is scattered from a larger distance into the close neighborhood of the ion nucleus, and where (ii) a target electron is scattered from

<table>
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<th>shell</th>
<th>$B^0$</th>
<th>$B^{1+}$</th>
<th>$P^0$</th>
<th>$P^{11+}$</th>
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<tr>
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<td>0.499</td>
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</tr>
</tbody>
</table>

Table 5.3: Shell radii in units of $a_0$, defined by the maxima of $4\pi r^2|\varphi_1(r)|^2$, where $\varphi_1(r)$ are the CR wave-functions \[50\] with the extended basis sets (→ Fig. 3.10 and Tab. 3.2).
Figure 5.5: Electronic stopping $S/Z_1^2$. Bold lines: ZBL [261]. Dashed: original Kaneko theory. Thin continuous: Kaneko theory with energy cuts as in Fig. 5.1. Lines labeled with ‘n’: no dead sphere. Lines labeled with ‘K’, ‘L’ or ‘M’: obtained by (H.3), where $r_c$ has been set equal to the radius of the corresponding ion shells acc. to Tab. 5.3. The abscissa $N$ shows the number of electrons that remain bound to the ion. The kinks are caused by the steps in the size parameter, Fig. 3.4.

the vicinity of the ion nucleus into a region outside the dead sphere.

If we confine the whereabouts of target elements this way through the mere presence of the
heavy ion and transfer this aspect to the local polarization, we have made a first step towards a
non-linear theory, which calculates the susceptibility including the electrons bound to the ion. Even
if we assume that a completely impenetrable sphere exists for target electrons around the site of the
ion, we do not expect that the cut radius is equal to the sphere radius, because for farther jumps
in this hopping model for the polarization (as described) the polarization would better be booked
at only half the step width of these “jumps,” i.e., nearby the center of mass of these electron-hole
pairs.

The calculation of the new stopping powers is presented in App. 1. The best fit of the
dead-sphere radius to improve the predictions of the model is close to the ion-size parameter $\tilde{\Lambda}$
(Fig. 5.5 and 5.8), which itself is a function of the ionization degree and hence the ion velocity (Fig.
3.4). This is the decisive hint that the physical picture of an unpolarizable inner region around the
ion nucleus is correct. In the case of $^{15}$P, $r_c$ is comparable with the radius of the L shell at $v \approx 0$,
and tends towards the radius of the K shell, if only two electrons remain bound. In the case of
$^{33}$As, $r_c$ has about the size of the radius of the M shell and approaches the radius of the L shell for
$N \approx 12$. In the case of $^{5}$B, however, the best result is obtained without any dead sphere. This is
also reasonable, because beyond $v \approx 2v_0$ only $N \leq 2$ electrons remain bound. Their density is not
much larger than the density of the target electrons, their repulsion too small and localization too
weak to prevent a penetration by target electrons.

Sect. 5.5 deals with some more examples for $r_c \propto \tilde{\Lambda}$ in Fig. 5.8 which — despite use of the
stepped $\tilde{\Lambda}$ (→ Fig. 3.4) — fit a convincingly large velocity region of stopping data.

5.4.2 How Local is the Stopping Force? A Comment on the LPDA.

If we repeat the calculation of App. 1 for punctiform ions $\rho_m(k) = Z_1e$ instead of the BK charge
cloud, we simply get with 3.721.1

$$\int_0^\infty dk' \left[ \frac{\sin(k' - k)r_c}{k' - k} + \frac{\sin(k' + k)r_c}{k' + k} \right] = \int_{-\infty}^\infty dk' \frac{\sin(k' + k)r_c}{k' + k} = \pi,$$

$$\Rightarrow \frac{dE}{dx} = \frac{Z_1^2e^2}{2\varepsilon_0v^2\pi^2} \int_0^\infty \frac{dk \sin kr_c}{k} \int_0^{kv} \omega \operatorname{Im} \frac{1}{\epsilon(k, \omega)} d\omega$$

(5.4)
generalizing (1.6). This helps to investigate the contribution of polarization charges in different distances to the total stopping force. The polarization charges in the neighborhood of the punctiform ion are divided into concentric spherical shells, and we obtain for example Fig. 5.6.

Figure 5.6: Electronic stopping in the FEG and in RPA (Sect. 1.3) at two different values of $v_F$ with dead-sphere radii $r_c$ between 0 and $2r_s$ for a point charge acc. to (5.4). $r_s$ is the one-electron radius (1.5) at the corresponding electron density. [The curves without dead sphere ($r_c = 0$) are also part of Fig. 1.2] Negative values, i.e., accelerating forces, indicate in essence that the next half period of the “wake field” has been reached.

It shows that the removal of the polarization charges in a distance of $2r_s$, twice the spacing between target electrons, removes also the main contribution to the electronic stopping. In other words: due to the $1/r$ potential between the polarization charges and the ion, the stopping force “arises in the close vicinity.” This is obviously also true above the onset of the plasmon excitation, which is indicated by a kink left from the maxima.

From this point of view one may comment on the ansatz of a local plasma density approximation (LPDA) and the success (at least for protons), Fig. (3-11)–(3-14) in [261] and [128]: Though the polarization charges and the wake field extend much further into the solid-state target, the excitations from within two electron distances to the ion dominate the stopping. The basic objection
against the LPDA that in particular plasmons build a “long-range” interaction and that the polarization extends over several atomic distances and electronically very inhomogeneous regions, is thus defeated. In addition, the stopping force reveals a self-scaling of its region of influence, as Fig. 5.6 points out by comparison of two systems with a ratio of electron densities of $5^3 : 1$. The region shrinks suitably in absolute units in dense electron systems. If in a LPDA calculation a punctiform ion passes through the inner shells of a target atom with locally large $v_F$, the region of important influence is reduced, and the assumption of homogeneity made by the LPDA does not necessarily deteriorate.

For heavy ions the LPDA should become increasingly worse, if the assumption of the “dead sphere” is basically correct, because the target electrons which stop the ion through their polarization would have to stay farther away and outside the sphere, and their density should be increasingly uncorrelated with the (unperturbed) target electron density at the site of the nucleus.

The objection against the LPDA that it over-estimates the energy losses by inner-shell excitations, because it neglects the binding energies [120, 186], is not touched by this remark.

The assumption that the stopping force of an ion may be calculated via the electron density at the momentary site of the ion is called LPDA throughout this thesis. A name collisions with the LSDA in DFT is thought to be avoided and the acronym LDA to be reserved for the spin-independent formulation of DFT. Hints of the literature at prospective transformation between the LPDA and the LSDA are not known to me, the corresponding section of [243] does also contribute to the problem either. The LPDA takes all the information on the target structure from the electron density at the ion site and implicitly assumes a homogeneity. The LSDA on the other hand means a representation of the energy as a space integral over a density functional which is believed to be local — a weaker assumption among others, because the result depends absolutely on the electron densities at all places. Even after a time derivative of this energy, this space integral similar to (1.4) would persist. The approximate equivalence between the LSDA and the LPDA can only be demonstrated via the detour that the local density at the ion site itself is a functional of the extended electron density according to DFT, and both may be transformed into each other within an approximation, which has not been formulated up to now.
5.5 Susceptibilities of $p$ and $d$ Sub-Shells

We return to the Kaneko model and observe that the theory predicts the maximum of the EL of $^{33}$As ions in Fig. 5.5 and even more of $^{92}$U ions in [127, Fig. 1] at a smaller velocity than ZBL. Is another weakness of the model hidden here? The maximum of light ions, however, is predicted rather accurately and practically determined by the EL due to the free target electrons. If $Z_1$ grows, the position of the maximum is rather determined by the contributions of the lower-lying $p$ and $d$ sub-shells. This leads to the impression that a poorer treatment of sub-shells with nonzero angular momentum quantum number is the reason for a worse prediction of the maximum for heavy ions. This section investigates a possible reason.

The Gaussian approximation (4.2) to the momentum distribution was derived by an application of statistical physics [124]. It simply reflects the Boltzmann factor with an energy term given by the dispersion of free electron in an isotropic system. The ansatz automatically ignores relations to quantum numbers in atomic systems. Subsequently this momentum distribution is interpreted directly as a representation of atomic wave-functions in momentum space. The wave packets of plane waves are meant to remain the basis of this representation, which means that we still obtain closed formulas for the susceptibility. (This major advantage of the theory rests on the fact that we do not have to deal with squares of transition matrix elements in the numerator of the RPA expression and in (4.3) but rather squares of momentum densities). An approximately Gaussian shape of $|\varphi_1(p)|^2$ is obtained for all angular momentum quantum numbers $l$, if the wave-function $\varphi_1(r)$ is averaged over all directions $r$, which is equivalent to a replacement of the angular dependence $\propto Y_{lm}(\hat{r})$ by the constant $\propto Y_0^0(\hat{r})$ in real space (3.24). Because the calculation of the susceptibility in the Kaneko ansatz deals only with the momentum representation of the wave-function, this average should be calculated as late as possible. That means we first make the transition to the momentum representation of the atomic wave-functions and average over the directions of $p$ afterwards, i.e., replace $Y_{lm}(\hat{p})$ by $Y_0^0(\hat{p})$. The factor $(ip)^l$ in (3.24) recommends the generalized ansatz

$$w(p) = c_l^2 p^{2l} \exp \left\{ - \left( \frac{p}{\bar{q}} \right)^2 \right\}, \quad (5.5)$$

if the sum is approximated again by a Gaussian. The shells with free electrons and with $s$ electrons...
are not touched. Another fitting form, i.e., using rational functions, was used by Moneta et al.\cite{170} in $1/r$-potentials. This form is even simpler than the original Kaneko ansatz, because it is completely degenerate with respect to the angular momentum and magnetic quantum numbers. The Kaneko theory is not degenerate because it attributes an individual parameter $\bar{q}_1$ to each sub-shell of each element of the PSE.

To fix the free normalization factors $c_l$, we re-analyze the transformation of the atomic densities with strong local variations of the density to the momentum distribution in the original theory. The equations (3.15) and (4.1)–(4.6) may be summarized as

$$\frac{dE}{dx} = \frac{1}{2\pi^2 \epsilon_0 v^2} \int_0^\infty \frac{dk}{k} |\rho_m(k)|^2 \int_{\epsilon_\text{sh}=\text{bnd,free}}^{kV} \omega d\omega \sum_{\text{sh=bnd,free}} \rho_{\at} \rho_{\text{sh}} \text{Im} \left[ \frac{1}{\epsilon_{\text{sh}}(k, \omega)} - 1 \right],$$

if $\rho_{\text{sh}}$ is defined via

$$\rho_{\text{bnd}} \equiv \frac{1}{4} \left( \bar{q}_1 / \sqrt{\pi} \right)^3 \quad \text{and} \quad \rho_{\text{free}} \equiv \frac{k_F^3}{3\pi^2 N_{\text{free}}} = \rho_{\at}. \tag{5.7}$$

The comparison with the basic equation (1.6) shows: the polarization of shells of bound electrons are calculated as a response of a virtual, homogeneous target with shells of packing density $\rho_{\text{bnd}}$ — this also provides the background for the existence “inner-shell plasmons” in the theory (→ Sect. 4.2). The polarizations are then diluted geometrically in (5.6) to obtain their actual density $\rho_{\at}$. In an equivalent manner one might also dilute the susceptibility and define a “macroscopic” susceptibility $\tilde{\chi}^R$ of each shell by

$$\tilde{\chi}^R = \frac{\rho_{\at}}{\rho_{\text{sh}}} \chi^R. \tag{5.8}$$

An alternative we do not follow here is use of the Clausius-Mossotti or Lorenz-Lorentz formula, which is often used at all frequencies, but would be also needed here (if used na"ively) at all wave numbers \cite{84,134}. The familiar derivations \cite{253} are based on a homogeneous polarizability of all particles in the target, which as a dipole approximation. But we soon leave this approximation in the application as the wave number increases, because the wavelengths $2\pi/k$ are no longer large compared to the shell radii in the case of inner shell excitation. The tight-binding approximation which is also involved may usually be regarded as well fulfilled. A feature of the Clausius-Mossotti formula is the appearance of a breakthrough to metallic conductivity of the macroscopic dielectric
function, if the product of polarizability and particle packing density increases beyond a certain value. This case of a contact between the dielectric particles seems to be represented by the “inner-shell plasmons” of the Kaneko theory, which perhaps may be removed using this insight.

If the pre-factor \( \rho_{at}/\rho_{sh} \) in (5.6) is removed at the same time, a susceptibility is defined for each shell equivalent to (1.6). It is macroscopic, because the distribution of the shells over the atoms in the solid is taken into account. This procedure “pulls” the pre-factor in \( \text{Im} \chi_R \) first into the numerator of \( \text{Im}1/\epsilon_{sh} \), and second (on the background of the RPA calculation (4.3)) to the front of the occupation probability in momentum space. Including (4.7) and (5.7) this yields

\[
\frac{\rho_{at}}{\rho_{sh}} w(p) = 4\pi^{3/2} q_1^{-3} \rho_{at} w(p) = \frac{1}{2} \left| \varphi_1(p = 0) \right|^2 w(p) \rho_{at} \approx \frac{1}{2} \left| \varphi(p) \right|^2 \rho_{at} \quad (\text{sh = bnd, free}).
\]

The factor \( \frac{1}{2} \) reminds us that the states with free electrons as well as the orbitals of bound electrons were assumed to be occupied by two electrons of opposite spin. \( \left| \varphi(p) \right|^2 \) now indicates that the atomic wave-functions, which were normalized to the integral \( \int \left| \varphi_1(p) \right|^2 d^3p = (2\pi)^3 \), have been distributed on the solid lattice, each occupied with two electrons.

To correspond to these deliberations, the normalization factor for (5.5) have to be fixed via

\[
4\pi^{3/2} q_1^{-3} \int d^3p w(p) = 4\pi^{3/2} c_l^2 2^{-l} q_1^{2l+3} q_1^{-3} (2l + 1)!! = \frac{1}{2} (2\pi)^3 N_{sh},
\]

\[
\Rightarrow \quad c_l^2 = \begin{cases} 
1, & l = 0 \text{ (sshell)} \\
2/(3q_1^2), & l = 1 \text{ (pshell)} \\n4/(15q_1^4), & l = 2 \text{ (dshell)}
\end{cases}.
\]

\( \int d^3pw(p) \), the total probability to find an electron with any momentum, automatically does not differ from the original theory, and likewise the quantity \( \int d^3r|\varphi(r)|^2 \). The generalized calculation of the linear susceptibility within the RPA is provided in App. \[158\]. The characteristic wave numbers \( q_1 \) have been re-determined by setting the wave numbers \( p_m \) of the maxima of the fits \( w(p) \) equal to the wave numbers of the maxima of the atomic values \( \left| \varphi_1(p) \right|^2 \):

\[
p_m = \sqrt{l} q_1 \quad \text{if} \quad l \neq 0.
\]

Table \[5.4\] list some of these values of \( q_1 \), which follow by a search for the maximum of the values \( \left| \varphi_1(p) \right|^2 \) derived from the CR tables. Similar to Sect. \[5.2\] we note that this is an fit to one point of the
atomic momentum distribution, which cannot be extracted directly from the tabulated expectation values of the moments of RHF calculations [87].

<table>
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<th>Fe $^5$D</th>
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</tbody>
</table>

Table 5.4: Values of $\bar{q}_1 a_0$ by insertion of the CR values of the extended basis [50] into (5.11). Values for s shells stay as in table 5.1. Numbers in parentheses are not used for targets in the solid state.

The quality of the fit to atomic wave-functions that is achieved with this generalization is shown in Fig. 5.7. One sees that the Gaussian declines too fast for large wave numbers, and that this is not well cushioned by the increase of the powers. To conserve the normalization, the values for small $p$ become too large. A logarithmic plot shows that a function linear in $p$ in the argument of the exponential might be more appropriate. This alternative is not followed in this thesis.

Fig. 5.8 illustrates that the influence of the new susceptibility on the sub-shell and total stopping cross sections of two targets is much weaker than one would expect. This seems to relate to the feature of susceptibilities according to (4.3) which do not depend on how many states are free (occupied) at momentum $\hbar k$, but on how many with distance $\hbar k$ apart are free (occupied). This “differential” point of view produces for these curves (5.5), which are always smooth, rather small differences for different $l$. The same observation has also been made in the framework of the kinetic theory [189], where the variation of the momentum distribution by the phase effect (the difference between the electronic configuration of free atoms and of solids) was discussed.

The fit (5.5) was derived from wave-functions of isolated target atoms. The wave packets differ for $l > 0$ even more from the step function, the “Fermi ice block”, than the original $l = 0$ theory. An improvement of results for solid transition metals with the new susceptibilities would be accidental, because the electrons in the $d$ bands ought to be more similar to free electrons than to electrons in $p$ orbitals. Therefore an example has been included in Fig. 5.10, where one of the Cu $3d^{10}$ electrons has been moved to the “shell” of free target electrons. The results improve a little compared to the original $3d^{10}$ configuration. This supports the insight that the “free” character of
the 3d electrons in the Kaneko model should rather be supported than diminished.

5.6 Coulomb Interaction Between Induced Charges

Eq. (4.1) is based on the independence of target shells. The polarization charge of each shell is calculated as if the excitation would be induced solely by the field of the ion. Because the Maxwell equations are linear, they add the induced fields and stopping powers and yield (4.1). (With this regard there is a certain similarity with the Matthiessen rule of the summation of cross section of electrons by several impurities and phonon branches and the Bragg rule of the stopping in non-elemental targets.) We shall now (i) distribute the polarization charges of the inner shells through the solid via equation (5.8) corresponding to the true atomic density, and (ii) introduce a unification of these susceptibilities to include — in the framework of the linear response — the Coulomb

Figure 5.7: Bold: the values $|\varphi_1(p)|^2$ of atomic RHF calculations [50]. Thin: the modified fits $(2\sqrt{\pi}/\bar{q}_1)^3\{2p^2/(3\bar{q}_1^2)\} \exp\{-p/\bar{q}_1\}^2$ or $(2\sqrt{\pi}/\bar{q}_1)^3\{4p^4/(15\bar{q}_1^4)\} \exp\{-p/\bar{q}_1\}^2$, respectively, of equation (5.5). Dashed: $(2\sqrt{\pi}/\bar{q}_1)^3 \exp\{-p/\bar{q}_1\}^2$ of the original theory. All momentum distributions are normalized to $\int d^3p = (2\pi)^3$ and given in units of $a_0^3$ as in Fig. 4.1. The two values of $\bar{q}_1$ stem from Tab. 5.4.
interaction between the polarization charges. The substitution (5.8) affects consistently \( \text{Re} \chi^R \) and \( \text{Im} \chi^R \) in the denominator of \( \text{Im}(1/\epsilon_{\text{bnd}}) \). This step alone modifies the energy loss function and the contribution of each shell. At small ion velocities \( dE/dx \) generally becomes larger, as \( \text{Re} \chi^R(k,\omega) \) is positive in essence. At larger velocities the tendency is opposite, because the integral (5.6) covers more and more areas with \( \text{Re} \chi^R(k,\omega) < 0 \). Fig. 5.10 shows this step of including the \( \rho_{\text{at}}/\rho_{\text{sh}} \) in \( \text{Im}(1/\epsilon_{\text{sh}}) \) via (5.8) in (5.6), but still with the summation over independent shell contributions. The stopping changes from the bold dotted to the thin dashed curves.

The following observation provides the motivation for step (ii): the total induced charge is according to (5.6) in the original theory

\[
\int \rho_p(r) d^3r = \rho_m(k = 0) \sum_{\text{sh=bnd,free}} \frac{\rho_{\text{at}}}{\rho_{\text{sh}}} \left[ \frac{1}{\epsilon_{\text{sh}}(k = \omega = 0)} - 1 \right] \neq -Qe.
\]
The ion charge $Qe$ is thereby over-compensated, because $\epsilon_{\text{sh}}(k = \omega = 0) \rightarrow \pm \infty$ without the energy cut for shells of bound as well as of free electrons. But it also is over-compensated after introduction of the energy-cuts, because $\epsilon_{\text{sh}}(k = \omega = 0) \not\rightarrow 1$ holds for the shells of bound electrons. An example for these $\epsilon_{\text{sh}}$ is given by inspection of the neighborhood of the origins of Fig. 5.4. This artifact does not necessarily result in a break-down of the stopping data, because $dE/dx$ is indifferent against any monopolar part of a multipole expansion of $\rho_p(\mathbf{r})$ around the ion site. With other words, the term $-1$ in (5.6) does not contribute to stopping, and the total induced charge is exactly this monopolar part.

The polarization charge of each shell ought better be calculated under the influence of the ionic field and of the remaining shells. More precisely, a unified dielectric function ought to be constructed via

$$
\epsilon = 1 + \sum_{\text{sh=free,bnd}} \tilde{\chi}^R
$$

and be inserted in (1.6) only then. This dielectric function $\epsilon$ also becomes $\pm \infty$ for $k, \omega \rightarrow 0$, through the contribution of the free target electrons, which means an exact compensation of the ion charge and charge neutrality for the total system. The indicated flaw of the original theory is thus removed. Because the summation of the individual susceptibilities means an excitation of each shell by the unified field of the ion charge and polarization charges, it is equivalent to a Hartree approximation to the interaction between the polarization charges. If it is switched on, we obtain spectra like in Fig. 5.9 for the “unified” dielectric function, and the stopping like for example the bold dash-dotted curve in Fig. 5.10 via integration.

Overlooking LPDA-type assumptions or the kinetic theory, where newer work also compiles the EL by adding contributions of target shells, one may remark that

- there is no additional expense — up to details of the integration — to implement the screening influence of all individual shells if the macroscopic susceptibility of each shell is known.

- these considerations are clearly based on electrodynamics, because summation of susceptibilities is the implementation of the Coulomb interaction between different polarization charges. It means an interaction of particles (electrons, holes) in excited states and is not included in
the lowest order of the common perturbation theory.

Figure 5.9: Energy loss function of Si. (a) The original theory \( \sum_{\text{sh}} |\text{Im}(1/\epsilon_{\text{sh}})| \). The three maxima at small \( k \) represent the three plasmons that enter (bottom to top), the plasmon of the “free” shell, of the 2s shell and the 2p shell. According to (1.25) and (4.9) these energies are 0.61, 2.76 and 4.43 a.u. The image emerges by adding plots similar to Fig. 5.3b. (b) With the unified susceptibility \( |\text{Im}(1/\epsilon)| \) and energy-cuts including the KK analysis acc. to (5.12). Two horizontal steps are yet visible, the energy cuts of the 2p and 2s shell at 3.95 and 5.85 a.u. (Tab. 5.2). The energetic order of the energy cuts is different from the order of the plasmon energies, which in essence originates in the lifting of the 2p plasmon by the ratio \( N_{2p}/N_{2s} = 3 : 1 \). All shells are calculated with the original simple Gaussian distribution of momenta without regard to the results of Sect. 5.5.

At this point the energy cuts and the (numerical) KK analysis of the individual \( \tilde{\chi}^R \) become essential to reduce the influence of the quasi-static polarizability of the inner target shells on the low-velocity stopping power. Therefore all dash-dotted curves in Fig. 5.10–5.11 have been calculated including both. Without the KK analysis, \( \text{Re} \epsilon \) would become much larger and the EL much smaller by the contributions of the virtual transitions, as one may already observe in Fig. 5.4.

Another qualitative difference to the independent treatment of the shells is the possibility
of the extinction of the plasmon by the free electrons, if its energy \(2\sqrt{3}r_s^{-3/2}E_0\) becomes larger than the excitation gap \(E_g\) of an inner shell. In the case of the \(^{29}\text{Cu}\) target for example, the plasmon of the free electrons is almost eliminated, because it may decay into 3d single-electron excitations. The formal reason is that for a given point in \((k, \omega)\) space — that means for energy and momentum conservation during a conversion of the photon energy in electron-hole excitations — the two spectra with infinite life-time of the plasmon (\(\text{Im} \tilde{\chi}^R = 0\)) and finite life-time of the 3d excitation (\(\text{Im} \tilde{\chi}^R > 0\)) combine to a finite life-time (\(\sum \text{Im} \tilde{\chi}^R > 0\)). In the other cases only a re-normalization of the plasmon dispersion curves takes place, as the implicit form \(\epsilon_{\text{free}} = 0\) becomes \(\epsilon = 0\) \([210]\).

Fig. 5.10 presents a target with the largest uncertainty within the theory, the case of a transition metal. The same group of calculations with a \(^{14}\text{Si}\) target is summarized in Fig. 5.11 and shows much smaller variation of the results. The dispersion of the free plasmons for example is changed only minimally due to the re-normalization by the virtual transitions into the other shells.
The $3d$ shells of transition metals with $\rho_{at}/\rho_{sh} \sim 1$ and gap energies which have been assumed to be very small here interfere massively with the shell of free electrons, if the mutual interaction is switched on. The energy loss functions of deeply buried target shells are generally separated better in $(k, \omega)$ space, and therefore less affected by the mutual screening/amplification.

![Proton stopping in $^{14}\text{Si}$](image)

**Figure 5.11**: Proton stopping in $^{14}\text{Si}$. Bold solid line: ZBL [261]. The other lines are defined as in Fig. 5.10. To enhance the clearness of the graph, the thin dash-dotted line is not plotted.

Heavy ions, which suppress the contributions of the energy loss function at small $k$ because of $\rho_m(k \to 0) \to Qe \ll Z_1 e$, are less sensitive to the model of the exterior target shells, as already discussed in Sect. 4.3. The double-maximum of the shells of free and $3d$ electrons in Fig. 5.10 for example does no longer exist for $Z_1 \gtrsim 5$.

### 5.7 Summary

The Kaneko theory permits real excitation of target shells by arbitrary momentum and energy transfers. Considering the *de facto* present band gaps yields a systematic reduction and improve-
ment of the electronic energy losses. An implementation that simply cuts off the imaginary part of the dielectric function below the excitation energies is possible.

All effective charge theories, not just the Kaneko theory, do not calculate the target polarization self-consistently, insofar a polarizable target is assumed to exist everywhere, independent of and also “underneath” the point where the ion resides at the moment. However, the electrons that are bound to heavy ions occupy this space, which relates to their shell radius, themselves. Two contributions to the polarization, the scattering into or outside this region do actually not exist and ought to be eliminated from the calculation. This region, which looks like dead with respect to the target polarization, adapts its size to the ion diameter, including the ionization degree, as a fit to experimental energy losses proposes. The model of a “dead sphere” systematically decreases the energy losses of heavy ions similar to the field energies of Fig. 3.20 in a sensible way.

Atomic calculations suggest that the momentum distribution is not Gaussian but a higher moment of a Gaussian for sub-shells with nonzero angular momentum quantum number. A re-calculation of the susceptibilities of these sub-shells based on the generalized distributions, however, has remarkably small influence on the energy loss functions and the energy loss.

The Kaneko theory calculates susceptibilities of independent target shells and uses them as if no interaction between their polarization charges would exist. The calculations presented here add the susceptibilities of target shells, which is equivalent to a Coulomb interaction between the polarization charges, and calculate the energy losses based on the combined susceptibility. The influence of this change is weak if they possess an excitation spectrum with well-separated single-shell excitations. For transitions metals on the contrary, this coupling between the $s$ electrons with “neighbored” $d$ electrons leads to drastic changes. This hints at insufficiencies of the model for shallow $d$ bands of transition metals. The related uncertainty of the predicted energy loss is larger for light ions than for heavy ions.
Chapter 6

Summary and Outlook

The dielectric description of the electronic energy loss (EL) of ions is characterized by the combination of the atomic theory for the ion and solid state physics for the target via Maxwell theory. If the projectiles are bare ions, they are an external potential in the eyes of the target electrons and the mutual interaction is not made complicated by the Pauli principle. The electrons of incompletely stripped ions are only treated in a Hartree approximation.

Improvements of the theory are based on improvements of the two components “ion” and "dielectric response“ (Chapt. 2, 4) or their mutual interdependence (Chapt. 3). The energy loss may hide dependences (Sect. 5.5) by an integration over energy and momentum that are exchanged between ion and target, and accepts for example the Brandt-Kitagawa with locally divergent electron density. In contrast to the energy loss of photons, the optical excitation, a complete implementation of the dynamic dielectric function at all wavelengths is required.

The dissertation shows:

• Fundamental statements of many-particle solid-state theory about the electron gas and its dynamic excitation lead after another half-automatic integration step to statements about the electronic energy loss. Because this integration is a specialty of the theory of the electronic energy loss by ions, ion beam physics has to implement the dielectric function on its own account. The free electron gas model finds broad application within the ion stopping and is not limited to metallic targets.
• The ionization degree inside solids represents and follows from the stability with respect to ionization by target electrons in a universal way. The stability is put into detail by summation over various energy contributions, the transferable kinetic energy, a field ionization term and the chemical potential of the target on one hand, and the barrier of the ionization energies of the ion on the other.

• The youngest, most realistic model of this formulation of the ion energy loss, the Kaneko theory, is the one with the least number of fit parameters. It opens a new potential of development, as incomplete physical descriptions are less hidden in fitted parameters. The energy losses of heavy ions can be calculated within this dielectric theory without scaling of proton energy losses or definitions of effective charges.

Returning to the opening discussion of Sect. 1.1 some basic tasks remain to be done with respect to the energy loss of heavy ions. (Not so basic and more complex are for example ion cluster \[64, 94, 237\], ion-surface scattering \[9, 107\] and the processes that are induced by the target electrons thereafter \[52\].)

On the Hartree-Fock level the determination of the ionization degree ought to be possible at general ion velocity and atomic number in the jellium model of the target. The argumentation in the present work uses the energy concept and is entirely classical with respect to the interaction between the target electrons and the electrons bound to the ion. The increasing number of thin-film experiments, which yield the energy loss of ions in frozen charge states, will permit the decomposition of the effective ionization degree into an ionization degree and a target dependence \[192\]. The uncertainty that was formulated in section 3.2.3 would then be removed, if the influence of charge state changes and internal excitations of ions on foil entry and exit is also investigated more closely.

The obvious deficit of the Kaneko theory is the existence of the branch of collective excitations for all shells, caused by the homogeneous ansatz in real space. The partial removal via the energy-cut in this work provides mere corrections. A theory is wishful that commences from the models for the momentum distributions of the shells and establishes Bethe-like oscillator strengths of the isolated target atoms as general as the Kaneko theory does. This could provide the basis to
build a susceptibility for a lattice-periodic ordering of target atoms.

The electronic energy loss of point-like ions is better known theoretically than the energy loss of incompletely stripped ions, because within quantum-mechanics the ion may be treated as an external potential in the semi-classical approximation. Effective charge theory describes heavy ions with the knowledge of atomic theory as a pragmatic starting point. The screening influence of target electrons must be introduced as a correction. The electronic energy loss of targets with atomic structure, channeling and impact-parameter dependence are most often treated in the local-plasma approximation nowadays. Usually it is no longer used as by ZBL in the pure form, but shell by shell, i.e., with consideration of the additional quantum numbers of target electrons. This shows the unspoken concession that the electron excitation is not a local phenomenon but dominated by complete orbitals like a resonance phenomenon. This LPDA concept may probably be generalized to ions with finite diameter, but becomes even less plausible in these cases.

The theory of binary collisions between ions and atoms in the framework of plasma physics will develop in form of \textit{ab initio} theories of few-electron systems as computer powers grow. It is difficult to transfer these methods to solid state physics, because the electrons in the solid cannot be introduced as a perturbation or an electric boundary problem to these calculations.

The path to a quantum-mechanically founded, numerically feasible and at medium velocities correct theory of the electronic energy loss of heavy ions in solids is not yet given.
Appendix A

The Integration of the First-Order Feynman Diagrams

A.1 Calculation of the “Exchange” Diagram b)

A.1.1 Reduction of Integrals

The law of residues yield the integral over $l_0$, the frequency part of the four-momentum $l$. A linear transformation of $l$ maps these two products of $\Theta$-functions onto one:

$$
\int \frac{d^4l}{(2\pi)^4} G_0^0(k - l) G_0^0(k + q - l) \frac{1}{l^2}
$$

$$
= \int \frac{d^4l}{(2\pi)^4} \left[ \frac{\Theta(|k - l| - k_F)}{k_0 - l_0 - \omega_{k-1} + i\eta} + \frac{\Theta(k_F - |k - l|)}{k_0 - l_0 - \omega_{k-1} - i\eta} \right] 
\times \left[ \frac{\Theta(|k + q - l| - k_F)}{k_0 + q_0 - l_0 - \omega_{k+q-1} + i\eta} + \frac{\Theta(k_F - |k + q - l|)}{k_0 + q_0 - l_0 - \omega_{k+q-1} - i\eta} \right] \frac{1}{l^2}
$$

$$
= -i \int \frac{d^3l}{(2\pi)^3} \Theta(|l + q| - k_F) \Theta(k_F - l) 
\times \left[ \frac{1}{(k + l + q)^2} \frac{1}{q_0 - \omega_1 + \omega_{q+1} - i\eta} + \frac{1}{(k - l)^2} \frac{1}{q_0 - \omega_1 + \omega_{q+1} - i\eta} \right].
$$
The integral over \( k_0 \) is likewise tractable by the law of residues and leads to

\[
\Pi_b^{(1)} = \frac{e^2}{\epsilon_0 \hbar^2} \int d^3l d^3k \left[ \frac{\Theta(k - k_F)\Theta(k - |k + q|)}{q_0 - \omega_k + \omega_{k+q} + i\eta} + \frac{\Theta(k_F - k)\Theta|k + q| - k_F)}{q_0 - \omega_k - \omega_{k+q} + i\eta} \right] \\
\times \left[ \Theta(|l + q| - k_F)\Theta(k_F - l) \right] \left( \frac{1}{(k + 1 + q)^2 q_0 - \omega_l + l_{q+1} + i\eta} + \frac{1}{(k - 1)^2 q_0 - \omega_l + l_{q+1} - i\eta} \right) .
\]

The substitution \( k \to -k - q \) in the first term of the first factor and then measuring all momenta in units of \( k_F \) plus the definition \([1.16]\) yield

\[
\Pi_b^{(1)} = \frac{2}{\epsilon_0} \left( \frac{m}{\hbar^2} \right)^2 \int d^3l d^3k \left[ \Theta(k + q) - 1 \right] \Theta(|l + q| - 1) \Theta(1 - l) \Theta(1 - \nu) \left( \frac{\nu - \frac{q}{2} - l_z + i\eta}{(k + q + 1)^2 \nu - \frac{q}{2} - l_z + i\eta} \right) \left[ \Theta(k - k_F)\Theta(k_F - l) \right] \left( \frac{1}{(k + 1 + q)^2 q_0 - \omega_l + l_{q+1} + i\eta} + \frac{1}{(k - 1)^2 q_0 - \omega_l + l_{q+1} - i\eta} \right) \left[ \Theta(|l + q| - k_F)\Theta(k_F - l) \right] \left( \frac{1}{(k + 1 + q)^2 q_0 - \omega_l + l_{q+1} + i\eta} + \frac{1}{(k - 1)^2 q_0 - \omega_l + l_{q+1} - i\eta} \right) .
\]

Here, “nf” means “negative frequency” and is a placeholder that adds the preceding expression with replacement of the frequency \( \nu \) or \( q_0 \) by \( -\nu \) or \( -q_0 \), respectively, at all places. (“nf” does not imply that one of the two terms vanishes for a given sign of the frequency.) Switching to cylinder coordinates with axis in the direction of \( q \)

\[
l_x \equiv y \cos \varphi_l ; \quad l_y \equiv y \sin \varphi_l ; \quad l_z \equiv x \\
k_x \equiv \xi \cos \varphi_k ; \quad k_y \equiv \xi \sin \varphi_k ; \quad k_z \equiv z
\]

(A.1)

\((k + q + l)^2 = x^2 + y^2 + z^2 + \xi^2 + q^2 + 2y\xi \cos(\varphi - \varphi_l) \pm 2zx + 2qx + 2qz\)

and Jacobi determinant \( y\xi \) permits to evaluate the integration over the angle with \([97\text{ 3.613.1}]\)

\[
\int_2^{2\pi} \int_0^{2\pi} \frac{d\varphi d\varphi_l}{(k + q + l)^2} = \frac{1}{\sqrt{(x^2 + y^2 + z^2 + \xi^2 + q^2 \pm 2zx + 2qx + 2qz)^2 - (2\xi y)^2}} .
\]

This reduces the integration region to the shaded area in Fig. [A.1] that consists of two Fermi half spheres, which overlap in general. At \( q > 2 \) it comprises a half unit circle, at \( q = 0 \) it vanishes.

The following type of integral may be solved by the substitution \( y^2 = u \) of the \( l \)-component perpendicular to \( q \) and \([97\text{ 2.261}]\):

\[
\int_0^{\sqrt{b(x)}} y dy = \frac{1}{2} \ln \left| \sqrt{((x + q + z)^2 + u + \xi^2)^2 - 4\xi^2 u} + (x + q + z)^2 + u - \xi^2 \right|_{u = b(x)} \left| u = 0 \right.
\]

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The central problem of the remaining threefold integral \( \int dxdzd\xi d\xi \) is the logarithm of \( \xi \), which was the \( k \)-component perpendicular to \( q \) before. The substitution \( \xi^2 = v \) simplifies to integrals of the form

\[
\int_{c(z)}^{c(z)} dv \ln |\sqrt{[(x + q \pm z)^2 + u + v]^2 - 4uv + (x + q \pm z)^2 + u - v}|,
\]

that are further treated with the Euler substitution

\[
\sqrt{[(x + q \pm z)^2 + u + v]^2 - 4uv - v} \equiv t.
\]

We are left with a logarithm of an argument which is linear in \( t \) multiplied with an algebraic function in \( t \), which is accessible via a decomposition into partial fractions and \([97, 2.727.3 \text{ and } 2.723]\). After the definition of an auxiliary function

\[
K(s; b, c) = K(s; c, b) \equiv s^2 + b + c \quad (A.2)
\]

\[
T(s; b, c) = T(s; c, b) \equiv \sqrt{K^2(s; b, c) - 4bc} \quad (A.3)
\]

the solution of

\[
F(s; b, c) \equiv \int_{0}^{c} \{ \ln |T(s; b, y) + K(s; b, -y)| - \ln |2s^2| \} dy \quad (A.4)
\]

can be summarized as

\[
F(s; b, c) = F(s; c, b) = \frac{1}{2}(T - K) + b \ln \left| \frac{b}{\frac{1}{2}(T - K) + b} \right| + c \ln \left| \frac{c}{\frac{1}{2}(T - K) + c} \right|
\]
\( F \) without indices never means a Hypergeometric Function in this thesis. \( F(s; b, c) \) has a logarithmic singularity at \( s = 0 \). The remaining double integrals are re-written in terms of four Cartesian coordinates. Fig. [A.1] helps to find the integration limits which are determined by the \( \Theta \)-functions:

\[
\Pi_b^{(1)}(\xi) = \frac{2mk_F}{\hbar^2} \chi^2 \int_{\max(-1,-q/2)}^1 dx \int_{\max(-1,-q/2)}^1 dz \int_{\max(0,1-(z+q)^2)}^1 d\xi \int_{\max(0,1-(x+q)^2)}^1 dy \\
\times \left[ \frac{1}{\nu^2 - \frac{q^2}{4} - z + i\eta} \sqrt{((x + z + q)^2 + \xi + y)^2 - 4\xi y} \right. \\
\left. \quad + \frac{1}{\nu^2 - \frac{q^2}{4} - z + i\eta} \sqrt{((x - z)^2 + \xi + y)^2 - 4\xi y} \right] + \text{nf} \quad (A.5)
\]

\[
= \frac{4mk_F}{\hbar^2} \chi^2 \int_{\max(-1,-q/2)}^1 dx \int_{\max(-1,-q/2)}^1 dz \\
\left[ \frac{G(x + z + q, x, z)}{(\nu^2 - \frac{q^2}{4} - z + i\eta)(\nu^2 + \frac{q^2}{4} + x - i\eta)} \right. \\
\left. \quad + \frac{G(x - z, x, z)}{(-\nu^2 - \frac{q^2}{4} - z + i\eta)(\nu^2 + \frac{q^2}{4} + x - i\eta)} \right] + \text{nf} \quad (A.6)
\]

\[
G(s, x, z) \equiv \begin{cases} 
F(s; 1 - x^2, 1 - z^2) & (x > 1 - q \land z > 1 - q) \\
F(s; 1 - x^2, 1 - z^2) - F(s; 1 - x^2, 1 - (z + q)^2) & (x > 1 - q \land z < 1 - q) \\
F(s; 1 - x^2, 1 - z^2) - F(s; 1 - (x + q)^2, 1 - z^2) & (x < 1 - q \land z > 1 - q) \\
F(s; 1 - x^2, 1 - z^2) + F(s; 1 - (x + q)^2, 1 - (z + q)^2) & (x < 1 - q \land z < 1 - q) \\
-F(s; 1 - x^2, 1 - (z + q)^2) - F(s; 1 - (x + q)^2, 1 - z^2) & (x < 1 - q \land z < 1 - q)
\end{cases} \quad (A.7)
\]

This means we always start the \( \xi \) and \( y \) integration at \( \xi = y = 0 \) to use \( (A.4) \), and subtract the region of the lower Fermi half circle if \( z \) or \( x \) are between \(-q/2\) and \(1 - q\). The factor \( 4mk_F / \hbar^2 \) has been split off, because the remaining terms constitute the part that has to be subtracted from the \( f_1 \) and \( f_2 \) functions in \( (1.19) \) and \( (1.20) \) to make the transition from the zeroth order polarization to the sum of first and zeroth order polarization.

Integration of expression \( (A.5) \) over \( \nu \) with the help of the law of residues would not yield a contribution from the second term, and the first term would obtain the form which is known from \( [88 \text{ Eq. 9}] \) and \( [194 \text{ Eq. 3.1}] \) and the contribution of diagrams a) to e) to the exchange-correlation energy.
A.1.2 The Real Part

After decomposition of the real part of (A.6) by repetitive application of the formula by Sochozki-Plemelj, which is commonly named according to Dirac by physicists,

\[
\text{Re}\left(\frac{\nu - q}{q/2 - z + i\eta} \frac{\nu + q}{q/2 + x - i\eta}\right)
= \left[\frac{P}{(\nu - q/2 - z)(\nu + q/2 + x)} + \pi^2 \delta(\nu - q - z)\delta(\nu + q + x)\right] G(x + z + q, x, z)
\]

the 2-dimensional \(\delta\)-distribution does not contribute within the integration region and may be removed. The decomposition

\[
\text{Re}\left(\frac{\nu - q}{q/2 - z + i\eta} \frac{-\nu + q}{q/2 + x - i\eta}\right)
= \left[\frac{P}{(\nu - q/2 - z)(-\nu + q/2 + x)} + \pi^2 \delta(\nu - q - z)\delta(-\nu + q + x)\right] G(x - z, x, z)
\]

yields two logarithmically divergent terms. They are treated with the formula derived in App. A.4.2

\[
\ldots = \left[\frac{P}{-\nu + q + x} \frac{P}{x - z} + \frac{P}{\nu - q/2 - z} \frac{P}{x - z} + \text{nf}\right] G(x - z, x, z);
\]

The numerical evaluation ought also take advantage from the symmetry of the integrand with respect to the interchange \(x \leftrightarrow z\) (if the “nf” part is added) and use eventually

\[
\Pi_b^{(1)} = \frac{4mk_F}{\hbar^2} \frac{\chi^2}{4q^2} \int_{\text{max}(-1,-q/2)}^{1} dx \int_{\text{max}(-1,-q/2)}^{1} dz \left\{ \frac{P}{(\nu - q/2 - z)(\nu + q/2 + x)} G(x + z + q, x, z) + \left[\frac{P}{-\nu + q + x} \frac{P}{x - z} + \text{nf}\right] G(x - z, x, z) \right\}.
\]

To smooth the integrand it is also essential to include some kind of pre-evaluation of the principal values according to the scheme

\[
P \int_{c}^{1} f(x) dx = \begin{cases} 
\int_{c}^{2x_0-1} \frac{f(x)dx}{x_0-x} + \lim_{\delta \to 0} \int_{2x_0-1}^{x_0-\delta} \frac{f(x)-f(2x_0-x)}{x_0-x} dx & \text{; for } x_0 > (1+c)/2 \\
\lim_{\delta \to 0} \int_{x_0+\delta}^{2x_0-c} \frac{f(x)-f(2x_0-x)}{x_0-x} dx + \int_{2x_0-c}^{1} \frac{f(x)}{x_0-x} dx & \text{; for } x_0 < (1+c)/2
\end{cases}
\]

generalized to two dimensions [48].
A.1.3 The Imaginary Part

The imaginary part is extracted as follows:

\[
\text{Im} \left( \frac{G(x + z + q, x, z)}{(\frac{\nu}{q} - \frac{q}{2} - z + i\eta)(\frac{\nu}{q} + \frac{q}{2} + x - i\eta)} \right) = \pi \left[ \frac{P\delta(\frac{\nu}{q} - \frac{q}{2} + x)}{\frac{\nu}{q} - \frac{q}{2} - z} - \frac{P\delta(\frac{\nu}{q} - \frac{q}{2} - z)}{\frac{\nu}{q} + \frac{q}{2} + x} \right] G(x + z + q, x, z)
\]

\[
\text{Im} \Pi^{(1)}_b = \frac{4mk_F}{h^2} \frac{\pi \chi^2}{4q^2} \int_{\max(-1,-q/2)}^{1} \int_{\max(-1,-q/2)}^{1} dx dz \\
\times \left[ \delta(\frac{\nu}{q} - \frac{q}{2} - x)G(x + z + q, x, z) - \delta(\frac{\nu}{q} - \frac{q}{2} - z)G(x + z + q, x, z) + \frac{\delta(\nu - \frac{q}{2} - x)}{\frac{\nu}{q} - \frac{q}{2} - z} - \frac{\delta(\nu - \frac{q}{2} - z)}{\frac{\nu}{q} - \frac{q}{2} - x} \right] + \text{nf}
\]

\[
= \begin{cases} 
\frac{4mk_F}{h^2} \frac{\pi \chi^2}{4q^2} \int_{\max(-1,-q/2)}^{1} dz \left[ \frac{G(z + \frac{|\nu|}{q} + \frac{|\nu|}{q} - \frac{q}{2}, q)}{\frac{|\nu|}{q} - \frac{q}{2} - z} + \frac{G(z - \frac{|\nu|}{q} + \frac{|\nu|}{q} - \frac{q}{2}, q)}{\frac{|\nu|}{q} - \frac{q}{2} - z} \right] & \text{if } -1 \leq \frac{|\nu|}{q} - \frac{q}{2} \leq 1 \\
0 & \text{else}
\end{cases}
\]

\[
= \text{Im} \Pi^{(1)}_b(q, \nu) = \text{Im} \Pi^{(1)}_b(q, -\nu).
\]

\[
\text{Im} \Pi^{(1)}_b(q, \nu = 0) = 0.
\]

This formula has been integrated numerically with the routine D01AJF of the NAG library. The law of residues applied to [A.6] yields

\[
\int_{-\infty}^{\infty} \Pi^{(1)}_b(q, \nu) d\nu = -2i \frac{mk_F \pi \chi^2}{h^2 q} \int_{\max(-1,-q/2)}^{1} dz \int_{\max(-1,-q/2)}^{1} dx G(x + z + q, x, z)
\]

\[
\Rightarrow \int_{-\infty}^{\infty} \text{Re} \Pi^{(1)}_b(q, \nu) d\nu = 0
\]

as it must be to let the correlation energy stay real [\text{S2} (12.21)]. This also provides a check for the subsequent results.
A.2 Calculation of the “Self-Energy” Diagrams c) And d)

A.2.1 Reduction of Integrals

The \( l \)-integral is proportional to the first-order self energy \( \Sigma^\ast(1) \), and is solved by integration over \( l_0 \) (law of residues) and subsequent transition to cylinder coordinates with \( k \) pointing into the direction of the cylinder axis \([82, \text{Prob. 4.9}] [109, (A4)]\):

\[
\int \frac{d^4 l}{(2\pi)^4} G^0(k - l) U_0(l) = \frac{e^2}{\epsilon_0} \int \frac{d^4 l}{(2\pi)^4} \left[ \frac{\Theta(|k - l| - k_F)}{k_0 - l_0 - \omega_{k-1} + i\eta} + \frac{\Theta(k_F - |k - l|)}{k_0 - l_0 - \omega_{k-1} - i\eta} \right] \frac{e^{i(k_0 - l_0)\eta}}{l^2}.
\]

The exterior \( k \)-integration is proportional to

\[
\int \frac{d^3 k}{(2\pi)^3} \left[ \frac{\Theta(k - k_F)}{k_0 - \omega_k + i\eta} + \frac{\Theta(k_F - k)}{k_0 - \omega_k - i\eta} \right] \left[ \frac{\Theta(|k + q| - k_F)}{k_0 + q_0 - \omega_{k+q} + i\eta} + \frac{\Theta(k_F - |k + q|)}{k_0 + q_0 - \omega_{k+q} - i\eta} \right] \times \left[ 1 - \frac{k^2}{4k} \ln \left( \frac{k + 1}{k - 1} \right)^2 + 1 \right] e^{ik_0\eta}.
\]

The first two brackets deliver four terms with overlapping \( \Theta \)-functions. The \( k_0 \)-integral is attacked with the law of residues, where the path is closed in the upper \( k_0 \) half-plane. One of the four terms does not possess a pole there and yields zero, one has a simple pole at \( k_0 = \mp q_0 + \omega_{k\pm q} + i\eta \) that contributes, one has a pole of second order at \( k_0 = \omega_k + i\eta \) that contributes, and the last has one pole of first and one of second order, that cancel each other. We measure again all momenta in units of \( k_F \) and introduce the dimensionless frequency \( \nu \) via \([1.16]\):

\[
\cdots = i \left( \frac{m}{\hbar} \right)^2 \frac{1}{k_F} \int \frac{d^3 k}{(2\pi)^3} \left[ \frac{\Theta(k - 1)\Theta(1 - |k \pm q|)}{(\pm \nu \mp kq - \frac{q^2}{2} + i\eta)^2} - \frac{\Theta(1 - k)\Theta(|k \pm q| - 1)}{(\pm \nu \mp kq - \frac{q^2}{2} + i\eta)^2} \right] \times \left[ 1 - \frac{k^2}{4k} \ln \left( \frac{k + 1}{k - 1} \right)^2 + 1 \right].
\]

With the linear transformation \( k \to k \pm q \) in two terms one can show that the last constant term \( '1' \) does not contribute to \( \Pi_{c+d}^{\ast(1)} \), and with the transformation \( k \to -k \) that

\[
\Pi_{d}^{\ast(1)}(q, \nu) = \Pi_{c}^{\ast(1)}(q, -\nu),
\]

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to obtain
\[ \Pi_{c+d}^{(1)} = -\frac{2e^2}{\epsilon_0\hbar^2(2\pi)^2} \left( \frac{m}{\hbar} \right)^2 \int \frac{d^3k}{(2\pi)^3} \left[ \frac{\Theta(k-1)\Theta(1-|k+q|)}{(\nu - kq - \frac{q^2}{2} - i\eta)^2} - \frac{\Theta(1-k)\Theta(|k+q|-1)}{(\nu - kq - \frac{q^2}{2} + i\eta)^2} \right] \times \frac{1 - k^2}{4k} \ln \left( \frac{k + 1}{k - 1} \right)^2 + nf. \] (A.10)

Again with the law of residues one can show that
\[ \int_{-\infty}^{\infty} \Pi_{c}^{*(1)}(q,\nu)d\nu = \int_{-\infty}^{\infty} \Pi_{d}^{*(1)}(q,\nu)d\nu = 0, \] (A.11)
and therefore these polarization diagrams do not contribute to the correlation energy of the electron gas in accordance with [82, (12.21)]. This sum rule also provides a helpful check for subsequent results.

Switching to spherical coordinates yields a factor \(2\pi\) by the integration over the azimuthal angle. The \(\Theta\)-functions provide the following new integration limits:
\[ \int d^3k (2\pi)^3 \Theta(1-k) \Theta(1-|k+q|) = \frac{1}{(2\pi)^2} \int_{\text{max}(q-1,1)}^{q+1} k^2 dk \int_{\text{arccos} \frac{1-k^2-q^2}{2kq}}^{\pi} \sin \theta d\theta d\phi; \]
\[ \int d^3k (2\pi)^3 \Theta(1-k) \Theta(|k+q|-1) = \frac{\Theta(q-1)}{(2\pi)^2} \int_{0}^{\text{min}(q-1,1)} k^2 dk \int_{\text{arccos} \frac{1-k^2-q^2}{2kq}}^{\min(q-1,1)} \sin \theta d\theta + \frac{\Theta(2-q)}{(2\pi)^2} \int_{|q-1|}^{1} k^2 dk \int_{0}^{\text{arccos} \frac{1-k^2-q^2}{2kq}} \sin \theta d\theta. \]

**A.2.2 The Imaginary Part**

The integration over \(\theta\) becomes elementary, and the results may be split again into real and imaginary parts,
\[ k \int_{\text{arccos} \frac{1-k^2-q^2}{2kq}}^{\pi} \frac{\sin \theta d\theta}{(\frac{\nu}{q} - k \cos \theta - \frac{q}{2} - i\eta)^2} = \frac{1}{\frac{\nu}{q} - \frac{1}{2q} + \frac{k^2}{2q} - i\eta} - \frac{1}{\frac{\nu}{q} + k - \frac{q}{2} - i\eta} \]
\[ = \frac{P}{\frac{\nu}{q} - \frac{1}{2q} + \frac{k^2}{2q}} + i\pi \sqrt{1-2\nu} \delta(k - \sqrt{1-2\nu}) - \frac{P}{\frac{\nu}{q} + k - \frac{q}{2}} - i\pi \delta(\frac{\nu}{q} + k - \frac{q}{2}). \] (A.12)
value of $k$, $\sqrt{1 \pm 2\nu}$ or $\pm \frac{\nu}{q} \pm \frac{q}{2}$, falls within the limits of the integration interval. The result is identical with \[109\] (2.13) for positive $\nu$. For negative $\nu$ it has the opposite sign, as the retarded polarization was computed there, but the time-ordered is computed here:

$$\text{Im} \, \Pi_{c+d}^{(1)} = \frac{4m_{\text{F}} \pi \chi^2}{\hbar^2} \frac{2q|\nu|}{4q^2} \ln \left| \frac{\sqrt{1 + 2|\nu|} + 1}{\sqrt{1 + 2|\nu|} - 1} \right|$$

$$+ \left[ 1 - (\frac{\nu}{q} + \frac{q}{2})^2 \right] \ln \left[ \frac{\nu^2 + q^2 + 1}{\nu^2 + q^2 - 1} \right] - \left[ 1 - (\frac{\nu}{q} - \frac{q}{2})^2 \right] \ln \left[ \frac{\nu^2 - q^2 + 1}{\nu^2 - q^2 - 1} \right] \right] ;$$

if $\frac{q^2}{2} - q \leq |\nu| \leq q + \frac{q^2}{2}$ and $-\frac{q^2}{2} + q \leq |\nu| \leq q$ \(\text{(A.13)}\)

$$\text{Im} \, \Pi_{c+d}^{(1)} = 0 \quad \text{if} \quad 0 \leq |\nu| \leq -\frac{q^2}{2} + q.$$

$\text{Im} \, \Pi_{c+d}^{(1)}$ is discontinuous on the curve $|\nu| = -\frac{q^2}{2} + q$. Adding the information of \(\text{(A.8)}\) we see that

$$\text{Im} \, \Pi_{c+d}^{(1)}(q, \nu) \equiv \text{Im} \, \Pi_{b+c+d}^{(1)}(q, \nu) = 0 \quad \text{for} \quad |\nu| > q + \frac{q^2}{2} \quad \text{or} \quad |\nu| < \frac{q^2}{2} - q.$$

The band in the $\nu - q$-plane with non-zero imaginary part of the polarization stays the same as within the RPA (1.20). The improved description also contains undamped plasmons. It is known that the replacement of the Greens function $G^0$ of the unperturbed problem by a RPA type of function for example, quasi an attempt at a self-consistent solution and mixing of another classes of diagrams \[8, 219\], keeps these life times finite.

### A.2.3 The Real Part

The principal values of \(\text{(A.12)}\) and the equivalent parts of \(\text{(A.10)}\) may be rewritten as

$$\text{Re} \, \Pi_{c+d}^{(1)} = -\frac{4m_{\text{F}} \chi^2}{\hbar^2} \frac{\nu^2 + q^2}{2q^2} \left[ \int_{|q-1|}^{q+1} \left( \frac{P}{\nu - \frac{1}{2}q + \frac{k^2}{2q}} - \frac{P}{\nu + \frac{k^2}{2q}} \right) + \int_{\text{max}(0,1-q)}^1 \left( \frac{P}{\nu + k - \frac{q}{2}} - \frac{P}{\nu - k - \frac{q}{2}} \right) \right]$$

$$\times \left[ (1 - k^2) \ln \left| \frac{k + 1}{k - 1} \right| \right] dk + \text{nf.}$$
If one defines the underivative
\[ \partial_x \mathcal{L}_c(x) \equiv \frac{\ln |c-x|}{x}, \]
the result can be formulated using \( a \) defined in (1.18) as
\[
\int_M^1 \left( \frac{P}{\nu + k - \frac{q}{2}} - \frac{P}{\nu - k - \frac{q}{2}} \right) (1 - k^2) \ln \left| \frac{k + 1}{k - 1} \right| dk \\
= (1 - a^2) \left[ \mathcal{L}_{a-1}(a + 1) - \mathcal{L}_{a-1}(a + M) - \mathcal{L}_{a+1}(a + 1) + \mathcal{L}_{a+1}(a + M) + \mathcal{L}_{-a-1}(1 - a) \\
- \mathcal{L}_{-a-1}(M - a) - \mathcal{L}_{1-a}(1 - a) + \mathcal{L}_{1-a}(M - a) \right] + (M - 1) \left[ (M + 1) \ln \left| \frac{M + 1}{M - 1} \right| + 2 \right],
\]
\[ M \equiv \max(0, 1 - q) \]
and
\[
- \int_{|q-1|}^{q+1} \frac{P}{\nu + k - \frac{q}{2}} (1 - k^2) \ln \left| \frac{k + 1}{k - 1} \right| dk \\
= (a^2 - 1) \left[ \mathcal{L}_{-a-1}(q + 1 - a) - \mathcal{L}_{-a-1}(|q - 1| - a) - \mathcal{L}_{1-a}(q + 1 - a) + \mathcal{L}_{1-a}(|q - 1| - a) \right] \\
+ (\frac{q}{2} + a)(q + 2) \ln(q + 2) - (\frac{|q - 1| - 1}{2} + a)(|q - 1| + 1) \ln||q - 1| + 1| + q + 1 - |q - 1| \\
- (\frac{q}{2} + 1 + a)q \ln q + (\frac{|q - 1| + 1}{2} + a)(|q - 1| - 1) \ln||q - 1| - 1| \quad . (A.14)
\]

The subsequent sum of the parts with negative frequencies lets some of \( a \) terms in (A.14) that do not belong to the first term, cancel, and they can be replaced by \( q/2 \). The term “+nf” simply doubles their contribution. An actual implementation of the \( \mathcal{L} \)-function is presented in appendix A.4.1.

If \( 1 - 2\nu \geq 0 \), the expression
\[
\int \frac{P}{\nu - \frac{q}{2} + \nu - \frac{q}{2}} (1 - k^2) \ln \left| \frac{k + 1}{k - 1} \right| dk
\]
can be further decomposed into partial fractions, to obtain an integral-free formula for \( \text{Re} \Pi^{(1)}_{c+d} \).

### A.3 Assemblage of the First-Order Diagrams

In replacement of a direct calculation using the representation of App. A.1.2, the KK relation
\[
\pi \text{ Re} \Pi^R(q, q_0) = P \int_{-\infty}^{\infty} \frac{\text{Im} \Pi^R(q, q_0')}{q_0' - q_0} dq_0'
\]

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for the retarded polarization $\Pi^R$

$$\text{Re} \, \Pi^R(q, q_0) \equiv \text{Re} \, \Pi(q, q_0) \quad ; \quad \text{Im} \, \Pi^R(q, q_0) \equiv \text{sign}(q_0) \text{Im} \, \Pi(q, q_0)$$

provides an alternative to calculate the real part of the polarization out of the imaginary part.

The intermediate results are shown in Figs. A.2 and A.3. The choice of axes means that the region $a < -u$ does have no values, because they would relate to the actually undefined values for $q < 0$.

![Figure A.2: The imaginary part of the first-order polarization in units of $4mk_F^2/h^2$.](image)

The imaginary part $\text{Im} \Pi^{(1)}$ is zero for $|a| > 1$ and does not need to be shown in this parameter region. Fig. A.2 shows $\text{Im} \, \Pi^{(1)}$ divided by $4mk_F^2/h^2$ and Fig. A.3 $\text{Re} \, \Pi^{(1)}$ in the same units. Their most important feature is that $\text{Im} \Pi^{(1)}$ is dominantly negative for $u < 1$, i.e., for velocities below the Fermi velocity. The contribution of diagram b) is negative there, but the contribution of diagrams c) and d) positive and of comparable magnitude.

Fig. A.3 displays the equivalent real part in the same units covering a larger parameter region, which contains also the interval $-u < a < -1$ which is needed to calculate the plasmon
Figure A.3: The real part of the first-order polarization in units of $4mk_F\chi^2/h^2$. The straight line $a = 1 - 2u$ is the discontinuity that was derived in App. [A.2.2]

A.4 Mathematical Aids

A.4.1 The Generalized Dilogarithm

An underivative of $\ln|c-x|/x$, which is continuous in separated intervals, is obtained via integration of the power (Laurent) series representations

$$
\int \frac{\ln|c-x|}{x} dx = \ln |c| \ln |x| + \frac{\ln^2 |\xi|}{2} - \int \frac{\ln|\xi|}{\xi} d\xi
$$

$$
= \ln |c| \ln |x| + \frac{\ln^2 |\xi|}{2} + 1 + (\xi - 1) \ln |1 - \frac{1}{\xi}| + \sum_{n=1}^{\infty} \frac{1}{n^2(n+1)\xi^n} + \text{const}; \quad (\xi^2 > 1) \quad (A.15)
$$

$$
\xi \equiv x/c
$$
using [97] 1.513.5, 1.513.3] and
\[
\int \frac{\ln|c-x|}{x} dx = \ln|c| \ln|x| - 1 - \frac{1-\xi}{\xi} \ln|1-\xi| - \sum_{n=1}^{\infty} \frac{\xi^n}{n^2(n+1)} + \text{const}; \quad (\xi^2 < 1) \tag{A.16}
\]

together with [97] 1.511]. To obtain an undervative that is also continuous at \(\xi = \pm 1\), the constants may be chosen as [97] 0.233]
\[
\text{const} = \begin{cases} 
-\pi^2/6 = -\zeta(2) & ; \xi > 1 \\
+\pi^2/3 & ; \xi < -1 \\
+\pi^2/6 & ; -1 < \xi < 1.
\end{cases}
\]

With this special choice of the adaptation of the power series of (A.15) and (A.16), which deliver a uniquely defined \(L\), we get the special values
\[
L_c(c) = \ln^2|c|; \quad L_c(-c) = \ln^2|c| + \frac{\pi^2}{4}; \quad L_c(0) = \pm \infty;
\]
and more generally
\[
L_c(x) \equiv P \int_c^x \frac{\ln|c-x'|}{x'} dx' + \ln^2|c|.
\]
The substitution \(x' \rightarrow -x'\) in the integral provides the functional equation
\[
L_{-c}(-x) = L_c(x).
\]
A numerical integration, which was suggested in [109] (B51)] is no longer necessary. If we start with the Dilogarithm as defined in [2] 27.7],
\[
\text{Li}_2(x) \equiv -\int_1^x \frac{\ln t}{t-1} dt \quad (x > 0),
\]
use of [97] 4.231.2] associates both functions via
\[
L_c(x) = \ln |c| \ln |x| + \frac{\pi^2}{6} + \text{Li}_2(1 - \frac{x}{c}),
\]
if \(1 - x/c > 0\). Insofar the integral presented here is generalization of the Dilogarithm.
A.4.2 Variable Substitution in the Two-Dimensional Principal Value Integral

The proof of the formula

\[ P \left( \frac{dx}{x} \right) P \left( \frac{dy}{y} \right) = P \left( \frac{dx}{x} \right) P \left( \frac{dy}{x+y} \right) + P \left( \frac{dy}{y} \right) P \left( \frac{dx}{x+y} \right) - \pi^2 \delta(x) \delta(y) \]  

(A.17)

(P ... principal value) proceeds as follows: the left side is a two-dimensional integral, which excludes stripes of width \(2\epsilon\) along the \(x\)- and \(y\)-axis (Fig. A.4a) from the integration, then evaluates the limit \(\epsilon \to 0\). The integral \(P \int dx/(x+y)\) of the left hand side must be corrected by the values of the integral over the rectangular triangles \(I_1 + I_3 - I_5 - I_6\) by comparison with \(P \int dx/x\), the first term of the right hand side, because \(I_1\) and \(I_3\) are excluded from the quadratic region of integration of the left hand side, but not from \(P \int dx/(x+y)\), the stripe along the minor diagonals (Fig. A.4b).

Figure A.4: a) Stripes of width \(2\epsilon\) and their overlap in the principal value integral \(P \int dx/x P \int dy/y\). b) Vertical stripe of width \(2\epsilon\), which is not included in \(P \int dx/x\), and its overlap with the stripe, which is not included in \(P \int dy/(x+y)\). c) Horizontal stripe of width \(2\epsilon\), which is not included in \(P \int dy/y\), and its overlap with the stripe, which is not included in \(P \int dx/(x+y)\).

\(I_5\) and \(I_6\) are not included in \(P \int dx/x\), but included in \(P \int dx/(x+y)\). The corresponding corrections to move from \(P \int dy/y\) to \(P \int dy/(x+y)\), the second term of the right side, are shown in Fig. A.4; their sum is \(I_2 + I_4 - I_5 - I_6\). The integrals over the triangles are

\[ I_1 = \int_{-\epsilon}^{\epsilon} dx \int_{\epsilon-x}^{\epsilon} dy \frac{1}{xy} = \int_{-\epsilon}^{\epsilon} dx \ln \frac{\epsilon - x}{\epsilon} = I_2 = I_3 = I_4 ; \]

\[ I_5 = \int_{\epsilon-x}^{\epsilon} dx \int_{\epsilon-x}^{\epsilon} dy \frac{1}{xy} = \int_{0}^{\epsilon} dx \ln \frac{\epsilon}{\epsilon - x} = I_6. \]
The total correction is
\[ 4(I_1 - I_5) = 4 \int_{-\epsilon}^{\epsilon} dx \frac{\ln(1 - \frac{x}{\epsilon})}{x} = -\pi^2, \]
as shown by a power series expansion, term-by-term integration and \[ \text{[97] 0.234.2}, \]

\[ \frac{\ln(1 - \frac{x}{\epsilon})}{x} = -\sum_{n=1}^{\infty} \frac{x^{n-1}}{n\epsilon^n} \]

\[ \Rightarrow \int_{-\epsilon}^{\epsilon} \frac{\ln(1 - \frac{x}{\epsilon})}{x} dx = -\sum_{n=1}^{\infty} \frac{x^n}{n^2\epsilon^n} \bigg|^{\epsilon}_{-\epsilon} = -2 \sum_{n=1}^{\infty} \frac{1}{n^2} = -\frac{\pi^2}{4}. \]

The product of \( \delta \)-functions in \((A.17)\) is a correction of the systematic neglect of the quantities \( I_1, \ldots, I_4 \) with a negative sign of \( xy \) and a preference of the quantities \( I_5 \) and \( I_6 \) with a positive sign of \( xy \) (and closer to the origin) by the right side.
Appendix B

Complements and Extensions of the Brandt-Kitagawa Ion Model

B.1 Adding an Exchange-Energy Term

A straightforward improvement of the BK theory is expected by consideration of the exchange energy in the density functional \[101, 139\]

\[
E_x = \int n(r) \epsilon_x(n) d^3r
\]

\[
\epsilon_x = -\frac{3}{2\pi\alpha r_s} E_0
\]

; \quad r_s \equiv \frac{3}{4\pi n a_0}

The equivalent extension of the Thomas-Fermi atom is known under the name Thomas-Fermi-Dirac atom [235]. The integral is calculated using the BK electron density (3.1) with [97, 3.38.4] and [2, 6.1.13] via

\[
\int \frac{n(r)}{r_s(r)} d^3r = 4\pi \sqrt{\frac{4\pi}{3}} a_0 \int_0^\infty r^2 n^{4/3} dr = \frac{1}{\sqrt{3}} \left( \frac{N^{4/3}}{\Lambda_x a_0} \right)^{8/3} \int_0^\infty r^{2/3} \exp \left( \frac{-4r}{3(\Lambda_x/a_0)} \right) dr
\]

\[
\Rightarrow \quad \frac{E_x}{E_0} = -\psi \frac{N^{4/3}}{\Lambda_x a_0} \quad ; \quad \psi \equiv \frac{9 \Gamma(2/3)}{16\pi^{2/3}} \approx 0.3551.
\]

The total internal energy (3.5) is complemented to read

\[
E_{BKx} \equiv E_{ee} + E_{ne} + E_{\text{kin}} + E_x,
\]

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\[
\frac{E_{BKx}}{E_0} = -2 \frac{Z_1 N}{\Lambda_x/a_0} + \lambda_x \frac{N^2}{2 \Lambda_x/a_0} + 2\phi \frac{N^{5/3}}{(\Lambda_x/a_0)^2} - \frac{N^{4/3}}{\Lambda_x/a_0},
\]
if we let the factor \(\lambda_x\) take the place of the prior \(\lambda\), which again is varied to let the chemical potential of the neutral atom become zero. The calculation proceeds without hindrances and completely similar to the original calculation by Brandt and Kitagawa:

\[
\frac{\partial E_{BKx}}{\partial \Lambda_x} = 0 \implies \frac{\Lambda_x Z_1^{1/3}}{a_0} = \frac{2\phi (1 - q)^{2/3}}{1 - \frac{\lambda_x}{4} (1 - q) + \frac{\phi}{2 Z_1^{2/3}} (1 - q)^{1/3}}, \quad (B.2)
\]

\[
\frac{\partial E_{BKx}}{\partial N} \bigg|_{N=Z_1} = 0 \implies \lambda_x = \frac{4}{7} + \frac{6 \phi}{7 Z_1^{2/3}}, \quad (B.3)
\]

— the correction factor \(\lambda_x\) to the Hartree term is closer to one than the original factor \(\lambda\), and hence agrees better with more accurate functionals — and finally

\[
\frac{E_{BKx}}{E_0 Z_1^{7/3}} = -\frac{(1 - q)^{1/3}}{2\phi} \left[ 1 - \frac{\lambda_x}{4} (1 - q) + \frac{\phi}{2 Z_1^{2/3}} (1 - q)^{1/3} \right]^2. \quad (B.4)
\]

The modified energies are shown in Fig. B.1.

---

Figure B.1: Total binding energy \(E_{BKx}/(E_0 Z_1^{7/3})\) of electrons as a function of the ionization degree \(q\) with inclusion of an exchange term in the BK energy function for \(Z_1 = 7, 15, 24\) and \(36\) (thin lines) acc. to \((B.4)\), and the original energy, \((3.10)\) (bold line).

The exchange terms generally reduce the strength of the Hartree term \([101]\) — they have the opposite sign. The effective energy of the neutral Brandt-Kitagawa atom is shifted by \(-0.362 Z_1^{5/3} E_0\)—
0.0657\,Z_1 E_0$, whereas the equivalent exchange term of the Thomas-Fermi-Dirac atom adds up to $-0.4416\,Z_1^{7/3} E_0$ \cite{235}. If the charge distribution is kept fixed, the repulsive electron-electron interaction is reduced by the exchange term, the quantity $\Lambda$ decreases and the energy minimum is reduced. The improvement of the energy functional leads to further obvious deterioration compared with the quantum-mechanical total electron energy (\to Fig. \ref{fig:3.14}). The decrease of $\Lambda$ implies a smaller effective ionization degree and a smaller EL compared with the original BK ion model. This may correctly be derived from (3.17) as (3.2) stays valid.

### B.2 Hydrogen-Like Electron Density Distributions

The class of electronic radial density function of the BK theory (3.1) may be replaced by the class of hydrogen-like density distributions.

\[ \tilde{n}_e = \frac{\beta^3}{8\pi} N e^{-\beta r} \quad ; \quad \int \tilde{n}_e d^3r = N. \]

The reasons to consider a different class of model functions are

- atomic wave-functions are often expanded as radial wave-functions that are products of exponentials and powers of $r$. The existence of approximations to RHF wave-functions by so-called single-zeta-functions demonstrates the validity of this ansatz \cite{50,161,138}. The description of light ions (ions with small density of bound electrons) is commonly done with this $1s$-shape \cite{121}. If the wave-functions are described with this form, the density also obtains the $1s$-type.

- The original functions (3.1) are singular at the origin, though the total number $N$ of electrons is finite. If one imagines $n_e$ to be the one-particle density and

\[ \psi = \sqrt{\frac{N}{4\pi r^3}} e^{-r/(2\Lambda)} \]

the corresponding wave-function, the expectation value of the kinetic energy is divergent in the ultra-violet:

\[ \int \psi \Delta \psi d^3r = -\infty \quad . \] (B.5)
Note that the expectation value is not given by the finite value of
\[
\int \frac{d^3k}{(2\pi)^3} k^2 n_e(k) \quad \text{with} \quad n_e(k) \equiv \int d^3r n(r) e^{-ikr},
\]
but by using the Greens integral theorem by
\[
\int \psi \Delta \psi d^3r = -\int d^3r (\nabla \psi)^2 = \int \frac{d^3k}{(2\pi)^3} k^2 |\psi(k)|^2 \quad \text{with} \quad |\psi(k)|^2 \neq n_e(k).
\]

- Results that depend on the special type of density distributions are artificial to some extend. Other forms of distributions provide helpful tests of the inherent uncertainty of predicted numbers and curves.

However,

- we must use the same ion model for a consistent description of the ion stopping, calculation of the ionization degree and the energy loss. Calculations that use some model to derive the ionization degree as a function of the ion velocity must use the same model to derive the effective charge fraction from the ionization degree.

Let the energies of these 1s-type charge densities be described again by the BK density functionals,
\[
E_{ne} = -\frac{Z_1 e^2}{4\pi\epsilon_0} \int \frac{n_e(r)}{r} d^3r = -\frac{Z_1 e^2}{4\pi\epsilon_0} \frac{\beta N}{2},
\]
\[
E_{kin} = \frac{3}{10} \frac{h^2}{m} \int d^3r \left(\frac{3\pi^2}{2}\right)^{2/3} n_e^{5/3} = \frac{3}{10} \frac{h^2}{m} \left(\frac{3\pi^2}{2}\right)^{2/3} \left(\frac{\beta^3 N}{8\pi}\right)^{5/3} \frac{4\pi}{\beta\beta^2} \frac{N^{5/3}}{8},
\]
\[
E_{ee} = \frac{\lambda}{2} \frac{e^2}{4\pi\epsilon_0} \int d^3r_1 d^3r_2 \left(\frac{3\beta N}{8\pi}\right)^2 \frac{e^{-\beta r_1} e^{-\beta r_2}}{|r_1 - r_2|} = \frac{\lambda}{2} \frac{e^2}{4\pi\epsilon_0} \frac{\beta^2 N^2}{\pi} \frac{5}{64},
\]
with
\[
\int_1^r \frac{dz}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 z}} = \frac{r_1 + r_2 - |r_1 - r_2|}{r_1 r_2} ; \int_0^\infty r_2 e^{-\beta r_2} \frac{r_1 + r_2 - |r_1 - r_2|}{r_1 r_2} d r_2 = \frac{4}{r_1 \beta^3} \left(1 - e^{-\beta r_1}\right) - \frac{2}{\beta^2} e^{-\beta r_1}.
\]
Adding the three terms yields
\[
\frac{E}{E_0} = \beta a_0 \left[-Z_1 N + 2bN^{5/3} \beta a_0 + \frac{\lambda}{2} \frac{5}{32\pi} N^2\right] ;
\]
\[\phantom{E/E_0} \]
\[
b \equiv \left( \frac{3}{5} \right)^4 \frac{(3\pi)^{2/3}}{8} \approx 0.072282
\]

Following the original work the size parameter \( \beta \) is determined by minimization of the internal ion energy at all ionization degrees, and the coupling parameter \( \tilde{\lambda} \) by assigning chemical potential zero to the neutral atom:

\[
\frac{\partial (E/E_0)}{\partial (\beta a_0)} = 0 \quad \Rightarrow \quad \beta a_0 = \frac{Z_1^{1/3}}{4b} \left[ \left( \frac{Z_1}{N} \right)^{2/3} - \frac{5\tilde{\lambda}}{32\pi} \left( \frac{N}{Z_1} \right)^{1/3} \right]. \quad (B.6)
\]

In the same manner as the original BK definition of \( \Lambda \), (B.6) guarantees the validity of the virial theorem in the special version with \( 1/r \) potentials \([168, 198]\) for arbitrary \( \beta \):

\[
E_{ee} + E_{ne} = -2E_{\text{kin}};
\]

\[
\frac{\partial (E/E_0)}{\partial N} = -Z_1\beta a_0 + \frac{10}{3} b N^{2/3} (\beta a_0)^2 + \tilde{\lambda} N \beta a_0 \frac{10}{32\pi} \Rightarrow \beta a_{0|N=Z_1} = \frac{Z_1^{1/3}}{4b} \left[ 1 - \frac{5}{32\pi} \right] \Rightarrow \tilde{\lambda} = \frac{32\pi}{35}
\]

The final formulas for the screening parameter and total energy have the same \( q \)-dependence than the original charge densities, but with different coefficients:

\[
\frac{E}{E_0} = -\frac{Z_1^{7/3}}{8b} (1-q)^{1/3} \left[ 1 - \frac{1-q}{7} \right]^2 \quad ; \quad \frac{1}{\beta a_0} = \frac{4b}{Z_1^{1/3}} \frac{(1-q)^{2/3}}{1 - \frac{1-q}{7}} \quad \text{.} \quad (B.7)
\]

The ion energy \( E \) of the original theory is 17% lower than the energy of the charge distribution here. As Fig. 3.14 shows, the energies of the 1s-type densities are much closer to the energies of the Clementi-Roetti tables.

The total charge distribution including the ion nucleus \([3.2]\) becomes \([171]\)

\[
\tilde{\rho}_m(k) \equiv \tilde{\rho}_e(k) + \rho_n(k) = Z_1 e \frac{q - 1 + [1 + (k/\beta)^2]^2}{[1 + (k/\beta)^2]^2} \quad ; \quad \tilde{\rho}_e(k) = -Ne e \frac{1}{[1 + (k/\beta)^2]^2} \quad (B.8)
\]

for the 1s-type charge distributions. The influence on the stopping is described by the Lindhard stopping number \([3.16]\). Using the Lindhard function for \( \epsilon(k, \omega) \) results in Fig. B.2.

The 1s charge distributions establish smaller energy losses \( dE/dx \sim L/v^2 \) than the original BK distributions. An effective charge theory has to assume larger \( q \) values at a given velocity \( v \) for the distributions of 1s-type to compensate this effect while fitting to experimental stopping data. The differences are not large, as one sees comparing Figs. B.3 and 3.9.
This switch to a different class of ion charge distributions is discussed in an appendix here, because it is in some sense transparent in the view of the energy criterion. On one hand the absolute value of the total electron energy is 17% below the BK energy, which is equivalent to a scaling of the velocity axis within the energy criterion — we just substitute \( 4 \beta \) for \( \beta \) in (3.33). This
predicted increase of the ionization degree is accompanied by a decrease of the stopping power at fixed $q$. A numerical example: With $Z_1 = 15$, $v_F = v_0$ and $y = 0.81$ the energy criterion (3.33) predicts $q = 0.572$, but $q = 0.626$ for hydrogen-like ions. This is a ratio of 1.20. The ratio of the Lindhard numbers of both cases with the different values of $q$ and different form factor is only 1.12, which means that half of the increase of the stopping, which is expected by a restricted view on the ionization degree, is not found in the effective charge fraction.

Conclusions:

- The ionization degrees of the ZBL and BK formulas $q(v)$ are not absolute, physical values at small velocities, but depend also on the underlying ion model. The results at high ionization degrees, however, are hardly dependent on the class of ion charge distributions.
- Within the given uncertainties of experimental heavy-ion stopping data one cannot decide whether the original BK form or the hydrogen-like form of the charge distribution represents bound electrons better, though the ionization degrees seem to promise this.

### B.3 Quantization of the Brand-Kitagawa Ion

The commitment to a electron density distribution is the entrance to density functional theory, though the solution to the Schrödinger equation of the quasi particles is already provided, which is usually the result of the calculations [20, 26, 66, 90, 101, 108, 139, 238]. It is impossible to find a one-particle potential $\varphi(r)$ for the given density

$$\sum_{i=1}^{N} |\psi_i|^2 = n_e,$$

which is already apparent from the divergence-$\gamma$ for $N = 1$ noted in (B.5). Instead, we start from the effective one-particle potential given by (3.1)

$$\varphi(r) = -\frac{Z_1 e^2}{4\pi \epsilon_0} \frac{1}{r} + \frac{\lambda e^2}{4\pi \epsilon_0} \int \frac{n(r')}{|r-r'|} d^3r' = -\frac{Z_1 e^2}{4\pi \epsilon_0} \frac{1}{r} + \frac{\lambda e^2 N}{4\pi \epsilon_0} \frac{1-e^{-r/\Lambda}}{r}.$$  (B.9)

The Kohn-Sham equation then reads

$$\left[ -\frac{\hbar^2}{2m} \Delta + \varphi(r) \right] \psi_i = \epsilon_i \psi_i.$$
After the familiar expansion of $\psi_i$ over spherical harmonics this becomes the known radial Schrödinger Equation with states that are $2(2l+1)$-fold degenerate with respect to spin and magnetic quantum number, where index $l$ denotes the angular momentum quantum number \[163, (9.20)\]:

$$
\left[ \frac{d^2}{d(r/a_0)^2} + 2 \frac{Z_1 - \lambda N (1 - e^{-r/\Lambda})}{r/a_0} - \frac{l(l+1)}{(r/a_0)^2} \right] y_l(r) = -\frac{\epsilon_i}{E_0} y_l(r). \quad (B.10)
$$

This type of Sturm-Liouville eigenvalue problems is handily solved by using the subroutine D02KDF of the NAG library \[178\]. The boundary conditions are known and derived from the hydrogen problem with the central point charges $Z_1$ \((r \to 0)\) or $Z_1 - \lambda N$ \((r \to \infty)\ \[163, (11.15)\]:

$$
y_l(r)/y_l'(r) \approx -1/\sqrt{\epsilon_i/E_0} \quad (r \to \infty); \quad y_l(r)/y_l'(r) \approx r/\left[2(l+1)/\sqrt{\epsilon_i/E_0}\right] \quad (r \to 0).
$$

A problem with artificially assumed “hard walls” does not emerge \[115\].

---

Figure B.4: The occupied bound states of the quantized BK ion for $Z_1 = 15$ (left) and $Z_1 = 36$ (right), and their energies $\epsilon/E_0$ as a function of the number $N$ of bound electrons acc. to \[B.10\]. The higher occupied orbital is labeled with the principal quantum number, the angular momentum quantum number $l$ and the occupation number.

The total energy of the quantized BK ion in Fig. \[B.5\] is calculated by summation of the energies of the occupied states under consideration of the degeneracies, and subtraction of the
electron-electron interaction energy, which otherwise would have been counted twice \[36\ (10)\] (2.10)]:

\[
E = \sum_{i=1}^{N} \epsilon_i - E_{ee} ; \quad E_{ee}/E_0 = \frac{1}{2} \frac{N^2}{\Lambda/a_0}, \tag{B.11}
\]

Figure B.5: Total energies \[E/[E_0Z_1^{7/3}]\] of the quantized BK ions for various atomic numbers (chemical symbols) acc. to (B.11) and of the original statistical theory (3.10) (solid line) \(\rightarrow\) Fig. 3.14. \(q\) denotes the ionization degree.

The discrete, quantized model

- possesses larger ionization energies of low order, which can be calculated by the energy differences of total energies \[B.11\] for states with \(N - 1\) and \(N\) electrons. This may be attributed to the partial occupation of tunneling states in the quantum-mechanical treatment, which therefore is able to pack more electrons into lower lying states, as discussed in \[80\]. [The ionization energies are not simply the energies of the highest occupied states, because the removal of one electron from one of these does not only lift this electron but layers the lower states at the same time (Fig. B.4).]

- shows as expected a better agreement with the original statistical model at larger atomic numbers. It does not reproduce the total energies \[3.10\], because the L(S)DA of the kinetic energy \[3.4\] has been replaced by the operator-valued expression in \[B.10\].
• produces a larger slope \( dE/dq \) for intermediate ionization degrees \( q \), and lower slope for very large ionization degrees. An interpretation of these ionization energies as velocities therefore leads (according to the energy criterion) to smaller ionization degrees at small and medium velocities than in the original model. Because these results are based on the coupling factor \( \lambda = 4/7 \) of the original model, and this was chosen to let the chemical potential of the neutral atom (the tangent to the energy at \( q = 0 \)) vanish, this factor would have to be re-fitted to some given first ionization energy for consistency.

• does not reproduce the crossing of energy levels which actually happens in the PSE, but even up to \( Z_1 = 54 \) the energies of levels with higher principal quantum numbers are always above the energies of levels with smaller principal quantum numbers.

but

• does not possess much value for our discussion, because the central advantage of the original model, the knowledge of physical parameters in analytical formulas, is lost, and because in this case tabulated values derived from better atomic calculations are available.
Appendix C

Electronic Energy Loss by TRIM85

C.1 The Section of the Program

Lines STO01960, RSTO1340 and 00002750 of the ZBL documentation [261, Ch.8] contain an insecure comparison of floating point numbers that may lead to an incorrect branching and prohibit the reproduction of the test values of [261, Fig. 8] on a hardware with a different precision of the representation of numbers in the memory and in the registers. To

- avoid this program error,
- simplify an independent reading of the current thesis,
- program in a structured way wherever supported by standard FORTRAN77, simplify the implementation in other programming languages and obtain ANSI and POSIX conformance
- eliminate formal parameters and local variables not used

the following version is proposed. (The equivalent version in C was used to obtain the results quoted in the thesis.)

```
1    subroutine pstop(z1,m1,z2,m2,e,pcoef,se)
2    real e,m1,m2,pcoef(8),pe,pe0,se,s1,sh,velpwr
3    integer z1,z2
4    parameter (pe0=25.)
```
pe = amax1(pe0, e)
sl = pcoef(1)*pe**pcoef(2) + pcoef(3)*pe**pcoef(4)
sh = pcoef(5)/pe**pcoef(6) * alog(pcoef(7)/pe+pcoef(8)*pe)
se = sl*sh/(sl+sh)
if (e .le. pe0) then
  if (z2 .le. 6) then
    velpwr= .25
  else
    velpwr=.45
  endif
  se = se*(e/pe0)**velpwr
endif
end

subroutine histop(z1,m1,z2,m2,e,ee,vfermi,lfctr,pcoef,se)
real a,b,e,ee,eee,v,vfermi,vmin,vr,vrmin,lfctr,1,10,11,m2,m1,
+ pcoef(8),power,q,se,sp,yr,yrmin,zeta
integer z1,z2
logical lowbra
parameter(yrmin=.13)
vrmin=1.
v = sqrt(e/25.)/vfermi
if( v.ge.1.) then
  vr=v*vfermi*(1.+2./(v*v))
else
  vr= .75*vfermi*(1.+2.*v*v/3.-v**4/15.)
endif
yr = amax1(yrmin,vrmin/z1**.6667)
if( vr/z1**.6667 .gt. yr) then
  yr = vr/z1**.6667
  lowbra=.false.
else
  lowbra=.true.
endif
a = -.803*yr**.3+1.3167*yr**.6+.38157*yr+.008983*yr*yr
q = amin1(1., amax1(0., 1. - exp(-amin1(a, 50.))))

b = (amin1(0.43, amax1(0.32, 0.12 + 0.025*z1)))/z1**.3333

l0 = (0.8 - q*(amin1(1.2, 0.6 + z1/30.)))/z1**.3333

if (q.lt. 0.2) then
   l1 = 0.
elseif (q.lt.(amax1(0., 0.9 - 0.025*z1))) then
   l1 = b*(q-.2)/abs(amax1(0., 0.9 - 0.025*z1)-0.2000001)
elseif (q.lt. amax1(0., 1. - 0.025*amin1(16., 1.*z1))) then
   l1 = b
else
   l1 = b*(1.-q)/(0.025*amin1(16., 1.*z1))
endif

l = amax1(l1, l0*lfctr)

zeta = q + .5/(vfermi**2) *(1.-q)*alog(1+(4.*l*vfermi/1.919)**2)
a = -(7.6-amax1(0., alog(e)))**2

zeta = zeta*(1+ 1./z1**2 *(.18+.0015*z2)*exp(a))

if (lowbra) then
   vrmin = amax1(vrmin, yrmin*z1**.6667)
   vmin = .5*(vrmin+sqrt(amax1(0., vrmin**2-0.8*vfermi**2)))
eee = 25.*vmin**2
   call pstop(z1,m1,z2,m2,eee,pcoef,sp)
   power = .5
   if ((z2.eq.6).or. ((z2.eq.14).or.(z2.eq.32)).and.(z1.le.19))
       / power = .375
   se = sp*(zeta*z1)**2 * (e/eee)**power
else
   call pstop(z1,m1,z2,m2,e,pcoef,sp)
   se = sp*(zeta*z1)**2
endif
end

subroutine scoef(z1, mm1, m1, m2, rho, atrho, vfermi, lfctr, pcoef)

real a, atrho, lfctr, mm1, m1, m2, rho, vfermi, pcoef(8)

integer z1, l

open(20, file='scoef.dat')
The results of this thesis were obtained with a slightly modified ZBL data file: the factor in the last column (screening length) was set to 0.92 for \( ^{54}\text{Xe} \) \cite{98}. Note also that TRIM85 differs from the description on pages 107 and 220 of \cite{261} in the case of \( Z_2 = 6 \). The program chooses the alternate power in the case of \( Z_2 = 6 \) for all \( Z_1 \) (→ the program lines 62–63 above and STO02060 and STO02070 in \cite{261}).

### C.2 Heavy Ions of High Energy

The ZBL parameterization of the ionization is based on experimental data of effective ion velocities up to \( y \approx 2.3 \) for \( ^{18}\text{Ar} \) or \( y \approx 1.7 \) for \( ^{29}\text{Cu} \) \cite{261, Figs. (3-21),(3-22)}. Mann and Brandt used \( ^{54}\text{Xe} \) data up to \( y \approx 1.05 \) \cite{154, Fig. 3}, which is in the energy range reported in \cite{103, Fig. 16}. The validity of these fits may nowadays be checked by comparison with heavy ion data at even higher energies. Fig. C.1 demonstrates that the deviation between the data by Hubert \textit{et al.} \cite{111, 112} and the ZBL predictions is negligible for our purposes up to 45.9 MeV/u for \( ^{54}\text{Xe} \) and up to 28.7 MeV/u for \( ^{36}\text{Kr} \) projectiles.

The ZBL values have been calculated by omission of the multiplication with the proton data in 64 and 67 of App. C.1. For C ions the validity up to \( y \approx 4.5 \) has bee reported in \cite{1, Fig. (5)]. More comparisons with experimental values in the medium and low energy region are given in \cite{49, 98, 145, 197, 223}. 

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Figure C.1: Effective ionization degrees $\gamma$ as a function of the effective velocity $y_r = v_r/(v_0Z_{\gamma}^{2/3})$ for varying projectile-target combinations: Bold solid lines are the fits of [112], the dashed thin lines results of the ZBL program [261 pp. 219].
Appendix D

The Internal Energy of the Thomas-Fermi Ion

The TF equation with total potential of the nucleus and of the bound electrons and \( \varphi \) reads

\[
a_0^2 \Delta \left( \frac{e\varphi(r)}{E_0} \right) = \frac{8}{3\pi} \left( \frac{e(\varphi - \mu)}{E_0} \right)^{3/2}, \tag{D.1}
\]

where \( \mu \) is the potential at distance \( r_c \), the ion radius. The electron density is

\[
n_e(r) = \frac{1}{3\pi^2a_0^3} \left( \frac{e(\varphi - \mu)}{E_0} \right)^{3/2}. \tag{D.2}
\]

With the standard variable transformation at this place

\[
x(c) \equiv \frac{r(c)}{a_0} \left( \frac{128Z_1}{9\pi^2} \right)^{1/3} \quad \tilde{\varphi} \equiv \frac{e(\varphi - \mu)}{2E_0 \frac{r}{a_0} Z_1^3} \tag{D.3}
\]

(D.1) becomes

\[
d^2\tilde{\varphi}(x)/dx^2 = \tilde{\varphi}^{3/2}/\sqrt{x}, \tag{D.4}
\]

subject to the boundary conditions

\[
\tilde{\varphi}(0) = 1 \quad x_c d\tilde{\varphi}/dx|_{x_c} = -q \quad \tilde{\varphi}(x_c) = 0 \tag{D.5}
\]

at the origin and at the scaled ion radius \( x_c \). This boundary value problem with undetermined right abscissa \( x_c \) has been solved with the help of routine \texttt{d02hbf} in the NAG library \[178\], to obtain \( r_c \) as a function of \( q/Z_1^{1/3} \).
The kinetic energy $E_{\text{kin}}$ of the electrons, their potential energy $E_{\text{ne}}$ in the nuclear potential and their interaction energy $E_{\text{ee}}$ for the TF ion obey \cite{235}, (3.20b)]

$$\frac{3}{5}E_{\text{kin}} + E_{\text{ne}} + 2E_{\text{ee}} + \mu N = 0,$$

$$E_{\text{TF}} \equiv E_{\text{kin}} + E_{\text{ne}} + E_{\text{ee}},$$

which may be combined linearly to

$$E_{\text{TF}} = \frac{1}{6}E_{\text{kin}} + \frac{1}{2}E_{\text{ne}} - \frac{1}{2}\mu N. \quad (D.6)$$

$E_{\text{ne}}$ becomes by insertion of \eqref{D.2} and \eqref{D.3}

$$E_{\text{ne}} = \int Z_1 e^{-e} \rho_n(r) dr = \frac{Z_1 e^2}{\epsilon_0} \int_0^{\infty} r \rho_n(r) dr = -\frac{16\sqrt{2}}{3\pi} Z_{1/3} E_0 \left(\frac{9\pi^2}{128}\right)^{1/6} \int_0^{x_c} dx \frac{d^2 \phi}{dx^2}$$

$$= -\left(\frac{32}{\pi}\right)^{2/3} Z_{1/3} E_0 \left[\frac{d \phi}{dx}\bigg|_{x_c} - \frac{d \phi}{dx}\bigg|_{x=0}\right]. \quad (D.7)$$

With $N = Z_1 (1 - q)$, \eqref{D.3} and \eqref{D.5} one gets

$$\mu N = \frac{Q e^2}{4\pi \epsilon_0 r_c} Z_1 (1 - q) = Z_{1/3} E_0 2q (1 - q) \left(\frac{128}{9\pi^2}\right)^{1/3} \frac{1}{x_c} = -\left(\frac{32}{\pi}\right)^{2/3} (1 - q) Z_{1/3} E_0 \frac{d \phi}{dx}\bigg|_{x_c} \quad (D.8)$$

By multiple alternate insertion of \eqref{D.4} and partial integration we first have

$$\int_0^{x_c} dx \frac{d^2 \phi}{dx^2} = \int_0^{x_c} dx \frac{\phi^{5/2}}{\sqrt{\pi}} = 2\sqrt{\pi} \phi^{5/2}\bigg|_0^{x_c} - 2 \int_0^{x_c} \sqrt{x} \phi^{3/2} \frac{d \phi}{dx} dx = -5 \int_0^{x_c} \sqrt{x} \phi^{3/2} \frac{d \phi}{dx} dx$$

$$= -5 \int_0^{x_c} x \frac{d^2 \phi}{dx^2} dx = -\frac{5}{2} \int_0^{x_c} x \frac{d \phi}{dx} \left(\frac{d \phi}{dx}\right)^2 dx$$

$$= -\frac{5}{2} \left(\frac{d \phi}{dx}\right)^2 \bigg|_0^{x_c} + \frac{5}{2} \int_0^{x_c} \left(\frac{d \phi}{dx}\right)^2\bigg|_{x=0} + \frac{5}{2} \int_0^{x_c} \left(\frac{d \phi}{dx}\right)^2\bigg|_{x=x_c},$$

and second by a single partial integration

$$\int_0^{x_c} dx \frac{d^2 \phi}{dx^2} = -\frac{d \phi}{dx}\bigg|_{x=0} - \int_0^{x_c} \left(\frac{d \phi}{dx}\right)^2 dx.$$

Equation of both expressions allows the elimination of the integral as follows:

$$\frac{7}{2} \int_0^{x_c} \left(\frac{d \phi}{dx}\right)^2 dx = -\frac{d \phi}{dx}\bigg|_{x=0} + \frac{5}{4} x_c \left(\frac{d \phi}{dx}\bigg|_{x=x_c}\right)^2. \quad (D.9)$$
The kinetic energy becomes by (D.2) and then by (D.4)
\[
E_{\text{kin}} = \frac{3}{10} (3\pi^2)^{2/3} \frac{\hbar^2}{m} \int d^3 r n_e^{5/3} = Z_1^{7/3} E_0 \frac{3}{10} (3\pi^2)^{2/3} \frac{\hbar^2}{m} \int d^3 r n_e^{5/3}
\]
\[
= Z_1^{7/3} E_0 \frac{16}{5\pi} \left( \frac{9\pi^2}{128} \right)^{1/6} \int_{x_c}^{x} \phi d^2 \frac{d\phi}{dx^2} dx,
\]
and via insertion of (D.9) one obtains an integral-free representation also here. This energy together with (D.7) and (D.8) are inserted in (D.6) and yield the expression we are looking for
\[
E_{\text{TF}} = \frac{3}{7} \left( \frac{32}{3\pi} \right)^{2/3} \left[ \frac{d\phi}{dx} \bigg|_{x=0} - q \frac{d\phi}{dx} \bigg|_{x=x_c} \right] E_0 Z_1^{7/3},
\]
that extracts the energy of the TF ion from the numerical solution of the TF differential equation without subsequent integration.
Appendix E

Screened Energies at Small Velocities

The explicit calculations for some analytical approximation of the energy terms in Sect. 3.6.1 follow. They are the analogue to the often quoted approximations to the energy loss of [150], avoid numerical integrations, and most of all become useful if the overall theories are more complicated like for example in App. H.2 At small velocities \( v \) and therefore small \( \omega \), the subsequent limits of (1.14), (1.19) and (1.20) are derived starting from analytical approximations to \( 1/\epsilon(z,u) \) for the case of the Lindhard function [150, (14)] [2, 4.1.24]

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

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

[The Thomas-Fermi potential with screening wave number \( k_{TF} \equiv 2/(\pi a_0 \chi) \) would result from the slightly different \( 1/\epsilon(z,u) \approx z^2/(\chi^2 + z^2) = k^2/(k_{TF}^2 + k^2) \).] If we continue this approximation of small \( z \) to infinity — an extrapolation that was also used in [171] — the law of residues yields

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

\[
= \frac{\pi}{2 \left(1 - \beta^2 \chi^2 - \frac{\chi^2}{3}\right)} \left[ \frac{1}{\beta} - \sqrt{\frac{\chi^2}{1 - \frac{\chi^2}{3}}} \right] \quad ; \quad \beta z \equiv k\Lambda \quad , \quad \beta = 2k_{TF} \Lambda \quad , \quad \text{(E.1)}
\]
and the Thomas-Fermi potential yields

\[
\cdots \approx \frac{\pi}{2(1-\beta^2\chi^2)} \left[ \frac{1}{\beta} - \chi \right] = \frac{\pi}{2\beta(1 + \beta\chi)},
\]

(E.2)
supposed that \( \chi^2 < 3 \) \((v_F > .106v_0)\), which keeps the zeros of the denominator away from the real axis. Likewise

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

\[
= \frac{\pi}{2\left(1-\beta^2\chi^2 - \frac{\chi^2}{3}\right)} \left\{ \frac{1-\chi^2/\beta}{1-\beta^2\chi^2 - \frac{\chi^2}{3}} - \frac{1}{2\beta} \right\} ,
\]

(E.3)
or with the more extensive Thomas-Fermi approximation

\[
\cdots \approx \frac{\pi}{2(1-\beta^2\chi^2)} \left\{ \frac{1}{\beta} - \chi - \frac{1}{2\beta} \right\} = \frac{\pi}{4\beta(1 + \beta\chi)^2} .
\]

(E.4)

The quality of this approximation is better for smaller \( r_s \) (smaller \( \chi^2 \)) and practically independent of \( q \): at \( r_s = 2 \) it is better than 8% \((Z_1 = 15, \text{eq. (E.1)})\), 4% \((Z_1 = 15, \text{eq. (E.3)})\), 9% \((Z_1 = 38, \text{eq. (E.1)})\), 6% \((Z_1 = 38, \text{eq. (E.3)})\).
Appendix F

Schrödinger Particle in the External Potential Under Motion

The one-particle Schrödinger equation (SE)

\[ i\hbar \frac{\partial}{\partial t} \psi(r, t) = \left( -\frac{\hbar^2}{2m} \Delta + V(r, t) \right) \psi(r, t) \]

with a time-dependent external potential that moves with constant velocity \( \mathbf{v} \),

\[ V(r, t) = V(r' - \mathbf{v} t, t') = V'(r', t') \]

may be solved via a Galilei Transformation

\[ r' \equiv r + \mathbf{v} t \quad ; \quad t' \equiv t. \]

Defining

\[ i\hbar \frac{\partial}{\partial t} \psi(r, t) = i\hbar \frac{\partial}{\partial t} \psi(r' - \mathbf{v} t, t) \equiv i\hbar \frac{\partial}{\partial t} \psi'(r', t) \]

it reads

\[ i\hbar \frac{\partial}{\partial t} \psi' = \left( -\frac{\hbar^2}{2m} \Delta_{r'} + V' \right) \psi' - i\hbar \mathbf{v} \nabla_{r'} \psi', \]

meaning that \( \psi' \) obeys neither a SE nor a continuity equation, but must first undergo an additional gauge transformation

\[ \psi'(r', t') = e^{i\int (r', t')} \Phi(r', t') \]
with (for example) \[215\]
\[
f(r', t') = -\frac{m}{\hbar} v r' + \frac{m}{2\hbar} v'^2 t',
\]
to obtain \(\Phi\). This wave-function obeys a SE in a time-independent potential if a Galilei reference frame is chosen which moves with the same velocity as the external potential:

\[
\frac{i\hbar}{\partial t} \Phi = \left( -\frac{\hbar^2}{2m} \Delta r' + V' \right) \Phi.
\]

If this SE possesses the known energy eigenvalues \(\epsilon'\),

\[
\Phi = z(r') e^{-i\epsilon' t' / \hbar}
\]
we obtain by substitution into the original SE

\[
-\frac{\hbar^2}{2m} \Delta r \psi = \left( \frac{1}{2} m v'^2 + \epsilon' - V \right) \psi + im\hbar e^{-imvr'/\hbar} e^{-i(\frac{1}{2} m v'^2 + \epsilon')/\hbar} \nabla r' z(r')
\]

This has been simply written down as \(\omega' = \omega + \frac{v^2}{2} + k v\) in \[100\]. After the computation of expectation values the last term vanishes, if \(V'\) is spherical symmetric. Hereby the time-dependent potential has been transformed into an increase of the energy of the operators of the kinetic and potential energy by \(\frac{1}{2} m v'^2\) in comparison with the eigenvalues \(\epsilon'\) in the reference system with the static potential.
Appendix G

A Heuristic, Implicit Stripping Criterion

dE/dx \propto v \text{ is a rule for the EL at small velocities} [164]. This is the conclusion by the Lindhard-Winther theory of point charges in the electron gas, remains valid for frozen charge states of the BK ion in the homogeneous electron gas (Fig. 3.10) and in the (original) Kaneko theory [124], and also in the kinetic theory [230]. Multiplied with v it reads $dE/dt \propto v^2$ and means that the energy transfer is proportional to the energy $E \propto v^2$ of the incoming projectile, which in its turn is valid for each binary collision for arbitrary pair potentials [261-2-16]. An implicit stripping criterion is hidden in the slightly different heuristic rule

$$dE/dt \propto v^2 N.$$

The rule is verified in Fig. G.1 in the notation $Sv \propto y^2(1 - q)$, where some powers of $Z_1$ are omitted and the effective velocity of (3.28) has been introduced.

The remarkable aspect of the rule is that it is valid non only in the low-velocity region of frozen charge states, but up to ionization degrees of $q \approx 0.9$. If finally this internal degree of freedom $q$ is exhausted and the ion completely stripped, the rule becomes invalid and the curve bends back to the upper left in Fig. G.1. This limit is obviously reached first by the lightest ion of the examples, 5B. The rule contains an implicit stripping criterion, because the stopping power on
the left side of (G.1) also depends on \( N \), respectively \( q \). An increase of \( v \) lets the ion decrease \( N \) such that \( dE/dt \) is increased and (G.1) remains valid.

A functional which is minimized to control this adaptation of the internal degree of freedom to the velocity — as the energy criterion in Sect. 3.5 does — cannot be derived by direct inspection. One might argue as follows, based on standard assumptions: for ion models like the BK model the size parameter obeys \( \Lambda \propto N^{2/3} \) — if one neglects the weak variation in the denominator of (3.8). The geometric cross section is therefore \( \propto \Lambda^2 \propto N^{4/3} \). The factor \( N \) of the left side in (G.1) might represent this ion size, and the collision frequency and eventually the EL are of course proportional to this area in a heuristic scattering theory. This observation, however, does not lead to a stripping criterion by its own, because it is valid for any ionization degree. One would need to argue further that the ion wishes to minimize the contact with the rushing target electrons like a branch in the wind. The ion may reduce this collision frequency by reduction of its cross section and this means electron release and increase of \( q \). This in turn increases the stopping force which works against the “intended” minimization of the contact. The number of electrons which is actually adjusted could be a compromise of the internal degree of freedom. This thesis does not contain an argument of which nature this geometric cross section might be. A transformation of this idea into the two
energies of different sign in the energy criterion may exist.
Appendix H

On Generalizations of the Kaneko Theory

H.1 Calculation of the Stopping Power With the Dead Sphere

The integration volume in (5.3) is represented by subtraction of the dead sphere from the total volume. The Fourier representation (1.1) and (1.2) are inserted:

\[ \Phi_{\text{ind}}(r, t) = \frac{1}{4\pi\epsilon_0} \int d^3r' - \int_{|r' - vt| < r_c} d^3r' \int \frac{d^3kd\omega}{(2\pi)^3} e^{i(kr' - \omega t)} \left[ \frac{1}{\epsilon(k, \omega)} - 1 \right] \rho_m(k) \delta(\omega - kv). \]

This real-space representation is inserted into the EL \( \frac{dE}{dx} = \left( \frac{dE}{dt} \right)/v \) with \( E_{\text{ind}} = -\nabla\Phi_{\text{ind}} \):

\[ \frac{dE}{dt} = v \int d^3r \rho_m(r) E_{\text{ind}}(r) = -i \int \frac{d^3k'}{(2\pi)^3} \rho_m(-k') e^{ik'vt} k'v \int e^{-ik'r} \Phi_{\text{ind}}(r, t) d^3r. \]

We use \( \int d^3r e^{i\mathbf{k}\cdot\mathbf{r}}/|\mathbf{r} - \mathbf{r}'| = 4\pi e^{i\mathbf{k}'\cdot\mathbf{r}'}/k^2 \) [116, (2.3)] and obtain

\[ \frac{dE}{dx} \bigg|_{r_c=0} + \frac{i}{v\epsilon_0} \int \frac{d^3k'}{(2\pi)^3} \rho_m(-k') \frac{k'v}{k^2} \int \frac{d^3kd\omega}{(2\pi)^3} \left[ \frac{1}{\epsilon(k, \omega)} - 1 \right] \rho_m(k) \delta(\omega - kv) \int_{r' < r_c} d^3r' e^{i(k - k')r'}. \]

Introduction of spherical coordinates with notations like \( k' = k' (\cos \varphi_{k'}, \sin \theta_{k'}, \sin \varphi_{k'}, \cos \varphi_{k'}) \) replaces the \( \varphi_{k'} \) integrals by a Bessel Function acc. to [97] 8.411.7.

\[ \int_0^{2\pi} e^{-ik'r' \sin \theta_{k'} \cos(\varphi_{k'} - \varphi_{k'})} d\varphi_{k'} = 2\pi J_0(k' r' \sin \theta_{k'} \sin \theta_{k'}). \]
The same type of formula applied to the integration over $\varphi'$ and $\rho_m(-k') = \rho_m^*(k')$ yields

$$\frac{dE}{dx} = \frac{dE}{dx}_{r_c=0} + \frac{i}{\epsilon v_0 (2\pi)^3} \int_0^\infty dk' \rho_m^*(k') k' \int_0^\pi \sin \theta' d\theta' \cos \theta' \cdot J_0 \left( k' r \sin \theta \sin \theta' \right) e^{-ik' r \cos \theta' \cos \theta'}$$

$$\times \int_0^\infty dk \int_{-k}^{k} d\omega \left[ \frac{1}{\epsilon(k, \omega)} - 1 \right] \rho_m(k) \int_0^r r^2 dr \int_0^\pi \sin \theta' d\theta' J_0 \left( kr \sqrt{1 - \frac{\omega^2}{k^2 v^2}} \sin \theta \right) e^{ikr \frac{\omega}{v} \cos \theta'}.$$

The integral $\int_0^\pi d\theta'$ first and then $\int_0^\pi d\theta'$ are mapped onto the integration intervals $[0, \pi/2]$ via the substitution $\theta \rightarrow \pi - \theta$ applied in the sub-intervals $[\pi/2, \pi]$:

$$\int_0^\pi J_0(k' r \sin \theta \sin \theta') e^{i(k' r \cos \theta' - \frac{\omega}{v} \cos \theta')} \sin \theta' d\theta' J_0(r \sqrt{k^2 - \frac{\omega^2}{v^2}} \sin \theta)$$

$$= 2 \int_0^{\pi/2} J_0(k' r \sin \theta \sin \theta') \cos \left[ (k' r \cos \theta' - \frac{\omega}{v}) \cos \theta' \right] \sin \theta' J_0(r \sqrt{k^2 - \frac{\omega^2}{v^2}} \sin \theta) d\theta'$$

$$+ 2 \int_0^{\pi/2} \cos \theta' \sin \theta \sin \theta' \cos \theta' \sin(k' r \cos \theta' \cos \theta') \sin(r \frac{\omega}{v} \cos \theta') \sin(k' r \cos \theta' \cos \theta') \sin(r \frac{\omega}{v} \cos \theta') \quad (H.1)$$

The $\theta'$ and subsequently the $\theta$ integral can then be treated by [97 6.738], which delivers Spherical Bessel Functions $j_1$:

$$\int_0^{\pi/2} \sin \vartheta \cos \vartheta \sin(a \cos \vartheta) J_0(ab \sin \vartheta) d\vartheta = \frac{1}{\sqrt{1 + b^2}} j_1(a \sqrt{1 + b^2}).$$

$$\frac{dE}{dx} = \frac{dE}{dx}_{r_c=0} - \frac{1}{\epsilon_0 \pi^3 v^2} \int_0^\infty dk' \rho_m^*(k') k' \int_0^r r^2 j_1(k' r) \int_0^\infty dk \rho_m(k) j_1(kr) \int_0^{k' \omega} \omega d\omega \frac{1}{\epsilon(k, \omega)}. \quad (H.2)$$

Eq. (5.54.1) in [97] computes the underivative of the $r$ integral.

$$\int dr r^2 j_1(k' r) j_1(k r) = \frac{r^2}{k'^2 - k^2} \left[ k j_1(k' r) j_0(k r) - k' j_0(k' r) j_1(k r) \right].$$

The result is decomposed into partial fractions

$$\frac{r^2}{k'^2 - k^2} \left[ \frac{k j_1(k' r) j_0(k r)}{k'^2 - k^2} - \frac{k' j_0(k' r) j_1(k r)}{k'^2 - k^2} \right] = -\frac{\sin(k r_c)}{k'^2 r_c} \frac{\sin(k' r_c)}{k'^2} + \frac{\sin(k' r_c) - k r_c}{2k' - k} + \frac{\sin(k' r_c) + k r_c}{2k' + k}.$$

The remainder three-fold integral may be reduced to a double integral, if we specialize to the case of the BK ion model (3.2), for example. The law of residues then yields

$$\int_0^\infty \rho_m(k') \left[ \frac{\sin(k' + k) r_c}{k' + k} + \frac{\sin(k' - k) r_c}{k' - k} \right] dk' = \pi \int Z_1 e(q - 1) e^{-r_c/\Lambda} \frac{k A \sin(k r_c) - \cos(k r_c)}{1 + (k A)^2} + \rho_m(k).$$
\[
\frac{dE}{dx} = \frac{Z_1 e}{2\epsilon_0 v^2 \pi^2} \int_{0}^{\infty} dk \frac{\rho_m(k)}{k} \times \left[ \frac{(1 - q)e^{-r_c/\Lambda}}{1 + (k\Lambda)^2} \left\{ k\Lambda \sin kr_c - \cos kr_c \right\} + \frac{\sin kr_c}{kr_c} \left\{ q + (1 - q)e^{-r_c/\Lambda} \right\} \right] \int_{0}^{kv} \omega \Im 1 e^{i(kr - \omega t)} d\omega \quad (H.3)
\]

$Z_1 e$ multiplied with the term in square brackets becomes $\rho_m(k)$ in the limit $r_c \to 0$, and (H.3) becomes (1.6).

This sharp cut of the polarization charge at distance $r_c$ from the ion nucleus constitutes a rather artificial model and was chosen to manage the $r$ integral in (H.2) analytically. It produces geometric resonances: if $kr_c \sim 1$, the term in square brackets may become negative, hence delivering an accelerating contribution to $dE/dx$. Future work ought to try smoother “transition functions” for $\rho_p(r)$.

A corresponding, lengthy expression may be written down if $\rho_m(k)$ is of the hydrogen-like shape. At small $N$ this ought to replace the statistical ion model (3.1) [132, 121], but it becomes hardly relevant here, because the dead-sphere model looses its validity in this case.

### H.2 Field Energies With the Dead Sphere

Some examples for the steps are presented that introduce the “dead sphere” into the calculation of the energy of the bound electrons in the Coulomb field of the induced charges, which has an associated term in the energy loss. Among the partial energies $E_\Phi$ and $E_\rho$ that were itemized in Sect. 3.6.1 only the generalization of (3.41) will be demonstrated. This means, the induced charge $\rho_p$ is created only by the nuclear charge $Z_1 e$ and then confined to the volume outside a sphere with radius $r_c$.

Again with the “dead sphere” (5.3) we rewrite (3.40)

\[
E_\Phi = \int d^3 r \rho_p(r) \frac{Z_1 e}{4\pi \epsilon_0} \int_{|r' - vt| > r_c} d^3 r' \frac{1}{|r - r'|} \int \frac{d^3 k d\omega}{(2\pi)^3} e^{i(kr' - \omega t)} [\frac{1}{\epsilon(k, \omega)} - 1] \delta(\omega - kv).
\]

From here on all integrations that do not run over a component of (later) $k'$ may be performed exactly as in App. [H.1] because the only intrinsic difference is the missing factor $k'v$. When the integration intervals of $d\theta_r$ and $d\theta_{k'}$ have been “convoluted” onto $[0, \pi/2]$, we obtain instead of
(H.1) (due to the missing factor \( \cos \theta_{k'} \)) the form

\[
2 \int_0^{\pi/2} \sin \theta_{k'} d\theta_{k'} J_0(k'r \sin \theta_{k'}) \cos(k'r \cos \theta_{k'} \cos \theta_r) \cos(\omega r \cos \theta_r).
\]

Tracking the symmetry of the factor with respect to \( \omega \rightarrow -\omega \), \( \int_0^{kv} d\omega \) may be reduced to \( \int_0^{kv} d\omega \), which in essence creates the real part of \( 1/\epsilon - 1 \). The substitution \( u \equiv \cos \theta_{k'} \) leads for \( \int d\theta_{k'} \) to an integral which has been solved in [97, 6.677.6]. This is repeated for \( N \)

Using [97, 3.728.1–2] this leads for \( \int d\theta_{k'} \) to an integral which has been solved in [97, 6.677.6]. This is repeated for \( \int_0^{\pi/2} d\theta_r \) and results in

\[
E_{\Phi} = \frac{Z_1 e}{\epsilon_0 v \pi^3} \int_0^\infty \frac{dk'}{k'} \rho_e^{\prime}(k') \int_0^\infty \sin(k'r) dr' \int_0^\infty \sin(kr) dk \int_0^{kv} d\omega \text{Re} \left[ \frac{1}{\epsilon(k, \omega)} - 1 \right].
\]

The integral over \( dr' \) is elementary [97, 2.532.1], and using \( \lim_{r \rightarrow \infty} \sin[(k' \pm k)r]/(k' \pm k) = \pi \delta(k' \pm k) \) one has arrived at three-fold integrals. For explicit results we specialize to the BK ion model (3.2) and can compute (by passing the two poles on the real axis in the upper half-plane) with the law of residues

\[
\int_0^\infty \frac{dk'}{k'} \frac{1}{1 + (k'\Lambda)^2} \left[ \frac{\sin(k' \pm k) r_c}{k' \pm k} - \frac{\sin(k' \mp k) r_c}{k' \mp k} \right] = \text{Im} \int_0^\infty \frac{dk'}{k' \mp 1 + (k'\Lambda)^2} \frac{1}{k' \pm k} e^{i(k' \pm k) r_c} = \frac{\pi \Lambda e^{-r_c/\Lambda}}{1 + (k\Lambda)^2} \left[ \sin(kr_c) - k\Lambda \cos(kr_c) \right] - \frac{\pi}{k} e^{-r_c/\Lambda} \cos k r_c. \quad (H.4)
\]

A double integral remains

\[
E_{\Phi} = \frac{Z_1 e^2}{2\epsilon_0 \pi^2} \int_0^\infty dk \left[ \frac{\cos kr_c}{k} - \frac{\Lambda e^{-r_c/\Lambda}}{1 + (k\Lambda)^2} (\sin kr_c + k\Lambda \cos kr_c) \right] \int_0^{kv} d\omega \text{Re} \left[ \frac{1}{\epsilon(k, \omega)} - 1 \right].
\]

As example we may insert the TF static screening (described at the beginning of App. E) at small \( v \), \( \text{Re}(1/\epsilon) \approx z^2/(\chi^2 + z^2) \) with the definitions of (E.1),

\[
E_{\Phi} = \frac{Z_1 e^2}{2\epsilon_0 \pi^2} \chi^2 \frac{\beta}{\Lambda} \int_0^\infty dz \cos(\beta r_c z/\Lambda) + (1 - e^{-r_c/\Lambda})(\beta z)^2 \cos(\beta r_c z/\Lambda) - e^{-r_c/\Lambda} \beta z \sin(\beta r_c z/\Lambda)/(1 + (\beta z)^2)(\chi^2 + z^2).
\]

Using [97, 3.728.1–2] this leads for \( N = Z_1 \) to the representation

\[
\frac{E_{\Phi}}{E_0 Z_1^{7/3}} = \frac{4}{\pi Z_1^{1/3}} \exp \left( -2r_c/(\pi a_0) \right) \left[ \frac{1}{\chi} - \frac{\beta e^{-r_c/\Lambda}}{1 + \beta \chi} \right]. \quad (H.5)
\]
H.3 Generalized Susceptibilities of \( l \neq 0 \) Sub-Shells

The RPA formula \([4.3]\) is written in cylinder coordinates after insertion of \([5.5]\), with the axis pointing into the direction of \( k \), \( \mathbf{p} \equiv \mathbf{p}_\parallel + \mathbf{p}_\perp, \mathbf{p}_\parallel k = 0 \) and \( \mathbf{p}_\parallel k = \pm p_\parallel k \):

\[
\int d^3p \left[ (\mathbf{p} + \mathbf{k})^{2l} e^{-(\mathbf{p}+\mathbf{k})^2/\hbar^2} - p^{2l} e^{-p^2/\hbar^2} \right] \delta \left( \omega - \frac{\hbar(\mathbf{p} + \mathbf{k})^2}{2m} / \hbar k^2 + \frac{\hbar^2}{2m} \right) \\
= \frac{2\pi m}{\hbar k} \int_0^\infty dp_\perp p_\perp \exp \left( - \left[ \frac{(m\omega/\hbar k + k/2)^2 + p_\perp^2}{\hbar^2} \right] \left[ \frac{(m\omega/\hbar k - k/2)^2 + p_\perp^2 + k^2 + 2m}{\hbar k} \left( \omega - \frac{\hbar k^2}{2m} \right) \right] \right) \\
- \left\{ k/2 \leftrightarrow -k/2 \right\}.
\]

We take the integrals from \([97]\) 3.416.2–3,

\[
\text{Im} \chi^R = \frac{\chi^2}{8\pi^3} \left\{ \begin{array}{ll}
\mathcal{C}_0^2 \left\{ e^{-(u-z)^2} - (z \leftrightarrow -z) \right\}, & l = 0 \\
(c_1q)^2 \left\{ [1 + (u-z)^2]e^{-(u-z)^2} - (z \leftrightarrow -z) \right\}, & l = 1 \\
(c_2q^2)^2 \left\{ [2 + 2(u-z)^2 + (u-z)^4]e^{-(u-z)^2} - (z \leftrightarrow -z) \right\}, & l = 2.
\end{array} \right.
\]

The KK analysis

\[
\text{Re} \chi^R(z, u') = -\frac{P}{\pi} \int_{-\infty}^\infty \frac{\text{Im} \chi^R(z, u) du}{u' - u} \quad (H.6)
\]

\( \rightarrow [218] \) needs integrals of the form \( \int_{-\infty}^\infty t^2 e^{-t^2}/(u' \pm z - t) dt \). In the case without energy cut one may start from \([124]\)

\[
\frac{P}{\pi} \int_{-\infty}^\infty dt \frac{e^{-t^2}}{t - x} = -\frac{2x}{\sqrt{\pi}} e^{-x^2} F(1, 1/2; 3/2; x^2) \equiv -\frac{2}{\sqrt{\pi}} G(x) \quad (H.7)
\]

as an “anchor”, to calculate recursively \([177]\)

\[
P \int_{-\infty}^\infty \frac{t^{n+1} e^{-t^2}}{t - x} dt = xP \int_{-\infty}^\infty \frac{t^n e^{-t^2}}{t - x} dt + \int_{-\infty}^\infty t^n e^{-t^2} dt
\]

for \( n = 0, \ldots, 3 \) and obtain

\[
\text{Re} \chi^R = \frac{\chi^2}{8\pi^3} \left\{ \begin{array}{l}
2c_0^2 \left\{ G(u - z) - (z \leftrightarrow -z) \right\}, \\
(c_1q)^2 \left\{ 2 \left[ 1 + (u-z)^2 \right] G(u - z) - (u - z) - (z \leftrightarrow -z) \right\}, \\
(c_2q^2)^2 \left\{ -\frac{5}{2}(u - z) - (u - z)^3 + 2 \left[ 2 + 2(u-z)^2 + (u-z)^4 \right] G(u - z) - (z \leftrightarrow -z) \right\},
\end{array} \right.
\]

as closed-form representations for \( l = 0, 1 \) and 2 (from top to bottom).
Appendix I

Scattering Phase Method, Inverse Scattering Geometry

Representing a different ansatz to calculate effective charges and energy losses, the method of the summation of scattering phases ought to be mentioned, without producing new results [6, 7, 72, 73, 74, 81, 179, 182, 230]. The theory starts from a calculation of the distribution of bound and scattered electrons on the basis of Density Functional Theory [85, 101, 119, 139]. It has also been called dielectric theory in the literature, because the definition of an energy functional may also be considered the definition of an effective dielectric function of the electronic system. As long as the electron distribution of the ion stays spherically symmetric, the quantum-mechanical scattering theory may compute from a set of scattering phases of the electrons at the Fermi surface in a straight-forward manner

- the momentum transfer, hence the so-called transport cross section and eventually the energy loss,

- the partitioning of the $Z_1$ charges into $N$ bound and $Q$ scattered electrons via the Levinson theorem and the Friedel sum rule [47, 81, 83, 135, pp. 358-204].

The Friedel sum rule means that states are filled by electrons in scattering states, which occupy a part of phase space depending on the time that they spend in the scattering potential. This is
done under consideration of the Pauli principle. This method of computation is not fundamentally different from effective charge theory. The energy of the ion charge $\rho_m$ in the field of the induced surrounding charge $\rho_p$ is

$$E = \int \frac{1}{4\pi\varepsilon_0} \frac{\rho_m(r)\rho_p(r')}{|r - r'|} d^3r d^3r' = \int \rho_m \Phi_{\text{ind}} d^3r = \int \rho_p \Phi_0 d^3r. \quad (I.1)$$

In the stationary state the total time derivative of this energy is

$$\frac{dE}{dt} = \int \frac{d}{dt}\rho_m \Phi_{\text{ind}} d^3r + \int \frac{d}{dt}\rho_m \Phi_{\text{ind}} d^3r \quad \text{zero, as indicated in Sect. 1.2, because the position of these charges relative to each other does not change. Effective charge theory computes the energy transfer as the partial derivative at } d\Phi_0/dt = 0, \text{ as an ion current in a stationary field,}$$

$$\int \left( \frac{\partial}{\partial t} \rho_m \right) \Phi_{\text{ind}} d^3r = v \int \text{grad} \rho_m \Phi_{\text{ind}} d^3r = -v \int \rho_m \text{grad} \Phi_{\text{ind}} d^3r = \int j_m E_{\text{ind}} d^3r.$$ 

Within the scattering phase method (inverse scattering geometry) the ion is at rest, the electrons move relative to it with velocity $-v$, and one starts from the last term in in (I.1):

$$\frac{dE}{dt} = \int \frac{d}{dt}\rho_p \Phi_0 d^3r + \int \rho_p \frac{d}{dt}\Phi_0 d^3r \quad \text{; } \frac{\partial E}{\partial t} = \int \left( \frac{\partial}{\partial t} \rho_p \right) \Phi_0 d^3r = -v \int \text{grad} \rho_p \Phi_0 d^3r.$$

The advantage inherent to density functionals in place of the Hartree energy (I.1) is also the uniform treatment of bound and scattered electrons, which means (i) the automatic regard of nonlinearities beyond the order $\rho_p \propto \rho_m$, and (ii) the inclusion of the polarizability of the ion such that the implicitly existing dielectric function contains the mutual influence of the phase space occupancies by both “kinds” of electrons.

Within density functional theory the splitting of the $Z_1$ electrons, which are moving into the volume upon adding the ion, in $N$ bound and $Q$ scattered is a merely intermediate result, but no longer an input as in effective charge theory.

The density functional applications have only become known for small velocities, because only the static DFT has been used \[20, 66, 90, 238\]. The Friedel sum rule, however, may be generalized to moving ions: the number of scattering states can be calculated by the difference between the Friedel sums at wave numbers $mv/h$ and $mv/h + k_F$. 

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[24] Bausells J., *Effect of charge state fluctuations of ions moving in solids in high-energy ion implantation*, J. App. Phys. 69 (1) (1991) 155–61. (5) is quoted from [26] without being critic. The remarks at the end of my Sect. 3.4 apply. Their FIG. 5 seems to contradict the procedure described. If occupancies are re-distributed over some neighboring ionization degrees at fixed mean ionization degree, the mean stopping increases because it is $\propto Q^2$, as shown in FIG. 4 there. Therefore the mean range ought to become smaller, in contrast to what is shown in FIG. 5.


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Automatic Quadrature for Cauchy Principal Value Integrals, ibid. 56 (194) (1991) 741–54; →


[123] Kaneko T., Free-electron Approximation Study on Slowing Down of Ions Colliding with Targets, Nucl. Instr. Meth. B 33 (1988) 147–50. The $x$ in (3) should read $\chi$. Table 1 has been updated in [130].
[124] Kaneko T., *Partial and Total Electronic Stoppings of Solids and Atoms for Energetic Ions*, phys. stat. sol. (b) 156 (1989) 49–63. The factor 2 in the denominator of (2.12) should read 4. The right hand side of (2.15) should be multiplied by $4\pi$ (CGS units) and of (2.22) by $-1$. A square is missing in the exponential function of the denominator of (2.27).


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[157] Mathar R., M. Posselt, *Dielectric Theory of Electronic Energy Loss in a Homogeneous Electron Gas: Effect of First-Order Polarization*, Forschungszentrum Rossendorf, Inst. of Ion Beam Physics and Materials Research, Annual Report 1992, FZR 93-06, March 1993, 56–8. Due to an error in the calculation the Fig. 2 is incorrect there and to be replaced by Fig. 2.3 here.

[158] Mathar R., M. Posselt, *Electronic Stopping of Heavy Ions in Solids*, Arbeitstreffen des Verbandes “Festkörperphysik und Materialforschung mit nuklearen Methoden”, Braunschweig, 4–6 Okt. 1994. In (22) the $\bar{q}$ have to be moved to the denominators. In App. B, first line, $\pm p \perp k$ must be replaced by $\pm p \parallel k$.


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Siddiqui A. M., V. Harikumar, A. P. Pathak, Double Screening Problem in Dechanneling by Point Defects, phys. stat. sol. (b) 185 (1994) 77–85. The $\rho_m(k)/k^2$ is re-written as $\rho_n(k)$ divided by a “first” screening dielectric function there, if one associates the point defect with our ion.


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reproduced …considered unproven” is not convincing looking at the good agreement with
the curves of my Fig. 3.5


(1988) 215–28. After (4) $C_2$ should be quoted to be 0.480.

[264] van Dijk P. W. L., L. J. van IJzendoorn, M. de Koning, P. Bobbert, W. van Haeringen, M.
J. A. de Voigt, *Stopping powers for channeled helium ions in silicon using electron densities

Review articles covering the EL are [29] and [55], and for the target excitations related to atoms
[51] [116] and [5] with emphasis on relativistic velocities. The Firsov model is extensively treated
in [54] [57]. The contributions in [74] offer a good overview on more present-day research activities.
[247] reports on electronic excitations within plasma physics, when both colliding partners are ions.
List of Abbreviations

ANSI American National Standard Institute
BCA binary collision approximation
BK Brandt-Kitagawa [36]
CR Clementi-Roetti [50]
DFT density functional theory
EL electronic energy loss
FEG free electron gas
FT Fourier Transformation
KK Kramers-Kronig
HF Hartree-Fock
HKS Hohenberg-Kohn-Sham [108, 139]
LPDA local plasma density approximation
L(S)DA local (spin) density approximation
LW Lindhard-Winther [150]
MFLOPS million floating point operations per second
NAG The Numerical Algorithms Group [178]
POSIX Portable Operating System Interface for computer environments
PSE Periodic System of Elements
RPA random phase approximation
RHF Roothaan-Hartree-Fock
SE Schrödinger equation
SI  Système Internationale, international unit system
STO  Slater Type Orbital
TF  Thomas-Fermi [235]
TRIM85  Transport of Ions in Solids, program in [261]
ZBL  Ziegler-Biersack-Littmark [261]
a.u.  atomic units
u  atomic mass unit
List of Symbols

\( j!! \) \( = 1 \cdots (j - 4) \cdot (j - 2) \cdot j \)

\( a \) the parameter \( (1.18) \)

\( a_0 \) Bohr radius, one atomic unit of length

\( \phi \) constant of the BK theory \( (3.6) \)

\( b \) “Stripping Parameter” of the velocity criterion

\( \psi \) constant of the BK theory with exchange term \( (B.1) \)

\( c_l \) normalization coefficients of wave packets \( (5.5) \)

\( C() \) auxiliary function in the BK model at small \( v \) \( (3.17) \)

\( C \) expansion coefficients for atomic orbitals in Sect. 3.2.3

\( dE/dx \) stopping force; electronic energy loss

\( e \) elementary charge, 1 atomic charge unit

\( E_0 \) 1 Rydberg, one half of the atomic energy unit

\( E_{BK} \) internal energy of the BK ion

\( E_{BKx} \) internal energy of the BK ion with exchange term, Sect. B.1

\( E_{cm} \) kinetic energy of bound electrons with target as the reference system, Sect. 3.5.1

\( E_{CR} \) internal energy of Clementi-Roetti ions

\( E_{ee}, E_{\text{kin}} \) electron-electron interaction energy and kinetic energy of the BK ion

\( E_g \) energy gap of shell of a target, Sect. 5.3

\( E_i \) internal energy (electron binding energy) of an ion (generally)

\( E_{\text{kin}} \) kinetic energy of the Thomas-Fermi ion (App. D)

\( E_M \) \( (3.43) \)
$E_{ne}$: electron-nucleus interaction energy of the BK ion

$E_{TF}$: internal energy of the Thomas-Fermi ion, App. D

$E_x$: exchange energy, Sect. B.1

$E_{\Phi}$: interaction energy between $\rho_e$ and the part of $\rho_p$ induced by $\rho_n$, (3.40)

$E_{\rho \rho}$: total electric energy

$E_{\rho}$: interaction energy between $\rho_e$ and the part of $\rho_p$ induced by $\rho_e$ (3.42)

$f_1, f_2$: scaled real and imaginary part of the susceptibility of a target shell

$F();$: macro function (A.4)

$\text{$_1F'_1();$}$: Confluent Hypergeometric Function

$G^0$: unperturbed Greens Function of the FEG, Sect. 2.2

$G();$: auxiliary function to represent Re$\Pi^{(1)}$, (A.7)

$G():$ auxiliary function of the Kaneko theory, (H.7)

$h (\hbar)$: (reduced) Plank constant

$i$: imaginary unit

$I_1, I_Q$: first ionization energy, $Q$th ionization energy

$I();$: auxiliary function in the BK model at small $v$, defined after (3.17)

Im: imaginary part

$j_m$: electric current of the ion, (1.5)

$j_0(), j_1(), J_0$: Spherical Bessel Functions of First Kind, Bessel Function

$k_F$: Fermi wave number in the FEG

$K();$: macro function (A.2)

$l$: factor that corrects ion sizes (used by ZBL), angular momentum quantum number

$L$: Lindhard number, Kaneko number, Avogadro Constant

$\mathcal{L}$: Logarithm-Integral, App. A.4.1

$m$: electron rest mass

$M$: defined before (A.14) for Chapt. 2.2, ion mass in Chapt. 3

$n$: electron density in the FEG

$n_e$: electron density distribution of the ion
\( \tilde{n}_e \) electron density distribution of a hydrogen-like ion

\( N \) number of electrons bound to the ion

\( \bar{N} \) number of electrons bound to the ion that absorb the momentum of a target electron

(Sect. 3.8)

\( N_{sh}, N_{bnd}, N_{frei} \) number of electrons in a target shell

\( nf \) preceding term with inverse sign of the frequency variable

\( O(\ldots) \) of the order \ldots

\( P \) polarization, Cauchy Principle Value

\( \mathbf{P} \) polarization

\( q \) absolute value of the wave number, 4-vector of the wave number, ionization degree

\( \langle q'^{t} \rangle \) expectation value of the \( t \)th moment of the momentum, Sect. 5.2

\( \bar{q}(\bar{q}_{1}) \) characteristic wave number of the target shell and of the target orbital

\( Q \) unitless charge number of the ion

\( \text{Re} \) real part

\( r_s \) Wigner one-electron radius in atomic units; stripping radius of the velocity criterion

\( r_c \) dead sphere radius

\( S \) stopping cross section (of a target atom, in the FEG: of a target electron)

\( S_{sh}, S_{bnd}, S_{frei} \) stopping cross section of a target shell

\( \text{sign} \) sign function

\( t \) time

\( \langle T \rangle \) expectation value of the kinetic energy

\( T(;,;) \) macro function [A.3]

\( u \) frequency scaled with the Fermi wave number or characteristic wave number

\( U, (U_0) \) screened (bare) Coulomb potential

\( v \) ion velocity

\( \bar{v} \) characteristic velocity of the target shell

\( v_0 \) Bohr velocity, one atomic velocity unit

\( \mathbf{v}_G \) relative velocity of the reference frames during a Galilei transform
\( v_e \) electron orbital velocity, Sect. 3.4

\( v_k \) velocity of a K-shell electron, Sect. 3.5.2

\( v_F \) Fermi velocity

\( V_{\text{mol}} \) molar volume, (4.11)

\( V, V' \) exterior potentials in the Schrödinger equation, App. F

\( \tilde{v}_F \) virtual Fermi velocity after homogenization of all target electrons, (4.11)

\( v_r \) effective ion velocity

\( w \) occupation probability in momentum space, (4.2), (5.5)

\( x (x_c) \) reduced radial variable (ion radius) in the TF ion model

\( y (y_r) \) reduced (effective) ion velocity

\( y_l \) radial wave-function in a central potential (Sect. B.3)

\( Y_l^m \) Spherical Harmonics

\( Z_1 \) atomic number of the ion

\( Z_2 \) atomic number of a target atom

\( z \) wave number scaled with Fermi wave number or characteristic wave number

\( \alpha \) constant \( \sqrt{4/(9\pi)} \) of the FEG theory (never the fine structure constant)

\( \beta \) combination after (2.53)

\( \chi \) density parameter acc. to (1.8) and after (4.3)

\( \chi^R (\tilde{\chi}^R) \) (diluted) retarded electric susceptibility

\( \delta() \) Dirac Delta Distribution

\( \epsilon \) dielectric function

\( \epsilon_0 \) permittivity of vacuum

\( \epsilon_{\text{sh}} \) Kaneko’s dielectric function of a target shell

\( \epsilon_x \) chemical potential of the exchange energy, Sect. B.1

\( \Gamma \) Gamma Function

\( \gamma \) effective ionization degree

\( \Phi_{\Phi}, \Phi_{\rho} \) parts of \( \Phi_{\text{ind}} \) acc. to (3.47)
The normalization and sign convention of the four-dimensional Fourier transformation is generally asymmetric in this work,

\[
\begin{align*}
    f(\mathbf{r}, t) &= \int \frac{d^3k \omega}{(2\pi)^4} e^{-(ikr - \omega t)} f(\mathbf{k}, \omega), \\
    f(\mathbf{k}, \omega) &= \int d^3r dt e^{i(\mathbf{kr} - \omega t)} f(\mathbf{r}, t),
\end{align*}
\]

which means

\[
\int d^3r |f(\mathbf{r})|^2 = 1 \quad \Leftrightarrow \quad \int d^3k |f(\mathbf{k})|^2 = (2\pi)^3.
\]
All equations are given in SI units, thus that the transition to Hartree atomic units is done among others by the replacements $m = \hbar = e = a_0 = k_0 = v_0 = e^2/(4\pi\epsilon_0) \rightarrow 1$ and $2E_0 \rightarrow 1$. 
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