Theory and Simulation of the Interaction of Ions with Plasmas:
Nonlinear stopping, ion-ion correlation effects and collisions of ions with magnetized electrons.

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Chapter 1

Introduction

The interaction of charged particles with matter has been an issue of extensive investigations throughout the whole century. Its theoretical treatment starts with the classical description of the energy loss of fast projectiles considered by Bohr [Boh13]. Later a quantum mechanical treatment of the energy transfer to bound electrons was established by Bethe [Bet30] and refined by Bloch [Blo33]. Further considerable improvements of the theoretical description have been achieved by Fermi and Teller [Fer47] and finally Lindhard [Lin54] and till nowadays an enormous number of publications are dedicated to specific questions on the energy loss for a variety of possible projectile and target conditions.

A complete theoretical description of the energy loss of charged particles in matter comprises a large spectrum of physical processes. A first challenge is the proper description of the target. Depending on density and temperature, it may be a solid, fluid, gas or plasma, and one has to know the degree of ionization, the degeneracy of the electrons, the various types of ions in the target and the related bound states. This requires already a rather complete solution of many-body and atomic physics. Here the composition of dense plasmas and their optical and transport properties as opacity or conductivity are topics of actual theoretical and experimental interest. Once the target is specified, one is concerned with the projectile–target interaction in mainly two respects:

1. The energy loss of the projectile in elastic collisions with free target electrons and target ions and in inelastic collisions due to ionization of target ions and excitation of bound electrons.
2. The changes in the electronic configuration of the projectile ion by various processes like radiative and dielectronic recombination of free electrons, collisional ionization and excitation by target ions and electrons, and the charge transfer by bound–bound transitions between target ions and projectile. Most of these processes give also small contributions to the energy loss.

Because the time scales are usually quite different, the stopping itself can be separated from the dynamics of the projectile ionization. This yields a substantially simplified description of stopping compared to a full scheme which includes all processes simultaneously. The stopping power is then determined for a given electronic configuration of the projectile and the changes of the configuration during the slowing down process are calculated separately, typically by using the corresponding rate equations for all the various atomic processes, see e.g. [Pet91a, May93, Cou94, May96]. Combining the stopping power for a fixed projectile charge state with the evolution of the charge state then yields the energy losses over the time or path of interest. If necessary, one can add the energy loss related to the changes in the electronic configuration...
of the projectile, which is usually small.

The remaining task is to calculate the stopping power for a given charge state which includes stopping contributions by target nuclei, by the ionization or excitation of target ions and by free electrons. This still requires a lot of many-body and atomic physics. Nuclear stopping yields relevant contributions only for very small projectile velocities of the order of the thermal velocity of the nuclei in the target. For the largest part of the slowing down process it can thus be neglected. The calculation of stopping by bound electrons, see e.g. Refs. [Bon67, Hil74, Vie82, Gar87, Cra89, Bou92, May96], requires in general an accurate knowledge of energy levels and related transition probabilities (oscillator strengths) in the target ions. At least a mean ionization potential of the target has to be provided for determining the stopping power at high velocities using the Bethe stopping formula [Bet30]. The existence of bound electrons in the target strongly affects the charge state of the projectile, mainly by the very efficient bound–bound charge transfer. Thus a decreasing amount of bound electrons, that is, an increasing degree of ionization, is accompanied by less charge transfer between the projectile and the target. For this reason the charge states of the projectile are usually higher in a plasma compared to a gas. For a sufficiently high degree of ionization the stopping is dominated by the free electron stopping which is very efficient because energy can be transferred much easier to free electrons than to bound ones. Both effects together result in an enhanced stopping in plasmas compared to a cold gas as it was theoretically predicted [Nar82] and experimentally observed [Die90, Die92, Jac95, Jac96, Gar92, Ser92, Cha93, Cou94].

For a theoretical description of the energy loss of ions in a plasma there exist two standard approaches. One of them considers the ion as a weak perturbation of the target and the stopping is caused by the polarization cloud which the moving ion creates in its wake. This is essentially a linear response treatment which becomes invalid if the ion strongly couples to the target as e.g. for a highly charged projectile. Alternatively the stopping is calculated as the result of the energy transfers in successive binary collisions between the projectile and the electrons. Here it is essential to consider appropriate approximations for the shielding of the Coulomb potential by the plasma while no restriction on the strength of the projectile-target coupling has to be made.

One major topic of this paper is the theoretical description of the energy loss of ions in regimes where these standard approaches and approximations cease to be valid. These studies are of actual interest in at least two areas of application:

1. In heavy ion inertial fusion (HIF) a D-T pellet is compressed until ignition. In the so-called indirect scheme, the compression is planned to be driven by X-rays which are produced in a hot plasma created through the stopping of an ion beam in a converter. The plasma in the converter has densities of $10^{21} \ldots 10^{24} \text{ cm}^{-3}$ and heats up eventually to temperatures of hundred eV, but will be nonideal in the initial stages of the heating process. The current status of HIF has been reported in Refs. [Bar96, Hof98, Blu98].

2. In most experiments with charged particle beams it is desired that the beams are well concentrated and have a low temperature, that is, they should have a small (single-particle) phase space volume. One method to achieve this is electron cooling as proposed by Budker [Bud67]. In this scheme the ion beam is mixed with a comoving electron beam which has a very small longitudinal momentum spread corresponding to a temperature of a few K. In the rest frame of the beams the cooling process may be viewed as the stopping of ions in an electron plasma. Although the density is low, $n = 10^7 - 10^8 \text{ cm}^{-3}$, the electrons can be strongly correlated because of the low longitudinal temperature. Moreover the coupling between electrons and ions can become nonlinear since often very highly charged ions, up to
U^{92+}, are used in recent experiments with heavy ion beams. Reviews on electron cooling have been given in [Sor83, Pot90, Mes94] and the proceedings [Bos94, Mal96, Ber00] present the status of the physics of cold and highly correlated beams.

Here we concentrate on the many–body and plasma physics aspects of ion stopping at strong coupling rather than on the atomic physics of the projectile and the target ions. Hence we focus in chapters 2 and 3 on stopping of a point–like projectile with a given, fixed charge by free electrons. This comprises a discussion of the different coupling regimes in the envisaged system where a heavy ion passes through an electron plasma (Sec. 2.1) and an overview on the available analytical and numerical treatments of the energy loss and their applicability in the the various coupling regimes (Secs. 2.2- 2.4). A comparison of the predictions of the analytical approaches with numerically obtained simulation results for classical projectile-target systems is then presented in Sec. 3.2. From this we finally conclude in Sec. 3.3 on the essential features of ion stopping at strong coupling and the validity of the investigated theoretical approaches.

The restriction to free electrons becomes of course more and more realistic for increasing degrees of ionization, that is usually at high temperatures. Also in dense plasmas bound states disappear through a lowering of the continuum edge. For investigations concerning electron cooling even the real target is a free electron target. But then additional questions arise about the influence of the magnetic field, which guides the electron beam through the cooling section. Here binary ion-electron collisions in the presence of an external magnetic field are an important issue for describing heavy ion stopping under these conditions. An outlook on this puzzling and still unsolved problem of nonlinear ion stopping in a magnetized electron target is given in Ch. 5, where we present and discuss some first results and observations from recent numerical evaluations. These studies are still in progress.

A further topic, which has recently attracted a lot of attention, is the interaction of fullerene–like, carbon–like or metallic clusters with solids and hot plasma targets. Here the cluster structures themselves, their stability during acceleration and possible applications are subject of extensive investigations. In particular, cluster–ion–beams are proposed as an alternative driver for the heavy ion inertial fusion (HIF) scenario, see e.g. [Deu92, Eli95]. In this proposals the interest lies mainly in particles with energies of a few keV per nucleon which interact mostly with the target electrons. Because such clusters will fragment very fast on a femto second time scale when hitting the target, one has to consider an ion debris with some atomic units relative distances between the ions. This raises the question about ion-ion correlation effects on the stopping of these ion clouds due to the proximity of the comoving ions. We investigate this topic in Ch. 4 in the framework of the dielectric linear response description of stopping, where the basic features and phenomena of correlated stopping are reported and discussed in Sec. 4.1. We outline, in particular, the conditions and prerequisites for an enhancement of the stopping on an cluster or cloud of ions compared to the uncorrelated stopping of single ions. This is important for an advantageous use of cluster-ion-beams instead of usual heavy ion beams for heating the absorber or converter of an HIF target. In this context, however, at least one more point is to be checked. The proximity of the ions in the envisaged ion-clusters causes as well strong repulsive forces between the involved ions. This results in a Coulomb-explosion of the cluster which is usually rather fast on the time scale of the whole slowing down process and the correlation effects on the stopping rapidly drop down with an increasing spread of the cluster. This competition of stopping enhancement and Coulomb-explosion is subject of Sec. 4.2, in particular, with respect to the final enhancement of the specific energy deposition by ion-ion correlation effects.
Chapter 2

Stopping of heavy ions by free electron targets

We now discuss the theoretical description of the stopping of heavy ions by free electrons where we concentrate on the many-body physics at strong coupling. As a first task detailed definitions of the target-projectile system, the stopping power and the various coupling regimes are established in Sec. 2.1. We will distinguish different weak and strong coupling regimes in two respects: the ideality of the target plasma and the linearity of the ion-target coupling. The target parameters density \(n\) and temperature \(T\) define the degree of ideality while the projectile properties charge \(Z\) and velocity \(v\) have a strong impact on the degree of linearity. Stopping can thus take place in an ideal or nonideal plasma at linear, semilinear or nonlinear ion-target coupling. The description of the energy loss in these different cases deals mainly with the question of how rigorously one has to treat the electron-electron interaction in the presence of the ion. In Sec. 2.2 we review the existing analytical descriptions which are basically the dielectric linear response treatment and the binary collision approaches as well as several extensions of them. These approaches are essentially applicable for linear and semilinear coupling and ideal or weakly nonideal targets. For the nonlinear and/or nonideal regimes more complete methods, as e.g. MD simulations or density functional theory, are needed. These numerical approaches are presented in Sec. 2.3. The validity and applicability of these analytical and numerical treatments with respect to the various coupling regimes are summarized in an overview given in Sec. 2.4.

2.1 The projectile-target system

The hamiltonian for the simplified system consisting of a non-relativistic projectile with nuclear charge \(Ze\) in a non-relativistic free electron target, where the projectile-target interaction is switched on instantaneously at a certain time, can be written as

\[
\hat{H}(t) = \hat{H}_0 + \frac{P^2}{2M} - \theta(t-t_0) \sum_i e\phi_p(\hat{r}_i - \hat{R}) ,
\]

in terms of the position \(\mathbf{R}\), momentum \(\mathbf{P}\), mass \(M\) and potential \(\phi_p(\mathbf{r}) = Ze/4\pi\varepsilon_0|\mathbf{r}|\) of the projectile and the step function \(\theta(t)\). The hamiltonian \(\hat{H}_0\) of the unperturbed electron (charge
\[ -e, \text{ mass } m \) target has the form
\[
\hat{H}_0 = \sum_i \frac{\hat{p}_i^2}{2m} + \sum_i \sum_{j \neq i} \frac{e^2}{4\pi\epsilon_0|\mathbf{r}_i - \mathbf{r}_j|} + U_0 ,
\] (2.2)
where \( U_0 \) is a constant representing the potential energy related to the interaction of the electrons with a static homogeneous charge neutralizing background as well as to the background–background interaction.

On this level of description of the projectile–target system with \( Ze \) as the nuclear charge, bound states of the projectile are still included as well as all changes of its electronic configuration as far as free electrons are involved, e.g. in the case of ionization by electron–projectile collisions and recombinations due to three– or many–body interactions. In the forthcoming discussion of the energy loss we usually approximate, however, the actual projectile configuration by a point-like one with a fixed total charge also denoted by \( Ze \).

### 2.1.1 Definitions of energy loss and stopping power

The key observable in experiments exploring the interaction of charged particles with matter is usually the energy loss \( \Delta E \) of the projectile ion. It is obtained by comparing the kinetic energy of the ion before and after passing through the target. The more detailed quantity is the stopping power which is defined as the energy change per unit path–length \( \frac{dE}{ds} \) and which represents the actual decelerating force on the ion. The knowledge of the stopping power as function of energy allows then to determine e.g. the time evolution of the slowing down of the ion and the range of the projectile in matter. For sufficiently small path length \( \Delta s \) and energy change \( \Delta E \), as it is often the case for experiments with heavy projectiles and thin targets as well as for simulation studies, the stopping power can directly be derived as \( \frac{dE}{ds}(v) = \frac{\Delta E}{\Delta s} \).

For most theoretical approaches the stopping power is more conveniently defined either by the change of the kinetic energy of the ion
\[
\frac{dE}{ds} = \frac{1}{v} \frac{d}{dt} \langle \mathbf{P}^2/2M \rangle ,
\] (2.3)
or by the decelerating force as the change in the momentum of the projectile projected on the direction of motion
\[
\frac{dE}{ds} = \frac{\mathbf{v} \cdot \mathbf{F}}{v} = \frac{\mathbf{v} \cdot \frac{d}{dt}(\mathbf{P})}{v} .
\] (2.4)
Both definitions are equivalent if the projectile travels along a straight line as it will be the case for sufficiently high projectile energies and/or large masses. Problems show up at very low projectile energy of the order of the mean kinetic energy of the target particles where the motion of the projectile represents a thermalization in the target and takes the character of Brownian motion with stochastically changing momenta.

We concentrate now on the proper deceleration processes where the ion travels along a straight or smoothly varying path and work out a microscopic clearcut definition of a stopping power for the ion–target system Eq. (2.1) and a fully quantum mechanical treatment. There the state of the system is described by the density operator \( \hat{\rho}(t) \). For \( t < t_0 \) the ion is still absent and the target as defined by \( \hat{H}_0 \), Eq. (2.2), is assumed in a stationary state \( \hat{\rho}_0 = \hat{\rho}(t < 0) \) with \( [\hat{H}_0, \hat{\rho}_0] = 0 \), i.e. typically in an equilibrium state like, e.g., \( \hat{\rho}_0 = \exp(-\beta \hat{H}_0)/\text{Tr} \exp(-\beta \hat{H}_0) \). For times \( t > t_0 \) the ion is present and the system evolves according to \( i\hbar \partial \hat{\rho}(t)/\partial t = [\hat{H}, \hat{\rho}(t)] \).
where $\hat{H}$ now denotes the full projectile–target Hamilton operator Eq. (2.1). With definition (2.4) the stopping power for $t > t_0$ reads

$$\frac{dE}{ds} = \left. \frac{\mathbf{v}}{v} \cdot \frac{d}{dt} \text{Tr} \hat{\rho}(t) \hat{\mathbf{P}} \right|_{t=t_0} = \left. \frac{\mathbf{v}}{v} \cdot \frac{1}{i\hbar} \text{Tr}[\hat{H}, \hat{\rho}(t)] \hat{\mathbf{P}} \right|_{t=t_0} = \left. \frac{\mathbf{v}}{v} \cdot \frac{1}{i\hbar} \text{Tr} \hat{\rho}(t)[ \hat{\mathbf{P}}, \hat{H} ] \right|_{t=t_0}$$

$$= - \frac{\mathbf{v}}{v} \cdot \frac{1}{i\hbar} \text{Tr} \hat{\rho}(t)[ \hat{\mathbf{P}}, \sum_i e \phi_p(\hat{\mathbf{r}}_i - \hat{\mathbf{R}}) ]$$

$$= \frac{\mathbf{v}}{v} \cdot \text{Tr} \hat{\rho}(t) \sum_i e \nabla_r \phi_p(\hat{\mathbf{r}}_i - \hat{\mathbf{R}}).$$

and represents the expectation value $\langle \hat{\mathbf{F}} \rangle$ of the total force on the ion $\hat{\mathbf{F}} = \sum_i e \nabla_r \phi_p(\hat{\mathbf{r}}_i - \hat{\mathbf{R}})$ projected along the direction of motion. Here $\langle \hat{\mathbf{F}} \rangle$ recurs only to the ion and one electron coordinate. Introducing thus the reduced density

$$\rho_2(\mathbf{r}, \mathbf{R}, t) = \sum_i \int d^3r_i \delta^3(\mathbf{r} - \mathbf{r}_i) \prod_{j \neq i} \int d^3r_j \langle \mathbf{r}_1, \ldots, \mathbf{r}_i, \mathbf{R}_N | \hat{\rho}(t) | \mathbf{r}_1, \ldots, \mathbf{r}_i, \mathbf{R}_N \rangle,$$

the stopping power can be finally written as

$$\frac{dE}{ds} = - \int d^3r \int d^3R \rho_2(\mathbf{r}, \mathbf{R}, t) \frac{\mathbf{v}}{v} \cdot e \nabla_r \phi_p(\mathbf{r} - \mathbf{R}). \tag{2.5}$$

This very general expression allows to determine the stopping power from any kind of theoretical treatment which provides the probability to find at time $t$ an electron at location $\mathbf{r}$ and the projectile at $\mathbf{R}$. Expression (2.5) can be simplified for high projectile mass and energy where we can assume a classical behavior of the projectile with simultaneously known position and velocity. The projectile trajectory is given by the density $\delta^3_{\mathbf{R}}(\mathbf{R} - vt)$ where $\mathbf{v} = \mathbf{v}(t)$ varies only slowly on the time scale of the target–projectile and intra–target interactions. This allows for the approximation $\rho_2(\mathbf{r}, \mathbf{R}, t) \approx \rho_1(\mathbf{r}, t) \delta^3(\mathbf{R} - vt)$ where $\rho_1(\mathbf{r}, t)$ is the electronic density at location $\mathbf{r}$. Now the stopping power can be expressed in terms of the electric field $\mathcal{E}$ at the projectile location $\mathbf{R} = vt$ created by the electronic charge density $\varrho(\mathbf{r}, t) = -e\rho_1(\mathbf{r}, t)$

$$\frac{dE}{ds} = \int d^3r \varrho(\mathbf{r}, t) \frac{\mathbf{v}}{v} \cdot \nabla_r \phi_p(\mathbf{r} - vt) = Z \frac{e}{v} \cdot \mathcal{E}(\mathbf{v}t, t), \tag{2.6}$$

when employing $\phi_p(\mathbf{r}) = Ze/4\pi\epsilon_0|\mathbf{r}|$.

Expression (2.6) corresponds to the straightforward definition of the stopping power in a simple classical picture for the ion where the force on the ion is directly related to the electric field. Here it was derived from a fully quantal approach together with the additional assumptions of high projectile mass. The expression (2.6) becomes a rigorous result in the limit of infinite projectile mass ($M \to \infty$) where the ion moves with constant velocity and acts just as an external potential at position $\mathbf{vt}$. The Hamiltonian (2.1) then reduces to the simpler one $\hat{H}'(t) = \hat{H}_0 - \theta(t - t_0) \sum_i e \phi_p(\hat{\mathbf{r}}_i - \mathbf{vt})$. Since there is no change in momentum or energy of the projectile, the stopping power must be derived from the energy transfer to the target. Guided by expression (2.3) the stopping power at $t > t_0$ is defined through

$$\frac{dE}{ds} = -\frac{1}{v} \frac{d}{dt} \langle \mathcal{E} \rangle = -\frac{1}{v} \frac{d}{dt} \text{Tr} \hat{\rho}(t) \hat{\mathcal{H}}'(t) = -\frac{1}{v} \text{Tr} \hat{\rho}(t) \frac{\partial}{\partial t} \hat{\mathcal{H}}'(t) \tag{2.7}$$
$$\begin{align*}
&\frac{1}{\nu} \text{Tr} \langle \rho(t) \frac{\partial}{\partial t} \sum_i e \phi_p(\hat{r}_i - \nu t) \rangle = - \text{Tr} \rho(t) \sum_i e \frac{\mathbf{v}}{\nu} \cdot \nabla_{\hat{r}_i} \phi_p(\hat{r}_i - \nu t) \\
&= - \int d^3r_1 \ldots d^3r_N \langle \{ \mathbf{r}_1, \ldots, \mathbf{r}_N | \rho(t) | \mathbf{r}_1, \ldots, \mathbf{r}_N \} \rangle \sum_i e \frac{\mathbf{v}}{\nu} \cdot \nabla_{\hat{r}_i} \phi_p(\hat{r}_i - \nu t),
\end{align*}$$

that is, again in terms of the expectation value of the total force on the ion. But here \( \langle \mathbf{F} \rangle \) is entirely defined by the target and recurs solely to one electron coordinate. Hence, by introducing the charge density

$$\varrho(\mathbf{r}, t) = -e \sum_i \int d^3r_i \delta^3(\mathbf{r} - \mathbf{r}_i) \prod_{j \neq i} \int d^3r_j \langle \{ \mathbf{r}_1, \ldots, \mathbf{r}_N | \rho(t) | \mathbf{r}_1, \ldots, \mathbf{r}_N \} \rangle$$

and the electrical field \( \mathcal{E} \) we immediately recover the result (2.6). In addition, the steady excitation leads after a transient period due to switching on the interaction at \( t_0 \) to a final stationary state. Then the constant stopping power depends only on the velocity of the inert ion

$$\frac{dE}{ds} \xrightarrow{t \to \infty} Zr \nu \frac{\mathbf{v}}{\nu} \cdot \mathcal{E}(\nu t) \quad ,$$

in contrast to definitions (2.5) and (2.6), where the stopping power can explicitly depend on time due to the feedback of the stopping on the projectile velocity \( \mathbf{v}(t) \). Employing the second stopping definition (2.4), the equivalent derivation of the final stopping expression (2.8) for an infinitely heavy projectile starts from the change of the total momentum of the target particles and the simplified Hamiltonian \( H' \) as used in Eq. (2.7). For the related force \( \mathbf{F} \) we thus have

$$\begin{align*}
\mathbf{F} &= - \frac{d}{dt} \langle \sum_i \hat{p}_i \rangle = - \frac{d}{dt} \text{Tr} \rho(t) \sum_i \hat{p}_i = - \frac{1}{i \hbar} \text{Tr} [\hat{H}', \rho(t)] \sum_i \hat{p}_i = - \frac{1}{i \hbar} \text{Tr} \rho(t) \langle \sum_i \hat{p}_i | H' \rangle \\
&= \frac{1}{i \hbar} \text{Tr} \rho(t) \sum_i [\hat{p}_i, e \phi_p(\hat{r}_i - \nu t)] = - \text{Tr} \rho(t) \sum_i e \nabla_{\hat{r}_i} \phi_p(\hat{r}_i - \nu t)
\end{align*}$$

(2.9)

In several theoretical descriptions the state of a system is characterized by a phase space distribution function \( f_N(\mathbf{p}_1, \ldots, \mathbf{p}_N, \mathbf{p}_1, \ldots, \mathbf{r}_N, \mathbf{R}, t) \), e.g. for classical ensembles [Lib90]. The desired expectation values are then obtained from a phase space integral. Starting from definition (2.4), this reduces for the stopping power to an integral over the one–particle distribution for the projectile \( f(\mathbf{P}, \mathbf{R}, t) \),

$$\begin{align*}
\frac{dE}{ds} &= \frac{\mathbf{v}}{\nu} \int d^3p_1 \ldots d^3p_N d^3p \int d^3r_1 \ldots d^3r_N d^3R \mathbf{P} \frac{\partial f_N}{\partial t} \\
&= \frac{\mathbf{v}}{\nu} \int d^3p \mathbf{P} \int d^3R \frac{\partial f(\mathbf{P}, \mathbf{R}, t)}{\partial t}
\end{align*}$$

(2.10)

where the time evolution of \( f(\mathbf{P}, \mathbf{R}, t) \) is to be determined from corresponding kinetic equations.

The definitions of the stopping introduced above are not restricted to an electron target plasma. They apply as well for more complex target systems as gases, solids, fluids and two–or multi–component plasmas. To extend the previous considerations to any kind of target consisting of electrons and one or more species of nuclei one has just to replace the target hamiltonian \( H_0 \) (2.2) by a more general one.
2.1.2 Important parameters and regimes

The energy loss of an ion traveling through an electron target plasma is determined by the direct interaction of the ion with the target electrons and by the interparticle correlations within the target. Hence, it is necessary to characterize the ion–target system in two respects - the strength of the ion–target coupling and the electron–electron correlations in the plasma target - which results in a double sorting of strengths distinguishing ideal and nonideal target conditions as well as linear, semilinear, and nonlinear ion–target coupling. This will be described in the following two subsections with some emphasis, since a proper definition and demarcation of the different regimes is essential for classifying and evaluating the theoretical approaches to the stopping power reviewed in the subsequent Secs. 2.2 and 2.3.

2.1.2.1 The electron target

An electron plasma is characterized by several length scales and velocities related to its density $n$ and temperature $T$ and the electron-electron interaction. While the density defines a mean interelectron distance, the Wigner–Seitz radius $a = (4\pi n/3)^{-1/3}$, and the Fermi velocity $v_F = \hbar(3\pi^2 n)^{1/3}/m$, the temperature introduces the thermal wavelength $\Lambda = h/(mk_B T)^{1/2} = h/mv_{th}$ and the thermal velocity $v_{th} = (k_B T/m)^{1/2}$, where $m$ is the electron mass. The characteristic velocities $v_F$ and $v_{th}$ also establish the Fermi energy $E_F = mv_F^2/2$ and the thermal energy $k_B T = mv_{th}^2/2$. The ratio of these energies or the related velocities or, alternatively, the ratio of the characteristic length $a$ and $\Lambda$ define the degree of degeneracy

\[
\Theta = \frac{k_B T}{E_F} = \frac{2v_{th}^2}{v_F^2} = 2\alpha^2 \left(\frac{a}{\Lambda}\right)^2 = \frac{k_B T}{13.6eV} (\alpha r_s)^2, \tag{2.11}
\]

where $\alpha = (4/9\pi)^{1/3} = 0.521\ldots$, $r_s = a/a_0$ and $a_0$ is the Bohr radius. This parameter $\Theta$ represents a measure for the importance of the Pauli exclusion principle. The electrons have to obey Fermi–Dirac statistics for $\Theta \ll 1$ and can be treated classically within Boltzmann statistics for $\Theta \gg 1$.

For the Coulomb interaction no natural length scale exist. The scattering of two electrons with relative velocity $v_{ee}$ introduces, however, by the Rutherford cross section $d\sigma/d\Omega = b_{ee}^2/[4\sin^4(\theta/2)]$ the classical collision diameter $b_{ee} = e^2/4\pi\epsilon_0\mu v_{ee}^2$, where $\mu = m/2$ is the reduced mass. The ratio of $b_{ee}$ to the wavelength of relative motion $\lambda_{ee} = h/\mu v_{ee}$ defines the Coulomb parameter

\[
\eta_e = \frac{b_{ee}}{\lambda_{ee}} = \frac{e^2}{4\pi\epsilon_0 h v_{ee}}. \tag{2.12}
\]

Replacing the relative velocity $v_{ee}$ by its average $\langle v_{ee}\rangle$ defines the length $\langle b_{ee}\rangle$ and the averaged Coulomb parameter

\[
\langle \eta_e \rangle = \frac{e^2}{4\pi\epsilon_0 h \langle v_{ee}\rangle} = \frac{\alpha r_s}{\sqrt{2 + \Theta}} \quad \Theta \gg 1 \quad \sqrt{\frac{13.6eV}{k_B T}}, \tag{2.12}
\]

which labels the electron plasma as a whole. For the last expressions in equation (2.12) we approximated the relative velocity by $\langle v_{ee}\rangle = 2^{1/2} \langle v_e \rangle$ and the averaged electron velocity by the interpolation $\langle v_e \rangle = (v_F^2 + v_{th}^2)^{1/2}$. The Coulomb parameter is concerned with the quantum mechanical nature of the electron interaction. Classical motion is a good approximation if $\eta_e, \langle \eta_e \rangle \gg 1$ and a quantum mechanical treatment is necessary for $\eta_e, \langle \eta_e \rangle < 1$. 

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The last, but for our concerns most important parameter, is the parameter of ideality \( \xi \) which quantifies the amount of interparticle correlations within the electron plasma. It is established from the comparison of an estimate of the mean interaction energy \( E_{\text{pot}} = e^2/4\pi\varepsilon_0a \) and of the kinetic energy \( E_{\text{kin}} = m\langle v_e^2 \rangle = m(v_F^2 + v_{th}^2) \) as the ratio

\[
\xi = \frac{E_{\text{pot}}}{E_{\text{kin}}} = \frac{e^2}{4\pi\varepsilon_0am(v_F^2 + v_{th}^2)} = \frac{2\alpha^2 r_s}{2 + \Theta}, \tag{2.13}
\]

For small \( \xi \ll 1 \) the behavior of the electron plasma is dominated by the kinetic energy of the electrons and we are in an ideal, collisionless regime where collective plasma phenomena prevail. Large \( \xi \geq 1 \) correspond to a strongly coupled, nonideal electron plasma with increasing importance of interparticle correlations. The parameter of ideality \( \xi \) alternatively represents the ratio of the averaged classical collision diameter \( \langle b_{ee} \rangle \) to the typical electron spacing \( a \), that is, \( \xi = \langle b_{ee} \rangle / a \).

For nondegenerate plasmas, \( \Theta \gg 1 \), the parameter of ideality \( \xi \) becomes identical to the classical plasma parameter \( \Gamma \), defined as

\[
\Gamma = \frac{e^2}{4\pi\varepsilon_0ak_BT} = \frac{2\alpha^2 r_s}{\Theta} \quad 1 \ll \Theta \quad \xi. \tag{2.14}
\]

The various regimes of target conditions are visualized in the \( n-T \) plane of the electron plasma in Fig. 2.1. The dash–dotted curve represents the critical degree of degeneracy \( \Theta = 1 \). The degenerate regime \( \Theta < 1 \) where the Pauli principle becomes important extends towards higher densities, i.e. below the dash-dotted division line. The solid curve corresponds to the critical ideality \( \xi = 1 \). Nonideal plasmas are located in the triangle below the solid curve. The long-dashed curve indicates the classical plasma parameter \( \Gamma = 1 \). It deviates from the line \( \xi = 1 \) only in the degenerate regime \( \Theta < 1 \). The electronic Coulomb parameter \( \langle \eta_e \rangle = 1 \) is drawn as dotted line in the nondegenerate region. A classical treatment of the electrons is possible in the region below that line, and above the dash-dotted degeneracy line \( \Theta = 1 \).
2.1.2.2 The ion–target coupling

The characteristic length scales involved in the interaction of the projectile with the electron plasma are the classical collision diameter \( b_0 = |Z|e^2/4\pi\epsilon_0\mu v_r^2 \), now defined from the scattering of an ion with charge \( Ze \) and an electron at the ion-electron relative velocity \( v_r \), the wavelength \( \lambda_r = \hbar/\mu v_r \) related to this relative motion and the screening length \( \lambda \). Here \( \mu \) is the reduced mass for the ion-electron relative motion, \( \mu^{-1} = M^{-1} + m^{-1} \). For the corresponding averaged quantities \( \langle b_0 \rangle \) and \( \langle \lambda_r \rangle \) the relative velocity \( v_r \) is replaced by its average \( \langle v_r \rangle := \langle |\mathbf{v}_e - \mathbf{v}| \rangle \). Here \( \langle v_r \rangle \) together with its dimensionless form \( \langle v_r \rangle' \) and the averaged electron velocity \( \langle v_e \rangle \) are approximated and interpolated as

\[
\langle v_r \rangle = \left( \langle v_e \rangle^2 + v^2 \right)^{1/2}
\]

\[
\langle v_r \rangle' = \frac{\langle v_r \rangle}{\langle v_e \rangle} = \left( 1 + \frac{v^2}{\langle v_e \rangle^2} \right)^{1/2}
\]

\[
\langle v_e \rangle = \left( v_F^2 + v_{th}^2 \right)^{1/2} = v_F \left( 1 + \frac{\Theta}{2} \right)^{1/2},
\]

in terms of the Fermi velocity \( v_F \), the thermal velocity \( v_{th} \) and the ion velocity \( v \). While the first two lengths, \( b_0, \langle b_0 \rangle \) and \( \lambda_r, \langle \lambda_r \rangle \) are basically related to the ion-electron two-body problem, the influence of the target on the interaction interferes by the screening with \( \lambda \) as a measure of the medium response. For our purpose of deriving ion–target coupling regimes, we ignore all details of the dynamic polarization and possible particularities and assume that the screening length depends on the target parameters \( n, T \) and the ion velocity \( v \) in the well–known form 

\[
\lambda = \langle v_r \rangle \omega_p,
\]

where \( \omega_p = (e^2 n/m\epsilon_0)^{1/2} \) is the plasma frequency and \( \omega_p^{-1} \) the typical response time of the target.

All the relevant parameters for classifying the ion-target coupling are now obtained from the various ratios of the length scales defined by \( b_0, \lambda_r \) and \( \lambda \). The first one is the analogue to \( \eta_e \) as defined previously, that is, the Coulomb–parameter

\[
\eta_p = \frac{b_0}{\lambda_r} = \frac{|Z|e^2}{4\pi\epsilon_0\hbar v_r}.
\]

Here \( \eta_p = 1 \) determines the transition point from a quantum–mechanical to a classical description for a pure Coulomb ion-electron interaction. While a fast interaction with a large kinetic energy \( \eta_p \ll 1 \) can be described by a plane wave in first order Born approximation, low energetic collisions \( \eta_p \gg 1 \) allow for a treatment based on classical trajectories, particularly for high ion charges \( Ze \). With respect to the ion-target interaction, \( \eta_p \) should be replaced with \( \langle \eta_p \rangle \) defined by

\[
\langle \eta_p \rangle = \frac{|Z|e^2}{4\pi\epsilon_0\hbar \langle v_r \rangle} = \frac{|Z|\alpha \langle r_s \rangle}{\sqrt{1 + \frac{\Theta}{2}}}.
\]

Here the quantum or classical regimes for the ion–target interaction are not solely determined by this generalization of the genuine Coulomb-parameter (2.16). Since we now deal with a screened interaction, one has to check a second ratio of lengths

\[
\frac{\lambda}{\lambda_r} = \frac{\langle v_r \rangle^2}{\hbar \omega_p} = \frac{ \langle v_e \rangle^2 }{ \hbar \omega_p } \langle v_r \rangle'^2 = \sqrt{\frac{3\pi}{4\alpha \langle r_s \rangle}} \left( 1 + \frac{\Theta}{2} \right) \langle v_r \rangle'^2 = \langle v_r \rangle'^2 \sqrt{\frac{3\pi\alpha}{4} \frac{1 + \Theta}{\xi}}.
\]

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Only for large values of $\lambda/\lambda_r$ the border line between quantal and classical ion-target collisions is in fact $(\eta_p)$, as we will show when discussing the transport cross section for a screened Coulomb interaction in Sec. 2.2.2.2. This is, however, usually the case, since $\lambda/\lambda_r < 1$ is restricted to low projectile velocities, $\langle v_r \rangle \approx 1$, and highly degenerate and nonideal targets with $\Theta < 1$ and $\xi > 1$, see Fig. 2.1. In the following we thus presume $\lambda \gg \lambda_r$.

We now turn to the major goal of this subsection which is the definition of a suitable measure of the strength of the perturbation on the target caused by the ion to classify the ion–target coupling. This strength or coupling parameter should decide whether one can treat the system in perturbation theory or not. To derive such a quantity, we compare, as previously for the definition of the ideality parameter $\xi$ (2.13), an appropriate chosen interaction energy $E_{ep}$ with the kinetic energy of the relative motion $E_r = \mu (v_r)^2 / 2$. Taking the quantum diffraction effects at short distances into account, the largest value of $E_{ep}$ corresponds to the expectation value of the ionic Coulomb potential when an electronic wavepacket of width $\lambda_r$ is centered on the ion which is roughly given by $|E_{ep}| = |Z| e^2 / 4 \pi \epsilon_0 \lambda_r$. As the coupling strength parameter we thus introduce

$$\frac{|E_{ep}|}{2E_r} = \frac{|Z| e^2}{4 \pi \epsilon_0 \lambda_r} \frac{1}{\mu (v_r)^2} = \langle b_0 / \lambda_r \rangle = \langle \eta_p \rangle,$$

(2.19)

which is just the averaged Coulomb parameter (2.17). Since $|E_{ep}|$ is here the maximum potential energy, a small value of $\langle \eta_p \rangle$ implies an even smaller local coupling energy everywhere in the target. This defines a regime of a weak perturbation at all distances, which is called the regime of

$$\text{linear ion–target coupling} \quad \langle \eta_p \rangle \ll 1 \quad (2.20)$$

where lowest order perturbation theory is applicable and which can be handled with linear response techniques. The corresponding parameter of linearity marking out this regime is given by Eq. (2.19) as the averaged Coulomb-parameter $\langle \eta_p \rangle$. A more detailed derivation of this definition and demarcation of the linear coupling is reported in [Zwi99] which is essentially based on the same arguments but uses a more elaborated expression for the potential field around the ion.

To confirm the previous considerations two alternative checks for the significance of $\langle \eta_p \rangle$ (and $\eta_p$) as a measure of linear ion–electron coupling are sketched. One variant to characterize the coupling strength in the binary ion–electron system starts from a look at the quantal Coulomb scattering. There the stationary Schrödinger equation reads (for $Z > 0$)

$$\left( \Delta \tilde{r} + \frac{2\eta_p}{\tilde{r}} \right) \psi_c(\tilde{r}) = 0$$

with $\tilde{r} = r / \lambda_r$ and the pure Coulomb wave $\psi_c(\tilde{r}, \eta_p)$ [Mes70, Schi68]. Here, a straightforward measure of the coupling strength is established by comparing the probability of finding the electron at the ion position with the free particle case $\eta_p = 0$. From the known behavior of the Coulomb wave one easily derives the relative deviation

$$\frac{\left| \psi_c(\tilde{r} = 0, \eta_p) \right|^2}{\left| \psi_c(\tilde{r} = 0, \eta_p = 0) \right|^2} - 1 = \frac{2 \pi \eta_p}{1 - \exp(-2 \pi \eta_p)} - 1 \xrightarrow{\eta_p \ll 1} \pi \eta_p,$$

which turns out to be small for $\eta_p \ll 1$.

A further check for the strength of the perturbation is provided by inspecting the change of the electron density when an ion is added to a free electron target of density $n$. As a particular
critical test we regard the induced density $\delta n(r) = n(r) - n$ at the ion location for the most severe case of an ion at rest ($v = 0$). In the framework of the linear response treatment, to be discussed in Sec. 2.2.1, the induced density can be computed explicitly from the linear response relation (2.43) and by using the RPA dielectric function $\varepsilon_R$ (2.38). A numerical survey yields

$$\frac{|\delta n(r = 0)|}{n} = \left| \frac{Z}{n(2\pi)^3} \int d^3k \left[ \frac{1}{\varepsilon_R(k, \omega = 0)} - 1 \right] \right| = \langle \eta_p \rangle h(\xi, \Theta) \approx \langle \eta_p \rangle,$$

with $\langle \eta_p \rangle = \langle \eta_p \rangle(v = 0)$ as defined in Eq. (2.17), and a function $h(\xi, \Theta)$ which is of the order of unity for any degree of degeneracy $\Theta$ and any $\xi < 1$. The small relative change of the density resulting for $\langle \eta_p \rangle \ll 1$ indicates a weak perturbation by the ion and linear coupling.

In summary, the Coulomb–parameter and parameter of linearity $\langle \eta_p \rangle = 1$ separates the regimes of weak and strong perturbation, that is of linear and nonlinear ion target coupling. In coincidence it also decides on the validity of a classical treatment of the ion–target interaction, provided that $\lambda \gg \lambda_r$. More precisely, $\eta_p$ or $\langle \eta_p \rangle$ demarcates under this condition the regimes of quantum–mechanical and classical two–particle scattering in a screened Coulomb field. In view of the ion-target interaction one has to be additionally aware of the appearance of other quantum interference effects in a many–body system. It is interesting to note, however, that a truly linear coupling will occur only in the quantal regime where the quantum smoothing over distances $\sim \lambda_r$ provides the required suppression of the $1/r$ singularity of the naked Coulomb potential. The location of the division line $\langle \eta_p \rangle = 1$ in the $n - T$ plane of target conditions is illustrated in Fig. 2.2 for an ion with $Z = 10$ and three different velocities, low $v \ll \langle v_e \rangle$, high $v \approx 10 \langle v_e \rangle$ and very high $v = 100 \langle v_e \rangle$ as indicated. The last two curves would also correspond to an ion with $Z = 1$ at $v \ll \langle v_e \rangle$ and $v \approx 10 \langle v_e \rangle$, respectively. The linear coupling and quantum regime $\langle \eta_p \rangle < 1$ extends here towards higher temperatures and densities in each case. The ion–target coupling is thus linear in most of the ideal plasma regime ($\xi < 1$) for sufficiently low $Z$ or sufficiently high velocities. For high charges and/or low velocities the linear regime is reached only for extreme temperatures and densities. This reflects mainly the impact of the target conditions on $\langle v_e \rangle$ for different projectiles at a given velocity ratio $v/\langle v_e \rangle$. A more appropriate dependence of $\langle \eta_p \rangle$ in view of the experimental situation, where an ion or ion beam hits the target, is given in Fig. 2.3. It shows the parameter of linearity $\langle \eta_p \rangle$ as a function of
the projectile energy and for different charge states \( Z = 1, 5, 20 \) and 50 for classical targets with \( \Theta \gg 1 \), \( k_B T = 10 \) eV (thick curves) and \( k_B T = 50 \) eV (thin solid curves). The target conditions influence \( \langle \eta_p \rangle \) only at low projectile energies where \( \langle v_r \rangle \to \langle v_e \rangle (n, T) \). Here, we see even more clearly that a linear ion-target coupling is granted only for low charges or sufficiently high projectile energies.

The transition to a nonlinear regime with increasing \( \langle \eta_p \rangle \geq 1 \) proceeds gradually and there comes first an intermediate regime where the coupling remains weak almost everywhere except for a small volume next to the projectile position. Simple approaches can still work in this transitional regime and we thus single it out by its own name and call it the regime of \emph{semilinear ion–target coupling}. As the ion-target interaction zone is demarcated by some multiple of the screening length \( \lambda \), a similar but less demanding criterion for a weak perturbation than Eq. (2.20) is established here through the ratio of \( \langle b_0 \rangle / \lambda \), or equivalently, the energies \( |Z| e^2 / 4 \pi \varepsilon_0 \lambda \) and \( \mu \langle v_r \rangle^2 \), that is, by the parameter

\[
\frac{\langle b_0 \rangle}{\lambda} = \frac{|Z| e^2}{4 \pi \varepsilon_0 \lambda} \frac{1}{\mu \langle v_r \rangle^2} = \frac{|Z| e^2 \omega_p}{4 \pi \varepsilon_0 m \langle v_r \rangle^3} = \frac{2 |Z| \omega_p}{\sqrt{3 \pi} \langle v_r \rangle^3} \left( \frac{\alpha r_s}{1 + \frac{\mu}{2}} \right)^{3/2}.
\]

The last expression is obtained by setting \( \mu = m \) for heavy ions and \( \lambda = \langle v_r \rangle / \omega_p \), disregarding again all eventual changes of the screening behavior for our estimates. The parameter \( \langle b_0 \rangle / \lambda \) together with the parameter of linearity (2.19) now demarcates the regime of

\[
\text{semilinear ion–target coupling} \quad \langle \eta_p \rangle > 1, \quad \frac{\langle b_0 \rangle}{\lambda} \ll 1.
\]

This definition of the semilinear coupling regime is related to the ordering of length scales \( \lambda_r < \langle b_0 \rangle \ll \lambda \). Thus the local strength of the perturbation \( |E_{ep}| / E_r = \langle b_0 \rangle / r \) at a distance \( r \) from the ion remains weak in the largest part of the interaction region except for a small volume of strong perturbation, \( \propto \langle b_0 \rangle^3 \).

Large values of the ratio \( \langle b_0 \rangle / \lambda \) then define the regime of essentially

\[
\text{nonlinear ion–target coupling} \quad \frac{\langle b_0 \rangle}{\lambda} \gtrsim 1.
\]
Figure 2.4: The regions of ion–target coupling for an ion of charge $Z = 10$ in an electron plasma. The dashed curves represent $\langle \eta_p \rangle = 1$ and separate the linear regime ($\langle \eta_p \rangle < 1$) from the semilinear regime ($\langle \eta_p \rangle > 1$, $\langle b_0 \rangle / \lambda < 1$) located between the linear regime and the boundary ($\langle b_0 \rangle / \lambda = 1$, dotted curves) to the proper nonlinear one. The corresponding relative velocities are $\langle v_r \rangle' = 1$ (left plot) and 10 (right plot) in units of $\langle v_e \rangle = (v_F^2 + v_{th}^2)^{1/2}$. The solid curve is the boundary $\xi = 1$ between ideal and nonideal electron targets.

where $\langle b_0 \rangle / \lambda > 1$ already implies $\langle \eta_p \rangle \gg 1$ for the usual cases with $\lambda \gg \lambda_r$. In the nonlinear regime we hence have the sorting $\lambda_r \ll \lambda < \langle b_0 \rangle$.

The location of the semilinear regime ($\langle b_0 \rangle / \lambda < 1$, $\langle \eta_p \rangle > 1$) in the $n$–$T$ plane between the two boundaries $\langle \eta_p \rangle = 1$ and $\langle b_0 \rangle / \lambda = 1$ to linear and (essentially) nonlinear coupling is shown in Fig. 2.4 for an ion with $Z = 10$ and the different relative velocities $\langle v_r \rangle' = 1$ (left part) and 10 (right part). The dashed curves ($\langle \eta_p \rangle = 1$) and the dotted curves ($\langle b_0 \rangle / \lambda = 1$) enclose a large region of densities and temperatures where the ion–target coupling for highly charged ions is semilinear, in particular for nondegenerate plasmas $\Theta \gg 1$. In this case we have $\langle v_n \rangle = v_{th}$ and (at least at $\xi < 1$) for the screening length $\lambda = v_{th}(1 + (v/v_{th})^2)^{1/2}/\omega_p = \lambda_D(1 + (v/v_{th})^2)^{1/2}$, where $\lambda_D$ is the Debye length. Here the critical ratio (2.21) reads

$$\frac{\langle b_0 \rangle / \lambda}{\langle \eta_p \rangle / \lambda} = \frac{\sqrt{3}|Z| \Gamma^{3/2}}{(1 + \frac{v^2}{v_{th}^2})^{3/2}} = \frac{|Z|}{4\pi n \lambda_D^3 (1 + \frac{v^2}{v_{th}^2})^{3/2}} = \frac{|Z|}{N_D \lambda_D^3 (1 + \frac{v^2}{v_{th}^2})^{3/2}},$$

(2.24)

where $\Gamma$ is the classical plasma parameter (2.14) and $N_D = 4\pi n \lambda_D^3 / 3$ is the number of electrons in a Debye sphere. In condition (2.22) together with expression (2.24) we recover the well–known condition to describe the stopping in classical plasmas by the dielectric formalism. There the ion charge state has to be small compared to the number of electrons $N_D$ in a Debye sphere or, more precisely, to the number $N_D(1 + (v/v_{th})^2)^{3/2}$ in the dynamical screening sphere [Pet91], in order to ensure that each electron contributes only slightly to the screening or, more generally, to the target response.

In summary, there exist for given target conditions and ion charge two critical velocities, $v_1$ from Eq. (2.21) and $v_2 > v_1$ from Eqs.(2.17) and (2.20): the ion–target coupling is linear for ion velocities $v \geq v_2$, semilinear for $v_1 \leq v < v_2$ and nonlinear for $v < v_1$. Of course, $v_1$ or both
velocities $v_1$ and $v_2$ may be zero in certain cases and only semilinear and linear or only linear coupling occurs, respectively. In fact, reality is a bit more involved because the effective ion charge depends on the projectile velocity and hence $v_1$ and $v_2$ should also vary with velocity. Nevertheless, the critical velocities serve as a useful sorting criterion delivering this sequence of the three different coupling regimes.

The criteria outlined above have been concerned exclusively with the electronic component of the target plasma while its ionic component has been assumed tacitly as a homogeneous static charge neutralizing background. The given definitions of various regimes and the related arguments can, however, be applied and extended to a much wider spectrum of ion–target systems with more complex targets, including for instance bound target electrons as well. For that purpose one has mainly to replace the identified characteristic lengths, velocities and energies with the corresponding new and additional ones.

### 2.2 Analytical Approaches

There are basically two complementary approaches to the problem: The continuum approach formulated in terms of the dielectric function $\varepsilon(k, \omega)$ considers the stopping in a first order perturbational treatment due to the polarization cloud which the moving ion creates in its wake. This linear response description, to be discussed in Sec. 2.2.1, properly accounts for the many-body effects in the target like the shielding of the projectile and the excitation of plasma waves as long as the ion-target coupling is linear. The particle aspects, on the other hand, are pronounced in the binary collision approach, Sec. 2.2.2, where the stopping is deduced as result of independent successive binary ion–electron collisions. As it rests on a purely kinetic description for the electrons, this treatment is appropriate for an ideal target with sufficiently weak interaction between the electrons while it is a priori not restricted to linear ion–target coupling. The collective phenomena as screening and plasmon excitations, however, have to be included by using an effective ion–electron interaction which needs to be determined carefully e.g. by using the linear response approach. This complementarity of both approaches becomes particularly important in the semilinear regime. There the perturbation caused by the ion is just beyond weak with a spatial distinction such that the perturbation remains truly weak in the largest part of the ion–target interaction region with $\langle b_0 \rangle < r < \lambda$, see definition (2.22) while a strong perturbation occurs only within a small radius $\sim \langle b_0 \rangle \ll \lambda$ around the ion. This suggests an approach which relies on linear response and adds corrections from the small region of nonlinear effects. Such a procedure is much less expensive than a fully nonlinear description of stopping, and it applies to a rather large area of projectile and target parameters covered by the semilinear regime, see Fig. 2.4. Here an efficient and successful treatment of stopping by specifically combining the both basic approaches is presented in Sec. 2.2.3.

#### 2.2.1 Linear Response

In the linear ion–target coupling regime the projectile represents a weak perturbation such that its effect on the target can be treated within linear response. It is the main feature of this approach that it separates the correlations within the target from those between the ion and the target. All necessary information about the internal structure of the target is condensed in the dielectric function $\varepsilon(k, \omega)$ which provides the dynamic response related to a momentum transfer $\hbar k$ and an energy transfer $\hbar \omega$ between projectile and target. We will discuss this linear response formulation in the following subsections. First, in Sec. 2.2.1.1 we define the
key quantities of linear response and their interrelations. In Sec. 2.2.1.2 we recall the RPA formulation for the dielectric function which is appropriate for ideal targets. Nonideal targets require an incorporation of higher correlations. Here, different concepts to derive a dielectric function for nonideal targets, like the technique of the local field corrections (LFC), are outlined in Sec. 2.2.1.3. After this overview on the required and available tools we then establish the linear response formulation of the stopping power in Sec. 2.2.1.4. Finally, in Sec. 2.2.1.5, we comment on extensions of this description into the semilinear regime, in particular on the very common use of appropriate chosen cutoff parameters.

2.2.1.1 Elementary formulations of linear response

As basis for all further considerations we recall quickly the main aspects and quantities of linear response theory. Most directly related to the concept of linear response is the density–density response function \( \chi \) which is defined from the relation between an external perturbing potential \( U_{\text{ext}} \) and the resulting density response \( \delta n \) as

\[
\delta n(r, t) = \int d^3r' dt' \chi(r, t; r', t') U_{\text{ext}}(r', t')
\]

and which is to be computed from first order time dependent perturbation theory (see e.g. [Fet71, Section 13]). This involved operator definition becomes a simple algebraic equation for systems with a spatially homogeneous ground state. Then the response function \( \chi \) depends only on the differences \( r - r' \), \( t - t' \), and Fourier transformation in space and time (see A.1) yields

\[
\delta n(k, \omega) = \chi(k, \omega) U_{\text{ext}}(k, \omega)
\]

which we will consider as the defining relation for the response \( \chi \). Note that we are using the same symbols for the space-time dependent quantities as well as for the corresponding momentum-frequency dependent ones. This should not cause confusion as the distinction is usually clear from the context.

An alternative formulation of linear response uses the concept of the dielectric function \( \varepsilon \) which is defined from the relation between the external perturbation \( U_{\text{ext}} \) and the resulting total potential \( U_{\text{tot}} \) as

\[
U_{\text{tot}}(k, \omega) = \frac{1}{\varepsilon(k, \omega)} U_{\text{ext}}(k, \omega)
\]

which is here already written in its simpler form in Fourier space. This equation is the analogue of equation (2.26) defining the response function \( \chi \). Both quantities are, in fact, fully equivalent and represent merely a different emphasis in their definition. The response density \( \delta n \) of equation (2.26) yields the induced potential

\[
U_{\text{ind}}(k, \omega) = V(k) \delta n(k, \omega)
\]

where \( V(k) \) is the Fourier transformed two-body interaction potential, in case of electron systems the repulsive Coulomb potential \( V(k) = e^2/\varepsilon_0 k^2 \). The induced potential adds up together with the external potential to the total potential, i.e. \( U_{\text{tot}} = U_{\text{ext}} + U_{\text{ind}} \). Combining all this information establishes the expected one-to-one relation

\[
\chi(k, \omega) = \frac{1}{V(k)} \left( \frac{1}{\varepsilon(k, \omega)} - 1 \right)
\]

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\[ \varepsilon(k, \omega) = \frac{1}{1 + V(k)\chi(k, \omega)} \quad . \quad (2.30) \]

The response functions \( \chi, \varepsilon \) carry similar physical information as the dynamical structure factor

\[ S(k, \omega) = \int d^3r \int_{-\infty}^{\infty} dt \, \langle \delta n(r + r', t + t) \delta n(r', t') \rangle \exp(-i(k \cdot r - \omega t)) \quad , \quad (2.31) \]

representing the Fourier transformation of the density-density correlation function \( \langle \delta n(r' + r, t' + t) \delta n(r', t') \rangle \), where \( \langle ... \rangle \) denotes the expectation value in the ground state. In homogeneous systems where the response is independent of the initial location \( r' \) and time \( t' \), the momentum dependence characterizes the spatial transport and the frequency dependence gives access to resonances, relaxation times and other spectral features.

The fluctuation–dissipation theorem establishes a direct relation between the dynamical structure factor \( S(k, \omega) \) and the response function \( \chi \) which reads \([\text{Pin64, Pin66, Lan80}]\)

\[ S(k, \omega) = -\frac{2}{\hbar} \frac{\omega}{1 - \exp(-\hbar \omega/k_B T)} \, \text{Im} \{ \chi(k, \omega) \} = -\frac{2}{\hbar} f_B(-\hbar \omega) \, \text{Im} \{ \chi(k, \omega) \} \quad , \quad (2.32) \]

where the two first expressions apply for a fully quantum mechanical treatment and the last one for the classical limit. The factor \( f_B(x) = \left[ \exp(x/k_B T) - 1 \right]^{-1} \) is the Bose function. Equivalently, the dynamical structure factor is related to the dielectric function \( \varepsilon \) through

\[ S(k, \omega) = -\frac{2}{\hbar} \frac{\omega}{1 - \exp(-\hbar \omega/k_B T)} \, \text{Im} \{ \chi(k, \omega) \} \]

\[ \text{h} \to 0 \quad -\frac{2k_B T}{\omega} \text{Im} \{ \chi(k, \omega) \} \quad (2.32) \]

\[ \text{where the two first expressions apply for a fully quantum mechanical treatment and the last one for the classical limit. The factor } f_B(x) = \left[ \exp(x/k_B T) - 1 \right]^{-1} \text{ is the Bose function. Equivalently, the dynamical structure factor is related to the dielectric function } \varepsilon \text{ through} \]

\[ S(k, \omega) = \frac{2}{\hbar V(k)} f_B(-\hbar \omega) \, \text{Im} \left[ \frac{1}{\varepsilon(k, \omega)} \right] \text{h} \to 0 = -\frac{2k_B T}{\omega V(k)} \, \text{Im} \left[ \frac{1}{\varepsilon(k, \omega)} \right] \quad . \quad (2.33) \]

Note that both relations (2.32) and (2.33) are not directly reversible as the relation between \( \chi \) and \( \varepsilon \) was. The structure function provides only the imaginary part of \( \chi \) or \( 1/\varepsilon \). The full information is nonetheless contained also in the dynamical structure factor \( S(k, \omega) \) and may be regained by Kramers-Kronig relations.

Finally, there is one more quantity, the static structure factor \( S(k) \), which represents the instantaneous density-density correlation \( \langle \delta n(r + r') \delta n(r') \rangle \). It is connected to the spatial correlations between particles as contained in the pair distribution function \( g(r) \) by Fourier transformation (see e.g.\([\text{Han86}]\))

\[ S(k) = 1 + n \int d^3r \,( g(r) - 1) \exp(-i k \cdot r) \quad . \quad (2.34) \]

The same symbol \( S \) is used for both, the static and the dynamic, structure factor. This usage suggests a close correspondence and, in fact, the static structure factor is obtained from the time-dependent (dynamic) density-density correlation as the limit of instantaneous response \( t \to 0 \). This results in the relation

\[ S(k) = \frac{1}{n} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} S(k, \omega) \quad . \quad (2.35) \]

There is, of course, also a simple relation between the static structure factor and the density-density response function \( \chi \) or the dielectric function \( \varepsilon \) which can be easily established by combining Eq. (2.35) with the relations (2.32) or (2.33).
Each one of these four response or correlation functions has a natural relation to a particular observable of the system. The structure factors $S$ are employed in connection with scattering experiments on homogeneous systems. For example, the dynamical structure function is typically related to the neutron scattering analysis of solids [Ash76]. It applies for any scattering analysis with good energy resolution which provide the double differential cross section $d^2\sigma/(d\Omega dE) \propto S(k,\omega)$, where the prefactor depends on the kinematics of the projectile and the scattering angle $\Omega$ is related to the transferred momentum $\hbar k$ in the standard fashion. The static structure function $d\sigma/d\Omega \propto S(k)$ is related to scattering without energy resolution as it is typically met in a X-ray scattering analysis of solids. For example, the cross section for photo-absorption is $\sigma_{\text{abs}} \propto \omega \text{Im}\{\chi(k = \omega/c, \omega)\}$.

Transport properties as the electrical resistivity or thermal conductivity can also be related to these basic response functions [Ich85b].

### 2.2.1.2 The RPA dielectric function for ideal targets

For ideal electron targets $\xi \ll 1$, the response functions $\chi(k,\omega)$ and $\varepsilon(k,\omega)$ are derived within the weak coupling limit of interparticle correlations, well–known as the random phase approximation (RPA). Starting point to derive the RPA density–density response function $\chi_R$, denoted by the subscript $R$, is the free density–density response function $\chi_0$.

$$\chi_0(k,\omega) = -2 \int \frac{d^3p}{(2\pi\hbar)^3} \frac{f_0(p + \hbar k) - f_0(p)}{\frac{\omega}{\varepsilon} - \zeta(p + \hbar k) + \zeta(p) + \text{i}0}, \quad (2.36)$$

where $f_0(p) = 1/(\exp((\zeta(p) - \mu)/k_B T) - 1)$ is the Fermi-Dirac distribution with chemical potential $\mu$ and the free electron dispersion $\zeta(p) = p^2/2m$. The free density–density response function $\chi_0$ (2.36) is often called the Lindhard function [Lin54]. The RPA density–density response function $\chi_R$ is computed from this free response and the two-body Coulomb interaction $V(k) = e^2/\varepsilon_0 k^2$ by the RPA equation

$$\chi_R(k,\omega) = \frac{\chi_0(k,\omega)}{1 - V(k)\chi_0(k,\omega)} \quad . \quad (2.37)$$

The RPA dielectric function $\varepsilon_R$ then follows from $\chi_R(k,\omega)$ using relation (2.29) as

$$\varepsilon_R(k,\omega) = 1 - V(k)\chi_0(k,\omega) = 1 - \frac{e^2}{\varepsilon_0 k^2} \chi_0(k,\omega) \quad . \quad (2.38)$$

The RPA response functions $\chi_R$ (2.37) and $\varepsilon_R$ (2.38) provide the dynamical response of an ideal electron target for any degree of degeneracy, for a cold electron gas in solids (using the jellium approximation) as well as for dilute, hot classical plasmas [Gou78, Ari84]. For the homogeneous and isotropic electron targets which we predominantly consider here the response functions $\chi_0$ (2.36), $\chi_R$ (2.37) and $\varepsilon_R$ (2.38) depend only on the absolute value of $k$.

### 2.2.1.3 Dielectric functions for nonideal targets

The RPA equation (2.37) incorporates already the most important long range correlations from the Coulomb interactions. In particular, it gives a pertinent description of the collective plasmon mode. There remain, however, several deficiencies in particular from neglecting short
range correlations which account for close two-electron collisions. There exists a variety of formulations which aim to cure these deficiencies and a widespread literature on this topic. We will not dwell on all the details of the various approaches and merely raise some of the schemes. A more detailed outline is given in [Zwi99].

One approach is the technique of the local field correction (LFC), which intends to incorporate correlations beyond mean field while maintaining the simple structure of the mean field (RPA) equation (2.37). The exact response function $\chi$ will then contain more information about higher correlations than the RPA response function $\chi_R$ which has anticipated already a great deal of the most crucial long range correlations. The extra correlations are thus defined by

$$\chi(k, \omega) = \frac{\chi_0(k, \omega)}{1 - V(k)(1 - G(k, \omega)) \chi_0(k, \omega)}.$$ \hspace{1cm} (2.39)

where the correlations enter in terms of a modified residual interaction, $V \rightarrow V(1 - G)$, to be used in the RPA equation (2.37). This modification is summarized in the function $G(k, \omega)$ which is called the local field correction. By relation (2.29) the modified dielectric function takes the form

$$\varepsilon(k, \omega) = 1 - \frac{V(k)}{1 + V(k) G(k, \omega) \chi_0(k, \omega)}.$$ \hspace{1cm} (2.40)

The RPA expressions (2.38) and (2.37) are recovered for vanishing LFC $G(k, \omega) \rightarrow 0$.

The form of definition (2.39) suggests that correlation effects can be treated in terms of an effective interaction for RPA calculations and it hints the direction for the construction of approximations. The LFC depends generally on momentum and frequency where the spectral structure of $G(k, \omega)$ reflects the dynamics of the higher many-body correlations from which one can hope that these are faster than the dominant modes described in RPA (usually the plasmon mode). This suggests a first step of approximation, the static LFC $G(k)$ where the $\omega$-dependence is neglected.

Here, one line of development has been initiated by Singwi-Tosi-Land-Sjölander in [Sin68]. This STLS approach has been first derived in a classical environment and later generalized to quantum systems in [Schw91, Schw93]. It starts from incorporating the two-particle density and thus the static structure factor $S(k)$ in the derivation of the response function $\chi$ which is based solely on the one-particle density in the usual RPA approach. From a given static structure factor $S(k)$ and the resulting $\chi$ one can then deduces a static LFC via a generalized RPA equation of the type (2.39). A known static LFC $G(k)$, on the other hand, allows to compute $\chi(k, \omega)$ via Eq. (2.39) which defines $S(k, \omega)$ according to Eq. (2.32) from which the frequency integration (2.35) delivers a static structure factor $S(k)$. This closes the circle and establishes a selfconsistent scheme which has been widely used in several applications where a correlated electron plasma plays a role. The STLS scheme is conceptually obvious and technically still fairly simple, but the emerging response and correlation functions violate some basic consistency conditions, like several sum-rules. This is a typical problem when constructing approaches which include correlations.

A widely used approach, which spends more effort to achieve compatibility with these consistency conditions, is the hypernetted–chain (HNC) approximation; see [Ich87] for a review in the context with plasma applications. The HNC scheme allows to compute the static pair correlation function $g(r)$ for a plasma and thus the static structure factor $S(k)$. This detailed and reliable information can now be incorporated into the computation of the dielectric response by choosing a static LFC $G(k)$ such that the LFC corrected RPA equation (2.39) together with
the relations (2.32) and (2.35) yields the static structure function \( S(k) \) as it is prescribed from HNC. This choice then guarantees to recover the static properties of the HNC approach in the LFC corrected formulation which now can be applied for dynamical processes.

The static LFC works very well for many purposes but in other cases, as e.g. in the description of the detailed line broadening of the plasmon peak, a dynamical LFC is desirable. Such an extended approach may still be deduced from static HNC calculations by considering limiting cases and interpolation as e.g. proposed and extensively studied by Ichimaru and collaborators with respect to all sorts of observables. A detailed discussion of results using these static and dynamic LFC with HNC input is found in [Ich85a, Ich85b, Ich87, Mit85, Tan85, Yan85].

Another possibility is to include correlations in terms of instantaneous (quasi)particle collisions. A particular simple scheme for that is provided by the relaxation–time approximation as suggested by Mermin [Mer70]. The resulting dielectric function for a given electron–electron collision frequency \( \nu \) takes the form

\[
\varepsilon(k, \omega) = 1 + \frac{(\omega + i\nu) (\varepsilon_R(k, \omega + i\nu) - 1)}{\omega + i\nu(\varepsilon_R(k, \omega + i\nu) - 1)/ (\varepsilon_R(k, 0) - 1)},
\]

expressed in terms of the RPA dielectric function \( \varepsilon_R \) (2.38). The collision frequency \( \nu \) is typically used as a model parameter but also can be deduced for classical targets from MD–simulations [Spr95]. In some cases the \( \nu \) was determined by fitting \(-\text{Im}[1/\varepsilon(k = 0, \omega)]\) to experimental optical energy loss functions of carbon and silicon and then via Eq. (2.41) used for investigation on the stopping power in these materials [Ash80, Ash87, Abr94, Per96a, Per96b]. Treating the collision frequency as a free parameter, the modified dielectric function (2.41) allows useful qualitative estimates of the influence of electron–electron collisions on the stopping power. The predicted effect is a shorter life time and smaller mean free path of the plasmons resulting in considerable modifications of the wake field behind the passing ion [Ash85]. This is of particular importance for vicinity effects on the energy loss of multi-ion arrangements discussed in chapter 4.

A recent line of development where also special attention is paid to the compliance of consistency conditions is presented in [Roe98, Roe98a]. Within a generalized linear response approach the dielectric function is expressed in terms of equilibrium correlation functions of relevant observables. This allows to derive dielectric functions including higher correlations beyond the RPA by systematically improving the evaluation of the required correlation functions and by increasing the number of employed observables. Depending on the actual treatment and choices, the LFC approach and the dielectric function (2.41) are recovered from this general formulation.

In summary, existing LFC treatments based on HNC and quantum HNC [Jac82], on the STLS approach and extended STLS schemes [Schw91, Schw93], on informations from Greens–function–Monte–Carlo methods [Uts82], diffusion Monte Carlo [Mor95, Sen96], or the relaxation–time approximation to incorporate electron-electron collisions are able to provide modified dielectric functions for a variety of nonideal target conditions. They can be used subsequently for stopping power calculations [based on Eq. (2.44)] to study ion stopping in a nonideal target at linear or to some extent semilinear ion–target coupling. Their domain of application is thus the parameter space with \( \xi \sim 1 \) and \( \langle \eta_p \rangle \sim 1 \), i.e. the regime of low projectile charge states \( Z \) or high velocities. Due to this very limited region in particular in view of heavy ions with high charge states we do not consider this issue further. The existing studies on stopping in nonideal target show that the LFCs [Say83, Wang95] or electron–electron collisions
via function (2.41) [Ash80] generally increase the stopping at low ion velocity while for high ion velocities the simple RPA dielectric description, see e.g. [May85], becomes sufficient again.

### 2.2.1.4 Linear response stopping power

After having prepared all the needed ingredients we now turn to establish and to discuss the relations between the stopping power $dE/ds$ and the response functions.

According to its definition (2.6) or (2.7), the stopping power is determined by the electric field $\mathbf{E}$ at the ion position which is caused by the charge density $\rho$ of the target. For an initial homogeneous system with $\rho_0 = \rho(t < t_0) = -en$ and $\mathbf{E}_0 = 0$ the relevant electric field is created by the charge density $\rho_{\text{ind}}(\mathbf{r}, t) = \rho(\mathbf{r}, t) - \rho_0$ which is induced by the perturbing ion potential $\phi_p(\mathbf{r}, t) = \theta(t - t_0) Z e / 4 \pi \varepsilon_0 |\mathbf{r} - \mathbf{v} t|$. Rewriting definition (2.6) in terms of the Fourier transformed $\rho_{\text{ind}}$ and $\phi_p$, the stopping power on an ion with charge $Ze$ and velocity $\mathbf{v}$ is

$$
\frac{dE}{ds} = Ze \mathbf{v} \cdot \mathbf{E}(\mathbf{r} = \mathbf{v} t)
$$

$$
= -\frac{i}{(2\pi)^4} \int d^3k \int d\omega \ k \cdot \mathbf{v} \ \rho_{\text{ind}}(k, \omega) \ \phi_p(-k) \exp(i \mathbf{k} \cdot \mathbf{v} - \omega t).
$$

This is still a general result for an initially homogeneous system. Assuming a linear ion–target coupling with sufficiently weak perturbation, we now employ the linear response relations (2.26) and (2.29). Identifying $\rho_{\text{ind}} = -e \delta n$, $U_{\text{ext}} = -e \phi_p$ and $V(k) = e^2 / \varepsilon_0 k^2$ we obtain the induced charge density as

$$
\rho_{\text{ind}}(k, \omega) = e^2 \phi_p(k, \omega) \chi(k, \omega) = \varepsilon_0 k^2 \phi_p(k, \omega) \left[ \frac{1}{\varepsilon(k, \omega)} - 1 \right].
$$

Inserting this relation together with the Fourier transformed $\phi_p(k, \omega) = 2 \pi \delta(\omega - k \cdot \mathbf{v}) \phi_p(k) = 2 \pi Ze \delta(\omega - k \cdot \mathbf{v}) / \varepsilon_0 k^2$ into Eq. (2.42) and taking advantage of the symmetry $\varepsilon^*(k, \omega) = \varepsilon(-k, -\omega)$ and the same one for $\chi$ finally yields

$$
\left( \frac{dE}{ds} \right)_\text{lr} = \frac{1}{(2\pi)^3} \int d^3k \ k \cdot \mathbf{v} \ |\varepsilon \phi_p(k)|^2 \ \text{Im} [\chi(k, \omega)]
$$

$$
= \frac{Z^2 e^2}{\varepsilon_0 (2\pi)^3} \int d^3k \ k \cdot \mathbf{v} \ \text{Im} \left[ \frac{1}{\varepsilon(k, k \cdot \mathbf{v})} \right].
$$

These are the basic expressions for the stopping power in the regime where the ion–target coupling is linear, $\langle \eta_p \rangle \ll 1$, or, with some restrictions and modifications to be discussed later, semilinear. Provided that the corresponding dielectric function $\varepsilon$ is available, they are applicable to any targets; ideal and nonideal electron plasmas at any $\xi, \Theta$, as well as targets beyond the present considerations like two component plasmas of different degrees of ionization and degeneracy or solids and atomic or molecular gases. In these cases also inelastic contributions from ionization and excitation of bound states are included within linear response. Note that transient effects caused by switching on the ion–target interaction have been disregarded in deriving relation (2.44) by considering the limit $t_0 \to -\infty$. This limit is practically reached after a transient period of the order of the response time of the electron target $\omega_p^{-1}$ [See95, See97, Zwi97a]. The induced electric field in the frame co–moving with the ion takes then a stationary value provided that the ion velocity ($\dot{v} \propto dE/ds$) varies slowly on the time scale for transient effects. This is usually ensured for a high projectile mass $M/m \gg 1$. 

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The most important features of the linear response stopping power (2.44) are its general dependencies on the basic projectile parameters, charge $Ze$ and velocity $v$. As on sees immediately, the stopping power grows quadratically with $Z$, which is a trivial consequence of the underlying first order perturbation theory. The dependence on the velocity is more involved. We have to distinguish two regimes. For ion velocities low compared to the mean electron velocity $\langle v_e \rangle$ the stopping power is linear in $v$

$$
\left( \frac{dE}{ds} \right)_{lr} = - \frac{Z^2 e^2 n}{\epsilon_0 (2\pi)^3 \omega_p} v \left[ C(\xi, \Theta) + O(v^2) \right], \quad v \ll \langle v_e \rangle , \quad (2.45)
$$

where the dimensionless friction coefficient $C(\xi, \Theta)$ depends on the target conditions and hence on the interparticle correlations. It can be obtained immediately from Eq. (2.44) as

$$
C(\xi, \Theta) = \frac{4\pi \omega_p}{3m} \int_0^{\infty} dk k^2 \left( \frac{\partial}{\partial \omega} \text{Im} \left[ \frac{1}{\epsilon(k, \omega)} \right] \right)_{\omega=0}, \quad (2.46)
$$

when assuming an isotropic target with $\epsilon(k, \omega) = \epsilon(k, \omega)$. For anisotropic targets the friction depends on the direction of motion and tensors have to be considered in this case. In the limit of large velocities, on the other hand, the stopping power goes like

$$
\left( \frac{dE}{ds} \right)_{lr} = - \frac{Z^2 e^4 n}{4\pi \epsilon_0 m v^2} \left[ \ln \left( \frac{2m v^2}{\hbar \omega_p} \right) + O(1/v^2) \right], \quad v \gg \langle v_e \rangle , \quad (2.47)
$$

and depends on the target conditions only through the electron density $n$. The approach to the limit (2.47) for sufficiently high $v$ follows directly from the $f$–sum–rule for the dynamical structure factor which is related to particle number conservation [Pin66, Section 2.2]. Thus, only the energy loss at low velocities provides information about the correlations within the target.

We continue this paragraph with an alternative derivation of the stopping power (2.44) which illustrates a different aspect of linear response and offers an additional interpretation of stopping. It directly falls back on first order perturbation theory and the concept of a scattering rate $R$ (see e.g.[Akh75]). We consider a scattering event of the projectile with the target where a change in the ion momentum $\hbar \mathbf{k} = \mathbf{P} - \mathbf{P}'$ and an energy transfer to the target of $\hbar \omega(\mathbf{k}) = (P^2/2M - P'^2/2M) = (P^2 - (\mathbf{P} - \hbar \mathbf{k})^2)/2M = \hbar \mathbf{k} \cdot \mathbf{v} - \hbar^2 k^2/2M = E_0' - E_0$ takes place. Here $E_0$ is the energy of the eigenstates of the target defined by the hamiltonian $\hat{H}_0$ (2.2). The corresponding transition rate is then obtained from time dependent perturbation theory according to Fermi’s ‘Golden Rule’ by

$$
\frac{d\Pi}{dt} \bigg|_{P,E_0 \rightarrow P',E_0'} = \frac{2\pi}{\hbar} \left| \langle E'_0, \mathbf{P}' | \sum_j e^{\phi_p(\mathbf{r}_j - \mathbf{R})} | E_0, \mathbf{P} \rangle \right|^2 \delta(\hbar \omega - E'_0 + E_0)
$$

Here $\sum_j e^{\phi_p(\mathbf{r}_j - \mathbf{R})}$ is the ion-target interaction, see Eq. (2.1), which can be reformulated in terms of the particle density operator $\hat{n}_\mathbf{k} = \sum_j \exp(-i\mathbf{k} \cdot \mathbf{r}_j)$ by Fourier-transformation as $\sum_j e^{\phi_p(\mathbf{r}_j - \mathbf{R})} = \int (d^3k/(2\pi)^3) e^{\phi_p(\mathbf{k})} \exp(-i\mathbf{k} \cdot \mathbf{R}) \hat{n}_{-\mathbf{k}}$. This leads to

$$
\frac{d\Pi}{dt} \bigg|_{P,E_0 \rightarrow P',E_0'} = \frac{2\pi}{\hbar} \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3k'}{(2\pi)^3} e^{\phi_p(\mathbf{k})} e^{\phi_p^*(\mathbf{k}')} \langle \mathbf{P}' | e^{-i\mathbf{k} \cdot \mathbf{R}} | \mathbf{P} \rangle \langle \mathbf{P} | e^{i\mathbf{k}' \cdot \mathbf{R}} | \mathbf{P}' \rangle \times \langle E'_0 | \hat{n}_{-\mathbf{k}} | E_0 \rangle \langle E_0 | \hat{n}_\mathbf{k} | E'_0 \rangle \delta(\hbar \omega - E'_0 + E_0)
$$

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ensemble average above is, however, nothing else than the density-density correlation function which defines the dynamic structure factor \( S \) as well as the relation of the projectile momentum projected in the direction of flight \( \hbar \) likewise of energies at variance to the leading contribution (2.44) resulting from the polarization. The present can be interpreted as a fluctuation contribution to the momentum change of the projectile response function. Again we consider here the limit of heavy projectiles (where Eq. (2.32) was used to relate the dynamical structure factor to the density-density correlation function).

In deriving the second expression we replaced \( \delta(\hbar\omega - E'_0 + E_0) \) by its Fourier representation and used the properties of the momentum eigenstates \( \langle k | \exp(i\mathbf{k} \cdot \mathbf{R}) | k' \rangle = \langle P | P' + \hbar \mathbf{k} \rangle = \delta(P - P' - \hbar \mathbf{k}') \) together with the definition \( \hbar \mathbf{k} = P - P' \). The last step involves \( \exp(iE_0 t/\hbar) | E_0 \rangle \) = \( \exp(i\mathbf{H}_0 t/\hbar) | E_0 \rangle \) and the abbreviation \( \hat{n}_k(t) = \exp(i\mathbf{H}_0 t/\hbar) \hat{n}_k \exp(-i\mathbf{H}_0 t/\hbar) \). From this transition rate for the specific transition \( | E_0, P \rangle \rightarrow | E'_0, P' \rangle \) we obtain a scattering rate \( R \) (events per time and \( P \)-space volume \( (2\pi \hbar)^3/V \)) after an unweighted summation over all possible excited states \( E'_0 \) of the target and a statistically weighted one over the initial states \( E_0 \)

\[
R(P \rightarrow P + \hbar \mathbf{k}, \omega(k)) = \frac{1}{\hbar^2} \frac{1}{(2\pi \hbar)^3} |e\phi_p(k)|^2 \frac{1}{V} \int_{-\infty}^{\infty} dt e^{i\omega t} \langle \hat{n}_k(t) \rangle \langle \hat{n}_k = k \rangle \]

where \( V \) is the target volume. In contrast to their previous use the brackets here denote an ensemble average \( \langle \ldots \rangle = \text{Tr} \hat{\rho}_0 \ldots \) where \( \hat{\rho}_0 \) is the statistical operator of the target. The ensemble average above is, however, nothing else than the density-density correlation function which defines the dynamic structure factor \( S(k, \omega) \) by Fourier transformation, see Eq. (2.31).

The stopping power is deduced from the scattering rate \( R \) by integrating over all the changes of the projectile momentum projected in the direction of flight

\[
\frac{dE}{ds} = -\int d^3(k \cdot v) R(k, \omega(k)) = -\frac{1}{(2\pi)^3} \int d^3 k \cdot \mathbf{v} |e\phi_p(k)|^2 \frac{1}{\hbar} S(k, \omega(k))
\]

\[
= -\frac{1}{(2\pi)^3} \int d^3 k \cdot \mathbf{v} |e\phi_p(k)|^2 2f_B(-h\omega(k)) \text{Im} [\chi(k, \omega(k))] ,
\]

where Eq. (2.32) was used to relate the dynamical structure factor to the density-density correlation function. Again we consider here the limit of heavy projectiles \( (M \gg m) \) which allows to neglect the recoil effects, taking \( \omega(k) = k \cdot v \). Using now the symmetries of \( \chi(k, \omega) \) as well as the relation \( f_B(x) + f_B(-x) = -1 \) for the Bose function yields the stopping power in the form (2.44). Retaining the recoil yields by a factor \( 1/M \) suppressed additional terms. They can be interpreted as a fluctuation contribution to the momentum change of the projectile at variance to the leading contribution (2.44) resulting from the polarization. The present procedure views the energy loss as an average over absorption and emission of momenta or likewise of energies \( h\omega \) when using the alternative definition of stopping via \( dE/ds = dE/dt/v = -\int d^3(k \cdot v) \hbar\omega R(k, \omega)/v \). This provides also a simple way to describe the straggling, i.e. the deviation of the energy loss per path–length from its mean value. The relative straggling (as compared with \( dE/ds \)) is there given by the second \( \omega \)-moment of the scattering rate \( R \) [Ari81].

### 2.2.1.5 Extensions and approximations for semilinear coupling

In the semilinear coupling regime the coupling strength is just beyond what is required for the linear response treatment which represents the first order in a perturbation expansion with respect to the external perturbation \( \phi_p \). This suggests that an extension to the (weak)
semilinear coupling can be achieved by taking into account higher orders in the perturbation series. The second order terms are called the Barkas correction [Bar63]. They are quadratic in $\phi_p$ and hence their contribution to stopping is $\propto Z^3$. More precisely, the Barkas correction gives a contribution of the order $Z/((\langle v_r \rangle)^3$ relative to the leading $Z^2$ term of the linear response theory. Thus it is a small correction in the linear, and to some extent in the semilinear, regime. But the perturbation series diverges as soon as one proceeds towards the nonlinear regime. The approach shares the general features of a perturbation series: it is designed to enhance the accuracy of the description within a regime inside its range of validity, i.e. the regime of weak coupling. We will not dwell on these typically rather expensive descriptions and calculations. A general discussion on this subject is found in [Ash72, Esb90, Pit95]. Investigations on the Barkas contribution in a classical electron target ($\hbar \to 0$) and for semilinear ion–target coupling are presented in [Pet91, Say92, Dav93].

A technically fairly simple and widely used approximation to extend the linear response expression (2.44) into the semilinear regime is the use of appropriate cutoff parameters. At semilinear coupling, see definition (2.22), the perturbation caused by the ion remains truly weak in the largest part of the ion–target interaction region and violates the linear coupling only in a small vicinity of the ion $r < \langle b_0 \rangle \ll \lambda$, corresponding to high transferred momenta. This suggest to approximate the stopping power by using the linear response result but to cut the effective velocity dependent screening length $\lambda$.

This can be achieved by comparison of the stopping power (2.50) with a binary collision approach using an appropriate screened potential. For the detailed procedure see [Pet91, Say92, Dav93].

But the perturbation series diverges as soon as one proceeds towards the nonlinear regime. The approach shares the general features of a perturbation series: it is designed to enhance the accuracy of the description within a regime inside its range of validity, i.e. the regime of weak coupling. We will not dwell on these typically rather expensive descriptions and calculations. A general discussion on this subject is found in [Ash72, Esb90, Pit95]. Investigations on the Barkas contribution in a classical electron target ($\hbar \to 0$) and for semilinear ion–target coupling are presented in [Pet91, Say92, Dav93].
be written as a function of velocity times a logarithmic term (Coulomb logarithm). In both approximations the functions in front of the logarithmic terms are roughly equal and their ratio is
\[ \left( \frac{dE}{ds} \right)_{bc} \approx \frac{\left( \frac{dE}{ds} \right)_{lr}}{\lambda_m^2} \approx \ln \left[ \frac{4 \lambda^2}{\lambda^2 (1 + \gamma^2 \langle \eta_b \rangle^2)} \right] / \ln |k_m \lambda|, \] (2.51)
where \( \lambda_m = \hbar/\langle v_c \rangle \) is the averaged wavelength of relative motion, \( \langle \eta_b \rangle \) the averaged Coulomb-parameter (2.17) and \( \ln \gamma = 0.577 \ldots \) is Euler’s constant. From Eq. (2.51) we read off the desired cutoff as
\[ k_m = \frac{2}{\lambda_r} \frac{1}{\sqrt{1 + \gamma^2 \langle \eta_b \rangle^2}}. \] (2.52)

In the linear coupling and quantum mechanical plane wave regime \( \langle \eta_b \rangle \ll 1 \), the cutoff \( k_m \) becomes identical to the intrinsic cutoff \( 2/\lambda_r \) provided from the behavior of the dielectric function \( \varepsilon_R \) at large \( k \). Thus Eq. (2.50) merges into the exact RPA linear response result in this case. In the opposite limit \( \langle \eta_b \rangle = \langle b_0 \rangle/\lambda_r \gg 1 \) the cutoff tends to \( k_m \approx 1/\langle b_0 \rangle \), in agreement with the initial assumption when introducing \( k_m \) in Eq. (2.50). Expression (2.52) may thus be identified with the commonly used cutoff \( k_m \approx \min(1/\langle b_0 \rangle, 2/\lambda_r) \) in classical dielectric approaches where the electrons are treated as classical particles, see e.g. [Pet91]. These approaches employ accordingly a classical dielectric function provided from the Fried–Coné plasma dispersion function [Fri61] which is the limit \( \hbar \to 0 \) of the RPA free density–density response (2.36). As this classical dielectric function fails at large \( k \)-values a cutoff is needed to render the \( k \)-integration in the stopping power (2.44) finite.

We emphasize, however, that the cutoff (2.52) is introduced in Eq. (2.50) to account for physical effects and not just to avoid divergences. The general linear response expression (2.44) yields a convergent integral by virtue of quantum effects which provide an intrinsic cutoff at \( 2/\lambda_r \) at any degeneracy \( \Theta \), including classical targets with \( \Theta \gg 1 \). It is, however, only valid for linear coupling \( \langle \eta_b \rangle \ll 1 \). The physical cutoff discussed here intends to correct for a small region of strong perturbation and thus to extend the applicability of the linear response expression into the semilinear regime. We remind that the linear regime never occurs in an entirely classical system where \( \Theta \) and \( \langle \eta_b \rangle \) are infinite. The need of a cutoff is decided by the question whether we are in the linear or the semilinear regime, that is, by the parameter \( \langle \eta_b \rangle \), independent of the degree of degeneracy \( \Theta \).

It emerges as a new feature in the semilinear regime that the \( Z^2 \)-charge dependence of the stopping power is modified by correction terms which carry the charge dependence of binary collisions, which will be discussed in detail in the following section. This charge dependence is then recovered in the resulting approximations and yields for parameters \( \langle \eta_b \rangle > 1 \) and \( \langle b_0 \rangle \ll \lambda \), i.e. in the semilinear regime, a logarithmic dependence on \( Z \) in addition to the leading pure quadratic one at linear coupling. We can also read off this additional \( Z \)-dependence from expression (2.51) and the definitions of \( k_m(Z) \) (2.52) and \( \langle \eta_b \rangle(Z) \) (2.17). More specific, the low velocity limit of the corrected linear response stopping power
\[ \left( \frac{dE}{ds} \right)_{lr}^{k_m} = - \frac{Z^2 e^2}{\varepsilon_0 (2\pi)^3} \varepsilon_B \frac{\langle \xi, \Theta, |Z| \rangle + O(v^3)}{v} \langle \xi, \Theta, |Z| \rangle + O(v^3) \right] , \quad v \ll \langle \xi, \Theta, |Z| \rangle , \] (2.53)
is now described by a dimensionless friction coefficient \( \tilde{C}(\xi, \Theta, |Z|) \) with a logarithmic dependence on \( Z \)
\[ \tilde{C}(\xi, \Theta, |Z|) \propto \ln \left( \frac{8\pi \varepsilon_0 m \langle v_c \rangle^2 \lambda(v=0)}{\gamma |Z| e^2} \right) . \] (2.54)
Figure 2.5: Normalized stopping power $dE/ds/Z^2$ in units of $ne^4/4\pi\epsilon_0mv^2$ as a function of the velocity $v$. In the left part the target conditions are $r_s = a/a_0 = 10$ and $\Theta = 45.2$ corresponding to a classical plasma and $v$ is given in units of the thermal velocity $v_{\text{th}}$, while in the right part a degenerate electron plasma with $r_s = 0.1$ and $\Theta = 0.41$ is considered and $v$ is scaled in the Fermi velocity $v_F$. In both cases the solid curves represent the linear response stopping power (2.44). The other curves result from the modified stopping power (2.50) using the cutoff $k_m(Z)$ as defined in Eq. (2.52) for different parameter of linearity (2.17) $\langle \eta_p \rangle (\langle v_r \rangle = v_{\text{th}}) = 1$ (dotted curve), 2 (dash-dotted) and 5 (dashed) in the left plot and $\langle \eta_p \rangle (v_F) = 0.5$ (dotted), 1 (dash-dotted) and 2 (dashed) in the right one. This is equivalent to charge states $Z = 1, 2$ and 5 (left) and $Z = 10, 20$ and 40 (right) at the given target conditions. In all cases we have small values of the ratio $\langle b_0 \rangle/\lambda$ defining the semilinear regime.

For velocities larger than $\langle v_e \rangle$ but still small enough to fulfill $\langle \eta_p \rangle > 1$ we get the classical high velocity result of Bohr [Boh13]

$$\left( \frac{dE}{ds} \right)_{\text{lr}}^{k_m} \sim - \frac{Z^2 e^4}{4\pi\epsilon_0mv^2} n \ln \left( \frac{8\pi\epsilon_0mv^3}{\gamma|Z|e^2\omega_p} \right), \quad v \gg \langle v_e \rangle, \quad \langle \eta_p \rangle > 1,$$

(2.55)

whereas still higher velocities lead back to linear coupling and the high velocity limit (2.47). We want to point out that the conditions for semilinear coupling imply large arguments of the logarithms in the above expressions.

In Fig. 2.5 we compare the linear response stopping power (2.44) for two different target conditions and increasing coupling, that is, for an increasing charge state and $\langle \eta_p \rangle$, with the modified stopping expression (2.50) using the cutoff (2.52). Significant reductions of stopping require very large ion charges in the dense and degenerate target, but only rather low charge states at classical target conditions.
2.2.2 Binary Collisions

In the binary collision approach the ion-target interaction is treated as an effective two-body problem. As long as the interaction between two electrons in the potential field of the ion is negligible compared with the ion-electron interaction of each electron, as it is certainly the case in an ideal plasma ($\xi \ll 1$), this mapping of the full interaction to entirely independent binary ion–electron collisions is achievable in principle by introducing an effective ion-electron interaction. Deriving this effective interaction which has to account for all the many-body contributions, as e.g. dynamic polarization effects, is the crucial issue of this description. This needs in particular some input from external sources and theories. Provided that an effective interaction which is consistent with the envisaged target and projectile parameters is available, the binary collision treatment holds, however, for arbitrary strengths of ion–electron collisions ($\eta_p$). In the first part 2.2.2.1 of this section we will describe the binary collision approach in general and derive and discuss the resulting stopping power expressions. An important ingredient for the binary collision description is the calculation of the required transport cross section. We will address this problem in the second part 2.2.2.2 for the specific case of an Yukawa-like screened Coulomb potential as a widely used parameterization of the effective ion-electron interaction.

2.2.2.1 Stopping by binary collisions

The binary collision approach starts with a completely kinetic description of the system through the momentum distribution $\tilde{f}(P)$ of the ion and the distribution $f(p)$ of the electrons. The time evolution of the ion distribution is determined from scattering events $(P,p) \rightarrow (P',p')$ of the ion with electrons in terms of a collision integral $I_{ie}$ as $\partial_t \tilde{f}(P) = I_{ie}$. Here, we use the quantum version of a Boltzmann collision integral for ion–electron collisions which includes Pauli blocking factors for the final electron states and allows to treat all degrees of degeneracy of the electron target. The force $F$ on the ion, i.e. the time derivative of its momentum, can be expressed now as the integral (see also the definition (2.10) of stopping)

$$\begin{align*}
F &= \frac{d}{dt}(P) = V \int \frac{d^3P}{(2\pi\hbar)^3} P \frac{\partial \tilde{f}(P)}{\partial t} = V \int \frac{d^3P}{(2\pi\hbar)^3} P I_{ie} \\
&= \frac{2V}{\mu^2} \int \frac{d^3P d^3P' d^3p d^3p'}{(2\pi\hbar)^6} P w(P,p;P',p') \\
&\quad \times [(\tilde{f}(P') f(p')(1-f(p)) - \tilde{f}(P) f(p)(1-f(p'))],
\end{align*}
$$

(2.56)

where $\mu = m\bar{M}/(m + \bar{M})$ is the reduced mass, $V$ a spatial volume and

$$w(P,p;P',p') = \sigma(P,p;P',p') \delta^3(P+p-P'-p') \delta \left(\tilde{\zeta}(P) + \zeta(p) - \tilde{\zeta}(P') - \zeta(p')\right)$$

with the energies $\tilde{\zeta}(P) = P^2/2M$ of the ion and $\zeta(p) = p^2/2m$ of the electrons and the cross section $\sigma$ for the collisions $(P,p) \rightarrow (P',p')$. For the projectile ion with a given velocity $v$, the corresponding distribution is $\tilde{f}(P) = [(2\pi\hbar)^3/V]\delta^3(P-Mv)$. This allows to integrate over two momenta. Assuming a cross section with the symmetry $\sigma(P,p;P',p') = \sigma(P',p';P,p)$ and substituting $(P'-p') = q$, the stopping power $dE/ds = \mathbf{v} \cdot \mathbf{F}$ becomes

$$\begin{align*}
\frac{dE}{ds} &= -\frac{2}{\mu^2} \int \frac{d^3p d^3q}{(2\pi\hbar)^3} \mathbf{v} \cdot \mathbf{q} \sigma(Mv,p;Mv-q,p+q) \\
&\quad \times \sigma(P,p;P',p') \delta^3(P+p-P'-p') \delta \left(\tilde{\zeta}(P) + \zeta(p) - \tilde{\zeta}(P') - \zeta(p')\right) \\
&\quad \times [(\tilde{f}(P') f(p')(1-f(p)) - \tilde{f}(P) f(p)(1-f(p'))],
\end{align*}
$$

(2.57)
Alternatively to this expression in terms of the transferred momentum $\mathbf{q}$, one can obtain a more common representation by a transformation to center of mass momentum $\mathbf{K} = \mathbf{Mv} + \mathbf{p} = \mathbf{K}'$ and relative momenta $\mathbf{p}_r = \mathbf{p} - (\mu/M)\mathbf{K} = (\mu/m)\mathbf{p} - \mathbf{\mu v}$, and $\mathbf{p}_r' = \mathbf{p}_r + \mathbf{q}$. The cross section $\sigma$ is usually independent of the center of mass motion, that is, $\sigma = \sigma(\mathbf{p}_r; \mathbf{p}_r')$. This yields

$$\frac{dE}{ds} = \frac{2}{\mu^2} \left( \frac{m}{\mu} \right)^3 \int \frac{d^3p_r}{(2\pi \hbar)^3} \delta(\frac{p_r^2}{2\mu} - \frac{p_r'^2}{2\mu}) \mathbf{\hat{v}} \cdot [\mathbf{p}_r - \mathbf{p}_r'] \sigma(\mathbf{p}_r; \mathbf{p}_r') \left( f(1 + \frac{m}{M})\mathbf{p}_r + m\mathbf{v} \right) - f \left( 1 + \frac{m}{M} \right) \mathbf{p}_r + m\mathbf{v} \right) \mathbf{f} \left( \mathbf{p}_r' + \frac{m}{M} \mathbf{p}_r + m\mathbf{v} \right) \right].$$

The cases of heavy ions and spherical scattering potentials allow further simplifications. For a heavy ion, where $m/M \to 0$, the reduced mass becomes $\mu \approx m$ and the quadratic term $f \left( 1 + \frac{m}{M} \right) \mathbf{p}_r + m\mathbf{v} \mathbf{f} \left( \mathbf{p}_r' + \frac{m}{M} \mathbf{p}_r + m\mathbf{v} \right)$ connected with Pauli–blocking cancels out for differential cross sections $\sigma(\mathbf{p}_r; \mathbf{p}_r')$ which are invariant under an exchange of $\mathbf{p}_r$ and $\mathbf{p}_r'$. There remains

$$\frac{dE}{ds} = 2 \int \frac{d^3p_r}{(2\pi \hbar)^3} f(\mathbf{p}_r + m\mathbf{v}) \frac{p_r^2}{m} \int d\Omega' \mathbf{\hat{v}} \cdot [\mathbf{p}_r - \mathbf{p}_r'] \sigma(\mathbf{p}_r; \mathbf{p}_r') \mathbf{f}(\mathbf{p}_r + m\mathbf{v}) \mathbf{f} \left( \mathbf{p}_r' + \frac{m}{M} \mathbf{p}_r + m\mathbf{v} \right).$$

It is worth to remark, that the stopping power (2.59) obtained under these conditions within the present kinetic–probabilistic description agrees completely with a rigorous, fully quantum mechanical treatment developed in [Boe89, Scho88], which starts with definition (2.7) of the energy transfer and evaluates it for non–interacting electrons.

For spherically symmetric scattering potentials with $\sigma(\mathbf{p}_r; \mathbf{p}_r') = \sigma(\mathbf{p}_r, \vartheta)$, the stopping power appears finally in the very compact form

$$\left( \frac{dE}{ds} \right)_{bc} = 2 \int \frac{d^3p_r}{(2\pi \hbar)^3} f(\mathbf{p}_r + m\mathbf{v}) \frac{p_r^2}{m} \mathbf{\hat{v}} \cdot \mathbf{p}_r \sigma_{tr}(\mathbf{p}_r).$$

Here the transport cross section $\sigma_{tr}(\mathbf{p}_r) = 2\pi \int_0^1 d\cos(\vartheta) \left[ 1 - \cos(\vartheta) \right] \sigma(\mathbf{p}_r, \vartheta)$ has been introduced after integrating over the scattering angle $\vartheta$, with $\cos(\vartheta) = (\mathbf{p}_r \cdot \mathbf{p}_r')/p_r^2$. Usually, one is interested in ion stopping in an electron plasma in thermal equilibrium and the electron distribution $f$ is the Fermi–Dirac distribution $f_0$ for free electrons. As a remarkable feature, the final results for the stopping power Eqs.(2.59) and (2.60) depend linearly on the electron distribution $f = f_0$ for any degree of degeneracy $\Theta$. The influence of the quadratic Pauli–blocking term in Eq. (2.58), $f_0 \left( 1 + \frac{m}{M} \right) \mathbf{p}_r + m\mathbf{v} \mathbf{f}_0 \left( \mathbf{p}_r' + \frac{m}{M} \mathbf{p}_r + m\mathbf{v} \right)$, becomes negligible in the limit of small mass ratios $m/M \to 0$. In the general case of arbitrary $m/M$ this Pauli–blocking term becomes unimportant only in the high temperature limit $\Theta \gg 1$, when $f_0$ merges into a Maxwell distribution and this quadratic term can be neglected. There the stopping power is given by expressions analogous to Eqs.(2.59) and (2.60) where $f(\mathbf{p}_r + m\mathbf{v})/m$ is replaced by $(m/\mu)^3 f(1 + m/M)\mathbf{p}_r + m\mathbf{v}/\mu)$.

The case of arbitrary $m/M$ and $\Theta \gg 1$ is also assumed for a commonly used different derivation of the energy loss in terms of binary collisions [Fer84, Sig82, Ord94]. There the starting point is the change of momentum $\Delta \mathbf{P}(p_r, b, \varphi)$ or energy $\Delta E(p_r, b, \varphi)$ of the ion in a scattering event with given momentum $p$, impact parameter $b$ and scattering angle $\varphi$ in the relative system. To obtain the stopping power, for instance, from definition (2.3) as the energy
change per time, one averages the elementary $\Delta E(p_t, b, \varphi)$ multiplied with the incident particle flux $p_t f (mp_t/\mu + mv)/\mu$ over all relative momenta, impact parameters and angles \( \varphi \), that is,

\[
\frac{dE}{ds} = \frac{1}{v} \frac{dE}{dt} = \frac{1}{v} \left( \frac{m}{\mu} \right)^3 \int \frac{d^3 p_t}{(2\pi \hbar)^3} f \left( \frac{mp_t}{\mu} + mv \right) \frac{p_t}{\mu} \int_0^{2\pi} d\varphi \int_0^\infty db \Delta E(p_t, b, \varphi)
\]

where we used the kinematic relation $\Delta E = -(v + p_t/M) \cdot \Delta p_t$. For symmetry reasons we further have $\int_0^{2\pi} d\varphi \Delta p_t(p_t, b, \varphi) = 2\pi p_t (\Delta p_t(p_t, b))$ where $2\pi \int_0^\infty db \Delta p_t(p_t, b) = -p_t \sigma_{tr}(p_t)$ by use of the classical relationship between impact parameter, scattering angle \( \vartheta \) and the differential cross section. In the limit of large projectile mass we obtain again the previous expression (2.60).

For spherical potentials simple and compact expressions in terms of the transport cross sections can be easily derived in the low and high projectile velocity range, respectively. At low velocities, an expansion with respect to \( v \) of the shifted electron distribution in the stopping power (2.60) yields

\[
\left( \frac{dE}{ds} \right)_{bc} = v \frac{1}{3\pi^2 m v^3} \int_0^\infty dp p^5 \frac{\partial f_0}{\partial \zeta(p)} (p) \sigma_{tr}(p) , \quad v \ll \langle v_e \rangle .
\]

For high velocities an even simpler expression is obtained by substituting $p_t \rightarrow (p - mv)$ and approximating $p_t = |p_t| \approx m v$. This leads to

\[
\left( \frac{dE}{ds} \right)_{bc} = - mn v^2 \sigma_{tr}(mv) , \quad v \gg \langle v_e \rangle ,
\]

where the density \( n \) emerges through $2 \int d^3 p f_0(p) = n (2\pi \hbar)^3$.

To express the stopping power in terms of the electron distribution and an effective electron-ion cross section goes in fact beyond a mere binary collision approximation and is successfully employed also in different regimes. The key issue is then to find an appropriate effective ion-electron potential and to compute the related effective cross section. A main ingredient to that are collective effects of the electron cloud like dynamic screening and plasma waves. These effects are, of course, best under control in the linear response regime. We thus regard, as an exercise and test, the cross section for the case of linear ion-target coupling. The required effective ion-electron potential \( \phi_{ei} \) is then for ideal plasmas (\( \xi \ll 1 \)) simply provided by the linear response of the medium in terms of the RPA dielectric function with \( \phi_{ei}(k, \omega) = \phi_p(k)/\varepsilon_R(k, \omega) = Ze/|e_0 k^2 \varepsilon_R(k, \omega)| \), see Eq. (2.27). Because we deal with linear coupling \( \eta_p \ll 1 \), the cross section \( \sigma \) can be evaluated in first order Born approximation, where

\[
\sigma(hk) = \frac{\mu^2}{4\pi^2 \hbar^4 |e \phi_{ei}(k, \omega(k))|^2} = \frac{\mu^2}{4\pi^2 \hbar^4} \frac{Z^2 \epsilon^4}{\phi_k^0 |\varepsilon_R(k, \omega(k))|^2} ,
\]

for a momentum transfer \( h k = q = p' - p \) and the related energy transfer \( h \omega(k) = \tilde{\omega}(Mv) - \tilde{\omega}(Mv - h k) = \omega(p + h k) - \omega(p) \). As the cross section in first order Born approximation depends only on the transferred momentum \( q \) it is favorable to insert it into Eq. (2.57). Rewriting
the product of Fermi-Dirac distributions as $f_0(p)(1 - f_0(p + \hbar k)) = -[f_0(p) - f_0(p + \hbar k)]$

and its relation $\text{Im}[\chi_0(k, \omega)] = -(\epsilon_0 k^2 / \epsilon^2) \text{Im}[\varepsilon_R(k, \omega)]$ to the imaginary part of the RPA dielectric function $\varepsilon_R$ (2.38). It is to be remarked, that in the derivation of the stopping power (2.65) the assumption of a target in thermal equilibrium with $f(p) = f_0(p)$ was essential, while the mass ratio between projectile and target particles may be arbitrary. In the limit of heavy projectiles, $m/M \to 0$, projectile recoil can be neglected and $\hbar \omega(k) = \tilde{\zeta}(Mv) - \tilde{\zeta}(Mv - \hbar k) \approx \hbar k \cdot v$. This allows to exploit the symmetry of the dielectric function $\varepsilon_R(k, \omega) = \varepsilon_R^*(k, -\omega)$ and the relation $f_B(x) + f_B(-x) = -1$. In the resulting expressions the function $f_B$ is thus simply replaced by a factor $-1/2$ and we obtain the so called Born–RPA stopping power [May85] which is identical to the linear response stopping power in the form of Eq. (2.44) for $\varepsilon = \varepsilon_R$. In the case of an ideal target the linear response stopping power (2.44) can thus be interpreted as result of binary ion–electron encounters in the linear coupling regime and with the effective ion-electron potential $\phi_e(k, \omega) = Z e / \epsilon_0 k^2 \varepsilon_R(k, \omega)$ containing the dynamic screening from linear response. More generally, the binary collision stopping power evaluated in first order Born approximation, Eq. (2.65), represents for any given interaction $-e \phi_e(k, \omega)$ the linear response stopping of a non-interacting electron target, that is, expression (2.44) after replacing $\phi_p$ with $\phi_e$ and $\chi$ with $\chi_0$. This equivalence results of course form the treatment of both approaches at the same level of approximation, that is, in first order of the perturbation.

The binary collision approach in general, Eqs. (2.56)-(2.60), applies, however, to any strength of the ion–electron interaction, $\langle \eta_p \rangle$, provided that the full many–body dynamics can be mapped into an effective interaction. This should be feasible at least for situations with weak electron–electron correlations, but one has yet to determine this effective interaction which includes the dynamic and nonlinear response of the medium. This requires, for instance, to solve the ladder $T$-matrix equation with a fully dynamically screened interaction. But generally applicable tools for this task are not available at present, and we have to consider approximations. Static effective interactions are sufficient at low ion velocities and e.g. the well developed techniques of density functional theory can be employed in that limit, as will be outlined in Section 2.3.3. A widely used, simpler alternative is to parameterize the screened Coulomb potentials in terms of Yukawa functions. The related transport cross section $\sigma_v$ have been extensively studied in particular in connection with ion stopping over the last decades, see
2.2.2.2 Transport cross sections

The transport cross section $\sigma_{\text{tr}}$ of a screened Coulomb potential is the central quantity of the binary collision stopping formula (2.60) and of various important transport properties like e.g. conductivities. Its evaluation is a major task in determining stopping powers once an effective projectile-electron interaction is defined. In this paragraph we will outline several properties of the transport cross section resulting from the very common choice of the Yukawa–like shielded Coulomb interaction

$$ V_{\text{ei}}(r) = -\frac{Ze^2}{4\pi\epsilon_0 r} \exp\left(-\frac{r}{\lambda}\right). \quad (2.67) $$

In particular, we will discuss the different approximations to calculate $\sigma_{\text{tr}}$ and their regimes of validity and resume the question already raised in Sec. 2.1.2.2 on the border line between quantum and classical description for the binary ion-electron encounters in the screened Coulomb field (2.67). The screening length $\lambda$ is here a fixed, given parameter.

In the non-relativistic regime, $\sigma_{\text{tr}}$ can be evaluated from the quantum phase shifts [Wil69] obtained from a solution of the Schrödinger equation for the relative motion of the two particles with velocity $v_r$, i.e. energy $\mu v_r^2/2$, which reads in reduced units ($\tilde{r} = r/\lambda$)

$$ \left( \Delta_F + \left( \frac{\lambda}{\lambda_r} \right)^2 + 2\frac{Z}{|Z|\kappa} e^{-\tilde{r}} \right) \psi(\tilde{r}) = \left( \Delta_F + \left( \frac{\lambda}{\lambda_r} \right)^2 \left[ 1 + 2\frac{Z}{|Z|\lambda} \left( \frac{b_0 e^{-\tilde{r}}}{\tilde{r}} \right) \right] \right) \psi(\tilde{r}) = 0. \quad (2.68) $$

Here we recover all the characteristic length scales $b_0 = |Z|e^2/(4\pi\epsilon_0\mu v_r^2)$, $\lambda_r = h/\mu v_r$, $\lambda$, and related ratios introduced and discussed in the general considerations on the ion-target coupling in Sec. 2.1.2.2. A specific combination of them is represented by $\kappa = \eta_b \lambda/\lambda_r = b_0 \lambda/\lambda_r^2 = |Z|e^2\mu \lambda/(4\pi\epsilon_0 h^2)$ which only depends on the charge and the screening length but not on the relative motion. In the attractive case ($Z > 0$) the number of bound states is determined by the number of nodes of the solution of Eq. (2.68) in the limit of vanishing energy $\lambda_r \to \infty$ and is hence a function only of $\kappa$ [Pat81]. The actual number of bound levels in the screened Coulomb potential increases almost linearly with $\kappa$, roughly like $\kappa/2$, and may serve to discriminate between a short-range ($\kappa < 1$) or long-range nature of the interaction. The solution of Eq. (2.68) depends only on $\lambda/\lambda_r$, and the parameter $\kappa$ or $b_0/\lambda$, respectively, and hence also the phase shifts $\delta_\ell (\lambda/\lambda_r, b_0/\lambda)$ which are determined from its asymptotic behavior. The $\delta_\ell$ are related to the desired transport cross section scaled in $4\pi\lambda^2$ by

$$ \frac{\sigma_{\text{tr}}(v_r)}{4\pi\lambda^2} = \frac{1}{2} \int_{-1}^{1} d\cos(\vartheta) \left[ 1 - \cos(\vartheta) \right] \frac{d\sigma(v_r, \vartheta)}{\lambda^2 d\Omega} = \left( \frac{\lambda_r}{\lambda} \right)^2 \sum_{\ell=0}^{\infty} (\ell + 1) \sin^2 \left[ \delta_{\ell+1} - \delta_\ell \right]. \quad (2.69) $$

In general the numerical evaluation of Eq. (2.68) and the determination of a large number of phase shifts is needed for $\sigma_{\text{tr}}$. This requires a large computational effort in particular in view of the subsequent integration over the velocity distribution for calculating the stopping power. Thus some approximations for certain limiting cases are highly desirable, as for instance an evaluation of the $\delta_\ell$ for large quantum numbers $\ell$ by use of the WKB scheme, see e.g. [Rog71]. More details on these questions can be found in [May00] where also some very useful fit formulas for $\sigma_{\text{tr}}$ (2.69) are presented and critically reviewed. Here we only consider more closely the first
Born approximation, Born I (BI), and the classical limit of expression (2.69) and their regimes
of applicability.

Since the BI differential cross section \( (d\sigma /d\Omega)_{BI} \) is directly given in terms of the Fourier
transform \( V_{el}(k) \) of the scattering potential (2.67), see Eq. (2.64), an analytic expression for
the related transport cross section can be easily obtained which reads in our variables

\[
\frac{\sigma_{tr}(v_{t})}{4\pi \lambda^{2}} \bigg|_{BI} = \frac{1}{2} \left( \frac{b_{0}}{\lambda} \right)^{2} \left\{ \ln \left[ 1 + 4 \left( \frac{\lambda}{\lambda_{r}} \right)^{2} \right] - \frac{1}{1 + 4 \left( \frac{\lambda}{\lambda_{r}} \right)^{2}} \right\} .
\]

(2.70)

Here, the factor \( b_{0}^{2} \) carries the \( Z^{2} \)-dependence characteristic for the stopping power in first
order of the perturbation and the linear coupling regime. The general \( Z \)-dependence of \( \sigma_{tr} \),
see e.g. [Schl98, Ger99], is, however, rather intricate, as we will see below and in the next
chapter. A further special case is the already mentioned additional logarithmic \( Z \)-dependence
in the semilinear regime. It is a typical feature of the classical first order perturbation theory
resulting in the stopping expression first obtained by Bohr. The corresponding Bohr-expression
of the transport cross section [Hah71]

\[
\frac{\sigma_{tr}(v_{t})}{4\pi \lambda^{2}} \bigg|_{Bohr} = \left( \frac{b_{0}}{\lambda} \right)^{2} \left\{ \ln \left[ \frac{2\lambda}{\gamma b_{0}} \right] - \frac{1}{2} \right\},
\]

(2.71)

represents the high velocity limit of the general classical description, where

\[
\frac{\sigma_{tr}(v_{t})}{4\pi \lambda^{2}} \bigg|_{class} = \frac{1}{2} \int_{0}^{\infty} \frac{b^{2}}{\lambda^{2}} \left[ 1 - \cos(\vartheta(b)) \right] = \int_{0}^{\infty} \frac{b^{2}}{\lambda^{2}} b \sin^{2} \left( \frac{\vartheta(b)}{2} \right)
\]

(2.72)

is defined in terms of the center–of–mass scattering angle \( \vartheta \) and the impact parameter \( b \) or
\( \bar{b} = b/\lambda \). Both are connected through the standard classical mechanics relation [Gol80, Chapter
3] which is for a relative kinetic energy of \( \mu v_{t}^{2}/2 \) given by

\[
\vartheta(\bar{b}) = \pi - 2\bar{b} \int_{\bar{r}_{m}}^{\infty} \frac{d\bar{r}}{\bar{r}^{2}} \left[ 1 + 2 \frac{Z}{\lambda} \frac{b_{0} e^{-\bar{r}}}{\lambda} - \bar{b} \right]^{-1/2}, \quad \text{where} \quad 1 + 2 \frac{Z}{\lambda} \frac{b_{0} e^{-\bar{r}_{m}}}{\lambda} - \bar{b}^{2} = 0 \quad (2.73)
\]

Here the integrals (2.72) and (2.73) must also be calculated numerically, in general. The
classical cross section \( \sigma_{tr}|_{class} \) only depends on the sign of \( Z \) and the parameter \( b_{0}/\lambda \) and
represents the \( \lambda/\lambda_{r} \rightarrow \infty \) limit at fixed \( b_{0}/\lambda\) of the quantal expression (2.69).

The remaining most interesting question concerns the regimes of applicability of these limiting
cases and approximations and their relation to the previously discussed stopping regimes.
Here we only present some simple arguments. A more detailed analysis of this subject can
be found in Ref.[Boh48]. Starting point are again the characteristic length scales \( b_{0}, \lambda_{r} \) and
\( \lambda \). Due to the scaling behavior of Eqs.(2.68) and (2.69) the problem is completely determined
by two different ratios of these lengths as e.g. \( \eta_{p} = b_{0}/\lambda_{r} \) and \( \lambda/\lambda_{r} \), which we have chosen
for the parameter plane in Fig. 2.6 indicating the different expected regimes. The applicability
of a classical description requires, of course, that both \( \lambda \) and \( b_{0} \) are (much) larger than
\( \lambda_{r} \). The regime of a classical binary collision description will hence be located at \( \eta_{p} > 1 \) and
\( \lambda/\lambda_{r} > 1 \), where the Bohr result (2.71) can be used at large velocities or more precisely at
small values of the classical perturbation parameter \( b_{0}/\lambda < 1 \). Throughout the classical regime
we furthermore have $\kappa = \eta_p \lambda/\lambda_r > 1$ and thus typically a large number of bound states in the attractive screened Coulomb potential, that is, a long-range interaction. From the classical regime we reach the Born I quantum scattering regime for decreasing $\eta_p$ in the region $\eta_p < 1$ and $\lambda/\lambda_r > 1$. There the ion-electron interaction can be safely considered as weak. Still for $\eta_p < 1$ but with decreasing $\lambda/\lambda_r < 1$ we came in the regime of a short-range interaction with $\kappa < 1$ and increasingly lower relative energy $b_0 > \lambda$. Here we expect that higher order terms like the second order Born II contribution are necessary for a correct description of the scattering process, since for short-range potentials, Born I would only be sufficient in the case of high relative energies. Penetrating now into the parameter region of increasing $\eta_p > 1$ at $\lambda/\lambda_r < 1$ corresponds to an increase of the coupling strength for a short-range potential at lower and lower energies and a rising number of possible bound states ($\kappa > 1$) and related scattering

![Figure 2.6: The classical and quantum domains for binary ion-electron collisions in the screened Coulomb potential (2.67) in the double logarithmically scaled $\eta_p$-$\lambda/\lambda_r$-plane. The high energy region is located above the dash–dotted line $b_0 = \lambda$. The dashed lines represent constant values of the parameter $\kappa = \eta_p \lambda/\lambda_r$ which is independent of the relative velocity and a measure of the number of bound states in the attractive potential.](image-url)
resonances. This clearly requires a complete quantum treatment beyond any perturbation expansion. In view of the introduced ion-target coupling regimes we obtain the following picture for the ion-electron interaction in a screened Coulomb potential. We reconsider Fig. 2.6 and start in the right part at \( \eta_r > 1 \) in the upper half-plane \( \lambda/\lambda_r > 1 \) but below the dash-dotted line \( b_0 = \lambda \). This represents the region of the nonlinear coupling where a classical description of scattering is valid. We next come into the classical semilinear regime located above the

![Graphs showing transport cross section \( \sigma_{tr} \) normalized by \( 4\pi \lambda^2 \) for the attractive \((Z > 0)\) screened Coulomb potential \((2.67)\) as a function of \( b_0/\lambda \) for different fixed \( \kappa = b_0 \lambda/\lambda_r^2 = |Z|e^2\mu\lambda/(4\pi\epsilon_0\hbar^2) \) as indicated. Compared are in each case the exact result obtained from Eq. \((2.68)\) represented by the solid curve, the entirely classical results \((2.72)\) given by the dash-dotted one and the Born I expression \((2.70)\) (dashed curve). The classical result only depends on \( b_0/\lambda \) but not on \( \kappa \).]
Figure 2.8: Normalized transport cross section $\sigma_{tr}/4\pi\lambda^2$ for the screened Coulomb potential (2.67) as obtained from the classical description given by Eqs. (2.72) and (2.73) as a function of $b_0/\lambda$ for attractive ($Z > 0$, solid curve) and repulsive ($Z < 0$, dash-dotted curve) interaction. The dashed curve represents the approximation

$$\frac{\sigma_{tr}}{4\pi\lambda^2} = \frac{1}{2} \left( \frac{b_0}{\lambda} \right)^2 \ln \left[ 1 + \left( \frac{2\lambda}{\gamma \exp(\gamma/b_0)} \right)^2 \right]$$

deduced from the classical high energy limit (2.71).

dash–dotted line where $b_0 < \lambda$ but still $\eta_p > 1$. From there we reach the quantum linear coupling regime at $\eta_p < 1$ and $\lambda/\lambda_r > 1$ by crossing the line $\eta_p = 1$. This is the usual and commonly accepted transition from the classical to the quantum Born I regime for decreasing $\eta_p$ or increasing velocity. In the latter case one goes, for fixed further parameters, along a line of constant $\kappa$ (like the dashed and long-dashed ones) towards left top. For nonideal targets at low $\Theta$, see Eq. 2.18, we may have, however, a very strong screening leading to $\lambda < \lambda_r$ and thus into the lower half-plane of Fig. 2.6. The next regime located at $\eta_p < 1$ and $\lambda/\lambda_r < 1$ then represents a quantum semilinear regime, while the quantum nonlinear regime is reached after crossing $\eta_p = 1$ towards larger values of $\eta_p$.

The previously established arguments for the applicability of the different approximations are checked and confirmed by a comparison between the classical result (2.72), the Born I expression (2.70) and the exact result (2.69) [May99b]. It is presented in Fig. 2.7 for different values of $\kappa = 0.1, 1, 10, 1000$ and for an attractive interaction ($Z > 0$) as a function of $b_0/\lambda$ which is proportional to the inverse of the relative energy $\mu v^2_r/2$. The plotted curves correspond to a section through Fig. 2.6 along lines of fixed $\kappa$. We note in particular the expected agreement of the exact and the classical result for $\kappa \gg 1$ and $\eta_p > 1$, the occurrence of resonances at $\kappa \gg 1$ and low energies $b_0/\lambda \gg 1$ and the merging of the exact and the Born I result at large velocities, that is, $b_0/\lambda \ll 1$ in all cases. Before closing this paragraph we still compare in Fig. 2.8 the frequently used approximation for the classical regime

$$\sigma_{tr}/4\pi\lambda^2 = (b_0/\lambda)^2 \ln[1 + (2\lambda/\gamma \exp(\gamma/b_0))^2]/2,$$

which represents a non-divergent modification of the Bohr expression (2.71), with the exact classical result obtained from Eqs. (2.72) and (2.73) for an attractive and repulsive interaction (2.67). Like the fully quantum mechanical $\sigma_{tr}$ (2.69) the exact classical result depends on the sign of the charge at variance with the Born I and the Bohr expressions. This difference in the cross sections for different signs of $Z$ is, however, only important for nonlinear coupling $b_0/\lambda > 1$ and unimportant in the truly semilinear regime $b_0/\lambda \ll 1$. We further remark that the contributions of resonances in the attractive case survive in the classical limit and yield the non-monotonous increase of $\sigma_{tr}$ with some hump at $b_0/\lambda \approx 4$. 

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2.2.3 The combined Model

In Sec. 2.2.1.5 we have seen that corrections of the linear response description by binary collisions using the Bloch correction or the introduction of a cutoff $k_m$ provide simple recipes to extend the linear response formalism into the semilinear regime with a minimum of calculational effort. The whole scheme, however, is based on several approximations as expression (2.51) which are well justified only close to the linear regime. To proceed further towards the nonlinear coupling regime one should prefer more complete approaches to incorporate the binary collision contributions from the strong coupling region. Recently more elaborated schemes have been proposed in [Ger96, Mora96, Schl98, Ger99, Zwi99, May00]. They adopt the treatment to derive convergent collision integrals needed for the calculation of transport properties in the framework of kinetic theory introduced by Gould and De Witt [Gou67]. There the cross section in the collision integral is estimated by composing three terms: The linear response or Born I approximation for the dynamically screened Coulomb interaction and the binary collision result for the related statically screened interaction are added while the linear response (Born I) cross section for the statically screened interaction is subtracted to compensate for its appearance in the other terms, see also e.g. [Red97]. Translating this to stopping powers and still generalizing it a bit establishes a combined expression

$$\left(\frac{dE}{ds}\right)_{\text{com}} = \left(\frac{dE}{ds}\right)_{\text{lr}} + \left(\frac{dE}{ds}\right)_{\text{bc}} - \left(\frac{dE}{ds}\right)_{\text{lr}}^0. \quad (2.74)$$

Here $(dE/ds)_{\text{lr}}$ represents the stopping power (2.44) which involves a fully dynamically screened interaction in linear response, $(dE/ds)_{\text{bc}}$ equals expression (2.60) where the transport cross section $\sigma_{\text{tr}}$ is determined from a static, spherically symmetric effective ion-electron interaction $V_{\text{ei}} = -e\phi_{\text{ei}}(k)$ which is also used in the linear response of a non-interacting target

$$\left(\frac{dE}{ds}\right)_{\text{lr}}^0 = \frac{1}{(2\pi)^3} \int d^3k \, \hat{v} \cdot k \, |V_{\text{ei}}(k)|^2 \, \text{Im}[\chi_0(k,\omega(k))]. \quad (2.75)$$

By construction the combined expression (2.74) guarantees a smooth merging into the correct high velocity asymptotic. For increasingly high velocities, where $\langle \eta_p \rangle \rightarrow 0$, the complete binary collision result turns into its first order Born approximation, see Sec. 2.2.2.2 and is hence identical to expression (2.75) [compare Eq. (2.65)]. Thus the two terms $(dE/ds)_{\text{bc}} - (dE/ds)_{\text{lr}}^0$ cancel gradually and leave solely the fully dynamic linear response contribution $(dE/ds)_{\text{lr}}$. The effective interaction $V_{\text{ei}}$, however, has still to be fixed. Two different choices for $V_{\text{ei}}$ have actually been considered.

The first one [Ger96, Mora96, Schl98, Ger99] directly translates the original proposal to calculate the cross section as a $T$-matrix expression with a dynamically screened first order Born approximation but statically screened ladder terms of higher order. Here the corresponding dynamically screened ion-electron potential is for ideal targets $\phi_{\text{ei}}(k,\omega) = \phi_{p}(k)/\varepsilon_{\text{R}}(k,\omega)$. The related stopping power in first Born approximation and for heavy ions ($M/m \gg 1$) is the linear response $(dE/ds)_{\text{lr}}$ (2.44) part in the combined expression (2.74). The static interaction used for the higher order terms is taken as the static limit of $\phi_{\text{ei}}(k,\omega)$, that is,

$$V_{\text{ei}}(k) = -\frac{e\phi_{p}(k)}{\varepsilon_{\text{R}}(k,\omega = 0)} = -\frac{Ze^2}{\varepsilon_0 k^2 \varepsilon_{\text{R}}(k,0)}, \quad (2.76)$$

which leads to

$$\left(\frac{dE}{ds}\right)_{\text{lr}}^0 = -\frac{Z^2e^2}{\varepsilon_0(2\pi)^3} \int d^3k \, \hat{v} \cdot k \, \text{Im}[\varepsilon_{\text{R}}(k,\omega)] \frac{\varepsilon_{\text{R}}(k,\omega)}{k^2|\varepsilon_{\text{R}}(k,0)|^2}. \quad (2.77)$$
by use of \( \text{Im}[\varepsilon_R(k, \omega)] = - (e^2/\epsilon_0 k^2) \text{Im}[\chi_0(k, \omega)] \). The last contribution, that is, the binary collisions part \((dE/ds)_{bc}\) is evaluated for the static interaction (2.76) which represents in the limit of classical targets the well-known Debye-screened Coulomb potential

\[
V_{ei}(k) \equiv \Theta(\lambda_D/\lambda) \frac{Ze^2}{\epsilon_0 k^2 + 1/\lambda_D^2} \quad \leftrightarrow \quad V_{ei}(r) = -\frac{Ze^2}{4\pi\epsilon_0 r} \exp\left(-\frac{r}{\lambda_D}\right),
\]

where \( \lambda_D \) is the Deybe length. In this scheme the dynamically screened potential \( \phi_p(k)/\varepsilon_R(k, \omega) \) turns into the statically screened \( \phi_p(k)/\varepsilon_R(k, 0) \) at low velocities. Consequently both contributions \((dE/ds)_{ir}\) and \((dE/ds)_{ir}^0\) merge and cancel out in \((dE/ds)_{\text{com}}\). The remaining binary collision term takes into account all the strong coupling effects. The resulting stopping power can thus be expected to be rather close to the exact one provided that linear response accurately reproduces the true statically screened interaction. More general expressions for arbitrary mass ratios using the effective interaction (2.76) are given and evaluated numerically for some specific target conditions and projectile parameters in [Ger96, Mora96, Ger99].

For the second choice [Zwi99, Zwi00, May00] of an effective interaction \( V_{ei} \), a velocity dependent screening length \( \lambda(v) \) is introduced and determined from linear response in the framework of the combined expression (2.74). The use of an interaction which depends on the projectile velocity \( v \) is of course clearly restricted to the limit of sufficiently heavy projectiles, where the ion velocity \( v \) enters the description as an external parameter and not as a dynamic variable of the ion-target system. Here the effective interaction

\[
V_{ei}(r) = -\frac{Ze^2}{4\pi\epsilon_0 r} \exp\left(-\frac{r}{\lambda(v)}\right) \quad \leftrightarrow \quad V_{ei}(k) = -\frac{Ze^2}{\epsilon_0 k^2 + 1/\lambda^2(v)},
\]

is employed to evaluate the contributions \((dE/ds)_{ir}^0\) and \((dE/ds)_{bc}\), while \( \lambda(v) \) is still to be determined. To that end we view the whole linear response part \((dE/ds)_{ir} - (dE/ds)_{ir}^0\) as a correction to the binary collision term \((dE/ds)_{bc}\) and intend to rely on binary collisions only. This fixes the desired screening length \( \lambda(v) \) by demanding \((dE/ds)_{ir} - (dE/ds)_{ir}^0 = 0\), that is,

\[
\left. \frac{dE}{ds} \right|_{ir} = \frac{1}{(2\pi)^3} \int d^3k \cdot \hat{\mathbf{k}} \left| \frac{Ze^2}{\epsilon_0 (k^2 + 1/\lambda^2(v))} \right|^2 \text{Im}[\chi_0(k, \omega(k))].
\]

which has to be resolved numerically for \( \lambda(v) \). This concept allows to include dynamic effects by mapping the dynamically screened interaction contained in the linear response description into a spherically symmetric velocity dependent effective interaction. Similar ideas have also been proposed and investigated for atomic stopping by bound electrons in [May97, May99a].

Both schemes for the combined expression \((dE/ds)_{\text{com}}\) have the important feature that no external parameter appears in contrast to all the cutoff approaches. They are, however, essentially based on the assumption that the collective effects, static ones as well as dynamic ones, are well described by linear response. Since the collective phenomena take place on the scale of the actual screening length, i.e. at small momenta \( k \), the strong interaction region must thus be small on this scale and hence restricted to high momenta. This immediately leads back to the definition of the semilinear regime, Eqs. (2.22), as the proper domain for such type of approximations. It may be extended to (weakly) nonideal plasmas by replacing the RPA dielectric function with the appropriate one which includes correlations within the target, see Section 2.2.1.3. Of course, no assurance exists that the real dynamic situation can be treated in a satisfactory manner by a velocity dependent, but statically screened and spherically
symmetric ion–electron interaction as assumed in the second scheme. This can be justified only a posteriori. In any case all approximations for the semilinear regime and extensions into the nonlinear one which are based on assumptions and models for an appropriate effective potential need to be checked by fully dynamic many–body treatments as e.g. the simulation techniques presented in the next Sec. 2.3. A specification of the combined schemes to entirely classical systems is discussed in Sec. 3.2 together with a comparison to simulation results.

2.3 Numerical Approaches

The regimes of linear and semilinear coupling allowed to separate the ion–target coupling from the interactions within the target. The common concept was the linear response formulation which describes the energy loss or provides the effective interaction for binary collisions for a large variety of target conditions by the same basic relations just adapting the dielectric function to the particular target condition. This changes if we proceed to nonlinear ion–target coupling. Now each parameter region for projectile and target requires its own methods. In this section, we discuss the most relevant of these numerical methods to compute stopping in the semilinear and nonlinear regime. We start in Sec. 2.3.1 with particle simulations of the Vlasov–Poisson equation which is designed to study strong ion-target coupling in classical, ideal targets. The appropriate tool for classical, but nonideal targets is given by molecular dynamics (MD) simulations which are presented in Sec 2.3.2. For fully degenerate targets (Θ ≪ 1), density functional methods are a widely used tool in all fields of electron physics. Some basic aspects of density functional approaches, the local density approximation (LDA) and its time dependent extension (TDLDA) are outlined in Section 2.3.3.

2.3.1 Particle simulations of Vlasov–Poisson for classical ideal targets

Classical (Θ ≫ 1, ⟨η_e⟩ > 1) and ideal (Γ ≪ 1) electron plasmas allow a mean–field treatment of the electrons because correlation effects are negligible. The electron cloud is described in terms of a phase–space distribution \( f(r,u,t) \) and it is propagated by the Vlasov equation

\[
\frac{\partial f}{\partial t} + u \cdot \frac{\partial f}{\partial r} + \frac{e}{m} \phi_p \cdot \frac{\partial f}{\partial u} = 0
\]  

(2.81)

using the electrostatic potential \( \phi = \phi_p + \phi_{\text{ind}} \) as given by the Poisson equation

\[
\Delta \phi(r,t) = -\frac{\rho_p}{\epsilon_0} - \frac{\rho_{\text{ind}}}{\epsilon_0} = -\frac{Ze}{\epsilon_0} \delta^3(r - vt) + \frac{e}{\epsilon_0} \left[ \int f(r,u,t) d^3u - n \right].
\]  

(2.82)

In absence of the external perturbation by the ion, represented here by its charge density \( Ze \delta^3(r - vt) \), the number density of the target electrons is \( n \) and serves here as a homogeneous neutralizing background. The electrostatic approximation is valid for non–relativistic ion and electron velocities. The induced electric field \( E_{\text{ind}} = -\nabla \phi_{\text{ind}} \) at the ion position or alternatively the induced electron density provided by a solution of Eqs.(2.81),(2.82) yields the stopping power by virtue of Eq. (2.6).

The Vlasov–Poisson equation requires ideal targets but is applicable for any strength of the ion–electron potential. The regime of weak coupling is also accessible and we look first at the Vlasov equation in this regime. The relative strength of the ionic perturbation can be estimated as

\[
\frac{e}{m} \frac{\partial \phi_p}{\partial r} \cdot \frac{\partial f}{\partial u} / u \cdot \frac{\partial f}{\partial r} \approx \sqrt{3} Z \Gamma^{3/2} \frac{u_{\text{th}}^3}{u_s^3} \frac{r_s}{|r - vt|}
\]  

(2.83)
where we have introduced typical scales of velocity $u_s$, time $t_s = \omega_p^{-1}$ and length $r_s = u_s t_s = u_s / \omega_p$ and the classical plasma parameter $\Gamma$ (2.14) which is related to the density $n$, the thermal velocity $v_{\text{th}}$ and the plasma frequency $\omega_p = (e^2 n / m_0)_{\text{th}}^{1/2}$ through $\Gamma^{3/2} = \omega_p^3 / 4 \pi n m_0^{3/2}$.

A natural choice for the velocity scale is the thermal velocity, $u_s = v_{\text{th}}$ which yields as the obvious strength of the perturbation the factor $\sqrt{3} Z \Gamma^{3/2} = |Z| / 3 N_D$, where $N_D$ is the number of particles in the Debye sphere, see Eq. (2.24). Weak perturbations with $|Z| / N_D \ll 1$ allow an expansion in orders of the perturbation $Z / N_D$. In the lowest order, the linearized Vlasov–Poisson equation provides the classical dielectric description [Ich73, Section 3.4] which comprises the classical version of all linear response quantities and observables like the stopping power. There results in particular the dielectric function $\varepsilon_{\text{cl}}(k, \omega)$ for classical electron plasmas [Pet91, Fri61]

$$\varepsilon_{\text{cl}}(k, \omega) = 1 + \frac{e^2 n}{m_0 k^2} \int d^3 u \ k \cdot \frac{\partial f_0(u)}{\partial u} \frac{1}{\omega - k \cdot u + i0}$$  \hspace{1cm} (2.84)

where $f_0(u) = (m/2\pi k_B T)^{3/2} \exp(-m u^2 / 2k_B T)$ is a Maxwell distribution. This classical dielectric function $\varepsilon_{\text{cl}}$ is the limit $\hbar \to 0$ of the RPA dielectric function $\varepsilon_R$ (2.38) and reproduces correctly the long wavelength (small $k$) behavior of $\varepsilon_R$ at $\Theta \gg 1$ where quantum effects can be safely neglected [Ari84]. The second order of the expansion in $Z / N_D$ yields the $Z^3$-Barkas contribution mentioned in Sec. 2.2.1.5.

Choosing as a more relevant velocity scale the mean relative motion between ion and electron, $u_s = \langle v_t \rangle = v_{\text{th}} \langle v_t \rangle$ suggests that the essential expansion parameter is $Z / N_D (\langle v_t \rangle)^3$ instead of $Z / N_D$ [Esb90, Say92]. Because the Coulomb potential of the ion diverges in this classical approach at $r \to v t$ whatever small the prefactor may be, see Eq. (2.83), the linearized Vlasov–Poisson equation is only applicable for relative distances $r / \lambda > \sqrt{3} Z \Gamma^{3/2} (\langle v_t \rangle)^3$, where $\lambda = r_s = \langle v_t \rangle / \omega_p$ is the dynamic screening length in an ideal plasma. Since this condition is only relevant for radii $r < \lambda$ we recover here the definition of the semilinear regime $\sqrt{3} Z \Gamma^{3/2} (\langle v_t \rangle)^3 = \langle b_0 \rangle / \lambda \ll 1$ (2.24). The linearization or, more general, the expansion of the Vlasov–Poisson equations is hence applicable in the parameter region of the semilinear coupling regime. There it provides approximations for the linear response stopping power of the form of Eq. (2.50) depending on a cutoff $k_m$, see Sec. 2.2.1.5, as the condition for linear coupling is always violated in a sufficiently small vicinity of the ion.

Numerical solutions of Eqs. (2.81) and (2.82) are unavoidable in the regime of nonlinear coupling. The Poisson equation Eq. (2.82) is usually solved on a spatial grid. There are various methods available for that task. A particularly efficient one employs fast Fourier transformation to obtain the electrostatic potential for a given charge density [Lau94]. There are two different schemes for the propagation of the Vlasov equation (2.81), either by finite element techniques on a grid in phase space or by particle–in–cell (PIC) techniques [Hoe81]. The direct solution of the Vlasov equation in six-dimensional phase space is extremely demanding concerning memory requirement, still beyond nowadays technical limits. There exist, however, solutions of the Vlasov–Poisson equations for a reduced four dimensional phase space $(r, z, v_r, v_z)$ corresponding to a cylindrical simulation box, achieved with the help of massively parallel supercomputers [Boi96]. The more efficient alternative PIC treatment where the phase-space distribution is represented by a swarm of pseudo-particles which follow the Newtonian equations of motion in the potential $\phi$ composed of the mean–field $\Phi (= \phi_{\text{ind}})$ produced from their own charges and, in our case, the external ionic field $\phi_p$. The (moderate) effort to solve the Poisson equation on the spatial, i.e. three-dimensional, grid remains the same. But the propagation of the Vlasov equation is much accelerated which usually allows to perform the computation on work stations.
because the numerical expense depends only linearly on the number of pseudo-particles. This number is to be adapted to the spatial grid (rather than the full phase-space grid) to achieve a sufficiently smooth representation of the electron density \( \rho(r,t) = \int f(r,u,t)du \) on the grid. Typically, a few pseudo-particles per grid cell are sufficient. Their number can be enhanced, if necessary, to suppressed the amount of unavoidable fluctuations or noise. Two basically different scenarios are conceivable. In the one case, one pseudo-particle stands as a “macro particle” for many physical electrons. This is the genuine PIC scheme. In the other case, one physical electron is represented by many pseudo-particles. This is the regime of test–particle simulations commonly used for numerical solutions of nuclear dynamics [Ber88, Rei95]. There the phase-space distribution \( f(r,u,t) \) is represented by \( i = 1, ..., N_T \) test-particles through

\[
f(r,u,t) = \frac{N}{N_T} \sum_i w(r - r_i(t)) w_u(u - u_i(t)). \tag{2.85}
\]

Here the \( w \) and \( w_u \) are smooth and fairly well concentrated, normalized wave–packets in phase space and \( N \) is the number of physical particles with \( N \ll N_t \). The test particles have smaller mass \( m_T = mN/N_T \) and charge \( q_T = eN/N_T \), but the physical charge to mass ratio \( q_T/m_T = e/m \). The genuine PIC technique was applied recently to determine the stopping power in cylindrical 2–D spatial geometry [Hof94, Dav98] while the test-particle scheme was used in full 3–D space simulations [Zwi96a, Zwi97a, Zwi97b, Zwi98a, Zwi99]. The results of these last named investigations will be discuss in Ch. 3. For this reason we illustrate the test–particle scheme used there in a bit more detail. Introducing characteristic units for time, velocity, length and energy, given by the inverse of the plasma frequency, the thermal velocity, the Debye length and the thermal energy, i.e.

\[
t_s = \omega_p^{-1}, \quad u_s = v_{th} = (k_B T/m)^{1/2}, \quad r_s = \lambda_D = v_{th}/\omega_p, \quad E_s = k_B T, \tag{2.86}
\]

and using \( \sqrt{3} \Gamma^{3/2} = e^2 \omega_p/(4\pi \epsilon_0 k_B T v_{th}) \) results in the dimensionless coupled equations of motion for the test-particle \( \{\tilde{r}_i = r_i/r_s, \tilde{u}_i = u_i/u_s, i = 1, ..., N_T\} \) and ionic \( \{\tilde{R} = R/r_s, \tilde{v} = v/u_s\} \) coordinates and the Poisson equation

\[
\begin{align*}
\frac{d\tilde{r}_i}{dt} &= \tilde{u}_i, & \frac{d\tilde{u}_i}{dt} &= -\frac{\partial}{\partial \tilde{r}_i} \left[ \hat{\Phi}(\tilde{r}_i) - \frac{\sqrt{3} \Gamma^{3/2}}{|\tilde{r}_i - \tilde{R}|} \right] \\
\frac{d\tilde{R}}{dt} &= \tilde{v}, & \frac{d\tilde{v}}{dt} &= \sqrt{3} \Gamma^{3/2} \frac{mN}{MN_T} \frac{\partial}{\partial \tilde{R}} \sum_i \frac{1}{|\tilde{r}_i - \tilde{R}|} \tag{2.87}
\end{align*}
\]

\[
\hat{\Delta} \hat{\Phi}(\tilde{r},t) = -\hat{\varrho}(\tilde{r},t) = \frac{N}{N_T} \sum_i \hat{w}(\tilde{r} - \tilde{r}_i),
\]

where \( \hat{\Phi} = e\Phi/k_B T, \hat{\varrho} = \rho/\epsilon_n, \hat{w} = w/n \) and \( \hat{\Delta} = \lambda_D^2 \Delta \). As one sees immediately, the scaled PIC (test-particle) equations depend only on the coupling parameter \( \Gamma^{3/2} \). In the actual numerical treatment the Poisson-equation is solved in Fourier space using fast Fourier transformation to switch forth and back simultaneously with the particle propagation where periodic boundary conditions for the cubic simulation box are used. The forces on the particles are retrieved from the grid using the same weight functions \( w \) again. See [Hoc81, Ber88, Rei95] for more details on the PIC treatment in general, and [Zwi99] for further technical remarks specifically on the previous scheme, Eqs. (2.87).
The problem with the Coulomb singularity at small distances is also present in these numerical solutions. In the usual approaches the ionic \(1/r\) potential is smoothed for \(r \to 0\), either explicitly [Boi96a] or implicitly by the finite resolution of the spatial grid or the width of the pseudo-particles. In the test-particle simulations described by Eqs. (2.87) no smoothing and restriction of the resolution at small distances occurs in the ion-test-particle interaction. This use of the full ionic Coulomb potential is made possible by switching to piecewise analytical solutions for the 2-body Coulomb problem of a test-particle close to the ion. This scheme was taken over from the MD simulations for ion stopping and will be outlined in the next section.

High resolution at small distances limits, however, the size of the simulation box for a given number of test-particles (which is usually fixed by technical limitations). The box size, in turn, sets an upper limit on the wave length in the description. Thus, a high spatial resolution can run into a conflict with long-range phenomena. The appropriate compromise depends on the actual problem. The stopping power at high velocities requires a reasonable treatment of the dynamic screening at long wavelengths while nonlinear effects become negligible. There one can go for the opposite strategy to pack several electrons into one numerical macro-particle, i.e. \(N_T/N \ll 1\) to increase the size of the simulation box. A very high resolution on a scale much smaller than the static screening length is, however, necessary for studies in the low velocity regime. Stopping power calculations based on numerical solutions of the Vlasov-Poisson equations with limited spatial resolution at short distances, as e.g. reported in [Boi96, Dav98], yield considerably smaller values for the nonlinear stopping power at low velocities compared with the results which are obtained from Eqs. (2.87) and which will be presented in the next chapter.

### 2.3.2 Molecular dynamics simulations

We again consider entirely classical projectile–target systems \((\Theta \gg 1, \langle \eta_0 \rangle > 1, \langle \eta_p \rangle > 1)\) but now without restriction on the coupling strength within the target, that is, on the ideality \(\xi(\Theta \gg 1) = \Gamma\). Molecular dynamics (MD) simulations, see e.g. [All87], provide a suitable tool to study the full many-body dynamics of these systems. During the last decades they have been successfully applied to various strongly coupled systems like classical Coulomb systems as the one component plasma (OCP) or (binary) ionic mixtures [Han75, Han79]. They allow in particular to investigate non-equilibrium properties of highly correlated systems without restrictions on the strength of the interaction and are thus a powerful tool to compute the stopping power on a heavy ion for the ion–electron system as described by the classical version of the hamiltonian (2.1). The procedure is conceptually very simple: the ion \((\mathbf{R}, \mathbf{v})\) and the electrons \(\{\mathbf{r}_i, \mathbf{u}_i, i = 1 \ldots N\}\) just follow the classical equations of motion with mutual Coulomb interactions

\[
\frac{d\mathbf{r}_i}{dt} = \mathbf{u}_i, \quad \frac{d\mathbf{u}_i}{dt} = -\frac{1}{m} \frac{\partial}{\partial \mathbf{r}_i} \left[ \sum_{j \neq i} \frac{e^2}{4\pi\varepsilon_0|\mathbf{r}_i - \mathbf{r}_j|} - \frac{Ze^2}{4\pi\varepsilon_0|\mathbf{r}_i - \mathbf{R}|} \right]
\]

\[
\frac{d\mathbf{R}}{dt} = \mathbf{v}, \quad \frac{d\mathbf{v}}{dt} = -\frac{1}{M} \frac{\partial}{\partial \mathbf{R}} \sum_i \frac{Ze^2}{4\pi\varepsilon_0|\mathbf{r}_i - \mathbf{R}|^3}
\]

(2.88)

which have to be integrated numerically.

The MD simulations contain without restriction all correlation effects, dynamic screening, close collisions, and multi-particle correlations. They do not rely on a spatial grid for the
Coulomb force and thus there is no restriction in the spatial resolution. On the other hand the expense grows quadratically with the particle number \( N \) because the Coulomb force is to be evaluated separately for each pair of particles. The available computing power thus limits the computation to at most a few thousand particles. Methods which overcome the quadratic growth of expense have been developed. There the particles are collected in spatial cells and the Coulomb force from remote cells is only computed globally using tree structures for the necessary bookkeeping. These “tree codes” [Bar86, Sal94, Spr95a, Pfa92] have, however, an enormous overhead of bookkeeping which makes them competitive only for particle numbers \( \gtrsim 8000 \). In order to approximate an infinite plasma by a finite particle number, the electrons are packed into an elementary cubic simulation box of length \( L \) and this box is continued periodically in all three spatial directions. Thus, a particle is replaced by a cubic lattice of particles and the Coulomb interaction by the Ewald sum of Coulomb interactions [Nij57, Han73] while the neutralizing background of positive charges is simplified in the jellium approach as a homogeneously distributed positive background. The limited simulation box introduces a largest length scale on which collective phenomena can be explored. This limitation is unimportant for strongly coupled targets (\( \Gamma > 1 \)) and low projectile velocities because the screening length \( \lambda \) scales basically like \( \lambda \propto \langle v_r \rangle L / \Gamma^{1/2} \). It becomes a real problem, however, at high projectile velocities where a spatially extended wake field is induced by the ion. But then one leaves anyway the regime of nonlinear coupling and can continue with simpler methods. It is a general feature, that MD simulations are particularly suited for the case of strong coupling and become inefficient, if not impossible, just where weak coupling approaches are valid.

In the next chapter we will report on the MD-simulation stopping results obtained from the simulation scheme used in [Zwi93a, Zwi93b, Zwi94a, Zwi95, Zwi96a, Zwi96b, Zwi97a, Zwi97b, Zwi97c, Zwi98a] and summarized in [Zwi99]. We thus discuss this scheme a bit closer. Using the same classical scaling, Eqs. (2.86), as before leads to the dimensionless version of the coupled equations (2.88)

\[
\frac{d\tilde{r}_i}{dt} = \tilde{u}_i , \quad \frac{d\tilde{u}_i}{dt} = -\frac{\partial}{\partial \tilde{r}_i} \left[ \sqrt{3} \Gamma^{3/2} \sum_{j \neq i} \frac{1}{|\tilde{r}_i - \tilde{r}_j|} - \sqrt{3} Z \Gamma^{3/2} \frac{|\tilde{r}_i - R|}{M} \right],
\]

\[
\frac{d\tilde{R}}{dt} = \tilde{v} , \quad \frac{d\tilde{v}}{dt} = \sqrt{3} Z \Gamma^{3/2} \frac{m}{M} \frac{\partial}{\partial \tilde{R}} \sum_{i} \frac{1}{|\tilde{r}_i - R|},
\]

from which one can read off immediately the coupling parameters. The parameter \( |Z| \Gamma^{3/2} \) characterizes the strength of the ion–electron coupling and the plasma parameter \( \Gamma \) the importance of the electron–electron interactions. This additional dependence on \( \Gamma \) was absent in the test-particle scheme Eqs. (2.87) where the direct electron interaction contained in the MD-Eqs.(2.89) is replaced by the mean–field potential \( \Phi(\mathbf{r}) \) and its selfconsistent determination via the Poisson equation. The parameter \( \Gamma \) which accounts for the correlations in the target becomes meaningless in a mean-field description.

As in the Vlasov-Poisson equation the Coulomb singularity at the ion position produces large forces at small distances whatever small \( |Z| \Gamma^{3/2} \) may be. The classical equations of motion (2.89) come never into a completely linear regime (\( \eta_p < 1 \)) and weak perturbations correspond already to semilinear coupling where the ion–electron coupling strength \( |Z| \Gamma^{3/2} \) demarcates for low ion velocities the semilinear regime (\( |Z| \Gamma^{3/2} \ll 1 \)) from the nonlinear regime (\( |Z| \Gamma^{3/2} \geq 1 \)), see Eqs. (2.21)-(2.24). Equations (2.89) are solved with standard numerical algorithms. The
use of the full Coulomb force requires to single out particles which come very close together, in particular for the attractive ion–electron interaction, where the arising large forces need a strong reduction of the time step and thus slows down the numerical propagation. This is avoided by introducing a separate treatment of close collisions, which takes advantage of the fact that the timescales in the close collision region are much shorter than those for the system as a whole. The most frequent binary systems of close colliding particles are propagated with the analytically known trajectories of the Rutherford problem while the few remaining close multi-particle collisions are propagated as subsystems with a much reduced time step. More details on this scheme and other technical aspects of the MD-simulation are given in the appendix of [Zwi99]. Observables are measured in the MD-simulations as time averages over a certain time interval and/or as ensemble averages over different initial configurations. To compute the stopping power, an equilibrium state of the electron system is produced first by a MD propagation without the ion. Then the ion is added and its energy loss $\Delta E$ and its traveling distance $\Delta s$ are determined over a sufficient long time $\tau$, typically $\tau \approx 60 \ldots 90 \omega_p^{-1}$. The accuracy and stability of the runs are monitored using the total energy. Since the energy loss of the ion is distributed over a "very finite" number of electrons the induced heating has to be cooled out in order to obtain the stopping power for a well defined target temperature $T$. Here a repeated cooling restores the initial temperature $T$ by drawing new velocities from the corresponding Maxwell distribution for electrons at distances $r > \lambda$ far away from the ion. This is done once in time intervals of $10 \ldots 20 \omega_p^{-1}$. The ratio $\Delta E/\Delta s(\tau)$ is the time averaged stopping power which includes the transient period after adding the ion where the stopping power has not yet reached a stationary value. But this period is small, usually $\sim \omega_p^{-1}$ [See95, See97], and affects the results only weakly. Since heavy ions have negligible change in velocity during the measuring time interval, $\Delta E/\Delta s$ represents immediately the stopping power for the given (initial) ion velocity $v$. From several runs with the same $\Gamma, Z, v$, but different samplings of the initial state, an ensemble average over the time averaged $\langle \Delta E/\Delta s \rangle$ is performed and yields finally the stopping power. The error can be deduced from the fluctuations in the ensemble of events.

The MD–simulations are based on a pure classical treatment. As a consequence, no ground state of the classical ($\hbar \to 0$) ion–target system exists and the dynamics at long time scales ends up in a Coulomb collapse where some electrons get deeper and deeper bound in the ion potential by transferring energy and momentum in interactions with the surrounding electrons. This problem is not explored in the dynamic non–equilibrium simulations of stopping where only a short time interval after switching on the ion–electron interaction is of interest. But MD-simulations are strictly restricted to parameters where the ion–target system behaves classically which inhibits an investigation of stopping in regimes where the wave nature of the electrons becomes crucial. This can be taken into account in a generalization of the MD-simulations, the wave–packet molecular dynamics (WPMD) where the pointlike electrons of the classical MD are replaced by Gaussian wave–packets. The WPMD adds quantum effects of wave nature and allows to treat weakly degenerate targets ($\Theta \lesssim 1$). This method is still under development. Its actual status is reported in detail in [Zwi99] together with some first results from its application to stopping.

### 2.3.3 Local energy-density functionals: LDA and TDLDA

Nonideal, $\xi \gtrsim 1$, and highly degenerate, $\Theta \ll 1$, targets which are nonlinearly coupled to the projectile ion, $\eta_p \gg 1$, require a fully quantal treatment and inclusion of correlations. But
a detailed quantum many-body calculation is even nowadays prohibitively complicated when spatial inhomogeneities are involved. Density functional approaches aim to incorporate higher correlations into mean field calculations by virtue of an effective interaction, where quite general theorems guarantee the existence of such effective interactions [Hoh64, Koh65, Run84]. A very efficient and widely used scheme to deal with inhomogeneous systems, as atoms, molecules, surfaces, or in our particular case the inhomogeneity from the projectile ion $U_{ext}$, are the Kohn-Sham equations with exchange and correlations in Local-Density Approximation (LDA). For extensive reviews see [Dre90, Jon89]. We discuss it here for the fully degenerate case ($\Theta = 0$) which is the typical regime of application for the LDA. It is based on a variational formulation starting from an expression for the total energy in the form

$$E_{tot} = E_{kin} (\{ \varphi_\alpha \}) + E_{Coul} (n(r)) + E_{xc} (n(r)) + \int d^3 r \ n(r) \ U_{ext}(r) \ (2.90)$$

and referring to the local electron density

$$n(r) = \sum_\alpha |\varphi_\alpha(r)|^2 \ . \ (2.91)$$

Note the dependencies: the Coulomb energy depends naturally on the local density, the exchange-correlation energy is approximated by a local density form, and the full dependence on the single electron wavefunction $\varphi_\alpha$ is carried through for the kinetic energy which serves to maintain the quantum shell structure. The Kohn-Sham equations are obtained by variation with respect to the $\varphi_\alpha^*$ which yields

$$\left( \frac{\hat{p}^2}{2m} + U_{Coul}(r) + U_{xc}(r) + U_{ext}(r) \right) \varphi_\alpha = \epsilon_\alpha \varphi_\alpha, \quad (2.92)$$

$$U_{xc}(r) = \frac{\delta E_{xc} (n(r))}{\delta n(r)}, \quad (2.93)$$

where $\delta/\delta n(r)$ is the functional derivative. This is a nonlinear equation because the potentials depend themselves on the wavefunctions through the density (2.91). In that respect, the Kohn-Sham equations are similar to the Hartree-Fock equations, but simpler because only local potentials occur. The existence of a local-density representation is guaranteed by the Hohenberg-Kohn [Hoh64] and Kohn-Sham theorem [Koh65]. The actual form of the exchange-correlation functional $E_{xc}$, however, can only be deduced in an approximate way. Most popular is the LDA whose construction is conceptually very simple and can be summarized as

$$E_{xc} (n(r)) = \int d^3 r \ n(r) \epsilon_{xc} (n(r)) , \quad \epsilon_{xc}(n) = \frac{E_{xc}(n)}{N} \ . \ (2.94)$$

In practice, one computes the energy $E_{xc}/N$ of a homogeneous electron cloud at various fixed densities $n$, and transfers the result point by point independently to the actual local density $n(r)$. Key quantity is thus the exchange-correlation energy $\epsilon_{xc}(n)$ to be obtained from a careful calculation of correlated electron matter. This has been done by using various methods of increasingly elaborated refinement of its correlational content [Bar72, Gun76, Cep80, Vos80], and constitute the Kohn-Sham equations with exchange-correlation functionals in LDA a versatile and robust approach to mean-field calculations of inhomogeneous electron systems.
The success of this Kohn-Sham scheme in static applications suggests a naive extension to dynamic situations by using the time-dependent analogue of equation (2.92). This yields the time-dependent LDA (TDLDA) with the basic equation

\[
\hat{p}^2/2m + U_{\text{Coul}}(\mathbf{r}, t) + U_{\text{xc}}(\mathbf{r}, t) + U_{\text{ext}}(\mathbf{r}, t) \phi_\alpha = i\hbar \partial_t \phi_\alpha
\]  

(2.95)

where the exchange-correlation potential \( U_{\text{xc}} \) is again defined as in equation (2.93). TDLDA has been successfully applied, e.g., to compute the plasmon response of metal clusters [Bra93, Eka84] and applications are still showing up, nowadays even in the highly excited regime [Cal97].

The TDLDA, consisting of the dynamic Kohn-Sham equation (2.95) and the instantaneous exchange-correlation potential (2.93), is not only local in coordinate space but also local in time since \( U_{\text{xc}} \) refers to the density \( n(\mathbf{r}, t) \) at the same instant in time as the wavefunctions \( \phi_\alpha \). That may be very well justified for slow processes. But there may arise situations where the time scale of the mean-field motion interferes with times for the correlation processes contained in \( U_{\text{xc}} \). An appropriate definition of \( U_{\text{xc}} \) should include retardation effects and has then to recur to the density \( n(\mathbf{r}', t') \) at past times \( t' \leq t \) and possibly other places \( \mathbf{r}' \neq \mathbf{r} \). Such generalized concepts for a dynamic exchange-correlation potential have been much discussed over the past decades. The essence is that one can extend the \( U_{\text{xc}} \) to become nonlocal in space and time, that is, \( U_{\text{xc}} = U_{\text{xc}}(\{n(\mathbf{r}', t'), t' \leq t\}) \). The construction of such generalized potentials is, however, very intricate because there are further, dynamic boundary conditions to be obeyed as, for example, the causality requirement \( t' < t \). This inhibits a variational formulation in terms of an energy-density functional \( E_{\text{xc}} \) and subsequent functional derivatives. Modeling has thus to take place at the level of \( U_{\text{xc}} \) and a consistent definition of energy or related quantities needs to be constructed separately. Here, considerable progress has been made in recent years. For a detailed discussion of this wide and involved topic, we refer the reader to the review articles [Gro90, Gro94, Gro96]. We remark in this context that a truly dynamic Kohn-Sham scheme is closely related to the technique of local field corrections (LFC) discussed in Sec. 2.2.1.3. Expressing the linearized dynamic Kohn-Sham equations in terms of the response function \( \chi \) establishes a connection between the exchange-correlation potential \( U_{\text{xc}}(\mathbf{r}, t) \) and the local field correction \( G(\mathbf{k}, \omega) \) as outlined in [Zwi99]. Hence the experience in designing LFC may help to construct \( U_{\text{xc}} \), and vice versa. This is what actually takes place in the present development of density functional theory [Pet96].

LDA and TDLDA calculations have been successfully applied to the impurity problem of an additional charge in highly degenerate \( \Theta \ll 1 \) electron targets. Particularly simple is the static case with the ionic charge at rest for which e.g. LDA calculations for the nonlinear screening of a proton were performed [Alm76]. The computation of the stopping power on moving ions in these schemes typically employs the general results (2.60), or (2.59) respectively, obtained in the binary collision picture and expressed in terms of the transport cross section \( \sigma_{tr} \) and a shifted electron (Fermi) distribution [Boe89, Scho88]. For \( \Theta = 0 \) and \( v \ll v_F \) the friction coefficient has been calculated using Eq. (2.62) for positively charged ions and antiprotons, see e.g. [Ech86, Nag89], and an application for the stopping power of an antiproton in the low velocity regime \( v < v_F \) is found in the paper [Zar95]. The transport cross section is evaluated with a selfconsistent potential built around the ion due to the screening by the electronic scattering states. The electronic exchange-correlation effects in these selfconsistent calculations are computed in LDA. The calculations used the relation (2.60) which is restricted to spherical scattering potentials and works well in the regime \( v \leq v_F \) where deformations
<table>
<thead>
<tr>
<th>ion–target coupling</th>
<th>target conditions</th>
<th>ideal</th>
<th>nonideal</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>$\xi \ll 1$</td>
<td>$\xi \gtrsim 1$</td>
</tr>
<tr>
<td>$\langle \eta_p \rangle \ll 1$</td>
<td>linear response description, any $\Theta$, $\langle \eta_e \rangle$</td>
<td>$\varepsilon(k,\omega)$ from RPA</td>
<td>$\varepsilon(k,\omega)$ from RPA &amp; LFC</td>
</tr>
<tr>
<td></td>
<td>effective $\frac{d\sigma}{d\Omega}$ with screening</td>
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<td></td>
<td>from $\varepsilon(k,\omega)$</td>
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<tr>
<td>$\langle b_0 \rangle / \lambda \ll 1$</td>
<td>combined expression $(dE/ds)_{\text{com}}$</td>
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<td></td>
<td>binary collisions</td>
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<tr>
<td>$\langle \eta_p \rangle \gtrsim 1$</td>
<td>Vlasov for $\Theta \gg 1$, $\langle \eta_e \rangle \gg 1$</td>
<td>effective $\frac{d\sigma}{d\Omega}$ from LDA</td>
<td>MD for $\Theta \gg 1$, $\langle \eta_e \rangle &gt; 1$</td>
</tr>
<tr>
<td>nonlinear</td>
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<td></td>
<td>TDLDA for $\Theta \ll 1$, any $\langle \eta_e \rangle$</td>
</tr>
<tr>
<td>$\langle b_0 \rangle / \lambda \gtrsim 1$</td>
<td></td>
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</tbody>
</table>

Table 2.1: Summary of the methods sorted according to the appropriate regime of application.

remain small. This encourages future work without restriction to spherical potentials, using e.g. expression (2.59) for general potentials instead of Eq. (2.60). Provided that the required exchange–correlation potentials are available the presented density functional methods can be applied as well to further target regimes. In any case, however, one has to bear in mind that the accessible parameter regime is mainly limited by the required spatial resolution. As soon as the length scales introduced by the wave nature of the electrons, i.e. $\lambda_r$, and the target response, i.e. the screening length $\lambda$, start to differ substantial, a numerical solution of the Kohn-Sham equation, Eq. (2.92) or (2.95) becomes prohibitively expensive and thus imposes a restriction to target regimes with $\lambda \approx \lambda_r$ as met for $\Theta \ll 1$ and $\xi \gtrsim 1$, see Eq. (2.18).

2.4 Overview on the various methods

Table 2.1 summarizes the presentation of methods in keywords sorted in tabular form, which is, hopefully, self-explanatory. Nonetheless, a few more remarks are in order. There are basically two opposite approaches to the problem: On the one hand, the continuum approach formulated in terms of the dielectric function $\varepsilon(k,\omega)$, and on the other hand, the particle as-
pects pronounced in the binary collision description. These both classes provide complementary points of view. While the collisional approaches provide correction terms for the linear response approach, the linear response formulation gives the appropriate screening for computing the effective cross sections. The more elaborate the treatment, the more does it contain from both aspects. And the most complete theories, as e.g. MD-simulations, finally contain each side with equal weight.

Before closing this section, we ought to mention that there exist a few more approaches which we have not reviewed here. For linear coupling and ideal or moderately nonideal plasmas a Fokker–Planck equation can be used as starting point [Li93]. A more general approach is provided by (quantum) kinetic theory [Kra88, Str92, Ger96] which allows successive improvement by incorporating various levels of approximations for the used collision integrals. The usually employed Lenard–Balescu or Boltzmann collision integrals are designed to describe stopping at linear and semilinear coupling in ideal targets. Non–Markovian extensions include higher correlations which provide access to nonideal targets. Also hydrodynamic descriptions have been used to determine the energy loss [Cra95]. Their validity is a question of time–scales rather than coupling strengths: a hydrodynamic approach is suitable whenever the relaxation times are fast enough such that the ion–target system is in local equilibrium. We already briefly mentioned the wave–packet molecular dynamics (WPMD) simulation which aims to extend the classical MD-simulations towards the quantum regimes. Here we refer the reader again to Ref. [Zwi99]. Therein also one more promising concept of expressing the stopping power at low velocities in terms of a force–force correlation function [Duf95a, Duf95b] is outlined. It offers an access to nonlinear stopping by means of a (simpler) equilibrium descriptions of the ion–target system.

Furthermore, this presentation, the various definitions and the classification of parameter regimes is biased on one–component plasmas. The theories for target plasmas with two or more components are complicated by new conditions and regimes and are beyond the scope of this paper.
Chapter 3

Nonlinear stopping in classical electrons

In this section we discuss the semilinear and nonlinear stopping power in classical systems as obtained by test-particle simulations of the Vlasov-Poisson equation (Sec. 2.3.1) and MD-simulations (Sec. 2.3.2) and the comparison of these results with the analytical approaches described in Sec. 2.2. The basic scenario throughout this section is a completely classical system with classical ion–electron collisions $\langle \eta_p \rangle \gg 1$, see Eq. (2.17), nondegenerate targets $\Theta \gg 1$, see Eq. (2.11), and classical electron–electron collisions, $\langle \eta_e \rangle \gg 1$, see Eq. (2.12). The singularity of the Coulomb potential will not be removed by quantum effects and the projectile represents always a strong perturbation on the electrons for sufficiently small distances. According to the classification scheme for the ion–target coupling, Section 2.1.2, the regime of linear coupling is essentially related to quantum effects and does not exist for a classical ion–target system. There we can deal only with semilinear and nonlinear coupling and the weak coupling limit for a classical system is the semilinear regime. Any features of nonlinear ion stopping have to be compared with the behavior of stopping at semilinear coupling as reference point. Here the decisive parameter is the demarcation between semilinear and nonlinear coupling in classical targets, as defined in Eq. (2.24),

$$\frac{\langle b_0 \rangle}{\lambda} = \frac{\sqrt{3} |Z| \Gamma^{3/2}}{(1 + (v/v_{th})^2)^{3/2}} = \frac{|Z|}{3N_D} \frac{1}{(1 + (v/v_{th})^2)^{3/2}}. \quad (3.1)$$

Classical weak coupling, i.e. the semilinear coupling regime, is given for $\langle b_0 \rangle/\lambda \ll 1$, and strong coupling, of course, in the opposite case. As we have already seen from the appropriate scaled equations of motion in Secs. 2.3.1 and 2.3.2 the dynamics of entirely classical ion-target systems is completely characterized by $\Gamma$ and $Z$, which is a consequence of the absence of a length scale in the Coulomb interaction.

3.1 Scaling and redefinitions

Before proceeding, we first specialize several important relations to the classical case in order to define properly the key quantities for the subsequent discussions. The stopping power for the classical weak coupling regime is to be derived from the approximations for the semilinear regime like the linear response with cutoff (Sec. 2.2.1.5) and the combined schemes of Sec. 2.2.3.
For the classical ion-target system at issue we employ again the characteristic units of Eq. (2.86) for time, velocity, length and energy, i.e. \( t_s = \omega_D^{-1}, u_s = v_{th}, r_s = \lambda_D = v_{th}/\omega_p \) and \( E_s = k_BT \).

Using this scaling parameters, we rewrite the linear response stopping result with cutoff, Eq. (2.50), in the dimensionless form

\[
\left( \frac{dE}{ds} \right)_{\text{lr}}^{\text{km}} \frac{\Gamma^{3/2} \lambda_D}{\sqrt{3} k_BT} = (\Gamma \Gamma^{3/2})^2 \frac{\lambda_D^2}{2\pi^2} \int_{k<k_m} d^3k k \cdot \hat{v} \text{ Im} \left[ \frac{1}{\varepsilon_R(k, \mathbf{k} \cdot \mathbf{v})} \right], \tag{3.2}
\]

where the RPA dielectric function \( \varepsilon_R \) (2.38) and the cutoff \( k_m \) (2.52) are replaced by their classical limits \( \varepsilon_{cl} \) (2.84) and

\[
k_m = \frac{2}{\gamma(b_0)} = \frac{1}{\lambda_D} \frac{2}{\gamma \sqrt{3} |Z| \Gamma^{3/2}} \left( 1 + \frac{v^2}{v_{th}^2} \right), \tag{3.3}
\]

respectively. The dimensionless stopping power (3.2) depends only on the quantities \( |Z| \Gamma^{3/2} \) and \( v/v_{th} \) and neither on \( Z \) and \( \Gamma \) separately nor on the sign of the ion charge.

By applying the same characteristic units, the scaled binary collision stopping power for spherically symmetric potentials, Eq. (2.60), reads

\[
\left( \frac{dE}{ds} \right)_{\text{bc}}^{\text{km}} \frac{\Gamma^{3/2} \lambda_D}{\sqrt{3} k_BT} = \int d^3v_i \frac{(v_i + v)^2}{2v_{th}^2} \exp \left( -\frac{(v_i + v)^2}{2v_{th}^2} \right) \frac{v_i \cdot \mathbf{v}_i}{v_{th}} \sigma_{tr}(v_i) \left( \frac{v}{v_{th}} \right)^2, \tag{3.4}
\]

Throughout the following discussion, we employ the classical limit of the transport cross section Eq. (2.72) together with Eq. (2.73) for the shielded Coulomb interaction (2.67) which reads in terms of the classical scaling parameters

\[
V_{cl}(r) = -k_BT \frac{\sqrt{3} Z \Gamma^{3/2}}{r/\lambda_D} \exp \left( -\frac{r}{\lambda_D} \right) \leftrightarrow V_{cl}(k) = -4\pi k_BT \lambda_D \frac{\sqrt{3} Z \Gamma^{3/2}}{k^2 + 1/\lambda_D^2}, \tag{3.5}
\]

As already discussed in detail in Sec. 2.2.2.2 the classical transport cross section \( \sigma_{tr}/4\pi \lambda^2 \) for interaction (3.5) is a function of \( b_0/\lambda \) and the sign of the charge. Thus the resulting scaled stopping power (3.4) is in the present scaling a function of \( v/v_{th}, \lambda/\lambda_D \) and \( Z \Gamma^{3/2} \), including here the sign of \( Z \).

In the high velocity limit \( (v \gg v_{th}) \) both stopping powers reduce to the compact expressions

\[
\left( \frac{dE}{ds} \right)_{\text{lr}}^{\text{km}} \frac{\Gamma^{3/2} \lambda_D}{\sqrt{3} k_BT} \sim - (\Gamma \Gamma^{3/2})^2 \frac{\lambda_D^2}{2\pi^2} \left( \frac{v_{th}}{v} \right)^2 \ln \left[ \frac{2}{\gamma \sqrt{3} |Z| \Gamma^{3/2}} \left( \frac{v}{v_{th}} \right)^3 \right], \tag{3.6}
\]

\[
\left( \frac{dE}{ds} \right)_{\text{bc}}^{\text{km}} \frac{\Gamma^{3/2} \lambda_D}{\sqrt{3} k_BT} \sim - \left( \frac{v}{v_{th}} \right)^2 \frac{\sigma_{tr}(v)}{12\pi \lambda_D^2}, \tag{3.7}
\]

which represent Eqs. (2.55) and (2.63), respectively, rewritten in terms of the dimensionless system parameters \( \Gamma, Z, \) and \( v/v_{th} \). We remind here the high velocity limit of the cross section \( \sigma_{tr}(v) \sim v^{-4} \).

In the limit of low velocities the stopping power becomes \( \propto v \) and can thus be parameterized in terms of a dimensionless friction coefficient \( R(Z, \Gamma) \) as

\[
\frac{dE}{ds} \frac{\Gamma^{3/2} \lambda_D}{\sqrt{3} k_BT} = - \left( \frac{v}{v_{th}} \right) R(Z, \Gamma), \quad v \ll v_{th}. \tag{3.8}
\]
The friction coefficient $R$ deduced from the classical linear response stopping power with cutoff (3.2) is, of course, again only a function of $|Z| \Gamma^{3/2}$ and takes the form $[\text{Ahk75, Pet91, Zwi94b}]

\[ R_{\text{bc}}^{|Z| \Gamma^{3/2}} = \frac{(Z \Gamma^{3/2})^2}{3\sqrt{2\pi}} \left[ \ln(k_m^2 \lambda_D^2 + 1) - \frac{k_m^2 \lambda_D^2}{k_m^2 \lambda_D^2 + 1} \right] \]

which replaces here the general friction coefficient $\tilde{C}(\xi, \Theta, |Z|)$ of Eq. (2.53) which carries the full dependencies for arbitrary target conditions. In the last step we employed $k_m \gg 1$ which is justified for low velocities and in the semilinear coupling regime, where $|Z| \Gamma^{3/2} \ll 1$. In case of the binary collision stopping power (3.4) the friction coefficient is

\[ R_{\text{bc}}(Z \Gamma^{3/2}) = \frac{4\pi}{3} \int_0^\infty \frac{dv_e v_e^5}{(2\pi)^{3/2} v_{\text{th}}^6} \exp \left( -\frac{v_e^2}{2v_{\text{th}}^2} \right) \frac{\sigma_{\text{tr}}(v_e)}{12\pi^2 \lambda_D^2}, \]

and represents together with definition (3.8) the scaled version of the general result (2.62).

To establish next the classical limit of the combined expression $(dE/ds)_{\text{com}}$, Eq. (2.74), some additional considerations are necessary. There, the statically screened interaction to be used in $(dE/ds)_{\text{bc}}$ and $(dE/ds)_0^{|Z| \Gamma^{3/2}}$ is given either by Eq. (2.78) or Eq. (2.79) and hence by interaction (3.5) where $\lambda$ is substituted by $\lambda_D$ or the velocity dependent $\lambda(v)$ defined via Eq. (2.80), respectively. The two linear response stopping expressions $(dE/ds)_l$ and $(dE/ds)_0^{|Z| \Gamma^{3/2}}$ do not exist, however, in the classical limit where the RPA dielectric function $\varepsilon_R$ (2.38) is replaced with its classical limit $\varepsilon_{\text{cl}}$ (2.84) as already mentioned in Sec. 2.2.1.5. A way out is to calculate the difference $(dE/ds)_l - (dE/ds)_0^{|Z| \Gamma^{3/2}}$ and not each contribution separately. This cures the problems of the classical description related to its invalid predictions for high transferred momenta $k$, since the statically and dynamically screened potentials become identical for high $k$ and cancel out. The classical limit of the combined expression (2.74) hence reads

\[ \left( \frac{dE}{ds} \right)_{\text{com}} = \left\{ \left( \frac{dE}{ds} \right)_l - \left( \frac{dE}{ds} \right)_0^{|Z| \Gamma^{3/2}} \right\} + \left( \frac{dE}{ds} \right)_{\text{bc}} \]

It corresponds to the first scheme presented in Sec. 2.2.3, if $\lambda$ is equal to the Debye length $\lambda_D$ in the screened interaction (3.5). The second combined scheme relies on binary collisions only and uses instead of $\lambda = \lambda_D$ a velocity dependent screening length $\lambda = \lambda(v)$ in $\varepsilon_{\text{cl}}$ (3.5) and $(dE/ds)_{\text{bc}}$ (3.4) to approximate the dynamic polarization effects. This screening length $\lambda(v)$ is defined implicitly by the classical limit of $(dE/ds)_l - (dE/ds)_0^{|Z| \Gamma^{3/2}} = 0$, Eq. (2.80), that is,

\[ \int d^3k \frac{k \cdot \hat{v}}{k^2} \left| \varepsilon_{\text{cl}}(\hat{k}, k, \hat{v}) \right| \frac{1}{\left| \varepsilon_{\text{cl}}(\hat{k}, k, \hat{v}) \right|^2} = \int d^3k \frac{k \cdot \hat{v}}{k^2} \left| \varepsilon_{\text{cl}}(\hat{k}, k, \hat{v}) \right| \frac{1}{\left| 1 + (\lambda(k)v)^2 \right|^2}. \]

A numerical solution yields $\lambda(v/v_{\text{th}})/\lambda_D$ as shown in Fig. 3.1 together with the frequently used approximation $\lambda(v) = \lambda_D(1 + (v/v_{\text{th}})^2)^{1/2}$ which fairly reasonably gives the right general behavior for purposes of discussing qualitative aspects and defining regimes. The simple approximation clearly fails, however, in reproducing the specific dependence showing up in the intermediate velocity range and underestimates the slope of the high velocity asymptotic $\lambda(v) \sim \exp(1/2)(v/v_{\text{th}})$ resulting from Eq. (3.12).
3.2 Comparison of simulations and theoretical predictions

We now discuss the results obtained from a large number of performed test–particle and MD-
simulations and compare it with the predictions of the theoretical approaches presented in
Sec. 2.2 and recent experimental results for electron cooling [Ste97, Win96, Win97, Win98, Wol94]. This will be split up in several subsequent parts. In Sec. 3.2.1 we first address the
semi- and nonlinear coupling regime in ideal targets which is the domain of the nonlinear
Vlasov-Poisson description. There, the important observation is that the stopping power in
the regime of nonlinear ion–target coupling depends on the ion charge as $Z^x$, with $x$ around
$\sim 1$. This is clearly different from the $Z^2 \ln(\text{const}/|Z|)$–behavior in the semilinear coupling
regime, see Eq. (3.9), but in good agreement with experimental results on electron cooling as
shown in 3.2.2. The reduced growth of $dE/ds$ with $Z$ in the nonlinear regime is connected
with a charge dependence of the screening length, which will be subject of Sec. 3.2.3. The last
part, Sec. 3.2.4, will then be dedicated to the influence of a target nonideality on nonlinear
stopping. Here the comparison of test-particle simulations with full MD-simulations exhibits
an additional reduction of the stopping power in the nonlinear regime due to electron-electron
correlations.

3.2.1 Nonlinear ion-electron coupling

Figs. 3.2-3.4 show the stopping power $dE/ds$ as function of the ion velocity $v$. The stopping
power $dE/ds$ is normalized by division through $(ZT^{3/2})^2$ and scaled in units of $3^{1/2}k_BT/\Gamma^{3/2}\lambda_D$
as suggested by the linear response expression Eq. (3.2). The ion velocity $v$ is scaled in units
of the thermal velocity $v_{th} = (k_BT/m)^{1/2}$. For graphic reasons and as reference for the forthcoming discussion we start with a comparison of the different theoretical expressions for the
stopping power in the semilinear regime. The dashed curves in Fig. 3.2 represent the combined expression $(dE/ds)_{\text{com}}$ (3.11) for a statically screened interaction (3.5) with $\lambda = \lambda_D$, while the dotted curves show the linear response stopping power (3.2) with cutoff (3.3). The solid curves are the results from the binary collision expression (3.4) with the velocity dependent screening length $\lambda(v)$ provided from Eq. (3.12) or, equivalent, $(dE/ds)_{\text{com}}$ (3.11) with
\[(dE/ds)^0 - (dE/ds)^0_{lr} = 0.\] In all cases a positively charged ion is considered. For the lowest displayed coupling strength \(Z\Gamma^{3/2} = 0.11\) we are within the semilinear regime for all velocities and both combined expressions (dashed and solid) are almost identical except of a small deviation around the maximum of the stopping power. This deviation vanishes quickly for still smaller coupling. With respect to these approaches the linear response result with cutoff (dotted) exhibits higher stopping powers at medium velocities, a bit lower ones at low velocities.

Figure 3.2: Normalized stopping power \(dE/ds/(Z\Gamma^{3/2})^2\) in units of \(3^{1/2}k_B T / \Gamma^{3/2}\lambda_D\) as function of the ion velocity \(v\) in units of the thermal velocity \(v_{th} = (k_B T/m)^{1/2}\) for a positively charged ion at various \(Z\Gamma^{3/2}\). The dashed curves represent the combined expression (3.11) for the screened interaction (3.5) with \(\lambda = \lambda_D\). The dotted curves are the linear response stopping power (3.2) with cutoff (3.3) and the solid curves exhibit the second combined expression where the velocity dependent screening length \(\lambda(v)\) from Eq.(3.12) is used for the screened interaction (3.5).
and agrees for high velocities. This is simply a consequence of the approximative derivation of the cutoff \(k_m\), see Section 2.2.1.5, which is best substantiated for large \(k_m\), that is, for high projectile velocities and/or for decreasing coupling parameter. In fact, the difference further diminishes for still smaller \(|Z|^{3/2}\). For increasing coupling strength, increasing deviations develop between the three descriptions. At \(ZT^{3/2} = 0.36\) we are at the fringe to the nonlinear regime at low ion velocities, while for the highest shown coupling strength \(ZT^{3/2} = 11.2\) nonlinear coupling is expected for \(v \leq 2.5v_{th}\) if we assume \((b_0)/\lambda = 3^{1/2}|Z|^{3/2}/(1+v^2/v_{th}^2)^{3/2} = 1\) as the division line between semilinear and nonlinear coupling. At medium velocities the combined expression with \(\lambda = \lambda_D\) (dashed) stays always above the binary collision approach with the velocity dependent screening \(\lambda = \lambda(v)\) (solid) with an increasing deviation for growing \(ZT^{3/2}\). Both descriptions agree in all cases at low and sufficiently high velocities. At sufficiently high velocities they also meet the linear response description with cutoff (dotted curves), which, however, considerably deviates at low velocities and for increasing coupling where it exhibits a drastically smaller stopping power. Its apparent cubic behavior at low velocities for \(ZT^{3/2} = 2\) and 11.2 is deceiving insofar as there exists a non–vanishing linear term, however very small. This can be easily read off from the friction coefficient Eq. (3.9), which decreases \(R \propto k_m^{1/2}\) for small \(k_m\) (3.3). We remind however, that the assumption of large \(k_m\) was essential for establishing the correction of the linear response stopping power by cutoffs, see Section 2.2.1.5. Agreement with the other approaches could be achieved of course by treating \(k_m\) in Eq. (3.2) as a free, velocity dependent fit function.

The filled circles in Fig. 3.3 show the stopping power \(dE/ds\) as function of the ion velocity \(v\) obtained from test-particle simulations of Vlasov-Poisson for coupling strengths \(ZT^{3/2} = 0.11, 0.23, 1.1\) and 4.6. The dotted curves are simple fits to the simulation results added in order to guide the eye. The errorbars are related to an ensemble averaging over different microscopic initial configurations. They represent already as an conservative estimate the standard deviations and not the smaller mean error of the mean. The simulation runs have typically been done with \(N_T = 175000\) test-particles where each physical target electron has been split into \(N_T/N = 350\) test-particles, see Sec. 2.3.1. The density and mean field have usually been handled on a \(32\times32\times32\) grid in coordinate space. All these numbers have been varied to check the stability of the results. The simulation results are compared to the two combined expressions (3.11) with either \(\lambda = \lambda_D\) (dashed curves) or \(\lambda = \lambda(v)\) from Eq. (3.12) (solid curves) in the screened interaction (3.5). We first concentrate on the low and medium velocity regime up to \(v/v_{th} = 3 \ldots 4\). For the lowest coupling strength \(ZT^{3/2} = 0.11\) both theoretical descriptions agree very well with the Vlasov results within the errors. For increasing \(ZT^{3/2} = 0.23\) the combined expression with velocity dependent screening length \(\lambda(v)\) (solid) again reproduces well the simulation results while the combined expression with fixed screening length \(\lambda = \lambda_D\) provides a bit higher values around the stopping power maximum. This trend proceeds for increasing coupling. At \(ZT^{3/2} = 1.1\) the combined scheme with \(\lambda = \lambda(v)\) still excellently fits the simulation data while using \(\lambda = \lambda_D\) predicts around 20 % to large values at the maximum. For the even larger coupling strength \(ZT^{3/2} = 4.6\) this deviation increases to around 40 % whereas the combined expression with velocity dependent screening length again agrees quite well with the Vlasov results but shows now larger deviations than for \(ZT^{3/2} = 1.1\). For \(ZT^{3/2} > 5\) (not shown) also the combined expression with \(\lambda(v)\) increasingly fails to fit the simulation results. A comparison of Fig. 3.2 with Fig. 3.3 also reveals the pure prediction of \((dE/ds)^{k_m}_{th}\) provided by the linear response result with cutoff (3.2) for \(ZT^{3/2} > 0.1.\) We now turn to the high velocity regime and weaker coupling. In contradiction to what is expected, a significant deviation between the simulations and the theoretical predictions can be seen for
all coupling strengths. It is to be remarked, however, that the simulations (test-particle and MD) are inapplicable at high velocities when the dynamic screening length $\propto v$ exceeds the finite length $L$ of the simulation box. For the simulations at issue the actual values for the box size are $L/\lambda_D = 13, 13.6, 18, \text{ and } 20$ for $Z\Gamma^{3/2} = 0.11, 0.23, 1.1 \text{ and } 4.6$, respectively. This explains the shift of the start of these deviations towards larger $v$ for increasing coupling. To allow nevertheless some comparison at high $v$, one can imitate the finite simulation box in the theoretical predictions. To that end, the linear response stopping power is calculated for a periodically continued system and not for an infinitely extended one as done for the plotted (dashed and solid) combined expressions. Now we have a moving lattice of projectile-ions instead of a single ion. The corresponding linear response expression is discussed in the context of ion-ion correlations in Sec. 4.1.3.4 of the next chapter [Eqs. (4.4) and (4.32)]. Adding at high velocities the difference between this linear response stopping for a periodic system and

![Figure 3.3: Normalized stopping power $dE/ds/(Z\Gamma^{3/2})^2$ in units of $3^{1/2}k_B T/\Gamma^{3/2}\lambda_D$ as function of the ion velocity $v$ in units of $v_{th} = (k_B T/m)^{1/2}$ for $Z > 0$ and different $Z\Gamma^{3/2} = 0.11, 0.23, 1.1 \text{ and } 4.6$. The filled circles with errorbars are the results of Vlasov (test–particle) simulations, which have been fitted by the dotted curves. The dashed and the solid curves are respectively, as in Fig. 3.2, the predictions of the combined expression (3.11) for $\lambda = \lambda_D$ or $\lambda = \lambda(v)$ from Eq.(3.12). The long-dashed curves represent the high velocity limit of the solid curves when taking into account the finite size of the simulation box as explained in the text.](image-url)
the usual one for an infinitely extended target as a correction term to the combined expression with \( \lambda = \lambda(v) \) results in the long-dashed curves shown in Fig. 3.3. These are in a similar good agreement with the combined scheme at high velocities as found for low and medium ones. We remark that the more or less pronounced humps which could be seen in the simulation results are related to the periodicity of the simulation cube. They can be viewed as the residues of the resonant peaks discussed in Sec. 4.1.3.4 which get strongly damped with increasing coupling strength.

In Fig. 3.4 we present again test-particle simulation results of Vlasov-Poisson, now for \( |Z| \Gamma^{3/2} = 0.46 \) and different signs of the ion charge. The unrealistic case of highly charged negative ions \( (Z < 0, \text{ squares}) \) yield at low \( v \) a significantly lower stopping than the positively charged ions \( (Z > 0, \text{ filled circles}) \). This is qualitatively and quantitatively well reproduced by the combined expression with \( \lambda = \lambda(v) \) (dash-dotted and solid curves) which depends on the sign of \( Z \) via the binary collision contribution, see Fig. 2.8 in Sec. 2.2.2.2, while the pure linear response approach only depends on \( Z^2 \).

From all this together we can conclude that the combined expression, Eq. (3.11), with \( \lambda = \lambda_D \), works well up to a coupling parameter \( Z \Gamma^{3/2} \lesssim 1 \) in agreement with the definition of the semilinear coupling regime for which it was designed. For larger coupling, more precisely in the range \( Z \Gamma^{3/2} \approx 1 \ldots 5 \), the combined scheme with \( \lambda = \lambda(v) \), that is, a binary collision treatment with velocity dependent screening length, yields still a very good prediction for the stopping power. For even larger coupling all discussed approximations fail.

We now focus on stopping at low velocities, parameterized in terms of the friction coefficient \( R(Z, \Gamma) \), see Eq. (3.8), and investigate the dependence on the ion charge \( Z \), particularly in the regime of nonlinear ion–target coupling. The stars in Fig. 3.5 show the \( Z \Gamma^{3/2} \) dependence of \( R \) computed with test-particle simulations of Vlasov-Poisson for positively charged ions. The solid curve is again the combined expression (3.11). Here in the low velocity limit where \( \lambda(v) \to \lambda_D \) both schemes are equal. They fit the simulation results quite well up to around \( Z \Gamma^{3/2} \approx 5 \) in agreement with the previous observations. The remaining differences at higher coupling parameters can be mainly explained by nonlinear screening effects where the selfconsistent potential in the Vlasov calculations differs from the screened effective interaction (3.5) as
determined by the linear response. This will be discussed in Sec 3.2.3. The weak hump which appears at \( Z_\Gamma^{3/2} \approx 2 \ldots 10 \) in the combined expression, that is, in the binary collision stopping is due to electron scattering events with scattering angles larger than \( 180^\circ \) (resonant states). The dashed curve represents the prediction of the linear response description with cutoff (3.9). Starting at weak coupling \( |Z|_\Gamma^{3/2} \ll 1 \), it first follows the trend of the \( Z_\Gamma^{3/2} \) dependence for quite a while, but then it fails grossly for nonlinear coupling with \( |Z|_\Gamma^{3/2} \gtrsim 1 \). The curve bends over and finally falls off like \( (Z_\Gamma^{3/2})^{-2} \) for large \( |Z|_\Gamma^{3/2} \).

For a given plasma parameter \( \Gamma \) the dependence of \( R \) on the coupling parameter \( Z_\Gamma^{3/2} \) just reflects the dependence of the low velocity stopping power on the charge state \( Z \). It can be read off from the fit (dotted curve) through the simulation data

\[
R \approx \frac{(Z_\Gamma^{3/2})^2}{8} \left[ \ln \left( 1 + \frac{0.14}{(Z_\Gamma^{3/2})^2} \right) + \frac{1.8}{1 + 0.4(Z_\Gamma^{3/2})^{1.3}} \right], \tag{3.13}
\]

which reveals a gradually decrease of the power \( x = x(Z) \) of a local charge dependence like \( Z^x \). Starting from the expected \( R \sim Z^2 \ln(\text{const}/Z) \) behavior in the truly semilinear regime at \( Z_\Gamma^{3/2} \ll 1 \) the charge dependence changes towards the very weak \( R \sim Z^{0.7} \) reached at the highest studied \( Z_\Gamma^{3/2} \gg 1 \).

### 3.2.2 Comparison with experimental results

Experiments on the stopping of highly charged heavy ions in dense and highly ionized target plasmas are in progress [Hof88, Hof90, Die90, Die92, Gar92, Ser92, Cha93, Cou94, Jac95, Jac96, Stet97]. But the plasma densities are not yet sufficiently high to reach the regime of nonlinear projectile–target coupling. There exist, however, experimental results from measuring the cooling force for electron cooling in heavy ion storage rings. In the electron cooler the ions of the stored ion beam are merged with a cold electron beam once in each cycle. Thermal energy is transferred from the ions to the cold electron plasma. This produces colder ion beams of lower phase–space volume [Pot90]. The cooling of the ions can be related to the energy loss of an ion when moving through the electron cloud and the measured cooling force represents the stopping power averaged over the velocity distribution of the ions. The cooling
forces at low ion–electron relative velocities observed experimentally show a $Z^x$ dependence with $x$ between 1.5 and 1.7 [Ste97, Win96, Win97, Wol94], more recent experiments at the experimental storage ring (ESR) at GSI, Darmstadt, yield even smaller values $x \approx 1.3$ [Win98]. This agrees qualitatively with the presented simulation results for isotropic electron plasmas. In the electron cooler, however, the situation is more complex because one has two different electron temperatures in the transversal and the longitudinal direction and because there is a longitudinal magnetic field which guides the electron beam. The typical parameters in the electron cooler at the test storage ring (TSR) in Heidelberg are $n \approx 3 \cdot 10^6 \text{cm}^{-3}$, $k_B T_\perp \approx 0.1 \text{eV}$, $k_B T_\parallel \approx 1 \ldots 5 \cdot 10^{-4}\text{eV}$ and $Z = 1 \ldots 16$ [Wol94], where $T_\perp$ denotes the temperature transversal to the beam direction and $T_\parallel$ longitudinal with the beam. These parameters stay safely in the regime of ideal target and linear ion–target coupling for the transversal temperature whereas the longitudinal temperature yields $\Gamma_\parallel \lesssim 0.7$ and $Z \Gamma_\parallel^{3/2} \lesssim 9$. The ESR in Darmstadt has the parameters $n \approx 10^6 \text{cm}^{-3}$, $k_B T_\perp \approx 0.15 \text{eV}$, $k_B T_\parallel \approx 5 \cdot 10^{-5}\text{eV}$ and $Z = 6 \ldots 92$ [Ste97, Win96]. That is again an ideal target and the ion–target coupling is linear for the transverse temperature but $\Gamma_\perp \lesssim 0.4$ and $Z \Gamma_\parallel^{3/2} \lesssim 23$ for the longitudinal degree of freedom. The longitudinal conditions in both devices corresponds to a target close to the nonideal regime and to nonlinear coupling. In addition there comes the longitudinal magnetic field. This hinders the transversal motion of the electrons and thus freezes the hot transverse electronic degrees of freedom. There should remain an effective temperature for the ion–electron interaction which stays close to the longitudinal temperature. In Fig 3.6, we compare the measured friction coefficients (symbols) with the test-particle simulations [dotted curve, according to Eq. (3.13)] of an isotropic plasma by interpreting the experiments in terms of an effective temperature. An effective temperature of $T = 7.1 T_\parallel$ (open squares) had been used to adjust the data from [Win96] and of $T = 3.1 T_\parallel$ (filled circles) for comparison with [Wol94]. The experimental trends are well reproduced which provides an experimental confirmation for the typical $Z$-dependence as seen in the simulations.
3.2.3 Nonlinear screening

We discussed in the previous Secs. 3.2.1 and 3.2.2 the \(Z\)-scaling of the stopping power and found a trend \(Z^2 \ln(\text{const}/Z) \rightarrow Z^{0.7}\). This trend is partially related to the development of screening with \(Z\) of a highly charged, slow ion. We have investigated that in detail in specific simulations. The Coulomb interaction between an ion at rest \((v=0)\) and the electrons was switched on at time \(t = 0\) and the ion subsequently attracts electrons. The electron density about the ion grows and reaches an almost stationary state on a time scale of \(\omega_p^{-1}\). The screening function \(\Upsilon(r)\) is then extracted as the total electric potential about the ion divided by the bare ion potential. The linear response theory yields \(\Upsilon(r) = \exp(-r/\lambda_D)\) (Debye–Hückel). The screening function deduced from Vlasov and MD simulations for nonlinear coupling is also close to an exponential function \(\Upsilon = \exp(-r/\lambda)\) but with a much different screening length \(\lambda = \lambda(Z, \Gamma) > \lambda_D\). This suggests that the corresponding effective ion–electron interaction is well approximated by the potential (3.5) when \(\lambda\) is replaced by \(\lambda(Z)\). The results for the observed screening length are shown in the left part of Fig. 3.7. The rather large errorbars reflect here not only the different initial states but mainly the imperfectness of matching the potential as obtained from the simulations to the simple exponential form \(\exp(-r/\lambda)/r\). One sees that the screening length increases with the coupling strength, particularly for \(Z\Gamma^{3/2} > 10\).
This trend of the static screening is in good agreement with the trend of the friction coefficient. Remind Fig. 3.5 where the friction coefficients at strong coupling $Z\Gamma^{3/2} \gg 1$ lie well above the results from the combined scheme (solid curve) where an interaction (3.5) with the linear response screening $\Upsilon(r) = \exp(-r/\lambda_D)$ was used. To be more quantitatively, a rough estimate for $\lambda(Z\Gamma^{3/2})$ reproducing the test-particle simulation results yields a behavior $\lambda(Z\Gamma^{3/2}) = \lambda_D(1 + 0.09(Z\Gamma^{3/2})^{0.7})$ as plotted in Fig. 3.7 (dotted curve in the left part). Taking this screening length as an input for the ion–electron interaction (3.5) in the combined expression Eq. (3.11) or, equivalently, in the binary collision approximation Eq. (3.10) results in the dash-dotted curve in the right part of Fig. 3.7 which agrees fairly well with the simulation results (stars). The enhanced friction is here clearly related to the enhanced screening length.

The observed nonlinear screening is also accompanied by a behavior of the electron density near the ion which differs from the linear response (Debye–Hückel) prediction for the density enhancement over the uniform density of the homogeneous system in absence of the ion. These deviations from the linear response result are in particular connected with an increasing number of trapped electrons for increasing coupling strength and nonideality of the target. This can be concluded from the negative energies of these electrons in the field of the ion and the surrounding electrons as observed in a number of MD-simulation studies on the local electron density around an ion [Zwi96b, Zwi97b, Zwi97c, Spr98, Spr99b]. Because such processes are quite sensitive to the collisions and correlations between the electrons they are correctly treated only in the MD–simulations whereas Vlasov simulations are insufficient in this case. The electron trapping is also of interest with respect to electron–ion recombination. There the actual electron density near the ion and the population of loosely bound electron states are one crucial issue to explain the puzzling enhancement of radiative recombination rates by factors of 4...5 as observed for a large number of ions in recent experiments with highly charged ions in heavy ion storage rings [Bai95, Gao95, Schr96, Uwi96]. These experiments used the electron beam in the cooler as an electron target to study spontaneous or laser–induced radiative electron–ion recombination. For a more detailed outline concerning the electron density and the electron trapping near the ion see [Zwi99].

### 3.2.4 Nonideal targets

The effects of the nonideality of the target are revealed by comparing the results from MD with those from the Vlasov simulations, because collisions between the electrons are included in the fully correlated MD–simulation but are excluded in the mean–field description as provided by the Vlasov–Poisson equation, see Secs. 2.3.1 and 2.3.2. We note again the explicit dependence on $\Gamma$ which is present only in the MD simulations and which characterizes target correlations in addition to the $Z\Gamma^{3/2}$-dependence related to the ion-target coupling which appears in both treatments. Fig. 3.8 shows again the normalized stopping power $dE/ds/(Z\Gamma^{3/2})^2$ in units of $3^{3/2}k_BT/\Gamma^{3/2}\lambda_D$ as a function of the ion velocity $v$ in units of $v_{th} = (k_BT/m)^{1/2}$. The filled circles are from test-particle simulations of Vlasov-Poisson for the coupling strengths $Z\Gamma^{3/2} = 0.11, 0.36, 2$ and 11.2. The open squares represent the results from MD-simulations with the same coupling strengths $Z\Gamma^{3/2}$ corresponding here to a fixed ion charge state $Z = 10$ and plasma parameters $\Gamma = 0.05, 0.11, 0.34$ and 1.08 of the electron target, respectively. The errorbars are again related to an ensemble averaging over different microscopic initial configurations and represent as a conservative estimate the standard deviations and not the (smaller) mean error of the mean. The MD-simulations exhibit quite large errors compared to the test-particle simulation, see Figs. 3.3 and 3.4. The large number of test-particles, which are
used to represent a smooth charge density, considerably reduces the fluctuations. The errorbars are here of the order of the size of the symbols and suppressed for graphical clearness. To guide the eye, the simulation results are fitted by the dotted and the dashed curves in each case. Typical MD simulations are carried out with $N = 500$ electrons on small work stations. The influence of the particle number $N$ on the results was checked by the occasional use of $N = 250$ and $N = 5000$ electrons. The test-particle simulations are done with the same $N_T = 175000$ and ratio $N_T/N = 350$ as for the previously discussed situations but with different lengths $L$ of the simulation cube. For the comparison with the MD-results the length has been adapted in the test-particle simulations to the same values as given in the MD-scheme for $N = 500$ and the desired $\Gamma$ via the relation $L/\lambda_D = (4\pi N/3)^{1/3}(3\Gamma)^{1/2}$. For the actual parameters we thus have $L/\lambda_D = 5, 7.3, 13,$ and $23$ for $\Gamma = 0.05, 0.11, 0.34$ and $1.08$, respectively. Since the same box size is used here in both simulation schemes the insufficient treatment of the

![Diagram](image1)

**Figure 3.8:** Normalized stopping power $dE/ds/(Z\Gamma^{3/2})^2$ in units of $3^{1/2}k_B T/T^{3/2}\lambda_D$ as function of the ion velocity $v$ in units of $v_{th} = (k_B T/m)^{1/2}$ for $Z\Gamma^{3/2} = 0.11, 0.36, 2$ and $11.2$, corresponding here to a fixed ion charge state $Z = 10$ and plasma parameters $\Gamma = 0.05, 0.11, 0.34$ and $1.08$, respectively. The open squares with errorbars are results of MD–simulations, the filled circles of Vlasov (test–particle) simulations. The errorbars for the Vlasov results are of similar size as the symbols and are suppressed for reasons of clearness. The fits to the simulation results (dotted and dashed curves) are introduced to guide the eye.
stopping power at high velocities due to the finite size of the simulation volume is unimportant for the comparison and the subsequent discussion of the effect of the nonideality of the target. For the smallest plasma parameter $\Gamma = 0.05$ and coupling strength $Z\Gamma^{3/2} = 0.11$ shown in Fig. 3.8, no difference between the Vlasov simulations and the fully correlated MD-simulations can be detected within the errors. At the next higher $\Gamma = 0.11$ ($Z\Gamma^{3/2} = 0.36$) some deviations start to appear at low velocities and around the stopping power maximum. With increasing nonideality of the target $\Gamma = 0.34$ ($Z\Gamma^{3/2} = 2$), and $\Gamma = 1.08$ ($Z\Gamma^{3/2} = 11.2$) this trend proceeds and a more and more pronounced difference develops at low velocities up to the velocity where the stopping is maximal. This clearly documents an influence of the nonideality of the target plasma, which tends to reduce the nonlinear stopping power at low and medium velocities. The high velocity stopping remains unaffected. This influence of the nonideality of the plasma has been investigated for a variety of simulation runs at various $Z$ and $\Gamma$. They allow to conclude that nonideal effects start to appear at $\Gamma \gtrsim 0.1$. Furthermore, all these simulations show the appropriate linear increase of the stopping power with $v$ at low velocities almost up to the maximum of $dE/ds$ at a $v_m \gtrsim v_{th}$, where $v_m$ shifts towards higher velocities with increasing coupling $|Z|\Gamma^{3/2}$. In view of this long linear increase it is to be noted that the low velocity stopping power $dE/ds \propto R(Z, \Gamma) v$ obtained for a one–component electron target provides already the stopping power in a (fully ionized) two component plasma for $v_{th}^{\text{ions}} < v \lesssim v_{th} \ldots 3 \times v_{th}$. Here $v_{th}^{\text{ions}}$ is the thermal velocity of the target ions with $v_{th}^{\text{ions}} \ll v_{th}$ due to the high ion mass.

In Fig. 3.9 we turn again to the low velocity stopping in terms of the friction coefficient

![Graph showing dimensionless friction coefficient R(Z, \Gamma) as function of |Z|\Gamma^{3/2}.](image)

Figure 3.9: Dimensionless friction coefficient $R(Z, \Gamma)$ (3.8) as function of $|Z|\Gamma^{3/2}$. The symbols with errorbars are MD–simulation results for different $Z > 0$ and $\Gamma = 0.11$ (circles), 0.34 (triangles), 1.08 (diamonds), 3.41 (crosses) and for different $Z < 0$ and $\Gamma = 1.08$ (stars). The various curves show the friction coefficient $R$ of the linear response description (3.9) (dashed), of the combined expression (3.11) with $\lambda = \lambda_D$ for positively (solid) and negatively (dash-dotted) charged ions, and from the fit (3.13) to the Vlasov simulations (dotted).
The symbols with errorbars indicate the MD results for various $Z > 0$ and $\Gamma = 0.11$ (circles), $\Gamma = 0.34$ (triangles), $\Gamma = 1.08$ (diamonds), and $\Gamma = 3.41$ (crosses) and for negatively charged ions ($Z < 0$) at $\Gamma = 1.08$ (stars). The dashed curve represents again the linear response description with cutoff (3.9). The dotted curve shows the fit function (3.13) and thus the Vlasov simulation results which only depend on $Z^{3/2}$ as it does for the combined expression (3.11) with interaction (3.5) (reminding that $\lambda(v) = \lambda_D$ at low $v$) given by the solid curve for $Z > 0$ and the dash-dotted curve for $Z < 0$. The friction coefficients from the full MD-simulations ($Z > 0$) exhibit a very similar general trend of the charge dependence as compared to the mean-field treatment (dotted curve). Thus we can conclude that the weaker charge dependence $Z^x$ with $x(Z) < 2$ is mainly due to the nonlinear ion-target coupling. The additional electron–electron correlations included in the MD simulations yield, however, a different offset of the MD results for different $\Gamma$ and thus a separate dependence on $\Gamma$ and $Z$ as expected from a full many–body dynamics. In particular, their $Z$–dependence fits for targets with $\Gamma \geq 0.34$ well on a simple power law $R \propto Z^x$ with $x(Z) < 2$ is mainly due to the nonlinear ion-target coupling. The nonideality of the target starts to affect the stopping power for plasma parameters $\Gamma > 0.1$. In addition to the previously mentioned change of the detailed charge dependence the nonideality of the target generally reduces nonlinear stopping compared to ideal targets in the low and medium velocity regime up to the stopping power maximum.

(iii) These specific features of nonlinear stopping are related to a nonlinear shielding of the ion at strong ion-target coupling. The nonlinear effective screening length is larger than the Debye length and increases with increasing ion charge or coupling strength $Z^{3/2}$. A
nonideality of the target again introduces a separate dependence on \( Z \) and \( \Gamma \), the general growth of the screening length is, however, the same as for ideal targets.

(iv) The standard approximations for semilinear coupling like the linear response stopping with cutoff are applicable in the truly semilinear regime up to \( Z \Gamma^{3/2} < 0.1 \).

(v) The combined expression (3.11) which uses the static linear response effective interaction (with \( \lambda = \lambda_D \)) describes well the semilinear stopping up to the border line to the essentially nonlinear regime \( Z \Gamma^{3/2} = 1 \).

(vi) The combined expression with a velocity dependent effective interaction, \( \lambda = \lambda(v) \), as provided from linear response by Eq. (3.12) is finally applicable also in the weak nonlinear regime up to \( Z \Gamma^{3/2} \leq 5 \).

The suggested combined expression with velocity dependent effective interaction thus represent a reliable approach to calculate the stopping power of highly charged, slow ions in most cases where the coupling does not exceed \( Z \Gamma^{3/2} \approx 5 \). For even higher ion charges the nonlinear screening has to be incorporated into the velocity dependent effective interaction. This requires, however, to develop first an analytical approach which is capable to treat nonlinear screening effects and to provide the appropriate effective interaction. Such a scheme still assumes ideal targets. But strong ion-target coupling appears not only for very high charges. It usually involves both high \( Z \) and \( \Gamma \approx 1 \) or larger. Thus one has to deal with the target nonideality as well. As a straightforward extension of the combined expression to nonideal targets one can simply replace the RPA dielectric function by a dielectric function which describes the response properties of nonideal targets, see Sec. 2.2.1.3. Again Eq. (2.80) defines the corresponding effective interaction which now depends separately on \( Z \) and \( \Gamma \). The resulting stopping power has then to be compared with the MD-simulation results for nonideal targets. This procedure still relies on the binary collision description with effective interaction and ceases to be valid if the electron-electron correlations become strong compared to the ion-electron interaction. This is expected for rather strong nonidealities of the target. Then a different ansatz for a stopping theory is needed.

All the previous discussion and the drawn conclusion concerned entirely classical systems, and one has to raise the question about quantum effects. Let us therefore consider the general combined expression with velocity dependent effective interaction Eqs. (2.74) - (2.80) which does not involve any restriction to classical systems. Here we can identify mainly two effects. One is related to the effective interaction provided by the linear response description. It changes, of course, in the degenerate regime where Pauli-blocking becomes important and, for instance, the Thomas-Fermi length \( v_F / \omega_p \) replaces the Debye length \( v_{th} / \omega_p \) as the actual screening length. Once the effective interaction, i.e. \( \lambda(v) \), is given, the expected influence of quantum effects solely depends on the actual parameter domain for the binary collisions as shown in Fig. 2.6. As discussed in Sec. 2.2.2.2 this is determined by the values of \( \lambda / \lambda_e \) and \( \eta_p \), that is, by the amount of quantum diffraction effects and not further related to Pauli-blocking which does not affect the binary collisions of electrons with heavy ions as shown in Sec. 2.2.2.1. A conclusive investigation on the quantum diffraction requires a very careful analysis of the different aspects, in particular, of the influence of a change of the screening length. Thus one has to study, for instance, the transition from the classical to the quantum regime along a line of constant \( \lambda \) (or \( \kappa \)) in the diagram of Fig. 2.6. Such work has still to be done.

The major problem with applying the combined expression to the quantum regimes is, however, its a priori unknown range of validity. As for the classical systems more complete
treatments are needed to verify its predictions. At present only the density functional approaches discussed in Sec. 2.3.3 are available for applications in extremely degenerate systems and at sufficiently low projectile velocities. There remains a large gap in the target parameter plane to be covered. According to the general discussion of the target regime given in Sec. 2.1.2, this gap is mainly located in the nonideal region where an incorporation of the electron-electron correlations is essential. To bridge this gap coming from the entirely classical regime suggests to map quantum features into a classical MD-simulation, e.g. by means of effective potentials which are typically derived from the quantum mechanical density matrix of the electrons in equilibrium, see [Kel63, Deu77, Deu78, Deu81]. There all quantum effects are basically mediated through some short-range cutoff of the Coulomb interaction. Another line of development are the already mentioned WPMD-simulations where the classical electrons are replaced by gaussian wave packets where their widths are treated as dynamic variables. This incorporates quantum effects into the classical MD on a deeper level than the simple use of effective potential. Both extensions of the classical MD simulations towards the quantum regime have been applied to stopping power calculations as reported in detail in [Zwi99]. Up to now, however, the resulting stopping do not correctly merge into the known weak coupling high velocity limit. Here further investigations and improvements are necessary.
Chapter 4

Correlated ion stopping

In the previous discussion of the energy loss of a single ion two types of correlations have been of importance: the correlation or coupling between projectile and target and correlations within the target plasmas. However, in many situations like the interaction of an ion beam with a target several ions are stopped simultaneously. This naturally raises the question of a third type of correlation effect due to the mutual influence of the ions in a given ion arrangement. Interesting candidates for these correlation effects are, for instance, the ion clouds created by the very fast fragmentation and ionization of large cluster-ions when hitting the target. The question about possible stopping enhancements is important in connection with the proposed use of cluster-ion-beams for inertial confinement fusion (ICF) as outlined in the introduction, Ch. 1. Like in the case of single ion stopping, the whole slowing down process of some arrangement of ions involves the stopping power, the evolution of the charge states of the ions, and as an additional aspect the Coulomb-explosion of these clouds of ions driven by the mutual repulsion between the charges. A complete description of the stopping of these ion-clusters of course requires a simultaneous treatment of all these processes including correlation effects on both the stopping power and the charge state. First attempts on this task are reported in [Nar93, Nar95] for the energy loss of C_{60}-Clusters. As in the case of single ions we disregard here completely the charge state evolution and concentrate in Sec. 4.1 on an overview of ion-ion correlation effects with respect to the stopping power for a given ion configuration, i.e. for given relative positions and charges of the ions at some instant during the slowing down process. It will be demonstrated that the quality and quantity of the correlation effects are mainly determined by two ratios: the typical length scale of or in the ion–cluster $\lambda_c$ to the screening length of the target plasma $\lambda$ and the ratio of the ion–cluster velocity $v$ to the mean velocity $\langle v_e \rangle$ of the target electrons. Because the stopping power on the ions results from the actual electric field at their locations, the ion-ion correlation effects are directly related to the specific polarization of the target plasma by a given arrangement of projectile ions. For an overall size of the ion-cluster which is small compared to the screening length $\lambda$ all ions together create the target response. The induced field is the same as produced by a single large charge and yields an enhancement of the stopping. In the opposite case where the distances between the ions are large with respect to $\lambda$ each ion acts more or less like an isolated ion on the target. The excited wake fields may, however, interfere constructively or destructively and thereby enhance or reduce the stopping compared to the case of uncorrelated stopping. The different underlying physics results in different features of correlated stopping. This will be illustrated in Sec. 4.1.3 for some specific examples and summarized in Sec. 4.1.4. In the forthcoming discussion cor-
related stopping of ion-clusters will be entirely treated within the linear response description. For small ion-clusters with $\lambda_c \ll \lambda$ and a high total charge, however, a treatment within semilinear or nonlinear regime would be desirable. Unfortunately, the previously discussed methods to treat semilinear and nonlinear stopping, in particular the numerical simulations are up to now not advanced enough for a treatment of ion-cluster stopping in general. The crucial issue is here the additional length scale introduced through the extension of the cluster and its spatially strongly varying interaction potential. This typically exceeds the usually available computational capacity for both MD- or PIC-Simulations and LDA-treatments. There are only very few attempts for a nonperturbative investigation of correlated stopping as e.g. a LDA-approach for the rather specific case of dicluster stopping at low velocities and in fully degenerate electron targets [Nag90, Urb93]. Thus the linear response description is the only available tool at present to study the phenomena related to ion-ion correlations in a wide range of possible cluster parameters and target conditions. While the quantitative results obtained within the linear treatment certainly have to be handled with care, the predicted qualitative features and conclusion may be supposed as basically correct. This point will be resumed in the summary and outlook Sec. 4.3.1.

In a second step we address in Sec. 4.2 the importance of possible stopping enhancements for the averaged specific energy deposition of an ion–cluster. This is a main concern for a cluster-ion-beam driven inertial confinement scenario. It basically involves an integration of the actual stopping power as a function of velocity over the full range of the ion-cluster in the target. There the calculation of the corresponding stopping power requires a knowledge of the time evolution of the ion configuration which is subject to a Coulomb-explosion. A simple model to include the Coulomb-explosion of ion–clusters is presented in Sec. 4.2.1. It predicts rather small enhancements of the total energy deposition of typically a few percent in all studied cases. While a strongly enhanced correlated stopping may be present at a first stage after the entrance in the target when the clusters are smaller than the screening length, the Coulomb–explosion very rapidly enlarges the cluster to a size where the ions represent individual projectiles.

### 4.1 Basic features of correlated stopping

We study the basic phenomena and features related to correlated stopping in the framework of the dielectric linear response formalism. Similar investigations on this topic started with dicluster stopping [Bas82] and proceed to arbitrarily large $N$-cluster stopping in fully degenerate electron jellium targets [Deu92, Ari91, Vic92, Deu95]. More recently also correlation effects in partially degenerate [Bre93] and classical electron plasmas [Dav93a, Dav93b, Deu95a, Zwi96c] have been studied. A more general overview is reported in [Zwi97d]. Here we consider correlated stopping only in ideal free electron targets with a density $n$ and temperature $T$ and $\xi < 1$ (2.13). We allow, however, for any degree of degeneracy $\Theta$ to include classical plasmas as well as the electron jellium in solids in order to cover the full range of target conditions which are important for the stopping of a cluster-ion beam. Except for one explicitly mentioned example, we thus performed all presented calculations by using the RPA dielectric function (2.38).
4.1.1 Basic Equations and provisional conclusions

The linear response formulation of stopping discussed for a single ion in Sec. 2.2.1.4 can be easily extended to an ion–cluster projectile of \( N \) ions with charges \( \{ Z_i e \} \) located at \( \{ r_i \} \), which all move through the target with the same projectile velocity \( \textbf{v} \) ('frozen configuration' of relative positions). Assuming point-like ions the perturbing charge density of this projectile is

\[
\rho_p(\mathbf{r}, t) = \int d^3r' \rho_p(\mathbf{r}') \delta^3(\mathbf{r}' - (\mathbf{r} - \mathbf{v}t)) = \sum_i Z_i e \delta^3(\mathbf{r}_i - (\mathbf{r} - \mathbf{v}t)) \quad .
\] (4.1)

where \( \rho_p(\mathbf{r}) = \sum_i Z_i e \delta^3(\mathbf{r}_i - \mathbf{r}) \) is the charge density in the cluster rest frame. The total stopping power on the whole cluster, \( F_c \), is derived from the general definitions and expressions, (2.42) and (2.43), by replacing the single ion potential \( \phi_p(\mathbf{k}) = Z e/\epsilon_0 k^2 \) with the cluster potential \( \phi_p(\mathbf{k}) = \rho_p(\mathbf{k})/\epsilon_0 k^2 \) as [Bre93, Ari78]

\[
F_c = \sum_i Z_i e \mathbf{v} \cdot \mathcal{E}(\mathbf{r} = \mathbf{r}_i + \mathbf{v}t) = \frac{1}{\epsilon_0 (2\pi)^3} \int d^3k \frac{\mathbf{k} \cdot \mathbf{v}}{k^2} \text{Im} \left[ \frac{-1}{\mathcal{E}(\mathbf{k}, \mathbf{k} \cdot \mathbf{v})} \right] \rho_p(-\mathbf{k}) \rho_p(\mathbf{k}) .
\] (4.2)

For the point-like ions the structure function of the charge density has the explicit form

\[
\rho_p(-\mathbf{k}) \rho_p(\mathbf{k}) = e^2 \left[ \sum_n Z_n^2 + \sum_{n \neq m} Z_n Z_m \exp(i \mathbf{k} \cdot (\mathbf{r}_n - \mathbf{r}_m)) \right] .
\] (4.3)

The restriction to point–like ions mainly serves to focus on the basic phenomena and to simplify the related expression. Within the linear response description a generalization to extended ions with an individual charge distribution \( q_i(\mathbf{r}) \), with \( \int d^3r q_i(\mathbf{r}) = Z_i e \), and a projectile density \( \rho_p(\mathbf{r}) = \sum_i q_i(\mathbf{r}_i - \mathbf{r}) \) can be easily introduced through replacing Eq. (4.3) by \( \rho_p(\mathbf{r}, t) = \sum_i q_i(\mathbf{r}_i - (\mathbf{r} - \mathbf{v}t)) \) and \( \rho_p(-\mathbf{k}) \rho_p(\mathbf{k}) = \sum_n \sum_m \exp(i \mathbf{k} \cdot (\mathbf{r}_n - \mathbf{r}_m)) q_n(-\mathbf{k}) q_m(\mathbf{k}) \) (see e.g. [Bre93]).

For many purposes, as the determination of correlation effects on the heating of a target by a cluster-ion-beam, one is mainly interested in an averaged stopping power rather than the stopping of individual clusters, which may differ in the detailed structure, the size, the orientation, the charge states of the ions and so on. It is thus useful to introduce an ensemble-average of (4.2) over varying configurations \( \{ Z_i \}, \{ \mathbf{r}_i \} \). For simplification we further assume equal charges of the ions \( Z_i = Z \), which leads to the ensemble-averaged stopping per particle [Ari91, Vic92]

\[
\langle F_c \rangle / N = \frac{Z^2 e^2}{\epsilon_0 (2\pi)^3} \int d^3k \frac{\mathbf{k} \cdot \mathbf{v}}{k^2} \text{Im} \left[ \frac{-1}{\mathcal{E}(\mathbf{k}, \mathbf{k} \cdot \mathbf{v})} \right] S(\mathbf{k}) .
\] (4.4)

Here \( S(\mathbf{k}) = \langle \rho_p(-\mathbf{k}) \rho_p(\mathbf{k}) \rangle / N Z^2 e^2 \) is the static structure factor of the ensemble of ion-clusters which is related to the pair–distribution function \( g(\mathbf{r}_i - \mathbf{r}_j) \) of the ion–clusters through

\[
S(\mathbf{k}) = 1 + \int d^3r g(\mathbf{r}) \exp(-i \mathbf{k} \cdot \mathbf{r}) ,
\] (4.5)

and normalized as \( S(\mathbf{k} = 0) = 1 + \int d^3r g(\mathbf{r}) = N \). It should be emphasized, that the averaging procedure contained in Eq. (4.4) yields the stopping power averaged over an ensemble.
of clusters and not the stopping of an extended charge density \( \langle \rho_p(r) \rangle \) resulting from an average on the cluster densities (4.1). The stopping of an extended charge distribution \( \langle \rho_p(r) \rangle \) tends to zero for a growing extension of the charge distribution \( \langle \rho_p(r) \rangle \to 0 \), while (4.4) approaches the stopping of isolated, individual ions in the case of an increasing spread of the cluster \( g(r) \to 0, S(k) \to 1 \).

From the basic linear response expressions, (4.2) and (4.4), for the stopping of ion-clusters one may already conclude on some general features. The linearity and the connected superposition principle allow to reformulate (4.2) as a contribution of single isolated ions and a correlation part \( C \), which is entirely built up by two-ion contributions

\[
C_2(r) = \frac{e^2}{\varepsilon_0 (2\pi)^3} \int d^3k \frac{k \cdot \hat{v}}{k^2} \text{Im} \left[ \frac{-1}{\varepsilon(k, k \cdot v)} \right] \exp(i k \cdot r),
\]

(4.6)

where each \( C_2 \) already exhibits all basic features of correlated stopping. The total stopping power \( F_c \) (4.2) thus represents the sum

\[
F_c = \sum_n Z_n^2 F_1 + C = \sum_n Z_n^2 F_1 + \sum_n \sum_{m \neq n} Z_n Z_m C_2(r_n - r_m),
\]

(4.7)

where \( F_1 = C_2(0) \) is the stopping power on a single ion with charge state \( Z = 1 \), see Eq. (2.44). These relations mainly motivated the extensive studies on ion-pairs [Deu92, Bas82, Dav93a, Dav93b, Dav92] and simple structures built up by a few pairs [Deu95, Deu95a].

To quantify the ion-ion correlation effects we define an enhancement factor \( \alpha \) as the total cluster stopping \( F_c \) divided by the sum of isolated particle stopping \( \sum_n Z_n^2 F_1 \)

\[
\alpha = \frac{F_c}{\sum_n Z_n^2 F_1} = 1 + \frac{C}{\sum_n Z_n^2 F_1}.
\]

(4.8)

From the definitions (4.6) and (4.7) we can deduce the boundaries \( |C_2| \leq |F_1| \) and \( |C/F_1| \leq (\sum_n Z_n)^2 - \sum_n Z_n^2 \). Since the total stopping \( F_c \), (4.2) and (4.4), has the same sign as \( F_1 \), we get

\[
0 \leq \alpha \leq \frac{(\sum_n Z_n)^2}{\sum_n Z_n^2}.
\]

(4.9)

Here \( \alpha < 1 \) indicates a reduction of stopping by correlations while the upper limit represents the complete coalescence of the clusters. For clusters of equal charges (4.9) simplifies to \( 0 \leq \alpha \leq N \).

These definitions and relations are independent of the target conditions and apply to hot classical plasmas as well as to electron jellium \( (T = 0) \) provided that the coupling is within the linear regime. For semilinear or nonlinear coupling the simple superposition underlying the sum (4.7) is invalid. There the pair–correlations depend on the entire cluster structure and thus differ from the universal linear response expression for \( C_2 \) (4.6). Although the semi- and nonlinear regimes may be easily reached in the case of small clusters with a large total charge, a proper treatment of correlated stopping beyond linear coupling is still an open problem. Some attempts and proposals will be discussed in Sec. 4.3.1. As we know from the previous chapters semilinear and nonlinear coupling reduces the stopping power with respect to the linear response value. The amount of correlation effects \( |\alpha - 1| = |C/F_1|/\sum_n Z_n^2 F_1| \) as obtained in the linear response treatment thus represents an upper limit of what can be expected for strong projectile target coupling.
4.1.2 Essential assumptions and their validity

Before proceeding, we briefly discuss some prerequisites, in addition to the requirement of linear projectile-target coupling, which are involved in the approach (4.2) for the description of correlated stopping. As mentioned earlier in Sec. 2.2.1.4, the stopping power expression (4.2) is based on an induced electric field which is stationary in the comoving cluster frame on a time scale $\omega_p^{-1}$. In order to consider the stopping power (4.2) as a snapshot in the whole slowing down process all changes in the cluster configuration and velocity have to be slow on this time scale. The decrease $\dot{v} \propto F_c$ of the velocity $v$ due to the stopping power $F_c$ and the changes $\dot{Z}$ in the charge states due to ionization and recombination are usually varying slowly on this time scale for most cases of interest. This is, however, not immediately obvious for the spread $v_i - v$ of the individual ion velocities around the cluster mean velocity and the related changes of the relative positions. First studies on the influence of small velocity spreads were performed by Lontano et al.\cite{Lon95} for classical target plasmas. There the dielectric response description yields an explicitly time-dependent stopping power which strongly impedes some general conclusions on the resulting effects. Main sources for a velocity spread are the Coulomb-explosion due to the repulsion of the ions, the straggling in the stopping power, various stopping powers caused by different ion charges of the cluster members and also collisions with target ions.

The contribution to the velocity spread by the Coulomb-explosion can be roughly estimated from the initial Coulomb-energy of the ion-cluster after fragmentation and ionization have already taken place. For an ion-cluster with $N$ ions of (averaged) charge $Ze$, mass $M$ and an initial size $r_0$, the kinetic energy $E_c$ (per u) gained by the ions during the repulsion is approximately

$$E_c \lesssim 0.0272 \frac{Z^2 N}{M/u} \left( \frac{a_0}{r_0} \right) \text{keV}, \quad (4.10)$$

where u is the atomic mass unit and $a_0$ is the Bohr radius. For most heavy ion-clusters of interest, the energy $E_c$ is much lower than the initial energy of the ions $E_o$ (typically 10 - 1000 keV per u) and the spread of velocities is small compared to the actual cluster velocity $v$ during the largest part of the slowing down. We resume these questions on the Coulomb-explosion in Sec. 4.2.

The straggling strongly depends on the projectile velocity and target parameters as well as on correlation effects, mostly in a very similar manner as the stopping power itself \cite{Bre93} and no general statements on the importance of straggling on the velocity spread are available at present. In particular, it is not evident, that straggling is negligible in this context.

Large changes in the individual velocities are expected for different ion charges $Z_e$ distributed around some mean value $\langle Z_e \rangle$ due to the quadratic dependence ($\dot{v_i} \propto Z_e^2$). In particular for small ion charges, the individual stopping may deviate relatively strongly from the stopping in the average.

While the contribution of nuclear stopping by the target ions is always negligible compared to the electronic stopping for projectile velocities much higher than the thermal velocities of the target ions, their collisions with the projectile ions can, nevertheless, contribute significantly to the velocity spread within the cluster. To estimate the importance of these collisions one has to compare the time scale of the cluster deceleration with the time scale for scattering events between the target ions (with density $n_t$ and charge $Z_te$) and the projectile ions (with $Ze$) at the cluster velocity $v$. Disregarding the screening by the electrons a typical collision rate $\nu$ is estimated from the Rutherford cross section. Accounting for all collisions with, for example, deflection angles in the center of mass system larger than 90$^\circ$ yields $\nu = \pi n_t (Z_t Ze^2 / 4 \pi \epsilon_0 \mu)^2 v^{-3}$,
where $\mu$ is the reduced mass. This rate strongly depends on the charge states of all involved ions and on the cluster velocity.

The given examples and estimates only broach a number of unsolved questions in connection with the approximation of given fixed ion velocities $v_i = v$ and hence fixed relative positions. As we are interested in the basic phenomena and elementary features related to correlated stopping, we do not dwell on these open problems. We urge, however, to keep them in mind for final conclusions on correlated stopping with respect to quantitative statements. Here much more detailed investigations, e.g. on the amount and influence of the velocity spread, are clearly needed.

### 4.1.3 Some selected examples

We now turn to evaluate the basic linear response expression for correlated stopping, (4.2) and (4.4), for some specific examples, chosen to cover the whole spectrum of effects brought about by ion-ion correlations. As a first structure we consider in Sec. 4.1.3.1 a spherical ion cloud of Gaussian shape. Here we call it a Gaussian cluster. This ion configuration can be viewed as a rather suitable model to describe the overall, averaged behavior of ion distributions as produced in the fragmentation process of cluster-ions when impacting the target. Furthermore, it allows for a relatively easy mathematical treatment. As an ion arrangement of practical interest we deal with an extended ion beam in Sec. 4.1.3.2. Then we turn to the opposite extreme of well-defined highly regular ion configurations. In Sec. 4.1.3.3, chains of ions, as they may result from the impact of linearly extended organic molecules, are investigated. In Sec. 4.1.3.4 we finally consider a rigid ion lattice which was already mentioned in context with the periodic boundary conditions used in the numerical simulations described in Secs. 2.3.1 and 2.3.2.

#### 4.1.3.1 Gaussian ion clouds

As the first example we investigate the stopping enhancement of a spherical ion cloud, where the ions are distributed independently of each other around the center of the cluster with a Gaussian probability density. Its parameterization is given by

$$g(r) = (N - 1) \left( \frac{1}{4\pi\sigma^2} \right)^{3/2} \exp\left( -\frac{r^2}{4\sigma^2} \right), \quad S(k) = 1 + (N - 1) \exp(-k^2\sigma^2), \quad (4.11)$$

where $r$ is the distance between two ions and $\sigma$ is the rms–radius and a measure for the cluster size. Rewriting (4.4) by setting $k \cdot v = kv \cos \vartheta = \omega$ the ensemble-averaged stopping power per ion for the Gaussian cluster takes the form

$$\langle F_c \rangle = \frac{Z^2 e^2}{v^2 2\pi^2 \epsilon_0} \int_0^\infty \frac{dk}{k} \int_0^{kv} d\omega \omega \text{Im} \left[ \frac{1}{\varepsilon(k, \omega)} \right]$$

$$+ (N - 1) \frac{Z^2 e^2}{v^2 2\pi^2 \epsilon_0} \int_0^\infty \frac{dk}{k} \int_0^{kv} d\omega \omega \text{Im} \left[ \frac{1}{\varepsilon(k, \omega)} \right]$$

$$= Z^2 \left[ F_1 + (N - 1) C_2 \right].$$

In the linear (Born) regime, which we are considering here, no cutoff in the $k$-integration is needed when using a proper dielectric function, as e.g. the RPA $\varepsilon(k, \omega)$ (2.38), where Im(1/ε(k, ω)) provides an intrinsic cutoff at $\sim 1/\lambda$, see the discussion in Sec. 2.2.1.5.
In the following we discuss the correlated stopping of Gaussian clusters mainly in terms of the enhancement \( \alpha \). It reads

\[
\alpha = \frac{\langle F_c \rangle}{NZ^2F_1} = 1 + (N - 1) \frac{C_2}{F_1},
\]  

(4.13)

and is here independent of the charge state \( Z \) due to the assumed linear coupling. In the limits of large velocities \( v \gg \langle v_e \rangle \) (any \( \Theta \)) and of low velocities in highly degenerate \( \Theta \ll 1 \) and classical plasmas \( \Theta \gg 1 \) an analytical evaluation of the stopping power (4.12) using the RPA dielectric function (2.38) is possible. By an interpolation between these analytical expressions we derived a formula for the enhancement \( \alpha \) (4.13) and \( \langle F_c \rangle \) from Eq. (4.12) for all \( v \) and \( \Theta \), given by

\[
\alpha = 1 + (N - 1) \frac{\zeta(v, \sigma)}{\zeta(v, 0)},
\]  

(4.14)

with

\[
\zeta(v, \sigma) = \frac{\beta^2 \exp(-\sigma^2 \delta^2)}{\beta^2 + \delta^2} - 1 + E_1(\sigma^2 \delta^2) - E_1\left(\frac{4\sigma^2}{\lambda v^2}\right)
\]

\[
- (1 + \sigma^2 \beta^2) \exp(\sigma^2 \delta^2) \left(E_1(\sigma^2(\beta^2 + \delta^2)) - E_1(\sigma^2 \delta^2)\right),
\]  

(4.15)

where \( E_1(z) = \int_z^\infty \exp(-t)/t dt \) is the exponential integral. The coefficients \( \beta, \delta \) are adapted to fit the exact solution in the known limits and are given by

\[
\beta^2 \lambda_0^2 = 3 + \frac{3}{2} \Theta + 0.408 v^2 \left(\frac{3.819}{1 + v^2} + \frac{3}{2} \Theta\right) \frac{1}{(1 + \frac{3}{2} \Theta)(1 + v^2)}, \quad \delta = \frac{2(1 + v^2)}{\lambda v + 2\lambda_0 v^3}.
\]  

(4.16)

Here \( v \) is the cluster velocity in units of the averaged electron velocity \( \langle v_e \rangle \) (2.15) and \( \lambda_0 = \langle v_e \rangle/\omega_p \) is the static screening length.

The interpolation formula (4.14) agrees by construction with Eq. (4.12) for high and low velocities where it was fitted to analytically obtained expressions. For intermediate velocities the deviations are about some percent. As an example, Fig. 4.1 shows the enhancement \( \alpha \) as function of the cluster size \( \sigma \) obtained by Eqs. (4.14)–(4.16) (curves) compared to the exact numerical solutions of Eq. (4.12) (crosses) for a cluster of \( N = 10 \) ions for different velocities \( v \) and two sets of target parameters, corresponding to an electron jellium and a classical plasma. Expressions (4.14)–(4.16) allow in particular an accurate and fast calculation of the stopping enhancement and thus avoid the very expensive full calculations needed otherwise. This is quite important for studies of the effects of the Coulomb explosion for various target and cluster conditions like the investigations presented in Sec. 4.2. In addition, Eqs. (4.14)–(4.16) are much more suitable for discussing the basic aspects of correlated stopping and the physics behind it than the original expression Eq. (4.12). We will inspect the behavior of \( \zeta \) (4.15) more closely for this purpose. We first recall the expansion of the exponential integral \( E_1(z) \) for small and large arguments (\( \ln \gamma = 0.577\ldots \))

\[
E_1(z) \sim \begin{cases} 
- \ln(z) - \ln \gamma + O(z) & , \quad z \ll 1 \\
\frac{\exp(-z)}{z} \left[ 1 - \frac{1}{z} + \frac{2}{z^2} + O\left(\frac{1}{z^3}\right)\right] & , \quad z \gg 1.
\end{cases}
\]  

(4.17)

and the behavior of the parameters (4.16). The coefficient \( \beta \) is for all \( v \) and \( \Theta \) of the order of the inverse of the static screening length, \( \beta(v, \Theta) \sim 1/\lambda_0 \), while \( \delta \) interpolates with increasing...
velocity $v$ between $2/\lambda_r$ and $1/\lambda_0 v$. For projectile velocities much larger than $\langle v_e \rangle$ the $\delta$ thus represents the inverse of the adiabatic or dynamic screening length $\lambda_0 v$ (with $v$ scaled in $\langle v_e \rangle$). The relation $\lambda_r \ll \lambda_0$ which holds for ideal targets, see Eq. (2.18), hence implies $\beta \ll 1/\lambda_r$, $\delta \lesssim 1/\lambda_r$ and results in $\beta \ll \delta$ at low $v$ and $\beta \gg \delta$ at large $v$. Different relations between the cluster size $\sigma$ and the different length introduced by $1/\beta$, $1/\delta$ and $1/\lambda_r$ are directly related to the following three different correlation regimes.

**Short range correlations - complete coalescence:** This regime corresponds to a cluster which is as a whole smaller than the electron wavelength $\sigma \ll \lambda_r$ and thus appears as point–like to the target. Here $\sigma \beta \ll \lambda_r \beta \ll 1$, $\sigma \delta \ll \lambda_r \delta < 1$ and all exponential integrals in $\zeta$ (4.15) asymptotically behave as $E_1(z) \sim -\ln(z) - \ln \gamma$, i.e.

$$\zeta(v, \sigma \ll \lambda_r) \sim \frac{\beta^2}{\beta^2 + \delta^2} - 1 + \ln \left( \frac{4(\beta^2 + \delta^2)}{\lambda_r^2 \beta^2 \delta^2} \right) = \zeta(v, 0). \quad (4.18)$$

This is just the case of complete coalescence $\sigma = 0$ where the largest possible enhancement $\alpha = N$ is reached. The approach to this limit is shifted towards lower cluster sizes $\sigma$ with increasing velocity $v$ ($\sigma / \lambda_r \propto \sigma / \langle v_e \rangle$). This can be seen both in Fig. 4.1 and in the second example for the enhancement $\alpha$ of a $N = 60$ ion-cluster in Fig. 4.2.

**Long range correlations - single ion stopping:** If the cluster is much larger than the screening length $\lambda$, that is, $\sigma \gg \lambda \approx \lambda_0 \max(1, v) \approx \max(1/\beta, 1/\delta)$, the related inequalities $\sigma \beta, \sigma \delta \gg 1$ yield the asymptotic behavior

$$\zeta(v, \sigma \gg \lambda) \sim \frac{1}{\sigma^4 \beta^4} - \exp(-\sigma^2 \delta^2) \left( 1 - \frac{\beta^2}{\beta^2 + \delta^2} \right). \quad (4.19)$$

The contribution of ion-ion correlations here vanishes for large $\sigma$ like $1/\sigma^4$ and the limit of long range correlations is for the spherical structureless Gaussian cluster just the limit of isolated ions $\alpha = 1$. Reaching this limit requires increasingly larger cluster sizes at increasing $v$, see again Figs. 4.1 and 4.2.
Intermediate range regime: For a cluster which is not point-like, that is $\sigma \gg \lambda_r$ and smaller than the screening length, $\sigma \ll \lambda \sim \max(1/\beta, 1/\delta)$, one has

$$
\zeta(v, \lambda_r \ll \sigma \ll \lambda) \sim \begin{cases} 
\frac{-\delta^2}{\beta^2+\delta^2} - \ln \gamma - \ln \left(\frac{\sigma^2\beta^2\delta^2}{\beta^2+\delta^2}\right), & \sigma\beta, \sigma\delta \ll 1 \\
-1 - \ln \gamma - 2\ln(\sigma\beta), & \sigma\beta \ll 1, \sigma\delta \gg 1 \\
-\ln \gamma - 2\ln(\sigma\delta), & \sigma\beta \gg 1, \sigma\delta \ll 1
\end{cases} \quad (4.20)
$$

The logarithmic increase of the enhancement with decreasing cluster size $\sigma$ is nicely pictured by the examples presented in Fig. 4.1 and Fig. 4.2 where $\sigma$ is given on a logarithmic scale.

In summary we have for a given velocity $v$ a dependence of the enhancement $\alpha$ with growing cluster size $\sigma$, which is characterized by the maximum value $\alpha = N$ for small clusters $\sigma \ll \lambda_r$, by a change to a logarithmic decrease starting at $\sigma \approx \lambda_r$ and persisting until $\sigma$ reaches the dynamic screening length $\lambda$. For even larger $\sigma$ one finally approaches the isolated, single ion limit $\alpha = 1$.

Another interesting case is the behavior of the enhancement as a function of the velocity $v$ for a fixed cluster size $\sigma$, in particular the limit of large velocities $v \gg 1$. Assuming sufficiently high $v$ to guarantee a cluster which is both, extended, $\sigma \gg \lambda_r \propto 1/v$, but small compared to the dynamic screening length $\sigma \ll \lambda_0 v = 1/\delta$. Then $\sigma\delta \ll 1$ and $\delta \ll \beta$ and we have $\zeta(v, \sigma) \sim -\ln \gamma - 2\ln(\sigma/\lambda_0 v)$, see Eq. (4.20), and $\zeta(v, 0) \sim 2\ln(2\lambda_0 v/\lambda_r)$, Eq. (4.18). This results in the enhancement

$$
\alpha = 1 + (N-1) \frac{2\ln(v\lambda_0/\sigma) - \ln \gamma}{2\ln(\lambda_0 v/\lambda_r) + \ln 4} \quad v \gg 1 \quad \frac{\ln(v)}{\ln(v^2)} \to \frac{N+1}{2} \quad (4.21)
$$

Here the last terms represent the high velocity limit $\alpha(v \to \infty) \to (N+1)/2$ which has to be viewed primarily as a mathematical one, as we deal with a non–relativistic description of correlated stopping. Depending on the given parameters of the cluster and the target this limit
Figure 4.3: Enhancement $\alpha$ for a Gaussian cluster as function of the cluster velocity $v$ in units of the averaged electron velocity $\langle v_e \rangle = (v_e^2 + v_{th}^2)^{1/2}$ for different cluster sizes and target parameters:

- $N = 20$, $T = 12\text{eV}$, $n = 4 \times 10^{20}\text{cm}^{-3}$, $\sigma/\lambda_0 = 0.05$ (solid curve), $\sigma/\lambda_0 = 0.5$ (dotted), $\sigma/\lambda_0 = 5$ (dash–dotted).
- $N = 100$, $\sigma/\lambda_0 = 5$, $T = 12\text{eV}$, $n = 4 \times 10^{20}\text{cm}^{-3}$ (short–dashed), $T = 0$, $n = 1.61 \times 10^{24}\text{cm}^{-3}$ (long–dashed).

may, however, be reached already for non–relativistic velocities and has an interesting physical meaning. As it has been stated [Lin64], the stopping of a single ion at high velocities is to one half due to single particle excitations and to the other half due to collective excitations of plasma waves. The wavelength $\lambda_p$ of the plasmons excited with the phase velocity $v$ is $\lambda_p = 2\pi v/\omega_p$, or, in scaled velocities $\lambda_p = 2\pi \lambda_0 v$ and clusters with $\sigma \ll \lambda_0 v$ appear as point–like to these plasma waves. Hence, the stopping by collective excitations is the same as the stopping by collective excitations of a single ion with the total charge $NZe$. The single particle excitations resolve the cluster structure ($\sigma \gg \lambda_r\bar{v}$) and the stopping is $N$ times the single ion contribution for a charge $Ze$. This yields in summary an enhancement $\alpha = \langle F_c \rangle/NZ^2F_1 = ((NZ)^2/2 + NZ^2/2)/NZ^2 = (N+1)/2$. The velocity dependence of the enhancement is shown in Fig. 4.3 for different cluster sizes $\sigma$, numbers $N$ of ions and target parameters. While the trend is visible, the high velocity limit $(N+1)/2$ lies still far away for the given parameters as it can be reached only through the weak logarithmic $v$–dependence of $\alpha$, see Eq. (4.21). For large numbers $N$ of ions and relatively large clusters considerable enhancements arise at high velocities, which remain, however, small compared to the ultimate limit $\alpha \sim N/2$. This type of stopping enhancement for high velocities has been documented also for other cluster configurations [Vic92, Per96a] with comparable values of the cluster size with respect to the screening length.

In the simple model of the Gaussian ion distribution no internal structure of the ion cloud is so far included. Some additional structure is, however, rather likely for a real ion debris as a consequence of the initial arrangement before fragmentation and the following mutual repulsion. To estimate the related effects on correlated stopping, some additional spacing between the ions is modeled in a quite simple and general manner by again a Gaussian profile through the pair–distribution function

$$g(r) = \frac{N-1}{(4\pi\sigma^2)^{3/2}} \frac{(s^2 + \sigma^2)^{3/2}}{(s^2 + \sigma^2)^{3/2} - s^3} \exp(-r^2/4\sigma^2) \left[ 1 - \exp(-r^2/4s^2) \right].$$

Here $\sigma$ is as before the measure for the cluster size as a whole, while $s$ defines a typical inter–ion spacing, where $s^3 \approx \sigma^3/N$. The choice of a Gaussian probability for this inter–ion spacing
is mainly motivated to benefit from the efforts for the description of the Gaussian cluster. It nevertheless reproduces the essentials connected with an internal structure, that is, a zero probability to find two ions at the same position and a strongly reduced one for distances smaller than the typical spacing \( s \). For further simplification we chose \( \sigma^2/s^2 = N^2/3 - 1 \) which results in \( (s^2 + \sigma^2)^{3/2} = N s^3 \) and the structure factor

\[
S(k) = 1 + N \left[ \exp(-k^2\sigma^2) - \frac{1}{N} \exp(-k^2\left(\frac{\sigma}{N^{1/3}}\right)^2) \right],
\]

while the corresponding enhancement reads

\[
\alpha_s = 1 + N \frac{\zeta(v,\sigma)}{\zeta(v,0)} - \frac{\zeta(v,\sigma/N^{1/3})}{\zeta(v,0)} - \frac{\zeta(v,\sigma/N^{1/3})}{\zeta(v,0)} + \frac{(N-1)\zeta(v,\sigma)}{\zeta(v,0)}.
\]

Because \( \zeta(v,\sigma) \) is a monotonically decreasing function of \( \sigma \) the difference \( \Delta \alpha \) is always negative and the additional internal structure of the cluster reduces the enhancement. Some examples for this reduction are plotted in Fig. 4.4 as function of the cluster velocity \( v \) at different cluster sizes and target conditions. For small clusters \( \sigma \ll \lambda_0 \) (long–dashed curve) the internal structure is negligible even at sufficiently high velocities where the electrons may resolve the structure \( \lambda_r \ll \sigma/N^{1/3} \). For large clusters of the order of the dynamic screening length \( \sigma \sim \lambda_0 v \) pronounced reductions occur at certain velocities depending on the cluster size \( \sigma \) and ion number \( N \). These minima in \( \Delta \alpha \) are located at velocities \( v_m \), where \( \lambda_0 v_m \) is proportional to the mean interparticle spacing \( \sigma/N^{1/3} \) (solid, short–dashed and dotted curves). A variation of the target conditions at given \( \sigma/\lambda_0 \) and \( N \) only slightly affects the \( v_m \)–location (dash–dotted curve). The reduction in the stopping for large clusters and medium or high velocities is a consequence of destructive interference between the excited plasma waves and has been reported also for other types of clusters with internal structure [Vic92, Per96a].
Figure 4.5: Stopping enhancement (reduction) $\alpha_s$ for an infinitely extended ion beam with a homogeneous density $n_b$ in a classical target plasma of $T = 20\text{eV}$, $n = 10^{21}\text{cm}^{-3}$ as a function of the mean ion spacing $s \propto n_b^{-1/3}$ between the ions in units of $\lambda_D$ for different velocities $v/v_{th} =$ 1 (full curve), 4 (dash-dotted), 8 (dashed), 12 (dotted).

4.1.3.2 Ion beams

Specific ion arrangements where an internal structure can be important are ion beams or bunches of ions which may be considered as very large clusters. Here, for sufficiently large $\sigma$ at a given velocity, the beam or bunch as a whole is then larger than the dynamic screening length $\sigma \gg \lambda_D v$ and the correlation contribution from the cluster as a whole vanishes $\sim 1/\sigma^4$, see Eq. (4.19). In the particular case of a constant ion density, that is, $s = \sigma/N^{1/3} = \text{const}$ while $\sigma, N \rightarrow \infty$, the remaining correlation effects due to the internal structure always result in a reduction of the stopping power as can be seen immediately by inspecting Eq. (4.24). For $\sigma, N \rightarrow \infty$, $s = \text{const}$, the cluster contribution $N\zeta(v,\sigma)/\zeta(v,0) \sim N/\sigma^4 \sim N^{-1/3}/s^4$ goes to zero and $\alpha_s \sim [1 - \zeta(v,\sigma/N^{1/3})/\zeta(v,0)] \leq 1$. This behavior of beams or large clusters was also reported e.g. in [Bri95]. As a simple example we assume an infinitely extended ion beam with a homogeneous density $n_b \propto s^{-3}$, see [Zwi96c]. The corresponding pair-distribution and structure factor follow from Eqs. (4.22) and (4.23) by taking $\sigma, N \rightarrow \infty$, $s = \sigma/N^{1/3} = \text{const}$ as

$$g(r) = \frac{1}{(4\pi s^2)^{3/2}} \left[ 1 - \exp\left(-\frac{r^2}{4s^2}\right) \right], \quad S(k) = 1 + N\delta_{k,0} - \exp(-k^2s^2).$$

The related reduction $\alpha_s = [1 - \zeta(v,s)/\zeta(v,0)] \leq 1$ depends only on the inter-ion spacing $s$ and increases with the density of the beam as illustrated in Fig. 4.5. The very small $s \ll \lambda_D$ are, however, typically connected with very high (unrealistic) beam densities. The observed behavior of $\alpha_s$ reflects both the destructive interference of plasmon excitations with wavelengths larger than $s$ and the amount of target plasma volume per particle which is available for the medium response and thus the stopping force.

4.1.3.3 Ion chains

As an antipode to the rather general and statistical description of correlated stopping of Gaussian ion clouds, we now turn to chains of ions as an example of a well defined, highly regular structure. In particular, such arrangements allow for significant interference effects of the
excited wake fields. A study of $N$–ion chains thus adds further aspects to the spectrum of fundamental features of correlated ion stopping.

We now consider a chain of $N$ (point–like) ions with charge $Ze$ and an equal distance $L$ between two neighboring ions. Choosing its extension in the $z$–direction the charge density is
\[
\rho_p(r) = Ze \delta(x) \delta(y) \sum_{n=1}^{N} \delta(nL - z),
\]
resulting in the structure function
\[
\frac{\rho_p(-k) \rho_p(k)}{Z^2e^2} = \sum_{n=1}^{N} \sum_{m=1}^{N} \exp(ik_z(n - m)L)
\]
\[
= N + 2 \sum_{\nu=1}^{N-1} (N - \nu) \cos(\nu k_z L) = \frac{\sin^2(Nk_z L/2)}{\sin^2(k_z L/2)},
\]
which enters the expression (4.2) for the total stopping power $F_c$.

For such a highly anisotropic structure we expect a strong dependence of the stopping on the orientation of the chain with respect to its velocity. For velocities parallel to the chain, that is $v = v \hat{e}_z$ and $\omega = k \cdot v = k_z v$, the stopping per ion is given by
\[
\frac{F_c}{N} = Z^2 F_1 + \frac{Z^2e^2}{\nu^22\pi^2\epsilon_0} \frac{2}{N} \sum_{\nu=1}^{N-1} (N - \nu) \int_{0}^{\infty} \frac{dk}{k} \int_{0}^{kv} d\omega \omega \cos(\nu L \omega/v) \Im \left[ \frac{-1}{\varepsilon(k,\omega)} \right]
\]
\[
= \frac{1}{N} \frac{Z^2e^2}{\nu^22\pi^2\epsilon_0} \int_{0}^{\infty} \frac{dk}{k} \int_{0}^{kv} d\omega \omega \frac{\sin^2(N\omega L/2)}{N\omega L/2} \Im \left[ \frac{-1}{\varepsilon(k,\omega)} \right],
\]
with the single ion stopping $F_1$ as in Eq. (4.12). For a chain extended perpendicular to its velocity ($\nu \perp \hat{e}_z$) the stopping power takes the form
\[
\frac{F_c}{N} = Z^2 F_1
\]
\[
+ \frac{Z^2e^2}{\nu^22\pi^2\epsilon_0} \frac{2}{N} \sum_{\nu=1}^{N-1} (N - \nu) \int_{0}^{\infty} \frac{dk}{k} \int_{0}^{kv} d\omega \omega J_0(\nu L \sqrt{k^2 - (\omega/v)^2}) \Im \left[ \frac{-1}{\varepsilon(k,\omega)} \right],
\]
where $J_0$ is the Bessel function of the first kind.

We consider again the enhancement $\alpha = F_c/NZ^2F_1$ for the total stopping, now for parallel and transversal (perpendicular) chains, Eqs. (4.29) and (4.30). A first example of a chain of $N = 10$ ions is shown in Fig. 4.6 as function of the inter–ion distance $L$ for different velocities, target conditions and orientations. In general, we recover the behavior as seen for the Gaussian cluster with a transition from vanishing ($\alpha = 1$) to maximal ($\alpha = N$) enhancement when $L$ decreases from $L \gg \lambda_0$ to $L \ll \lambda_0$. We remark that for the parallel chain the onset of the increase of $\alpha$ for decreasing $L$ is located at the same value $L/\lambda_0$ for the same velocity $v/\langle v \rangle$ but different target conditions (solid and dash–dotted curves). The qualitative agreement with the Gaussian cluster is almost perfect for transversal chains (long–dashed curve) and for parallel
chains at low velocities $v \lesssim 1$ (not shown). The parallel chains behave at $v > 1$ quite similar for $L < \lambda$ but show new features for large $L$ where some resonant structures appear. They are shown in more detail in Fig. 4.7. These structures are due to interferences of the wake fields exited at high projectile velocities. In general these interferences of plasma waves are destructive and yield a reduction of stopping compared to the isolated ion value, i.e. $\alpha < 1$, see e.g. in the region $L \approx 5 \ldots 10$, Fig. 4.6, and between the peaks at larger $L$, Fig. 4.7.  

Constructive interference, which results in a significant enhancement of stopping, occurs at certain values of $L$, where the ions in the chain are in phase with the excited waves. Here, the wave with the strongest amplitude complies with the dispersion relation $\text{Re}[\omega(k)] = k \cdot v$ and travels in phase with the ion chain if $k = 2\pi n/L$. Taking $\text{Re}[\omega(k \ll 1)] = \omega_p$ and a velocity $v = 6\langle v_e \rangle$, the resonance condition $\text{Re}[\omega/\omega_p] = 2\pi n v/L$ reads $L/\lambda_0 = 12\pi n = 37.7, 75.4, \ldots$. These two possible values agree roughly with the peak locations in Fig. 4.7. The remaining discrepancy results from the fact, that we have for $k \geq 2\pi/L$ higher plasmon frequencies $\text{Re}[\omega(k)] > \omega_p$ as used for our first estimate. This shifts the peaks to lower $L$ and introduces a dependence on the plasma conditions (solid and dash–dotted curves), because the dispersion relation for $k > 0$ explicitly depends on $n, T$. The plasmon mode which is selected by the
resonance condition dominates more and more the resonance for an increasing number of ions which contribute to this wave excitation and thus enforce the resonant enhancement and shift it toward the corresponding values $L = 2\pi n v / \text{Re}[\omega(k)] \approx \omega_p(1 + 3k^2\lambda_D^2)^{1/2}$, yields $v / v_{th} = [(L / 2\pi \lambda_D)^2 + 3]^{1/2} = 8.14$ in perfect agreement with the observed edge. For lower velocities only plasma waves with shorter wave length $L/n$ ($n > 1$) can be in phase. These waves when exited by one ion in the chain reach only a smaller number of other ions because they are more strongly damped. For an increasing number $N$ of ions the relative contribution of the shorter waves to the total stopping thus decreases. For the same reason the enhancement due to the wave with length $L$ saturates to a maximum for $N \to \infty$. Beyond the edge towards higher $v$ a wave with length $L$ does not longer obey the resonance condition but is still excited, however, with decreasing amplitude for increasing $v$. For velocities larger than shown in Fig. 4.8 the destructive interference finally results in a reduction ($\alpha < 1$) as at low velocities.

The dependence on the number of ions is addressed once more in Fig. 4.9 for parallel chains. For large $L$ we recover the resonant structure with its slight $N$–dependence, while the enhancement for small $L$ strongly grows with increasing $N$ (note the logarithmic scale for $\alpha$). The larger enhancements for larger $N$ at small $L$, however, drop down earlier for increasing $L$. A chain does not longer appear as point-like if its total length exceeds a size $NL \approx \lambda_0$, which happens already at lower $L$ for larger $N$. Together with further resonance effects this yields rather strong variations of the enhancement with respect to the ion number at ion spacings around $L \approx \lambda_0$. This is nicely demonstrated by the enhancement as function of $N$ for different fixed inter–ion distances $L$ as shown in Fig. 4.10. The enhancement grows monotonically with $N$ at small $L$ (long–dashed curve), but shows strong oscillations for medium $L$ (solid and short-dashed). For large $L$ outside the resonance (not shown) the enhancement rapidly decreases to values $\alpha < 1$ for small $N$ and than remains constant for large $N$. This is at
4.1.3.4 Rigid ion lattice

A structure which exhibits in a most extreme manner the discussed resonant enhancement of stopping at large ion distances is a rigid infinite ion lattice. We discuss it here in context with the periodic boundary conditions used in the simulations of the stopping power, see Secs. 2.3.1 and 2.3.2. It also demonstrates further characteristics of correlated stopping connected to a nonideality of the target and some disorder in highly regular ion structures. For a simple cubic lattice of point-like ions with a lattice constant $L$, the charge density

$$\rho_p(r) = Ze \sum_n \delta(nL - r),$$

and the structure factor

$$S(k) = \frac{\rho_p(-k) \rho_p(k)}{NZ^2 e^2} = \sum_n \exp(ik \cdot nL) = \left(\frac{2\pi}{L}\right)^3 \sum_g \delta(k - g)$$

are sums over delta-functions located at the lattice vectors $nL$ and the reciprocal vectors $g = 2\pi n/L$, respectively. The stopping power per particle for such an ion lattice, moving as a whole with a velocity $v$ through the target plasma, is then calculated from the
basic expression (4.4). There the integral over $k$ turns into a sum over reciprocal lattice vectors $g$ when inserting the structure function (4.32). The expected resonant enhancement as a function of the lattice velocity is plotted in Fig. 4.11 for lattices with $L = 16 \lambda_D$ and $L = 22 \lambda_D$ in a classical target. As for the ion chains there is, in general, a reduction of stopping at high velocities except for some peaks at velocities $v$ which comply with the resonance condition $\text{Re}[\omega(g)] = g \cdot v$. In the presented examples, the ion lattice moves with $v = v(1,1,1)/\sqrt{3}$. For the smallest reciprocal lattice vectors $g = 2 \pi n/L$ with $g = g/L$ (corresponding to $n = \{(\pm 1, 0, 0), (0, \pm 1, 0), (0, 0, \pm 1)\}$) this results in velocities $v/v_{th} = \text{Re}[\omega(2\pi/L)/\omega_p \sqrt{3(L/\lambda_D)}/2\pi]$. For $g \lambda_D = 2\pi \lambda_D/L = 2\pi/22$ and $2\pi/16$ the dispersion relation for a classical Maxwell plasma yields $\text{Re}[\omega(2\pi \lambda_D/L)/\omega_p] \approx 1.14$ and 1.27 and the velocities for the location of the resonances at $v/v_{th} = 6.9$ and 5.6, respectively. The second much smaller peak around $v/v_{th} = 3.9$ also visible in Fig. 4.11 for $L = 22 \lambda_D$ (solid curve) is associated with the next larger reciprocal vectors $g$ with $g = 2\pi \sqrt{2}/L$. A comparison of the height of the three observable peaks nicely shows the increasing suppression of the resonant stopping enhancement with increasing values of $g$, where the growing $\text{Im}[\omega(g)]$ yields an increasing damping of the interfering plasma waves. Within the RPA description this damping is solely given by collisionless Landau-damping. For a primarily qualitative discussion of additional collisional damping in a nonideal target we recalculate the stopping power for the rigid ion lattice [Eqs. (4.4) and (4.32)] by replacing the RPA dielectric function for ideal targets (2.38) with the modified dielectric function in the relaxation–time approximation (2.41). The result is a suppression of both, the resonant stopping enhancement and the reduction due to destructive interference. This suppression strongly increases with the electron-electron collision-frequency $\nu$ as demonstrated in Fig. 4.12 and in Ref. [Ash87]. A similar influence on the interference of the plasma waves as provided by collisional damping is expected by an incoherence of their phases due to deviations of the ions from the lattice sites. For a qualitative estimate we assume again an isotropic Gaussian probability with a rms deviation $s$ for finding an ion around a given lattice site. Then the structure factor (4.32) is

$$S(k) = \left\langle \frac{\rho_p(-k) \rho_p(k)}{NZ^2e^2} \right\rangle = 1 - \exp(-k^2 s^2) + \left(\frac{2\pi}{L}\right)^3 \sum g \exp(-g^2 s^2) \delta(k - g). \quad (4.33)$$
Enhancement $\alpha$ for a rigid ion lattice with $L = 22 \lambda_D$ as in Fig. 4.11 (solid curve) and with an additional damping due to electron–electron collisions in the target with a collision–frequency $\nu/\omega_p = 0.02$ (dotted), 0.04 (dash–dotted) and 0.08 (short dashed) (see text).

Enhancement $\alpha$ for a rigid ion lattice with $L = 22 \lambda_D$ as in Fig. 4.11 (solid curve) and with an additional deviation of the ions from their lattice sites with a rms–deviation $\sigma/L = 0.05$ (dotted), 0.1 (dash–dotted) and 0.2 (short dashed).

In the case $s \to \infty$ this represents an infinitely extended ion beam without any internal structure, that is, without any correlation effects [$S(k, s \to \infty) \to 1$]. The enhancement $\alpha$ for finite deviations $s < L$ are shown in Fig. 4.13. A significant suppression of the interference effects occurs if $\sigma/L$ exceeds about 0.1. This indicates that a stopping enhancement due to constructive interference of the wake fields not necessarily requires perfectly regular structures as lattices or chains.

### 4.1.4 General conclusions on correlated ion stopping

Besides the generic examples discussed in the previous section a various number of different ion configurations has been studied, see e.g. [Vic92, Deu95, Bre93, Dav93a, Dav93b, Deu95a, Ari78, Dav92, Per96a, Bri95]. Taking all the available information together we obtain a general picture of correlated stopping where the following different regimes and scenarios can be identified:

**Short range correlations:** The size $\lambda_c$ of the whole ion–cluster is much smaller than the static screening–length $\lambda_0$ and smaller than the relevant spatial resolution $\lambda_r$ of the electrons, that is, $\lambda_c < \lambda_r \ll \lambda_0$. This defines the limit of complete coalescence where the ion–clusters acts on the target as a single point–like ion with a charge equal to the sum of the charges of all its constituents. Correlated stopping is there characterized through:

- The energy loss of the ion-cluster grows, at fixed cluster size, monotonically with the number $N$ of its constituents, that is, with increasing total charge. The corresponding increase in the enhancement is linear in $N$ provided that the cluster-target coupling
remains linear. For semilinear and nonlinear coupling considerable lower enhancement factors are expected. This will be discussed in Sec. 4.3.1.

- For a given total charge, the stopping is independent of the exact cluster structure.
- The stopping is always enhanced compared to that of uncorrelated individual ions.

**Long range correlations:** The size of the whole ion–cluster and/or the typical correlation length $\lambda_c$ (distances between the ions) is of same order or larger than the dynamic screening length, that is, $\lambda_r \ll \lambda_0 (v/\langle v_e \rangle) \leq \lambda_c$. Here each ion of the cluster basically acts as an individual charge with, however, possible correlation effects via the interference of the excited long ranged wake fields. This may yield enhanced or reduced stopping due to constructive or destructive interference, respectively. The typical features of this type of correlated stopping are:

- The dependence on the number $N$ of ions is weak. The reduction or the enhancement of stopping due the interferences saturates when more and more ions contribute for a fixed inter-ion distance $\lambda_c$. In particular, the maximal stopping per ion remains always of the order of a few times the stopping of individual ions even for a large or infinite number of ions, see e.g. the resonant enhancement for the rigid lattice.

- In general a reduction of stopping by destructive interference occurs. It reflects the suppression of plasmon excitations with wave–lengths larger than the typical distances $\lambda_c$.

- Enhancements of stopping by constructive interference are possible for velocities $v$ where the ion–cluster is in phase with the excited plasma waves and the resonance condition $\text{Re}[\omega(\mathbf{k}_c = 2\pi/\lambda_c)] = \mathbf{k}_c \cdot \mathbf{v}$ is complied. Because the damping of the plasma waves has to be sufficiently small these interferences only occur for high velocities. Then the resonance condition allows for small $k_c$–values with a vanishing $\text{Im}[\omega(\mathbf{k}_c)]$ and damping.

- There is a strong dependence of the correlation effects on the cluster structure $\mathbf{k}_c$ and the ion–cluster velocity $\mathbf{v}$ by this resonance condition.

- The correlation effects due to interferences are very sensitive on the target conditions. They are strongly suppressed in a nonideal plasma where the interelectron correlations reduce the plasmon mean–free–path.

**Intermediate range correlations:** When the cluster sizes and correlation lengths are of the order of the screening length and hence lie in between both previous regimes, the physics of correlated stopping in this intermediate regime carries features of the long and short range regimes. Its main characteristic is the transition between some reduction of stopping with occasional resonant, but moderate enhancements to the large possible enhancements for small clusters. Typically, the enhancement increases logarithmically with decreasing size of the cluster. Some more specific features are:

- The size and geometry of the cluster strongly affect the dependence on the ion number $N$. In general there is an increase of the enhancement with $N$ as for short range correlations.

- Depending on the cluster structure reductions of stopping due to destructive interference may occur but no enhancement by constructive interference. The velocity dependence of correlated stopping is thus less pronounced than in the long range correlation regime.
4.2 Stopping enhancement versus Coulomb-explosion

Some femto seconds after the penetration of a cluster-ion into a dense target a collisional loss of bonding electrons leads to ionization and destabilization of the cluster-ion which fragments into a debris of comoving neighboring ions. In the previous sections we investigated thoroughly the correlation effects for a given fixed ion configuration as it appears at some instant during the slowing down process of this ion debris. Now we are interested in the overall effect of ion-ion correlations on the whole slowing down, or more precisely, on the total range $R_c$ for decelerating the ion-cluster and its averaged specific energy deposition $E_0/\pi a^2 R_c$. Here $E_0$ denotes the total initial energy of a cluster-ion-beam and $a$ its radius or the focus spot size on the target. Such an analysis requires in principle a complete knowledge of the full time evolution of the ion-cluster, including basically the velocity change by the stopping itself, the charge state evolution of the ions and the Coulomb-explosion driven by the repulsion between the ions. Due to the Coulomb-explosion an ion-cluster which is initially small enough for an enhanced energy loss will increasingly spread during time until the limit of isolated uncorrelated ions is reached. We concentrate only on the essentials of this process and treat the Coulomb-explosion of the cluster by introducing a time dependent cluster size $\sigma(t)$ in the stopping power expression of the Gaussian cluster, Sec. 4.1.3.1. We restrict our analysis again to stopping by ideal electron targets and completely neglect the evolution of the charge states of the ions. This allows a revealing overview on the effects of the Coulomb explosion for various target and cluster conditions. Within these simplifications we obtain as the central result a overall enhancement of the energy deposition due to correlation effects of typically only some percent. In all relevant cases, Coulomb–explosion is much faster than the stopping process [Zwi98b].

4.2.1 The model

As a suitable ion configuration we focus on the spherical Gaussian ion cloud discussed in Sec. 4.1.3.1, which is characterized by its rms-radius $\sigma$ as a measure for the cluster size, the number $N$ of ions with equal fixed charges $Ze$ and the overall cluster velocity $v$. Since a constant $Z$ is assumed during the slowing down the actual stopping power $F_c(t)$ on this Gaussian cluster only depends on its velocity $v(t)$ and size $\sigma(t)$ and is given by Eq. (4.12) or by the single ion stopping (2.44) combined with the interpolation formula Eqs. (4.14)–(4.16). The latter possibility provides rather accurate calculations of correlated stopping at relatively low computational effort. This allows to scan a wide range of target conditions and cluster parameters. Starting with the initial cluster velocity $v_0 = v(t=0)$ at range zero, the actual velocity $v(t)$ and subsequent the total range $R_c$ is determined by integrating the equations of motion for the ion-cluster

$$
\dot{\sigma}(t) = \frac{1}{NM} F_c(v(t),\sigma(t)) , \quad R_c = \int dt \, v(t) ,
$$

where $M$ denotes the ion mass. The function $\sigma(t)$ incorporates the time evolution of the Coulomb-explosion in the calculation scheme and has to be known. To provide $\sigma(t)$, we performed molecular dynamics (MD) simulations similar to those employed for the stopping power, see Sec. 2.3.2, but here for the ion motion in the center–of–mass frame of the cluster. To account for the presence of the electron target which moves with velocity $v$ relative to the cluster, the repulsive forces between the ions are calculated from the screened Coulomb potential

$$
V(r) = \frac{(Ze)^2}{4\pi\epsilon_0 r} \exp(-r/\lambda) .
$$
The screening length $\lambda$ is either taken as the static one $\lambda = \langle v_e \rangle / \omega_p$ or, in order to approximate the dynamic polarization effects related to the relative motion, the dynamic screening $\lambda = \langle v_t \rangle / \omega_p$. It is approximated by the interpolation $\langle v_t \rangle / \omega_p = \left( \langle v_e \rangle^2 + v^2 \right)^{1/2} / \omega_p$ between the static screening length $\langle v_e \rangle / \omega_p$ and the adiabatic screening $v / \omega_p$. From these MD-simulations we obtained the time evolution of the rms-size of the ion-cluster $\sigma(t)$, which is then parameterized by some simple analytical function to be used in the evaluation of the range via Eqs. (4.34). With dynamic screening, $\lambda = \langle v_t \rangle / \omega_p$, the slowing down of the cluster feeds back to the Coulomb-explosion since $\sigma(t) = \sigma(t,v(t))$ and both processes have to be treated simultaneously. Once all the ingredients are prepared and available a final numerical evaluation of the cluster motion using Eqs. (4.34) yields the desired range $R_c$ for a given cluster with initial energy, i.e. $v_0$, and initial cluster size $\sigma_0 = \sigma(t = 0)$ and target parameters $n, T$. Due to the moderate computational effort of this scheme, results for a large number of cluster parameters and in particular target conditions can be obtained: a meaningful selection is presented in the next section. Although this description strongly simplifies the real situation, the presented model shows rather good agreement with more sophisticated studies which have been performed for a few selected cases [Nar93, Nar95]. It is to remark, however, that in these studies also the interaction (4.35) between the ions has been used. A replacement of this simple interaction by a more realistic one, which fully accounts for the dynamic polarization and screening, is certainly a major subject for an improvement of the treatment of Coulomb-explosion. This will be noted more detailed in Sec. 4.3.2.

### 4.2.2 Cluster stopping with Coulomb-explosion

Before discussing results concerning the influence of the Coulomb-explosion, we first turn to the range $R_c$ of an ion-cluster when Coulomb–explosion is absent and the cluster size is time–independent $\sigma = \sigma_0$. In Fig. 4.14 we plotted the ratio $R_t / R_c$ of the range of a single ion $R_t$ and the range $R_c$ of a Gaussian cluster with $N = 60$, $Z = 2$, $E_0 = 100$keV/u and $\sigma_0 = 3.5 \times 10^{-10}$m for a wide range of target densities $n$ and temperatures $T$. The ratio $R_t / R_c$ also represents the enhancement of the specific energy deposition due to ion-ion correlation effects in the cluster stopping and is directly related to the previously regarded stopping power enhancements $\alpha$ (4.8). An enhanced stopping results in a reduced range of the ion-cluster. For the general behavior of $\alpha$ we refer to Sec. 4.1.3.1 and Figs. 4.1 and 4.2, and remind the observed essentials: the stopping enhancement increases with decreasing ratio $\sigma / \lambda_0$ at a given velocity, whereas with increasing velocities $v / \langle v_e \rangle$ at fixed cluster size the enhancement increases for large clusters and decreases for small ones. While the velocity dependence is basically averaged out through the integration (4.34) when calculating the range, the remaining dependence on the ratio $\sigma / \lambda_0$ is fully recovered in Fig. 4.14. Here a decreasing $n$ and increasing $T$ results in a rising screening length $\lambda_0(n,T)$. In particular, no range reduction at all (i.e. stopping enhancement) occurs at very high densities. There the ion-cluster is too large compared with the screening length. Considerable enhancement of the specific energy deposition only occur for low and medium dense targets. Hence, in the high density area, nothing will change when Coulomb–explosion is included, see Fig. 4.15. At low densities and high temperatures, however, the large screening length yields an almost unscreened ion–ion repulsion and a very efficient, that is, very fast Coulomb–explosion. The large stopping enhancements as found without Coulomb–explosion only emerge for the very beginning of the slowing down process and vanish later on due to the very fast explosion of the cluster. Since the total stopping time rises with decreasing $n$ and increasing $T$ no enhancement occurs on an increasingly large part of the range. The total
Figure 4.14: Ratio $R_1/R_c$ of the individual ion range $R_1$ to the ion-cluster range $R_c$ as function of density $n$ and temperature $T$ of the electron target for an ion-cluster of $N = 60$ carbon ions with charge $Z = 2$ and an energy loss from an initial energy $E_0 = 100\text{keV/u}$ down to $0.01E_0$. The cluster size of the Gaussian cluster is $\sigma = \sigma_0 = 3.5 \times 10^{-10}\text{m}$ and constant during the slowing down.

relative range reduction diminishes to at most some percent in the medium density regime.

Similar results for different cluster parameters yield the same general prediction of a range reduction due to correlated stopping by not more than some percent. For instance, in Fig. 4.16 the charge state of the ions was doubled compared with Fig. 4.15 to $Z = 4$. The qualitative behavior remains practically unchanged and no significant quantitative changes occur except for the $n,T$–region with strongest range reduction. There $R_1/R_c$ grows by around a factor of 2. The decisive quantity for the value of $R_1/R_c$ is the ratio of the slowing down time to the Coulomb–explosion time. While their actual dependence on $Z$ is different in detail, they both become shorter for increasing charge and the resulting charge dependence of $R_1/R_c$ is relatively weak in general. This gives some justification for the rather crude assumption to use a given, fixed ion charge during the whole slowing down and for all target conditions. This should be acceptable here for a global estimate of the importance of correlation effects on the overall specific energy deposition.

A further approximation concerns the effective interaction (4.35) for the repulsive ion–ion force driving the Coulomb–explosion. While the Coulomb–explosion was treated using the dynamic screening length $\lambda = \langle v_r \rangle / \omega_p$ in Fig. 4.16, a static screening with $\lambda = \langle v_e \rangle / \omega_p$ yields the range reduction of Fig. 4.17. As the static screening provides a weaker repulsive force between the ions than the dynamic one, the Coulomb–explosion is faster in the dynamically screened case. This results in a further decrease of $R_1/R_c$ in Fig. 4.16 compared with Fig. 4.17.

In the last example which is devoted to the dependence on the ion number and initial cluster size we consider the deceleration and Coulomb-explosion driven by a dynamically screened ion–ion interaction for a large sodium cluster of $N = 1000 \text{Na}^{5+}$–ions with $E_0 = 100\text{keV/u}$ and $\sigma_0 = 10 \times 10^{-10}\text{m}$. Without Coulomb-explosion the range reduction and hence $R_1/R_c$ is approximatively 13 times larger than the values shown in Fig. 4.14 for the $N = 60$ carbon cluster. With Coulomb–explosion, however, the range ratio $R_1/R_c$ and thus the overall specific energy deposition shows essentially the same enhancements as in the previous cases, here up to around 10%, as shown in Fig. 4.18.
Figure 4.15: Range ratio $R_1/R_c$ as function of the target conditions $n, T$ for an ion-cluster of $N = 60$ carbon ions with $Z = 2, E_0 = 100\text{keV/}\text{u}$ and initial cluster size $\sigma(t = 0) = \sigma_0 = 3.5 \times 10^{-10}\text{m}$ as in Fig. 4.14. Now Coulomb-explosion is included by a growing cluster size $\sigma(t)$ as deduced from MD simulations using the effective interaction (4.35) with dynamic screening $\lambda = \langle v_e \rangle / \omega_p$.

Figure 4.16: Range ratio $R_1/R_c$ as function of the target conditions $n, T$ with Coulomb-explosion at the same parameters and conditions as in Fig. 4.15, except that the ion charge state is $Z = 4$.

Figure 4.17: Range ratio $R_1/R_c$ as function of the target conditions $n, T$ for an ion-cluster of $N = 60$ carbon ions with $Z = 4$ and $E_0$, $\sigma_0$ as in Fig. 4.15, but now with Coulomb-explosion for an effective ion–ion interaction (4.35) with static screening $\lambda = \langle v_e \rangle / \omega_p$.

Figure 4.18: Range ratio $R_1/R_c$ including Coulomb-explosion with dynamically screened effective interaction (4.35) as in Figs. 4.15 and 4.16, here for an ion-cluster of $N = 1000$ sodium ions with $Z = 5, E_0 = 100\text{keV/}\text{u}$ and an initial cluster size $\sigma_0 = 10 \times 10^{-10}\text{m}$.

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4.3 Conclusions and open problems

We comprehensively reviewed the effects on the energy loss of arrangements or clusters of ions due to the vicinity of the ions and the related possible ion-ion correlations in a non-relativistic velocity regime within the framework of the linear response description of stopping by ideal free electron targets. As demonstrated, the ratios of overall cluster size and nearest neighbor distance, respectively, to the screening length $\lambda$ in the target allow, in connection with the ratio of overall cluster velocity $v$ to the averaged electron velocity $\langle v_e \rangle$, a classification of correlated stopping. While for an overall size of the ion-cluster smaller than $\lambda$ the cluster behaves as a single highly charged ion with a large enhancement of the stopping, the correlation effects at large ion distances and cluster sizes strongly depend on the actual structure and the velocity. There, the excited wake fields interfere in general destructively, but for sufficiently regular ion configurations and at certain velocities also constructively. This results either in a reduction or an enhancement of the stopping power compared to the uncorrelated case. In particular, we displayed the considerable qualitative and quantitative differences as well as the common features of correlated stopping for ion arrangements as distinct as a Gaussian spherical distribution, an infinitely extended ion beam, $N$–chains of ions and a rigid ion lattice.

We remind, however, that all these results have been obtained under the assumption of a linear projectile-target coupling which allowed to employ the linear response formalism. Thus there are clearly additional efforts needed to extend the description of correlated stopping into the semilinear and nonlinear regime. While the observed qualitative features are expected to remain essentially unchanged for stronger coupling, considerable quantitative changes may emerge. Some preliminary attempts and estimates together with an outlook on this question are added below in Sec. 4.3.1.

We also addressed the effects of correlated stopping on the overall specific energy deposition which is an important issue in context with the use of cluster-ion beams as drivers for heating a target in an inertial confinement fusion scenario. Important enhancements of the stopping power due to correlation effects require ion-clusters which are smaller than the screening length in the target plasma. For a considerable reduction of the cluster range and an increase of the specific energy deposition this condition has to be complied for a large fraction of the whole range. The related time scale for the slowing down thus has to compete with the time scale for Coulomb–explosion which inflates the ion–cluster. For realistic interionic distances of the order of $10^{-10}$ m in the initial ion debris and neglecting Coulomb–explosion, considerable range reductions and energy deposition enhancements are restricted to the density regime $n < 10^{22} \ldots 10^{23}$ cm$^{-3}$. In these regimes, however, the Coulomb–explosion is much faster than the stopping process and reduces the enhancement of energy deposition for all studied cluster parameters to some percent. This is the essential result of the presented investigations under reserve of the underlying assumptions: (1) the neglect of the charge evolution of the ion charges ($Z_i(t) \rightarrow Z$), (2) the absence of collisions with the target ions, which could affect the evolution of the ion-cluster size $\sigma(t)$, (3) the approximation (4.35) used for the repulsive ion–ion interaction instead of a fully dynamically screened one.

Here, the changes due to a variation of charge states and collisions of the ion-cluster with the target ions are not very likely to change the ratio of stopping and Coulomb-explosion time substantially. In particular, we even expect a tendency that they further accelerate the spread of the cluster in disfavor of the energy deposition enhancement. The dynamic target polarization with determines the effective ion–ion interaction, however, may be able to produce a contrary behavior where some electron density induced within the cluster counterbalances the
repulsive forces and thus keeps the ions for a sufficiently long time together. This is certainly an important issue for future investigations and will be briefly discussed in Sec. 4.3.2.

4.3.1 Nonlinear stopping

The linear response description is strictly valid only for a sufficiently weak perturbation of the target caused by the ion projectiles. Already an exact definition of the linear coupling regime is, however, more demanding for an ion-cluster than for the case of a single ion, as discussed in Sec. 2.1.2.2. Only for large ion–clusters with a negligible enhancement the single ion criterion \( \langle \eta_p \rangle (Z, \langle v_t \rangle) = Z e^2 / 4 \pi \epsilon_0 \hbar \langle v_t \rangle \ll 1 \) (2.17) again defines linear coupling through the (averaged) charge \( Z e \) of the ions and the relative velocity \( \langle v_t \rangle \). In the opposite case of complete coalescence of a \( N \)-ion-cluster linear coupling is simply defined by \( \langle \eta_p \rangle (NZ, \langle v_t \rangle) \ll 1 \). In all other cases the corresponding criterion lies in between these limits and depends on the cluster configuration and size. As discussed in Sec. 2.1.2.2, linear coupling is not very likely whenever high total charges at relatively low velocities are involved. The extension of the description of ion-cluster stopping into the semilinear and nonlinear regime is hence an important issue for further theoretical efforts. As already mentioned, the additional length scale introduced by the cluster size rises the computational requirement to a level which generally prohibits the use of all the numerical methods to treat semilinear and nonlinear stopping of a single ion, which have been discussed in the previous chapters. At present, only some qualitative estimates and approximations concerning semilinear and nonlinear stopping can be given. Again only the two opposite cases of very extended, uncorrelated clusters and of complete coalescence allow definitive statements. There the stopping power on the whole cluster is either \( N \) times the value of a single ion of charge state \( Z \) or the stopping power of a single ion of charge \( NZ \).

While in the first case linear coupling may still apply for each of the uncorrelated ions, the highly correlated ion-cluster in the second case is very likely to couple in a nonlinear manner. Since nonlinear stopping has, however, a much weaker dependence on the ion charge than linear stopping, the enhancement for complete coalescence will be considerably reduced compared to \( \alpha = (\sum_n Z_n)^2 / \sum_n Z_n^2 \) (4.9) as predicted by the linear theory. As the degree of nonlinearity increases with a decreasing cluster size one thus expects enhancements which first rise with

![Figure 4.19: Enhancement \( \alpha \) for a Gaussian cluster of \( N = 60 \) ions as function of the cluster size \( \sigma \) in units of \( \lambda_0 = \langle v_e \rangle / \omega_p \) for a cluster velocity \( v/\langle v_e \rangle = 10 \) and for \( T = 12eV, n = 4 \times 10^{20} cm^{-3} \) and an ion charge state \( Z = 5 \) (solid curve), for \( T = 300eV, n = 10^{22} cm^{-3}, Z = 1 \) (dashed), and \( T = 0, n = 1.61 \times 10^{24} cm^{-3}, Z = 1 \) (dash–dotted). The dotted curves represent the respective enhancement for pure linear stopping when nonlinear effects which appear in the semilinear regime are neglected.](image-url)
a shrinking cluster size as in the linear treatment but then saturate at some lower level. An attempt to extend correlated stopping at least into the semilinear regime has been presented in [Zwi97d]. There again a cutoff $k_m$ is introduced in the linear response expression to cure the insufficient treatment of the close collision contributions as discussed for the single ion case in Sec. 2.2.1.5. The essential idea is now to determine this cutoff from an appropriate effective potential for the electrons which is generated by the entire cluster. The resulting cutoff depends on the cluster size and structure and provides an interpolation between large uncorrelated clusters and complete coalescence. For details on this treatment see [Zwi97d]. Here we only show in Fig. 4.19 one example of a comparison of the enhancements obtained within the purely linear treatment and this correction for semilinear coupling. We essentially recover the deduced qualitative behavior, but better founded descriptions and approximations for the semi- and nonlinear regime are, however, necessary. We propose in particular an extension of the combined scheme introduced for single ion stopping in Sec. 2.2.3 for future investigations on this topic.

4.3.2 Dynamic polarization

To improve the description of the Coulomb-explosion one has certainly to replace the approximative ion-ion interaction (4.35) with a more realistic model which better takes into account the dynamic target polarization due to the cluster. This may result, for instance, in some induced electron density inside the cluster and a very different ion-ion interaction. In principle, the Coulomb-explosion can be treated by combining linear response with MD-simulations: The force on each ion of a given ion configuration is calculated in linear response in the same manner as the stopping power on the ions, Eq. (4.2), that is here, as the forces due to the surrounding ions and the polarized target. In a subsequent time-step of a MD-simulation the new ion configuration is obtained for which again the new forces have to be calculated from linear response and so forth. Very recently such a full calculation has been performed for a fast C$_{60}$ ion-cluster in a solid Al target [Wan00]. But due to the enormous required computational effort such a scheme can only be applied to a very limited number of target parameters and cluster configurations.

Thus one has to think about simpler alternatives and approximations. In this context the cluster self-energy $E_s$

$$E_s = \frac{1}{2\varepsilon_0 (2\pi)^3} \int d^3k \frac{\varrho_p(-k) \varrho_p(k)}{k^2 \varepsilon(k, k \cdot v)} (4.36)$$

was proposed in [Mis98] as an appropriate global cluster quantity to derive the driving force for Coulomb-explosion. The self-energy $E_s$ (4.36) represents the total potential energy of a cluster with charge density $\varrho_p(r)$ including the fully dynamic polarization of the target at a relative velocity $v$. Within the linear response description the target polarization is completely provided by the dielectric function $\varepsilon(k, \omega)$ of the target medium. In the particular case of $\varepsilon = 1$ the self-energy $E_s$ is just the total Coulomb energy of the ion-cluster at issue in vacuum. For instance, for the Gaussian cluster where the structure factor $S(k)$ (4.11) only depends on the rms-radius $\sigma$, the self-energy $E_s(v, \sigma)$ then allows to derive an approximative equation of motion for $\sigma(t)$. In Ref. [Mis98] the self-energy $E_s$ was calculated for some selected ion configurations in solid density targets at different velocities. The most important result of these investigations was the possible occurrence of a negative self-energy which suggests that the dynamic target polarization can stabilize an ion-cluster under certain conditions against Coulomb-explosion. This was also confirmed for one specific example in the mentioned full calculation [Wan00], 92
where such a stabilizing behavior and even a compression of the trailing part of the cluster was found. In view of an enhancement of the specific energy deposition there remains, however, to show whether the necessary target and cluster conditions for such a stabilizing effect coincide with those where a significant stopping enhancement over the whole range occurs.
Chapter 5

Collisions of ions with magnetized electrons

The transport properties of a plasma in an external magnetic field are subject of extensive investigations in a wide field of plasma physics applications, in particular in connection with magnetic confinement fusion. Among the topics of interest also the stopping power of ions in a magnetized plasma has been considered in various studies, usually, however, for weak coupling situations where standard methods as the dielectric description or a perturbation treatment of binary collisions are applicable. Already in these regimes the presence of a magnetic field considerably complicates the description of stopping because of the introduced new parameters and dependencies and the reduced symmetry of this problem as compared to the case of an isotropic nonmagnetized plasma discussed earlier. It becomes still more demanding at nonlinear ion-target coupling for highly charged, slow ions and, in addition, for an anisotropic velocity distribution of the electrons as it is the case for electron cooling, see Sec. 3.2.2. Although electron cooling is now a well established method a lot of observations are not yet really understood. Here, an improvement of the theoretical understanding has to start with the energy loss of a highly charged heavy ion in a magnetized anisotropic electron plasma which can be viewed as the basic process of the interaction between the ion beam and the electron plasma in the cooling section of a storage ring. We first briefly introduce and outline the problem of ion stopping in magnetized electrons in Sec. 5.1. As an important step towards the final goal of a comprehensive theoretical description of the semilinear and nonlinear stopping by magnetized electrons we consider in Sec. 5.2 binary ion-electron collisions in an external magnetic field. This study of the binary collisions is strongly motivated by the achievements obtained for the nonlinear energy loss in isotropic, nonmagnetized electron plasmas by using the combined description which we propose to extent to anisotropic, magnetized electron targets. As we have seen in the earlier chapters a correct evaluation of the binary collision contribution plays an important role for the success of the combined scheme. In the presence of a magnetic field this requires a fully numerical treatment of binary ion-electron collisions in a statically screened Coulomb potential. This task is in progress. Some first results on the collisions of ions with magnetized electrons are reported which already provide some preliminary observation and conclusions (Sec. 5.4), but the nonlinear stopping of ions in magnetized electron plasmas needs much more further efforts and investigations.
5.1 Introducing and general remarks

When considering ion stopping in magnetized electrons on the level of the definitions given in Sec. 2.1 the changes introduced by the magnetic field look rather moderate. In the projectile-target hamiltonian $\hat{H}$ (2.1) and the target hamiltonian $\hat{H}_0$ (2.2) the momenta $\hat{P}$ and $\hat{p}_i$ are just replaced by $\hat{P} - ZeA(R)/c$ and $\hat{p}_i + eA(r_i)/c$, respectively. Here, $c$ is the speed of light and $A$ is the vector potential which is related to the external magnetic field $B$ via $B = \nabla \times A$.

Because the momentum of the free projectile ion is not conserved any more, the definition of a stopping power has to be derived from the change of its kinetic energy, see Eq.(2.3), and reads

$$\frac{dE}{ds} = \frac{1}{v} \frac{d}{dt} \langle \left(\hat{P} - ZeA(R)\right)^2 \rangle. \quad (5.1)$$

Going through the same analysis as in Sec. 2.1 for a further evaluation of definition (5.1) we again end up with the simple connection to the electric field at the position of the ion, Eq.(2.6), when treating the heavy ion as a classical particle

$$\frac{dE}{ds} = \int d^3 r \, \rho(r,t) \frac{v}{v} \cdot \nabla r \phi_p(r - vt) = Ze \frac{v}{v} \cdot \mathcal{E}(vt,t). \quad (5.2)$$

The difference is, of course, that the electric field caused by the dynamic response of the ions now depends on the influence of the magnetic field on this process. This concerns as well the limit of infinite projectile mass ($M \to \infty$) assumed for the stopping definition (2.7) where the stopping power is given rigorously by the expectation value of the total force on the ion $\langle \hat{F} \rangle = \langle \sum_i e \nabla r \phi_p(r_i - vt) \rangle$, that is, by Eq. (5.2).

While the definitions of the stopping power are basically the same in the presence of a magnetic field, new parameters appear which are likely to change the definition of the coupling regimes considered in Sec.2.1.2 or which even add further ones. A comprehensive analysis of the parameter- and coupling regimes is still an unsolved task. In particular, the demarcation lines between the linear, semilinear and nonlinear coupling regime may now depend on the strength of the magnetic field as well. The direction of the magnetic field together with an anisotropy of the electron velocity distribution further complicates the situation by introducing some angular dependence into the definition of various quantities like averaged velocities, the screening length and the related coupling parameters, e.g. the plasma parameter. We do not dwell on this further and only mention the new length scale related to the cyclotron motion of the electrons in the magnetic field which is given by the averaged cyclotron or Larmor radius

$$\langle r_c \rangle = \frac{m \langle v_\perp^0 \rangle}{eB} = \frac{\langle v_\perp^0 \rangle}{\omega_c}. \quad (5.3)$$

Here $\langle v_\perp^0 \rangle$ is the averaged electron velocity perpendicular to the magnetic field and $\omega_c = eB/m$ is the cyclotron frequency. The length $\langle r_c \rangle$ upgrades now the set of characteristic lengths of both, the electron target and the ion-target coupling, which have been introduced and discussed in Sec.2.1.2. Its relation $\langle r_c \rangle/a$ to the mean interelectron spacing $a$, for instance, now decides whether the target has to be considered as weakly ($\langle r_c \rangle \gg a$) or strongly ($\langle r_c \rangle \lesssim a$) magnetized. In a similar manner the ratios $\langle r_c \rangle/(b_0)$ and $\langle r_c \rangle/\lambda$ allow to define different cases of slow and fast, as well as, weakly or strongly magnetized ion-electron collisions, see e.g. [Mes94].

Of course, ion stopping in magnetized plasmas can be treated within the linear response description. Assuming an infinitely heavy projectile which is not subject to a cyclotron motion...
yields again the basic stopping expression (2.44). Because the force on the ion is, in general, not directed along is actual path in an anisotropic and magnetized target, we reformulate it here for the force itself, that is,

\[ F_{lr} = \frac{Z^2 e^2}{\epsilon_0 (2\pi)^3} \int d^3k \frac{k}{k^2} \text{Im} \left[ \frac{1}{\epsilon_B(k, k \cdot v)} \right]. \] (5.4)

The subscript \( B \) on \( \epsilon_B \) indicates that we have to use the proper dielectric function which describes the response of a magnetized electron plasma with a possibly anisotropic velocity distribution. This dielectric function \( \epsilon_B \) can be derived analytically for ideal electron plasmas at the same level of approximations as the RPA dielectric function for isotropic nonmagnetized targets (2.38). Its fully quantal version, see [Wal68, Har69], is only rarely used, but its classical limit, which is the analogue of the classical dielectric function (2.84), is well known and can be found in most textbooks on plasma physics, e.g. in [Ich73]. The rather complex structure of the dielectric function \( \epsilon_B(k, \omega) \) requires, however, a very intricate numerical evaluation of the stopping expression (5.4). While certain approximations make a calculation of the stopping force (5.4) possible in some specific cases and limits, its complete numerical analysis is still an important subject for a more advanced understanding of the stopping at these conditions. Although the actual parameter of linearity may differ here from the previously established one for the nonmagnetized target, Eq. (2.20), the linear response expression (5.4) ceases to be valid when a highly charged, slow ion strongly perturbs the target. Here one can again extend the applicability of the linear response formulation by introducing certain upper cutoffs \( k_m \) into the \( k \)-integration, as it was discussed in Sec. 2.2.1.5, where \( k_m \) will now depend also on the magnetic field. Again a binary collision approach is needed to determine the contribution of close collisions and the appropriate cutoff or, even better, to be used in an extensions of the combined expression (2.74) and the determination of the velocity dependent screening length \( \lambda(v) \), Eq. (2.80), where \( \epsilon \) is replaced by \( \epsilon_B \). To derive the effective interaction used for the binary collisions is, however, as expensive and intricate as the evaluation of expression (5.4). This task is in progress. Here we assume, as in Sec. 2.2.3, that the spherically symmetric, statically screened effective ion-electron interaction \( V_{ei}(r) \) is known for all further considerations on binary ion-electron collisions in the next section. The description of binary-collisions is, however, strongly complicated in the presence of a magnetic field compared to the nonmagnetic case, where the transport cross section for the momentum transfer is a function only of the ion–electron relative velocity. With magnetic field, additional dependencies show up and the ion-electron motion separates not longer in a center-of-mass and relative part. The required changes of the energy and momentum are now functions of the transversal and longitudinal energies and the center-of-mass motion. This makes even binary collisions to a rather exhausting and challenging problem. Typically they are treated only on an approximative level based on the classical high velocity behavior of binary collisions, see Eq. (2.71), where the influence of the magnetic field enters through certain cutoffs with divide the possible impact parameters into several classes corresponding to slow and fast and/or nonmagnetized and magnetized collisions. For each of this impact parameter region a separate contribution to the total stopping is formulated, see e.g. [Mes94] for more details. These procedures allow valuable approximations for the binary collision stopping in a truly semilinear regime but become certainly doubtful if nonlinear coupling is involved. A more accurate description of ion-electron collisions in a magnetic field requires a fully numerical treatment as it is discussed in the next section. Alternatively, the ion stopping in a magnetized target can be treated by the simulation methods discussed in Sec. 2.3.1 and 2.3.2 which can be extended to the magnetized case by adding the
Lorentz-force to the corresponding equations of motion. This line of development is in progress as well and first results can be found in [Wal98, Wal00].

5.2 Ion-electron collisions in a homogeneous magnetic field

We now concentrate on the interaction between an ion (mass \( M \) charge \( Ze \), position \( \mathbf{R} \), velocity \( \mathbf{v} = \dot{\mathbf{R}} \)) and an electron (mass \( -e \), position \( \mathbf{r}_e \), velocity \( \mathbf{v}_e = \dot{\mathbf{r}}_e \)) in a static, homogeneous magnetic field \( \mathbf{B} = \nabla \times \mathbf{A}(\mathbf{r})/c \). As we have seen in Sec. 2.2.2.2, the semilinear and nonlinear ion-electron coupling regime usually coincide with the applicability of a classical description of the binary collisions. Since we are mainly interested in these strong coupling regimes and envisage the typical parameters met in electron cooling, we will study the ion-electron interaction in a magnetic field entirely within the framework of classical mechanics. This starts with the Lagrangian \( \mathcal{L} \) which defines the considered system

\[
\mathcal{L} = \frac{m}{2} \dot{v}_e^2 + \frac{M}{2} \dot{v}^2 - \frac{e}{c} \mathbf{A}(\mathbf{r}_e) \cdot \mathbf{v}_e + \frac{Ze}{c} \mathbf{A}(\mathbf{R}) \cdot \mathbf{v} - \Phi(\mathbf{r}_e - \mathbf{R})
\]

\[
= \frac{m}{2} \dot{v}_e^2 + \frac{M}{2} \dot{v}^2 - \frac{e}{2} (\mathbf{B} \times \mathbf{v}_e) \cdot \mathbf{v}_e + \frac{Ze}{2} (\mathbf{B} \times \mathbf{R}) \cdot \mathbf{v} - \Phi(\mathbf{r}_e - \mathbf{R}),
\]

(5.5)

for a two-body interaction \( \Phi = \Phi(\mathbf{r}_e - \mathbf{R}) \) and the specific choice \( \mathbf{A} = c(\mathbf{B} \times \mathbf{r})/2 \). Because the interaction depends only on the relative distance, we next perform a transformation to cms (\( \mathbf{R}_s, \mathbf{V}_s \)) and relative frame (\( \mathbf{r}_r, \mathbf{v}_r \)) defined through \( \mathbf{r}_r = \mathbf{r}_e - \mathbf{R}, \mathbf{v}_r = \mathbf{v}_e - \mathbf{v} \) and \( \mathbf{R}_s = (m \mathbf{r}_e + M \mathbf{R})/(m + M), \mathbf{V}_s = (m \mathbf{v}_e + M \mathbf{v})/(m + M) \). The Lagrangian (5.5) expressed in the new coordinates takes then the form

\[
\mathcal{L} = \frac{m + M}{2} \dot{V}_s^2 + \frac{\mu}{2} \dot{v}_r^2 - \Phi(\mathbf{r}_r) + \frac{(Ze - e)}{2} \mathbf{B} \times (\mathbf{V}_s - \mathbf{V}_r) \cdot \mathbf{V}_s
\]

\[
+ \frac{\mu^2}{2} \left( \frac{Ze}{M^2} - \frac{e}{m} \right) (\mathbf{B} \times \mathbf{r}_r) \cdot \mathbf{v}_r
\]

\[
- \frac{\mu}{2} \frac{Ze}{M} \left\{ (\mathbf{B} \times \mathbf{R}_s) \cdot \mathbf{v}_r + (\mathbf{B} \times \mathbf{r}_r) \cdot \mathbf{V}_s \right\},
\]

(5.6)

where \( \mu \) is the reduced mass \( \mu^{-1} = M^{-1} + m^{-1} \). This already offers some useful insight in the complications which here appear compared to the case without a magnetic field. There only the first three terms are present and the motion separates in a cms and a relative part in the usual way. This is, however, not the case when a magnetic field exists. Then the cms velocity \( \mathbf{V}_s \) is not a constant of motion and, in particular, the cms motion is coupled to the relative motion as given by the last term of \( \mathcal{L} \) (5.6). Thus the problem cannot be simply reduced to three relevant degrees of freedom, in general. This is possible, however, for electron-electron collisions which are, of course, of great interest when discussing transport properties of a magnetized plasma. Then we have formally \( Z = -1, M = m, \mu = m/2 \) and the prefactor of the coupling term in Eq. 5.6 cancels and allows to rewrite the Lagrangian as \( \mathcal{L}_{ee} = \mathcal{L}_s(\mathbf{V}_s, \mathbf{R}_s) + \mathcal{L}_r(\mathbf{v}_r, \mathbf{r}_r) \). We will resume this particular case later on.

To simplify the treatment of ion-electron collisions in a magnetic field and thus the unavoidable numerical solution of the related equations of motion, we consider an infinitely heavy ion, \( M \rightarrow \infty, \mu \rightarrow m \). In this case the ion moves with a constant velocity, \( \mathbf{V}_s = \mathbf{v} = \text{const} \),
\[ \mathbf{R}_s = \mathbf{R} = \mathbf{R}_0 + \mathbf{vt}, \] and acts as a time-dependent external potential. Taking the limit of an infinite ion mass in the general expression (5.6) we arrive via \( \mathcal{L}_r = \mathcal{L} - \frac{1}{2} \mathbf{v}^2 - (Z_e - e) (\mathbf{B} \times \mathbf{R}_0) \cdot \mathbf{v}/2 \) at the relevant part for the remaining relative coordinates

\[
\mathcal{L}_r = \frac{m}{2} \mathbf{v}_r^2 - \Phi(|\mathbf{r}_r|) - \frac{e}{2} (\mathbf{B} \times \mathbf{r}_r) \cdot \mathbf{v}_r \\
- \frac{e}{2} \left\{ (\mathbf{B} \times (\mathbf{R}_0 + \mathbf{vt})) \cdot \mathbf{v}_r + (\mathbf{B} \times \mathbf{r}_r) \cdot \mathbf{v} \right\},
\]
which is now explicitly time-dependent. Therefore the total energy in the relative system \( E_r \) is not conserved in general,

\[
\frac{dE_r}{dt} = \frac{d}{dt} \left( \frac{m}{2} \mathbf{v}_r^2 + \Phi(|\mathbf{r}_r|) \right) = -e (\mathbf{v} \times \mathbf{B}) \cdot \mathbf{v}_r,
\]
as can be easily derived from the equations of motion resulting from \( \mathcal{L}_r \) (5.7):

\[
\frac{dt}{dr} = \mathbf{v}_r, \quad \frac{d}{dt} m \mathbf{v}_r = -\nabla \Phi(|\mathbf{r}_r|) - e (\mathbf{v}_r \times \mathbf{B}) - e (\mathbf{v} \times \mathbf{B}).
\]
The numerical evaluation of these equations is the major task when investigating ion-electron collisions in a magnetic field and will be discussed below. In this context it is rather useful that there exists nevertheless a constant of motion which is given by

\[
K = \frac{m}{2} \mathbf{v}_r^2 + \Phi(|\mathbf{r}_r|) + e (\mathbf{v} \times \mathbf{B}) \cdot \mathbf{r}_r.
\]

### 5.2.1 Definitions and scaling

We now turn to the more specific situation of binary ion-electron collisions in the statically screened Coulomb-potential

\[
\Phi_{ei}(r) = -\frac{Ze^2}{4\pi\epsilon_0 r} \exp\left( \frac{-r}{\lambda} \right)
\]
which we have discussed in Sec. 2.2.2.2 for the unmagnetized case. Again the screening length is here a given, fixed parameter. We now choose the magnetic field in the z-direction of our coordinate frame, that is, \( \mathbf{B} = B \mathbf{e}_z \) and restrict the ion (and center-of-mass) velocity to the \( x-z \) plane, \( \mathbf{v} = (v_x, 0, v_z) \), for symmetry reasons. To proceed, we scale all lengths in units of the screening length \( \lambda \), all velocities in a characteristic velocity \( v_c \), the time in \( \lambda/v_c \) and the magnetic field in units of \( B_0 \), where \( v_c \) and \( B_0 \) are defined through the system parameters by

\[
v_c = \left( \frac{|Z|e^2}{4\pi\epsilon_0 m \lambda} \right)^{1/2}, \quad B_0 = \frac{mv_c}{e\lambda} = \left( \frac{|Z|m}{4\pi\epsilon_0 \lambda^3} \right)^{1/2}.
\]
This allows to cast the equations of motion (5.8) with interaction (5.10) in the dimensionless form

\[
\frac{d}{dt} \mathbf{r}_r = \mathbf{v}_r, \quad \frac{d}{dt} \mathbf{v}_r = -\frac{Ze^2}{|Z|} \frac{\exp(-r_c)}{r_c^2} \mathbf{r}_r - \frac{B}{B_0} \left( \begin{array}{c} -v_{ry} \\ -v_{rx} - v_x \end{array} \right),
\]
where we use the same symbols for position, velocity and time for the scaled as for the unscaled quantities. The scaled equations of motion only depend on the sign of the ion charge \( Z/|Z| \),

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an interaction time $\lambda/v_c$ cyclotron frequency of the electron gyration. It represents the ratio of two time scales, $\omega_c^{-1}$ and an interaction time $\lambda/v_c$, related to the magnetized motion and the screened Coulomb-interaction, respectively. The larger the values of $\lambda/v_c$ compared to $\omega_c^{-1}$ the stronger is the scattering process dominated by the Coulomb-field at a given magnetic field and initial particle velocity $v_r(0)$. The importance of the Coulomb-interaction compared to the case of noninteracting particle (at given $B$) depends, of course, on the kinetic energy of the relative motion and it quantified by the ratio $v_c/v_r(0)$. Large values indicate a strong ion-electron coupling and small values a weak one because the kinetic energy $mv_r^2/2$ of an electron with $v_r$ just corresponds to the half of its potential energy in the Coulomb field of the ion at a distance $\lambda$.

The parameter $v_c/v_r(0)$ thus represents the analogue of the coupling parameter $b_0/\lambda$ (2.21), which measures whether the kinetic or the interaction energy dominates the collision process.

Before solving the equations of motion (5.12) we still have to specify the initial conditions for $t = 0$. To that end, the initial velocities and positions are assumed as $\mathbf{v}_r(0) = (v_{rx}^0, v_{ry}^0, v_{rz}^0) = (v_0^0 \cos \varphi - v_x, v_0^0 \sin \varphi, v_0^0 - v_z)$ and $\mathbf{r}_r(0) = (r_{rx}^0, r_{ry}^0, r_{rz}^0) = (b_1 \cos \beta + \lambda_0 \sin \beta + r_c \sin \varphi, b_2 - r_c \cos \varphi, -b_1 \sin \beta + \lambda_0 \cos \beta)$. Here $\varphi$ is the initial phase of the cyclotron motion of the electron and $r_c = mv_{rz}^0/eB = v_{rz}^0/\omega_c$ its radius, while $v_{z}^0$ and $v_{r}^0$ are the initial electron velocities in the lab-frame perpendicular and parallel to the magnetic field lines, respectively. The initial distance $\lambda_0$ of the guiding center of the electronic motion has to be chosen as $\lambda_0 \gg \lambda$ to assure no initial interaction. The initial velocity of the guiding center is $\mathbf{g}_r(t = 0) = (-v_x, 0, v_{z}^0 - v_z)$. It defines the angle $\beta$ by $\sin \beta = -\mathbf{g}_r \cdot \mathbf{e}_r/|\mathbf{g}_r|$, and a surface perpendicular to $\mathbf{g}_r(t = 0)$ at a distance $\lambda_0$ from the ion on which the impact parameters $b = (b_1^2 + b_2^2)^{1/2}$ are located. A specific ion-electron collision thus depends on the parameters $v_z, Z/|Z|$ and $B/B_0$ via the equations of motion and in addition via the initial conditions on $v_{rz}^0 = [v_{z}^0 - v_z], v_{r}^0, \varphi$ and $b$ (i.e. $b_1, b_2$), or instead of $v_{r}^0$ on $r_c = v_{rz}^0 B_0/B$. The geometry for the ion–electron motion before collision is outlined in Fig. 5.1 both in the lab-frame and the relative system.
5.2.2 Energy and momentum transfer in single collisions

With respect to the final goal to determine the stopping on an ion in a magnetized electron plasma we are interested in the energy and momentum transfer in a binary ion-electron collision. In the general case of an arbitrary ion mass the total energy is conserved during the scattering process, that is, \( \Delta E = 0 = \Delta E_M + \Delta E_m \). Here \( \Delta E_M \) is the desired energy transfer which is the difference between the kinetic energy of the ion \( \Delta E_M = M(v^2 - v'^2)/2 \) after and before the collision where no interaction is present, that is, in our case for ion-electron distances \( \gg \lambda \). It can be obtained alternatively from the energy change of the kinetic energy of the electron by \( \Delta E_M = -\Delta E_m = -m(v'^2 - v^2)/2 \). Transforming to cm's and relative motion with \( \mathbf{v}_e = \mathbf{V}_s + \frac{\mu_e}{m} \mathbf{v}_r \), this reads in general \( \Delta E_M = -m([\mathbf{V}'_s + \mu \mathbf{v}'_r/m] - [\mathbf{V}_s + \mu \mathbf{v}_r/m]^2)/2 \). For an infinitely heavy ion which moves with a constant \( \mathbf{v} = \mathbf{V}_s \) it formally reduces to \( \Delta E_M = -m([\mathbf{v} + \mathbf{v}'_r]^2 - [\mathbf{v} + \mathbf{v}_r]^2)/2 \). Although no energy change of the ion occurs by definition in this case, we can identify \( \Delta E_M/\Delta s \) as a legal definition of the absolute value of the force on the ion when going through the electron target as has been already discussed in detail in Sec. 2.1, see Eqs. (2.7) and (2.9). A similar consideration for the conserved component of the total momentum parallel to the magnetic field yields the momentum change of the ion as \( \Delta P_z = -m([v_z + v'_r] - [v_z + v_r]) \). These expressions in terms of the relative coordinates thus provide the desired \( \Delta E_M \) and \( \Delta P_z \) from a solution of the equations of motion (5.12), together with the initial conditions as already specified. To gain greater insight in the complex collision process it is useful to split the energy change \( \Delta E_M \) into three partial contributions for the transversal (\( \perp \mathbf{B} \)) energy change \( \Delta E_{\perp} \), the longitudinal (\( \parallel \mathbf{B} \)) change of relative energy \( \Delta E_{r,\parallel} \), and the change of longitudinal momentum \( \Delta P_z \), which are explicitly given by

\[
\Delta E_{\perp} = -\frac{m v_e^2}{2} \left\{ [v_x + v'_r]^2 + v'^2_y - |v_\perp|^2 \right\}
\]

\[
\Delta E_{r,\parallel} = -\frac{m v_e^2}{2} \left\{ v'^2_{rz} - |v'_rz|^2 \right\}
\]

\[
\Delta P_z = -m v_e \left\{ [v_z + v'_r] - [v_z + v_r] \right\} = -m v_e \left\{ v'_r - v_{rz}^0 \right\}
\]

and

\[
\Delta E_M = \Delta E_{\perp} + \Delta E_{r,\parallel} + v_e v_z \Delta P_z,
\]

where the velocities are scaled in \( v_e \). Before proceeding to the stopping power we find it advantageous to study first the relative changes of energy and momentum averaged over all initial phases \( \varphi \) of the cyclotron motion and all impact parameters. These averages can be viewed as generalizations of the transport cross section for ion-electron collisions without magnetic field as discussed in detail in Sec. 2.2.2.2. We thus define the following partial transport cross sections, scaled in units of \( 4\pi \lambda^2 \),

\[
\sigma_{\Delta E_{\perp}}(v_{rz}^0, v_{\perp}^0, v_x) = \frac{2}{m v_e^2 |v_\perp|^2} \int \frac{d^2 b}{4\pi \lambda^2} \int \frac{d\varphi}{2\pi} \Delta E_{\perp}(v_{rz}^0, v_{\perp}^0, v_x, b, \varphi)
\]

\[
\sigma_{\Delta E_{r,\parallel}}(v_{rz}^0, v_{\perp}^0, v_x) = \frac{2}{m v_e^2 |v_{rz}^0|^2} \int \frac{d^2 b}{4\pi \lambda^2} \int \frac{d\varphi}{2\pi} \Delta E_{r,\parallel}(v_{rz}^0, v_{\perp}^0, v_x, b, \varphi)
\]

\[
\sigma_{\Delta P_z}(v_{rz}^0, v_{\perp}^0, v_x) = \frac{1}{m v_e v_{rz}^0} \int \frac{d^2 b}{4\pi \lambda^2} \int \frac{d\varphi}{2\pi} \Delta P_z(v_{rz}^0, v_{\perp}^0, v_x, b, \varphi).
\]

The notation cross section is, however, to be used with care, because the expressions (5.14) can be negative as well. Their evaluation is now subject of a classical-trajectory-Monte-Carlo
(CTMC) type numerical treatment where the trajectories through the interaction zone are calculated by a numerical integration of Eqs. (5.12) for some given initial conditions. We use here a modified Velocity-Verlet algorithm which has been specifically designed for particle propagations in a (strong) magnetic field and which is described in detail in [Spr99a]. To achieve the required accuracy the constant of motion $K$ (5.9) is monitored and the actual time-step is adapted continuously. The resulting relative deviations of $K$ are of the order of $10^{-6} \ldots 10^{-5}$. From the changes of the relative velocities $\mathbf{v}_r$ for a specific trajectory we then obtain the energy and momentum transfers (5.13) as a function of the initial conditions $b_1, b_2, \varphi$. The averages (5.14) are performed by a Monte-Carlo sampling which provides the required integrations over the phase $\varphi$ and the impact parameters $b$. The actual number of computed trajectories is adjusted by monitoring the convergence of the averaging procedure. Around $10^5$ trajectories are typically needed for one parameter set $v_{rz}^0, v_{\perp}^0, v_z, B/B_0$.

As the first case we consider the particular situation where $v_z = 0$. Here the ion motion is parallel to $\mathbf{B}$. It can be completely transformed into $v_{rz}$ and energy conservation yields $\Delta E_{\perp} = -\Delta E_{\parallel}$. While the partial transport cross sections (5.14) represent the averaged change of the considered quantity with respect to its initial value, we here discuss the averaged changes itself, that is, $\langle \Delta E_{\perp} \rangle = -|v_{\perp}|^2 \sigma_{\Delta E_{\perp}}$ and $\langle \Delta P_{\perp} \rangle = -v_{\perp}^2 \sigma_{\Delta P_{\perp}}$ scaled in $mv_{\perp}^2/2$ or $mv_{\perp}$, respectively. Their typical behavior for ion motion parallel to the magnetic field as a function of $|v_{rz}^0|^2$ is illustrated in Fig. 5.2 for different velocities of the cyclotron motion $v_{\perp}^0$ and varying magnetic fields $B/B_0$. Positive values of $\langle \Delta E_{\perp} \rangle$ are observed for all $v_{rz}^0$ for the low initial $v_{\perp}^0 = 0.2$ (left top) and correspond to an increase of the energy in the cyclotron motion and a blowing up of the spirals during the collision in the average. A considerably different behavior occurs for the higher initial velocity $v_{\perp}^0 = 5$ (right top). Here negative values of $\langle \Delta E_{\perp} \rangle$ at small longitudinal velocities $v_{rz}^0 < v_{\perp}^0$ indicate an oppositely directed flow of energy. In the average a shrinking of the spirals takes place. The same qualitative behavior was also found for other $v_{\perp}^0$. It reflects a flow from the higher to the lower one of the initial longitudinal or transversal energies during the collision process. Similar features are observed for the momentum change $\langle \Delta P_{\perp} \rangle$ (left and right bottom in Fig. 5.2), where positive values correspond to a deceleration of the relative motion parallel to $\mathbf{B}$. This is the case for all $v_{rz}^0$ at the low $v_{\perp}^0 = 0.2$. For the negative values at low $v_{rz}^0$ and $v_{\perp}^0 = 5$ the relative motion in longitudinal direction is accelerated by a gain of energy provided from the transversal (cyclotron) motion. In all cases, however, the absolute values of $\langle \Delta E_{\perp} \rangle$ and $\langle \Delta P_{\perp} \rangle$ are strongly reduced with increasing magnetic field $B$. These qualitative features, in particular the strong suppression of the energy and momentum transfer with increasing magnetic field, have also been found in a perturbative treatment of the equivalent case of an ion at rest [Gel97]. This approach is, however, only applicable to weak coupling situations, that is, for velocities which are large compared to the velocity $v_c$ (5.11), i.e. $v_{\perp}^0 > 1$. But the most interesting effects occur in the nonlinear coupling regime at low velocities.

For comparison we briefly regard the case of repulsive electron–electron collisions. Two examples for $\langle \Delta E_{\perp} \rangle$ and $\langle \Delta P_{\perp} \rangle$ with the same parameters as in the previous case are shown in Fig. 5.3. Again, an increase of $B$ yields a strong suppression of the energy transfer. This has already been well documented e.g. in investigations on the equilibration of transversal and longitudinal temperatures in a magnetized electron plasma [Gli92]. The momentum transfer $\langle \Delta P_{\perp} \rangle$ (right bottom) shows, however, a very different behavior at low $v_{\perp}^0$ compared with the previous ion–electron collisions, mainly a weaker dependence on $B$ and a convergence towards an always positive value for strong magnetic fields. This can certainly be ascribed to the repulsive force.
Figure 5.2: Normalized averaged changes of energy $-\langle \Delta E_\perp \rangle = -[v_\perp^0]^2 \sigma_{\Delta E_\perp}$ (top) and momentum $-\langle \Delta P_z \rangle = -v^0_z \sigma_{\Delta P_z}$ (bottom) as defined by Eqs. (5.13) and (5.14) as a function of the scaled initial kinetic energy $[v_\perp^0]^2$ of the relative motion parallel to the magnetic field $B$. Shown are the results for ion-electron collisions with $v_x = 0$, where the ion moves parallel to $B$, for initial velocities of the cyclotron motion of the electron $v_\perp^0 = 0.2$ (left) and $5$ (right), and for different magnetic field strengths $B$ as indicated. Here $\langle \Delta E_\perp \rangle$ is scaled in $mv_c^2/2$, $\langle \Delta P_z \rangle$ in $mv_c$, all velocities in units of $v_c$ and $B$ in units of $B_0$, with $v_c$ and $B_0$ as given by Eqs. (5.11).
Now we turn back to the case of attractive ion–electron collisions and allow for a transversal ion motion, \( v_x \neq 0 \), where a net energy transfer \( \Delta E_\perp \neq -\Delta E_{r,\parallel} \) occurs. This yields a characteristic behavior of \(-\langle \Delta E_\perp \rangle\) and \(-\langle \Delta P_z \rangle\) which differs considerably from the case \( v_x = 0 \). We discuss it here for an initial transversal velocity \( v_\perp^0 = 6 \) and for two different strength of the magnetic field \( B/B_0 = 6 \) and 30, see Fig. 5.4. While the relatively small component \( v_x \) of the ion velocity is unimportant at high \( [v_{r,z}^0]^2 \), the results strongly depend on the transversal ion motion \( v_x \) in the nonlinear regime of small initial energies \( [v_{r,z}^0]^2 \). In particular, the absolute value of the energy transfer \( \langle \Delta E_\perp \rangle \) can be much larger than for \( v_x = 0 \) and the transversal momentum transfer \(-\langle \Delta P_z \rangle\) even shows a totally different behavior for a nonvanishing \( v_x \) (bottom). Already a small \( v_x \) turns the acceleration of electrons observed at low \( [v_{r,z}^0]^2 \) and \( v_x = 0 \) into a deceleration. The related positive values of \(-\langle \Delta P_z \rangle\) first increase with growing \( v_x \), then reaches a maximum and decrease again at larger transversal ion motion. A nonvanishing transversal ion motion obviously introduces a very complex behavior of the energy and momentum changes which qualitatively and quantitatively differs strongly from the case of an ion motion along the magnetic field lines or for an ion at rest.

**5.3 Stopping power**

To obtain finally the stopping power one has still to average over the initial velocities \( v_{r,z}^0, v_\perp^0 \) according to their distribution \( f(v_{r,z}^0, v_\perp^0) \). The appropriate definition of the stopping power via an average over the energy loss of individual binary encounters is given by Eq. (2.61) and yields in our case the stopping power \( F \) projected on the direction of flight \( \mathbf{\hat{v}} \) in the form

\[
F = F \cdot \hat{v} = \frac{1}{v} \frac{dE}{dt} = \frac{n_e}{v} \int d^3v f(v_{||}, v_\perp) |g_r| \int d^2b \int_0^{2\pi} \frac{d\varphi}{2\pi} \Delta E_M(v_r, v, b, \varphi) \quad (5.15)
\]
Figure 5.4: Normalized averaged changes of energy $-\langle \Delta E_{\perp} \rangle = -[v_{0,\perp}^0]^2 \sigma_{\Delta E_{\perp}}$, $B/B_0 = 6$ and $B/B_0 = 30$, and momentum $-\langle \Delta P_z \rangle = -v_{0,rz}^0 \sigma_{\Delta P_z}$ (bottom), see definitions (5.13) and (5.14), as a function of the scaled initial kinetic energy $[v_{0,\perp}^0]^2$ of the relative motion parallel to the magnetic field $B$, now for ion-electron collisions with different transversal velocities $v_x$ of the ion, as indicated. The initial velocity of the cyclotron motion is $v_{\perp}^0 = 6$ in all plotted cases, and the magnetic field strength is $B = 6B_0$ in the left figures and $B = 30B_0$ in the right ones. The scaling is again provided by the system parameters $v_c$ and $B_0$ from Eqs. (5.11) as in Fig. 5.2.
\[
\lambda^2 n_e m v^2_e \int d^3v f(v_\parallel, v_\perp^0) \left| \mathbf{g}_r \right|_v \int d^2b \int_0^{2\pi} \frac{d\varphi}{2\pi} (\Delta E_\perp + \Delta E_{r,\parallel} + 2v_z \Delta P_z) \\
= 2\pi^2 n_e m v^2_e \int d^3v f(v_\parallel, v_\perp^0) \left| \mathbf{g}_r \right|_v (|v_\perp^0|^2 \sigma_{\Delta E_\perp} + |v_{r,z}^0|^2 \sigma_{\Delta E_{r,\parallel}} + 2v_z v_{r,z}^0 \sigma_{\Delta P_z}).
\]

Here we recall that \( \mathbf{g}_r \) denotes the velocity of the guiding center in the relative frame, which defines the impact parameter \( b \) with respect to a plane perpendicular to \( \mathbf{g}_r \). Thus \( n_e |\mathbf{g}_r| = n_e (|v_{r,z}^0|^2 + v_z^2)^{1/2} \) represents the current density of the incoming electron flux.

Applying the analogous considerations as used to derive Eq. (5.15) to the longitudinal momentum transfer, an expression for the stopping power in the direction of \( \mathbf{B} \) is established by

\[
F_z = \mathbf{F} \cdot \mathbf{e}_z = \frac{dP_z}{dt} = n_e \int d^3v f(v) |\mathbf{g}_r| \int d^2b \int_0^{2\pi} \frac{d\varphi}{2\pi} \Delta P_z(v_r, v, b, \varphi) = \lambda^2 n_e m v^2_e \int d^3v f(v_\parallel, v_\perp^0) |\mathbf{g}_r| \int d^2b \int_0^{2\pi} \frac{d\varphi}{2\pi} \Delta P_z(v_{r,z}, v_\perp^0, v_x, b, \varphi) = 4\pi^2 n_e m v^2_e \int d^3v f(v_\parallel, v_\perp^0) |\mathbf{g}_r| |v_{r,z}^0| \sigma_{\Delta P_z}(v_{r,z}^0, v_\perp^0, v_x).
\]

In both stopping power definitions, the first line refers to the unscaled quantities, while in the second and the third line the energies, momenta and velocities are scaled in \( m v^2_e/2, m v_e \) and \( v_e \), respectively, while \( b \) is scaled in \( \lambda \). The definition and evaluation of Eq. (5.15) in connection with the force in direction of \( \mathbf{B} \) (5.16) allows to reconstruct the total stopping force, which will be not directed parallel to \( \mathbf{v} \) in general, e.g. for anisotropic \( f(v_\perp^0, v_\parallel^0) \). The numerical evaluation and analysis of the binary collision stopping power is still in progress. Only some recent, preliminary results are available for the parallel stopping force (5.16), where the anisotropic velocity distribution \( f(v_\perp^0, v_\parallel^0) \) was assumed as a product of two Maxwell distributions for the parallel and the transversal degrees of freedom with different temperatures \( T_\parallel \) and \( T_\perp \), respectively. The specific parameters, which are characteristic for recent experiments performed at the TSR storage ring in Heidelberg [Beu00], are: \( Z = 6, n_e = 8 \times 10^6 \text{cm}^{-3}, k_B T_\parallel = 11.5 \text{ meV} \) and \( k_B T_\perp = 0.1 \text{ meV} \). The screening length assumed for the effective interaction (5.10) has been chosen as \( \lambda = 1 \times 10^{-4} \text{ m} \) which lies in between the values for the Debye lengths corresponding to \( T_\parallel \) and \( T_\perp \). This results in the values \( v_e = 3.9 \times 10^3 \text{ m/s}, B_0 = 0.01 \text{ T} \) of the scaling parameters (5.11). The thermal velocity of the parallel electron motion is \( v_{th,\parallel} = 4.2 \times 10^3 \text{ m/s} = 1.08 v_e \). Some examples, which demonstrate the typical dependencies of \( F_z \) (5.16) on the transversal ion motion \( v_x \) and the magnetic field \( B \), are shown in Fig. 5.5, where \( F_z \) is discussed as function of the longitudinal ion velocity \( v_z \). In the left part, we have a transversal ion motion of \( v_x = 0.3 \) and different magnetic fields \( B/B_0 = 1, 3 \) and 5. At low velocities \( v_x \approx 1 \) where the ion travels under an angle of around 15° with the magnetic field lines a strong enhancement of the stopping \( F_z \) occurs for nonvanishing magnetic field which increases with \( B \). For large \( v_x \gg 1 \), when the ion motion is almost parallel to \( \mathbf{B} \) the typical previously seen suppression of the momentum transfer with increasing \( B \) yields a growing reduction of \( F_z \). In the right part of Fig. 5.5 the magnetic field is \( B/B_0 = 3 \) while the transversal motion is \( v_x = 0, 0.1, 0.3, 0.5 \) and 1. Here almost no influence on \( v_x \) can be detected at large \( v_z \) where \( v_z \) completely dominates the ion motion. For low \( v_x \), however, we observe a strong increase of the stopping power \( F_z \) with increasing \( v_x \). For an interpretation of these results it should be noted, that the stopping \( F_z \) for a given \( v_x \) corresponds at different \( v_z \) to an ion motion with different angles with \( \mathbf{B} \) and various absolute values of the velocity \( v = (v_x^2 + v_z^2)^{1/2} \).
5.4 Conclusions and remarks

The presented results obtained from a fully numerical investigation of ion-electron collisions in a magnetic field mainly give an impression of the typical and important effects. These numerical studies on the stopping power are still in the beginning, and a large number of CTMC runs is required to provided the transport cross sections (5.14) as a function of all the initial velocities needed for the necessary integrations and to cover the whole space of parameters of interest like the strength of the magnetic field $B$, the ion charge $Z$ or the screening length $\lambda$ employed in the effective interaction. This has certainly to be studied further and in more detail before a similar comprehensive understanding of (nonlinear) stopping as in the simpler case of collisions without a magnetic field can be achieved. In particular, the dependence of the stopping on the ion charge in a magnetized plasma and at nonlinear coupling has still to be investigated. In our first studies, present here in part, we have not yet explored this question and mainly concentrated on the dependencies on the strength of the magnetic field and on the transversal ion motion. The preliminary results indicate, nevertheless, that special attention has to be paid to the actual ion motion when calculating the energy loss related to electron cooling in storage rings where the low velocity regime is of particular importance. Similar observations on this role of the transversal ion motion in connection with stopping in magnetized electrons has already been made in PIC-simulations on this subject [Wal98, Wal00].
Appendix A

Definitions and Notation

A.1 Definitions used for the Fourier–transformation

For the Fourier transformation of a function $f$ in space and time we used throughout this paper the definitions

$$f(r,t) \rightarrow f(k,\omega) = \int d^3r \int_{-\infty}^{\infty} dt f(r,t) \exp(-i(k \cdot r - \omega t)),$$

$$f(k,\omega) \rightarrow f(r,t) = \int \frac{d^3k}{(2\pi)^3} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} f(k,\omega) \exp(i(k \cdot r - \omega t)),$$

with the transform of a constant

$$f(r,t) = 1 \rightarrow f(k,\omega) = (2\pi)^3 \delta^3(k) 2\pi \delta(\omega).$$

A.2 Definitions of some important quantities

Wigner-Seitz radius

$$a = \left( \frac{4\pi n}{3} \right)^{-1/3}$$

Bohr radius

$$a_0 = \frac{\epsilon_0 \hbar^2}{\pi e^2 m} = 5.29 \cdot 10^{-11} \text{m}$$

$r_s$ parameter

$$r_s = \frac{a}{a_0} \approx \left[ \frac{n_e}{1.6 \cdot 10^{24} \text{cm}^{-3}} \right]^{-1/3}$$

parameter of degeneracy

$$\Theta = \frac{k_B T}{E_F} = 2 \frac{v^2_{th}}{v^2_F} = \frac{k_B T}{13.6 \text{eV}} \left( \alpha r_s \right)^2, \quad \alpha = \left( \frac{4}{9\pi} \right)^{1/3} = 0.521\ldots$$

parameter of ideality

$$\xi = \frac{2\alpha^2 r_s}{2 + \Theta}$$
plasma parameter
\[ \Gamma = \frac{e^2}{4\pi \epsilon_0 k_B T} \left( \frac{4\pi n}{3} \right)^{1/3} = \frac{e^2}{4\pi \epsilon_0 k_B a T} \frac{2a^2 r_s}{\Theta} \]

plasma frequency
\[ \omega_p = \left( \frac{e^2 n}{\mu \epsilon_0} \right)^{1/2} \]

Debye length
\[ \lambda_D = \left( \frac{\epsilon_0 k_B T}{\mu e^2} \right)^{1/2} = \frac{v_{th}}{\omega_p} = \frac{a}{\sqrt{3} \Gamma} \]

thermal velocity
\[ v_{th} = \left( \frac{k_B T}{m} \right)^{1/2} \]

Fermi velocity
\[ v_F = \frac{\hbar (3\pi^2 n)^{1/3}}{m} \]

Fermi energy
\[ E_F = \frac{1}{2} m v_F^2 = \frac{\hbar^2 (3\pi^2 n)^{2/3}}{2m} \]

averaged velocities (approximations)
\[ \langle v_r \rangle = \left( \langle v_e \rangle^2 + v^2 \right)^{1/2}, \quad \langle v_r \rangle' = \frac{\langle v_r \rangle}{\langle v_e \rangle} = \left( 1 + \frac{v^2}{\langle v_e \rangle^2} \right)^{1/2} \]
\[ \langle v_e \rangle = \left( v_F^2 + v_{th}^2 \right)^{1/2} = v_F \left( 1 + \frac{\Theta}{2} \right)^{1/2} \]

classical collision diameter
\[ b_0 = \frac{|Z| e^2}{4\pi \epsilon_0 \mu v_r^2} \frac{\mu v_r^2 - m \langle v_r \rangle^2}{2m} \langle b_0 \rangle = \frac{|Z| e^2}{4\pi \epsilon_0 m \langle v_r \rangle^2} = \frac{|Z| \alpha^2 r_s^2}{\langle v_r \rangle^2 (1 + \frac{\Theta}{2})} a_0 \]

The collision diameter \( b_0 \) is equal to the impact parameter for a classical collision in the (bare) Coulomb potential with 90° deflection angle at relative energy \( \mu v_r^2 / 2 \).

ion–electron Coulomb parameter
\[ \eta_p = \frac{|Z| e^2}{4\pi \epsilon_0 \hbar v_r} \frac{v_r - \langle v_r \rangle}{\langle v_r \rangle} \langle \eta_p \rangle = \frac{|Z| e^2}{4\pi \epsilon_0 \hbar \langle v_r \rangle} = \frac{|Z| \alpha r_s}{\langle v_r \rangle \sqrt{1 + \frac{\Theta}{2}}} \]

electron–electron Coulomb parameter
\[ \eta_e = \frac{e^2}{4\pi \epsilon_0 \hbar v_{ee}} \frac{v_{ee} - \langle v_{ee} \rangle}{\langle v_{ee} \rangle} \langle \eta_e \rangle = \frac{e^2}{4\pi \epsilon_0 \hbar \langle v_{ee} \rangle} = \frac{\alpha r_s}{\langle v_{ee} \rangle \sqrt{1 + \frac{\Theta}{2}}} \]
A.3 Notation

\[ a = (4\pi n/3)^{-1/3} \]
\[ a_0 = 0.529 \cdot 10^{-10} \text{m} \]
\[ b_0, \langle b_0 \rangle \] classical collision diameter
\[ C, \tilde{C} \] dimensionless friction coefficients
\[ C \] correlational part of correlated stopping
\[ E \] energy
\[ \mathcal{E} \] electric field
\[ e \] elementary charge, distinct from exp. function
\[ dE/ds \] stopping power
\[ F \] force on the ion
\[ F_1, F_c \] single ion stopping power, total stopping on a cluster
\[ f \] phase space distribution function
\[ f_0 \] phase-space distribution in ground state, usually Fermi or Maxwell
\[ f_B(x) \] Bose function
\[ G \] local field correction
\[ g \] spatial pair distribution function
\[ H \] Hamilton operator
\[ \text{Im}[...] \] imaginary part
\[ k, \tilde{k} \] wave number
\[ k_B \] Boltzmann constant
\[ k_m \] cutoff parameter
\[ m \] electron mass
\[ M \] projectile mass
\[ N \] particle number
\[ N_D \] number of electrons in a Debye sphere
\[ n \] bulk ground state electron density
\[ n(r) \] distribution of particle density
\[ \delta n \] small deviation from equilibrium density
\[ p, p, P, P \] momenta
\[ \mathbf{r}, \mathbf{R} \] coordinates in space
\[ \mathcal{R}(Z, \Gamma) \] dimensionless friction coefficient for classical systems
\[ r_s \] a/a_0
\[ S \] structure factor (function), dynamic as well as static
\[ T \] electron temperature
\[ t \] time
\[ U \] one-body potential, mean field
\[ V \] two-body interaction, usually Coulomb
\[ v, \mathbf{v} = |\mathbf{v}| \] ion velocity
\[ \mathbf{\hat{v}} = \mathbf{v}/v \] unit vector of ion velocity
\[ v_t, v_{th}, v_F \] relative, thermal, Fermi velocity
\[ v_e, \mathbf{u}, u \] electron velocities
\[ Z \] effective ion charge state or nuclear charge state

\[ \alpha = (4/9\pi)^{1/3} = 0.521... \]
\[ \alpha \] stopping power enhancement
\[ \Gamma \] (classical) plasma parameter
\[ \gamma, \ln \gamma \] ln \( \gamma = 0.577... \), Euler’s constant
\[ \delta(x), \delta^3(x) \] Dirac delta function
\[ \varepsilon \] dielectric function
\[ \varepsilon_R \] RPA dielectric function
\[ \varepsilon_0 \] dielectric constant in vacuum
\[ \varepsilon_{so} \] single-electron energy
\[ \zeta, \tilde{\zeta} \] kinetic energy, free particle dispersion
\[ \eta_e, \langle \eta_e \rangle \] Coulomb parameter for electron–electron collisions
\[ \eta_p, \langle \eta_p \rangle \] Coulomb parameter for projectile–electron collisions
\[ \Theta \] degree of degeneracy
\[ \theta(x) \] step function
<table>
<thead>
<tr>
<th>Symbol</th>
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<tr>
<td>$\Lambda$</td>
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<td>de Broglie wavelength $\hbar/\mu v_t$ or $\hbar/\mu \langle v_t \rangle$</td>
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<td>$\lambda, \lambda_D$</td>
<td>screening length, Debye length</td>
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<td>reduced mass</td>
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<td>charge density</td>
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<td>$\tilde{\rho}$</td>
<td>density operator</td>
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<td>$\sigma$</td>
<td>rms of Gaussian clusters</td>
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<td>quantum and/or ensemble averaging</td>
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