A relativistic optical-data model for inelastic scattering of electrons and positrons in condensed matter

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Abstract

A relativistic optical-data model for the calculation of non-radiative inelastic scattering of electrons and positrons in condensed matter is presented. The scattering is described within the first Born approximation, in terms of longitudinal and transverse interactions. Differential cross sections are determined by a generalized oscillator strength density, which is generated by extending a semi-empirical optical oscillator strength density to non-zero momentum transfers using a modified δ-oscillator as the extension algorithm. The Fermi density-effect correction is obtained from the optical oscillator strength and a simple approximation is proposed to account for its effect on the cross section differential in energy loss. The differential cross sections take relatively simple analytical forms, and various quantities of interest, such as total cross section, stopping power, straggling parameter and restricted inelastic transport cross section are evaluated by a single quadrature. Results are presented for electron and positron energies between 10 eV and 1 GeV.

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1. Introduction

Accurate and sometimes also detailed information on the interaction of electrons and positrons with matter is required in electron analytical techniques (e.g. Auger electron spectroscopy, X-ray photoelectron spectroscopy and electron probe
microanalysis), in electron microscopy and in positron surface spectroscopy. It is also of basic interest in dosimetry and medical physics (nuclear medicine, radiation treatment and protection), as well as in the design of particle detectors. Reliable interaction models are needed too for Monte Carlo simulation of radiation transport (see e.g. [1]). The most relevant interactions are elastic collisions, inelastic radiative interactions (i.e. emission of bremsstrahlung photons), and inelastic non-radiative collisions involving the excitation of atomic or molecular electrons. The present work deals with the third of these items. It should of course be remembered that the energy loss of electrons and positrons at highly relativistic energies (well above 1 MeV) is dominated by the contribution from bremsstrahlung; see [2] for a detailed review of radiative energy-loss processes.

Although the theory of inelastic collisions is well developed, much of the information required for practical quantitative work is available only in fragmentary form. Published databases provide stopping powers for electrons and positrons above 10 keV [3] and inelastic mean free paths for low-energy (from about 100 eV to a few keV) electrons [4], but information on the energy-loss dependence and angular dependence of the inelastic differential cross section (DCS) is for most materials available only from simplified analytical models. This information is important for Monte Carlo simulation purposes, especially in detailed and mixed (class II) simulation schemes [1].

The present work describes a semi-empirical optical-data model for the calculation of non-radiative inelastic collisions of electrons and positrons in condensed matter. The model can be applied in a wide range of incident electron or positron energies, from about 100 eV up towards 1 GeV. The underlying theory is the relativistic first Born approximation, as presented e.g. by Fano [5]. The interaction between the projectile and the stopping material is treated as a first-order perturbation, which in the relativistic case is split into longitudinal and transverse interactions. The response of the material to this perturbation is determined by its complex dielectric function, which is converted into a generalized oscillator strength (GOS) density. The GOS, which thus is a material-dependent quantity, is conveniently written as a function of the energy transfer and momentum transfer in an inelastic collision, alternatively as a function of energy transfer and scattering angle, and gives directly the inelastic DCS per atom or molecule [6]. Once the GOS is known – by calculations, modelling or from empirical data – interaction cross sections, stopping powers and other quantities of interest can be evaluated by simple quadratures. Although the GOS is, of course, a quantum-mechanical concept, the name derives from the classical picture of bound target electrons set into oscillation by, and thus absorbing energy from, the field of the incident charged particle [7].

In an “optical-data” model, such as the present one, the GOS is obtained by combining an empirical or semi-empirical optical oscillator strength (OOS) density with an algorithm that extends (extrapolates) the OOS to non-zero momentum transfers, i.e. into the GOS. Usually, the OOS density is obtained by merging experimental optical-data (refractive index and extinction coefficient) with empirical or calculated photoabsorption cross sections for inner atomic electron shells. Several optical-data models have previously been presented in the literature, differing in the set of optical data or in the choice of extension algorithm.

The relativistic formulation of the present optical-data model makes it applicable up towards GeV energies. The accuracy in the details of the adopted OOS density should not be important for global quantities like the stopping power and the straggling parameter at incident energies above ~10 keV. However, it may matter, to some extent, for the inelastic mean free path and for the details of the energy-loss distribution and the angular distribution since these quantities are more sensitive to the details of the GOS at small momentum transfers. The accuracy of the OOS becomes essential for a realistic description of inelastic collisions below ~10 keV.

For relativistic projectiles, the Born approximation (with appropriate consideration of the Fermi density effect) is expected to be very accurate. As regards the validity of the present model in the low-energy limit, it may be noted that optical-data models have been used by different authors to esti-
mate inelastic mean free paths and/or stopping powers of electrons with energies as low as 10 eV in condensed matter (see e.g. [8–18]). The results of the calculations agree reasonably well with available experimental measurements of these two quantities (which are affected by considerable uncertainties) and show the same energy dependence as the data. This indicates that the models, though based on the first Born approximation, may in practice be used with confidence for energies larger than, say, 100 eV.

On the other hand, the application of optical-data models to describe inelastic collisions of electrons and positrons at energies below some 100–200 eV is subject to criticism, insofar as these models are formally based on the first Born approximation and therefore neglect the contributions from higher-order terms in the (perturbative) Born series expansion of the cross sections. In particular, the terms of odd order in the projectile charge give rise to the so-called Barkas effect (see e.g. [19]), which yields different stopping powers for a particle and its antiparticle at energies around and below the stopping power maximum. The inaccuracies of the optical-data models for electrons and positrons in the very low energy region might then be roughly estimated from the differences in measured or calculated proton–antiproton stopping powers at the same particle velocities. In this respect, experiments carried out at CERN show that antiproton stopping powers are smaller than those of protons by about 30% near the maximum, located at 50–200 keV depending on the material, and up to 50% smaller at 20 keV [20,21]; these energies correspond to electrons or positrons of 25–100 eV and 10 eV, respectively. Non-perturbative calculations predict similar trends and values [22]. The straightforward translation of these facts to the inelastic mean free paths, stopping powers and straggling parameters of electrons and positrons is uncertain. Nonetheless, they suggest that results from optical-data models for electrons and positrons below 100–200 eV should only be considered as semi-quantitative estimates.

Non-relativistic optical-data models have so far been implemented in a few Monte Carlo codes to simulate inelastic collisions of electrons and positrons in condensed matter (see e.g. [23,24]). However, the extension of these or similar codes to higher relativistic energies requires the formulation of a fully relativistic optical-data model. In order to facilitate the eventual incorporation of the present model in a Monte Carlo code, we provide here a complete derivation of the cross sections needed for the random sampling of the energy loss and angular deflection of electrons and positrons in single inelastic events.

The paper is structured as follows. Section 2 summarizes the basic theory in a form suited to our purposes. In Section 3 we describe the optical-data model and derive explicit formulas for the DCSs for electrons and positrons. The density-effect correction to the stopping power is obtained from an algorithm due to Fano [5]; this algorithm only requires knowledge of the OOS. A simple approximation to account for the density effect on the DCSs is proposed. We also consider the angular deflections of the projectile’s trajectory caused by inelastic interactions. In Section 4, some calculation results are presented and compared with experimental data where those are available. Concluding remarks are given in Section 5. Finally, the appendices deal with the kinematics of inelastic collisions and the evaluation of restricted angular DCSs.

2. The Born approximation

In the early 1930s Bethe formulated the quantum theory of inelastic collisions of charged particles with individual atoms and molecules on the basis of the first-order plane-wave Born approximation [25,26]. The extension of the theory to inelastic collisions in condensed materials has been discussed by Fano [5]. The formal aspects of quantum theory for condensed matter are fairly involved. Fortunately, the results are essentially equivalent to those from the classical dielectric theory [27,28], in which the stopping power exerted on the charged particle is derived by using a Fourier decomposition of the field of the particle and the complex dielectric function $\epsilon(k, \omega)$, which describes the polarization and energy absorption of the medium when subjected to a monochromatic electromagnetic field with wavevector $k$ and frequency $\omega$. 
We consider inelastic collisions of fast electrons and positrons (rest mass \( m_e \), charge \( \mp e \)) in condensed matter. For the sake of simplicity in formulating the theory, we basically consider inelastic scattering in a single-element medium of atomic number \( Z \), mass density \( \rho \) and \( \mathcal{N} \) atoms per unit volume. At extremely relativistic energies, the collision stopping power of the medium is completely determined by the average electron density, \( \mathcal{N}/Z \), and can be expressed in terms of the quantity

\[
\Omega_p = \sqrt{4\pi Z \hbar^2 e^2 / m_e},
\]

which is the plasma energy of a homogeneous free-electron gas with the electron density of the medium. The present theory of inelastic collisions may be generalized to compounds (and mixtures) by interpreting \( Z \) as the number of electrons per molecule, and \( \mathcal{N} \) as the number of molecules per unit volume. Strictly speaking, though, this requires that the molecules may be regarded as randomly oriented, since the differential cross sections derived here are independent of the azimuthal scattering angle.

Let \( \mathbf{p} \) and \( E \) be the momentum and the kinetic energy of the projectile just before an inelastic collision, as seen from a reference frame where the stopping medium is at rest; the corresponding quantities after the collision are denoted by \( \mathbf{p}' \) and \( E' = E - W \), respectively, where \( W \) is the energy loss. Evidently, for positrons the maximum energy loss is \( W_{\text{max}} = E \). In the case of ionization by electron impact, owing to the indistinguishability between the projectile and the ejected electron, the maximum energy loss is \( W_{\text{max}} = (E + U_i)/2 \), where \( U_i \) is the ionization energy of the target electron. We recall that

\[
(cp^2)^2 = (E + 2m_e c^2) = (\beta \gamma m_e c^2)^2,
\]

where \( c \) is the velocity of light in vacuum, \( \gamma \) is the total energy in units of the rest energy, \( m_e c^2 \), and \( \beta \) is the velocity in units \( c \),

\[
\gamma \equiv \frac{E + m_e c^2}{m_e c^2} = \sqrt{\frac{1}{1 - \beta^2}},
\]

\[
\beta \equiv \frac{v}{c} = \sqrt{\frac{\gamma^2 - 1}{\gamma^2}} = \sqrt{\frac{E(E + 2m_e c^2)}{(E + m_e c^2)^2}}.
\]

The magnitude of the momentum \( \mathbf{p}' \) of the projectile after the inelastic collision is

\[
(c p')^2 = (E - W)(E - W + 2m_e c^2).
\]

The momentum transfer in the collision is \( \mathbf{q} \equiv \mathbf{p} - \mathbf{p}' \) and its magnitude is given by

\[
(cq)^2 = c^2(p^2 + p'^2 - 2pp' \cos \theta),
\]

where \( \theta \equiv \arccos(\mathbf{p} \cdot \mathbf{p}') \) is the polar scattering angle (Fig. 1).

After summing over degenerate final states of the target, the inelastic differential cross section (DCS) can be expressed in terms of \( W \) and \( \theta \). This corresponds to the DCS that would be obtained from experiments in which only the final state of the projectile is observed. Instead of the scattering angle, it is more convenient to use the recoil energy \( Q \) defined by [5]

\[
Q(Q + 2m_e c^2) = (cq)^2.
\]

When the collision is with a free electron at rest (binary collision), the energy loss is completely transformed into kinetic energy of the recoiling target electron, i.e. \( Q = W \). For interactions with bound electrons, the relation \( Q \approx W \) still holds if \( W \gg U_i \), i.e. when binding effects are negligible; we refer to these interactions as “hard ionizing collisions”.

The DCS per atom obtained from the relativistic quantum theory can be expressed as [5]

\[
\frac{d^3\sigma}{dWdQ} = \frac{d^3\sigma_L}{dWdQ} + \frac{d^3\sigma_T}{dWdQ},
\]

where

\[
\frac{d^3\sigma_L}{dWdQ} = \frac{2 \pi e^4}{m_e c^2 Q(1 + Q/2m_e c^2)} \frac{2Z}{\pi \Omega_p^2} \text{Im} \left( \frac{-1}{e(Q, W)} \right)
\]

\[
\frac{d^3\sigma_T}{dWdQ} = \frac{2 \pi e^4}{m_e c^2 Q(1 + Q/2m_e c^2)} \frac{2Z}{\pi \Omega_p^2} \text{Re} \left( \frac{-1}{e(Q, W)} \right)
\]

Fig. 1. Kinematics of inelastic collisions.
and

\[
\frac{d^2\sigma}{dWdQ} = \frac{2\pi e^4}{m_e v^2} 2(Q + m_e c^2) b^2 \sin^2 \theta_t \times \frac{2Z}{\pi Q_p^2} \text{Im} \left( \frac{1}{Q(Q + 2m_e c^2) - W^2 \epsilon(Q, W)} \right)
\]

(9)

are the contributions from longitudinal and transverse excitations, which are induced by the instantaneous Coulomb field and by the exchange of virtual photons, respectively. The quantity \( \theta_t \) is the angle between the initial momentum of the projectile and the momentum transfer (see Fig. 1) and is given by Eq. (113) in Appendix A. In writing the complex dielectric function as \( \epsilon(Q, W) = \epsilon_1(Q, W) + i \epsilon_2(Q, W) \) it is understood that \( Q \) and \( W \) are related to wavevector and frequency by \( q = \hbar k \) and \( W = \hbar \omega \); the DCS given by Eqs. (7)–(9) may in fact be obtained formally from the classical stopping power expression by assuming that momentum and energy are transferred from the projectile to the medium in quantized amounts \( \hbar k \) and \( \hbar \omega \). Expressions (7)–(9) and (113) constitute the basis of the present optical-data model calculations. However, knowledge of the dielectric function does not suffice to describe the energy spectrum and angular distribution of secondary knock-on electrons (delta rays).

The DCS obtained from the dielectric formulation generalizes the quantum result for atoms and molecules. This is seen by considering the case of a low-density medium, for which \( \epsilon_1 \approx 1 \) and \( \epsilon_2 \ll 1 \), in which case \( \text{Im}(-1/\epsilon) \approx \epsilon_2 \) and

\[
\text{Im} \left( \frac{1}{Q(Q + 2m_e c^2) - W^2 \epsilon(Q, W)} \right) \approx \frac{W^2 \epsilon_2}{[Q(Q + 2m_e c^2) - W^2 \epsilon_1]^2 + W^4 \epsilon_2^2} = \frac{W^2}{[Q(Q + 2m_e c^2) - W^2]^2} \text{Im} \left( \frac{-1}{\epsilon(Q, W)} \right).
\]

(10)

Inserting this approximation into Eq. (9) and using Eqs. (7)–(9), the DCS for our dilute medium simplifies to

\[
\frac{d^2\sigma}{dWdQ} = \frac{2\pi e^4}{m_e v^2} \left( \frac{1}{WQ(1 + Q/2m_e c^2)} \right. + \left. \frac{\beta^2 \sin^2 \theta_t W/2m_e c^2}{|Q(1 + Q/2m_e c^2) - W^2/2m_e c^2|^2} \right) \frac{df(Q,W)}{dW},
\]

(11)

where the last factor is the atomic generalized oscillator strength (GOS), defined as

\[
\frac{df(Q,W)}{dW} \equiv W(1 + Q/m_e c^2) \frac{2Z}{\pi Q_p^2} \text{Im} \left( \frac{-1}{\epsilon(Q, W)} \right).
\]

Expression (11) is consistent with the result from the first Born approximation for a single atom [5]. Eq. (12) thus establishes the connection between the GOS, an atomic property, and the dielectric function \( \epsilon \), a property of macroscopic matter, in the limit of low density.

In the derivation of Eqs. (7)–(9) explicit use is made of the assumption that the momentum transfer \( q \) is much smaller than the initial and final momenta of the projectile, i.e. \( q \ll p \) and \( q \ll p' \) (see e.g. [5]). This assumption is accurate when the incident particle is an ion, because in that case only small relative momentum transfers are allowed by energy and momentum conservation. For electron and positron collisions, however, relatively large momentum transfers occur with appreciable probability in “hard” collisions, i.e. where the energy transfer \( W \) is comparable to \( E \). Fernández-Varea et al. [29] have evaluated the longitudinal DCS for ionization of inner shells of free atoms without invoking the \( q \ll p' \) approximation; their result differs from expression (8) by a factor that reduces to unity for \( Q \ll W \ll E \) and also in the non-relativistic limit (i.e. when \( E, E' \ll m_e c^2 \)), even when \( q \) is comparable to the initial momentum. This factor introduces a significant correction (of the order of a few percent) to Eq. (8) only for hard collisions of relativistic projectiles. It is effective e.g. in the calculation of inner-shell ionization by impact of electrons and positrons with kinetic energy near the ionization threshold. Under these circumstances, however, the Born approximation is known to be very inaccurate (with and without the correcting factor). For hard interactions with
$Q \ll W$, which represent only a minor contribution to the integrated cross sections, we shall therefore retain the approximation $q \ll p_p'$, which leads to much simpler formulas. When $Q$ is comparable to $W$ (i.e. for close collisions) we will follow the usual procedure of invoking the approximation $Q \approx W$ and using, for electrons and positrons, the Möller [30] and Bhabha [31] cross sections, which describe binary collisions with free target electrons at rest.

We will now assume that the condensed-medium GOS (counted per atom) is defined by the expression (12). The longitudinal DCS (8) can then be written as

$$
\frac{d^2\sigma_L}{dWdQ} = \frac{2\pi e^4}{m_e^2} \frac{1}{WQ(1 + Q/2m_e^2)} \frac{df(Q, W)}{dW}.
$$

This expression is formally identical to that of the longitudinal DCS for a free atom. However, the GOS here pertains to the condensed medium and provides a complete description of the effect of condensation on the longitudinal interactions – for example, the possibility of plasmon excitation. In the limit $Q \rightarrow 0$, i.e. for vanishing momentum transfer, the GOS reduces to the optical oscillator strength (OOS) density $d(W)/dQ \equiv df(Q = 0, W)/dW$, which is related to the optical properties of the scattering medium through the prescription $W = h\omega$; to be precise, the OOS as defined here is given by Eq. (12) with $Q = 0$.

The transverse DCS (9) can also be expressed in an equivalent form that shows the dependence on the GOS more explicitly,

$$
\frac{d^2\sigma_T}{dWdQ} = \frac{2\pi e^4}{m_e^2} \frac{\beta^2 \sin^2 \theta, W/2m_e^2}{[Q(1 + Q/2m_e^2) - W^2/2m_e^2]^2} \times \frac{df(Q, W)}{dW} + \frac{d^2\Delta\sigma_T}{dWdQ}.
$$

The first term on the right-hand side is formally the same as the transverse DCS of a single atom [see Eq. (11)], but here it has the GOS of the condensed medium. The second term, $d^2\Delta\sigma_T/dWdQ$, is equal to the difference between the transverse DCS (9) and the first term,

$$
\frac{d^2\Delta\sigma_T}{dWdQ} = \frac{2\pi e^4}{m_e^2} \frac{2(Q + m_e^2)\beta^2 \sin^2 \theta,}{W(1 + Q/2m_e^2) - W^2/2m_e^2} \times \frac{2Z}{\pi\Omega_p^2} \text{Im} \left( \frac{\beta^2 \sin^2 \theta, W^2/2m_e^2}{Q(1 + Q/2m_e^2) - W^2/2m_e^2} \right)
$$

This quantity can be considered as a correction to the “atomic” DCS, which accounts for the effect of the polarizability of the medium on the transverse interactions, the so-called Fermi density effect [32]. For low-density materials ($\epsilon_1 \approx 1, \epsilon_2 \ll 1$) this correction vanishes.

3. Optical-data model

The GOS can be represented as a surface over the $(Q, W)$ plane, which is known as the Bethe surface [6]. Fig. 2 shows the Bethe surface for ionization of the hydrogen atom; this illustrates the conspicuous features of the GOS for ionization of inner shells. For large $Q$ the Bethe surface reduces to a ridge stretched out along the line $W = n/h\omega$. The surface is drawn in a $(Q/U, W/U)$ coordinate system, where $U = 1.36$ eV is the ionization energy of the ground state. All energies are in units of ionization energy $U_1 = 13.6$ eV. The GOS for ionization of (non-relativistic) hydrogenic ions is independent of $Z$ if energies are expressed in units of the ionization energy.

![Fig. 2. The GOS for ionization of the hydrogen atom (Z = 1) in the ground state. All energies are in units of the ionization energy U_1 = 13.6 eV. The GOS for ionization of (non-relativistic) hydrogenic ions is independent of Z if energies are expressed in units of the ionization energy.](image-url)
where the binding energy of the target electron is negligible compared with the energy transfer. In the region \( Q \ll W \), the Bethe surface is “flat” along the \( Q \) direction; this is the region where the dipole approximation is applicable. The GOS of the free-electron gas [27,33] also exhibits a Bethe ridge, but for low \( Q \) it is gradually replaced by a narrow resonance, the plasmon line, whose energy \( W_{\text{ph}}(Q) \) equals the plasma energy at \( Q = 0 \) [given by Eq. (1) with \( N/Z \) replaced by the electron density of the gas] and increases with \( Q \).

Closed, analytical calculations of the full GOS are possible only for the hydrogen atom (see e.g. [6]) and for the free-electron gas [27]. Numerical calculations of the GOS of many-electron free atoms are also available (see e.g. [34,35]), but they are based on approximate atomic wave functions, usually obtained from Dirac–Hartree–Slater self-consistent calculations (see e.g. [36]), and are adequate to describe excitations only of inner electron shells. An accurate (and necessarily numerical) calculation of the contribution to the GOS from valence-electron excitations in condensed matter seems at present to be very difficult. Moreover, using an inelastic DCS defined in terms of a numerical GOS makes it cumbersome to evaluate integrals of the DCS, and to perform Monte Carlo simulation (sampling) of inelastic interactions. It may therefore be concluded that an optimally accurate detailed GOS model is, for the present, conveniently obtained by means of optical-data models, where an approximate GOS for valence electron or outer shell excitations is constructed by extending – i.e., extrapolating – an experimentally-determined OOS to the region \( Q > 0 \) with the use of physically motivated “extension algorithms” [8,9,15,37]. This may also provide a suitable method for sampling inelastic interactions, i.e. the \( Q \) and \( W \) values, in a simulation. The contribution to the OOS from inner-shell excitations may be computed numerically from atomic wave functions or obtained from photoelectric data [15]. It should be noted, though, that also highly simplified models of the OOS are found to be sufficient for many purposes [38–41].

In terms of the real and imaginary parts of the frequency-dependent dielectric function in the

\[
W = Q,
\]

which corresponds to binary collisions where the binding energy of the target electron is negligible compared with the energy transfer. In the region \( Q \ll W \), the Bethe surface is “flat” along the \( Q \) direction; this is the region where the dipole approximation is applicable. The GOS of the free-electron gas [27,33] also exhibits a Bethe ridge, but for low \( Q \) it is gradually replaced by a narrow resonance, the plasmon line, whose energy \( W_{\text{ph}}(Q) \) equals the plasma energy at \( Q = 0 \) [given by Eq. (1) with \( N/Z \) replaced by the electron density of the gas] and increases with \( Q \).

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In terms of the real and imaginary parts of the frequency-dependent dielectric function in the
photoelectric cross sections extracted either from the LLNL Evaluated Photon Data Library [46,47] or from the XCOM program of Berger and Hubbell [48].

In the following we shall assume that the OOS of the considered material is known for all values of $W$. Since the empirical OOS is generated from available optical data and calculated inner-shell OOSs, it is affected by uncertainties in the original experimental data as well as by approximations in the calculated OOSs of inner shells. A basic consistency test is provided by the Thomas–Reiche–Kuhn sum rule or $f$-sum [42,50],

$$\frac{1}{Z} \int_{0}^{\infty} f(W) \, dW = 1.$$  \hspace{1cm} (18)

The $f$-sum rule checks the reliability of the OOS for intermediate $W$-values, where the integrand has the largest contributions. A test for the consistency of the low-$W$ behaviour of the OOS is provided by the perfect-screening sum rule or psi-sum [51,52],

$$\frac{\Omega_p^2}{Z} \int_{0}^{\infty} \frac{1}{W^2} f(W) \, dW + \frac{1}{\epsilon(0)} = 1,$$  \hspace{1cm} (19)

which expresses the fact that the material medium effectively screens static and low-frequency electromagnetic perturbations. For an electric conductor $\epsilon^{-1}(0) = 0$, whereas for an electric insulator $\epsilon^{-1}(0)$ is real and positive [51]. It should be kept in mind that empirical OOSs satisfy these sum rules only approximately, and this may have an effect on other “exact” integral properties of the OOS (see below).

While the first ingredient of an optical-data model is the OOS, the second ingredient is the extension algorithm, which generates the GOS from the OOS. We use here a new algorithm named the $N$-oscillator (Fig. 3), which is a generalization of the $\delta$-oscillator model used by Liljequist [38,39] and Salvat et al. [41]. The main reason for introducing the $N$-oscillator is that it largely removes the tendency – noted e.g. by Emfietzoglou [53] – of the $\delta$-oscillator to exaggerate stopping power and inelastic cross section at very low energies, without being much more complicated and without losing the desirable property of the $\delta$-oscillator of placing excitation thresholds correctly. An $N$-oscillator

![Figure 3](image-url)
with resonance energy \( W' \) is a very simple model of a contribution to the GOS, given by (see Fig. 3)

\[
F(W'; Q, W) = \delta(W - W' - BQ)\Theta(W' - Q) + \delta(W - Q)\Theta(Q - W'),
\]

where \( \delta(x) \) is the Dirac delta function, \( B \) is a constant that depends on the “resonance” energy \( W' \) and \( \Theta \) is the unit step function \([\Theta(x) = 0 \text{ if } x < 0 \text{ and } =1 \text{ if } x > 0]\). The first and second terms in this expression correspond to distant (“resonance”) and close (binary) collisions respectively.

In the expression \( \Theta(W - Q) \) is a contribution to the GOS, given by (see Fig. 3), which was proved to be adequate to describe the ionization of inner shells by electron impact [44]. Note further that the \( N \)-oscillator is normalized so that

\[
\int_0^\infty F(W'; Q, W) dW = 1 \quad \text{for any } Q.
\]

To generate the GOS density in the complete \( (Q, W) \) plane, we combine the empirical OOS density with the \( N \)-oscillator according to

\[
\frac{df(Q, W)}{dW} = \int_0^\infty \frac{df(W')}{dW'} F(W'; Q, W) dW'.
\]

When \( Q \to 0 \) the GOS reduces to the adopted empirical OOS; therefore Eq. (22) “extends” the OOS to finite values of \( Q \). This GOS model adequately describes the low-\( Q \) \( (Q < W) \) dipole-like region of the Bethe surface, but it gives a Bethe ridge with zero width, i.e. the broadening of the energy-loss spectrum of close interactions caused by the momentum distribution of the target electrons is neglected. This is not a serious drawback for electrons and positrons, but it introduces sizeable errors in the computed cross sections for slow, heavy charged particles, a fact that has been overlooked by some authors (e.g. [9]).

Notice that if the empirical OOS satisfies the \( f \)-sum rule, the GOS model (22) automatically satisfies the Bethe sum rule [6]

\[
\frac{1}{Z} \int_0^\infty \frac{df(Q, W)}{dW} dW = 1 \quad \text{for any } Q.
\]

In non-relativistic quantum theory, this sum rule can be derived (see e.g. [54]) by considering a central-field independent-electron model of the atom, such as the one resulting from Hartree–Fock–Slater self-consistent calculations [55]. Eq. (23) is also approximately valid for relativistic atomic models.

A perturbative calculation of relativistic corrections to the Bethe sum rule [56] indicates that these corrections increase with \( Z \) and decrease with \( \theta \); for the least favourable case analyzed in [56], \( Z = 86 \) and \( \theta = 0 \), they are less than 1.5%. For the sake of simplicity, here we shall assume that Eq. (23) holds in all cases. The Bethe sum rule, together with the physically sound shape of the GOS, ensures that the present optical-data model will yield reliable values of the stopping power of high-energy projectiles (see Section 3.2).

In the choice of the dispersion parameter \( B \) of the \( N \)-oscillator, we follow a method similar to that proposed by Fernández-Varea et al. [15,24]. For resonance energies \( W' > W_s \), where \( W_s \) is a suitably selected “switch” energy (see below), we use the \( \delta \)-oscillator model, i.e. \( B = 0 \). For \( W' < W_s \) we shall use the \( N \)-oscillator with

\[
B = 0.23717 + 0.32244 \rho^{1/3}.
\]

This \( W' \)-dependence of parameter \( B \) was determined by fitting the total cross sections and stopping cross sections obtained from the Lindhard theory for a free-electron gas with plasma resonance energy equal to \( W' \). Fig. 4 displays mean free paths and stopping powers \(^2\) of positrons in free-electron gases of different electron densities, corresponding to the indicated values of the plasma energy \( W' \), as functions of the kinetic energy \( E \) of the positron. The dashed curves were obtained from the non-relativistic Lindhard theory [27,33], using the numerical algorithm described by Salvat [57]. To account for (weak) relativistic effects, the non-relativistic Lindhard DCSs were multiplied by the global factor

\[
\frac{2E}{m_e c^2 \beta^2} = \frac{2(E + m_e c^2)^2}{m_e c^2 (E + 2m_e c^2)}.
\]

The continuous curves in Fig. 4 are results calculated using the \( N \)-oscillator with \( B \) given by Eq. (24) (as described in Section 3.1). It is seen that,

\(^2\) These quantities are defined in Section 3.1.
for energies $E$ larger than $\sim 5W'$, the $N$-oscillator does yield integrated cross sections in close agreement with the results from the Lindhard theory.

It is worth discussing the relation between the present optical-data model and previous ones. It seems that the first model of this kind was proposed by Penn [37]; it has been extensively used by Tanuma, Powell and Penn [4,10–12] to compute inelastic mean free paths of low-energy electrons in solids. In the original formulation of the Penn model, the medium is regarded as a statistical mixture of homogeneous electron gases of different densities, whose complex dielectric functions are approximated by means of the Lindhard [27] dielectric function of the free-electron gas. Penn’s approach is strictly equivalent to an optical-data model in which the extension algorithm is the GOS of a free-electron gas (the one associated with the Lindhard dielectric function). Although it is physically motivated for weakly bound electrons, the use of the Lindhard GOS complicates the calculations. A simplification of the Penn model was proposed by Ashley [8,9], who used an extension algorithm equivalent to $F_{\text{A}}(W'; Q, W) = \delta(W - (W' + Q))$ to compute mean free paths and stopping powers of low-energy electrons and positrons in a variety of substances. The Ashley model generates nearly the same GOS as the Penn model for small $Q$-values and it simplifies the calculations considerably; it has been frequently used, e.g. by Akkerman and Akkerman [17], Dingfelder et al. [58], Pimblott and Siebbeles [59] and Emfietzoglou [53]. Both methods predict that, for a given $W$, the GOS varies with $Q$ (dispersion), even when $Q$ is small. In particular, in the Ashley model the GOS is constant along the line $W = W' + Q$. This dispersion is plausible only for low-$W$ interactions (excitations of loosely bound electrons); for energy losses of the order of the ionization energy of bound shells, the GOS at a given $W$ is constant with $Q$ in the interval from $Q = 0$ up to $Q \approx W/2$ (see Fig. 2), where the dipole approximation is applicable. Incorrect dispersion leads to erroneous results in the case of collisions causing the ionization of an inner shell with ionization energy $U_i$; the Penn model allows ionizing collisions with $W < U_i$ (because the GOS of the free-electron gas does not vanish when $W$ is less than the plasmon energy – single electron excitations out of the Fermi sphere are possible down to zero energy transfer) and the Ashley model shifts the ionization threshold from $W = U_i$ to $W \approx 2U_i$ (for positron impact). The $\delta$-oscillator, on the other hand, provides an extension algorithm which is more appropriate for inner-shell ionization and keeps the threshold energy unaltered; Mayol and Salvat [44] have shown that it is equivalent to the Weizsäcker–Williams method of virtual quanta (see e.g. [60,28]). Unfortunately, all these models are essentially non-relativistic and, therefore, they are applicable only to electrons and positrons with moderate energies (less than about 50 keV).
An attempt to circumvent the computational difficulties with a free-electron gas GOS using the full Lindhard theory is represented by the two-modes model [15], which is an extension algorithm that closely reproduces the Lindhard theory stopping power and inelastic mean free path in a free-electron gas. It is in closer agreement with the Penn model, and thus with the Lindhard theory, than is the N-oscillator (with \( B \neq 0 \)), which in turn we find to be a better approximation than the Ashley model or the \( \delta \)-oscillator (see Fig. 2 in [61] and our Fig. 4). However, since the N-oscillator is adaptable to valence-electron (free-electron-like) excitations as well as to inner-shell ionizations and lends itself somewhat more easily to a fully relativistic treatment, we have preferred it over the two-modes model in the present work. In fact, most of the calculations with the N-oscillator can be done analytically (see below).

3.1. Differential and integrated cross sections

The contents of this section may be outlined as follows. The inelastic DCS \( \frac{d^2 \sigma}{dW \, dQ} \) is first expressed in terms of the OOS, combined with the DCS of an N-oscillator. Next, the DCS of the N-oscillator is split into parts due to close and distant interactions, and the latter are further split into longitudinal and transverse interactions. The calculations of the stopping power, the total cross section and the straggling parameter are outlined. The correction for the Fermi density effect modifies the transverse, distant interaction. Positrons and electrons are treated alike in distant interactions (exchange effects for the electrons are here neglected). In close interactions (on the Bethe ridge), the DCS for electrons is replaced by a modified Möller cross section, while for positrons it is replaced by the Bhabha cross section.

3.1.1. The basic DCS, excluding density effect

The DCS per atom resulting from our optical-data model, but still excluding the density effect, can be written as [see Eqs. (13), (14) and (22)]

\[
\frac{d^2 \sigma}{dW \, dQ} = \int_0^\infty \frac{d \sigma(W')}{dW'} \frac{d^2 \sigma_1(W')}{dW \, dQ} \, dW',
\]  

where

\[
\frac{d^2 \sigma_1(W')}{dW \, dQ} = \frac{2 \pi e^4}{m_e v^2} \left( \frac{1}{WQ(1 + Q/2m_e c^2)} \right. \\
+ \frac{\beta^2 \sin^2 \theta_W W/2m_e c^2}{[Q(1 + Q/2m_e c^2) - W^2/2m_e c^2]^2} \\
\times F(W'; Q, W)
\]  

may be regarded as the DCS for excitation of an N-oscillator with unit oscillator strength (in the sense of the Bethe sum rule) and resonance energy \( W' \) (“one-electron DCS”). This DCS is split into its close and distant contributions,

\[
\frac{d^2 \sigma_1(W')}{dW \, dQ} = \frac{d^2 \sigma_{1,\text{dis}}(W')}{dW \, dQ} + \frac{d^2 \sigma_{1,\text{clo}}(W')}{dW \, dQ}. 
\]

The one-electron DCS for close collisions \( (Q = W) \) with the oscillator is

\[
\frac{d^2 \sigma_{1,\text{clo}}(W')}{dW \, dQ} = \frac{2 \pi e^4}{m_e v^2} \frac{1}{W^2} \left( \frac{1}{1 + W/2m_e c^2} + \frac{\beta^2 \sin^2 \theta_W}{2m_e c^2} W \right) \\
\times \delta(W - Q) \Theta(W - W'),
\]

where \( \theta_c \) is the recoil angle \( \theta_c \) with \( Q = W \) [see Eq. (114)]; the two terms represent longitudinal and transverse interactions, respectively. In the case of electrons and positrons, this expression will eventually be replaced by the Möller and Bhabha cross sections, obtained from conventional quantum electrodynamics including exchange terms for electrons and annihilation-recreation for positrons.

The one-electron DCS for distant collisions with an oscillator (excluding the density-effect correction) is the sum of longitudinal (L) and transverse (T) contributions,

\[
\frac{d^2 \sigma_{1,\text{dis}}(W')}{dW \, dQ} = \frac{d^2 \sigma_{1,\text{dis,L}}(W')}{dW \, dQ} + \frac{d^2 \sigma_{1,\text{dis,T}}(W')}{dW \, dQ},
\]

which are given by

\[
\frac{d^2 \sigma_{1,\text{dis,L}}(W')}{dW \, dQ} = \frac{2 \pi e^4}{m_e v^2} \frac{1}{WQ(1 + Q/2m_e c^2)} \\
\times \delta(W - W' - BQ) \Theta(W' - Q)
\]

and

\[
\frac{d^2 \sigma_{1,\text{dis,T}}(W')}{dW \, dQ} = \frac{2 \pi e^4}{m_e v^2} \frac{\beta^2 \sin^2 \theta_W W/2m_e c^2}{[Q(1 + Q/2m_e c^2) - W^2/2m_e c^2]^2} \\
\times \delta(W - W' - BQ) \Theta(W' - Q),
\]
respectively. The contribution from distant transverse interactions is appreciable only for high-energy projectiles, whose kinetic energy is of the order of $m_e c^2$ or larger. Moreover, the most probable energy losses in these interactions are of the order of 10 eV, i.e. $W \ll m_e c^2$. Therefore, the minimum allowed recoil energy $Q_0$ given by Eq. (108), is much less than $W$. As discussed in Appendix A, in the DCS for distant transverse interactions we can approximate $\theta_r$ by $\tilde{\theta}_r$ (see Eqs. (115) and (116) and [5]). As $Q$ increases from $Q_-$ to $W$, $\cos^2 \tilde{\theta}_r$ varies from $\sim 1$ to $\sim 0$. Now, since the cross section (31) becomes very large – in fact, nearly diverges – at $Q_-$, no large error will be introduced if we set $B = 0$ (i.e. if we ignore the dispersion of the resonance line) in the calculation of the distant transverse DCS. Consequently, we will set

$$\frac{d^2 \sigma_{\text{dis},T}(W')}{dW dQ} \approx \frac{2\pi e^4}{m_e v^2} \frac{\beta^4 \sin^2 \tilde{\theta}_r}{W (1 - \beta^2 \cos^2 \tilde{\theta}_r)^2} \frac{d(-\cos^2 \tilde{\theta}_r)}{dQ} \times \delta(W - W') \Theta(W' - Q).$$ (32)

With these simplifications, the calculations become much easier.

### 3.1.2. Integrated cross sections

The energy-loss DCS is defined by

$$\frac{d \sigma}{dW} = \int_{Q_-}^{Q_+} \frac{d^2 \sigma}{dW dQ} dQ,$$ (33)

where $Q_-$ and $Q_+$ are the minimum and maximum kinematically allowed recoil energies given by Eq. (104).

We introduce the quantities

$$\sigma^{(n)} = \int_0^{W_{\text{max}}} W^n \frac{d \sigma}{dW} dW$$

$$= \sigma^{(0)} \int_0^{W_{\text{max}}} W^n \frac{1}{\sigma^{(0)}} \frac{d \sigma}{dW} dW = \sigma^{(0)} \langle W^n \rangle,$$ (34)

where $\langle W^n \rangle$ denotes the average value of $W^n$ in a single collision. Notice that $\sigma^{(0)}$ is the total inelastic cross section. $\sigma^{(1)}$ and $\sigma^{(2)}$ are known as the stopping cross section and the energy straggling cross section (for inelastic collisions), respectively. For computational purposes, it is convenient to write Eq. (34) in the form

$$\sigma^{(n)} = \int_0^{\infty} \frac{df(W')}{dW'} \sigma^{(n)}(W') dW',$$ (35)

where

$$\sigma^{(n)}(W') = \int_0^{W_{\text{max}}(W')} W^n \frac{d \sigma^{(1)}(W')}{dW} dW$$

$$= \int_0^{W_{\text{max}}(W')} dW W^n \int_{Q_-}^{Q_+} \frac{d^2 \sigma^{(1)}(W')}{dQ dW} dQ$$ (36)

are the total cross sections of order $n$ for a unit-strength $N$-oscillator with resonance energy $W'$. These are calculated as

$$\sigma^{(n)} = \sigma^{(n)}_{\text{dis}} + \sigma^{(n)}_{\text{clo}},$$ (37)

where

$$\sigma^{(n)}_{\text{dis}}(W') = \int_0^{W_{\text{max}}(W')} W^n \frac{d \sigma^{(1)}_{\text{dis}}(W')}{dW} dW$$ (38)

are the contributions due to distant ($k = \text{"dis"}$) and close ($k = \text{"clo"}$) interactions.

The mean free path $\lambda$ for inelastic collisions is given by

$$\lambda^{-1} = N \sigma^{(0)},$$ (39)

where $N$ is the number of atoms per unit volume. The stopping power $S$ and the energy straggling parameter $\Omega^2$ are defined by

$$S = N \sigma^{(1)} = \frac{\langle W \rangle}{\lambda},$$ (40)

and

$$\Omega^2 = N \sigma^{(2)} = \frac{\langle W^2 \rangle}{\lambda},$$ (41)

respectively. The quantity $\langle W \rangle = \sigma^{(1)}/\sigma^{(0)}$ is the average energy loss in a single collision. Evidently, the stopping power gives the average energy loss per unit path length. The product $\Omega^2 ds$ is the variance of the energy distribution of an originally monoenergetic beam after a short path length $ds$ (see e.g. [41]).

### 3.1.3. The density-effect correction

Let us now consider the density-effect correction, Eq. (15). This correction affects only distant (i.e. low-$Q$) transverse interactions; there is no need for a density correction for high-$Q$ transverse
excitations because the response of target electrons to these excitations is dominated by their inertia. It is thus convenient to introduce the variable $\vartheta_r$, Eq. (115) in Appendix A and write Eqs. (14) and (15) in the form

$$ \frac{d^2 \sigma_T}{dW \ dQ} = \frac{2\pi e^4}{m_e v^2 \pi \Omega_p^2} \left[ \frac{\beta^4 \sin^2 \vartheta_r}{(1 - \beta^2 \cos^2 \vartheta_r)^2} \right] \times \frac{d(-\cos^2 \vartheta_r)}{dQ} + \frac{d^2 \Delta \sigma_T}{dW \ dQ} \quad (42) $$

and

$$ \frac{d^2 \Delta \sigma_T}{dW \ dQ} = \frac{2\pi e^4}{m_e v^2 \pi \Omega_p^2} \left[ \frac{\beta^4 \sin^2 \vartheta_r}{\cos^2 \vartheta_r} \right] \left[ \frac{\beta^2 \cos^2 \vartheta_r}{1 - \beta^2 \cos^2 \vartheta_r} \right] \frac{d(-\cos^2 \vartheta_r)}{dQ} \left[ \frac{\epsilon_2}{(1 - \beta^2 \cos^2 \vartheta_r)^2} \right] \frac{d \Delta \sigma_T}{dW \ dQ}. \quad (43) $$

respectively. Since, for a given $W$, the various terms in these expressions increase rapidly when $Q$ decreases, to almost diverge at $Q_\ast$, we can replace the dielectric functions by their values at $Q = 0$, i.e. by the optical dielectric functions (until now, all calculations of the density effect have utilized this approximation; see e.g. [5,62]). Thus, the density-effect correction alters the transverse DCS only for low-$Q$ excitations and is completely determined by the optical dielectric function $\epsilon(W) = \epsilon_1(W) + i \epsilon_2(W)$.

To compute the corresponding energy-loss DCSs, we have to integrate the DCSs (42) and (43) over $Q$. The energy-loss DCS for distant transverse interactions is

$$ \frac{d \sigma_{\text{dist},T}}{dW} = \frac{2\pi e^4}{m_e v^2 \pi \Omega_p^2} \left[ \frac{\beta^4 \sin^2 \vartheta_r}{(1 - \beta^2 \cos^2 \vartheta_r)^2} \right] \frac{d(-\cos^2 \vartheta_r)}{dQ} \left[ \frac{\epsilon_2}{(1 - \beta^2 \cos^2 \vartheta_r)^2} \right] \frac{d \Delta \sigma_T}{dW} \quad (44) $$

The density-effect correction to the energy-loss DCS for distant transverse interactions can be evaluated analytically after removing the $Q$-dependence of the dielectric functions and replacing the upper integration limit $Q_\ast$ by $\infty$; we have [5]

$$ \frac{d \Delta \sigma_T}{dW} = \frac{2\pi e^4}{m_e v^2 \pi \Omega_p^2} \left[ \frac{\beta^2 \epsilon_2}{\epsilon_1^2} \right] \arctan \left( \frac{\beta^2 \epsilon_2}{1 - \beta^2 \epsilon_1} \right) + \frac{\epsilon_2}{\epsilon_1^2} \ln \left[ \frac{(1 - \beta^2 \epsilon_1)^2 + \beta^2 \epsilon_2^2}{\beta^2 \epsilon_2} \right] - \frac{\epsilon_2}{\epsilon_1^2} \ln \left( \frac{1}{1 - \beta^2} - \beta^2 \right) \right]. \quad (45) $$

The sum of the first and second terms in Eq. (45) equals the distant transverse DCS in the medium; the third term simply compensates for the free-atom-like transverse DCS that was added and subtracted in expression (14). The global density-effect correction on the stopping power is negative and vanishes for a low-density medium ($\epsilon_1 \to 1$, $\epsilon_2 \to 0$).

For practical calculations, it is advantageous to express the density-effect correction in terms of the inverse optical dielectric function $^3$

$$ \frac{1}{\epsilon(W)} \equiv \eta_1(W) - i \eta_2(W). \quad (46) $$

The real and imaginary parts of $\epsilon^{-1}(W)$ satisfy the Kramers–Kronig relation (see e.g. [63])

$$ \eta_1(W) = 1 - \frac{2}{\pi} \int_0^\infty \frac{W'}{W'^2 - W^2} \eta_2(W') dW', \quad (47) $$

where $P$ denotes the principal value of the integral. Moreover, from Eq. (12),

$$ \eta_2(W) = \text{Im} \left[ \frac{-1}{\epsilon(W)} \right] = \frac{\pi \Omega_p^2}{2Z} \frac{1}{W} \frac{df(W)}{dW}. \quad (48) $$

Thus, the functions $\eta_1(W)$ and $\eta_2(W)$ are both determined by the OOS. In terms of these functions, the density-effect correction (45) takes the form

$$ \frac{d \Delta \sigma_T}{dW} = \frac{2\pi e^4}{m_e v^2} \frac{df(W)}{dW} \left[ \frac{1}{2} \ln \left( \frac{\eta_1^2 + \eta_2^2}{\eta_1 (\eta_1 - \beta^2)^2 + \eta_2^2} \right) - \frac{\eta_1 - \beta^2}{\eta_2} \arctan \left( \frac{\eta_2}{\eta_1 (\eta_1 - \beta^2)^2 + \eta_2} \right) - \ln \left( \frac{1}{1 - \beta^2} - \beta^2 \right) \right]. \quad (49) $$

$^3 \eta_2 = \text{Im}(-1/\epsilon)$ is known as the energy-loss function.
and the energy-loss DCS for distant transverse interactions reads
\[
\frac{d\sigma_{\text{dist,T}}}{dW} = \frac{2\pi e^4}{m_e v^2} \frac{df(W)}{dW} \left\{ \frac{1}{2} \ln \left( \frac{\eta_1^2 + \eta_2^2}{(\eta_1^2 - \beta^2)^2 + \eta_3^2} \right) \right. \\
- \left. \frac{\eta_1 - \beta^2}{\eta_2} \arctan \left( \frac{\eta_3 \beta^2}{\eta_1 (\eta_1 - \beta^2) + \eta_2} \right) \right\}. \\
\tag{50}
\]

Although, in principle, the real and imaginary parts of the inverse dielectric functions are completely determined by the OOS, in practice we have to content ourselves with empirical OOSs which satisfy the sum rules only approximately. Inconsistencies in the adopted empirical OOS can affect the calculated \(\eta_i(W)\) and \(\eta_3(W)\) functions, where they can become magnified. For instance, in the case of electric conductors, from the Kramers–Kronig relation (47) we see that \(\eta_1(W)\) must tend to zero for small \(W\), because the “true” OOS satisfies the ps-sum rule (19). In reality, however, the empirical OOSs available verify the ps-sum rule only approximately and, therefore, the \(\eta_1(W)\) function calculated according to Eq. (47) behaves incorrectly for small \(W\) (it reaches a constant finite value when \(W\) decreases). Since these errors are difficult to control, it may be helpful to have alternative approximate methods to compute the density-effect correction to the stopping power and is completely defined by the OOS.

The calculation of the stopping power involves the integral
\[
\int_0^E W \frac{d\Delta\sigma_T}{dW} dW = -\frac{2\pi e^4}{m_e v^2} \frac{df(W)}{dW} \delta_F. \\
\tag{51}
\]

This equation defines \(\delta_F\), the Fermi density-effect correction to the stopping power, which has been studied extensively in the past [5,32,62,64]. Fano [5] has described a convenient method to compute \(\delta_F\) directly from the OOS. The recipe is
\[
\delta_F \equiv \frac{1}{2} \int_0^\infty \frac{df(W')}{dW'} \ln \left( 1 + \frac{L^2}{W'^2} \right) dW' - \frac{L^2}{Q_p} (1 - \beta^2), \\
\tag{52}
\]

where \(L\) is a real-valued function of \(\beta^2\) defined as the positive root of the following equation [64]:
\[
\mathcal{F}(L) \equiv \frac{1}{Z^2 \Omega_p^2} \int_0^\infty \frac{1}{W'^2 + L^2} \frac{df(W')}{dW'} dW' = 1 - \beta^2. \\
\tag{53}
\]

The function \(\mathcal{F}(L)\) decreases monotonically with \(L\), and hence, the root \(L(\beta^2)\) exists only if \(1 - \beta^2 < \mathcal{F}(0)\); otherwise \(\delta_F = 0\). Therefore, the function \(L(\beta^2)\) starts with zero at \(\beta^2 = 1 - \mathcal{F}(0)\) and grows monotonically with increasing \(\beta^2\). For an electrical conductor, \(\varepsilon^{-1}(0) = 0\) and \(\mathcal{F}(0) = 1\), by virtue of the ps-sum rule (19).

From Eq. (49) it is apparent that, at least for \(\beta \sim 1\) and \(\eta_1 \sim 1\), \(d\Delta\sigma_T/dW\) is roughly proportional to the OOS. This leads us to introduce the approximation
\[
\frac{d\sigma_{\text{dist,T}}}{dW} \simeq \frac{2\pi e^4}{m_e v^2} \frac{df(W)}{dW} \delta_F, \\
\tag{54}
\]

which is analytically simple and leads to the correct stopping power, although it may distort somewhat the \(W\)-dependence of the density correction for small energy losses. Therefore, when the inverse dielectric functions \(\eta_1(W)\) and \(\eta_3(W)\) are not available, it is reasonable to assume that
\[
\frac{d\sigma_{\text{dist,T}}}{dW} \simeq \frac{2\pi e^4}{m_e v^2} \frac{df(W)}{dW} \left[ \ln \left( \frac{1}{1 - \beta^2} \right) - \beta^2 - \delta_F \right]. \\
\tag{55}
\]

### 3.1.4. Distant interaction cross sections

From the discussion after Eqs. (42) and (43) it is clear that Eq. (42) is consistent with the DCS for distant transverse interactions (32) derived above for a single unit-strength oscillator. Accordingly, we can express the DCS for distant transverse interactions with an oscillator in a condensed medium as
\[
\frac{d^2\sigma_{\text{1,dist,T}}(W')}{dW dQ} \simeq \frac{2\pi e^4}{m_e v^2} \frac{2\pi \beta^2 \sin^2 \theta_r}{\pi \Omega_p^2} \text{Im} \left( \frac{1}{1 - \beta^2 \cos^2 \theta_r} \epsilon(W) \right) \\
\times \frac{d(-\cos^2 \theta_r)}{dQ} \delta(W - W') \Theta(W' - Q). \\
\tag{56}
\]
Let us now consider the calculation of integrated cross sections for distant interactions with a unit N-oscillator,
\[
\sigma^{(n)}_{\text{dis},L}(W') = \sigma^{(n)}_{\text{dis},L}(W') + \sigma^{(n)}_{\text{dis},T}(W').
\]
(57)
The contributions from longitudinal (K = “L”) and transverse (K = “T”) interactions are
\[
\sigma^{(n)}_{\text{dis},K}(W') = \int \int dQ W W' \frac{\partial^2 \sigma_{\text{dis},K}(W')}{\partial W \partial Q},
\]
(58)
where the integrals extend over the kinematically allowed domain.

The contribution due to distant transverse interactions can be readily calculated from the energy-loss DCS [cf. Eq. (50)]
\[
\frac{d\sigma_{\text{dis},T}(W')}{dW} = 2\pi^4 \frac{1}{m_e v^2} \frac{1}{W} \left( \frac{1}{2} \ln \left( \frac{\eta_1^2 + \eta_2^2}{(\eta_1 - \beta^2)^2 + \eta_2^2} \right) - \frac{\eta_1 - \beta^2}{\eta_2} \arctan \left( \frac{\eta_2 \beta^2}{\eta_1 (\eta_1 - \beta^2) + \eta_2} \right) \right) \times \delta(W - W'),
\]
(59)
obtained by integrating Eq. (56) over Q following the same steps as above. The integration over W is trivial and gives
\[
\sigma^{(0)}_{\text{dis},T}(W') = 2\pi^4 \frac{1}{m_e v^2} \frac{1}{W} \left( \frac{1}{2} \ln \left( \frac{\eta_1^2 + \eta_2^2}{(\eta_1 - \beta^2)^2 + \eta_2^2} \right) - \frac{\eta_1 - \beta^2}{\eta_2} \arctan \left( \frac{\eta_2 \beta^2}{\eta_1 (\eta_1 - \beta^2) + \eta_2} \right) \right),
\]
(60)
\[
\sigma^{(1)}_{\text{dis},T}(W') = W' \sigma^{(0)}_{\text{dis},T}(W'),
\]
\[
\sigma^{(2)}_{\text{dis},T}(W') = W'^2 \sigma^{(0)}_{\text{dis},T}(W').
\]
(61)

With the approximation (55), we have
\[
\frac{d\sigma_{\text{dis},T}(W')}{dW} \simeq 2\pi^4 \frac{1}{m_e v^2} \frac{1}{W} \left( \frac{1}{2} \ln \left( \frac{1}{1 - \beta^2} \right) - \beta^2 - \delta \right) \delta(W - W'),
\]
(62)
and
\[
\sigma^{(0)}_{\text{dis},T}(W') \simeq 2\pi^4 \frac{1}{m_e v^2} \frac{1}{W} \left[ \ln \left( \frac{1}{1 - \beta^2} \right) - \beta^2 - \delta \right].
\]
(63)

On the other hand, the DCS for distant longitudinal interactions with an oscillator is given by Eq. (30). To obtain the integrated cross sections for these interactions, it is convenient to first perform in Eq. (58) the integral over W, which gives
\[
\sigma^{(n)}_{\text{dis},L}(W') = \frac{2\pi^4}{m_e v^2} \frac{\pi}{Q^2} \int_{Q_{\text{min}}}^{Q_{\text{max}}} \frac{(W' + BQ)^n}{Q(-Q/2m_e^2)} dQ.
\]
(64)
The integral extends over the Q-interval where the resonance line \( W = W' + BQ \) lies below the energy-momentum conservation limit \( W = W_m(Q) \), Eq. (109). For sufficiently high energies, the equation \( W' + BQ = W_m(Q) \) has two real roots, \( \bar{Q}_- \) and \( \bar{Q}_+ \) (\( \bar{Q}_- < \bar{Q}_+ \)) and then \( Q_{\text{min}} = \bar{Q}_- \) and \( Q_{\text{max}} = \min(\bar{Q}_+, W') \); for low energies, for which this equation has no real roots, \( \sigma^{(n)}_{\text{dis},L}(W') = 0 \). The evaluation of the integrals (65) for \( n = 0 \), 1, and 2 is elementary,
\[
\sigma^{(0)}_{\text{dis},L}(W') \simeq \frac{1}{m_e v^2} \frac{1}{W} \ln \left( \frac{W'}{W' + BQ} \right) \int_{Q_{\text{min}}}^{Q_{\text{max}}} \frac{1}{W' + BQ} \ln \left( \frac{W' + BQ}{Q + 2m_e c^2} \right) dQ,
\]
(65)
\[
\sigma^{(1)}_{\text{dis},L}(W') \approx \frac{2\pi^4}{m_e v^2} \left[ \ln \left( \frac{W'}{Q + 2m_e c^2} \right) \right]_{Q_{\text{min}}}^{Q_{\text{max}}},
\]
(66)
and
\[
\sigma^{(2)}_{\text{dis},L}(W')
\approx \frac{2\pi^4}{m_e v^2} \left[ \ln \left( \frac{W'}{W' - 2m_e^2 c^2} \right) \ln \left( \frac{Q + 2m_e c^2}{Q + 2m_e c^2} \right) \right]_{Q_{\text{min}}}^{Q_{\text{max}}},
\]
(67)
For the \( \delta \)-oscillator (i.e. for \( B = 0 \)), these expressions take the following simpler forms:
\[
\sigma^{(1)}_{\text{dis},L}(W') = \frac{2\pi^4}{m_e v^2} \left[ \ln \left( \frac{Q}{Q + 2m_e c^2} \right) \right]_{Q_{\text{min}}}^{Q_{\text{max}}} W',
\]
(68)
\[
\sigma^{(0)}_{\text{dis},L}(W') = \sigma^{(1)}_{\text{dis},L}(W') / W',
\]
\[
\sigma^{(2)}_{\text{dis},L}(W') = \sigma^{(1)}_{\text{dis},L}(W') W'.
\]
(68)
It is interesting to observe that the stopping cross sections \( \sigma^{(1)}_{\text{dis},L} \) for the \( N \)- and \( \delta \)-oscillators differ only in the integration limits and that, for energies
\( E \) substantially larger that \( W' \), they are approximately equal. In other words, in the limit of high energies \( (E \gg W') \), the contribution of distant longitudinal interactions to the stopping cross sections is independent of the “slope” \( B \) of the resonance line, \( W = W' + BQ \), and is determined by the resonance energy \( W' \) of the oscillator.

3.1.5. Close interaction cross sections for electrons

When the projectile is an electron, the one-electron DCS must be corrected to account for the indistinguishability of the projectile and the target electrons (exchange correction). For distant low-\( Q \) interactions, this correction is expected to be small (see e.g. [65,66]) and will be disregarded. The cross sections for distant interactions of electrons are then given by the expressions obtained above, Eqs. (57)–(68).

The energy-loss DCS for close collisions of electrons with a unit-delta oscillator is given by the modified Møller formula [15,30], cf. Eq. (28),

\[
\frac{d\sigma_{1,\text{clo}}(W')}{dW} = \frac{2\pi e^4}{m_e v^2 W^2} \left[ 1 + \left( \frac{W}{E + W' - W} \right)^2 \right. \\
\left. - \frac{(1-a)W}{E + W' - W} + \frac{aW^2}{(E + W')^2} \right]\Theta(W - W'),
\]

where

\[
a = \left( \frac{E}{E + m_e c^2} \right)^2 = \left( \frac{\gamma - 1}{\gamma} \right)^2.
\]

The allowed energy losses in electron collisions lie in the interval from \( W' \) to a certain maximum value, which we set equal to

\[
W_{\text{max}}(W') = (E + W')/2.
\]

This can be justified by regarding \( W' \) as a kind of binding energy of the target electron and considering that after the interaction the kinetic energy of the recoiling target electron is \( W' - W' \), while that of the projectile is \( E - W \) [8]. We consider that the “primary” electron is that with the larger kinetic energy after the interaction and, therefore, the maximum energy transfer is \( (E + W')/2 \) (as when \( W = W_{\text{max}} \) the two electrons have the same final kinetic energy). This recipe preserves the ionization threshold of the oscillator at \( E = W' \), which is consistent with the interpretation of \( W' \) as its binding energy.

The one-electron total cross sections \( \sigma_{1,\text{clo}}^{(n)} \) are obtained from Eq. (38). The integrals are elementary; explicitly, for \( n = 0, 1 \) and 2 we have

\[
\sigma_{1,\text{clo}}^{(0)}(W') = \frac{2\pi e^4}{m_e v^2 \left[ \left( \frac{1}{W} + \frac{1}{E + W' - W} + \frac{1-a}{E + W'} \right)^2 \right. \\
\left. \times \ln \left( \frac{E + W' - W}{W} \right) + \frac{aW}{(E + W')^2} \right] W_{\text{max}}^{W'}
\]

(72)

\[
\sigma_{1,\text{clo}}^{(1)}(W') = \frac{2\pi e^4}{m_e v^2 \left[ \ln W + \frac{E + W'}{E + W' - W} + (2-a) \right. \\
\left. \times \ln(E + W' - W) + \frac{aW^2}{2(E + W')^2} \right] W_{\text{max}}^{W'}
\]

(73)

and

\[
\sigma_{1,\text{clo}}^{(2)}(W') = \frac{2\pi e^4}{m_e v^2 \left[ (2-a)W + \frac{2(E + W')^2 - W^2}{E + W' - W} \right. \\
\left. + (3-a)(E + W') \ln(E + W' - W) \right. \\
\left. + \frac{aW^3}{3(E + W')^3} \right] W_{\text{max}}^{W'}
\]

(74)

if \( W_{\text{max}} > W' \); otherwise they all vanish.

3.1.6. Close interaction cross sections for positrons

The cross sections for distant interactions of positrons with an oscillator are given by the expressions obtained above, Eqs. (57)–(68). Therefore, we only need to consider the cross sections for close collisions.

The energy-loss DCS for close collisions is given by the Bhabha [31] formula,

\[
\frac{d\sigma_{1,\text{clo}}(W')}{dW} = \frac{2\pi e^4}{m_e v^2 W^2} \left[ 1 - b_1 \frac{W}{E} + b_2 \left( \frac{W}{E} \right)^2 \\
- b_3 \left( \frac{W}{E} \right)^3 + b_4 \left( \frac{W}{E} \right)^4 \right] \Theta(W - W'),
\]

(75)
where

\[ b_1 = \left( \frac{\gamma - 1}{\gamma} \right)^2 \frac{2(\gamma + 1)^2 - 1}{\gamma^2 - 1}, \]
\[ b_2 = \left( \frac{\gamma - 1}{\gamma} \right)^2 \frac{3(\gamma + 1)^2 + 1}{(\gamma + 1)^2}, \]
\[ b_3 = \left( \frac{\gamma - 1}{\gamma} \right)^2 \frac{2(\gamma - 1)}{(\gamma + 1)^2}, \]
\[ b_4 = \left( \frac{\gamma - 1}{\gamma} \right)^2 \frac{\gamma - 1}{(\gamma + 1)^2}. \]

The allowed energy losses lie in the interval \((W', E)\).

As in the case of electrons, the one-electron total cross sections \(\sigma_{\text{clo}}^{(0)}\), for close collisions of positrons with an oscillator can be evaluated analytically. For the total, stopping and energy straggling cross sections we have

\[
\sigma_{\text{clo}}^{(0)}(W') = \frac{2\pi e^4}{m_e v^2} \left[ -\frac{1}{W} - b_1 \ln \frac{W}{E} + b_2 \frac{W}{E^2} - b_3 \frac{W^2}{2E^3} + b_4 \frac{W^3}{3E^4} \right] E^{W'},
\]

(76)

\[
\sigma_{\text{clo}}^{(1)}(W') = \frac{2\pi e^4}{m_e v^2} \left[ \ln W - b_1 \frac{W}{E} + b_2 \frac{W^2}{2E^2} - b_3 \frac{W^3}{3E^3} + b_4 \frac{W^4}{4E^4} \right] E^{W'},
\]

(77)

\[
\sigma_{\text{clo}}^{(2)}(W') = \frac{2\pi e^4}{m_e v^2} \left[ W - b_1 \frac{W^2}{2E} + b_2 \frac{W^3}{3E^2} - b_3 \frac{W^4}{4E^3} + b_4 \frac{W^5}{5E^4} \right] E^{W'},
\]

(79)

if \(E > W'\); otherwise they all vanish.

### 3.2. Stopping power of high-energy electrons and positrons

It is of interest to evaluate explicitly the collision (non-radiative) stopping power for projectiles with high energies \((E \gg W')\). We shall assume that \(W'\), which is of the order of the ionization energies \(U_i\) of the target atoms, is much less than \(2m_e c^2\) (for the most unfavourable case of the K shell of heavy elements, \(U_i\) is of the order of \(2m_e c^2/10\)). Under these circumstances, \(Q_- \ll 2m_e c^2\) and we can use the approximation [see Eq. (108)]

\[
Q_- \approx \frac{W^2}{(2m_e c^2 \beta^2)}.
\]

(80)

The contribution of close interactions is given by [see Eqs. (73) and (78)]

\[
\sigma_{\text{clo}}^{(1)} = \int_0^\infty \frac{df(W')}{dW'} \sigma_{\text{clo}}^{(1)}(W')dW'.
\]

(81)

Recalling that \(E \gg W'\), we have

\[
\sigma_{\text{clo}}^{(1)} \simeq \frac{2\pi e^4}{m_e v^2} \int_0^\infty \frac{df(W')}{dW'}
\]

\[
\times \left\{ \ln \frac{E}{W'} + 1 - \left[ 1 + \beta^2 + 2\sqrt{1 - \beta^2} \right] \ln 2
\]

\[
+ \frac{1}{8} \left( 1 - \sqrt{1 - \beta^2} \right)^2 \right\} \Theta(W_{\text{max}} - W')dW'.
\]

(82)

for electrons and

\[
\sigma_{\text{clo}}^{(1)} \simeq \frac{2\pi e^4}{m_e v^2} \int_0^\infty \frac{df(W')}{dW'}
\]

\[
\times \left\{ \ln \frac{E}{W'} - b_1 + b_2 - b_3 + \frac{b_4}{2} \right\}
\]

\[
\times \Theta(W_{\text{max}} - W')dW'.
\]

(83)

for positrons. The contribution from distant (longitudinal and transverse) interactions to the stopping cross section [see Eqs. (67) and (55)] can be expressed as

\[
\sigma_{\text{dis}}^{(1)}(W') \simeq \frac{2\pi e^4}{m_e v^2} \int_0^{W_{\text{max}}} \frac{df(W')}{dW'}
\]

\[
\times \left\{ \ln \frac{E}{W'} + \ln[2(\gamma + 1)] - \beta^2 - \delta_1 \right\} dW'.
\]

(84)

For high-energy projectiles \((E \gg W')\), the upper limit \(W_{\text{max}}\) of the integrals over \(W'\) can be replaced by \(\infty\). It is customary to introduce the mean excitation energy \(I\), defined by (see e.g. [5])

\[
\ln I = \left[ \int_0^\infty \frac{df(W')}{dW'} dW' \right]^{-1} \int_0^\infty \ln W' \frac{df(W')}{dW'} dW'.
\]

(85)
Then, adding both the distant and close stopping cross sections, and using the $f$-sum rule (18), we arrive at the familiar Bethe formula for the stopping power,

$$S \approx N \left( \sigma_{\text{dis}}^{(1)} + \sigma_{\text{clo}}^{(1)} \right)$$

$$\simeq N \frac{2\pi e^4}{m_e v^2} Z \left\{ \ln \left( \frac{E^2}{I} \right) + f^{(+)}(\gamma) - \delta_F \right\},$$

(86)

where

$$f^-(\gamma) = 1 - \beta^2 - \frac{2\gamma - 1}{\gamma^2} \ln 2 + \frac{\gamma - 1}{8} \left( \frac{\gamma - 1}{\gamma} \right)^2$$

(87)

and

$$f^{(+)}(\gamma) = 2 \ln 2$$

$$- \frac{\beta^2}{12} \left[ 23 + \frac{14}{\gamma + 1} + \frac{10}{(\gamma + 1)^2} + \frac{4}{(\gamma + 1)^3} \right]$$

(88)

for electrons and positrons, respectively. Apart from $\delta_F$, this formula can be derived from very general arguments that do not require knowledge of the fine details of the GOS; the only information needed is contained in the $f$-sum rule (18) and in the definition (85) of the mean excitation energy (see e.g. [5]). Since the GOS from our optical-data model is physically motivated, satisfies the $f$-sum rule and is assumed to reproduce the adopted value of $I$, it yields the Bethe stopping power formula.

It is striking that the “asymptotic” Bethe formula is in fact valid down to fairly small energies, of the order of 10 keV for high-$Z$ materials (see Section 4). When valid, it also accounts for the differences between the stopping powers of electrons and positrons, to the same degree of accuracy as our GOS model approximation.

In the high-energy limit ($\beta \rightarrow 1$), the $L$ value resulting from Eq. (53) is large and can be approximated as $L^2 = \Omega_p^2 / (1 - \beta^2)$. Inserting this value in expression (52), using the $f$-sum rule (18) and the relation (85), we obtain

$$\delta_F \approx \ln \left( \frac{\Omega_p^2}{(1 - \beta^2)I^2} \right) - 1, \quad \text{when } \beta \rightarrow 1.$$  

(89)

For ultrarelativistic projectiles, for which this approximation holds, the Bethe formula simplifies to

$$S \simeq N \frac{2\pi e^4}{m_e v^2} Z \left\{ \ln \left( \frac{E^2}{I^2} \right) + f^{(+)}(\gamma) + 1 \right\},$$

(90)

The mean excitation energy $I$ has disappeared from this formula, showing that at very high energies the collision stopping power depends only on the electron density $N Z$ of the medium.

### 3.3. Angular deflections in inelastic collisions

For practical Monte Carlo simulations of high-energy electron/positron transport (see e.g. [1]) it is of interest to consider the angular deflections of the projectile due to inelastic collisions. In these simulations, angular deflections caused by elastic collisions are described by multiple-scattering theories, such as those of Molière [67], Goudsmit and Saunderson [68,69] and Lewis [70]. Several Monte Carlo codes describe the energy loss resulting from multiple inelastic collisions by means of the theory of Landau [71] or one of its various improved versions. These energy straggling theories do not account for inelastic scattering (deflection), which must be described by other means. The inelastic DCS differential in the scattering angle can be calculated approximately from the Morse formula (Eq. (4.70) in [6]), which expresses the angular DCS in terms of the incoherent scattering function. This was the approach followed by Fano [72] in order to introduce scattering by (atomic) electrons in the multiple-scattering theory of Molière [67]. However, the DCS calculated in this way is only a rough approximation. Moreover, it accounts for all excitations and, hence, it is not adequate for mixed (class II) simulations, where the part of electron scattering due to hard inelastic collisions is explicitly simulated. The present optical-data model provides a more consistent method to determine the angular DCS, differential in the scattering angle, either in its complete form or restricted to collisions with energy loss less than a certain cutoff value $W_c$. 
It is convenient to measure angular deflections in terms of the variable
\[ \mu \equiv \frac{(1 - \cos \theta)}{2}, \]
which is related to the recoil energy through
\[ Q(\theta) = Q_0 + 2m_e c^2 \left( (c \rho - c \rho')^2 + 4c \rho c \rho' \mu \right). \]
The quantity of interest is the inelastic DCS, differential in \( \mu \), restricted to collisions with energy losses less than a chosen value \( W_c \), which is given by
\[ \frac{d\sigma(W_c)}{d\mu} = \int_0^{W_c} \frac{d^2\sigma}{dWdQ} dW, \] (93)
where
\[ Q = \sqrt{(c \rho - c \rho')^2 + 4c \rho c \rho' \mu + m_e^2 c^4 - m_e^2 c^2}. \] (94)
In principle, Eq. (93) has to be evaluated numerically. This task is facilitated to a large extent by using an optical-data model, because the one-electron cross sections have analytical expressions and the numerical work then reduces to integrals of these functions times the OOS. Explicit formulas for the restricted angular DCS using the present optical-data model are given in Appendix B. Notice that if we set \( W_c = W_{\text{max}} \) in Eq. (93), the integral of the angular DCS equals the total cross section,
\[ \sigma^{(0)} = \int_0^1 \frac{d\sigma(W_{\text{max}})}{d\mu} d\mu. \] (95)
This equality may be used to check the correctness of the numerical calculation of the restricted angular DCS (93).

As mentioned above, the deflections caused by inelastic collisions (only “soft” interactions, i.e., those with \( W < W_c \), in the case of class II simulation schemes) add to those produced by elastic collisions. The exact angular distribution after a given path length (ignoring energy losses) can be calculated by means of the multiple-scattering theory of Goudsmit and Saunderson [68,69] (see also [73]), in which the angular distribution is completely determined by the Legendre moments of the single-scattering distribution, i.e., by the transport cross sections. The contribution of inelastic scattering to the \( \ell \)th transport cross section is
\[ \sigma_{\text{inel,}\ell}(W_c) \equiv \int_0^1 [1 - P_{\ell}(\cos \theta)] \frac{d\sigma(W_c)}{d\mu} d\mu, \] (96)
where \( P_{\ell}(\cos \theta) \) is the Legendre polynomial of order \( \ell \). In certain simulation schemes (e.g., that adopted in the Monte Carlo simulation code PENelope [41]) the information needed to describe the effect of soft inelastic scattering reduces to the first and second inelastic transport cross sections, \( \sigma_{\text{inel,1}}(W_c) \) and \( \sigma_{\text{inel,2}}(W_c) \); these are given by
\[ \sigma_{\text{inel,1}}(W_c) = 2\sigma^{(0)}(W_c) \langle \mu \rangle \] and
\[ \sigma_{\text{inel,2}}(W_c) = 6\sigma^{(0)}(W_c) \langle \mu^2 \rangle, \]
where \( \sigma^{(0)}(W_c) \) is the total inelastic cross section for \( W < W_c \) and
\[ \langle \mu^n \rangle = \frac{1}{\sigma^{(0)}(W_c)} \int_0^1 \mu^n \frac{d\sigma(W_c)}{d\mu} d\mu. \] (98)
are the moments of the angular deflection in single soft inelastic collisions. In the high-energy limit, when \( \langle \mu^2 \rangle \ll \langle \mu \rangle \ll 1 \), the numerical calculation of the second inelastic transport cross section becomes unstable and we must rely on the asymptotic relation \( \sigma_{\text{inel,2}}(W_c) \approx 3\sigma_{\text{inel,1}}(W_c) \). The (restricted) inelastic first and second transport mean free paths are defined by
\[ \lambda_{\text{tr,1}}(W_c) = \frac{1}{\mathcal{N} \sigma_{\text{inel,1}}(W_c)} \] and
\[ \lambda_{\text{tr,2}}(W_c) = \frac{1}{\mathcal{N} \sigma_{\text{inel,2}}(W_c)}. \] (99)

4. Examples and discussion

As indicated in Section 3, the OOS of a condensed material is constructed by combining available “experimental” OOS data for low-energy losses with calculated OOS (or photoelectric cross sections) for inner-shell ionization in the high-\( W \) domain. A compilation of measured optical functions for a number of solids (metals, semiconductors and insulators) is given by Palik [42]. The experimental information is available either as the real and imaginary parts of the optical dielectric
function or as the refraction index and the extinction coefficient.

The substances considered in the present calculations are the metals aluminium, copper and gold and the semiconductor silicon. For Al we used the table of optical dielectric functions given by Shiles et al. [74] and Smith et al. [75], who performed a thorough study of the optical properties of this metal and tabulated its optical functions in the range from 0.01 eV to 10 keV. We extended the table to higher energies with the aid of total photoelectric cross sections obtained from the EPDL [46, 47]. For Si we have made use of the data tabulated by Smith et al. [75] by less than 1%.

For Cu and Au we prepared by Bichsel [76], which cover the whole energy range of interest. For Cu and Au we combined optical functions from Palik [42] with photoabsorption cross sections from the EPDL table to higher energies with the aid of total photoelectric conductors Al and Cu [for which \( e^{-1}(0) = 0 \)]. In the case of Si, and for any insulator or semiconductor, the ps-sum rule is satisfied exactly, because the value of \( e^{-1}(0) \) is calculated precisely according to Eq. (19). The calculated values of the mean excitation energy agree well with the ICRU Report 37 [3] recommended values, except for Au. Table 1 also lists the \( W_c \) energies adopted in the present calculations, which are placed at the smallest core-level ionization energy of each material [15].

The real and imaginary parts \( \eta_1(W) \) and \( \eta_2(W) \) of the inverse dielectric function are determined from the OOS. \( \eta_2(W) \) is obtained according to Eq. (48) and \( \eta_1(W) \) is computed using the Kramers–Kronig relation, Eq. (47). In the case of electric conductors, possible departures from the ps-sum rule (19) are partially corrected by “renormalizing” the integral as follows:

\[
\eta_1(W) = 1 - \left[ \int_0^\infty \frac{1}{W^2} \frac{df(W')}{dW'} \, dW' \right]^{-1}
\]

\[
\times P \int_0^\infty \frac{1}{W'^2 - W^2} \frac{df(W')}{dW'} \, dW'.
\]

If the OOS is known to enough accuracy, the functions \( \eta_1(W) \) and \( \eta_2(W) \) can be employed to compute the DCS for distant transverse interactions without relying on the approximation (55); these calculations can be used to check the accuracy of this approximation. Fig. 6 displays \( \epsilon_1(W) \) and \( \epsilon_2(W) \) of Al and Si evaluated from the OOSs shown in Fig. 5 using Eqs. (46)–(48). In the low-energy-loss range, the “reconstructed” optical dielectric functions agree well with the original experimental optical data from which the OOS was generated. For metallic Al the reconstructed \( \epsilon_1 \) and \( \epsilon_2 \) differ from the data tabulated by Smith et al. [75] by less than 1%.

Fig. 7 shows the density-effect correction \( \delta_F \) for Al, Si and Au computed from Eqs. (52) and (53), as a function of the kinetic energy of the projectile. In the case of Al, our results practically coincide with those of Inokuti and Smith [64] for energies of the order of 50 keV and larger, because we use essentially the same OOS (although our interpolation and integration algorithms are different). For lower energies, where the density effect is negligible, our \( \delta_F \) values differ substantially from those of Inokuti and Smith. The reason is that our numerical OOS deviates slightly from the ps-sum rule, see Table 1. This kind of low-energy inconsistency, which will very likely occur for all materials, does not affect the accuracy of the numerical results owing to the smallness of the density effect at these energies. For electric insulators and semiconductors such as Si, \( \delta_F \) vanishes for slow projectiles, see Fig. 7.

A remark regarding the effects of the approximation (55) is in order. Calculations avoiding this approximation [i.e. using the exact formula (50)] show that the stopping power \( S \), the energy straggling parameter \( \Omega^2 \) and the transport mean free paths \( \lambda_{tr,1} \) and \( \lambda_{tr,2} \) (unrestricted, with \( W_c = E \)) are practically not affected by the approximation (the largest relative error introduced in these quantities is less than 0.2% for \( E < 1 \) GeV). However, the use of Eq. (55) does influence the total cross section and the mean free path; the error in \( \sigma \) is negligible for energies less than \( \sim 250 \) keV, but increases with energy, and is about 2% at 500 keV and up to 20% at 1 GeV. This error arises from the fact that expression (55) gives an energy-loss
spectrum for distant transverse interactions that differs from the “true” spectrum obtained from Eq. (50). Nevertheless, the details of these low-\(W\) interactions are irrelevant for studies of high-energy electron and positron transport, which is practically determined by the integrated quantities \(S\), \(\Omega^2\), \(\lambda_{\text{tr},1}\) and \(\lambda_{\text{tr},2}\) (see e.g. [41]) that are not affected by the approximation. Therefore, the use of the approximation (55) in high-energy transport calculations is justified.

Fig. 8 depicts calculated mean free paths, stopping powers and energy straggling parameters for
electrons and positrons in Si, as functions of the kinetic energy. The energy straggling parameter, which has been divided by $E$ to fit in the plots, is nearly constant with $E$ in the interval from 1 keV to 100 keV, but at higher energies becomes approximately proportional to $E$. This rise is a relativistic effect and does not occur in the non-relativistic theory, which predicts that $X_2$ reaches a saturation value at high energies. The variation of the mean free path with energy reveals another interesting difference with non-relativistic theory.

In non-relativistic quantum mechanics the cross section can be regarded as a measure of the excitation probability of the target during the time it is exposed to the varying electromagnetic field of the projectile. In a non-relativistic formulation, projectiles with larger energies have larger velocities and interact with the target for a shorter time. Therefore, the excitation probability (or the cross section) decreases with $E$ and, consequently, the mean free path increases without limit when the energy of the projectile increases. Conversely, in the relativistic theory, the velocity of the projectile never exceeds the speed of light in vacuum and, for relativistic energies, the energy straggling parameter becomes approximately proportional to $E$.

### Table 1

<table>
<thead>
<tr>
<th>Material</th>
<th>$Z$</th>
<th>$\rho$ (g/cm$^3$)</th>
<th>ps-sum</th>
<th>$I$ (eV)</th>
<th>$I_{\text{ICRU}}$ (eV)</th>
<th>$E_F$ (eV)</th>
<th>$W_s$ (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al</td>
<td>13</td>
<td>2.70</td>
<td>0.991</td>
<td>164</td>
<td>166 ± 2</td>
<td>11.7</td>
<td>73</td>
</tr>
<tr>
<td>Si</td>
<td>14</td>
<td>2.33</td>
<td>1.000*</td>
<td>174</td>
<td>173 ± 3</td>
<td>12.5</td>
<td>99</td>
</tr>
<tr>
<td>Cu</td>
<td>29</td>
<td>8.96</td>
<td>1.019</td>
<td>323</td>
<td>322 ± 10</td>
<td>7.0</td>
<td>74</td>
</tr>
<tr>
<td>Au</td>
<td>79</td>
<td>19.32</td>
<td>1.127</td>
<td>737</td>
<td>790 ± 30</td>
<td>5.5</td>
<td>54</td>
</tr>
</tbody>
</table>

$\rho$ are the mass densities of the materials and $I_{\text{ICRU}}$ are the mean excitation energies recommended in the ICRU Report 37 [3]. $E_F$ and $W_s$ are the Fermi and switch energies, respectively, taken from [15].

* Not significant.

Fig. 6. Real and imaginary parts of the dielectric functions of Al and Si, obtained numerically from the OOSs displayed in Fig. 5. Notice that the absolute value of $\varepsilon_1$ is plotted multiplied by $10^{-3}$; the dashed and dotted curves represent positive and negative values of $\varepsilon_1$, respectively.
hence, the “interaction time” remains bound when the energy of the projectile increases. This implies that the cross section for high-energy projectiles is constant with $E$ and explains the “saturation” of the mean free path when $E \rightarrow 1$.

We see that differences between the mean free paths of electrons and positrons are small and limited to low energies. For energies up to about 0.5 MeV, the stopping power of positrons is larger than that of electrons, essentially because the maximum allowed energy loss in electron collisions is bound to be less than $(E + W)/2$; for the same reason, the energy straggling of positrons is larger than that of electrons (by a factor of $\sim 2$ for energies up to $\sim 100$ keV). At higher energies the relative differences are smaller, and the stopping power becomes slightly larger for electrons than for positrons. It should be kept in mind that our description of electron exchange is expected to be realistic only for hard close collisions, for which the Møller cross section (69) applies. A more accurate description of exchange effects would probably alter the low-energy portion of Fig. 8.

Fig. 9 displays inelastic mean free paths of electrons in Al, Si, Cu and Au calculated using the present optical-data model, together with available experimental data from several research groups. The experimental values were acquired by a variety of techniques such as photoelectron spectroscopy, the overlayer method, elastic-peak electron spectroscopy and transmission electron microscopy. The uncertainties tend to be large, especially at energies of about 100 eV and below, where $\lambda$ attains a minimum. Nevertheless, the global agreement between our theoretical results and the measurements is quite satisfactory. Our inelastic mean free paths are also in excellent agreement with the widely-used values from the optical-data model of Tanuma et al. [11], which cover the energy interval from 50 eV to 2 keV. Unfortunately, no experimental data seem to exist above a few hundred keV. At still larger energies the calculated inelastic mean free paths become constant due to the finite interaction time at relativistic velocities.

In Fig. 10 we compare calculated collision stopping powers for electrons in Al, Si, Cu and Au with experimental data reported by various authors. It should be kept in mind that measured stopping powers are affected by considerable uncertainties, which are evident from the discrepancies between data sets from different sources and which increase for decreasing energies. The calculation results for Al and Si are very close to the experimental values down to a few tens of eV. Notice that the OOSs of these two elements display a prominent plasmon peak (see Fig. 5). In the case of Cu, whose OOS is broader due to the strong interband transitions characteristic of transition metals, agreement is very good above $\sim 400$ eV, but the calculated stopping powers fall

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Fig. 7. Fermi density-effect correction to the stopping power of Al (solid curve), Si (dashed curve) and Au (dot-dashed curve).

Fig. 8. Comparison of calculated mean free paths $\rho\lambda$ (in $\mu g/cm^2$), stopping powers $S/\rho$ (in eV cm$^2/$$\mu g$) and energy straggling parameters $(\Omega^2/\rho)$ (in eV$^2$ cm$^2/$$\mu g$) of electrons (solid curves) and positrons (dashed curves) in Si, due to non-radiative inelastic scattering.
slightly below the measured data at lower energies. Agreement between theory and experiment is somewhat worse for Au. The mean excitation energy determined from the adopted OOS of Au is considerably lower than the currently accepted value, see Table 1, resulting in a stopping power which is too large. For instance, our calculated stopping power at 10 keV is 8% larger than the value tabulated in the ICRU Report 37 [3]. On the other hand, there is a notable scarcity of experimental information above 10 keV; this is, however, the energy interval where the Bethe formula, Eq. (86), becomes accurate if the adopted mean excitation energy is correct. At energies above ~1 MeV the contribution from the transverse interaction (including the density-effect correction) cannot be neglected, yielding an increase of the stopping power with energy. Here, the excellent agreement between our results and the measurements carried out by MacPherson [98] provides a clear indication of the consistency of our optical-data model calculation at relativistic energies.

Regarding Figs. 9 and 10, we recall that the fair accordance between our theoretical inelastic mean free paths and stopping powers and the experimental values below about 100 eV may be fortuitous due to the neglect of higher-order terms in the Born series.

Restricted angular DCSs and transport mean free paths can be calculated as described in Section 3.3 and using the formulas derived in Appendix B. In Fig. 11 we show angular DCSs for electrons and positrons of various energies in Al and Au, with the cutoff energy loss $W_c$ set equal to $E$ (i.e.
unrestricted). The plotted quantity is the inelastic DCS per unit solid angle,

$$\frac{d\sigma}{d\Omega} = \frac{1}{4\pi} \frac{d\sigma}{d\mu}. \quad (101)$$

The integral of this angular DCS over directions should then equal the total cross section $\sigma$ computed by integrating the (unrestricted) energy-loss DCS. Total cross sections obtained by these two different schemes are found to agree to more than five significant digits, which gives an indication of the accuracy of the adopted numerical integration methods. The DCSs in Fig. 11 exhibit the characteristic shape discussed by Fano [100], with a maximum at small angles that originates from the contribution of distant transverse interactions [this contribution vanishes at $\theta = 0^\circ$, see Eq. (121)]. The angular DCSs for positrons are smooth and vanish for $\theta \geq 90^\circ$. The DCSs for electrons have a sharp drop at an angle less than $90^\circ$ due to the fact that close collisions are restricted to $W \leq (E + W)/2$.

The angular DCSs for elastic and inelastic scattering of electrons in Al and Au are compared in Fig. 12. Inelastic DCSs were evaluated using the OOSs shown in Fig. 5. The elastic DCSs were calculated within the static-field approximation using the relativistic partial-wave code ELSEPA [101], and are plotted multiplied by $Z^{-1}$. It is apparent that, for intermediate and high energies, the angular distributions of elastically and inelastically scattered electrons have similar shapes in a wide angular interval. This justifies a simple approximation,
used by many authors, in which the angular DCS for inelastic scattering is set equal to $Z^{-1}$ times the elastic DCS. Fig. 13 displays the integrated (total) cross section ($\sigma$) and the first and second transport cross sections ($\sigma_1$ and $\sigma_2$) for inelastic and elastic collisions of electrons in Al and Au, as functions of the kinetic energy of the projectile.
5. Conclusions

We have proposed a new optical-data model to describe inelastic collisions of electrons and positrons in condensed matter. Unlike other semi-relativistic models, our approach is based on the fully relativistic plane-wave Born approximation, thus consistently including the contribution of transverse interactions, which are non-negligible for energies larger than a few hundred keV. By using the N-oscillator as the extension algorithm, relatively simple expressions for the various DCSs are obtained. For incident electrons, exchange effects are incorporated by employing the Møller DCS for close collisions; close collisions of positrons are described by means of the Bhabha DCS. The density-effect correction on the DCSs is calculated directly from the OOS. The model also allows the calculation of the angular DCS for inelastic interactions, as well as the angular DCS restricted to energy transfers smaller than a given threshold value. The latter is needed for mixed (class II) Monte Carlo simulation.

The basic ingredient of the optical-data model is the OOS. To obtain reliable results, the OOS should be available over a wide energy interval and fulfill various constraints in the form of sum rules. This limits the applicability of the model to materials (elements and compounds) for which optical or dielectric properties are relatively well known. To demonstrate the reliability of the method, we have calculated inelastic mean free paths and stopping powers of electrons in Al, Si, Cu and Au. The results from the calculations are generally in very good agreement with experimental data available from the literature, except for the stopping power below about 400 eV in Cu and below several keV in Au. In the case of Au, the reason for this departure may be attributed partly to inaccuracies in the input OOS.

Fig. 13. Integrated (total) cross section (σ) and first and second transport cross sections (σ₁ and σ₂) for inelastic and elastic collisions of electrons of the indicated energies in Al and Au. The inelastic cross sections (solid curves) were calculated from the OOSs shown in Fig. 5; the elastic cross sections (dashed curves) were obtained using the relativistic partial-wave analysis code ELSEPA [101].
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Appendix A. Kinematics of inelastic collisions

The recoil energy $Q$ is defined by

$$Q(Q + 2m_e c^2) = c^2 (p^2 + p'^2 - 2pp' \cos \theta), \quad (102)$$

where we use the notation introduced in Section 2 and Fig. 1. The kinematically allowed recoil energies lie in the interval $Q_- \leq Q \leq Q_+$, with end points given by this equation with $\cos \theta = +1$ and $-1$, respectively,

$$Q_+ (Q_+ + 2m_e c^2) = (cp \pm cp')^2. \quad (103)$$

That is,

$$Q_+ = \sqrt{(cp \pm cp')^2 + m_e^2 c^4 - m_e^2 c^2}$$

$$= \sqrt{[\sqrt{E(E + 2m_e c^2) \pm \sqrt{(E-W)(E-W+2m_e c^2)}]}^2 + m_e^2 c^4} - m_e c^2. \quad (104)$$

For $W < E$ we have $Q_- < W$ and $Q_+ > W$. When $W \ll E$, expression (104) is not suitable for evaluating $Q_-$ since it involves the subtraction of two similar quantities. In this case, it is more convenient to use the approximate relation

$$cp - cp' \approx c \left( \frac{dp}{dE} W - \frac{1}{2} \frac{d^2p}{dE^2} W^2 + \frac{1}{6} \frac{d^3p}{dE^3} W^3 \right)$$

$$= \frac{W}{\beta} \left[ 1 + \frac{1}{2\gamma(\gamma+1)} \frac{W}{E} + \frac{1}{2(\gamma+1)^2} \left( \frac{W}{E} \right)^2 \right]. \quad (105)$$

and calculate $Q_-$ as

$$Q_- = m_e c^2 \left[ \sqrt{\left( \frac{cp - cp'}{m_e c^2} \right)^2 + 1} - 1 \right]$$

$$\simeq m_e c^2 \left( x - \frac{x^2}{2} + \frac{x^3}{2} \right), \quad (106)$$

with

$$x = \frac{1}{2} \left( \frac{cp - cp'}{m_e c^2} \right)^2$$

$$\simeq \frac{W^2}{2\beta^2 m_e^4 c^4} \left[ 1 + \frac{1}{2\gamma(\gamma+1)} \frac{W}{E} + \frac{1}{2(\gamma+1)^2} \left( \frac{W}{E} \right)^2 \right]. \quad (107)$$

For $W \ll E$,

$$Q_- (Q_+ + 2m_e c^2) = (cp - cp')^2 \approx W^2 / \beta^2. \quad (108)$$

From (104), it is clear that the curves $Q = Q_-(W)$ and $Q = Q_+(W)$ intersect at $W = E$. Thus, they define a single continuous function $W = W_m(Q)$ in the interval $0 < Q < Q_+(0)$. By solving the equations $Q = Q_{\pm}(W_m)$ we obtain

$$W_m(Q) = E + m_e c^2$$

$$- \sqrt{\left[ \sqrt{E(E + 2m_e c^2) - \sqrt{Q(Q + 2m_e c^2)}} \right]^2 + m_e^2 c^4}, \quad (109)$$

which, when $W \ll E$, reduces to

$$W_m(Q) \approx \beta \sqrt{Q(Q + 2m_e c^2)}. \quad (110)$$

Now it follows that, for given values of $E$ and $Q$ [$< Q_+(0)$], the only kinematically allowed values of the energy loss are those in the interval $0 < W < W_m(Q)$.

The scattering angle $\theta$ is related to the energy loss through

$$\cos \theta = \frac{(cp)^2 + (cp')^2 - (cq)^2}{2(cp)(cp')} \quad (111)$$

The recoil angle $\theta_r$ between $p$ and $q$ (see Fig. 1) is given by

$$\cos \theta_r = \frac{(cp)^2 - (cp')^2 + (cq)^2}{2(cp)(cq)}, \quad (112)$$
which can also be written in the form
\[
\cos^2 \theta_r = \frac{W^2 / \beta^2}{O(Q + 2m_e c^2)} \left( 1 + \frac{Q(Q + 2m_e c^2) - W^2}{2W(E + m_e c^2)} \right)^2.
\]
(113)

For collisions on the Bethe ridge, i.e. when \( Q = W \), this expression reduces to
\[
\cos^2 \theta_r \equiv \cos^2 \theta_r (Q = W) = \frac{W E + 2m_e c^2}{E W + 2m_e c^2}.
\]
(114)

Distant transverse interactions occur with appreciable probability only for fast projectiles (with \( E \) of the order of \( m_e c^2 \)) and the most probable energy losses are also such that \( W \ll E + m_e c^2 \). Moreover, in this case, only recoil energies \( Q \ll W \) are observed. Then, for the distant transverse excitations, we may use the approximation
\[
\cos^2 \theta_r \simeq \frac{W^2 / \beta^2}{O(Q + 2m_e c^2)},
\]
(115)

which allows a considerable simplification of the formulas. From Eq. (108), it follows that
\[
\cos^2 \theta_r \simeq \frac{O(Q + 2m_e c^2)}{O(Q + 2m_e c^2)}.
\]
(116)

Appendix B. Expressions for the restricted angular DCS

For the sake of completeness, in this appendix we provide explicit formulas for the restricted angular DCS \( d\sigma(W_c)/d\mu \), Eq. (93), based on our optical-data model. To this end, we proceed by inserting Eqs. (25) and (27) into Eq. (93). The DCS is expressed again as a superposition of DCSs of \( N \)-oscillators weighted with the OOS,
\[
\frac{d\sigma(W_c)}{d\mu} = \int_0^\infty dW' \frac{d^2 \sigma_1(W', W_c)}{d\mu} dW',
\]
(117)

where the restricted DCS for collisions with an oscillator with resonance energy \( W' \) is given by
\[
\frac{d\sigma_1(W', W_c)}{d\mu} = \int_0^{W_c} \left( \frac{d^2 \sigma_1(W', W_c)}{dW dQ} \right) dQ d\mu.
\]
(118)

This DCS vanishes when \( W' > W_c \).

Disregarding the density-effect correction for a moment, the restricted angular DCS for distant transverse interactions with a unit oscillator with resonance energy \( W' \) is
\[
\frac{d\sigma_{1,T}(W', W_c)}{d\mu} = \int_0^{W'} \frac{d^2 \sigma_{1,T}(W')}{d\mu} dW' = 2\pi \epsilon^4 \beta^2 \sin^2 \vartheta_r \frac{W'}{W^2/2m_e c^2} \frac{m_e c^2}{Q_1(1 + Q_1/2m_e c^2 - W'^2/2m_e c^2)} \times \frac{2 \epsilon p \epsilon' p'_1}{Q_1 + m_e c^2}, \quad 0 < \mu < \mu_1,
\]
(119)

where
\[
(c\epsilon' p'_1)^2 = (E - W')(E - W' + 2m_e c^2),
\]
\[
Q_1 = \sqrt{(c\epsilon - c\epsilon' p'_1)^2 + 4c\epsilon p \epsilon' p'_1 \mu + m_e c^4 - m_e c^2},
\]
\[
\mu_1 = \frac{W'(W' + 2m_e c^2) - (c\epsilon - c\epsilon' p'_1)^2}{4c\epsilon p \epsilon' p'_1}.
\]
(120)

In accordance with the derivation of Eq. (32), here we have neglected the variation of the excitation energy of the oscillator with \( Q \). Consequently, for a given \( \mu, Q \) is given by Eq. (94) with \( W = W' \). Recalling the definition of \( \vartheta_r \), Eq. (115), we can write
\[
\frac{d\sigma_{1,T}(W', W_c)}{d\mu} = C_F \frac{2\pi \epsilon^4}{m_e c^2} \frac{1}{Q_1(1 + Q_1/2m_e c^2)} \times \frac{W'}{2m_e c^2} \frac{\beta^2 Q_1(1 + Q_1/2m_e c^2) - W'^2/2m_e c^2}{Q_1(1 + Q_1/2m_e c^2 - W'^2/2m_e c^2)} \times \frac{2 \epsilon p \epsilon' p'_1}{Q_1 + m_e c^2}, \quad 0 < \mu < \mu_1,
\]
(121)

where \( C_F = 1 \) if the density-effect correction is excluded. Notice that, as pointed out by Fano [100], the transverse contribution approximately vanishes for \( \mu = 0 \) (\( Q = Q_\perp \)) [see Eq. (108)] and, therefore, it has a maximum at intermediate angles, which is clearly visible in the angular DCSs for electrons and positrons with \( E \sim 10m_e c^2 \) (see Section 4).

In the derivation of the result (121) we have ignored the density-effect correction. We can account for this correction approximately by
reducing the transverse part of the DCS by the same factor as the energy-loss DCS is reduced, see Eq. (49). That is, Eq. (121) is still valid but now
\[
C_F = \left[ \frac{1}{2} \ln \left( \frac{\eta_1 + \eta_2}{(n_1 - \beta^2)^2 + \eta_2^2} \right) - \frac{\eta_1 - \beta^2}{\eta_2} \arctan \left( \frac{\eta_2 \beta^2}{\eta_1 (n_1 - \beta^2) + \eta_2} \right) \right] \times \left[ \ln \left( \frac{1}{1 - \beta^2} \right) - \beta^2 \right]^{-1},
\]
(122)
or
\[
C_F \simeq \left[ \ln \left( \frac{1}{1 - \beta^2} \right) - \beta^2 - \delta_F \right] \left[ \ln \left( \frac{1}{1 - \beta^2} \right) - \beta^2 \right]^{-1},
\]
(123)
if the approximation (55) is adopted.

The restricted angular DCS for distant longitudinal interactions with an oscillator is given by
\[
\frac{d^2\sigma_{1,\text{dis,l}}(W',W_c)}{d\mu} = \int_0^{\pi/2} d^2\sigma_{1,\text{dis,l}}(W') \frac{dQ}{dW} \frac{dQ}{d\mu} = \frac{2\pi e^4}{m_e v^2} \frac{1}{(W' + BQ_d)Q_d(1 + Q_d/2m_e c^2)} \times \frac{dQ}{d\mu}, 0 < \mu < \mu_d,
\]
(124)
where
\[
cp_d = \sqrt{(E - W' - BQ_{\text{max}})(E - W' - BQ_{\text{max}} + 2m_e c^2)},
\]
\[
Q_d = \sqrt{(cp - cp'_d)^2 + 4cp cp'_d \mu + m_e^2 c^4 - m_e c^2},
\]
\[
\mu_d = Q_{\text{max}}(Q_{\text{max}} + 2m_e c^2) - (cp - cp'_d)^2 / 4cp cp'_d.
\]
(125)
The quantity \(Q_{\text{max}}\) is the largest allowed recoil energy in distant longitudinal interactions [see Eq. (65)]. Noting that
\[
\frac{d(cp')}{dQ} = -\frac{B}{cp'}(E - W' - BQ + m_e c^2),
\]
(126)
we obtain
\[
\frac{d\mu}{dQ} = \frac{1}{2cp cp'} \left[ Q + m_e c^2 + \frac{d(cp')}{dQ} (cp - cp' - 2cp \mu) \right].
\]
(127)
When \(E \gg W'\), we can invoke the approximation [see Eq. (105)]
\[
\frac{1}{2} \ln \left( \frac{\eta_1 + \eta_2}{(n_1 - \beta^2)^2 + \eta_2^2} \right) \simeq \frac{W}{\beta} = \frac{W' + BQ_1}{\beta} \tag{128}
\]
and write
\[
\frac{d\mu}{dQ} \simeq \frac{1}{2cp cp'} \left[ Q + m_e c^2 - \frac{B}{\beta^2} (W' + BQ) + 2cp \frac{B}{cp'} (E - W' - BQ + m_e c^2) \mu \right].
\]
(129)
For a \(\delta\)-oscillator \((B = 0)\), the corresponding angular DCS is [cf. Eq. (124)]
\[
\frac{d^2\sigma_{1,\text{clo,l}}(W',W_c)}{d\mu} = \frac{2\pi e^4}{m_e v^2} \frac{1}{W'Q_1(1 + Q_1/2m_e c^2)} \times \frac{2cp cp'_1}{Q_1 + m_e c^2}, 0 < \mu < \mu_1,
\]
(130)
with \(cp'_1\), \(Q_1\) and \(\mu_1\) given by Eq. (120).

To determine the restricted angular DCS for close collisions \((W = Q)\) with an oscillator with resonance energy \(W'\), we write the energy-loss DCS [see Eqs. (69) and (75)] in the form
\[
\frac{d\sigma_{1,\text{clo}}(W)}{dW} = \frac{2\pi e^4}{m_e v^2} R^{(\pm)}(W) \Theta(W - W')
\]
(131)
with
\[
R^{(\pm)}(W) = \begin{cases} 
1 - b_1 \frac{W}{W'} + b_2 \left( \frac{W}{W'} \right)^2 - b_3 \left( \frac{W}{W'} \right)^3 + b_4 \left( \frac{W}{W'} \right)^4 & \text{for positrons,} \\
1 + \left( \frac{W}{E + W - W'} \right)^2 - \frac{(1 - \mu)W}{E + W - W'} + \frac{aw^2}{(E + W - W')^2} & \text{for electrons.}
\end{cases}
\]
(132)
In these collisions, the kinematics is the same as for binary collisions with free electrons at rest and the energy loss and the angular deflection \(\mu\) are related by
\[
W = \frac{E(E + 2m_e c^2)2\mu(1 - \mu)}{E2\mu(1 - \mu) + m_e c^2}.
\]
(133)
Therefore
\[
\frac{d\sigma_{1,\text{clo}}(W',W_c)}{d\mu} = \frac{d\sigma_{1,\text{clo}}(W')}{dW} \frac{dW}{d\mu} = \frac{2\pi e^4}{m_e v^2} R^{(\pm)}(W) \frac{2(cp)^2 m_e c^2(1 - 2\mu)}{[E2\mu(1 - \mu) + m_e c^2]^2}, \tag{134}
\]
\(\mu_1 < \mu < \mu_2\),
where

\[
(c\rho')^2 = \left( E - W_c \right) \left( E - W_c + 2m_e c^2 \right),
\]

\[
\mu_2 = \frac{W_c \left( W_c + 2m_e c^2 \right) - (c\rho - c\rho')^2}{4c\rho c\rho'};
\]

the restricted angular DCS vanishes for \( \mu > \mu_2 \).

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