Charged particles energy loss in matter: The multiple theories of the stopping power.

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October 30, 2018

Contents

Physics notation:

- $g, kg \rightarrow$ gram, kilogram, mass unit.
- $cm, m \rightarrow$ centimeter, meter, lenght unit.
- $C \rightarrow$ Coulomb, electrostacit charge unit.
- $J, eV \rightarrow$ Joule, electronvolt, energy units.
- $Gy \rightarrow$ Gray= J/kg, absorbed dose unit.
- $Z \rightarrow$ atomic number.
- $A \rightarrow$ atomic mass.
- $N_A \rightarrow$ Avogadro's number, $N_A = 6,022 \times 10^{23}\, mol^{-1}$.
- $c \rightarrow$ vacuum light speed, $c = 299.792.458\, m/s$.
- $m_e \rightarrow$ electron mass, $m_e = 9,109 \times 10^{-31}\, kg$.
- $e \rightarrow$ electron charge, $e = -1.602 \times 10^{-19}\, C$.
- $r_0 \rightarrow$ electron classic radius, $r_0 = \frac{e^2}{m_e c^2} = 2,817 \times 10^{-15}\, m$.
- $h, \hbar \rightarrow$ Planck's constant, $h = 6.626 \times 10^{-34}\, Js$, $\hbar = 1.054 \times 10^{-34}\, Js$.
- m_n, $m_p \rightarrow$ neutron and proton mass respectively, $m_n = 1.674 \times 10^{-27}\, kg$, $m_p = 1.672 \times 10^{-27}\, kg$.

Mathematics notation:

- $z^* \rightarrow$ that if $z \in \mathbb{C}$ then z^* is the complex conjugate.

List of Figures

Introduction

Chapter 1

Stopping power theory

1.1 Definition and conceptual topics

The first approach to the concept of stopping power is rather simple. Let us consider a physical system conformed by:

- A target, made of some material of interest, commonly named the **phantom**.
- A charged particle accelerated so that, in addition to its rest energy, it has an amount of kinetic energy T. Explaining how this **projectile** obtains its acceleration is not a goal of the present text.

We already know that the target material contains a bunch of elements of different nature, namely fundamental particles, atoms of molecules. We will call each of them the **scattering centers**. This is because when our projectile travels inside the target, it is capable of noticing the existence of those elements, and this action of "noticing" will be called **interaction** or **scattering**.

Each interaction presents a unique nature, and depends at least of three variables: the type of scattering center, the type of projectile and the kinetic energy it possesses. After this things are well stablished, there are usually different kinds of possible interactions between projectile and scatterer, and to each of them a probability of occurrence associated. Some of this interactions may cause the projectile to lose an amount of its energy, say dT. Obviously, $dT < 0$. If we are able to assume that for each step of length $d\xi$, the projectile loses, in average, dT, then, the possitively defined rate of energy loss per length unit is:

$$S(T) = -\frac{dT}{d\xi}\,. \tag{1.1}$$

The question: "when are we able to assume this?" is what this text intends to answer. The quantity S is called in literature **stopping power**. dT plays the role of the expectation value, with a suitable definition, of the energy lost if the projectile manages to travel a length unit $d\xi$ in the phantom. This definition, altough accurate, does not contain any information on how to deal with each of the ingredients we named before. For this reason, a seemingly more complex definition is needed, capable of making notorius the statistical nature of the energy deposition process.

The goal of the stopping power itself, is to somehow model all possible interactions the projectile, usually a particle of mass M and charge $Z_p e$, is subject to when traveling inside some material. As already explained, the matter is conformed by several different scattering centers, and to each of them there are several interaction types associated. Logically, treating them all independently to characterize, for example, the energy transferred, is not possible nor desirable. This is why thinking a solution in statistical terms is neccesary, using sets of interactions with similar characteristics presenting a certain probability of ocurrence. An example could be modelling the interaction of an electron with an ion and then apply the same rule for every other electron in the material, discriminating them with some statistical weight. This analysis will lead us to what is called the **electronic stopping power**.

The scattering centers might produce **elastic** or **inelastic** collisions. In the first, the energy and momentum magnitude of the projectile does not change, but it might suffer a deflection of angle θ_{scatt} from the direction of incidence. Even backscattering is a possibility, with $\theta_{scatt} \approx \pi$. When the problem being solved is the transport of particles, for example when the dosimetry of a heavy ion beam is being modelled, the elastic scattering plays an important role. The projectiles are deflected from the beam direction without depositing energy, but it will certainly lose it somewhere else. Therefore, understanding the so called **angular straggling** accurately is a need. In the present text, we will be concerned with the inelastic interactions, those that may also cause energy loss in the incident particle. The energy lost in one interaction is also attached to a probability, therefore the inelastic collisions presents an **energy straggling** that will undermine the stopping power definition.

As can be deduced from this explanation, a projectile travelling inside some material will follow tortuous paths rather than moving in a straight line (see figure 1.2), losing part of its energy at every inelastic collision until it spent it all, or a **capture** process ocurr. An example of this is the proton-boron fusion therapy technique. It consists on doping the cancerous tumor with an amount of ^{11}B boron non-radioactive isotope, that in comparison with the other scattering centers present in biological tissue, presents a high probability of induce a nuclear reaction with the protons of the clinical beam. After this capture process, the proton will no further deposite energy, but some reaction products will. On the other cases, the projectile looses small amounts of energy per collision until it comes to rest. In the next section, an explanation on how to think the stopping power statistically will be developed, introducing the physical magnitudes needed to fully describe the energy deposition of charged particles in matter.

For the sake of completitude, a word about the terminology used in english to refer to S. As already mentioned by Inokuti[1], using the SI unit system,

$$[S] = \frac{J}{m} = \frac{N \times m}{m} = N\,,$$

which is indeed a force unit. Therefore, the name "stopping power" seems quite inaccurate, being "power" defined as the energy per time unit. Inokuti indicates that this name for the projectile energy loss probably comes from the german word *Bremsvermögen*, that literally translates as "the capability of braking". The word "stop" is also questionable, because it usually refers to the notion of "coming to rest", while the german original verb *bremsen* refers to "braking" or "decelerating". This note is only to clear concepts, because the stopping power clearly quantifies the force exerted by the matter on the projectile with the aim of decelerating it, and consequently is sometimes referred as the "stopping force". Throughout the rest of the lecture, the most common name found in literature will be used, namely, stopping power.

1.2 Geometrical and statistical considerations

Lets assume that out phantom is a thick foil of volume V, width ξ, and with the greatest face presenting an area A. The projectile is part of a beam reaching the foil, designated by the letter J. This quantity is called the **current density of projectiles**:

$$[J] = \frac{\text{number of projectiles}}{\text{unit time} \times \text{unit area}}\,.$$

If each of the scattering centers of the foil present a transversal area σ to the projectiles, we may say that an interaction occurs if one of the particles in J crosses the surface σ. This area is denominated in literature the **cross section** of the interaction between projectile and scattering center, and it has profound physical implicancies.

Assuming that the rate of particles that are able to reach the entrance surface of the foil is constant, the fraction of them that can effectively interact with the scatterers in a time unit is σ/A. In the same unit of time, the total number of particles traversing the phantom surface can be estimated as $J \times A$. Consequently, the **net number of interactions** per unit time that occur can be estimated as

$\eta = J\,A\frac{\sigma}{A} = J\,\sigma$. Consider that inside the phantom there is a density N of scattering centers. Then, the total number of collisions inside it per unit time is:

$$\eta\,V\,N = J\,\sigma\,A\,\xi\,N = (J\,A)(N\,\xi\,\sigma)\,. \qquad (1.2)$$

Being $J\,A$ the number of projectiles entering the phantom in a time t, by discarding other possibilities, $N\,\xi\,\sigma$ should be in average the number of interactions per projectile. We will denote it as $\langle n\rangle = N\,\xi\,\sigma$. This has its own logic. If changing the perspective of the problem, what we intend to quantify here is the probability P_n of finding a number n of projectiles contained in the small volume $v = \sigma\xi$ associated with one scatterer, in a unit time t, provided the v volumes do not overlap. This approximation is not valid for example in crystal solids.

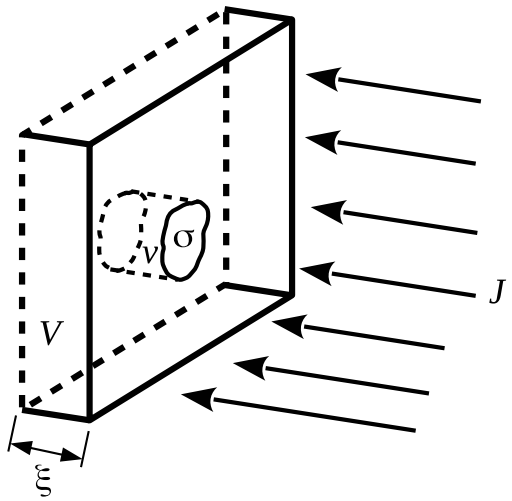

Figure 1.1: Sketch of a target phantom with the cross section area presented by the scattering centers.

This probability is solution of a known statistical problem of the kinetic theory of ideal gases, and it obeys the so called **Poisson's distribution**:

$$P_n = \frac{(Nv)^n}{n!}\,e^{-Nv}\,. \qquad (1.3)$$

The properties of this distribution are well known:

$$\sum_{n=0}^{\infty} P_n = 1\,, \qquad (1.4)$$

$$\sum_{n=0}^{\infty} nP_n = \langle n\rangle = Nv = N\xi\sigma\,. \qquad (1.5)$$

Then, what we called the average number of interactions per projectile estimated geometrically, is the mean of the Poisson distribution estimated by treating the problem statistically. This will be useful in a moment, but first lets try to approach the explanation using other tool.

A simple exercise solved by Monte Carlo experts is the **random walk**. There are several ways to describe the problem, but here we will use the one with direct association: consider a particle that, from a starting point in space, travels to another at some distance λ. The space where this particle travels is filled with an homogeneous and isotropic material, and we will consider that the source that emits this particles, do so in an isotropic way. When the particle stops, it is considered as if it is interacting with some constitutent of the material, and from that point it will travel again in another direction. Each step's direction is randomly drawn, to give the statistical meaning to the problem.

It can be shown that, after n steps, the particles have "walked" a mean distance r. Even more, this mean distance corresponds to the statistical mean of the Poisson's distribution. If the source location corresponds with $r = 0$, the radial distribution of interactions can be constructed. For this, the number of collisions is counted on several spherical shells of width dr centered at the source. This leads to the Poisson's distribution as shown in the second graphic of figure 1.2, normalized to the maximum number of collisions.

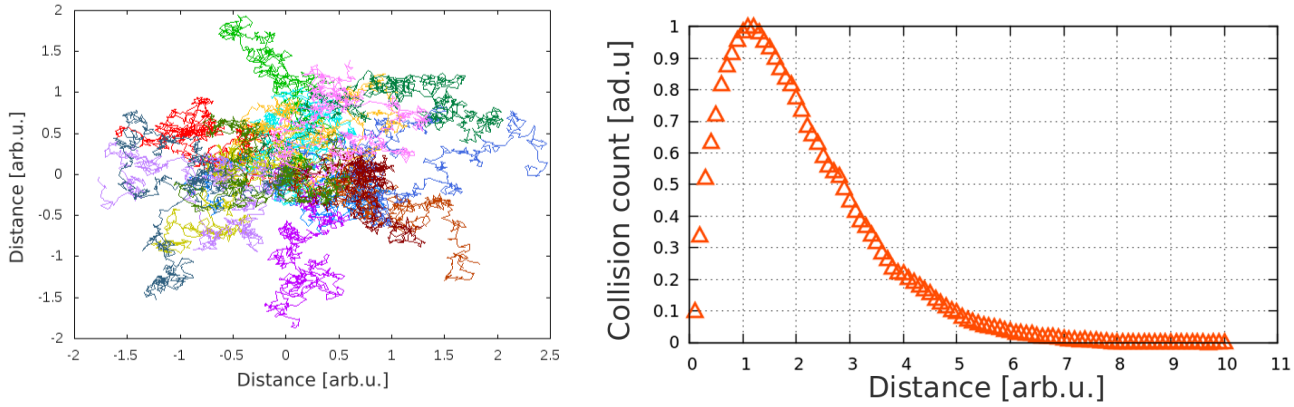

Figure 1.2: Left: Sample particle trajectories in a 2D random walk. Right: Poisson's distribution of the random walk.

In transport Monte Carlo codes, the particles are not allowed to travel λ each step, and they certainly does not stop after n collisions. Here, the interactions were elastic, so the limit of the simulation was the number of steps. In a more realistic case, the particle has a scalar number associated, its kinetic energy T, and it stops when the projectiles run out of energy. Nevertheless, this is an illustrative example of how the Monte Carlo codes work, and how they predict physical answers to problems like the mean number of collisions per projectile in matter.

Paying attention to what we have achieved, now we know the average of interactions of one projectile with different scattering centers inside a phantom, regardless of its form. This is exactly the statistical concept in which we want to sustain the study of physically relevant quantities as the stopping power. Therefore, we are ready to give the more sofisticated definition of stopping power.

1.3 Statistical stopping power

Consider the projectile entering a phantom whose material is conformed by different scattering centers which we will label using and index a. As already said, different interactions might occur with the same kind of scatterer, and we will correspondingly label them with a index b. In a discrete approximation, we let the scattering center a to be capable of absorbing finite amounts of energy w_{ab} in a b interaction. This is probably a more suitable approximation for a quantum treatment, but nevertheless easily generalizable. If the projectile travels a distance ξ in the phantom, it will suffer n_b interactions of type b, and it will have lost an energy:

$$\Delta_a = -\sum_b w_{ab} n_b \,. \tag{1.6}$$

Since w_{ab} is not a stochastic variable (it is fixed by scattering center and projectile types, and the last one energy), the mean energy loss by the projectile can be estimated as:

$$\langle \Delta_a \rangle = -\sum_b w_{ab} \langle n_b \rangle \,, \tag{1.7}$$

where $\langle n_b \rangle$ is the average number of collisions with scattering centers of type b per projectile, or $\langle n_b \rangle = N_a \xi \sigma_{ab}$. N_a is then the density of type a scattering centers and σ_{ab} the cross section of the corresponding interaction with the projectile. It is perhaps the correct time to clarify that σ_{ab} is a microscopic quantity, while the stopping power we are trying to define is a macroscopic magnitude. It is also worthy signaling the generality of this expression, where a may denote an electron, nucleus, atom or molecule. The energy lost by the projectile can then be expressed as:

$$\begin{aligned}\langle \Delta_a \rangle &= -\sum_b N_a \xi w_{ab} \sigma_{ab} \\ &= -N_a \xi \sum_b w_{ab} \sigma_{ab} \,.\end{aligned}$$

In general terms, the microscopic cross section is thought of as a probability distribution for the interaction to take place, and depends directly on the available kinetic energy T of the projectile, or the scattering angle θ_{scatt}, and consequently, a more adequate notation for the energy loss is:

$$\Delta T = -\sum_a N_a \xi \sum_b \int w_{ab} d\sigma_{ab} \,, \tag{1.8}$$

where the contribution of each type of scatterer was added. Thinking of a small displacement $\Delta\xi$, we are able to write our general definition of the stopping power:

$$\boxed{S(T) = -\frac{\Delta T}{\Delta \xi} = \sum_a N_a \sum_b \int w_{ab} \sigma_{ab}} \,. \tag{1.9}$$

It can be seen that the only information that is needed to evaluate this expression are the energetic levels and the interaction probability, namely, the differential cross section.

This formalism is completely deduced in terms of classical concepts, but this does not imply that its ingredients cannot (in fact they should) be defined in a quantum theoretical frame. On the other hand, this formula is valid at first orden, because it is simply the linear multiplication of the microscopic properties times the amount of scattering centers. This assumption means that the way the projectile interacts with one scatterer is totaly independent of how was the immediately previous interaction. This implies that there exists an independence of random events known as **Màrkov process**. Altough this is not rigorously true, the results of the theory with its corresponding corrections, fit very well with the experimental data.

Our formula for the stopping power also pre-suposes that the interaction between the projectile particles, if they are part of a beam, is negligible, as if there were a considerable amount of time between one particle and the next. If this were not this way, different projectiles of the same beam might present different kinetic energies and direction of movement.

In some fields of study, such us astrophysics, a useful definition is that of the *stopping cross section*, which is a macroscopic quantity sometimes measured experimentally, that for scattering centersof type a is defined as:

$$(\sigma_S)_a = \sum_b \int w_{ab} d\sigma_{ab} \,, \tag{1.10}$$

and consequently the stopping power reads:

$$S(T) = \sum_a N_a \, (\sigma_S)_a \,. \tag{1.11}$$

At this point, knowing the energy loss of the projectile consists of knowing the details of σ_{ab} and make the calculation term by term, interaction by interaction. This is still pretty tedious and un-practical. Thereby, an average definition of σ_{ab} over every interaction possible seems to be the logical next step. If this average proves not to be enough, the corresponding interaction enhancing the difference respect the experimental data can be studied, and corrections can be added to the mean stopping power formula. This is far simpler than studying each of the possible interactions.

Even though we will describe the energy loss of light particles as electrons and positrons, the problem that leads the ideas of the theory is that of the stopping of heavy ions of mass M and charge $Z_p e$ in all energy ranges, including relativistic effects. This kind of projectiles lose their energy mainly

by interaction with the atomic elecron cloud. Therefore, what we call a **swift ion** is that whose kinetic energy far exceeds the binding energy of this electrons. As we know, semi-classically speaking, this binding energies represent the **mean orbital velocity** of the electrons. Therefore, care must be taken when the ions are considered **slow**, or when the target atom presents high atomic number Z_t, because the inner shells have higher binding energies. This effect gives rise to the **shell correction** by Sternheimer[2] in 1952. We will try to expose several corrections of this kind throughout this lecture.

Back to the atomic electrons, there exists two possible situations of interaction with the heavy ion: either the atom excites from its ground state, moving the electron from one orbital to another, or it becomes ionized, removing the electron from the atom and its energy passes from a discrete to a continuous spectra. Then with only one interaction, the atom might:

1. Absorb a mininum amount of energy $\epsilon_{min} = \langle I \rangle$ known as **mean excitation potential**. The definition of this quantity is abstract and complicated, and depends strongly on the theoretical frames used to calculate σ_{ab}.

2. Absorb a maximum amount of energy ϵ_{max} corresponding to a frontal, collineal collision. This quantity is easily defined, and this will be our start point.

Respect to the theoretical frames named when introducing the mean excitation potential, we refer for example to the first calculation of the stopping power due to Bohr between 1913 and 1915, before the emergence of quantum mechanics. This calculation makes extensive use of the **impact parameter** b to characterize the energetic limits of the theory. After quantum mechanics was born, Bethe repeated the calculation, but he also proposed the first relativistic version of the deduction, between 1930 and 1932.

Chapter 2

Physics theory

2.1 Maximum energy transfer: frontal collision

The expression for the maximum energy transfer ϵ_{max} is obtainable from the relativistic arguments of energy and momentum conservation. Lets think about two particles of mass M and m, with m initially at rest. Then, we can use a reference frame attached to it to describe the dynamical variables. This is usually called the **laboratory frame**. In this system, M travels collineal to m with velocity $\vec{v}$.

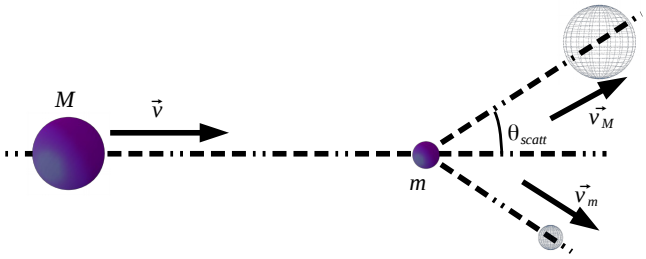

Figure 2.1: Simple sketch of a frontal collision.

The total energy before and after the collision should be written in a convenient way to make the calculation easier:

$$\begin{cases} E_i &= \gamma Mc^2 + mc^2 \\ E_f &= \gamma_M Mc^2 + \gamma_m mc^2 \quad = (\gamma Mc^2 - \Delta) + (mc^2 + \Delta)\,, \end{cases} \tag{2.1}$$

where $\gamma_i^2 = (1 - v_i^2/c^2)^{-1}$ is the Lorentz factor, and Δ is the amount of energy transfered in the collision from M to m. In the laboratory frame, the momentum before and after might be written as:

$$\begin{aligned} p_i &= p_M^i + p_m^i = \sqrt{\gamma^2 M^2c^2 - M^2c^2}\,, \\ p_f &= p_M^f - P_m^f = \sqrt{\frac{(E_M^f)^2}{c^2} - M^2c^2} - \sqrt{\frac{(E_m^f)^2}{c^2} - m^2c^2} \\ &= \sqrt{\frac{(\gamma Mc^2 - \Delta)^2}{c^2} - M^2c^2} - \sqrt{\frac{(mc^2 + \Delta)^2}{c^2} - m^2c^2}\,. \end{aligned}$$

The minus sign in the final momentum is because we are using the condition that the maximum energy transfer only occur if the projectil "bounces" in m. Then, using that lineal momentum must be conserved, we can start to clear Δ.

$$\begin{aligned} \sqrt{\gamma^2 M^2c^2 - M^2c^2} &= \sqrt{\frac{(\gamma Mc^2 - \Delta)^2}{c^2} - M^2c^2} - \sqrt{\frac{(mc^2 + \Delta)^2}{c^2} - m^2c^2} \\ \gamma^2\beta^2 M^2c^2 &= \frac{(\gamma Mc^2 - \Delta)^2}{c^2} - M^2c^2 + \frac{(mc^2 + \Delta)^2}{c^2} - m^2c^2 - \\ &\quad - 2\sqrt{\left(\frac{(\gamma Mc^2 - \Delta)^2}{c^2} - M^2c^2\right)\left(\frac{(mc^2 + \Delta)^2}{c^2} - m^2c^2\right)}\,, \end{aligned}$$

where in the left-hand-side (l.h.s.), $\beta = v/c$ and $\gamma^2 - 1 = \frac{\beta^2}{1-\beta^2} = \gamma^2\beta^2$ was used. Leaving the square root for the last, every other term in the right-hand-side (r.h.s.) goes to the l.h.s. Working in this member:

$$\begin{aligned}
&\gamma^2\beta^v M^2c^2 + M^2c^2 + m^2c^2 - \left(\gamma^2M^2c^2 - 2\gamma M\Delta + \frac{\Delta^2}{c^2}\right) - \left(m^2c^2 + 2m\Delta + \frac{\Delta^2}{c^2}\right) = \\
&= \gamma^2\beta^2M^2c^2 + M^2c^2(1-\gamma^2) + 2\gamma M\Delta - \frac{\Delta^2}{c^2} - 2m\Delta - \frac{\Delta^2}{c^2} \\
&= \gamma^2\beta^2M^2c^2 + M^2c^2(-\gamma^2\beta^2) + 2\Delta(M\gamma - m) - 2\frac{\Delta^2}{c^2} \\
&= 2\Delta(M\gamma - m) - 2\frac{\Delta^2}{c^2}\,.
\end{aligned}$$

The factor 2 will cancel with the on in the r.h.s. multiplying the square root. Now, lets work with this square root argument:

$$\begin{aligned}
&\left(\gamma^2M^2c^2 - 2\gamma M\Delta + \frac{\Delta^2}{c^2} - M^2c^2\right)\left(m^2c^2 + 2m\Delta + \frac{\Delta^2}{c^2} - m^2c^2\right) = \\
&= \left(M^2c^2\beta^2\gamma^2 - 2\gamma M\Delta + \frac{\Delta^2}{c^2}\right)\left(2m\Delta + \frac{\Delta^2}{c^2}\right) \\
&= 2mM^2c^2\beta^2\gamma^2\Delta - 4mM\gamma\Delta^2 + 2m\frac{\Delta^3}{c^2} + M^2\beta^2\gamma^2\Delta^2 - 2\frac{\gamma M}{c^2}\Delta^3 + \frac{\Delta^4}{c^4} \\
&= 2mM^2c^2\beta^2\gamma^2\Delta + M^2\beta^2\gamma^2\Delta^2 - 4mM\gamma\Delta^2 + 2\frac{\Delta^3}{c^2}(m - M\gamma) + \frac{\Delta^4}{c^4}\,.
\end{aligned}$$

All of this is what remains in the r.h.s. when squaring both sides. Applying this operation to the l.f.s.:

$$\left(\Delta(M\gamma - m) - \frac{\Delta^2}{c^2}\right)^2 = \Delta^2(M\gamma - m^2)^2 - 2\frac{\Delta^3}{c^2}(M\gamma - m) + \frac{\Delta^4}{c^4}\,.$$

Now we are able to equal both sides:

$$\begin{aligned}
\Delta^2(M\gamma - m)^2 + \cancel{2\frac{\Delta^3}{c^2}(m - M\gamma) + \frac{\Delta^4}{c^4}} &= 2mM^2c^2\beta^2\gamma^2\Delta + M^2\beta^2\gamma^2\Delta^2 - 4mM\gamma\Delta^2 + \\
&\quad + \cancel{2\frac{\Delta^3}{c^2}(m - M\gamma) + \frac{\Delta^4}{c^4}} \\
\Delta\left[(m - M\gamma)^2 - M^2\beta^2\gamma^2 + 4mM\gamma\right] &= 2mM^2c^2\beta^2\gamma^2 \\
\Delta\left[m^2 - 2mM\gamma + \gamma^2M^2 - M^2\beta^2\gamma^2 + 4mM\gamma\right] &= 2mM^2c^2\beta^2\gamma^2 \\
\Delta[m^2 + 2mM\gamma + \gamma^2M^2(1-\beta^2)] &= 2mM^2c^2\beta^2\gamma^2 \\
\Delta\left[m^2 + 2mM\gamma + M^2\right] &= 2mM^2c^2\beta^2\gamma^2\,,
\end{aligned}$$

and finally, we obtain Δ, that in this situation of the energy-momentum conservation corresponds to the maximum energy transferred ϵ_{max}:

$$\boxed{\epsilon_{max} = \Delta = \frac{2mc^2\beta^2\gamma^2}{1 + 2\frac{m}{M}\gamma + \left(\frac{m}{M}\right)^2}}\,. \tag{2.2}$$

If, e.g., the projectile is a proton, and the scattering center is an electron, we have:

$$\begin{matrix} M = m_p = 1.672 \times 10^{-27} & kg \\ m = m_e = 9.109 \times 10^{-31} & kg \end{matrix} \Rightarrow \frac{m}{M} \sim \frac{1}{1835} \sim 0\,. \tag{2.3}$$

In this approximation, namely when $M >> m$, the energy can be written as:

$$\boxed{\epsilon_{max} \simeq 2mc^2\beta^2\gamma^2}\,. \tag{2.4}$$

And the last useful case is, together with $M >> m$, using $\beta << 1$, or $v << c$ which is the non-relativistic limit. In this case:

$$\boxed{\epsilon_{max} \simeq 2mv^2}\,. \tag{2.5}$$

This energy transfers are representative of every collision that can be thought of as collineal, that is exactly using the minimum impact parameter b possible from a classical point of view.

As will be seen, the calculation of $\langle I \rangle$ is much more complex and representative of the theoretical frame, and a general expression derived from first principles is still not achieved. This energetic limit represent a break in the stopping power, associated to the point where its now valid treating the eletron as free, and atomic effects becomes relevant. From a classical point of view, this enforces the existence of a number b_1 separating the effects of **close** and **distant collisions**. From a quantum point of view, the discriminating parameter is the momentum transfer $\vec{q}$, and because of that they change names to **hard** and **soft collisions** respectively.

In next chapter, the full classical theory of stopping power will be studied.

2.2 Electric permittivity: energy loss function

2.2.1 General properties: Macroscopic Maxwell equations

The theory of the electric stopping power in a classical framework, consists on making a rough calculation of the electric field that the projectile generates on one and only one atomic electron at a time. If the transporting material is dense, there is a not-negligible chance that the distance $|\vec{r}|$ between the projectile and aforementioned electron is filled with several other scattering centers susceptible to the electromagnetic fields. Therefore, the electric field at the electron position is distorted respect its vacuum behavior. In other words, in a dense material, the projectile might interact with several scattering centers simultaneously, and polarization effects are not negligible anymore.

In a dense material, a microscopic treatment is unfeasible, and consequently classical electrodynamics seems to be the correct framework to make estimations on the energy loss per pathlength. The Maxwell equations for macroscopic fields with external free sources $(\rho, \vec{J})$ are:

$$\nabla \cdot \vec{D} = 4\pi\rho \;\; ; \;\; \nabla \times \vec{E} + \frac{1}{c}\frac{\partial \vec{B}}{\partial t} = 0\,;$$
$$\nabla \cdot \vec{B} = 0 \;\; ; \;\; \nabla \times \vec{H} - \frac{1}{c}\frac{\partial \vec{D}}{\partial t} = \frac{4\pi}{c}\vec{J},$$

where in general $\vec{D} = \hat{\epsilon}\vec{E}$ and $\vec{B} = \hat{\mu}\vec{H}$, where $\hat{\epsilon}$ and $\hat{\mu}$ are operators on the fields (not necessarily lineal), known as **electric permittivity** and **magnetic permeability** tensors respectively. This operators are usually defined in such a way that ρ and $\vec{J}$ represent the free charge densities and currents (without the induced distributions). Given that the magnetic forces do not work, the only force applied to the electron capable of inducing an energy transfer would be $\vec{F} = -e\vec{E}$. Therefore, we concentrate our efforts in solving the pair of equations:

$$\nabla \cdot \vec{D} = 4\pi\rho \;\; ; \;\; \nabla \times \vec{E} = 0\,.$$

The way of connecting $\vec{E}$ and $\vec{D}$ might be non-local both spatially and temporarily. This means that $\vec{D}(\vec{r}, t)$ might depend on the values of $\vec{E}(\vec{r}\,', t')$ with $\vec{r}\,' \neq \vec{r}$ and $t' \neq t$. In general, if the transporting material is not isotropic, we have:

$$D_a(\vec{r},t) = \sum_b \int d^3\vec{r}' \int dt' \epsilon_{ab}(\vec{r}',t') E_b(\vec{r}-\vec{r}', t-t') \,. \tag{2.6}$$

In the optical energy range (large wavelengths), the spatial non-locality can usually be neglected, and consequently:

$$D_a(\vec{r},t) = \sum_b \int dt' \epsilon_{ab}(t') E_b(\vec{r}, t-t') \,. \tag{2.7}$$

Also, if the transporting material is simple (isotropic), we have:

$$\vec{D}(\vec{r},t) = \int dt' \epsilon(t') \vec{E}(\vec{r}, t-t') \,. \tag{2.8}$$

It is also convenient keep in mind that the electric field exists even without a propagating material, and consequently, extracting the corresponding "vacuum" field is useful for calculation issues. Then:

$$\vec{D}(\vec{r},t) = \vec{E}(\vec{x},t) + \int dt'\, f(t') \vec{E}(\vec{r}, t-t') \,, \tag{2.9}$$

where $f(t')$ is a function that depends entirely on the material properties. All of this are approximations to merely simplify the model. If applying a Fourier transform to last expression, we have:

$$\begin{aligned}
\frac{1}{\sqrt{2\pi}} \int d\omega \vec{D}(\vec{r},\omega) e^{-i\omega t} &= \frac{1}{\sqrt{2\pi}} \int d\omega \vec{E}(\vec{r},\omega) e^{-i\omega t} + \int dt'\, f(t') \frac{1}{\sqrt{2\pi}} \int d\omega \vec{E}(\vec{r},\omega) e^{-i\omega(t-t')} \\
&= \frac{1}{\sqrt{2\pi}} \int d\omega \vec{E}(\vec{r},\omega) e^{-i\omega t} + \frac{1}{\sqrt{2\pi}} \int d\omega \vec{E}(\vec{r},\omega) \left[\int dt'\, f(t') e^{i\omega t'} \right] e^{-i\omega t} \,,
\end{aligned}$$

and using the orthogonality of $\{e^{i\omega t}\}$, this expression becomes a lineal equation in ω:

$$\begin{aligned}
\vec{D}(\vec{r},\omega) &= \vec{E}(\vec{r},\omega) + \vec{E}(\vec{r},\omega) \int dt'\, f(t') e^{i\omega t'} \\
&= \vec{E}(\vec{r},\omega) \left[1 + \int dt'\, f(t') e^{i\omega t'} \right] \\
&= \epsilon(\omega) \vec{E}(\vec{r},\omega) \,,
\end{aligned}$$

where the **dispersion relation** has been defined as:

$$\epsilon(\omega) = 1 + \int dt'\, f(t') e^{i\omega t'} \,. \tag{2.10}$$

For the convolution to be correctly defined, $f(t')$ must not diverge (it is finite) for every possible value t'. This means that the value of $\vec{D}$ at any time t must not be excesively affected by $\vec{E}(t')$ at remotes times t'. Under this conditions, the general expression (2.10) in isotropic media provides a lot of information at an optical level of the dispersion relation properties. First of all, $\epsilon(\omega)$ is a complex function, therefore it can be written as $\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega)$, where $\epsilon_1(\omega) = \mathbb{R}e(\epsilon(\omega))$ and $\epsilon_2(\omega) = \mathbb{I}m(\epsilon(\omega))$. This in turn implies that:

$$\begin{aligned}
\epsilon(\omega) &= 1 + \int f(t') \cos(\omega t') dt' + i \int f(t') \sin(\omega t') dt' \\
\epsilon^*(\omega) &= 1 + \int f(t') \cos(\omega t') dt' - i \int f(t') \sin(\omega t') dt' \\
&= 1 + \int f(t') \cos(-\omega t') dt' + i \int f(t') \sin(-\omega t') dt' \\
&= \epsilon(-\omega) \,.
\end{aligned}$$

This merely establishes that $\epsilon_1(-\omega) = \epsilon_1(\omega)$ (is even) and $\epsilon_2(-\omega) = -\epsilon_2(\omega)$ (is odd). If causality is to be respected, it is necessary that $t' < t$, because $\vec{D}(t)$ must only be affected by the past values of $\vec{E}$. Therefore, integration limits can be established thinking of all the possible previous moments t':

$$\epsilon(\omega) = 1 + \int_0^\infty f(t')e^{i\omega t'}dt' \,. \tag{2.11}$$

2.2.2 Analytical properties: $\epsilon(\omega)$ in the complex plane

In several occasions, it will be needed to make an extension $\epsilon(\omega) \to \epsilon(z)$ with $z \in \mathbb{C}$. Therefore it is useful to study some of the properties of (2.11) as an analytic funtion $\epsilon : \mathbb{C} \to \mathbb{C}$. First of all, if $z = z_1 + iz_2$, then:

$$\epsilon(z) = 1 + \int_0^\infty f(t')e^{iz_1t'}e^{-z_2t'}dt' \,. \tag{2.12}$$

But $f(t')$ is finite for every value of t', and in the upper half-plane $z_2 > 0$, therefore $\epsilon(z)$ does not diverge anywhere because of the $e^{-z_2t'}$ factor. Therefore, $\epsilon(z)$ is regular everywhere if $z \in \mathbb{C}(z_2 > 0)$. This property, derived from the causality condition, together with other properties enlisted by Landau[3] ensures that in the upper half-plane, $\epsilon(z)$ has no zeros (INTENTAR PROBAR ESTO POR COMPLETITUD!!). This is certainly useful provided most of the integrals to be evaluated depends on the following function:

$$\frac{1}{\epsilon(\omega)} = \frac{1}{\epsilon_1(\omega) + i\epsilon_2(\omega)} = \frac{\epsilon_1(\omega)}{|\epsilon(\omega)|^2} - i\frac{\epsilon_2(\omega)}{|\epsilon(\omega)|^2} \,, \tag{2.13}$$

which extended to the complex plane, shows no poles in the upper half-plane. Therefore, be means of the Cauchy-Goursat theorem[4], any closed curve in the upper half-plane gives a zero integral.

It is also useful to note that $1/\epsilon(\omega)$ shares its parity with $\epsilon(\omega)$, and also $\mathbb{I}m\left(\frac{1}{\epsilon(\omega)}\right) = -\frac{\epsilon_2(\omega)}{|\epsilon(\omega)|^2} < 0$. This imaginary part is usually named the **energy loss function** (ELF) and denoted by $\eta(\omega)$.

2.2.3 High frequency general behaviour

Independently of the material (whether it is a dielectric or a conductor), if $\omega \to \infty$, necessarily $\epsilon(\omega) \to 1$, because no polarization effect can occur if the electric field varies sufficiently fast. Given $\omega >> \overline{\nu}$, the polarization of the material can be calculated treating the electrons as free respect the interaction with the atomic nucleus and other electrons. Therefore, the equation for the electron's displacement $\vec{x}$ is $m_e\ddot{\vec{x}} = e\vec{E} = e\vec{E}_0e^{-i\omega t}$. Then:

$$m_e\dot{\vec{x}} = i\frac{e}{\omega}\vec{E}_0e^{-i\omega t} \quad \Rightarrow \quad \vec{x} = -\frac{e}{m_e\omega^2}\vec{E}_0e^{-i\omega t} = -\frac{e}{m_e\omega^2}\vec{E} \,.$$

If N is the atomic density, and each atom have Z_t electrons, the polarization $\vec{P}$ per volume unit will be simply $\vec{P} = NZ_t(e\vec{x})$, where $\vec{d} = e\vec{x}$ is the dipolar moment of each electron. Consequently:

$$\vec{P} = -\frac{NZ_te^2}{m_e\omega^2}\vec{E} \,.$$

On the other hand, we know that:

$$\begin{aligned}\vec{D} &= \vec{E} + 4\pi\vec{P} = \vec{E} - \frac{4\pi NZ_te^2}{m_e\omega^2}\vec{E} \\ &= \left(1 - \frac{4\pi NZ_te^2}{m_e\omega^2}\right)\vec{E} = \epsilon(\omega)\vec{E} \,.\end{aligned}$$

Then, if $\omega \to \infty$, we have that $\epsilon(\omega) \to 1 - \frac{\omega_p^2}{\omega^2}$ where the **plasmon frequency** $\omega_p^2 = \frac{4\pi NZ_te^2}{m_e}$ has been defined.

Chapter 3

Classic Stopping Power

3.1 Impulse transfer approximation

Consider our projectile is a heavy ion with mass M and charge $Z_p e$, whose initial velocity in the laboratory reference frame is $\vec{v}$. In this frame, the scattering material is at rest, and its constituents can be considered at rest also, regardless the electron movement in their orbits. This is so if the initial velocity of the ion is much more greater than the characteristic velocity of the electron in its orbit.

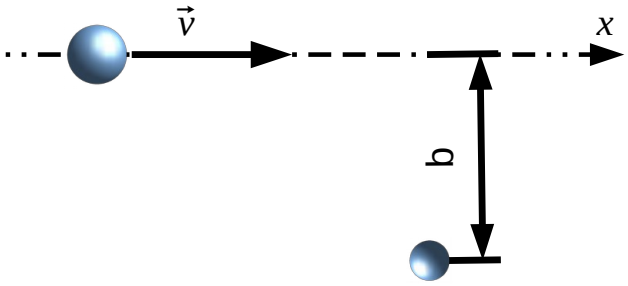

Figure 3.1: Definition of impact parameter in electron-ion interaction.

This is also useful to neglect the magnetic field effects generated by the moving projectile. It will also be used that $M >> m_e$, i.e., the ion is heavy enough so that its trajectory is slightly modified from the initial direction after the interaction with the electron. This is the small impulse approximation in which Bohr based its calculation.

We define the impact parameter b as the minimum traversal distance between the projectile's initial direction of movement and the electron's position.

The impulse transferred to the electron can be calculated using the classical definitions as:

$$\Delta p = \int_{-\infty}^{\infty} F dt = e \int_{-\infty}^{\infty} E_\perp dt = e \int_{-\infty}^{\infty} E_\perp \frac{dt}{dx} dx = \frac{e}{v} \int_{-\infty}^{\infty} E_\perp dx \,, \tag{3.1}$$

where the difference is measured long time before and after the collision takes place. Consequently, the projectile can be assumed to be in both situations far away in the x axis. The fact of choosing the component of the electric field perpendicular to the direction of movement is a consequence of the symmetry of the problem. At first, it might appear as if there is no symmetry, but it plays a fundamental role in the classical theory. In this approximation, we can think of the ion as belonging to a "wire" around which Gauss law can be used with a virtual cylindrical surface. See figure 3.2.

$$\int\limits_{cylinder} \vec{E} \cdot d\vec{a} = \int\limits_{cylinder} E_\perp da = 2\pi b \int_{-\infty}^{\infty} E_\perp dx = 4\pi q_{enc} \;\Rightarrow\; \int_{-\infty}^{\infty} E_\perp dx = \frac{2Z_p e}{b} \,,$$

and with this, the impulse transfer is:

$$\Delta p = \frac{2Z_p e^2}{vb} \,. \tag{3.2}$$

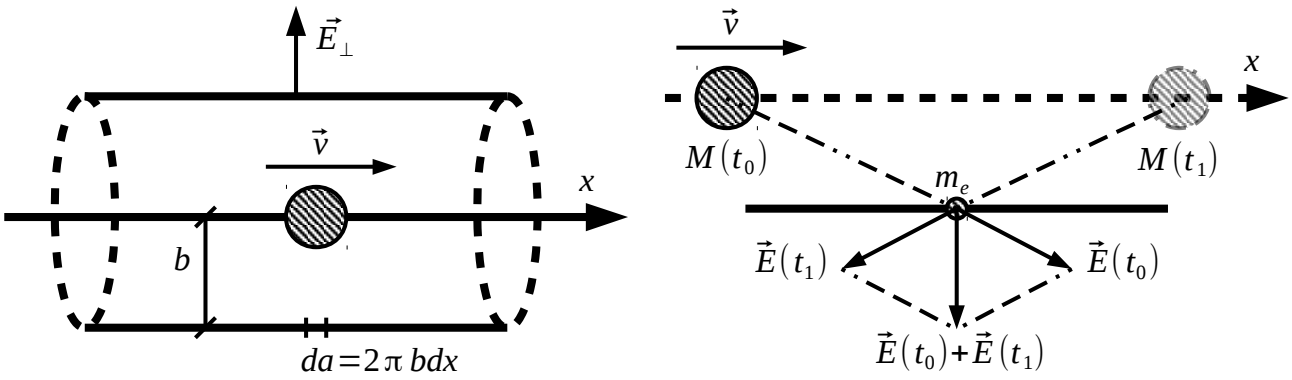

Figure 3.2: Gauss law with a cylindrical surface around the heavy ion path.

This enhances the evidence of the symmetry between two opposite times t_0 and t_1 before and after the collision takes place, using that $t = 0\,s$ is reached when the projectile is exactly at the impact parameter distance from the electron. The "net" field the electron feels is traversal due to this symmetry, canceling the longitudinal components when taking the full time interval in consideration.

The corresponding classical energy transfer to the atomic electron is then:

$$\Delta E(b) = \frac{\Delta p^2}{2m_e} = \frac{2Z_p^2 e^4}{m_e v^2 b^2}\,, \tag{3.3}$$

Then, adapting equation (1.9) to the information we are working with, $dS = N_e \Delta E(b) d\sigma(b)$, where we need an expression for the classical collision cross section, and N_e represents the electronic density. This is easily estimated as:

$$N_e = \frac{Z_t \rho N_A}{A_t} \;\;;\;\; [N_e] = \frac{g}{cm^3}\frac{mol}{g}\frac{1}{mol} = \frac{1}{cm^3}\,, \tag{3.4}$$

where Z_t and A_t are the material atomic and mass number respectively, ρ is its mass density, and N_A is Avogadro's constant.

The classical cross section is an already well known quantity and an elegant derivation may be found in Landau's[5] book on classical mechanics. As a function of the impact parameter, the expression for the differential cross section if the collision presents azymuthal symmetry in the incident direction axis is $d\sigma = 2\pi b db$. Putting everything together, we get:

$$dS = N_e \Delta E(b) d\sigma(b) = N_e \frac{2Z_p^2 e^4}{m_e v^2 b^2} 2\pi b db = \frac{4\pi N_e Z_p^2 e^4}{m_e v^2}\frac{db}{b} \tag{3.5}$$

The implicit association behind all of this deductions is that of the small angle coulomb scattering. Rutherford's exact formula establishing the relation between scattering angle θ_{scatt} and impact parameter b is:

$$\frac{2Z_p e^2}{pvb} = 2\tan\left(\frac{\theta_{scatt}}{2}\right) \sim \theta_{scatt}\,. \tag{3.6}$$

This can be geometrically deduced analyzing the impulse transfer vector as in figure 3.3.

$$\theta_{scatt} \approx \frac{\Delta p}{p} = \frac{2Z_p e^2}{pvb}\,. \tag{3.7}$$

We will see that using the exact Rutherford formula has other implications in the stopping power theory when relaxing the small angle approximation.

It is important to keep in mind that expression (3.5) is obtained thinking about the energy transferred to the electron, while the geometric picture in figure 3.3 is the momentum lost by the projectile, meaning these are quantities defined in different frames, although related.

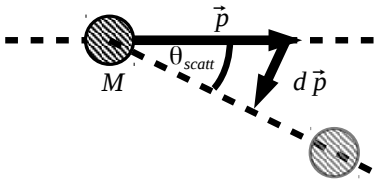

Figure 3.3: Relation between small scattering angle and small impulse transfer.

There is another way of obtaining expression (3.5) that does not concern our definition (1.9). Let's consider a uniform distribution of electrons in the target's material.

The "net" number of electrons from the cylindrical volume dV in figure 3.4 that "sees" the projectile is:

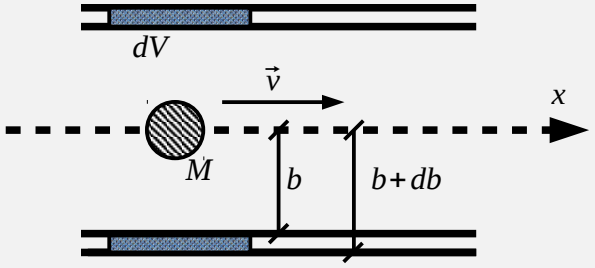

Figure 3.4: Volume containing the electrons that interact with the projectiles field.

$$N_{interactions} = N_e dV = N_e(2\pi b db dx)\,. \qquad (3.8)$$

Therefore, we define the energy lost by the projectile $-dT = N_e \Delta E(b) dV = N_e \Delta(b) 2\pi b db dx$,, and consequently the differential stopping power:

$$dS = -\frac{dT}{dx} = N_e \Delta E(b) 2\pi b db dx = \frac{4\pi N_e Z_p^2 e^4}{m_e v^2}\frac{db}{b}\,.$$

Here, the stopping power was written using the estimation of the net number of interactions with atomic electrons.

Next step consists of making the integration needed to get to know $S(T)$. The dependence in b^{-1} makes it impossible to integrate in the whole impact parameter interval $[0, \infty)$. This is because:

- When $b = 0$ the stopping power results infinite, but the projectile cannot deliver this amount of energy. This is the same divergence in Rutherford's formula for the long-range Coulomb interaction.
- When $b \to \infty$ the electrons are "infinitely far" from the projectile, and the collision characteristic time would be infinite.

In both cases the small impulse transference approximation is lost. Therefore, a pair of limits b_{min} and b_{max} are proposed so that the calculation remains physic. For example, we already know the maximum amount of energy than can be transferred to the electron in a close collision when $b \to 0$, equation (2.2). If $M >> m_e$ and the projectile can be considered relativistic, then:

$$\epsilon_{max} \simeq 2m_e v^2\gamma^2 = \frac{2Z_p^2 e^4}{m_e v^2 b_{min}} \quad \Rightarrow \quad b_{min} \simeq \frac{Z_p e^2}{m_e v^2 \gamma}\,. \qquad (3.9)$$

On the other hand, if the projectile is far away from the electron, the characteristic time of the collision, $T = \frac{b}{\gamma v}$ will be much greater than the time associated with the mean electron's orbital period $\tau = \frac{1}{\overline{\nu}}$, where $\overline{\nu}$ is the mean orbital frequency. If $T >> \tau$ then the electron is capable of doing many cycles orbiting around the nucleus while the projectiles slowly passes with practically no energy transfer. As we intend the projectile to lose energy, we choose:

$$T \leq \tau \quad \Rightarrow \quad \frac{b}{\gamma v} \leq \frac{1}{\overline{\nu}} \quad \Rightarrow \quad b \leq \frac{\gamma v}{\overline{\nu}} = b_{max}\,. \qquad (3.10)$$

With these limits, the integral can be handled:

$$\begin{aligned} S(T) &= \int_{b_{min}}^{b_{max}} dS(b) = \frac{4\pi N_e Z_p^2 e^4}{m_e v^2} \int_{b_{min}}^{b_{max}} \frac{db}{b} \\ &= \frac{4\pi N_e Z_p^2 e^4}{m_e v^2} \ln\left(\frac{b_{max}}{b_{min}}\right) \\ &= \frac{4\pi N_e Z_p^2 e^4}{m_e v^2} \ln\left(\frac{\gamma v}{\overline{\nu}} \frac{m_e v^2 \gamma}{Z_p e^2}\right) \\ &= \frac{4\pi N_e Z_p^2 e^4}{m_e v^2} \left\{\ln\left(\frac{m_e v^3}{Z_p e^2 \overline{\nu}}\right) - \ln(1-\beta^2)\right\} . \end{aligned} \tag{3.11}$$

It is convenient to rewrite the two big factors in this expression, defining some interesting parameters as follows:

$$\frac{4\pi N_e Z_p^2 e^4}{m_e v^2} = \frac{4\pi Z_t \rho N_A Z_p^2 e^4}{A_t m_e v^2} = K_0 \frac{\rho}{A_t} \frac{Z_t Z_p^2}{\beta^2} ;$$

$$\frac{m_e v^3}{Z_p e^2 \overline{\nu}} = \frac{2 m_e v^2}{\hbar \overline{\nu}} \frac{\hbar v}{2 Z_p e^2} = \frac{2 m_e v^2}{\langle I \rangle} \frac{1}{2\eta} ,$$

where $K_0 = \frac{4\pi N_A e^4}{m_e c^2}$ and $\eta = \frac{Z_p e^2}{\hbar v}$ is the **Sommerfeld parameter** measuring the Coulomb interaction importance. It also appears in the quantum mechanically treated Coulomb scattering problem. Taking all of this to the stopping power formula, we are able to give our first approximation using the classical picture, containing every feature Bohr presented in 1915:

Adiabatic Bohr's radius

The upper limit $b_{max} = \frac{\gamma v}{\overline{\nu}}$ is defined thinking of the distance to the electron where the energy transfer is negligible, in other words, the interaction process is **adiabatic**. This limit is proposed by Bohr[6] in 1915, and it presupposes that the electrons are orbiting the nucleus of the atom. It might seem as we are dabbling in quantum mechanics, but the modern picture of this last was not developed until 1925 with the famous Schrödinger's[7] equation. Nevertheless, the notion of periodic trajectories with quantized action was already there, proposed separately by Wilson[8] and Sommerfeld[9] by the condition:

$$\oint_{H(p,q)=E} p_i dq_i = n_i h , \tag{3.12}$$

where H is the Hamiltonian, q_i and p_i the generalized coordinates and conjugate momentum respectively, $n_i \in \mathbb{Z}$ and h is Planck's constant.
b_{max} is defined in a way that the electron accomplishes several periods of motion like these in the atom without energy transfer from the projectile, and thereby was called the **Bohr's adiabatic radius**.
Other important characteristic of this radius is the mean orbital period $\tau = \frac{1}{\overline{\nu}}$. According to modern quantum mechanics, each electron presents different binding energy for each orbital, and consequently different associated frequency ν. Bohr's calculation of the stopping power uses the idea of an average frequency, related to the mean excitation potential $\langle I \rangle = h\overline{\nu}$, but fails to give a first principle definition.

$$\boxed{S(T) = K_0 \frac{\rho}{A_t} \frac{Z_t Z_p^2}{\beta^2} \left\{\ln\left(\frac{2 m_e v^2}{\langle I \rangle}\right) - \ln(2\eta) - \ln(1-\beta^2)\right\}} . \tag{3.13}$$

It is worthwhile pointing out some features of the resulting formula:

1. This deduction is somehow simplistic, lacking of better arguments for the integral limits, and of a thoroughly accurate definition of $\overline{\nu}$, remaining $\langle I \rangle$ undetermined.

2. The term $\ln(1-\beta^2)$ is associated to the relativistic effects when the projectile presents high kinetic energy. It is made of a squared Lorentz factor, this is γ^2, and in following sections the provenance of both of them will be signaled.

3. The term with the Sommerfeld parameter $\ln(2\eta)$ is usually presented in literature together with the first logarithmic term, but it is interesting separating it to compare with the results of next sections. This term arises as a compromise between the classical and the quantum mechanical views of the stopping power as explained by Bloch[10] in 1933. The factor 2 accompanying the Sommerfeld parameter is not exactly 2 as obtained in this small impulse transfer approximation, and the careful study of next sections will clarify why.

3.2 Classic calculation of Bohr: close collisions

To give support to the parameter definitions of the last section, it is instructive to fulfill Bohr's calculation. In the close collision approximation, the high energetic projectile approaches the electron with and impact parameter $b < b_1$, where b_1 is some undetermined limit where it is not possible to assume the electron as free. Therefore, in this section we will be working in the interval $0 < b < b_1$, treating the electron as free given the characteristic time of the collision is much smaller than the orbital period.

The electron will suffer a momentum transfer from the projectile, whose Lorentz invariant Q^2 can be written in two useful inertial frames:

- Center of mass: located in the projectile, because $M >> m_e$. In this frame, the electron has velocity $\vec{v}$, and the four-momentum is:

$$p_i^{c.m.} = \begin{pmatrix} \gamma m_e c \\ \gamma m_e \vec{v} \end{pmatrix} \quad ; \quad p_f^{c.m.} = \begin{pmatrix} \gamma' m_e c \\ \gamma' m_e \vec{v}\,' \end{pmatrix},$$
$$p_f^{c.m.} - p_i^{c.m.} = \begin{pmatrix} 0 \\ \gamma m_e(\vec{v}\,' - \vec{v}) \end{pmatrix} \Rightarrow Q^2 = \left(p_f^{c.m.} - p_i^{c.m.}\right)^2 = -\gamma^2 m_e^2 \left(\vec{v}\,' - \vec{v}\right).$$

  The fact that the energy conserves in the center of mass was used, therefore $|\vec{v}\,'| = |\vec{v}|$, but anything is said on the possible deflection of the electron. This was implicitly done when assuming that $\gamma' = \gamma$. The Lorentz invariant is then:

$$\begin{aligned} Q^2 &= -\gamma^2 m_e^2 \left\{|\vec{v}\,'|^2 - 2\vec{v}\,' \cdot \vec{v} + |\vec{v}|\right\} = -\gamma^2 m_e v^2 \left\{2 - 2\cos(\theta_{scatt})\right\} \\ &= -2\gamma^2 m_e^2 v^2 \left\{1 - \cos(\theta_{scatt})\right\} = -4\gamma^2 m_e^2 v^2 \sin^2\left(\frac{\theta_{scatt}}{2}\right). \end{aligned}$$

- Laboratory frame: in this case, the electron is initially at rest inside the target material. Therefore the projectile moves with $\vec{v}$ towards the atomic electron. In this case:

$$p_i^{l.f.} = \begin{pmatrix} m_e c \\ 0 \end{pmatrix} \quad ; \quad p_f^{l.f.} = \begin{pmatrix} E/c \\ \vec{p} \end{pmatrix},$$
$$p_f^{l.f.} - p_i^{l.f.} = \begin{pmatrix} E/c - m_e c \\ \vec{p} \end{pmatrix} \Rightarrow Q^2 = \left(p_f^{l.f.} - p_i^{l.f.}\right)^2 \left(\frac{E}{c} - m_e c\right)^2 - |\vec{p}|^2.$$

  Using the relativistic formula $E^2 = m_e^2 c^4 + |\vec{p}|^2 c^2$ and defining the kinetic energy transferred to the electron as $T = E - m_e c^2$ it can be obtained:

$$Q^2 = \frac{E^2}{c^2} - 2m_e E + m_e c^2 - \frac{E^2}{c^2} + m_e^2 c^2 = -2m_e(E - m_e c^2) = -2m_e T.$$

As said, Q^2 is a Lorentz invariant, meaning it has the same numerical value in every frame:

$$\begin{aligned} -2m_eT &= -4\gamma^2 m_e^2 v^2 \sin^2\left(\frac{\theta_{scatt}}{2}\right) \\ T(\theta_{scatt}) &= 2\gamma^2 m_e v^2 \sin^2\left(\frac{\theta_{scatt}}{2}\right). \end{aligned} \tag{3.14}$$

We will rewrite the kinetic energy transferred to the electron (3.14) using Rutherford's formula (3.6) with $p = \gamma m_e v$ in the center of mass frame, and the following trigonometric identity:

$$\begin{aligned} \sin^2\left(\frac{\theta_{scatt}}{2}\right) &= \frac{1}{1+\frac{1}{\tan^2\left(\frac{\theta_{scatt}}{2}\right)}} = \frac{1}{1+\frac{\gamma^2 m_e^2 v^4 b^2}{Z_p^2 e^4}} = \\ &= \frac{Z_p^2 e^4}{\gamma^2 m_e^2 v^4}\frac{1}{\frac{Z_p^2 e^4}{\gamma^2 m_e^2 v^4}+b^2} = \frac{Z_p^2 e^4}{\gamma^2 m_e^2 v^4}\frac{1}{b_{min}^2+b^2}, \end{aligned}$$

where the definition (3.9) was used. With this, the kinetic energy transferred to the electron in terms of the impact parameter is obtained:

$$T(b) = \frac{2Z_p^2 e^4}{m_e v^2}\frac{1}{b_{min}^2+b^2}. \tag{3.15}$$

If $\theta_{scatt} \approx 0$, then according (3.6):

$$0 \approx \theta_{scatt} \sim \frac{2Z_p e^2}{\gamma m_e v^2 b} = 2\frac{b_{min}}{b} \quad \Rightarrow \quad b_{min} \approx 0, \tag{3.16}$$

and equation (3.15) is reduced exactly to the kinetic energy calculated in (3.3).

As the electron was initially at rest, then $T(b) = \Delta E(b)$ and the stopping power definition can be used with the classical cross section as before:

$$dS = N_e \Delta E(b) d\sigma(b) = N_e \frac{2Z_p^2 e^4}{m_e v^2}\frac{2\pi b db}{b^2+b_{min}^2} = K_0 \frac{\rho}{A_t}\frac{Z_t Z_p^2}{\beta^2}\frac{bdb}{b^2+b_{min}^2}. \tag{3.17}$$

The integration can be done in the interval of interest without further problems:

$$\begin{aligned} S(T) &= \int_0^{b_1} dS(b) = K_0 \frac{\rho}{A_t}\frac{Z_t Z_p^2}{\beta^2}\int_0^{b_1}\frac{bdb}{b^2+b_{min}^2} = \\ &= K_0 \frac{\rho}{A_t}\frac{Z_t Z_p^2}{\beta^2}\frac{1}{2}\int_{b_{min}^2}^{b_1^2+b_{min}^2}\frac{dx}{x} = K_0 \frac{\rho}{A_t}\frac{Z_t Z_p^2}{\beta^2}\frac{1}{2}\ln\left(1+\frac{b_1^2}{b_{min}^2}\right). \end{aligned}$$

The classic stopping power formula for close collisions is obtained:

$$\boxed{S_{b<b_1}(T) = K_0 \frac{\rho}{A_t}\frac{Z_t Z_p^2}{\beta^2}\frac{1}{2}\ln\left(1+\frac{\gamma^2 m_e^2 v^4}{Z_p^2 e^4}b_1^2\right)}. \tag{3.18}$$

As can be seen, this expression depends on an undetermined limit b_1 between the free electron approach and other approximation in which the atomic binding becomes important, where the energetic transference can produce excitation of the atoms if $b < b_{max}$, that is below the adiabatic limit. This is the distant collision approximation studied in next section.

Reinterpretation of the calculation

In this non-relativistc close collision calculation, the four-momentum conservation implied that:

$$T(\theta_{scatt}) = 2\gamma^2 m_e v^2 \sin^2\left(\frac{\theta_{scatt}}{2}\right) \approx 2m_e v^2 \sin^2\left(\frac{\theta_{scatt}}{2}\right) \;\; ; \;\; \gamma \approx 1\,. \tag{3.19}$$

meaning $T(\theta_{scatt})$ is the energy gained by the electron in the collision process. Also, $\sin^2\left(\frac{\theta_{scatt}}{2}\right) = \frac{Z_p^2 e^4}{m_e v^2}\frac{1}{b^2+b_{min}^2}$ was derived and used, writing the stopping power as:

$$dS = N_e \Delta E(b) d\sigma(b) = N_e \frac{2Z_p^2 e^4}{m_e v^2}\frac{1}{b^2+b_{min}^2} b db d\varphi = N_e 2m_e v^2 \sin^2\left(\frac{\theta_{scatt}}{2}\right) b db d\varphi\,. \tag{3.20}$$

According to Rutherford, $\tan\left(\frac{\theta_{scatt}}{2}\right) = \frac{Z_p e^2}{m_e v^2 b} \Rightarrow b = \frac{Z_p e^2}{m_e v^2}\frac{1}{\tan\left(\frac{\theta_{scatt}}{2}\right)}$. Using this:

$$db = \frac{Z_p e^2}{m_e v^2}\frac{1}{\tan^2\left(\frac{\theta_{scatt}}{2}\right)}\frac{1}{\cos^2\left(\frac{\theta_{scatt}}{2}\right)}\frac{d\theta_{scatt}}{2} \Rightarrow b db = \left(\frac{Z_p e^2}{m_e v^2}\right)^2 \frac{\cos\left(\frac{\theta_{scatt}}{2}\right)}{\sin^3\left(\frac{\theta_{scatt}}{2}\right)}\frac{d\theta_{scatt}}{2}\,. \tag{3.21}$$

Taking this to the stopping power:

$$\begin{aligned} dS &= N_e T(\theta_{scatt}) \left(\frac{Z_p e^2}{m_e v^2}\right)^2 \frac{\cos\left(\frac{\theta_{scatt}}{2}\right)}{\sin^3\left(\frac{\theta_{scatt}}{2}\right)}\frac{d\varphi d\theta_{scatt}}{2} \\ &= N_e T(\theta_{scatt}) \left(\frac{Z_p e^2}{m_e v^2}\right)^2 \frac{\cos\left(\frac{\theta_{scatt}}{2}\right)}{\sin^3\left(\frac{\theta_{scatt}}{2}\right)}\frac{\sin(\theta_{scatt}) d\varphi d\theta_{scatt}}{\sin(\theta_{scatt})2} \\ &= N_e T(\theta_{scatt}) \left(\frac{Z_p e^2}{m_e v^2}\right)^2 \frac{1}{\sin^4\left(\frac{\theta_{scatt}}{2}\right)} d\Omega \\ &= N_e T(\theta_{scatt}) \frac{d\sigma_{Ruth}}{d\Omega} d\Omega = N_e T d\sigma_{Ruth}\,, \end{aligned}$$

expression that is in accordance to the statistical interpretation of definition (1.9).

3.3 Classic calculation of Bohr: distant collisions

In this section, the b_{max} limits chosen in (3.10) will be correctly justified as the plausible representation of limit of adiabatic interaction (elastic collision) respect Coulombian interaction with atomic electrons. Here, some of the assumptions made in section 3.1 will be used again, for example the projectile will leave the interaction region with practically no deflection respect its initial movement direction. The electron will be considered as describing an harmonically bound trajectory around the nucleus. To describe this, a laboratory frame centered in the atomic nucleus responsible for the electron binding is used, and the electron's position is given by some vector $\vec{x}$.

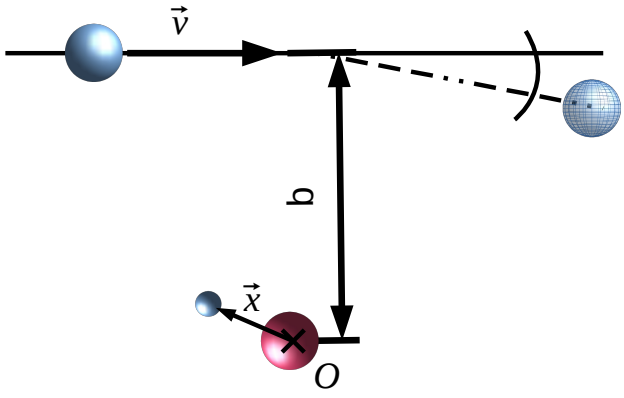

Figure 3.5: Simple sketch of the interaction with an harmonically bound atomic electron.

If the impact parameter is sufficiently great, $b >> |\vec{x}|$, then the energy transfer will be small and the electron's movement can be considered not relativistic. Also, the electric field of the projectile on the electron position can be approximated by it's value at the origin O, that is, the nucleus position. This is known as the **dipolar approximation**.

Being the electron non-relativistic, and considering its movement around the nucleus as an harmonic oscillation with small amplitude, we can approximate $|\dot{\vec{x}}| = |\vec{v}_{el}| \sim 0$, and consequently, $\vec{v}_{el} \times \vec{B} \sim 0$ is justified, neglecting the magnetic field effects.

It will also be included in the model, only for completing the theoretical view, a small **damping constant** $\Gamma \approx 0$, such that if the characteristic oscillation angular frequency is ω_0 then the harmonic force equation with the second Newton's law stands for:

$$m_e\vec{a} = \sum \vec{F}_{ext} = \vec{F}_\Gamma + \vec{F}_{\omega_0} + \vec{F}_{\vec{E}} \;\Rightarrow\; \ddot{\vec{x}} + \gamma\dot{\vec{x}} + \omega_0^2\vec{x} = -\frac{e}{m_e}\vec{E}\,. \tag{3.22}$$

We lack the expression of the electric field $\vec{E}$ that feels the electron due to the presence of the projectile. Obtaining this requires explicit relativistic calculations and will be dealt with later. Now, it is preferable to remember how this kind of force equations can be solved to obtain $\vec{x}$. The idea is rather simple, making a Fourier analysis that spectrally decomposes the involved functions in terms of the harmonic components of frequency ω. This is:

$$\mathfrak{F}\left(\vec{x}(t)\right) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\vec{x}(\omega)e^{-i\omega t}d\omega \;\;;\;\; \mathfrak{F}\left(\vec{E}(t)\right) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\vec{E}(\omega)e^{-i\omega t}d\omega\,. \tag{3.23}$$

The Fourier transform presents the following properties that will be used:

$$\mathfrak{F}(\dot{f}(t)) = -i\omega\mathfrak{F}(f(t)) \;\;;\;\; \mathfrak{F}(f^{(n)}(t)) = (-i\omega)^n\mathfrak{F}(f(t))\,. \tag{3.24}$$

Consequently, $\mathfrak{F}\left(\dot{\vec{x}}\right) = -i\omega\mathfrak{F}\left(\vec{x}\right)$ and $\mathfrak{F}\left(\ddot{\vec{x}}\right) = -\omega^2\mathfrak{F}\left(\vec{x}\right)$. Taking everything to the force equation for $\vec{c}$ we obtain:

$$-\frac{\omega^2}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\vec{x}(\omega)e^{-i\omega t}d\omega - \frac{i\omega\Gamma}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\vec{x}(\omega)e^{-i\omega t}d\omega + \frac{\omega_0^2}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\vec{x}(\omega)e^{-i\omega t}d\omega = \frac{e}{m_e}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\vec{E}(\omega)e^{-i\omega t}d\omega\,,$$

which is solver only when the integrands coincides. This leaves us with an algebraic equation for the spectral components of the electron's position $\vec{x}$ and the projectile's electric field $\vec{E}$:

$$\begin{aligned} -\omega^2\vec{x}(\omega) - i\omega\Gamma\vec{x}(\omega) + \omega_0^2\vec{x}(\omega) &= -\frac{e}{m_e}\vec{E}(\omega) \\ \vec{x}(\omega)\left(-\omega^2 - i\omega\Gamma + \omega_0^2\right) &= -\frac{e}{m_e}\vec{E}(\omega)\,, \end{aligned}$$

and therefore, the solution for the spectral amplitudes of the electron's position is:

$$\vec{x}(\omega) = \frac{e}{m_e}\vec{E}(\omega)\frac{1}{\omega^2 - \omega_0^2 + i\omega\Gamma}\,. \tag{3.25}$$

Then, Fourier transforming the integral equation, we obtained an easily solved algebraic equation in terms of the electric field amplitude for frequency ω. This is just an ingredient of the deduction of the stopping power, as we will like to quantify the energy transferred in the interaction. We know that the electric field exerts a work on a charge $q = -e$ that moves $d\vec{x}$ in its presence as viewed from O:

$$\begin{aligned} dW = \vec{F}(t)\cdot d\vec{x} = q\vec{E}(t) &= -e\vec{E}(t)\cdot d\vec{x} \\ &= -e\vec{E}(t)\cdot\frac{d\vec{x}}{dt}dt = -e\vec{E}(t)\cdot\dot{\vec{x}}dt\,. \end{aligned}$$

Then, the energetic transference along the trajectory $\vec{x}(t)$ of the electron whilst the time passes from very long before and very long after the interaction is:

$$\Delta E = -e\int_{-\infty}^{\infty}\vec{E}(t)\cdot\dot{\vec{x}}dt\,. \tag{3.26}$$

We are obviously assuming that $\vec{E}$ has a compact support in time. In this formula, the Fourier transforms of the integrand factors will be used, rewritten as follows not to mix up variables:

$$\vec{x}(t)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\vec{x}(\omega)e^{-i\omega t}d\omega\ \ ;\ \ \dot{\vec{x}}(t)=\frac{-i}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\vec{x}(\omega)\omega e^{-i\omega t}d\omega\ \ ;\ \ \vec{E}(t)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\vec{E}(\Omega)e^{-i\Omega t}d\Omega\,,$$

and therefore:

$$\Delta E=\frac{ie}{2\pi}\int_{-\infty}^{\infty}d\omega\;\omega\int_{-\infty}^{\infty}d\Omega\int_{-\infty}^{\infty}dt\;\vec{x}(\omega)\cdot\vec{E}(\Omega)e^{-i(\omega+\Omega)t}\,.$$

We already know that independently of the normalization used to define the Fourier transforms, the exponential function satisfies that $\int e^{-i(\omega+\Omega)t}dt=(2\pi)\delta(\omega+\Omega)$, where δ is the Dirac's delta. With this:

$$\Delta E=ie\int_{-\infty}^{\infty}d\omega\;\omega\int_{-\infty}^{\infty}d\Omega\;\vec{x}(\omega)\cdot\vec{E}(\Omega)\delta(\Omega-(-\omega))=ie\int_{-\infty}^{\infty}d\omega\;\omega\;\vec{x}(\omega)\cdot\vec{E}(-\omega)\,.$$

Moreover, $\vec{x}$ and $\vec{E}$ must be real quantities to be physical, and therefore $\vec{E}(-\omega)=\vec{E}^*(\omega)$. With this, we can keep on working the energy transfer, also replacing $\vec{x}(\omega)$ by equation (3.25).

$$\begin{aligned}\Delta E&=ie\int_{-\infty}^{\infty}d\omega\;\omega\;\vec{x}(\omega)\cdot\vec{E}^*(\omega)\\&=ie\int_{-\infty}^{\infty}d\omega\;\omega\frac{e}{m_e}\vec{E}(\omega)\cdot\vec{E}^*(\omega)\frac{1}{\omega^2-\omega_0^2+i\omega\Gamma}\\&=\frac{e^2}{m_e}\int_{-\infty}^{\infty}d\omega\;|\vec{E}(\omega)|^2\frac{i\omega}{\omega^2-\omega_0^2+i\omega\Gamma}\,.\end{aligned}$$

It is convenient to rewrite the complex function of ω appearing on the integrand using its real and imaginary parts.

$$\frac{i\omega}{\omega^2-\omega_0^2+i\omega\Gamma}=\frac{i\omega(\omega^2-\omega_0^2-i\omega\Gamma)}{(\omega^2-\omega_0^2)^2+\omega^2\Gamma^2}=\frac{\omega^2\Gamma}{(\omega^2-\omega_0^2)^2+\omega^2\Gamma^2}+i\frac{\omega(\omega^2-\omega_0^2)}{(\omega^2-\omega_0^2)^2+\omega^2\Gamma^2}\,.$$

If $\Gamma\sim 0$, both real and imaginary parts presents a high peak centered at ω_0. Therefore, assuming $|\vec{E}(\omega)|^2\approx|\vec{E}(\omega_0)|^2$ is not wrong, consequently the interaction proceeds mainly when there is a resonance of the electric field component whose frequency coincides with the characteristic atomic electron's frequency. After using this, the factor $|\vec{E}(\omega_0)|^2$ can be taken out the integral, and using that the imaginary part is odd in ω while the real part is even, the energy transfer is:

$$\Delta E=\frac{2e^2\Gamma}{m_e}|\vec{E}(\omega_0)|^2\int_0^{\infty}\frac{\omega^2}{(\omega^2-\omega_0^2)^2+\omega^2\Gamma^2}d\omega\,. \tag{3.27}$$

The remaining integral can be solved using that $\frac{\omega_0}{\Gamma}\to\infty$, or equivalently $\Gamma\sim 0$, but if not using this approximation nothing can be said at first. In his book Classical Electrodynamics, Jackson[11] says that the integral's solution is the same independently of the value of $\frac{\omega_0}{\Gamma}$ but this is not strictly true. The solution depends strongly on the limit $\omega_0/\Gamma >> 1$. Making a first the change of variables $u=\omega_0/\Gamma$, then $y=u-\frac{\omega_0}{\Gamma}$, and finally $z=2y$, the calculation can be handled as follows:

$$\int_0^\infty \frac{\Gamma\omega^2}{(\omega^2-\omega_0^2)^2+\omega^2\Gamma^2} = \int_0^\infty \frac{\Gamma\Gamma^2u^2\Gamma du}{(\Gamma^2u^2-\omega_0^2)^2+u^2\Gamma^4} = \int_0^\infty \frac{u^2}{\left(u^2-\frac{\omega_0^2}{\Gamma^2}\right)^2+u^2}du =$$
$$= \int_0^\infty \frac{du}{\frac{\left(u^2-\frac{\omega_0^2}{\Gamma^2}\right)^2+u^2}{u^2}+1} = \int_{-\omega_0/\Gamma}^\infty \frac{dy}{1+\frac{\left(y^2+2y\frac{\omega_0}{\Gamma}\right)^2}{y^2+2y\frac{\omega_0}{\Gamma}\frac{\omega_0^2}{\Gamma^2}}} =$$
$$= \int_{\omega_0/\Gamma}^\infty \frac{dy}{1+\frac{\left(y^2+2y\frac{\omega_0}{\Gamma}\right)^2}{\frac{\omega_0^2}{\Gamma^2}\left(\frac{\Gamma^2}{\omega_0^2}y^2+2y\frac{\Gamma}{\omega_0}+1\right)}} \sim \int_{-\infty}^\infty \frac{dy}{1+\frac{\left(y^2+2y\frac{\omega_0}{\Gamma}\right)^2}{\frac{\omega_0^2}{\Gamma^2}}} =$$
$$= \int_\infty^\infty \frac{dy}{1+\left(\frac{\Gamma}{\omega_0}y^2+2y\right)^2} \sim \int_{-\infty}^\infty \frac{dy}{1+4y^2} = \frac{1}{2}\int_{-\infty}^\infty \frac{dz}{1+z^2} =$$
$$= \frac{1}{2}\arctan(z)\Big|_{-\infty}^{\infty} = \frac{\pi}{2}\,.$$

When the symbol $\sim$ appears, the approximation $\Gamma << \omega_0$ was used, and thereby the integral value depends strongly on this assumption. With this calculation, the energy transfer stands for:

$$\Delta E = \frac{2e^2}{m_e}|\vec{E}(\omega_0)|^2\frac{\pi}{2} \quad \Rightarrow \quad \boxed{\Delta E = \frac{\pi e^2}{m_e}|\vec{E}(\omega_0)|^2}\,. \tag{3.28}$$

Despite all the approximations used, formula (3.28) is quite general. The only remaining unknown ingredient is the Fourier transform of the electric field generated by the projectile in O, that is the same the electron feels at $\vec{x}$ using the dipolar approximation. This is a completely different problem and that is why we take care of it last. Consider a second frame O' attached to the projectile. In this frame, the projectile is "at rest", and therefore writing the electric field it produces is easy. It will be assumed that at $t = t' = 0\,s$ the frames axis are parallel and coincident except O' is at a distance b from O. Figure 3.6 shows what happens for $t' < 0\,s$. The observation point O seen from O' have coordinates:

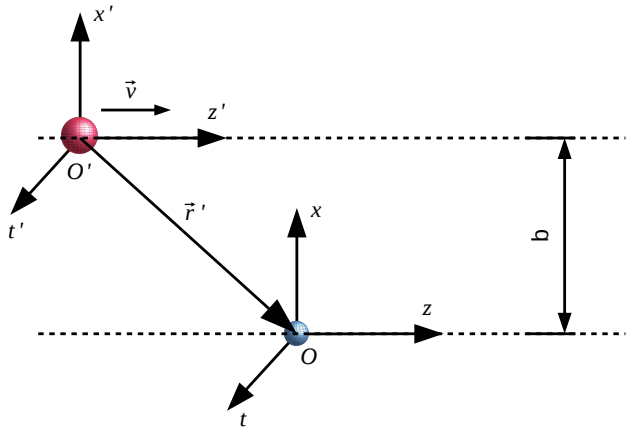

Figure 3.6: Frames O and O' used to calculate the electric field at eletron's position.

$$x'^{\mu} = \begin{pmatrix} t' \\ x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} t' \\ -b \\ 0 \\ -vt' \end{pmatrix} \quad \Rightarrow \quad r' = \sqrt{b^2+v^2t'^2}\,.$$

And with this, writing the electric field in components is straightforward:

$$\vec{E}\,'(x') = \frac{Z_p e}{r'^3}\vec{r}\,' = E'_x\hat{i}\,' + E'_z\hat{k}\,'$$
$$= -\frac{Z_p e b}{r'^3}\hat{i}\,' - \frac{Z_p e v t'}{r'^3}\hat{k}\,'\,.$$

Rewriting this in the frame O requires the corresponding Lorentz transformation. In this case, as $\vec{B}\,' = 0$, the transformation of the field is easy:

$$E_x = \gamma E'_x \;\;;\;\; E_y = 0 = E'_y \;\;;\;\; E_z = E'_z\,, \tag{3.29}$$

and with this:

$$\vec{E}(x') = -\frac{Z_p e b\gamma}{(b^2+v^2t'^2)^{3/2}}\hat{i} - \frac{Z_p e v t'}{(b^2+v^2t'^2)^{3/2}}\hat{k}\,, \tag{3.30}$$

where the versors transformation is trivial because the axis are parallel in Cartesian coordinates. It remains to apply the Lorentz transformation to the coordinates. The only coordinate of O' that remains variable is t'. We know (see Jackson[11]) that for this $ct' = \gamma(ct - \beta z)$, but the coordinate z of O as seen from O is exactly $z = 0$. Therefore $t' = \gamma t$. With this, the electric field produced by the projectile on the electron position as seen from the observer O in the atomic nucleus is:

$$\vec{E}(t) = -\frac{Z_p e b\gamma}{(b^2+\gamma^2v^2t^2)^{3/2}}\hat{i} - \frac{Z_p e \gamma v t}{(b^2+\gamma^2v^2t^2)^{3/2}}\hat{k}\,. \tag{3.31}$$

The dependence in t show the symmetry used in the small impulse approximation of section 3.1. In figure 3.7 both components are drawn using that every other parameter is a constant with unity value.

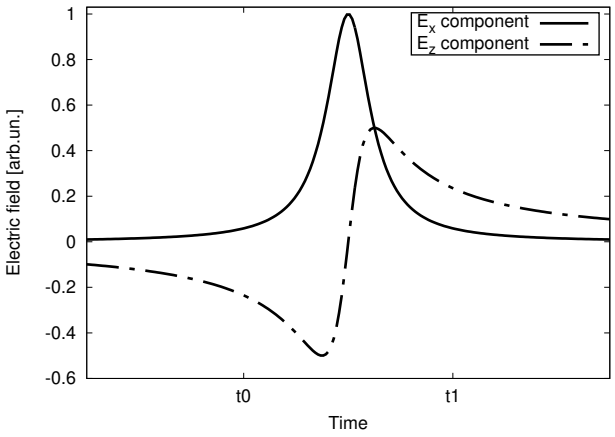

Figure 3.7: Electric field components affecting the electron as seen from atomic nucleus.

The parity of the electric force components becomes evident, and the symmetry used to keep the traversal component of the field shown in figure 3.2 is now supported by theoretical means. It is worthwhile to mention that the shape of the x-component (corresponding to the traversal of section 3.1) is that of a compact support signal in time. This helps to create the picture of a short duration perturbation applied to the atom. Now, the Fourier transform will be applied to both component of the fields separately, because this will lead to the appearance of special function related to the cylindrical symmetry of the problem, and different relations between them are needed to move forward. We begin with the x-component.

$$\begin{aligned} E_x(\omega) &= -\frac{Z_p e b\gamma}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\frac{e^{i\omega t}}{(b^2+\gamma^2v^2t^2)^{3/2}}dt = -\frac{Z_p e\gamma}{\sqrt{2\pi}b^2}\int_{-\infty}^{\infty}\frac{e^{i\omega t}}{\left(1+\left[\frac{\gamma v t}{b}\right]^2\right)^{3/2}}dt \\ &= -\frac{Z_p e}{\sqrt{2\pi}vb}\int_{-\infty}^{\infty}\frac{e^{i\frac{b\omega}{\gamma v}u}}{(1+u^2)^{3/2}}du\,, \end{aligned}$$

where $u = \frac{\gamma v}{b}t$ was used. According to Abramowitz and Stegun[12], the **modified Bessel functions of the second kind** satisfy:

$$K_\nu(xz) = \frac{\Gamma\left(\nu+\frac{1}{2}\right)(2z)^\nu}{\sqrt{\pi}x^\nu}\int_0^\infty \frac{\cos(xt)}{(t^2+u^2)^{\nu+1/2}}dt\,. \tag{3.32}$$

Replacing $t = u$, $z = 1$, $\nu = 1$ and $x = \frac{b\omega}{\gamma v}$ leads to:

$$K_1\left(\frac{b\omega}{\gamma v}\right) = \frac{2\Gamma(3/2)}{\sqrt{\pi}\frac{b\omega}{\gamma v}}\int_0^\infty \frac{\cos\left(\frac{b\omega}{\gamma v}u\right)}{(1+u^2)^{3/2}}du\,. \tag{3.33}$$

Using that $\cos(x)$ is even and $\sin(x)$ is odd, and $\Gamma(3/2) = \Gamma(1+1/2) = \frac{1}{2}\Gamma(1/2) = \frac{\sqrt{\pi}}{2}$, then:

$$K_1\left(\frac{b\omega}{\gamma v}\right) = \frac{\gamma v}{2b\omega}\int_{-\infty}^{\infty}\frac{e^{i\frac{b\omega}{\gamma v}}}{(1+u^2)^{3/2}}du \;\Rightarrow\; \int_{-\infty}^{\infty}\frac{e^{i\frac{b\omega}{\gamma v}}}{(1+u^2)^{3/2}}du = \frac{2b\omega}{\gamma v}K_1\left(\frac{b\omega}{\gamma v}\right). \tag{3.34}$$

Then, the x-component of the electric field can be written as:

$$E_x(\omega) = -\frac{2Z_p e\omega}{\sqrt{2\pi}\gamma v^2}K_1\left(\frac{b\omega}{\gamma v}\right). \tag{3.35}$$

A similar calculation can be used to estimate the z-component. In this case:

$$\begin{aligned} E_z(\omega) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\frac{(-Z_p e\gamma v t)e^{i\omega t}}{(b^2+\gamma^2v^2t^2)^{3/2}}dt = -\frac{Z_p e\gamma v}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\frac{te^{i\omega t}}{b^3\left(1+\left[\frac{\gamma v}{b}t\right]^2\right)^{3/2}} \\ &= -\frac{Z_p e}{\sqrt{2\pi}\gamma v b}\int_{-\infty}^{\infty}\frac{ue^{i\frac{b\omega}{\gamma v}u}}{(1+u^2)^{3/2}}du\,, \end{aligned}$$

where again $u = \frac{\gamma v}{b}t$. To continue the calculation, we use a recurrence relation[12]. If $\mathcal{L}_\nu(x) = e^{i\pi\nu}K_\nu(x)$, then:

$$\frac{d\mathcal{L}_\nu}{dx}(x) = \mathcal{L}_{\nu-1}(x) - \frac{1}{x}\mathcal{L}_\nu(x) \text{ and setting } \nu = 1;\; \frac{d\mathcal{L}_1}{dx}(x) = \mathcal{L}_0(x) - \frac{1}{x}\mathcal{L}_1(x)\,;$$

$$\mathcal{L}_0(x) = \frac{d\mathcal{L}_1}{dx}(x) + \frac{1}{x}\mathcal{L}_1(x) \;\Rightarrow\; K_0(x) = -\frac{dK_1}{dx}(x) - \frac{1}{x}K_1(x)\,.$$

Using equation (3.32) with $\nu = 1$ and $z = 1$ is easy to see that:

$$\frac{dK_1}{dx}(x) = -\frac{1}{2x^2}\int_{-\infty}^{\infty}\frac{e^{ixt}}{(1+t^2)^{3/2}}dt + \frac{1}{2x}\int_{-\infty}^{\infty}\frac{ite^{i\omega t}}{(1+t^2)^{3/2}}dt\,,$$

and therefore:

$$\begin{aligned} K_0(x) &= \cancel{\frac{1}{2x^2}\int_{-\infty}^{\infty}\frac{e^{ixt}}{(1+t^2)^{3/2}}dt} - \frac{i}{2x}\int_{-\infty}^{\infty}\frac{te^{ixt}}{(1+t^2)^{3/2}}dt - \cancel{\frac{1}{2x^2}\int_{-\infty}^{\infty}\frac{e^{ixt}}{(1+t^2)^{3/2}}dt} \\ &= \frac{1}{2ix}\int_{-\infty}^{\infty}\frac{te^{ixt}}{(1+t^2)^{3/2}}dt\,. \end{aligned}$$

Making the substitution $x = \frac{b\omega}{\gamma v}$, we finally obtain:

$$\int_{-\infty}^{\infty}\frac{ue^{i\frac{b\omega}{\gamma v}u}}{(1+u^2)^{3/2}}du = 2i\frac{b\omega}{\gamma v}K_0\left(\frac{b\omega}{\gamma v}\right), \tag{3.36}$$

and consequently, the z-component can be written as:

$$E_z(\omega) = -i\sqrt{\frac{2}{pi}}\frac{Z_p e\omega}{\gamma^2 v^2}K_0\left(\frac{b\omega}{\gamma v}\right). \tag{3.37}$$

Now that we have the components of the electric field in the Fourier decomposition, the amplitude $|\vec{E}(\omega_0)|$ can be evaluated to estimate the energy deposition by equation (3.28).

$$\begin{aligned} |\vec{E}(\omega_0)| &= E_x^2(\omega_0) + E_z^2(\omega_0) = 4\frac{Z_p^2e^2\omega_0^2}{2\pi\gamma^2v^4}K_1^2\left(\frac{b\omega_0}{\gamma v}\right) + \frac{2}{\pi}\frac{Z_p^2e^2\omega_0^2}{\gamma^4v^4}K_0^2\left(\frac{b\omega_0}{\gamma v}\right) \\ &= \frac{2}{\pi}\frac{Z_p^2e^2}{v^2b^2}\xi^2K_1^2(\xi) + \frac{2}{\pi}\frac{Z_p^2e^2}{\gamma^2v^2b^2}\xi^2K_0^2(\xi) = \frac{2}{\pi}\frac{Z_p^2e^2}{v^2b^2}\left\{\xi^2K_1^2(\xi) + \frac{\xi^2}{\gamma^2}K_0^2(\xi)\right\}. \end{aligned}$$

Now we are able to give an expression for the energy deposition in classical distant collision approximation:

$$\boxed{\Delta E = \frac{2Z_p^2 e^4}{m_e v^2 b^2}\left\{\xi^2 K_1^2(\xi) + \frac{\xi^2}{\gamma^2}K_0^2(\xi)\right\}}. \tag{3.38}$$

This formula represents the energy transfer to an atomic electron by a projectile of charge $Z_p e$ that passes an impact parameter b distance from the atomic nucleus. To estimate the material stopping power this quantity must be laboured as in previous sections, but in this case it is convenient to analyze the behavior of the modified Bessel functions of the second kind for the small and asymptotic argument limits[12]:

$$\xi << 1 \quad \longrightarrow \quad \begin{array}{ll} K_0 \sim & -\overline{\gamma} - \ln\left(\frac{\xi}{2}\right), \\ K_1 \sim & \frac{\Gamma(1)}{2}\frac{2}{\xi} = \frac{1}{\xi}, \end{array} \tag{3.39}$$

$$\xi >> 1 \quad \longrightarrow \quad K_\nu(\xi) \sim \sqrt{\frac{\pi}{2\xi}}e^{-\xi}, \tag{3.40}$$

where $\overline{\gamma} \approx 0.5772\cdots$ is known as the Euler-Mascheroni constant.

Consider, for example, the small argument limit of (3.38):

$$\begin{aligned} \Delta E(\xi << 1) &\sim \frac{2Z_p^2 e^4}{m_e v^2 b^2}\left\{\xi^2\frac{1}{\xi^2} + \frac{1}{\gamma}\xi^2\left(-\overline{\gamma} - \ln\left(\frac{\xi}{2}\right)\right)^2\right\} \\ &= \frac{2Z_p^2 e^4}{m_e v^2 b^2} + \mathcal{O}(\xi^2), \end{aligned}$$

that is exactly the energy deposition that we found in section 3.1 during the small impulse transfer deduction. Therefore, this calculation was valid only if $\xi = \frac{b\omega_0}{\gamma v} << 1$, or $\frac{b}{\gamma v} << \frac{1}{\omega_0} = T$ which is exactly the assumption we made, that is, the characteristic time of the collision is much smaller than the orbital period of the electron.

If we look in the complete opposite direction, towards large arguments, we can see that:

$$\begin{aligned} \Delta E(\xi >> 1) &\sim \frac{2Z_p^2 e^4}{m_e v^2 b^2}\left\{\xi^2\frac{\pi}{2\xi}e^{-2\xi} + \frac{1}{\gamma^2}\xi^2\frac{\pi}{2\xi}e^{-2\xi}\right\} \\ &= \frac{2Z_p^2 e^4}{m_e v^2 b^2}\left\{1 + \frac{1}{\gamma^2}\right\}\xi e^{-2\xi} \to 0 \ \text{ if } \ \xi \to \infty. \end{aligned}$$

In this case, if $\xi = \frac{b\omega_0}{\gamma v} = \frac{b}{b_{max}} >> 1$, then $b >> b_{max}$ with $b_{max} = \frac{\gamma v}{\omega_0}$, and consequently $\Delta E = 0$. This correctly justifies the choice of the adiabatic radius of Bohr as the limit of zero energy transfer in section 3.1.

To complete the stopping power deduction, our definition will be used again, but this time we have associated to each electron a different harmonic frequency ω_0. Naming them with an index label, ω_a, it is important to understand that the electron density must be written differently because of this. If only a fraction f_a of the Z_t electrons of the atom presents characteristic frequency ω_a, then $N_a = N f_a$ is the density of electrons oscillating with ω_a, being N the density of atoms. Therefore:

$$N_e = \sum_a N_a = \sum_a N f_a = N\sum_a f_a, \tag{3.41}$$

and on the other hand we already know that $N_e = N Z_t$, consequently we obtain the following sum rule:

$$\boxed{\sum_a f_a = Z_t}\,. \tag{3.42}$$

This is important for several reasons that will be explained later. Now, using this definition and the classical cross section again, the stopping power can be calculated:

$$\begin{aligned}
S_{b>b_1}(T) &= \sum_a N_a \int \Delta E_a(b) d\sigma(b) = 2\pi \sum_a N_a \int_{b_1}^{b_{max}} \Delta E(b) b db = \\
&= 2\pi N \sum_a f_a \int_{b_1}^{\infty} \Delta E(b) b db = \frac{4\pi N Z_p^2 e^4}{m_e v^2} \sum_a f_a \int_{b_1}^{\infty} \left\{ \xi_a^2 K_1^2(\xi_a) + \frac{\xi_a^2}{\gamma^2} K_0^2(\xi_a) \right\} \frac{db}{b} \\
&= \frac{4\pi N Z_p^2 e^4}{m_e v^2} \sum_a f_a \left\{ \int_{\xi_{1,a}}^{\infty} K_1^2(\xi_a) \xi_a d\xi_a + \frac{1}{\gamma^2} \int_{\xi_{1,a}}^{\infty} K_0^2(\xi_a) \xi_a d\xi_a \right\},
\end{aligned}$$

where $\Delta E(\xi >> 1) \sim 0$ was used, and $\xi_{1,a} = \frac{b_1 \omega_a}{\gamma v}$. It is convenient to work on the integrals separately. They can be found on tables such as Abramowitz and Stegun[12]:

$$\begin{aligned}
\int_{\xi_{1,a}}^{\infty} K_1^2(\xi_a) \xi_a d\xi_a &= \frac{\xi_a}{2} \left\{ \xi_a K_1^2(\xi_a) - \xi_a K_0^2(\xi_a) - 2 K_0(\xi_a) K_1(\xi_a) \right\} \Big|_{\xi_{1,a}}^{\infty}, \\
\int_{\xi_{1,a}}^{\infty} K_0^2(\xi_a) \xi_a d\xi_a &= \frac{\xi_a^2}{2} \left\{ K_0^2(\xi_a) - K_1^2(\xi_a) \right\} \Big|_{\xi_{1,a}}^{\infty}.
\end{aligned}$$

Using the asymptotic behavior $K_\nu(\xi) \sim e^{-\xi} \sim 0$, this results in:

$$\begin{aligned}
\int_{\xi_{1,a}}^{\infty} K_1^2(\xi_a) \xi_a d\xi_a &= \frac{\xi_{1,a}}{2} \left\{ \xi_{1,a} K_0^2(\xi_{1,a}) - \xi_{1,a} K_1^2(\xi_{1,a}) + 2 K_0(\xi_{1,a}) K_1(\xi_{1,a}) \right\}, \\
\int_{\xi_{1,a}}^{\infty} K_0^2(\xi_a) \xi_a d\xi_a &= \frac{\xi_{1,a}^2}{2} \left\{ K_1^2(\xi_{1,a}) - K_0^2(\xi_{1,a}) \right\}.
\end{aligned}$$

Taking this to $S_{b>b_1}$ and with some algebraic work done:

$$\begin{aligned}
S_{b>b_1}(T) &= \frac{4\pi N Z_p^2 e^4}{m_e v^2} \sum_a f_a \left\{ \frac{\xi_{1,a}^2}{2} K_0^2(\xi_{1,a}) - \frac{\xi_{1,a}^2}{2} K_1^2(\xi_{1,a}) + \xi_{1,a} K_0(\xi_{1,a}) K_1(\xi_{1,a}) + \right. \\
&\qquad \left. + \frac{1}{\gamma^2} \frac{\xi_{1,a}^2}{2} K_1^2(\xi_{1,a}) - \frac{1}{\gamma^2} \frac{\xi_{1,a}^2}{2} K_0^2(\xi_{1,a}) \right\} \\
&= \frac{4\pi N Z_p^2 e^4}{m_e v^2} \sum_a f_a \left\{ \frac{\xi_{1,a}^2}{2} K_0^2(\xi_{1,a}) \left(1 - \frac{1}{\gamma^2}\right) + \xi_{1,a} K_0(\xi_{1,a}) K_1(\xi_{1,a}) - \right. \\
&\qquad \left. - \frac{\xi_{1,a}^2}{2} K_1^2(\xi_{1,a}) \left(1 - \frac{1}{\gamma^2}\right) \right\} \\
&= \frac{4\pi N Z_p^2 e^4}{m_e v^2} \sum_a f_a \left\{ \xi_{1,a} K_0(\xi_{1,a}) K_1(\xi_{1,a}) - \frac{\beta^2 \xi_{1,a}^2}{2} (K_1^2(\xi_{1,a}) - K_0^2(\xi_{1,a})) \right\}. \qquad (3.43)
\end{aligned}$$

In general, the projectile velocity v is much greater than the electron orbital velocity, and therefore $\xi_{1,a} = \frac{b_1 \omega_a}{\gamma v} << 1$. It is convenient (although not mandatory) to approximate:

$$K_0(\xi_{1,a}) \sim -\overline{\gamma} - \ln\left(\frac{\xi_{1,a}}{2}\right) \;\; ; \;\; K_1(\xi_{1,a}) \sim \frac{1}{\xi_{1,a}}\,, \tag{3.44}$$

and using this in the bracketed factor of $S_{b>b_1}$:

$$\begin{aligned} & \xi_{1,a}K_0(\xi_{1,a})K_1(\xi_{1,a}) - \frac{\beta^2\xi_{1,a}}{2}(K_1^2(\xi_{1,a}) - K_0^2(\xi_{1,a})) \simeq \\ \simeq\ & -\overline{\gamma} - \ln\left(\frac{\xi_{1,a}}{2}\right) - \frac{\beta^2\xi_{1,a}^2}{2}\left(\frac{1}{\xi_{1,a}^2} - \left(\overline{\gamma} + \ln\left(\frac{\xi_{1,a}}{2}\right)\right)\right) \\ =\ & -\overline{\gamma} - \ln\left(\frac{\xi_{1,a}}{2}\right) - \frac{\beta^2}{2} + \mathcal{O}(\xi_{1,a}) \sim \ln\left(\frac{2e^{-\overline{\gamma}}}{\xi_{1,a}}\right) - \frac{\beta^2}{2}\,. \end{aligned}$$

When taking this to $S_{b>b_1}$, the summation over a puts a Z_t factor due to the sum rule (3.42) in every term independent of a, but the term that depends on a via $\xi_{1,a}$ must be worked in the following way:

$$\begin{aligned} \sum_a f_a \ln\left(\frac{2e^{-\overline{\gamma}}}{\xi_{1,a}}\right) &= \sum_a f_a \ln\left(\frac{2e^{-\overline{\gamma}}\gamma v}{b_1\omega_a}\right) \\ &= Z_t \ln\left(\frac{2e^{-\overline{\gamma}}\gamma v}{b_1}\right) - \sum_a f_a \ln(\omega_a) \\ &= Z_t \ln\left(\frac{2e^{-\overline{\gamma}}\gamma v}{b_1}\right) - Z_t \frac{\sum\limits_a f_a \ln(\omega_a)}{\sum\limits_a f_a}\,. \end{aligned}$$

We identify the second term as a logarithmic average of the characteristic frequencies, with a statistical weight given by the fraction of electrons with the respective frequency. We consequently define:

$$\boxed{\ln(\langle\omega\rangle) = \frac{\sum\limits_a f_a \ln(\omega_a)}{\sum\limits_a f_a} = \frac{1}{Z_t}\sum_a f_a \ln(\omega_a)}\,. \tag{3.45}$$

This is our very first theoretical definition of the mean excitation potential $\langle I\rangle = \hbar\langle\omega\rangle$. With this, the bracketed term we were working reads:

$$\xi_{1,a}K_0(\xi_{1,a})K_1(\xi_{1,a}) - \frac{\beta^2\xi_{1,a}}{2}(K_1^2(\xi_{1,a}) - K_0^2(\xi_{1,a}) \simeq Z_t\left\{\ln\left(\frac{2e^{-\overline{\gamma}}\gamma v}{b_1\langle\omega\rangle}\right) - \frac{\beta^2}{2}\right\}\,.$$

If, at this point, we decide to use $b_1 = b_{min} = \frac{Z_p e^2}{m_e\gamma v^2}$, which was the classical inferior limit defined in section 3.1 for the maximum energy transference in a frontal collision, it can be seen that:

$$\ln\left(\frac{2e^{-\overline{\gamma}}\gamma v}{\langle\omega\rangle b_{min}}\right) = \ln\left(\frac{2m_e v^2}{\hbar\langle\omega\rangle}\right) - \ln\left(\frac{Z_p e^2 e^{-\overline{\gamma}}}{\hbar\gamma^2 v}\right) = \ln\left(\frac{2m_e v^2}{\hbar\langle\omega\rangle}\right) - \ln\left(e^{\overline{\gamma}}\eta\right) - \ln(1-\beta^2)\,.$$

Gathering everything in the stopping power formula, which now does not depend on b_1, we obtain:

$$S(T) = \frac{4\pi N Z_p^2 e^4}{m_e v^2} Z_t\left\{\ln\left(\frac{2m_e v^2}{\hbar\langle\omega\rangle}\right) - \ln\left(e^{\overline{\gamma}}\eta\right) - \ln(1-\beta^2) - \frac{\beta^2}{2}\right\}\,. \tag{3.46}$$

Recognizing the constant $K_0 = \frac{4\pi N_A e^4}{m_e c^2}$ with $N = \frac{\rho N_A}{A_t}$ and then, the final expression reads:

$$\boxed{S(T) = K_0\frac{\rho}{A_t}\frac{Z_t Z_p^2}{\beta^2}\left\{\ln\left(\frac{2m_e v^2}{\hbar\langle\omega\rangle}\right) - \ln\left(e^{\overline{\gamma}}\eta\right) - \ln(1-\beta^2) - \frac{\beta^2}{2}\right\}}\,. \tag{3.47}$$

In comparison with formula (3.13), there are a lot of things to say about this result:

1. It presents a formal definition of the mean excitation potential for pure material and in the ideal gas approximation, namely low density:

$$\ln(\langle I\rangle) = \frac{\sum\limits_a f_a \ln(\hbar\omega_a)}{\sum\limits_a f_a} \,. \tag{3.48}$$

2. Introduction of a small correction $\beta^2/2$, small even at high energy of the projectile, but related with the spin when the correct connection of quantum mechanics with special relativity is used to determine the stopping power.

3. Consistent explanation of the term $\ln(1-\beta^2) = \ln(\gamma^2)$. One of the γ factors comes from the definition of maximum energy transfer in a frontal collision for a relativistic projectile ($b_{min} \sim \mathcal{O}(1/\gamma)$). The other factor comes from the change in the form of the electric field under a Lorentz transformation. This means that this term is purely relativistic. Another way of interpreting it is: as we are solving distant collisions, when the projectile has high energy $\beta^2 \sim 1$ and $-\ln(1-\beta^2) \to \infty$, meaning the electric field is more effective for transferring energy at distant collisions if the particle that generated it is relativistic.

4. Give $\overline{\gamma} \simeq 0.5572\cdots$, then $\exp(\overline{\gamma}) \simeq 1.781\cdots$, not exactly 2 as in formula (3.13). This term in fact is a nexus showing the validity of the classical or the quantum mechanical approach, and is sometimes called the Bohr factor $\kappa = e^{\overline{\gamma}}\eta$. More will be said when studying the Bloch correction.

5. It is important to note that a choice of b_1 was made, namely $b_1 = b_{min}$. This is not mandatory, and in the next section, a conciliation between the distant and close collisions stopping power formulas will be shown leaving b_1 undetermined.

3.4 Conciliation between classical close and distant collisions

For this part, we will consider that there exists only one type of electron with characteristic frequency ω_0. Then, the stopping power for the close and distant collisions might be read from formulas (3.18) and (3.43) respectively:

$$S_{b<b_1}(T) = \frac{4\pi N_e Z_p^2 e^4}{m_e v^2}\frac{1}{2}\ln\left(1+\left[\frac{\gamma m_e v^2}{Z_p e^2}b_1\right]^2\right) , \tag{3.49}$$

$$S_{b>b_1}(T) = \frac{4\pi N_e Z_p^2 e^4}{m_e v^2}\left\{\xi_1 K_0(\xi_1)K_1(\xi_1) - \frac{\beta^2\xi_1^2}{2}(K_0^2(\xi_1)-K_1^2(\xi_1))\right\} . \tag{3.50}$$

Here, $\xi_1 = \frac{b_1\omega_0}{\gamma v}$. It can be seen (see figure 3.8) that this expressions diverge in the corresponding limits where the approximation used to calculate them fails, namely:

$$\begin{matrix} S_{b<b_1} & \to\infty \\ b_1 & \to\infty \end{matrix} \quad ; \quad \begin{matrix} S_{b>b_1} & \to\infty \\ b_1 & \to 0 \end{matrix} \,.$$

The calculations for figure 3.8 were done by imposing b_1 the limits $b_{min} = \frac{Z_p e^2}{\gamma m_e v^2}$ and $b_{max} = \frac{\gamma v}{\langle\omega\rangle}$, where $\langle\omega\rangle$ was calculated from the mean excitation potential of each material, and the kinetic energy was set to $\beta = 0.5$.

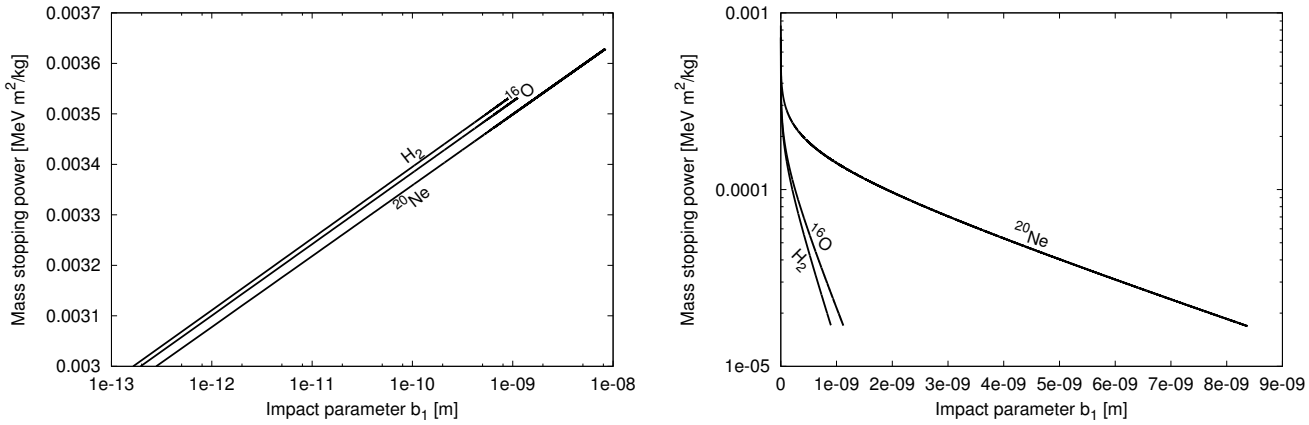

Figure 3.8: Mass stopping power for close and distant collisions respectively, as a function of b_1.

Then, we must analyze how to approximate $S_{b<b_1}$ and $S_{b>b_1}$ in the limits where the approximation remains valid. In the case of $S_{b<b_1}$, it is convenient thinking that $b_1 >> b_{min}$, that is the classical limit associated with the maximum energy transfer in a frontal collision, and therefore can be thought of as the "size" of the scattering center. In this approximation:

$$\begin{aligned} S_{b<b_1}(T) &\sim \frac{4\pi N_e Z_p^2 e^4}{m_e v^2}\frac{1}{2}\ln\left(\left[\frac{\gamma m_e v^2}{Z_p e^2}b_1\right]^2\right) \\ &= \frac{4\pi N_e Z_p^2 e^4}{m_e v^2}\ln\left(\frac{\gamma m_e v^2}{Z_p e^2}b_1\right) . \end{aligned}$$

For $S_{b>b_1}$, and as already done in section 3.3, we choose $b_1 << \frac{\gamma v}{\omega_0}$, corresponding to the limit of inefficient energy transfer or adiabatic process. Using the limiting forms of the modified Bessel functions of the second kind again we obtain:

$$\begin{aligned} S_{b>b_1} &\sim \frac{4\pi N_e Z_p^2 e^4}{m_e v^2}\left\{-\overline{\gamma} - \ln\left(\frac{\xi_1}{2}\right) - \frac{\beta^2\xi_1^2}{2}\left(\frac{1}{\xi_1^2} - \left(\overline{\gamma} + \ln\left(\frac{\xi_1}{2}\right)\right)^2\right)\right\} \\ &= \frac{4\pi N_e Z_p^2 e^4}{m_e v^2}\left\{\ln\left(\frac{2e^{-\overline{\gamma}}}{\xi_1}\right) - \frac{\beta^2}{2} + \frac{\beta^2\xi_1^2}{2}\left(\overline{\gamma} + \ln\left(\frac{\xi_1}{2}\right)\right)^2\right\} . \end{aligned}$$

The conciliation is simple adding this approximate forms of $S_{b<b_1}$ and $S_{b>b_1}$, which gives:

$$\begin{aligned} S(T) &= S_{b<b_1}(T) + S_{b>b_1}(T) \\ &= \frac{4\pi N_e Z_p^2 e^4}{m_e v^2}\left\{\ln\left(\frac{2e^{-\overline{\gamma}}}{\cancel{b_1}\omega_0}\gamma v\frac{\gamma m e v^2}{Z_p e^2}\cancel{b_1}\right) - \frac{\beta^2}{2} + \frac{\beta^2\xi_1^2}{2}\left(\overline{\gamma} + \ln\left(\frac{\xi_1}{2}\right)\right)^2\right\} \\ &= \frac{4\pi N_e Z_p^2 e^4}{m_e v^2}\left\{\ln\left(\frac{2m_e v^2}{\hbar\omega_0}\right) - \ln\left(e^{\overline{\gamma}}\eta\right) - \ln(1-\beta^2) - \frac{\beta^2}{2} + \frac{\beta^2\xi_1^2}{2}\left(\overline{\gamma} + \ln\left(\frac{\xi_1}{2}\right)\right)^2\right\} \end{aligned} \quad (3.51)$$

This is exactly the formula (3.47) without a mean frequency defined, and with an additional term, that in section 3.3 was neglected for being $\mathcal{O}(\xi_1^2)$.

So far, every stopping power formula we derived, presents the same form. It consists of a constant we called K_0, factors depending on the material and the projectile, and a number L, such that:

$$S(T) = K_0 \frac{\rho}{A_t} \frac{Z_t Z_p^2}{\beta^2} L(\beta)\,. \tag{3.52}$$

This factor L is called the **stopping number**. The leading form of the stopping number is:

$$L(\beta) = \ln\left(\frac{2m_e v^2}{\hbar\langle\omega\rangle}\right) - \ln(1-\beta^2) - \frac{\beta^2}{2}\,, \tag{3.53}$$

being every other term simply corrections for different effects. For example, the Bohr's stopping number is:

$$L_{Bohr}(\beta) = \ln\left(\frac{2m_e v^2}{\hbar\langle\omega\rangle}\right) - \ln\left(e^{\overline{\gamma}}\eta\right) - \ln(1-\beta^2) - \frac{\beta^2}{2}\,. \tag{3.54}$$

The correction term added in formula (3.51) will be called $L_{corr}(\beta, b_1) = \frac{\beta^2\xi_1^2}{2}\left(\overline{\gamma} + \ln\left(\frac{\xi_1}{2}\right)\right)^2$. This can be proved to be a very small correction almost independent of the value of b_1. For this, setting the b_1 limits as in figure 3.8, the correction ratio $100\frac{L_{corr}}{L_{Bohr}}$ was calculated.

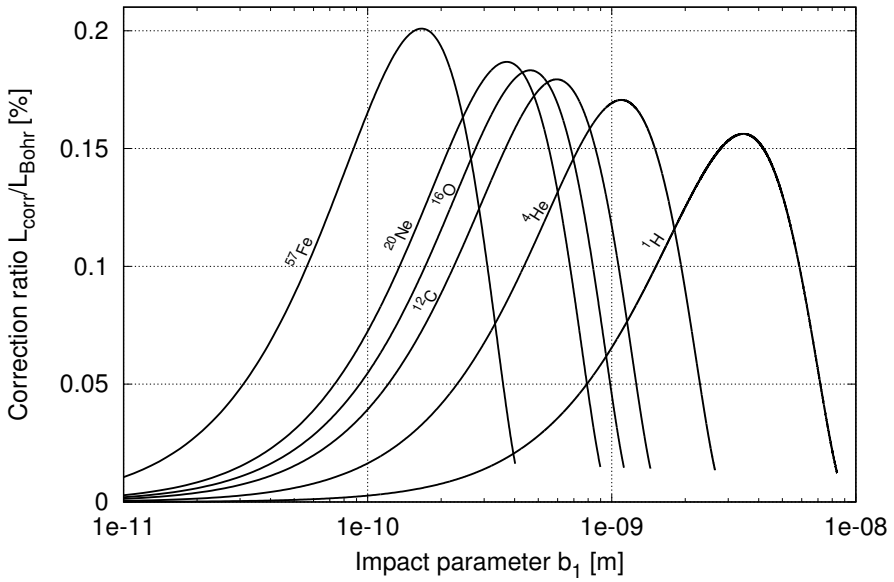

Figure 3.9: Correction term of compromise between close and distant collisions as a function of b_1.

Figure 3.9 is a plot of this ratio for a bunch of materials, showing a relative maximum correction of 0.2% respect the leading Bohr term for the heavier material. This express the non-sensibility of the classical theory to the choice of b_1. Therefore, this term can be safely neglected.

With the remaining formula (3.51), the definition of a mean frequency for different characteristic oscillation of the electrons can be deduced in the same exact form as already done in section 3.3.

Chapter 4

Quantum Stopping Power

Other problem concerning quantum mechanical application to the energy transfer is that the atom is known to absorb energy in definite energy jumps. Thereby, there exists cases where our evaluation of ΔE presents values too low to be absorbed by the atom. This means that the classical picture of "small energy transfer per collision" is not correct. An theoretical idea of solution to this problem is extending the notion of energy transfer as if it were a statistical quantity associated with many collisions instead to only one. This idea will be further explored later. Now I would like to focus on making a conciliation between the close and distant collisions approaches to give our final classical expression for the stopping power, not depending on an undetermined limit b_1.

4.1 Heisenberg uncertainty principle approximation

When studying the stopping power in the impulse transfer approximation, we derived equation (3.11), that we rewrite here:

$$S(T) = \frac{4\pi N_e Z_p^2 e^4}{m_e v^2} \ln\left(\frac{b_{max}}{b_{min}}\right) , \tag{4.1}$$

where the choices of limits was determined by classical arguments such as the maximum energy transferred in a single collision or the impact parameter from which the process becomes adiabatic. If we think in terms of quantum mechanics, particles presents the wave-particle duality in their behavior. If we were able to construct a wave packet giving some sense to a classical trajectory, that path can only be defined approximately due to the Heisenberg uncertainty principle $\Delta x \gtrsim \frac{\hbar}{p}$. If there exists an impact parameter lower than this, every classical concept fails. Then, the limit $b_1 \simeq \frac{\hbar}{p}$ seems to be more accurate respect a quantum compatible energy transference. Given that lighter particles present higher uncertainty, it is convenient to define the quantum limit b_1^q using the electron as reference. From the reference frame attached to the projectile, the electron moves slowly in its orbit, and therefore its lineal momentum is mainly $p = \gamma m_e v$. With this $b_1^q = \frac{\hbar}{\gamma m_e v}$. Comparing this with the limit defined classically we can see that:

$$\frac{b_{min}}{b_1^q} = \frac{Z_p e^2}{\gamma m_e v^2} \frac{\gamma m_e v}{\hbar} = \frac{Z_p e^2}{\hbar v} = \eta \, . \tag{4.2}$$

Again, the Sommerfeld parameter appears as connection between classical and quantum mechanical approximations.

If we use this limit in (3.11) instead of the classical b_{min}, we can see that:

$$\begin{aligned} S^{(q)}(T) &= \frac{4\pi N_e Z_p^2 e^4}{m_e v^2} \ln\left(\frac{b_{max}}{b_{min}^{(q)}}\right) \\ &= \frac{4\pi N_e Z_p^2 e^4}{m_e v^2} \ln\left(\frac{\gamma v}{\overline{\nu}} \frac{\gamma m_e v}{\hbar}\right) \\ &= K_0 \frac{\rho}{A_t} \frac{Z_t Z_p^2}{\beta^2} \left\{ \ln\left(\frac{m_e v^2}{\hbar \overline{\nu}}\right) - \ln(1-\beta^2) \right\} . \end{aligned}$$

This is merely an approximation of what we expect to obtain with the quantum mechanical calculation. This case does not predict the high energy correction $\beta^2/2$ and sub-estimates the leading logarithm by a factor 2. It will be shown that the factor 2 is corrected in the final quantum version of the stopping power, but the term $\beta^2/2$, does not appear unless the calculation is made a the relativistic quantum mechanics framework, that naturally includes spin.

4.2 Quantum calculation by Bethe

To analyze the stopping power from a quantum mechanical point of view, the perturbation theory will be used, together with the first Born approximation. We need to be capable of modeling the interaction of a projectile of charge $Z_p e$ and mass M with an atom of Z_t electrons forming a closed system with the atomic nucleus. Therefore, the hamiltonian of the system should be $\hat{H} = \hat{H}_{at} + \hat{H}_{part} + \hat{H}_{int}$ where:

- $\hat{H}_{at}$ is the full atomic hamiltonian, described by a set of coordinates for each electron, that we will call $A = \{\vec{r}_1, \cdots, \vec{r}_{Z_t}\}$, and eigenfunctions $\varphi_n(A)$.
- $\hat{H}_{part}$ is the projectile's hamiltonian thought of as a free particle, with eigenfunction $\exp(i\vec{k}\cdot\vec{r})$, i.e. and incident wave.
- $\hat{H}_{int}$ is the interaction hamiltonian, must contain a projectile-nucleus term, and the interaction with the Z_t atomic electrons.

The extended mathematical form that we will use is the next:

$$\hat{H}_{part} = \frac{p^2}{2M} \;;\; p = -i\hbar\nabla \,; \tag{4.3}$$

$$\hat{H}_{at} = \sum_{i=1}^{Z_t} \left\{ \frac{p_i^2}{2m_e} - \frac{Z_t e^2}{r_i} \right\} + \sum_{i=1}^{Z_t} \sum_{k=1}^{i-1} \frac{e^2}{|\vec{r}_i - \vec{r}_k|} \;;\; p_i = -i\hbar\nabla_i \,; \tag{4.4}$$

$$\hat{H}_{int} = \frac{Z_t Z_p e^2}{r} - \sum_{i=1}^{Z_t} \frac{Z_p e^2}{|\vec{r} - \vec{r}_i|} \,. \tag{4.5}$$

As already said, the interaction term will be worked in the perturbation theory, using as reference states the ones from the free hamiltonian $\hat{H}_0 = \hat{H}_{at} + \hat{H}_{part}$. This states can be written as $|\psi_n\rangle = |\varphi_n\rangle \otimes |\vec{k}\rangle$, so that using a coordinate representation:

$$\begin{aligned} \langle \vec{r}_1 \cdots \vec{r}_{Z_t} | \varphi_n \rangle &= \varphi_n(A) \,, \\ \langle \vec{r} | \vec{k} \rangle &= \exp(i\vec{k}\cdot\vec{r}) \,. \end{aligned}$$

The atom will be considered to be in its ground state φ_0, and the probability that the interaction causes a transition from ψ_0 to ψ_n is $T_{0n} = \langle \psi_n | \hat{H}_{int} | \psi_0 \rangle$. This calculation is by definition:

$$\begin{aligned} T_{0n} &= \int d^{Z_t}A\; d^3\vec{r}\; \left(e^{-i\vec{k}_n\cdot\vec{r}}\varphi_n^*(A)\right)\hat{H}_{int}\left(\varphi_0(A)e^{i\vec{k}_0\cdot\vec{r}}\right) \\ &= \int d^{Z_t}A\; d^3\vec{r}\; e^{-i(\vec{k}_n-\vec{k}_0)\cdot\vec{r}}\; \varphi_n^*(A)\hat{H}_{int}\varphi_0(A) \\ &= \int d^3\vec{r}\; e^{i\vec{q}\cdot\vec{r}}\; V_n(\vec{r})\;;\; \vec{q}=\vec{k}_0-\vec{k}_n\,. \end{aligned}$$

The last expression is the first order Born approximation term applied to the effective potential $V_n(\vec{r})$, defined by:

$$V_n(\vec{r}) = \int d^{Z_t}A\; \varphi_n^*(A)\hat{H}_{int}\varphi_0(A)\,. \tag{4.6}$$

Before working with this potential, is is convenient to re-write T_{0n} using the following property:

$$\nabla\left(e^{i\vec{q}\cdot\vec{r}}\right) = i\vec{q}e^{i\vec{q}\cdot\vec{r}} \;\Rightarrow\; \nabla^2\left(e^{i\vec{q}\cdot\vec{r}}\right) = -q^2e^{i\vec{q}\cdot\vec{r}} \;\Rightarrow\; e^{i\vec{q}\cdot\vec{r}} = -\frac{1}{q^2}\nabla^2\left(e^{i\vec{q}\cdot\vec{r}}\right)\,,$$

and consequently:

$$\begin{aligned} T_{0n} &= -\frac{1}{q^2}\int d^2\vec{r}\; V_n(\vec{r})\nabla^2\left(e^{i\vec{q}\cdot\vec{r}}\right) \\ &= -\frac{1}{q^2}\left[\int d^3\vec{r}\; e^{i\vec{q}\cdot\vec{r}}\;\nabla^2V_n(\vec{r}) + \int_{\partial V}\left(e^{i\vec{q}\cdot\vec{r}}\;\nabla V_n(\vec{r}) - V_n(\vec{r})\;\nabla\left(e^{i\vec{q}\cdot\vec{r}}\right)\right)\cdot\hat{n}dS\right]\,, \end{aligned}$$

where a Green identity has been used. The integration is performed in $V=\mathbb{R}^3$, therefore ∂V is a surface "closed at infinity". Both terms in the integrand vanishes when evaluated at infinity, because V_n takes values near the projectile, and ∇V_n represents the force applied to it due to the presence of the atom. Both quantities present compact support near the projectile. The remaining term depends on ∇^2V_n, thereby this is the moment to check this effective potential properties. From its definition, only $\hat{H}_{int}$ depends of $\vec{r}$ on V_n, and consequently:

$$\begin{aligned} \nabla^2V_n(\vec{r}) &= \int d^{Z_t}A\;\varphi_n^*(A)\;\left(\nabla^2\hat{H}_{int}\right)\;\varphi_0(A) \\ &= \int d^{Z_t}A\;\varphi_n^*(A)\;Z_pe\left[Z_te\nabla^2\left(\frac{1}{r}\right) - \sum_{i=1}^{Z_t}e\nabla^2\left(\frac{1}{|\vec{r}-\vec{r}_i|}\right)\right]\varphi_0(A) \\ &= -4\pi Z_pe^2\int d^{Z_t}A\;\varphi_n^*(A)\left[Z_t\delta(\vec{r}) - \sum_{i=1}^{Z_t}\delta(\vec{r}-\vec{r}_i)\right]\varphi_0(A)\,. \end{aligned}$$

The differential equation to be solved is thus:

$$\boxed{\nabla^2V_n(\vec{r}) = -4\pi Z_pe^2\left[Z_t\delta(\vec{r})\delta_{n,0} - \rho_n(\vec{r})\right]}, \tag{4.7}$$

that is a Green inhomogeneous equation. To complete the last steps of the calculation, the following properties has been used:

- $\nabla^2\left(\frac{1}{|\vec{r}-\vec{r}_i|}\right) = -4\pi\delta(\vec{r}-\vec{r}_i)$.
- $\int d^{Z_t}A\;\varphi_n^*(A)\varphi_0(A) = \delta_{n,0}$, atomic eigenfunctions orthogonality.
- $\rho_n(\vec{r}) = \sum_{i=1}^{Z_t}\int d^{Z_t}A\;\delta(\vec{r}-\vec{r}_i)\;\varphi_n^*(A)\varphi_0(A)$.

One of the possible ways of describing the inhomogeneous Green equation solution is by calculation of the asociated Green function, that in this particular case stands for:

$$V_n(\vec{r}) = Z_p e^2 \left\{ \frac{Z_t \delta_{n,0}}{r} - \int d^3\vec{r}\, \frac{\rho_n(\vec{r})}{|\vec{r} - \vec{r_i}|} \right\} . \tag{4.8}$$

From this, it is clear that ρ_n plays the role of electric charge distribution of the atom in the nth state. Also, if $n = 0$, there will be no atomic transition, and the corresponding interaction can be thought of as elastic. Then, to enforce energy transfer, $n \neq 0$, and this implies $\delta_{n,0} = 0$ always. The first term of V_n is consequently zero, and this is not unexpected as this term comes from the coulombian interaction between the nuclei. Using (4.8) in the matrix element of the transition leads to:

$$\begin{aligned} T_{0n} &= -\frac{1}{q^2} \int d^3\vec{r}\, e^{i\vec{q}\cdot\vec{r}}\, (-4\pi Z_p e^2)\, [-\rho_n(\vec{r})] \\ &= -\frac{4\pi Z_p e^2}{q^2} \int d^3\vec{r}\, \rho_n(\vec{r})\, e^{i\vec{q}\cdot\vec{r}} \\ &= -\frac{4\pi Z_p e^2}{q^2} F_n(\vec{q})\, . \end{aligned}$$

The **atomic form factor** for the nth excitation state has beed defined here as $F_n(\vec{q}) = \int d^3\vec{r}\rho_n(\vec{r})e^{i\vec{q}\cdot\vec{r}}$. The transition probability is closely related to the differential cross section by the so called Fermi's golden rule:

$$\frac{d\sigma_n}{d\Omega} = \frac{1}{(2\pi)^2\hbar^4} \frac{T_n^2}{c^2} \frac{v_n}{v_0} |T_{0n}|^2 , \tag{4.9}$$

where $T_n = \gamma M c^2$ and $\{v_0, v_n\}$ are the initial and final velocities of the projectile. If the transition probability calculated is replaced in (4.9), we obtain:

$$\frac{d\sigma_n}{d\Omega} = \frac{4Z_p^2 e^4}{\hbar^4 c^2} \frac{T_n^2}{q^4} \frac{v_n}{v_0} \left|F_n(\vec{q})\right|^2 , \tag{4.10}$$

and consequently, the total cross section of projectile-atom interaction leading to the nth characteristic excited state of the material's atom can be calculated to be:

$$\sigma_n = \left[\frac{2Z_p e^2 T_n}{\hbar^2 c^2} \right]^2 \frac{v_n}{v_0} \int_{4\pi} d\Omega \frac{\left|F_n(\vec{q})\right|^2}{q^4} . \tag{4.11}$$

This expression can be further transformed in a general way, but it is necessary to understand the behavior of the moment transference $\vec{q}$ and the energy conservation in the collision process, which will allow us to rewrite the integral of σ_n in terms of known quantities and the scattering angles. The atomic energies before and after the collision are E_0 and E_n respectively, and the projectile energies T_0 and T_n. They relate by $E_n - E_0 = -(T_n - T_0)$. Both, before and after the collision, the projectile is regarded as a free particle, and consequently $k_{0,n} = \frac{2MT_{0,n}^2}{\hbar^2}$. The momentum transfer satisfies:

$$\hbar^2 q^2 = \hbar^2 |\vec{k}_n - \vec{k}_0|^2 = \hbar^2 \left[(k_0^2 - k_n^2) + 4k_0 k_n \sin\left(\frac{\theta_{scatt}}{2}\right) \right] ,$$

where the identity $\cos(\theta_{scatt}) = 1 - 2\sin\left(\frac{\theta_{scatt}}{2}\right)$ was used. From the last expression:

$$2qdq = 8k_0 k_n \sin\left(\frac{\theta_{scatt}}{2}\right) \cos\left(\frac{\theta_{scatt}}{2}\right) \frac{d\theta_{scatt}}{2} \quad \Rightarrow \quad qdq = k_0 k_n \sin(\theta_{scatt}) d\theta_{scatt} .$$

With this, we can write:

$$\begin{aligned}\frac{v_n}{v_0}d\Omega &= \frac{v_n}{v_0}\sin(\theta_{scatt})d\theta_{scatt}d\varphi_{scatt}\\ &= \frac{v_n}{v_0}\frac{qdq}{k_0k_n}d\varphi_{scatt}\\ &= \frac{v_n}{v_0}\frac{qdq}{\left(\frac{T_0v_0T_nv_n}{\hbar^2c^4}\right)}d\varphi_{scatt}\\ &= \frac{\hbar^2c^4}{v_0^2}\frac{qdq}{T_0T_n}d\varphi_{scatt}\,,\end{aligned}$$

where the following deduction is used:

$$\begin{aligned}p_n &= \hbar k_n = \gamma M v_n\\ T_n &= \gamma Mc^2 = \sqrt{p_n^2c^2+M^2c^4}\\ \frac{dT_n}{dp_n} &= \frac{1}{2}\frac{1}{\sqrt{p_n^2c^2+M^2c^4}}2p_nc^2\\ &= \frac{p_nc^2}{T_n} = \frac{\gamma Mv_nc^2}{\gamma Mc^2} = v_n\\ \Rightarrow p_n &= \frac{T_nv_n}{c^2} \Rightarrow k_n = \frac{T_nv_n}{\hbar c^2}\,.\end{aligned}$$

Now we take this calculations to the cross section and perform the integration on φ_{scatt} using azymuthal symmetry. This is an approximation, because $F_n(\vec{q})$ does not need to by symmetric, but the summation in the stopping power runs only on the energy quantum number n and not in the angular momentum l and m. Therefore, we obtain the inelastic cross section:

$$\begin{aligned}\sigma_n &= 2\pi\left[\frac{2Z_pe^2}{\hbar^2c^2}\right]^2\frac{T_n^2\hbar^2c^4}{v_0^2T_0T_n}\int_{q_{min}}^{q_{max}}dq\frac{|F_n(q)|^2}{q^3}\\ &= 2\pi\left[\frac{2Z_pe^2}{\hbar^2c^2v_0}\right]^2\hbar^2c^2\frac{T_n}{T_0}\int_{q_{min}}^{q_{max}}dq\frac{|F_n(q)|^2}{q^3}\\ &= 2\pi\left[\frac{2Z_pe^2}{\hbar v_0}\right]^2\frac{T_n}{T_0}\int_{q_{min}}^{q_{max}}dq\frac{|F_n(q)|^2}{q^3}\,.\end{aligned}$$

As can be seen, it is also assumed that F_n does not depend on θ_{scatt}, and the integration limits are given by:

$$q^2 = k_0^2+k_n^2-2k_0k_n\cos(\theta_{scatt}) = \begin{cases}(k_0+k_n)^2 = q_{max}^2 & (1)\\ (k_0-k_n)^2 = q_{min}^2 & (2)\end{cases}\,, \tag{4.12}$$

where (1) imples $\theta_{scatt}=\pi$, or that the projectile "bounces" in the atom, scattering in the initial direction, and (2) that $\theta_{scatt}=0$, therefore the charged ion does not deflect upon the incident direction.

Consider N the atomic density, and using that the energetic "jumps" of the atoms are usually hundreds of eV, and the energy of the projectile is far greater: around millions of eV (MeV), allows for the assumption that after an atomic transition, $T_n \approx T_0$ (small energy transfer or soft collisions). Therefore, using the statistical definition of stopping power (1.9), we obtain the electronic stopping power for inelastic collisions:

$$\begin{aligned}S(T) &= N\sum_n(E_n-E_0)\sigma_n\\ &= 2\pi N\left[\frac{2Z_pe^2}{\hbar v_0}\right]^2\sum_n(E_n-E_0)\int_{q_{min}}^{q_{max}}dq\frac{|F_n(q)|^2}{q^3}\,.\end{aligned}$$

Rigorously speaking, $q_{min,max} = q_{min,max}(n)$ through k_n, but, as we said, $T_n \approx T_0$, and consequently $k_n^2 = \frac{2MT_n}{\hbar^2} \simeq k_m^2$ with $n \neq m$. Then, all the possible values of $q_{min,max}$ are similar, inviting us to define an "acceptable" average $\overline{q}_{min,max}$ that makes this limits independent of n, allowing the interchange of the integral symbol with the summation in $S(T)$. We will return to this "acceptable" definition the moment we intend to evaluate $S(T)$ using $\overline{q}_{min,max}$. It is now convenient to continue with the calculation, interchanging the integral and summation symbols:

$$S(T) = 2\pi N \left[\frac{2Z_p e^2}{\hbar v_0}\right]^2 \int_{\bar{q}_{min}}^{\bar{q}_{max}} \frac{dq}{q^3} \sum_n (E_n - E_0)|F_n(q)|^2 \,. \tag{4.13}$$

This is as far as we can go without specifying the form factor. By definition, it can be developed using the atomic eigenfunctions as follows:

$$\begin{aligned} F_n(q) &= \int d^3\vec{r}\, e^{i\vec{q}\cdot\vec{r}}\, \rho_n(\vec{r}) = \int d^3\vec{r}\, e^{i\vec{q}\cdot\vec{r}} \sum_{i=1}^{Z_t} \int d^{Z_t}A\; \delta(\vec{r}-\vec{r}_i)\varphi_n^*(A)\varphi_0(A) \\ &= \sum_{i=1}^{Z_t} \int d^{Z_t}A \varphi_n^*(A)\varphi_0(A) \int d^3\vec{r}\, e^{i\vec{q}\cdot\vec{r}}\; \delta(\vec{r}-\vec{r}_i) = \sum_{i=1}^{Z_t} \int d^{Z_t}A \varphi_n^*(A)\varphi_0(A)\; e^{i\vec{q}\cdot\vec{r}_i} \\ &= \int d^{Z_t}A \varphi_n^*(A)\varphi_0(A) \sum_{i=1}^{Z_t} e^{i\vec{q}\cdot\vec{r}_i} \,. \end{aligned}$$

This suggest that it is plausible to think of an operator defined by:

$$\hat{B} = \sum_{i=1}^{Z_t} e^{i\vec{q}\cdot\vec{r}_i} \,, \tag{4.14}$$

such that $F_n(q)$ is the corresponding matrix element in the atomic eigenstates basis, $F_n(q) = \langle\varphi_n|\hat{B}|\varphi_0\rangle = \hat{B}_{n0}$. With this in mind, we make the calculation:

$$\begin{aligned} \sum_n (E_n - E_0)|F_n(q)|^2 &= \sum_n (E_n - E_0)|\hat{B}_{n0}|^2 = \sum_n (E_n - E_0)\hat{B}^\dagger_{0n}\hat{B}_{n0} \\ &= \sum_n \left(\hat{B}^\dagger\right)_{0n} \left(E_n\hat{B}_{n0} - \hat{B}_{n0}E_0\right) = \sum_n \left(\hat{B}^\dagger\right)_{0n} \left\{\langle\varphi_n|\hat{H}_{at}\hat{B}_{n0} - \hat{B}_{n0}\hat{H}_{at}|\varphi_0\rangle\right\} \\ &= \sum_n \left(\hat{B}^\dagger\right)_{0n} \left[\hat{H}_{at}, \hat{B}\right]_{n0} = \langle\varphi_0|\hat{B}^\dagger \left[\sum_n |\varphi_n\rangle\langle\varphi_n|\right] \left[\hat{H}_{at}, \hat{B}\right] |\varphi_0\rangle \\ &= \left(\hat{B}^\dagger \left[\hat{H}_{at}, \hat{B}\right]\right)_{00} ; \end{aligned}$$

meaning that all the calculation reduces to determine this matrix element. Here, it is understand from context that $[\cdot,\cdot]$ is the usual operator commutator. Given $\hat{H}_{at}$ as in (4.4), it is clear that $[\hat{B}, V] = 0$ because they only depend on the electron position operators $\{\vec{r}_i\}$. Therefore, we only need to evaluate the commutator with the electron's kinetic energy operator. For this, consider a "nice" test function $\varphi = \varphi(\vec{r}_k) \in C^\infty$:

$$\begin{aligned} \left[\hat{H}_{at}, \hat{B}\right]|\varphi\rangle &= -\frac{\hbar^2}{2m_e} \sum_i \sum_j \left[\nabla_j^2, e^{i\vec{q}\cdot\vec{r}_i}\right] \varphi(\vec{r}_k) = -\frac{\hbar^2}{2m_e} \sum_i \sum_j \left\{\nabla_j^2 \left(e^{i\vec{q}\cdot\vec{r}_i}\varphi(\vec{r}_k)\right) - e^{i\vec{q}\cdot\vec{r}_i}\nabla_j^2\varphi(\vec{r}_k)\right\} \\ &= -\frac{\hbar^2}{2m_e} \sum_i \sum_j \Big\{ \cancel{e^{i\vec{q}\cdot\vec{r}_i}\nabla_j^2\varphi(\vec{r}_k)} + 2i\delta_{ij}e^{i\vec{q}\cdot\vec{r}_i}\vec{q}\cdot\nabla_j\varphi(\vec{r}_k) + \\ &\qquad + \varphi(\vec{r}_k)(-q^2)e^{i\vec{q}\cdot\vec{r}_i}\delta_{ij} - \cancel{e^{i\vec{q}\cdot\vec{r}_i}\nabla_j^2\varphi(\vec{r}_k)} \Big\} \\ &= \frac{\hbar^2}{2m_e} \sum_i \sum_j \delta_{ij} e^{i\vec{q}\cdot\vec{r}_i} \left\{q^2 - 2i\vec{q}\cdot\nabla_j\right\} \varphi(\vec{r}_k) \\ &= \frac{\hbar^2}{2m_e} \sum_i e^{i\vec{q}\cdot\vec{r}_i} \left\{q^2 - 2i\vec{q}\cdot\nabla_i\right\} |\varphi\rangle \,. \end{aligned}$$

Now that we know the commutator operator, the calculation of its matrix element is straightforward:

$$\begin{aligned}\left(\hat{B}^\dagger\left[\hat{H}_{at},\hat{B}\right]\right)_{00} &= \frac{\hbar^2}{2m_e}\sum_i\sum_j\langle\varphi_0|e^{-i\vec{q}\cdot\vec{r}_j}e^{i\vec{q}\cdot\vec{r}_i}\left\{q^2-2i\vec{q}\cdot\nabla_i\right\}|\varphi_0\rangle \\ &= \frac{\hbar^2}{2m_e}\sum_i\sum_j\int d^{Z_t}A e^{i\vec{q}\cdot(\vec{r}_i-\vec{r}_j)}\left\{q^2\varphi_0^2(A)-2i\varphi_0^*(A)\vec{q}\cdot\nabla_i\varphi_0(A)\right\} \\ &= \frac{\hbar^2}{2m_e}\sum_i\sum_j\int d^{Z_t}A e^{i\vec{q}\cdot(\vec{r}_i-\vec{r}_j)}\left\{q^2\varphi_0^2(A)-i\vec{q}\cdot\nabla_i\left(\varphi_0^2(A)\right)\right\}\,,\end{aligned}$$

where the fact that the fundamental state can always be choosen to be real, $\varphi_0^*(A)=\varphi_0(A)$, was used, together with the calculus identity $\nabla\left(\varphi^2\right)=2\varphi\nabla\varphi$.

Next step is, perhaps, the most subtle of the whole deduction. We will prove that in the last expression, if $i\neq j$, there exists a zero factor making zero the entire matrix element, implying that only those terms with $i=j$ remains. To check this, we "isolate" one of the integrals (remember that $A=\{\vec{r}_1,\cdots,\vec{r}_{Z_t}\}$):

$$\begin{aligned}&\int d^{Z_t}A\, e^{i\vec{q}\cdot(\vec{r}_i-\vec{r}_j)}\left\{q^2\varphi_0^2(A)-i\vec{q}\cdot\nabla_i\left(\varphi_0^2(A)\right)\right\} = \\ &\qquad = \int d^3\vec{r}_1\cdots d^3\vec{r}_{i-1}d^3\vec{r}_{i+1}\cdots d^3\vec{r}_{Z_t}e^{-i\vec{q}\cdot\vec{r}_j}\int d^3\vec{r}_i\; e^{i\vec{q}\cdot\vec{r}_i}\left\{q^2\varphi_0^2(A)-i\vec{q}\cdot\nabla_i\left(\varphi_0^2(A)\right)\right\}\,.\end{aligned}$$

To the $\vec{r}_i$ isolated integral, we separate the second term in order to calculate it clearly:

$$\begin{aligned}-i\int d^3\vec{r}_i\; e^{i\vec{q}\cdot\vec{r}_i}\vec{q}\cdot\nabla_i\varphi_0^2(A) &= -i\int d^3\vec{r}_i\left\{\nabla_i\cdot\left(\vec{q}e^{i\vec{q}\cdot\vec{r}_i}\varphi_0^2(A)\right)-\varphi_0^2(A)\nabla_i\cdot\left(e^{i\vec{q}\cdot\vec{r}_i}\vec{q}\right)\right\} \\ &= -i\int_{\partial\mathbb{R}^3}dS\vec{q}\cdot\hat{n}\; e^{i\vec{q}\cdot\vec{r}}\varphi_0^2(A)+i\int d^3\vec{r}_i\varphi_0^2(A)\nabla_i\left(e^{i\vec{q}\cdot\vec{r}_i}\vec{q}\right) \\ &= -\int d^3\vec{r}_i\;\varphi_0^2(A)\;q^2\;e^{i\vec{q}\cdot\vec{r}_i}\,.\end{aligned}$$

Here, Gauss theorem was used to move from $\mathbb{R}^3$ integral to the boundary at infinity $\partial\mathbb{R}^3$, and being φ_0 square-integrable, it presents compact support. This makes zero the surface integral term, because the complex exponential is bounded. The remaining term cancels with the first term of the $\vec{r}_i$ isolated integral. This proves that each term with $i\neq j$ is zero. Thereby the matrix element we seek is of the form:

$$\begin{aligned}\left(\hat{B}^\dagger\left[\hat{H}_{at},\hat{B}\right]\right)_{00} &= \frac{\hbar^2}{2m_e}\sum_{i=1}^{Z_t}\int d^{Z_t}A\left[q^2\varphi_0^2(A)-i\vec{q}\cdot\nabla_i\varphi_0^2(A)\right] \\ &= \frac{\hbar^2}{2m_e}\sum_{i=1}^{Z_t}q^2+\frac{i\hbar^2}{2m_e}\sum_{i=1}^{Z_t}\int d^{Z_t}A\vec{q}\cdot\nabla_i\varphi_0^2(A)\,.\end{aligned}$$

The second term is, again, zero by Gauss theorem:

$$\begin{aligned}\int d^{Z_t}A\vec{q}\cdot\nabla_i\varphi_0^2(A) &= \int d^3\vec{r}_1\cdots d^3\vec{r}_{i-1}d^3\vec{r}_{i+1}\cdots d^3\vec{r}_{Z_t}\int d^3\vec{r}_i\vec{q}\cdot\nabla_i\varphi_0^2(A)\\ &= \int d^3\vec{r}_1\cdots d^3\vec{r}_{i-1}d^3\vec{r}_{i+1}\cdots d^3\vec{r}_{Z_t}\int d^3\vec{r}_i\nabla_i\left(\vec{q}\cdot\varphi_0^2(A)\right)\\ &= \int d^3\vec{r}_1\cdots d^3\vec{r}_{i-1}d^3\vec{r}_{i+1}\cdots d^3\vec{r}_{Z_t}\int_{\partial\mathbb{R}^3} dS\;\hat{n}\cdot\vec{q}\,\varphi_0^2(A)\\ &= 0\,.\end{aligned}$$

Then, as q^2 does not depend on the index i, we finally obtain that:

$$\left(\hat{B}^\dagger\left[\hat{H}_{at},\hat{B}\right]\right)_{00} = \frac{Z_t\hbar^2}{2m_e}q^2 = \sum_n (E_n-E_0)|F_n(q)|^2\,. \tag{4.15}$$

This sum resembles the sum rule found on the classical derivation, formula (3.42), which establishes a connection between the fraction f_a of electrons with characteristic classical frequency ω_a and the quantum atomic form factor $F_n(\vec{q})$. More will be said later about this sum rules. Turning back to the stopping power calculation, what we achieved can be inserted in formula (4.13):

$$\begin{aligned}S(T) &= 2\pi N\left[\frac{2Z_pe^2}{\hbar v_0}\right]^2\int_{\overline{q}_{min}}^{\overline{q}_{max}}\frac{dq}{q^3}\frac{\hbar^2}{2m_e}q^2Z_t\\ &= \frac{\pi N}{m_e}\left[\frac{2Z_pe^2}{v_0}\right]^2 Z_t\ln\left(\frac{\overline{q}_{max}}{\overline{q}_{min}}\right)\\ &= K_0\frac{\rho}{A_t}\frac{Z_p^2Z_t}{\beta^2}\ln\left(\frac{\overline{q}_{max}}{\overline{q}_{min}}\right)\;\;;\;\; K_0=\frac{4\pi N_Ae^4}{m_ec^2}\,.\end{aligned} \tag{4.16}$$

It is worthwhile to mention the similarity of (4.16) with formula (3.11) but showing the main issue of the quantum derivation: using the momentum transfer rather than the impact parameter (experimentally infeasible quantity), to evaluate the energy transfer. Now it is time to evaluate the averages mentioned before, to determine the integration limits. We already said something about the momentum transference in (4.12). Then:

$$q_{min} = k_0 - k_n = \frac{p_0-p_n}{\hbar} = -\frac{\Delta p}{\hbar}\,.$$

Using that $v_0 = \frac{dT}{dp}\approx\frac{\Delta T}{\Delta p} = -\frac{\Delta E}{\Delta p}$ with $\Delta E = E_n - E_0$, then $\Delta p\approx -\frac{\Delta E}{v_0}$. With this:

$$q_{min} = \frac{\Delta E}{\hbar v_0}\;\;\Rightarrow\;\; \overline{q}_{min} = \frac{\overline{\Delta E}}{\hbar v_0} = \frac{\langle I\rangle}{\hbar v_0}\,. \tag{4.17}$$

Again, we are capable of identifying this recurrent average in the characteristic energy levels of the atom. Nevertheless, this is not a rigorously definition of $\langle I\rangle$ because this must be defined in order to interchange the integral with the summation. The corresponding quantum definition of $\langle I\rangle$ to fit this necessity is shown in chapter 6.

On the other hand, q_{max} is the maximum momentum transfer to the atom by excitation of one of its electrons. This quantity is already calculated in energy terms such that if $M >> m_e$ and $v_0 << c$, $\epsilon_{max}\approx 2m_ev_0^2$. Then:

$$v_0\approx\frac{\epsilon_{max}}{p_{max}}\;\Rightarrow\; p_{max}\approx\frac{\epsilon_{max}}{v_0} = 2m_ev_0\,, \tag{4.18}$$

and being $p_{max} = \hbar q_{max}$, then $q_{max} = \frac{2m_ev_0}{\hbar}\neq q_{max}(n)$. This is the inverse of the non-relativistic approximation of b_1^q in section 4.1. With these limits, the stopping power is:

$$\boxed{S(T) = K_0 \frac{\rho}{A_t} \frac{Z_p^2 Z_t}{\beta^2} \ln\left(\frac{2m_e v_0^2}{\langle I \rangle}\right)}. \tag{4.19}$$

Several remarks on the quantum stopping power expression should be made:

1. It only consists on the leading logarithmic term, but changing ϵ_{max} by the corresponding expression if $v_0 \sim c$ makes the $\ln(1-\beta^2)$ term appear.

2. As expected, the factor 2 missing in section 4.1 appears inside the leading term.

3. The quantum mechanics theoretical framework used is not compatible with special relativity. Therefore, the spin correction term $-\beta^2/2$ does not appear naturally.

4. The term $\ln(e^{\overline{\gamma}}\eta)$ is missing, and Bohr establishes a limit with his factor $\kappa = e^{\overline{\gamma}}\eta$ that forces to use the classical expression (3.47) when $\eta > 1$ and (4.19) when $\eta < 1$. This comes from the impact parameter comparison (4.2) because if $\eta < 1$, the quantum minimum impact parameter b_1^q is larger than the classical one, and we seem obliged to include quantum modifications. More information about this will be available when studying the Bloch correction.

5. The mean excitation potential is included, as a necessary condition to carry on with the calculation. Nothing is said about the formal definition but the complete deduction is shown in chapter 6.

Chapter 5

High Density Stopping Power

In the case of ideal gases, the problem of energy-loss per pathlength can be understood in a binary formulation: the projectile interacts with one atom at a time. This is not true in more dense materials, e.g. solids or liquids. In these cases, the distance $|\vec{r}|$ between the projectile and one scattering center probably contains other elements that might be susceptible to the electromagnetic fields generated by the charged ion. To put it in alternative description, the projectile might be able to overcome interaction with more than one scattering center simultaneously, and effects such as polarization of the material are not negligible. Obviously, a microscopic and individual analysis of each interaction is unfeasible, becoming the classical electrodynamics the suitable theoretical frame for a macroscopic treatment.

It will be shown in the following sections, that if the projecile does not have extremely large kinetic energy (meaning it is not relativistic), the result is essentially the same as quantum stopping power (aca agregar la fórmula correspondiente) if $\eta < 1$. This means that the treatment of dense transporting media corresponds to a distant collision situation, with the substantial changes appearing in the relativistic regime. To understand the limits and consequences of the previous models, and aimimg at generating an intuitive description, a dimensional analysis is mandatory.

5.1 Dimensional analysis of the problem

Let the distance between the projectile and the atom be measured with a vector $\vec{r}$ from the charged ion to the nucleus of the atom. In every practical situation, the distance from the nucleus to the electron is negligible compared with $|\vec{r}|$, and therefore it can be said that $\vec{r}$ is also the position of the electron respect to the projectile.

In the non-relativistic limit $|\vec{v}| << c$, the Lorentz factor is $\gamma \approx 1$, and therefore, Bohr's adiabatic radius becomes $b_{max} = \frac{\gamma|\vec{v}|}{\overline{\nu}} \approx \frac{|\vec{v}|}{\overline{\nu}}$, where $\overline{\nu}$ is the average characteristic frequency of the atomic electrons trajectories. It is important to keep in mind that for distances $|\vec{r}| > b_{max}$ the energy transfer is essentially zero.

On the other hand, a positively charged ion moving with velocity $\vec{v}$, generates an electromagnetic field in $\vec{r}$ that can be decomposed spectrally in terms of the frequency $\omega \sim \frac{|\vec{v}|}{|\vec{r}|}$, which is the inverse of the *"characteristic time of collision"*. The electrons in the different atoms can be excited by the components of the electromagnetic field of the projectile whose frequency satisfy $\omega \gtrsim \overline{\nu}$.

It is convenient to define some parameters as shown in figure 5.1. It will be understood by *"interatomic distance"* a, the separation length between a neigthbouring pair of atoms as measured from their nuclei. For the *"characteristic atomic dimension"* c, it corresponds the distance between the nucleus and the boundary of the surrounding electron cloud. With this dimensional characteristics it can be said that a material can be considered as "dense" if $a \sim c$, that is, the interatomic distance is similar to the dimension of the atoms.

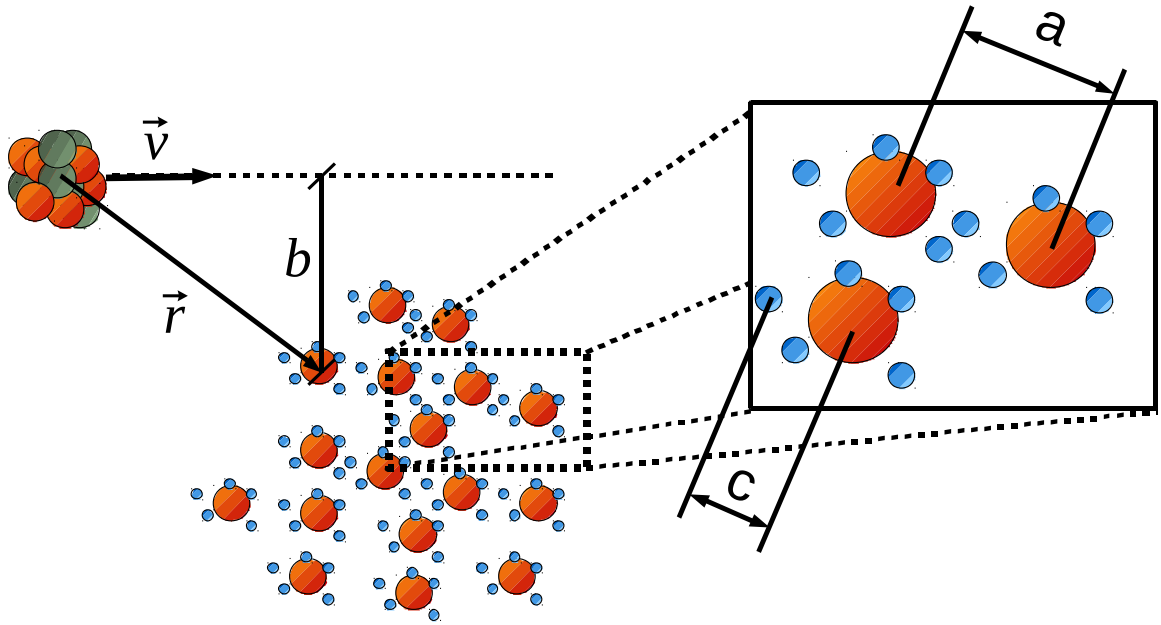

Figure 5.1: Simplified and classical scheme of the material scattering centers and the intuitive definition of the *"interatomic distance"* a and the *"characteristic atomic dimension"* c.

Therefore, the intuitive description that is intended to be cleared can be stated as follows: the charged ion can interact with the atomic electrons if $\omega \sim \frac{|\vec{v}|}{|\vec{r}|} \gtrsim \overline{\nu}$, which means that $\frac{|\vec{v}|}{\overline{\nu}} \gtrsim |\vec{r}|$. If $|\vec{r}| > a$, then the ion "sees" more than one atom simultaneously. This two relations together imply that $\frac{|\vec{v}|}{\overline{\nu}} \gg a$.

Here comes the key issue of the deduction: if the material is "dense", then $a \sim c$, and then $\frac{|\vec{v}|}{\overline{\nu}} \gg a \sim c$. Therefore, $|\vec{v}| \gg c\overline{\nu} = v_{el}$, that is, the projectile's velocity must be greater than the mean orbital velocity v_{el} of the majority of the atomic electrons . In this limit, the dense material can be treated macroscopically.

5.2 Dense material non-relativistic calculation

We stuck in the limits $v_{el} << |\vec{v}| << c$ for the projectile's velocity, ensuring the macroscopic treatment condition. We will also assume that the charged ion $(Z_p e)$ is heavier than the atomic electrons, $M >> m_e$. Therefore, we will solve the macroscopic Maxwell equation for the electric field, given the magnetic field does not work:

$$\nabla \cdot \vec{D} = 4\pi\rho \;\; ; \;\; \nabla \times \vec{E} = 0\,, \tag{5.1}$$

where the density ρ corresponds only to the projectile, that is $\rho = Z_p e\delta(\vec{r} - \vec{v}t)$. The zero rotational equation for the electric field implies the existence of a scalar field $\phi : \mathbb{R}^3 \to \mathbb{R}$ such that $\vec{E} = -\nabla\phi$. The spatial derivatives does not affect $\hat{\epsilon}$, and consequently, using the divergence equation:

$$\nabla \cdot \vec{D} = \nabla \cdot (\hat{\epsilon}\vec{E}) = -\nabla \cdot (\hat{\epsilon}\nabla\phi) = -\nabla^2(\hat{\epsilon}\vec{E}) = 4\pi Z_p e\delta(\vec{r} - \vec{v}t) \;\; \Rightarrow \;\; \nabla^2(\hat{\epsilon}\vec{E}) = -4\pi Z_p e\delta(\vec{r} - \vec{v}t)\,. \tag{5.2}$$

This equation can be solved by usual means using Fourier transform in the spatial part:

$$\hat{\epsilon}\phi(\vec{r}, t) = \frac{1}{(2\pi)^{3/2}} \int d^3\vec{k} (\hat{\epsilon}\phi)_{\vec{k}}(t)\, e^{i\vec{k}\cdot\vec{r}}\,,$$
$$\delta(\vec{r} - \vec{v}t) = \frac{1}{(2\pi)^3} \int d^3\vec{k}\, e^{i\vec{k}\cdot(\vec{r}-\vec{v}t)}\,,$$

expressions that taken to the equation gives:

$$-\frac{1}{(2\pi)^{3/2}}\int d^3\vec{k}(\hat{\epsilon}\phi)_{\vec{k}}(t)|\vec{k}|^2\, e^{i\vec{k}\cdot\vec{r}} = -\frac{4\pi Z_p e}{(2\pi)^3}\int d^3\vec{k}\, e^{i\vec{k}\cdot(\vec{r}-\vec{v}t)}\,. \tag{5.3}$$

As always, the orthogonality of the functions $\{e^{i\vec{k}\cdot\vec{r}}\}$ allows to isolate an algebraic equation of the form:

$$(\hat{\epsilon}\phi)_{\vec{k}}(t) = \frac{4\pi Z_p e}{(2\pi)^{3/2}}\frac{1}{|\vec{k}|^2}e^{-i\vec{k}\cdot\vec{v}t}\,. \tag{5.4}$$

This necessarily implies that $\phi_{\vec{k}}(t) \propto e^{-i\vec{k}\cdot\vec{v}t}$, meaning it depends of frequency factors of $\omega = \vec{k}\cdot\vec{v}$. As explained in section 2.2, Fourier transforming $\hat{\epsilon}$ results in a multiplying factor $\epsilon(\vec{k}\cdot\vec{v})\phi_{\vec{k}}(t)$, and consequently:

$$\phi_{\vec{k}}(t) = \frac{4\pi}{(2\pi)^{3/2}}\frac{Z_p e}{|\vec{k}|^2}\frac{1}{\epsilon(\vec{k}\cdot\vec{v})}e^{-i\vec{k}\cdot\vec{v}t}\,. \tag{5.5}$$

It is important to keep in mind that our starting equations does not use the Maxwell equation with $\nabla\times\vec{H}$. This equation depends on a source $\frac{4\pi}{c}\vec{j} = \frac{4\pi}{c}Z_p e\vec{v}\delta(\vec{r}-\vec{v}t)$, and given $v << c$, it can be neglected. Taking this equation into account, the vacuum field should be substracted from $\vec{E}$ on calculation. This logically does not modify the energy deposition, but it would have changed the $1/\epsilon(\vec{k}\cdot\vec{v})$ factor by $1/\epsilon(\vec{k}\cdot\vec{v})-1$, making the integrals to converge. This will be seen clearly when studying the relativistic case due to Fermi in 1940[13]. Nevertheless, when evaluating the following integrals, care should be taken of using the correct function. The electric field can be written as:

$$\vec{E} = \frac{1}{(2\pi)^{3/2}}\int d^3\vec{k}\vec{E}_{\vec{k}}\, e^{i\vec{k}\cdot\vec{r}}\ \ ;\ \ \phi = \frac{1}{(2\pi)^{3/2}}\int d^3\vec{k}\phi_{\vec{k}}\, e^{i\vec{k}\cdot\vec{r}}\,,$$

and since $\vec{E} = -\nabla\phi$, we have:

$$\frac{1}{(2\pi)^{3/2}}\int d^3\vec{k}\vec{E}_{\vec{k}}\, e^{i\vec{k}\cdot\vec{r}} = -\frac{i}{(2\pi)^{3/2}}\int d^3\vec{k}\phi_{\vec{k}}\vec{k}\, e^{i\vec{k}\cdot\vec{r}}\ \ \Rightarrow\ \ \vec{E}_{\vec{k}} = -i\vec{k}\phi_{\vec{k}}\,,$$

or, replacing the potential expansion coefficients:

$$\vec{E} = -\frac{4\pi}{(2\pi)^{3/2}}iZ_p e\int d^3\vec{k}\frac{\vec{k}}{|\vec{k}|^2}\frac{1}{\epsilon(\vec{k}\cdot\vec{v})}\, e^{i\vec{k}\cdot(\vec{r}-\vec{v}t)}\,. \tag{5.6}$$

It is worth mentioning the similarity of the procedure respect the distant collision deduction due to Bohr, where the energy loss is estimated by the amount of work done by the projectile's field in the atomic electron. In this case, the field generated inside the material due to the presence of the projectile is being calculated, and it is capable of generating a force in the present charges at a position $\vec{r}$. Given the third Newton law, of action-reaction, the projectile must feel (in its own position) a force of equal intensity that logically will oppose to its displacement, given by $\vec{F} = Z_p e\vec{E}(\vec{r}=\vec{v}t)$. This force is then:

$$\vec{F} = -\frac{i(Z_p e^2)}{2\pi^2}\int d^3\vec{k}\frac{1}{\epsilon(\vec{k}\cdot\vec{v})}\frac{\vec{k}}{|\vec{k}|^2}\,.$$

Choosing the laboratory frame such that the projectiles initial direction of movement is $\vec{v} = v\hat{i}$, the magnitude of the stopping force (the linear stopping power) is:

$$F = i\frac{(Z_p e)^2}{2\pi^2}\int d^3\vec{k}\frac{1}{\epsilon(\vec{k}\cdot\vec{v})}\frac{k_x}{|\vec{k}|^2}\,. \tag{5.7}$$

As stated in section 1.1, this stopping force is nothing more than the stopping power itself. Therefore, in this case, the magnitude (5.7) is equivalent to writing $S(T) = -Z_p e\vec{E}(\vec{r}=\vec{v}t)\cdot\frac{\vec{v}}{|\vec{v}|}$. Introducing

$\omega = \vec{k}\cdot\vec{v} = k_x v$, and joining the transversal components of the momentum transfer in a "cylindrical" variable $q = \sqrt{k_y^2 + k_z^2}$, we have that $d^3\vec{k} = dk_x dk_y dk_z = \frac{d\omega}{v} q dq d\varphi$. Therefore, we can carry on with the calculation:

$$\begin{aligned} S(T) &= i\frac{(Z_p e)^2}{2\pi^2}\frac{1}{v^2}\int d\omega \int q dq \int d\varphi \frac{\omega}{(q^2+k_x^2)}\frac{1}{\epsilon(\omega)} \\ &= i\frac{(Z_p e^2)}{\pi}\int d\omega \int q dq \frac{\omega}{(v^2q^2+\omega^2)}\frac{1}{\epsilon(\omega)}\,. \end{aligned}$$

We know that $k_j \in (-\infty,\infty)$, with $j = x,y,z$, and consequently $0 < k_j^2 < \infty$. Then $q \in [0,\infty)$. This transversal momentum transfer is asociated with the impact parameter of the projectile as $\frac{1}{q} \sim b$. If the collision were close (small b), the notion of simultaneous interaction with several scattering centers is lost. Therefore, to remain in a macroscopic description, there exists a limit b_1 such that $b > b_1$, which implies $\frac{1}{b_1} > \frac{1}{b} \sim q$. Then, there is a limit in the possible momentum transfer, meaning there exists q_1 such that $q < q_1$. If $q > q_1$, the problem can be treated as a binary collision with a free electron (close collision approximation). The stopping power with the corresponding limits stands for:

$$S(T) = i\frac{(Z_p e)^2}{\pi}\int_0^{q_1} q dq \int_{-\infty}^{\infty} \frac{\omega}{(v^2q^2+\omega^2)\epsilon(\omega)} d\omega\,.$$

It is important to keep in mind that, given $\omega/(v^2q^2\omega^2)$ is an odd function of ω, combining it with the properties seen in section 2.2:

$$\begin{aligned} &\frac{\omega}{(v^2q^2+\omega^2)}\mathbb{R}e\left(\frac{1}{\epsilon(\omega)}\right) \text{ is odd } \Rightarrow \int_{-\infty}^{\infty}\frac{\omega}{(v^2q^2+\omega^2)}\mathbb{R}e\left(\frac{1}{\epsilon(\omega)}\right)d\omega = 0\,, \\ &\frac{\omega}{(v^2q^2+\omega^2)}\mathbb{I}m\left(\frac{1}{\epsilon(\omega)}\right) \text{ is even } \Rightarrow \int_{-\infty}^{\infty}\frac{\omega}{(v^2q^2+\omega^2)}\mathbb{I}m\left(\frac{1}{\epsilon(\omega)}\right)d\omega = 2\int_0^{\infty}\frac{\omega}{(v^2q^2+\omega^2)}\mathbb{I}m\left(\frac{1}{\epsilon(\omega)}\right)d\omega\,, \end{aligned}$$

and consequently:

$$S(T) = i\frac{(Z_p e)^2}{\pi}2i\int_0^{q_1} q dq \int_0^{\infty}\frac{\omega}{(v^2q^2+\omega^2)}\mathbb{I}m\left(\frac{1}{\epsilon(\omega)}\right)d\omega\,,$$

and combining $i^2 = -1$ and that $\mathbb{I}m\left(\frac{1}{\epsilon(\omega)}\right) < 0$ (see section 2.2), finally we obtain:

$$S(T) = \frac{2}{\pi}(Z_p e)^2\int_0^{q_1} q dq \int_0^{\infty}\frac{\omega}{(v^2q^2+\omega^2)}\left|\mathbb{I}m\left(\frac{1}{\epsilon(\omega)}\right)\right| d\omega\,. \tag{5.8}$$

The q-integral can be performed taking into account that as $q \sim \frac{1}{b}$, then $b \sim \frac{1}{q} << b_{max} \approx \frac{v}{\overline{\nu}}$. This implies that $\frac{\overline{\nu}}{v} << q$. Therefore, the useful frequencies of the spectral decomposition of the field are those satisfying $\overline{\nu} \lesssim \omega$. Then, $\frac{\overline{\nu}}{v} \lesssim \frac{\omega}{v}$ and for sufficiently large q (but not greater than the distant collision limit q_1) we have that $\frac{\omega}{v} < q \Rightarrow \frac{\omega}{v} << q_1$. Then, using the intuitive change of variables:

$$u(q) = q^2 + \frac{\omega^2}{v^2} \;\;;\;\; du = 2qdq \;\;;\;\; u(0) = \frac{\omega^2}{v^2} \;\;;\;\; u(q_1) = q_1^2 + \frac{\omega^2}{v^2} \sim q_1^2\,,$$

and the integral in the transversal momentum transfer is:

$$\begin{aligned} \int_0^{q_1}\frac{q}{v^2q^2+\omega^2}dq &= \frac{1}{2v^2}\int_{\omega^2/v^2}^{q_1^2}\frac{du}{u} = \frac{1}{2v^2}\left\{\ln(q_1^2) - \ln\left(\frac{\omega^2}{v^2}\right)\right\} \\ &= \frac{1}{v^2}\ln\left(\frac{q_1 v}{\omega}\right)\,. \end{aligned}$$

With this, the stopping power is:

$$S(T) = \frac{2}{\pi}\left(\frac{Z_p e}{v}\right)^2 \int_0^\infty \omega \ln\left(\frac{q_1 v}{\omega}\right) \left|\mathbb{I}m\left(\frac{1}{\epsilon(\omega)}\right)\right| d\omega\,. \tag{5.9}$$

We next define the characteristic mean frequency for the energy transfer as follows:

$$\begin{aligned}
\int_0^\infty \omega \ln\left(\frac{q_1 v}{\omega}\right) \left|\mathbb{I}m\left(\frac{1}{\epsilon(\omega)}\right)\right| d\omega &= \int_0^\infty \omega \ln(q_1 v) \left|\mathbb{I}m\left(\frac{1}{\epsilon(\omega)}\right)\right| d\omega - \int_0^\infty \omega \ln(\omega) \left|\mathbb{I}m\left(\frac{1}{\epsilon(\omega)}\right)\right| d\omega \\
&= \left\{ \ln(q_1 v) - \frac{\int_0^\infty \omega \ln(\omega) \left|\mathbb{I}m\left(\frac{1}{\epsilon(\omega)}\right)\right| d\omega}{\int_0^\infty \omega \left|\mathbb{I}m\left(\frac{1}{\epsilon(\omega)}\right)\right| d\omega} \right\} \int_0^\infty \omega \left|\mathbb{I}m\left(\frac{1}{\epsilon(\omega)}\right)\right| d\omega \\
&= \{\ln(q_1 v) - \ln(\langle\omega\rangle)\} \int_0^\infty \omega \left|\mathbb{I}m\left(\frac{1}{\epsilon(\omega)}\right)\right| d\omega \\
&= \ln\left(\frac{q_1 v}{\langle\omega\rangle}\right) \int_0^\infty \omega \left|\mathbb{I}m\left(\frac{1}{\epsilon(\omega)}\right)\right| d\omega\,,
\end{aligned}$$

where:

$$\ln(\langle\omega\rangle) = \frac{\int_0^\infty \omega \ln(\omega) \left|\mathbb{I}m\left(\frac{1}{\epsilon(\omega)}\right)\right| d\omega}{\int_0^\infty \omega \left|\mathbb{I}m\left(\frac{1}{\epsilon(\omega)}\right)\right| d\omega}\,. \tag{5.10}$$

Then, the stopping power of a dense material with a momentum transfer not greater than q_1 (distant collision) is given by:

$$\boxed{S_{q<q_1}(T) = \frac{2}{\pi}\left(\frac{Z_p e}{v}\right)^2 \ln\left(\frac{q_1 v}{\langle\omega\rangle}\right) \int_0^\infty \omega \left|\mathbb{I}m\left(\frac{1}{\epsilon(\omega)}\right)\right| d\omega}\,. \tag{5.11}$$

This result is substantially different respect the Bohr and Bethe solutions. Also, this expression can no longer be transformed in a general way, because some specification needs to be made about the enery loss function $1/\epsilon(\omega)$.

In section 2.2.3, a general quantification of the electric permittivity at high frequencies is developed. This can be used to estimate the remaining integral in (5.11) by making some steps backward. Using the defined parity of the integrand:

$$\begin{aligned}
\int_0^\infty \omega \left|\mathbb{I}m\left(\frac{1}{\epsilon(\omega)}\right)\right| d\omega &= -\int_0^\infty \omega \mathbb{I}m\left(\frac{1}{\epsilon(\omega)}\right) d\omega = i\int_0^\infty \omega\, i\, \mathbb{I}m\left(\frac{1}{\epsilon(\omega)}\right) d\omega \\
&= \frac{i}{2}\int_{-\infty}^\infty \omega\, i\, \mathbb{I}m\left(\frac{1}{\epsilon(\omega)}\right) d\omega = \frac{i}{2}\int_{-\infty}^\infty \frac{\omega}{\epsilon(\omega)} d\omega\,.
\end{aligned}$$

In the last expression, it is possible to extend $\omega \to z \in \mathbb{C}$, using a closed curve in the upper half-plane, consisting on a real line from $-R$ to R and a semicircle σ_R (see figure 5.2), and given $1/\epsilon(z)$ has no poles when $\mathbb{I}m(z) > 0$ (see section 2.2.2), the Cauchy-Goursat theorem ensures that:

$$0 = \lim_{R\to\infty} \oint \frac{z}{\epsilon(z)} dz\,. \tag{5.12}$$

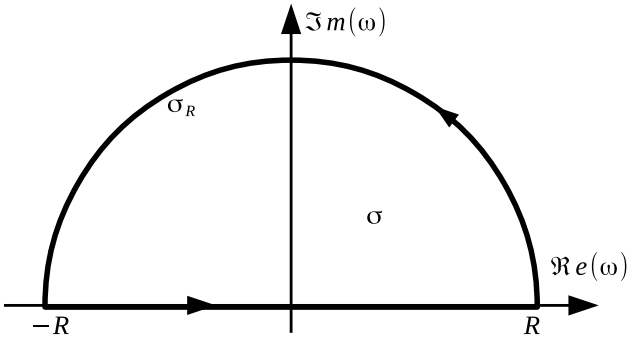

Figure 5.2: Complex plane contour for integration.

Rewriting this integral, it is easily seen that:

$$0 = \lim_{R\to\infty} \oint \frac{z}{\epsilon(z)} dz = \lim_{R\to\infty} \int_{-R}^{R} \frac{\omega}{\epsilon(\omega)} d\omega + \lim_{R\to\infty} \int_{\sigma_R} \frac{z}{\epsilon(z)} dz$$
$$= \int_{-\infty}^{\infty} \frac{\omega}{\epsilon(\omega)} d\omega + \lim_{R\to\infty} \int_{\sigma_R} \frac{z}{\epsilon(z)} dz$$
$$\Rightarrow \int_0^{\infty} \omega \left| \mathbb{I}m\left(\frac{1}{\epsilon(\omega)}\right)\right| d\omega = -\frac{i}{2} \lim_{R\to\infty} \int_{\sigma_R} \frac{z}{\epsilon(z)} dz\,.$$

The integral is carried out in a semicircle with very large radius R, then, the high frequency permittivity $\epsilon(\omega) \to 1 - \frac{\omega_p^2}{\omega^2}$ can be used. Here it is needed for the integral to converge, to remember that the electric field in vacuum must be substracted, changing the energy loss function as:

$$\frac{1}{\epsilon(\omega)} \to \frac{1}{\epsilon(\omega)} - 1 = \frac{\omega_p^2}{\omega^2 - \omega_p^2} \sim \frac{\omega_p^2}{\omega^2}\,.$$

With this:

$$\int_{\sigma_R} \frac{z}{\epsilon(z)} dz \sim \int_{\sigma_R} \frac{z\omega_p^2}{z^2} dz = \omega_p^2 \int_{\sigma_R} \frac{dz}{z}$$
$$= \omega_p^2 \int_0^{\pi} \frac{Ri\, e^{i\theta} d\theta}{Re^{i\theta}} = i\pi\omega_p^2\,,$$

and finally:

$$\Rightarrow \int_0^{\infty} \omega \left| \mathbb{I}m\left(\frac{1}{\epsilon(\omega)}\right)\right| d\omega = -\frac{i}{2} \lim_{R\to\infty} \int_{\sigma_R} \frac{z}{\epsilon(z)} dz = \frac{\pi}{2}\omega_p^2\,. \tag{5.13}$$

With all this, the stopping power formula (5.11) can be rewritten as:

$$S_{q<q_1}(T) = \frac{2}{\pi}\left(\frac{Z_p e}{v}\right)^2 \ln\left(\frac{q_1 v}{\langle\omega\rangle}\right) \frac{\pi}{2}\omega_p^2 = \frac{4\pi N Z_t e^2}{m_e}\left(\frac{Z_p e}{v}\right)^2 \ln\left(\frac{q_1 v}{\langle\omega\rangle}\right)$$
$$= \frac{4\pi N_A e^4}{m_e c^2}\frac{\rho}{A_t}\frac{Z_p^2 Z_t}{\beta^2} \ln\left(\frac{q_1 v}{\langle\omega\rangle}\right) = K_0 \frac{\rho}{A_t}\frac{Z_p^2 Z_t}{\beta^2} \ln\left(\frac{q_1 v}{\langle\omega\rangle}\right)\,.$$

As can be seen, this expression shares every structural feature with previous stopping power formulas, with a leading logarithmic term, and depending upon an average frequency. When $q > q_1$, the macroscopic assumption fails, and the formula given by Bethe (4.16) can be used with $\overline{q}_{min} = q_1$:

$$S_{q>q_1}(T) = K_0 \frac{\rho}{A_t}\frac{Z_p^2 Z_t}{\beta^2} \ln\left(\frac{q_{max}}{q_1}\right)\,, \tag{5.14}$$

and the complete stopping power for dense material can be given:

$$S(T) = S_{q<q_1}(T) + S_{q>q_1}(T) = K_0 \frac{\rho}{A_t}\frac{Z_p^2 Z_t}{\beta^2} \ln\left(\frac{q_{max} v}{\langle\omega\rangle}\right)\,,$$

and given the assumptions $M >> m_e$ and $v << c$, $q_{max} = \frac{\epsilon_{max}}{\hbar v} \approx \frac{2m_e v}{\hbar}$. This gives the final expression for the stopping power for dense material in the non-relativistic limit:

$$\boxed{S(T) = K_0 \frac{\rho}{A_t}\frac{Z_p^2 Z_t}{\beta^2} \ln\left(\frac{2m_e v^2}{\hbar\langle\omega\rangle}\right)}\,. \tag{5.15}$$

A few remarks on this formula:

1. It presents a different formal definition of the mean excitation potential $\langle I \rangle$, given by $\langle I \rangle = \hbar \langle \omega \rangle$ where:

$$\ln(\langle \omega \rangle) = \frac{\int_0^\infty \omega \ln(\omega) \left| \mathbb{I}m\left(\frac{1}{\epsilon(\omega)}\right)\right| d\omega}{\int_0^\infty \omega \left| \mathbb{I}m\left(\frac{1}{\epsilon(\omega)}\right)\right| d\omega}, \tag{5.16}$$

   which is dependent on the dispersion relation for the electric permittivity (due to polarization effects in matter). Further comparisons shed light on the oscillators strength nature, as shown in section 6.2.

2. It does not present the classical term $\ln(e^{\overline{\gamma}}\eta)$. Therefore, this is equivalent to the quantum formulation of the stopping power by Bethe, except for the definition of the mean excitation potential. The real difference will become evident when extending the calculation to the relativistic regimen.

3. The limit b_{max} cannot be freely choosen as before, making the term $\ln(1-\beta^2)$ appear, because the calculation is explicitly assuming the non-relativistic limit $v << c$.

4. The spin correction $-\beta^2/2$ is also not present.

5.3 Dense material calculation by Fermi

Chapter 6

Mean excitation potential theory

6.1 Quantum definition

To complete the deduction of Bethe for the stopping power in the quantum mechanical framework, it is important to define the mean excitation potential $\langle I \rangle$. For this, a set of mathematical properties associated with the atomic hamiltonian and its eigenstates is needed. First, we will explore those formulations to define, at the end of this section, the mean excitation potential as derived from quantum mechanics.

Consider the operator $\hat{B}$ defined by formula (4.14). The assumption that will be made is that of the **dipolar approximation** also used in section 3.3. This consisted on considering that the electrons present small variations in their positions respect the atomic nucleus, in comparison with the impact parameter b, i.e. $|\vec{x}| << b$. In the quantum theoretical frame, this position is represented by a quantum operator, therefore speaking of it as "smaller than" is inaccurate. We would need some anchor to the classical intuition for being able to make comparisons, such as averages or expectation values. Therefore, it is convenient to remember that the quantum energy transfer was parametrized using the momentum transfer rather than the impact parameter, and that the *distant collisions* corresponds to the *soft collisions* with small energy transfer. Consequently, $q \sim 0$, allowing the following Taylor representation:

$$e^{i\vec{q}\cdot\vec{r}_i} = 1 + i\vec{q}\cdot\vec{r}_i + \mathcal{O}(q^2)\,. \tag{6.1}$$

With this, the matrix elements of $\hat{B}$ can be written as follows:

$$\begin{aligned}
\hat{B}_{n0} &= \int d^{Z_t}A\varphi_n^*(A)\sum_{i=1}^{Z_t} e^{i\vec{q}\cdot\vec{r}_i}\varphi_0(A) \\
&= \int d^{Z_t}A\varphi_n^*(A)\varphi_0(A)\sum_{i=1}^{Z_t} 1 + i\vec{q}\cdot\sum_{i=1}^{Z_t}\varphi_n^*(A)\vec{r}_i\varphi_0(A) + \mathcal{O}(q^2) \\
&= Z_t\delta_{n,0} + i\vec{q}\cdot\sum_{i=1}^{Z_t}\varphi_n^*(A)\vec{r}_i\varphi_0(A) + \mathcal{O}(q^2)\,.
\end{aligned}$$

Now we force the transition, $\delta_{n,0} = 0$, and construct $|\hat{B}_{n0}|^2$:

$$\begin{aligned}
|\hat{B}_{n0}|^2 = \hat{B}_{0n}^\dagger\hat{B}_{n0} &= \left[i\vec{q}\cdot\sum_{i=1}^{Z_t}\varphi_n^*(A)\vec{r}_i\varphi_0(A) + \mathcal{O}(q^2)\right]\left[-i\vec{q}\cdot\sum_{i=1}^{Z_t}\varphi_n^*(A)\vec{r}_i\varphi_0(A) + \mathcal{O}(q^2)\right] \\
&= \left|\vec{q}\cdot\sum_{i=1}^{Z_t}\int d^{Z_t}A\;\varphi_n^*(A)\vec{r}_i\varphi_0(A)\right|^2 + \mathcal{O}(q^3) \approx \left|\vec{q}\cdot\vec{R}_{n0}\right|^2\,,
\end{aligned}$$

where $\vec{R} = \sum_{i=1}^{Z_t} \vec{r}_i$, and $\vec{R}_{n0} = \langle\varphi_n|\vec{R}|\varphi_0\rangle$. This is the position operator of the atomic dipolar moment, $\vec{d} = -e\vec{R}$. Taking this to the summation in the atomic energy levels:

$$\sum_n (E_n - E_0)|F_n(\vec{q})|^2 = \sum_n (E_n - E_0)|\hat{B}_{n0}|^2 \approx \sum_n (E_n - E_0)|\vec{q}\cdot\vec{R}_{n0}|^2 \,. \tag{6.2}$$

Defining the quantities $f^q_{n,0}$ such that:

$$\sum_n (E_n - E_0)|\vec{q}\cdot\vec{R}_{n0}|^2 = \frac{\hbar^2}{2m_e}\sum_n f^q_{n,0} \;\Rightarrow\; \boxed{f^q_{n,0} = \frac{2m_e}{\hbar^2}(E_n - E_0)|\vec{q}\cdot\vec{R}_{n0}|^2}\,. \tag{6.3}$$

This quantities are closely related to the fraction f_a of atomic electrons with characteristic frequency ω_a defined in the classical calculation of the stopping power, that obeyed the sum rule $\sum_a f_a = Z_t$. To define the mean excitation potential in a quantum mechanical scheme, we will need to know the value of $\sum_n f^q_{n,0}$. For this, it is useful to choose a coordinate system oriented such that $\vec{q} = q\hat{k}$, which helps to simplify the calculations. Therefore:

$$\begin{aligned}
\sum_n (E_n - E_0)|\vec{q}\cdot\vec{R}_{n0}|^2 &= q^2 \sum_n (E_n - E_0)\,|R^z_{n0}|^2 \\
&= q^2 \sum_n (E_n - E_0)\left|\langle\varphi_n|\sum_{i=1}^{Z_t} z_i|\varphi_0\rangle\right|^2 \\
&= q^2 \sum_n (E_n - E_0)\,|\langle\varphi_n|z|\varphi_0\rangle|^2 \quad , \quad z = \sum_{i=1}^{Z_t} z_i \,.
\end{aligned}$$

It can be found in almost any quantum mechanics textbook[14, 15, 16], when studying the interaction of atoms with electromagnetic fields, the concept of **oscillator strengths**, which are defined by:

$$f_{n,0} = \frac{2m_e}{\hbar^2}(E_n - E_0)\left|\langle n|\sum_j z_j|0\rangle\right|^2 \,, \tag{6.4}$$

where the index j indexes the summation over the atomic electrons. This quantities satisfy the same sum rule that their classical counterpart f_a, namely $\sum_n f_{n,0} = Z_t$. The summations are known in modern literature as **Thomas-Reiche-Kuhn sum rules**[17]. With them, the calculation of the summation of $f^q_{n,0}$ is straightforward. The $f^q_{n,0}$ were called by Bethe the **generalized oscillator strengths**. We define the total momentum of the electrons as $\vec{p} = \sum_j \vec{p}_j$, such that $p_z = \sum_j p^z_j$. Then:

$$[z, p_z] = \sum_{i=1}^{Z_t}\sum_{j=1}^{Z_t}[z_i, p^z_j] = i\hbar\sum_{i=1}^{Z_t}\sum_{j=1}^{Z_t}\delta_{i,j} = i\hbar Z_t \,. \tag{6.5}$$

On the other hand, the atomic hamiltonian can be written as:

$$\hat{H}_{at} = \sum_{i=1}^{Z_t}\frac{p_i^2}{2m_e} + V(A) = \frac{p_x^2 + p_y^2 + p_z^2}{2m_e} + V(A)\,, \tag{6.6}$$

from where it is direct that:

$$[z, \hat{H}_{at}] = \left[z, \frac{p_z^2}{2m_e}\right] = \frac{1}{2m_e}[z, p_z^2] = \frac{i\hbar}{m_e}p_z \,, \tag{6.7}$$

where the operator relation $[x, f(p_x)] = i\hbar\frac{\partial f(p_x)}{\partial p_x}$[15] was used. With this tools, it can be seen that:

$$i\hbar Z_t = [z, p_z] = \langle 0|[z, \hat{H}_{at}]|0\rangle = \sum_n \{\langle 0|z|n\rangle\langle n|p_z|0\rangle - \langle 0|p_z|n\rangle\langle n|z|0\rangle\} \,. \tag{6.8}$$

The momentum expectation values should be addressed separately, using the properties already found:

$$\begin{aligned}\langle n|p_z|0\rangle &= \frac{m_e}{i\hbar}\langle n|[z, \hat{H}_{at}]|0\rangle \\ &= \frac{m_e}{i\hbar}\left\{\langle n|z\hat{H}_{at}|0\rangle - \langle n|\hat{H}_{at}z|0\rangle\right\} \\ &= \frac{im_e}{\hbar}(E_n - E_0)\langle n|z|0\rangle \,,\end{aligned}$$

and with the same procedure, $\langle 0|p_z|n\rangle = -\frac{im_e}{\hbar}(E_n - E_0)\langle 0|z|n\rangle$. Then:

$$\begin{aligned}i\hbar Z_t &= \sum_n \{\langle 0|z|n\rangle\langle n|p_z|0\rangle - \langle 0|p_z|n\rangle\langle n|z|0\rangle\} \\ &= \sum_n \left\{\langle 0|z|n\rangle\frac{im_e}{\hbar}(E_n - E_0)\langle n|z|0\rangle + \frac{im_e}{\hbar}(E_n - E_0)\langle 0|z|n\rangle\langle n|z|0\rangle\right\} \\ &= \frac{2im_e}{\hbar}\sum_n (E_n - E_0)\left|\langle n|z|0\rangle\right|^2 \,.\end{aligned}$$

This proves the sum rule we needed, namely:

$$\sum_n f_{n,0} = \frac{2m_e}{\hbar^2}\sum_n (E_n - E_0)\left|\langle n|z|0\rangle\right|^2 = Z_t \,. \tag{6.9}$$

Taking this result to (6.3), it is easily obtained the sum rule for the generalized oscillator strengths:

$$\begin{aligned}\sum_n f^q_{n,0} &= \frac{2m_e}{\hbar^2}\sum_n (E_n - E_0)\left|\vec{q}\cdot\vec{R}_{n,0}\right|^2 \\ &= \frac{2m_e}{\hbar^2}q^2\sum_n (E_n - E_0)\left|\langle n|z|0\rangle\right|^2 \\ &= \frac{2m_e}{\hbar^2}\frac{\hbar^2}{2m_e}Z_t q^2 = Z_t q^2 \,.\end{aligned}$$

All of this mathematical developements will be of use when trying to obtain a definition of the mean excitation potential from the quantum mechanical framework. Lets start from formula (4.13) before and after interchanging the integral symbol with the summation. On one side we have:

$$\sum_n \int_{q_{min}}^{q_{max}} \frac{dq}{q^3}|\hat{B}_{n0}|^2(E_n - E_0) = \sum_n \int_{\frac{E_n - E_0}{\hbar v_0}}^{q_{max}} \frac{dq}{q^3}|\hat{B}_{n0}|^2(E_n - E_0) \,. \tag{6.10}$$

On the other side:

$$\sum_n \int_{\bar{q}_{min}}^{\bar{q}_{max}} \frac{dq}{q^3}|\hat{B}_{n0}|^2(E_n - E_0) = \sum_n \int_{\frac{\langle I\rangle}{\hbar v_0}}^{\bar{q}_{max}} \frac{dq}{q^3}|\hat{B}_{n0}|^2(E_n - E_0) \,. \tag{6.11}$$

What we need is that:

$$\sum_n \int_{q_{min}}^{q_{max}} \frac{dq}{q^3}|\hat{B}_{n0}|^2(E_n - E_0) = \sum_n \int_{\bar{q}_{min}}^{\bar{q}_{max}} \frac{dq}{q^3}|\hat{B}_{n0}|^2(E_n - E_0) \,. \tag{6.12}$$

But we already showed that $q_{max} = \overline{q}_{max} \neq q_{max}(n)$, therefore we may construct the following integral equation:

$$\begin{aligned}
\sum_n \int_{\frac{E_n-E_0}{\hbar v_0}}^{q_{max}} \frac{dq}{q^3}|\hat{B}_{n0}|^2(E_n-E_0) &= \sum_n \int_{\frac{\langle I\rangle}{\hbar v_0}}^{q_{max}} \frac{dq}{q^3}|\hat{B}_{n0}|^2(E_n-E_0) \\
0 &= -\sum_n \int_{\frac{E_n-E_0}{\hbar v_0}}^{q_{max}} \frac{dq}{q^3}|\hat{B}_{n0}|^2(E_n-E_0) + \sum_n \int_{\frac{\langle I\rangle}{\hbar v_0}}^{q_{max}} \frac{dq}{q^3}|\hat{B}_{n0}|^2(E_n-E_0) \\
&= \sum_n \left\{ \int_{q_{max}}^{\frac{E_n-E_0}{\hbar v_0}} \frac{dq}{q^3}|\hat{B}_{n0}|^2(E_n-E_0) + \int_{\frac{\langle I\rangle}{\hbar v_0}}^{q_{max}} \frac{dq}{q^3}|\hat{B}_{n0}|^2(E_n-E_0) \right\} \\
&= \sum_n \int_{\frac{\langle I\rangle}{\hbar v_0}}^{\frac{E_n-E_0}{\hbar v_0}} \frac{dq}{q^3}|\hat{B}_{n0}|^2(E_n-E_0)\,.
\end{aligned}$$

Then, replacing $|\hat{B}_{n0}|^2 = |\vec{q}\cdot\vec{R}_{n0}|^2$ with (6.3) (therefore applying the dipolar approximation), we have:

$$\begin{aligned}
0 &= \sum_n \int_{\frac{\langle I\rangle}{\hbar v_0}}^{\frac{E_n-E_0}{\hbar v_0}} \frac{dq}{q^3}\frac{q^2\cancel{\hbar^2}}{\cancel{2m_e}}\frac{f_{n,0}}{\cancel{(E_n-E_0)}}\cancel{(E_n-E_0)} \\
&= \sum_n \int_{\frac{\langle I\rangle}{\hbar v_0}}^{\frac{E_n-E_0}{\hbar v_0}} \frac{dq}{q} f_{n,0} \\
&= \sum_n f_{n,0}\left\{\ln\left(\frac{E_n-E_0}{\hbar v_0}\right) - \ln\left(\frac{\langle I\rangle}{\hbar v_0}\right)\right\} \\
&= \sum_n f_{n,0}\ln(E_n-E_0) - \sum_n f_{n,0}\ln(\langle I\rangle)\,,
\end{aligned}$$

which finally leads to:

$$\boxed{\ln(\langle I\rangle) = \frac{\sum\limits_n f_{n,0}\ln(E_n-E_0)}{\sum\limits_n f_{n,0}}}\,. \tag{6.13}$$

Note the similarity with the classical counterpart (3.45), but the radical change in the conceptual contents, meaning every magnitude used in the calculation presents essentially different interpretations. Moreover, the quantum mechanical determination includes the suitable definition of the oscillator strenghts.

6.2 Polarization effects: energy loss function

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