Impulsions électromagnétiques dans des milieux ultra-dispersifs nanostructurés: une approche théorique et numérique.

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To my parents Blanca Vergara Antonio and Modesto Garcia Rojas, everything that is good in me is because of you.
Mathematical analysis is as extensive as nature itself; it defines all perceptible relations, measures times, spaces, forces, temperatures; this difficult science is formed slowly, but it preserves every principle which it has once acquired; it grows and strengthens itself incessantly in the midst of the many variations and errors of the human mind. It’s chief attribute is clearness; it has no marks to express confused notations. It brings together phenomena the most diverse, and discovers the hidden analogies which unite them.

– Jean Baptiste Joseph Fourier

One cannot escape the feeling that these mathematical formulae have an independent existence and an intelligence of their own, that they are wiser than we are, wiser even than their discoverers, that we get more out of them than was originally put into them.

– Heinrich Hertz

We do not really deal with mathematical physics, but with physical mathematics; not with the mathematical formulation of physical facts, but with the physical motivation of mathematical methods. The oftmentioned “prestabilized harmony” between what is mathematically interesting and what is physically important is met at each step and lends an esthetic - I should like to say metaphysical – attraction to our subject.

– Arnold Sommerfeld

The scientist does not study nature because it is useful; he studies it because he delights in it, and he delights in it because it is beautiful. If nature were not beautiful, it would not be worth knowing, and if nature were not worth knowing, life would not be worth living. Of course I do not here speak of that beauty that strikes the senses, the beauty of qualities and appearances; not that I undervalue such beauty, far from it, but it has nothing to do with science; I mean that profounder beauty which comes from the harmonious order of the parts, and which a pure intelligence can grasp.

– Henri Poincaré
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Résumé en français

Cependant, il me semble que traduire d’une langue dans une autre, à moins que ce ne soit des reines de toutes les langues, la grecque et la latine, c’est comme quand on regarde les tapisseries de Flandre à l’envers.

—Miguel de Cervantes Saavedra, L’Ingénieux Hidalgo Don Quichotte de la Manche

L’étude de l’interaction entre une impulsion électromagnétique et un matériau dispersif est un vieux sujet qui remonte au moins à Sommerfeld et Brillouin [1]. Depuis lors de nombreux scientifiques ont apporté leur contribution mais il reste qu’un certain nombre de questions demeure, y compris dans des domaines supposés complètement défrichés. Le but de cette thèse est d’aborder de manière la plus systématique qui soit les problèmes les plus emblématiques du domaine de ce qu’il est convenu d’appeler l’électrodynamique classique dans la matière.

Le cadre général de cette thèse couvre les points suivants.

Le problème qui consiste à trouver un modèle précis, notamment dans le visible, est un problème qui trouve sa source dans les travaux de Lorentz [2] et reste aujourd’hui un domaine actif de recherches comme en témoignent les nombreux articles parus sur le sujet [3, 4]. Pour ce qui nous concerne, nous avons cherché à répondre à une question à la fois simple et pratique. Étant donné un certain nombre de données expérimentales tabulées dans un tableau où figurent les parties réelle et imaginaire de la permittivité en fonction de la fréquence, lesquelles données sont obtenues, par exemple, par ellipsométrie [5], comment trouver une procédure qui permette de trouver un modèle analytique qui réponde aux deux propriétés physiques fondamentales: réalité de la réponse temporelle et causalité. En d’autres
termes, on cherche la transformée de Fourier de la susceptibilité électrique \( \hat{\chi} \) sous la forme suivante:

\[
\hat{\chi}_{\text{trunc}}(\omega) = \sum_{j=1}^{l_p} \frac{A_j}{\omega - \Omega_j} - \frac{\bar{A}_j}{\omega + \bar{\Omega}_j}.
\]  

(1)

On notera que les modèles les plus utilisés tels que ceux de Drude, Drude-Lorentz model, Debye, celui des points critiques [6] ou la combinaison de tous ces modèles ne sont que des cas particuliers de ce modèle (assez) général. Les tableaux 1 et 2 donnent les valeurs des pôles \( \Omega_j \) ainsi que les amplitudes associées \( A_j = |A_j| \exp(i\phi_j) \) trouvées en appliquant la méthode utilisée au chapitre I à partir d’un certain nombre de données expérimentales. Les erreurs de type norme \( L_2 \) ou de type \( L_\infty \) exprimées en pourcentage sont aussi reportées et, ce, pour des données considérées dans l’article de Gold et Copper [7], à savoir l’aluminium, l’argent, le GaAs, le GaP et le silicium.

Maintenant équipé d’un modèle phénoménologique vérifiant les grands critères généraux de la Physique avec une concordance optimale sur l’axe réel des fréquences entre le modèle et les données expérimentales, on s’attache à déterminer les caractéristiques essentielles, comme la vitesse par exemple, liées à la propagation d’une impulsion électromagnétique dans un milieu arbitrairement dispersif. Cette problématique a été étudiée par un grand nombre de chercheurs comme par exemple [8, 9, 10, 11], pour ne citer que les contributeurs les plus fameux. Afin d’aborder ce problème, nous avons divisé l’exposé en deux chapitres. Dans le chapitre 2, nous reprenons à notre compte les concepts les plus fondamentaux comme par exemple la notion de vitesse de groupe [12, 13, 14, 2] lorsqu’une impulsion lumineuse traverse un milieu transparent et faiblement dispersif. Ainsi afin d’aborder les notions de propagation de paquets d’ondes dans des milieux quelconques (i.e. pouvant être extrêmement dispersifs et éventuellement absorbants), nous avons pensé qu’il était utile d’utiliser la notion de centrovélocité, notion qui a été définie par exemple dans [13]. Ceci est fait en considérant le cas d’une polarisation rectiligne où l’on se ramène à une seule inconnue scalaire \( u(t, y) \), laquelle représente selon les deux cas de polarisation \( s \) et \( p \), soit le champ électrique, soit le champ magnétique. On définit alors les centres de
### Table 1. Métaux

| Au (Johnson and Christy) $\lambda : 0.188 - 1.937\mu m$ | $\Omega_j [P_{rad/s}]$ | $|A_j| [P_{rad/s}]$ | $\phi_j [rad]$ |
|--------------------------------------------------------|------------------------|---------------------|----------------|
| $3.43E - 01 - 5.21E - 02i$ | 238.36 | 3.14 |
| $4.56E + 00 - 1.46E + 00i$ | 9.83 | 2.12 |

| Cu (Johnson and Christy) $\lambda : 0.188 - 1.937\mu m$ | $\Omega_j [P_{rad/s}]$ | $|A_j| [P_{rad/s}]$ | $\phi_j [rad]$ |
|--------------------------------------------------------|------------------------|---------------------|----------------|
| $4.46E - 01 - 4.61E - 02i$ | 156.78 | 3.12 |
| $3.11E + 00 - 7.71E - 01i$ | 5.16 | 1.07 |

| Al (Ordal et al.) $\lambda : 0.667 - 200\mu m$ | $\Omega_j [P_{rad/s}]$ | $|A_j| [P_{rad/s}]$ | $\phi_j [rad]$ |
|--------------------------------------------------------|------------------------|---------------------|----------------|
| $3.24E - 10 - 1.35E - 03i$ | 4284.43 | 1.57 |
| $1.13E - 01 - 7.16E - 02i$ | 228.84 | 3.08 |
| $4.24E - 01 - 7.94E - 01i$ | 139.21 | $-0.69$ |

| Ag (Babar et al) $\lambda : 0.2066 - 12.40\mu m$ | $\Omega_j [P_{rad/s}]$ | $|A_j| [P_{rad/s}]$ | $\phi_j [rad]$ |
|--------------------------------------------------------|------------------------|---------------------|----------------|
| $-9.14E - 16 - 6.52E - 02i$ | 1818.56 | $-1.57$ |
| $8.37E + 00 - 2.78E + 00i$ | 6.83 | 2.44 |
| $6.30E + 00 - 4.72E - 01i$ | 1.62 | 2.58 |
| $6.73E + 00 - 2.18E - 01i$ | 0.39 | 1.55 |
Table 2. Semi-conducteurs

| $\Omega_j$ [P rad/s] | $|A_j|$ [Prad/s] | $\phi_j$ [rad] |
|----------------------|-----------------|----------------|
| **GaAs (Jellison et al.) $\lambda : 0.234 - 0.840 \mu m$** | | |
| ($error_2 = 3.13\%$ and $error_{\infty} = 6.23\%$) | | |
| $7.17E + 00 - 8.55E - 01i$ | 18.54 | 2.92 |
| $4.65E + 00 - 1.00E + 00i$ | 12.34 | 2.96 |
| $4.30E + 00 - 2.57E - 01i$ | 2.37 | 1.54 |
| $7.66E + 00 - 2.40E - 01i$ | 1.79 | $-1.29$ |
| **GaP (Jellison et al.) $\lambda : 0.234 - 0.840 \mu m$** | | |
| ($error_2 = 3.16\%$ and $error_{\infty} = 6.78\%$) | | |
| $7.60E + 00 - 7.60E - 01i$ | 20.56 | 3.10 |
| $5.64E + 00 - 2.40E - 01i$ | 5.02 | 2.87 |
| $6.19E + 00 - 3.51E - 01i$ | 1.96 | 2.62 |
| $4.32E + 00 - 4.49E - 01i$ | 0.68 | 1.87 |
| **Si (Green and Keevers) $\lambda : 0.25 - 1.0 \mu m$** | | |
| ($error_2 = 1.08\%$ and $error_{\infty} = 3.08\%$) | | |
| $7.99E + 00 - 1.83E + 00i$ | 13.57 | $-2.98$ |
| $6.54E + 00 - 3.74E - 01i$ | 11.50 | $-2.78$ |
| $5.49E + 00 - 6.65E - 01i$ | 10.51 | 2.46 |
| $5.12E + 00 - 1.68E - 01i$ | 4.02 | 2.46 |
gravité des ondes de la manière suivante:

\[ Y_E(t) = \frac{N_E(t)}{D_E(t)} = \frac{\int_{y \in \mathbb{R}} y|u(t, y)|^2 dy}{\int_{y \in \mathbb{R}} |u(t, y)|^2 dy} \]  

\[ Y_H(t) = \frac{N_H(t)}{D_H(t)} = \frac{\int_{y \in \mathbb{R}} y|h(t, y)|^2 dy}{\int_{y \in \mathbb{R}} |h(t, y)|^2 dy} \]

En considérant la propagation d’une impulsion quelconque dans un milieu infini, nous avons montré que, quel que soit le milieu, les fonctions \( Y_E \) et \( Y_H \) sont des fonctions affines du temps. Il est alors facile d’en extraire une vitesse que l’on a nommé vitesse du centre de gravité du paquet d’ondes. Nous trouvons alors que dans le milieu où le nombre d’onde ne varie pas trop dans la bande des fréquences impliquées, la vitesse du paquet d’ondes et la vitesse de groupe sont une et même chose.

Avec ces résultats dans notre besace, nous sommes en mesure d’analyser le cas d’une impulsion électromagnétique qui vient illuminer un slab homogène réalisé avec un matériau dont la loi de dispersion est aussi générale que possible. Ce simple dispositif permet l’étude pratique de phénomènes fondamentaux et de revisiter le concept même d’énergie. Reprenant à notre compte les idées développées par A. Nicolet et F. Zolla dans [15] sur la densité d’énergie associée aux ondes électromagnétiques ainsi que celles de Van Groesen et Maniardi [16], qui ont trait à une généralisation du concept de centrovitesse utilisée au chapitre 2, nous les appliquons à ce cas pratique. Les solutions numériques obtenues ont été placées sous les fourches caudines des critères énergétiques ainsi revisités. Les positions des centres de gravité des différentes impulsions électromagnétiques (incidente, réfléchie, transmise et celle qui correspond à l’onde à l’intérieur du slab) ont été dûment calculées. Les résultats montrent (Fig 1 et Fig 2), conformément à la théorie, un comportement affine desdits centres de gravité ce qui permet du même coup d’obtenir la vitesse (célerité) de la lumière dans un milieu dispersif quelconque. Dès le chapitre 4, nous changeons de dimension et fort des résultats obtenus dans les chapitres précédents, nous nous attaquons vaillamment aux problèmes tridimensionnels. Le problème étant au sens propre comme au sens figuré d’une autre dimension, nous commençons par l’étude du problème académique suivant: l’étude du champ
Fig. 1. Position des centres de gravité pour le superstratum $Y_{I}(t)$, substratum $Y_{III}(t)$, dans le slab $Y_{II}(t)$ et leur comparaison avec $ct$ et $-ct$.

Fig. 2. Position du centre de gravité pour la propagation des impulsions dans le slab $Y_{II}(t)$. 
électromagnétique diffusé par une particule chargée ponctuelle oscillant à une fréquence fixe donnée, \( \omega_0 \), et placée à côté d’un objet dont les dimensions caractéristiques sont de l’ordre de grandeur des oscillations de ladite particule, cet objet étant éventuellement dispersif (Fig 3). Ce problème doit être abordé avec la plus grande circonspection. En premier lieu, il nous est apparu indispensable de calculer aussi précisément que possible le champ rayonné par la particule dans le vide, qu’il soit lointain ou proche. Et c’est là que le bât blesse car, contrairement à ce que l’on pourrait croire, le calcul exact n’est pas disponible dans la littérature. En effet, on pourrait songer à utiliser les très fameuses égalités dues à Liénard et Wiechert que nous rappelons ici.

\[
E = \frac{q}{4\pi\epsilon_0} \left[ \left( 1 - \beta^2 \right) \left( n - \beta \cdot n \right) \frac{a \times (n - \beta \times n)}{c^2 K^3 R} \right]_t,
\]

(4)

\[
B = \frac{q c \mu_0}{4\pi} \left[ \frac{a \times n}{K^2 R c^2} + \frac{a \cdot n (\beta \times n)}{c^2 K^3 R} + \left( 1 - \beta^2 \right) \frac{(\beta \times n)}{K^3 R^2} \right]_t.
\]

(5)

et qui semblent donner un résultat satisfaisant et compact (closed form, comme aiment à le dire nos amis anglosaxons!) mais ce résultat n’est, en fait, simple qu’en apparence puisqu’il fait appel au temps retardé, lequel dépend non seulement du temps de l’observateur mais aussi de sa position, ce qui rend rapidement le calcul du champ en espace libre inextricable. C’est pourquoi, nous proposons une approche nouvelle en faisant un développement polyharmonique exact des sources \( \rho \) et \( j \), ce qui nous permet de représenter les champs à calculer comme une superposition des champs harmoniques suivants:

\[
E(x, t) = \sum_{l \in \mathbb{Z}} e^{+il\omega_0 t} E_l(x),
\]

(6)

\[
B(x, t) = \sum_{l \in \mathbb{Z}} e^{+il\omega_0 t} B_l(x),
\]

(7)

avec les amplitudes complexes \( E_l \) et \( B_l \) associées aux différentes fréquences.
Fig. 3. Une particule chargée oscille proche du volume dispersif, dans ce cas: une nano-sphère. La version papier montre un instantané à \( t = 0 \) fs, et l’animation complète peut être consulté à https://youtu.be/KtI6nkfQyg0. Celle-ci est aussi montrée dans la version pdf en cliquant sur la figure.
Résumé en français

$l\omega_0$:

$$
E_l(x) = \frac{1}{4\pi\varepsilon_0} \int_{\mathbb{R}} \frac{q}{cR^3} \left( cQ_l(z', \vec{R})\vec{R} + K_l(z', \vec{R})(\mathbf{e}_z \times \vec{R}) \times \vec{R} \right) dz',
$$

(8)

$$
B_l(x) = \frac{\mu_0}{4\pi} \int_{\mathbb{R}} \frac{q}{R^2} K_l(z', \vec{R})\mathbf{e}_z \times \vec{R} dz'.
$$

(9)

Ces résultats ont été soigneusement comparées avec les expressions connues notamment pour ce qui concerne le champ lointain lorsque la vitesse de la particule est faible devant celle de la lumière. Nous retrouvons entre autres la bonne vieille approximation dipolaire, base de tant de travaux sur le champ électromagnétique. La seconde partie se veut être le point d’orgue de cette thèse puisqu’il s’agit d’étudier l’interaction du champ créé par la particule oscillante et ce matériau placé à proximité. Pour cela nous utilisons un procédé maintenant bien éprouvé à l’Institut Fresnel qui met à profit une formulation dont l’inconnue est le champ diffracté et qu’utilise toute la puissance de la méthode des éléments finis et, ce, grâce aux PML et au fait qu’avec cette formulation, les sources sont complètement localisées dans le matériau en question et que ces sources sont proportionnelles au champ diffusé par la charge en l’absence dudit matériau. On comprend alors pourquoi il était si important de calculer ce champ avec précision! Ces champs sont obtenus grâce à un solveur numérique GNU (GPL), getDP, développé par C. Geuzaine et P. Dular [17]. La figure 4 (resp. 5) montre la partie imaginaire (resp. réelle) des amplitudes complexes $E_l$ (resp. $B_l$) pour $l = 1, 2, 3$ et 4. Enfin, on ne peut être complet sans aborder un aspect plus géométrique de la résonance. Qu’advient-il lorsqu’il y a à la fois une résonance géométrique et physique des structures étudiées? Les dispositifs nanophotoniques d’aujourd’hui sont composés de silicium ou bien de métaux nobles qui sont utilisés dans les conditions de cette double résonance. Mais chercher les résonances de structures ouvertes n’est pas une mince affaire et conduit assez naturellement à considérer des résonances dans le plan complexe (QNM). Dans le chapitre 5, on determine à la main les QNM d’une cavité Fabry-Pérot. Ce simple exercice nous entraîne sur le terrain des coupures dans le plan complexe qu’il faut savoir choisir avec soin. Par la suite, le champ électromagnétique diffracté est exprimé sur la base des
Fig. 4. Les composantes harmoniques du champ électrique généré par une particule oscillante, $E_l$ for $l = 1, 2, 3, 4$
Fig. 5. Composantes harmoniques de la partie réelle du champ d’induction magnétique généré par une particule oscillante, $B_l$ for $l = 1, 2, 3, 4$ (coupé en vue canonique)
QNM, ce qui est fait en proposant une sorte de normalisation utilisant à la fois les PML et la biorthogonalité des vecteurs de base en jeu.
General introduction

Begin at the beginning, the King said, very gravely, and go on till you come to the end: then stop.

—Lewis Carroll, Alice in wonderland.

The study of the interaction between electromagnetic pulses with dispersive and possibly passive materials has a long tradition that can be traced, at least, to the works of Sommerfeld and Brillouin [1]. As time has passed many scientist have contribute to a better understanding of this kind of phenomena. However some well established concepts need to be revisited and some questions remain open. The aim of this thesis is then, to tackle in a very systematic way, some of the most representative problems in this area.

The general frame of this thesis encompasses the following points.

- The problem of giving an accurate model for electric permittivity, specially at optical frequencies range, goes back to the works of Lorentz [2] and remains as a topic of interest until recent years, see for instance [3, 4]. Having as starting point tabulated experimental data [18, 19], which in the case of the optical range can be obtained using ellipsometry [5], we develop in chapter 1 a mathematical procedure that allows to find analytical models that in the frequency domain fulfills two fundamental physical properties: reality in time domain and causality. Even more, well known models such as: Drude and/or Drude-Lorentz model, Debye model, critical points model [6], or a combination of these elementary resonances [3, 4], can be seen as particular cases of this new and general model.

- Provided with a causal model for the permittivity, we can focus on the task of determining the velocity of an electromagnetic pulse that
propagates in a highly dispersive medium. This issue has been studied by many [8, 9, 10, 11], for mentioning some of the most representative contributions. In order to tackle this problem, we divide the exposition of our ideas in two chapters: In chapter 2 we make a brief discussion about the usual concepts of group velocity [12, 13, 14, 2] when dealing with transparent and mild dispersion materials. In order to give a more general notion of what is the propagation velocity for a wave packet, we use the concept of centrovelocity, as it is defined in [13], and show how under certain assumptions it is possible to see the well known definition of group velocity as a particular case of the centrovelocity. With these ideas in mind, we are in position to analyze in chapter 3 the case of an EM pulse that illuminates normally a slab embedded in vacuum. This homogeneous slab is considered as a non magnetic temporally dispersive absorbing material. This simple setup will allow us to study very important concepts in wave propagation: the very definition of energy for a leaky dispersive material and the propagation velocity of an electromagnetic wave in this kind of material. This is made by using the ideas for energy density given by Nicolet et al. [15] and the approach given by Van Groesen and Maniardi [16] which is a generalization of the centrovelocity used in chapter 2.

- Chapter 4 goes beyond the 1D case and tackles the problem of describing the electromagnetic field generated by an oscillating charge and its interaction with some dispersive 3D-object. In order to handle this issue smoothly we have divided our procedure in two main parts: the first one deals with the pure description of an EM field generated by arbitrary charge density \( \rho \) and corresponding current density \( j \) [20, 21]. Next, one arrives to the well known results of the Liénard-Wiechert fields [2, 20, 22, 23, 24, 25] which despite to be a closed expression are less explicit than they appear to be [23]. To overcome this difficulty, we propose a polyharmonic representation of the electric and magnetic fields in the sense of distributions [26, 27, 28]. These results have been compared with the well know formula of far field
power [2]. The second part is related to the interaction of this polyharmonic EM field and a dispersive object (a sphere in this case). This problem is handled via the diffracted field formulation [29] and solved numerically by using FEM solver GetDP [17].

• Finally, one can not talk about electromagnetic pulses in dispersive (i.e. resonant) media without mentioning a more geometrical aspect of resonances: what happens if both materials and structures are resonant? Nanophotonic devices based on silicon or noble metals are countless examples of open resonators. Finding the resonant frequencies and consequently the resonant modes is a well known problem in physics, when the fields are not strictly confined and can leak to the whole universe [30], in this case we say that we are dealing with Quasi Normal Modes (QNMs). In chapter 5 we give a brief and straightforward way of deriving the QNMs of a Fabry-Perot cavity [12]. The problem of determining the right branch cut of the complex logarithm is studied and more important it is shown its importance when obtaining the complex resonant eigenfrequencies of the cavity. Finally, we deal with the issue of expressing EM fields in terms of a QNMs expansion. This is done by proposing a normalization of the QNMs by using Perfectly Matched Layers (PMLs) [31], and obtaining their bi-orthogonal vectors [32].
Chapter 1

Extracting an accurate model for permittivity from experimental data: Hunting complex poles from the real line.

All models are wrong, but some are useful.
—George E. P. Box, Robustness in the strategy of scientific model building

1.1 Introduction

As we know, Maxwell’s equations are a generalization of experimental facts [33, 2]. Depending on the specific situation that has to be modeled, it is necessary to take into account the electromagnetic properties of the material media. This can be done by using constitutive relations, which relate the fields \( E, H, D \) and \( B \). Keeping in mind that under the action of an external electromagnetic field the material is polarized and magnetization currents are induced in it [34], the following constitutive relations can be used [13, 35, 34]

\[
H = \frac{1}{\mu_0} B - M, \quad D = \epsilon_0 E + P_e,
\]

where \( P_e \) and \( M \) are the polarization and magnetization vectors respectively. The materials that will be considered in this work present a negligible magnetization, that is \( M = 0 \). More important, they are frequency dispersive, which mathematically can be formulated as

\[
P_e(r, t) = \frac{\epsilon_0}{2\pi} \int_{-\infty}^{t} \chi(t - \tau) E(r, \tau) d\tau,
\]
where the factor before the integral is just to keep the right units in MKS system and to be consistent with our Fourier Transform convention (See Appendix A equations (A.1)-(A.4)).

Equation 1.2 establishes that the polarization at some fixed point and instant depends on the past history of the electric field at that point, modulated by the function $\chi(t)$ which is called the susceptibility of the material [9]. The causal nature of this relation is ensured by requiring to $\chi(t)$ to have positive support i.e. $\chi(t) = 0$ for $t < 0$. Then, the polarization vector $P_e$ can be rewritten as

$$P_e(r, t) = \frac{\epsilon_0}{2\pi} \int_{-\infty}^{\infty} \chi(t - \tau) E(r, \tau) d\tau,$$

and consequently the electric displacement $D$ is given by

$$D(r, t) = \frac{\epsilon_0}{2\pi} \int_{-\infty}^{\infty} \epsilon_r(t - \tau) E(r, \tau) d\tau,$$

where $\epsilon_r(t)$ is the relative permittivity and it is defined as

$$\epsilon_r(t) = 2\pi \delta(t) + \chi(t).$$

We can see that in order to obtain an accurate model for the permittivity of highly dispersive materials, it is enough to study the electric susceptibility. In the next section we will use these results in order to fit experimental data with a model that respects reality and causality.

### 1.2 Statement of the problem

From a practical point of view, experimental values of complex permittivities are given as tabulated data [18, 19]. In the optical range, these values are obtained using ellipsometry [5]. When time harmonic numerical methods are used in electromagnetism, one selects a real frequency and uses the tabulated data, up to a simple interpolation, as it is. However, in time domain methods (e.g. Finite difference [36], discontinuous Galerkin [37]), the inverse Fourier Transform of the experimental data is needed since frequency dispersion in the time domain is generally tackled through an extra differential equation involving the polarization vector $P_e$. An analytical expression of the relative permittivity $\hat{\epsilon}_r(\omega)$ (or equivalently, of the susceptibility...
of the material $\hat{\chi}(\omega)$ fulfilling causality requirements has to be extracted from the data given in frequency domain. Same considerations hold when tackling generalized modal computations [38] of dispersive structures. This problem is well known and several closed forms have already been proposed: Drude and/or Drude-Lorentz model, Debye model, critical points model [6], or a combination of these elementary resonances [3, 4]. Nevertheless, the forms assumed in these permittivity models are material dependent. In this approach the closed form assumed for the permittivity is general enough to be material-independent. The only requirement is the causality principle handled via the general constitutive relation between the electric field $E$ and the polarization vector $P_e$.

1.3 Mathematical formulation of the problem

It is clear from equation (1.3) that $\chi(t)$ can be seen as the Green’s function of a differential equation that relates the electric field and the polarization vector. A quite general approach is to consider the following constitutive relation:

$$\sum_{l=0}^{N_d} q_l \frac{\partial E}{\partial t^l} = \epsilon_0 \sum_{k=0}^{N_n} p_k \frac{\partial P_e}{\partial t^k}$$

where the reality of both $P_e$ and $E$ requires $p_k$’s and $q_l$’s to be real numbers. Keeping causal solutions for $P_e$, it remains to carry out a Fourier transform.

$$\left(\sum_{l=0}^{N_d} q_l (-i\omega)^l\right) \hat{P}_e = \epsilon_0 \left(\sum_{k=0}^{N_n} p_k (-i\omega)^k\right) \hat{E}.$$  

(1.7)

Then, the electric susceptibility $\hat{\chi}(\omega)$ is given by

$$\hat{\chi}(\omega) = \frac{\sum_{k=0}^{N_n} p_k (-i\omega)^k}{\sum_{l=0}^{N_d} q_l (-i\omega)^l}.$$  

(1.8)

Using the fact that the electric susceptibility is expressed as a rational function, it is convenient to divide all the coefficients by $q_0$, and calling $P_k = p_k/q_0$, $Q_l = q_l/q_0$ equation (1.8) takes the form

$$\hat{\chi}(\omega) = \frac{\sum_{k=0}^{N_n} P_k (-i\omega)^k}{\sum_{l=0}^{N_d} Q_l (-i\omega)^l}, \quad Q_0 = 1.$$  

(1.9)
Consider now, some experimental data determined for instance by ellipsometry \([5]\) given by a set of corresponding points \((\omega_m, \hat{\chi}_{\text{Data}}^m)\) with \(m = 0, \ldots, M - 1\). For passive materials these data are such that \(\omega_m \in \mathbb{R}^+\) and \(\hat{\chi}_{\text{Data}}^m \in \mathbb{C}^+\) where \(\mathbb{C}^+ = \{\xi \in \mathbb{C} | \Im\{\xi\} > 0\}\). These data can be organized into the following vectors

\[
\omega = (\omega_0, \ldots, \omega_{M-1})^T, \quad \hat{\chi}_{\text{Data}}^m = (\hat{\chi}_{\text{Data}}^0, \ldots, \hat{\chi}_{\text{Data}}^{M-1})^T.
\]  

Let’s suppose that each \(\hat{\chi}_{\text{Data}}^m\) at \(\omega_m\) has a form as in Eq. (1.9), that is:

\[
\hat{\chi}_{\text{Data}}^m = \sum_{n=0}^{N_n} P_n (-i\omega_m)^k \sum_{l=0}^{N_d} Q_l (-i\omega_m)^l.
\]  

After some elementary manipulations and remembering that \(Q_0 = 1\), Eq. (1.11) reads:

\[
\hat{\chi}_{\text{Data}}^m = \sum_{n=0}^{N_n+N_d} r_n \xi_{m,n},
\]  

with

\[
\begin{aligned}
r_n &= \begin{cases} 
P_n & \text{if } n = 0, \ldots, N_n \\
Q_{n-N_n} & \text{if } n = N_n + 1, \ldots, N_n + N_d \end{cases},
\end{aligned}
\]  

and

\[
\xi_{m,n} = \begin{cases} 
(-i\omega_m)^n & \text{if } n = 0, \ldots, N_n \\
-\hat{\chi}_{\text{Data}}^m (-i\omega_m)^{n-N_n} & \text{if } n = N_n + 1, \ldots, N_n + N_d
\end{cases}.
\]  

This can be rewritten in matrix form as:

\[
\hat{\chi}_{\text{Data}} = \Xi \mathbf{r}
\]  

where \(\mathbf{r}\) is the column vector with entries \(r_n\), with \(n = 0, \ldots, N_n + N_d\) and \(\Xi\) is the \(M \times (N_n + N_d + 1)\) matrix with entries \(\xi_{m,n}\). This overdetermined system can be solved in the sense of least squares [39]. That is, to find the vector \(\mathbf{r}\) such that

\[
\| \Xi \mathbf{r} - \hat{\chi}_{\text{Data}} \|_2 = \min_{\mathbf{r} \in \mathbb{R}^{N_n+N_d+1}} \| \Xi \mathbf{r} - \hat{\chi}_{\text{Data}} \|_2.
\]  

This can be achieved, for instance, by the Householder transformation method [40, 41]. In practice, we consider the entries of \(\mathbf{r}\) to be complex, which relaxes
our numerical scheme involving complex polynomials in $(-i\omega)$. The imaginary part of these numbers remains several orders of magnitude smaller than their real part.

Once the $p_k$’s and $q_l$’s coefficients have been determined, it is possible to obtain the poles and zeros of $\hat{\chi}(\omega)$ by finding the roots of $\sum_{k=0}^{N_d} Q_l(-i\omega)^l$ and $\sum_{k=0}^{N_n} P_k(-i\omega)^k$ respectively. Let $\Omega_j, j = 1, \ldots, N_d$ be the obtained poles then $\hat{\chi}(\omega)$ can be expanded in partial fractions [42]:

$$\hat{\chi}(\omega) = \sum_{j=1}^{N_d} \frac{A_j}{\omega - \Omega_j} + g(\omega), \quad (1.17)$$

where $g$ is an holomorphic function representing a non resonant term of $\hat{\chi}$ and is approximated by a polynomial of degree $N_n - N_d$. Assuming that this non resonant term is negligible, the amplitude coefficients $A_j$’s can be obtained via the Tetrachotomy method [43] or as in the case of this chapter by another least squares procedure. Note that this latest assumption simply amounts to compelling the degree of the numerator to be smaller than the denominator’s.

### 1.4 Fitting data in practice

With the mathematical tools described above, the procedure summed up in Fig. 1.1 is used in order to hunt the complex poles of a given material:

- First, vectors $\omega$ and $\hat{\chi}^{Data}$, which are always given for positive frequencies only, are extended to negative frequencies such that the new vectors represent an electrical susceptibility with Hermitian symmetry. This guarantees the reality of the susceptibility in time domain.

- Second, we set $N_d = 2J$ for $J \in \mathbb{N}$ and $N_n \leq N_d$. This is done keeping in mind that each pole $\Omega_j$ have its corresponding symmetric $-\Omega_j$ and in order to ensure that the non resonant function $g$ is at most a constant. In practice a good choice is to keep $N_n = N_d$, which is the approach we will follow in the sequel.

- Next, when poles $\Omega_j$ and associated amplitudes $A_j$ are computed, it is handy to sort these pairs by considering the modulus of $A_j$. Once the
data sorted, the sign of the imaginary part of \( \Omega_j \) has to be checked. In the case of our choice for the Fourier Transform, the imaginary part of physical poles \( \Omega_j \) must be non positive. By the Titchmarsh’s theorem (See Appendix B) this requirement allow us to get a causal model. If the first \( J_p \) pairs of poles \((\Omega_j, -\Omega_j)\), with \( J_p \leq J \), have non negative imaginary part, then we can truncate the limit of the sum in Eq. (1.17), that is:

\[
\hat{\chi}_{\text{trunc}}(\omega) = \sum_{j=1}^{J_p} \frac{A_j}{\omega - \Omega_j} - \frac{\overline{A_j}}{\omega + \overline{\Omega_j}}. \quad (1.18)
\]

It is easy to see that this expression presents Hermitian symmetry.

- Finally, if the error between \( \hat{\chi}_{\text{trunc}}(\omega) \) and \( \hat{\chi}^{\text{Data}} \) according to a given norm is less than a certain tolerance, one can say the best fitting, according to this procedure, has been found. Otherwise it is necessary to repeat this procedure with \( J + 1 \) pairs of poles and so on.

It can be thought at first that the bigger the number of poles \( J \) the better will be the fitting. This is not true in general. As an illustrative example, the energy (\( L_2 \)) and maximum (\( L_\infty \)) norms fitting errors for Si [44] are shown in Figure 1.2. Notice that while the energy norm error decreases as \( J \) increases, the maximum norm error does not exhibit a monotonic behavior. This is mainly due to the fact that the experimental data can exhibit measurement artifacts, for instance when switching from one source to another, and these small artifacts are revealed by the presence of spurious poles sometimes lying in the wrong (upper) half of the complex plane. These sharp spikes make the \( \infty \)-norm increase once physical poles are found.

### 1.5 Results

Tables 1.1 and 1.2 show the values of the poles \( \Omega_j \) and associated amplitudes \( A_j = |A_j|\exp(i\phi_j) \) found when applying the method described above for different data sets. The errors for \( L_2 \)-norm and \( L_\infty \)-norm expressed in percentage are also given for each material. The materials and associated
CHAPTER 1. EXTRACTING AN ACCURATE MODEL FOR PERMITTIVITY

Initialization: $N_p = 1,$ $N_d = 2,$ and $N_n = 1$

Symmetrization of $\hat{\chi}^{\text{Data}}$:
$\hat{\chi}^{\text{Data}}(-\omega) = \overline{\hat{\chi}^{\text{Data}}(\omega)}$

Minimization of
$||N(i\omega) - \hat{\chi}^{\text{Data}}(\omega) D(i\omega)||_2$

Find $\tilde{p}_0, \ldots, \tilde{p}_{2N_p-1}$ and
$(\tilde{q}_0 = 1), \tilde{q}_1 \ldots \tilde{q}_{2N_p}$

Find $A_j$ and $\Omega_j$ with
$\hat{\chi}^{\text{Approx}}_{N_p}(\omega) \simeq \sum_{j=1}^{N_p} \frac{A_j}{\omega - \Omega_j} + \frac{\overline{A_j}}{\omega + \Omega_j}$

$N_p \rightarrow N_p + 1$

Test:
$\Omega_1, \ldots, \Omega_{N_p}$
are located in the lower half complex plane.

no

Stop! Apparition of a spurious pole
Best approximation of $\hat{\chi}^{\text{Data}}$ with $N_p - 1$ poles.

yes

Fig. 1.1. Algorithm for hunting poles in the complex plane
data set considered in this paper are: Gold and Copper [7], Aluminum [45], Silver [46], GaAs, GaP [47] and Silicon [44]. The poles obtained for metals are tabulated in Table 1.1. The frequency range of validity of each fitting is dictated by the tabulated wavelengths available in the corresponding reference given. In the case of Au and Cu, it is $\lambda: 0.188 - 1.937 \mu m$, whereas for Al and Ag the validity range are $\lambda: 0.667 - 200 \mu m$ and $\lambda: 0.2066 - 12.40 \mu m$ respectively. Finally, for the case of semiconductors, GaAs, GaP with $\lambda: 0.234 - 0.840 \mu m$ and Si with $\lambda: 0.25 - 1.0 \mu m$, the parameters are given in Table 1.2. These values were computed using the Python script freely available at Ref. [48].

### 1.6 Validation

In order to illustrate the relevance of our method, two comparisons are now presented between our results and those found in the literature. In the case of metals, the recent results reported by Barchiesi and Grosges (B&G) in [3] for Gold (using experimental data from [7]). In this case, $J$ is set to 8 and the sum is finally truncated to $J_p = 2$ (the same number of poles considered by B&G). We obtain errors of 3.01% using $L_2$-norm and 1.27% using
CHAPTER 1. EXTRACTING AN ACCURATE MODEL FOR PERMITTIVITY

$L\infty$–norm, while these are 9.98% and 6.65% respectively for B&G. The real and imaginary parts of experimental data and corresponding fittings are shown in Fig. 1.3a and 1.3b. For semiconductors, the fitting parameters obtained by Deinega and John (D&J) for Silicon by considering two poles allow to reach a $L_2$–norm error of 8.5% and a $L\infty$–norm error of 15.63%. On the other hand, our approach setting $J = 6$ and $J_p = 4$ (the double of poles than D&J) allow us to compute corresponding two and infinity norm errors of 1.08% and 3.08%. The fittings are shown in Fig. 1.4).

1.7 Partial conclusion

As a conclusion, we have proposed a simple yet systematic procedure for fitting experimental data of permittivities of resonant materials such as metals and semiconductors in the visible range. This procedure does not assume a priori any particular shape for the electric susceptibility $\hat{\chi}$. The final expression obtained for the permittivity preserves causality and stability. This fitting is more accurate than those presented in the reviewed literature. It can be used as it is in numerical codes such as FDTD.
### Table 1.1. Metals

| $\Omega_j$ $[P\text{ rad/s}]$ | $|A_j| [P\text{ rad/s}]$ | $\phi_j [\text{rad}]$ |
|-------------------------------|--------------------------|-----------------------|
| **Au (Johnson and Christy)** $\lambda : 0.188 - 1.937 \mu m$ ($error_2 = 3.01\%$ and $error_\infty = 1.27\%$) |                          |                       |
| $3.43E-01 - 5.21E-02i$         | 238.36                   | 3.14                  |
| $4.56E + 00 - 1.46E + 00i$     | 9.83                     | 2.12                  |
| **Cu (Johnson and Christy)** $\lambda : 0.188 - 1.937 \mu m$ ($error_2 = 6.70\%$ and $error_\infty = 2.88\%$) |                          |                       |
| $4.46E-01 - 4.61E-02i$         | 156.78                   | 3.12                  |
| $3.11E + 00 - 7.71E - 01i$     | 5.16                     | 1.07                  |
| **Al (Ordal et al.)** $\lambda : 0.667 - 200 \mu m$ ($error_2 = 8.36\%$ and $error_\infty = 11.55\%$) |                          |                       |
| $3.24E - 10 - 1.35E - 03i$     | 4284.43                  | 1.57                  |
| $1.13E - 01 - 7.16E - 02i$     | 228.84                   | 3.08                  |
| $4.24E - 01 - 7.94E - 01i$     | 139.21                   | $-0.69$               |
| **Ag (Babar et al) $\lambda : 0.2066 - 12.40 \mu m$ ($error_2 = 1.71\%$ and $error_\infty = 1.87\%$) |                          |                       |
| $-9.14E - 16 - 6.52E - 02i$   | 1818.56                  | $-1.57$               |
| $8.37E + 00 - 2.78E + 00i$    | 6.83                     | 2.44                  |
| $6.30E + 00 - 4.72E - 01i$    | 1.62                     | 2.58                  |
| $6.73E + 00 - 2.18E - 01i$    | 0.39                     | 1.55                  |
### Table 1.2. Semiconductors

| Ω_j [P rad/s] | |A_j|[Prad/s] | φ_j [rad] |
|---------------|----------------|----------------|
| **GaAs (Jellison et al.) λ : 0.234 – 0.840μm** | (error_2 = 3.13% and error_∞ = 6.23%) |
| 7.17E + 00 – 8.55E – 01i | 18.54 | 2.92 |
| 4.65E + 00 – 1.00E + 00i | 12.34 | 2.96 |
| 4.30E + 00 – 2.57E – 01i | 2.37 | 1.54 |
| 7.66E + 00 – 2.40E – 01i | 1.79 | –1.29 |
| **GaP (Jellison et al.) λ : 0.234 – 0.840μm** | (error_2 = 3.16% and error_∞ = 6.78%) |
| 7.60E + 00 – 7.60E – 01i | 20.56 | 3.10 |
| 5.64E + 00 – 2.40E – 01i | 5.02 | 2.87 |
| 6.19E + 00 – 3.51E – 01i | 1.96 | 2.62 |
| 4.32E + 00 – 4.49E – 01i | 0.68 | 1.87 |
| **Si (Green and Keevers) λ : 0.25 – 1.0μm** | (error_2 = 1.08% and error_∞ = 3.08%) |
| 7.99E + 00 – 1.83E + 00i | 13.57 | –2.98 |
| 6.54E + 00 – 3.74E – 01i | 11.50 | –2.78 |
| 5.49E + 00 – 6.65E – 01i | 10.51 | 2.46 |
| 5.12E + 00 – 1.68E – 01i | 4.02 | 2.46 |
Fig. 1.3. Comparison between the experimental data, the approach by Barchiesi and Grosges (B&G) and our fitting for the (a) real and (b) imaginary part of $\hat{\chi}$ for Gold.
Fig. 1.4. Comparison between the experimental data, the approach by Deinega and John (D&J) and our fitting for the (a) real and (b) imaginary part of $\hat{\chi}$ for Silicon.
Chapter 2

The propagation velocity of an EM pulse in transparent and gentle media

Let us first consider waves that have a definite velocity, like sound and light.

2.1 Introduction

This chapter is devoted to the study of the velocity associated to an electromagnetic pulse that propagates in an homogeneous medium. For the case of ideal transparent materials i.e. materials for which $\epsilon$ is a constant and monochromatic light, the most common associated velocity is the phase velocity, defined as [12, 13]:

$$v_\phi = \frac{\beta}{\omega}$$

(2.1)

where $\omega$ is the frequency of the electromagnetic pulse in sinusoidal (harmonic) regime and $\beta$ the corresponding wave number. As its name indicates this velocity represents the rate-of-change of phase with distance [12, 14]. However, when dealing with a more realistic situation, for instance in the case of a wave packet that propagates in a medium with mild dispersion (which we call gentle materials), this solution is not appropriate because different components of the wave travel with different speeds and tend to change phase with respect to one another [2]. The new definition that comes into play is the so called group velocity defined as [12, 13, 14, 2]:

$$v_g = \partial_\beta \omega(\beta_0),$$

(2.2)
where $\partial_\beta \omega(\beta_0)$ represents the partial derivative of $\omega$ with respect to the wave number evaluated at some $\beta_0$ that represents the dominant wave number in the modulated wave [2]. Notice that given the fact that usually $\beta$ is expressed in terms of $\omega$ it is assumed implicitly the existence of a function that goes from $\beta \to \omega$.

Having these ideas in mind, we are going to work on a different way of defining the propagation velocity of an electromagnetic pulse in transparent and gentle media. This approach follows the idea of finding the center of gravity of an electromagnetic pulse, as it can be seen e.g. in [13]. Nevertheless our method to accomplish this task is different from the one used by Petit in [13].

2.2 The electromagnetic pulse as a wave packet

Due to the fact that we are dealing with classical quantities, it is convenient to start by the Maxwell’s equations without sources:

$$\vec{\nabla} \times \mathbf{E} = -\partial_t \mathbf{B}, \quad (2.3)$$
$$\vec{\nabla} \times \mathbf{H} = +\partial_t \mathbf{D}, \quad (2.4)$$
$$\vec{\nabla} \cdot \mathbf{D} = 0, \quad (2.5)$$
$$\vec{\nabla} \cdot \mathbf{B} = 0. \quad (2.6)$$

Taking the Fourier Transform in time (See Appendix A equations (A.1)-(A.4)) of these equations one has:

$$\vec{\nabla} \times \hat{\mathbf{E}} = +i\omega \hat{\mathbf{B}}, \quad (2.7)$$
$$\vec{\nabla} \times \hat{\mathbf{H}} = -i\omega \hat{\mathbf{D}}, \quad (2.8)$$
$$\vec{\nabla} \cdot \hat{\mathbf{D}} = 0, \quad (2.9)$$
$$\vec{\nabla} \cdot \hat{\mathbf{B}} = 0. \quad (2.10)$$

We consider now, that this homogeneous medium has negligible magnetization (i.e. $\hat{\mathbf{B}} = \mu_0 \hat{\mathbf{H}}$) and that electric displacement vector $\hat{\mathbf{D}}$ is given by the constitutive relation $\hat{\mathbf{D}} = \varepsilon_0 \varepsilon_r(\omega) \mathbf{E}$, where $\varepsilon_r(\omega)$ is an even real-valued function. This represents a non absorptive medium with mild dispersion. In the sequel we will refer to these kind of materials as gentle ones, to make a distinction with the highly dispersive materials.
Taking the curl of the Faraday’s law in Eq. (2.7) we arrive to the vectorial Helmholtz equation:
\[ \vec{\nabla}^2 \hat{\mathbf{E}} = -\frac{\omega^2}{c^2} \hat{\epsilon}_r(\omega) \hat{\mathbf{E}}. \] (2.11)
For simplicity, we consider a linearly polarized solution along the z-axis which depends only on the space variable \( y \), that is:
\[ \hat{\mathbf{E}} = \hat{u}(\omega, y) \mathbf{e}_z. \] (2.12)
This implies that equation (2.11) is now
\[ \partial_y^2 \hat{u}(\omega, y) = -\frac{\omega^2}{c^2} \hat{\epsilon}_r(\omega) \hat{u}(\omega, y). \] (2.13)
Given the homogeneous nature of the medium (that is, there are no obstacles that can scatter the electromagnetic pulse), we are only interested in one of the propagative solutions of Eq. (2.13). Thus, without loss of generality, we set:
\[ \hat{u}(\omega, y) = \hat{A}(\omega) e^{-i\beta(\omega)y}, \] (2.14)
where
\[ \beta(\omega) = \sqrt{\frac{\omega^2}{c^2} \hat{\epsilon}_r(\omega)}. \] (2.15)
Notice that this square root is defined in the usual sense for real numbers \[49\]. The magnetic field can be retrieved by plugging equation (2.14) into equation (2.7), namely:
\[ \hat{\mathbf{H}} = \frac{\vec{\nabla} \times \hat{\mathbf{E}}}{i\omega\mu_0} = \frac{\partial_y \hat{u}}{i\omega\mu_0} \mathbf{e}_y \times \mathbf{e}_z = -\frac{\beta(\omega)}{\omega\mu_0} \hat{u}(\omega, y) \mathbf{e}_x = \hat{h}(\omega, y) \mathbf{e}_x. \] (2.16)
The solutions in time domain are then given as wave packets by taking the inverse Fourier transform
\[ u(t, y) = \int_{\omega \in \mathbb{R}} \hat{u}(\omega, y) e^{-i\omega t} d\omega \] (2.17)
\[ h(t, y) = \int_{\omega \in \mathbb{R}} \hat{h}(\omega, y) e^{-i\omega t} d\omega. \] (2.18)

### 2.3 The wave center of the electric field

In order to define in a different (and hopefully more general) fashion the velocity of a propagating pulse, we consider the approach given in [13].
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Making an analogy with mechanics, where the center of gravity is defined as an expected value of the position with respect to the mass density, we define the wave center of the electric field as per:

\[ Y_E(t) = \frac{N_E(t)}{D_E(t)} \]  

(2.19)

where

\[ N_E = \int_{y \in \mathbb{R}} y |u(t, y)|^2 dy \]  

(2.20)

\[ D_E = \int_{y \in \mathbb{R}} |u(t, y)|^2 dy \]  

(2.21)

and \( |\cdot|^2 \) denotes the square complex modulus which coincides with the square of the function when this one is real-valued.

In order to see expression (2.19) in a more illuminating way, we are going first to work with the denominator \( D_E(t) \), in the following manner:

\[ D_E(t) = \int_{y \in \mathbb{R}} u(t, y) \overline{u}(t, y) dy, \]

\[ = \int_{y \in \mathbb{R}} u(t, y) \int_{\omega \in \mathbb{R}} \overline{u}(\omega, y)e^{i\omega t} d\omega dy, \]

\[ = \int_{y \in \mathbb{R}} \int_{\omega \in \mathbb{R}} u(t, y) \overline{u}(\omega, y)e^{i\omega t} d\omega dy. \]  

(2.22)

Notice that the last equation holds by assuming the validity of Fubini’s theorem [50]. Using the definition of \( \hat{u} \) given by Eq. (2.14) in Eq. (2.22) we have:

\[ D_E(t) = \int_{\omega \in \mathbb{R}} \int_{y \in \mathbb{R}} u(t, y) \overline{A}(\omega)e^{i\beta(\omega)y}e^{i\omega t} d\omega dy, \]

\[ = \int_{\omega \in \mathbb{R}} \overline{A}(\omega)e^{i\omega t} \int_{y \in \mathbb{R}} u(t, y)e^{i\beta(\omega)y} dy d\omega. \]  

(2.23)

It is apropos to define the integral:

\[ M_u(t, \omega) := \int_{y \in \mathbb{R}} u(t, y)e^{i\beta(\omega)y} dy \]  

(2.24)

Thus equation (2.23) can be written as:

\[ D_E(t) = \int_{\omega \in \mathbb{R}} \overline{A}(\omega)e^{i\omega t} M_u(t, \omega) d\omega. \]  

(2.25)
Considering now the numerator $N_E(t)$ in Eq. (2.20) we have, after an analogous procedure:

$$N_E(t) = \int_{\omega \in \mathbb{R}} \tilde{A}(\omega) e^{+i\omega t} \left[ \int_{y \in \mathbb{R}} y u(t, y) e^{+i\beta(\omega)y} dy \right] d\omega. \quad (2.26)$$

The integral in square brackets can be written in terms of $M_u$ by noticing:

$$\partial_\omega M_u(t, \omega) = i \partial_\omega \beta(\omega) \int_{y \in \mathbb{R}} y u(t, y) e^{+i\beta(\omega)y} dy. \quad (2.27)$$

This allows to have the following identity:

$$\int_{y \in \mathbb{R}} y u(t, y) e^{+i\beta(\omega)y} dy = -i \left[ \partial_\omega \beta(\omega) \right]^{-1} \partial_\omega M_u(t, \omega). \quad (2.28)$$

Therefore the numerator written in Eq. (2.26) can be seen as:

$$N_E(t) = -i \int_{\omega \in \mathbb{R}} \tilde{A}(\omega) e^{+i\omega t} \left[ \partial_\omega \beta(\omega) \right]^{-1} \partial_\omega M_u(t, \omega) d\omega. \quad (2.29)$$

Plugging equations (2.23) and (2.29) into Eq. (2.19) the position of the electric wave center reads:

$$Y_E(t) = \frac{-i \int_{\omega \in \mathbb{R}} \tilde{A}(\omega) e^{+i\omega t} \left[ \partial_\omega \beta(\omega) \right]^{-1} \partial_\omega M_u(t, \omega) d\omega}{\int_{\omega \in \mathbb{R}} \tilde{A}(\omega) e^{+i\omega t} M_u(t, \omega) d\omega}. \quad (2.30)$$

This result is equivalent to the one obtained by Petit in [13] but contrary to his approach it is not necessary to define a new Fourier transform from $y \rightarrow \beta$ but rather to just assume the validity of Fubini’s theorem. Moreover from this expression, it is easy to see that this new representation of $Y_E(t)$ depends on two facts: 1) The existence of integral $M_u(t, \omega)$ and 2) the derivative of $\beta$ with respect to $\omega$ must be different of zero. The first issue can be tackled by using again Fubini’s theorem and the definition of $u$ in Eq. (2.17). Then Eq. (2.24) reads:

$$M_u(t, \omega) := \int_{\sigma \in \mathbb{R}} \tilde{A}(\sigma) e^{-i\sigma t} \int_{y \in \mathbb{R}} e^{i(\beta(\omega) - \beta(\sigma))y} dy d\sigma. \quad (2.31)$$

Due to the fact that $\beta$ was defined as a real-valued function the integral in $y$ can be computed as [51]:

$$\int_{y \in \mathbb{R}} e^{i(\beta(\omega) - \beta(\sigma))y} dy = 2\pi \delta(\beta(\omega) - \beta(\sigma)), \quad (2.32)$$
It is very important to remark here the role that plays to take the integral in the whole real line. Notice that if this integral was taken, for instance, in a semi infinite plane (diopter case) or in a slab, the result would be different from a $\delta$ distribution. This underlines the importance of the spatial domain in which propagates the electromagnetic pulse. Plugging Eq. (2.32) into Eq. (2.31) one arrives to the expression:

$$M_u(t, \omega) := 2\pi \int_{\sigma \in \mathbb{R}} \hat{A}(\sigma)e^{-i\omega t}\delta(\omega - \beta(\sigma))d\sigma.$$  (2.33)

This formula reveals something very important: The existence of $M_u(t, \omega)$ and the fact that $\partial_\omega \beta \neq 0$ are two ways of seeing the fact that the real-valued function $\beta$ must be invertible. As the reader may remember this is the same requirement that is implicitly asked for the group velocity. In the next lines we are going to explore physical situations which satisfy this requirement.

**Electric wave center in transparent media**

As we know, when dealing with transparent media the wave number $\beta$ is simply given by $\beta = \frac{\omega}{c}n$ where $n$ is the so called optical index [14, 20, 2] and for the case of transparent materials is a constant number. From the mathematical point of view, it is easy to see that this correspondence rule between $\omega$ and $\beta$ is invertible for all $\omega$. This implies:

$$M^T_u(t, \omega) = 2\pi \int_{\omega \in \mathbb{R}} \hat{A}(\omega)e^{-i\omega t}\delta\left(\omega - \frac{\omega}{c}n\right)d\omega,$$

$$= 2\pi \frac{c}{n} \int_{\eta \in \mathbb{R}} \hat{A}(\omega - \frac{c}{n}\eta)e^{-i(\omega - \frac{\omega}{c}n)t}\delta(\eta)d\eta,$$

$$= 2\pi \frac{c}{n} \hat{A}(\omega)e^{-i\omega t}.$$  (2.34)

where the superscript $T$ stands for transparent. Plugging this result into equations (2.23) and (2.29) the denominator and numerator functions are:

$$D^T_E(t) = \frac{c}{n}2\pi \int_{\omega \in \mathbb{R}} |\hat{A}(\omega)|^2d\omega,$$  (2.35)

$$N^T_E(t) = -\frac{c}{n}2\pi \int_{\omega \in \mathbb{R}} \hat{A}(\omega)e^{i\omega t}[\partial_\omega \beta(\omega)]^{-1}\partial_\omega(\hat{A}(\omega)e^{-i\omega t})d\omega.$$  (2.36)

After taking the derivative of $M_u(t, \omega)$ with respect to $\omega$ and some algebra we get that the electric wave center obeys an affine law of the form

$$Y^T_E(t) = Y^T_E + tV^T_E,$$  (2.37)
with

\[
\mathcal{V}_E^T = -\frac{i}{n} \frac{\int_{\omega \in \mathbb{R}} \hat{A}(\omega) \partial_\omega \hat{A}(\omega) d\omega}{\int_{\omega \in \mathbb{R}} |\hat{A}(\omega)|^2 d\omega},
\]

\[
\mathcal{V}_E^T = -\frac{c}{n'},
\]

(2.38)

(2.39)

where we have used the fact that \([\partial_\omega \beta(\omega)]^{-1} = \frac{c}{n}\). This result coincides with the usual textbook results for the group velocity as in [12, 14]. It is also important to say that \(D_E^T(t)\) is a constant in time.

**Electric wave center in gentle media**

So far, we have seen how the position of the electric wave center obeys an affine law when dealing with transparent media. In this paragraph we are going to show a similar result but just considering \(\beta\) as an even real-valued function. For this purpose we need to assume that \(\beta\) is invertible within the support of \(\hat{A}\). Under this hypothesis we have:

\[
M^G_u(t, \omega) = 2\pi \int_{\sigma \in \mathbb{R}} \hat{A}(\sigma) e^{-i\sigma t} \delta(\beta(\omega) - \beta(\sigma)) d\sigma,
\]

\[
= -2\pi \int_{\Omega} [\partial_\sigma \beta(\sigma)]^{-1} \hat{A}(\sigma) e^{-i\sigma t} \delta(\eta) d\eta,
\]

where the superscript \(G\) stands for gentle and \(\sigma\) is just a shorthand notation for \(\sigma(\eta) := \beta^{-1}(\beta(\omega) - \eta)\). Then:

\[
M^G_u(t, \omega) = -2\pi [\partial_\omega \beta(\omega)]^{-1} \hat{A}(\omega) e^{-i\omega t}.
\]

(2.40)

Upon substitution of Eq. (2.40) into equations (2.23) and (2.29) which can be seen as:

\[
D^G_E(t) = -2\pi \int_{\omega \in \mathbb{R}} |\hat{A}(\omega)|^2 [\partial_\omega \beta(\omega)]^{-1} d\omega.
\]

(2.41)

\[
N^G_E(t) = 2\pi i \int_{\omega \in \mathbb{R}} \hat{A}(\omega) e^{+i\omega t} [\partial_\omega \beta(\omega)]^{-1} \partial_\omega ([\partial_\omega \beta(\omega)]^{-1} \hat{A}(\omega) e^{-i\omega t}) d\omega.
\]

(2.42)
Taking the ratio as in Eq. (2.19) we notice that \( Y_E^G \) follows also an affine law \( Y_E^G(t) = Y_E^G + tV_E^G \) with

\[
Y_E^G = \frac{-i \int_{\omega \in \mathbb{R}} \hat{A}(\omega)[\partial_\omega \beta(\omega)]^{-1}\partial_\omega (\hat{A}(\omega))d\omega}{\int_{\omega \in \mathbb{R}} |\hat{A}(\omega)|^2[\partial_\omega \beta(\omega)]^{-1}d\omega},
\]

(2.43)

\[
V_E^G = -\int_{\omega \in \mathbb{R}} |\hat{A}(\omega)|^2[\partial_\omega \beta(\omega)]^{-2}d\omega
\]

\[
\int_{\omega \in \mathbb{R}} |\hat{A}(\omega)|^2[\partial_\omega \beta(\omega)]^{-1}d\omega.
\]

(2.44)

If now we make the assumption, as in [13], that \( \beta \) does not vary too much (i.e. can be approximated by a constant) with respect to the frequencies within the support of \( \hat{A} \), which more or less resembles to the assumption of evaluating \( \partial_\beta \omega \) in \( k_0 \), we get that the wave center velocity is then given by:

\[
Y_E^G = -[\partial_\omega \beta]^{-1} = -\partial_\beta \omega,
\]

(2.45)

where the last equality comes from the Inverse function theorem [50]. And thus we have recovered the group velocity result as a particular case of the centrovelocity.

### 2.4 The wave center of the magnetic field

Up to this point we have found a new way to see the propagation velocity of the electric field. It is then natural to ask ourselves about the propagation velocity associated to the magnetic field \( \mathbf{H} \). In the same fashion as for the electric field we consider a wave center given by:

\[
Y_H(t) = \frac{N_H(t)}{D_H(t)},
\]

(2.46)

where

\[
N_H = \int_{y \in \mathbb{R}} |h(t,y)|^2dy,
\]

(2.47)

\[
D_H = \int_{y \in \mathbb{R}} |h(t,y)|^2dy.
\]

(2.48)

*Mutatis mutandis* we get that the denominator can be written as:

\[
D_H(t) = \int_{\omega \in \mathbb{R}} \left( -\frac{\beta(\omega)}{\omega \mu_0} \right) \hat{A}(\omega)e^{+i\omega t}M_h(t,\omega)d\omega.
\]

(2.49)
and correspondingly the numerator is:

\[ N_H(t) = -i \int_{\omega \in \mathbb{R}} \left( \frac{-\beta(\omega)}{\omega \mu_0} \right) \overline{A}(\omega)e^{+i\omega t}[\partial_{\omega}\beta(\omega)]^{-1}\partial_{\omega}M_h(t, \omega)d\omega, \quad (2.50) \]

where \( M_h(t, \omega) \) is defined as:

\[ M_h(t, \omega) := 2\pi \int_{\sigma \in \mathbb{R}} \left( \frac{-\beta(\sigma)}{\sigma \mu_0} \right) \hat{A}(\sigma)e^{-i\sigma t}\delta(\beta(\omega) - \beta(\sigma))d\sigma. \quad (2.51) \]

Thus the magnetic wave center is given by:

\[ Y_H(t) = -i \int_{\omega \in \mathbb{R}} \left( \frac{-\beta(\omega)}{\omega \mu_0} \right) \overline{A}(\omega)e^{+i\omega t}[\partial_{\omega}\beta(\omega)]^{-1}\partial_{\omega}M_h(t, \omega)d\omega \int_{\omega \in \mathbb{R}} \left( \frac{-\beta(\omega)}{\omega \mu_0} \right) \overline{A}(\omega)e^{+i\omega t}M_h(t, \omega)d\omega. \quad (2.52) \]

**Magnetic wave center in transparent media**

As we saw before, for the case when wave number is \( \beta = \frac{\omega}{c}n \) where \( n \) is a constant, the integral in Eq. (2.51) is given by:

\[ M^T_h(t, \omega) = 2\pi \frac{c}{n} \hat{A}(\omega)e^{-i\omega t}\left( \frac{-\beta(\omega)}{\omega \mu_0} \right), \quad (2.53) \]

where again the \( T \) means transparent. Plugging this result into equations (2.49) and (2.50) the denominator and numerator functions are:

\[ D^T_H(t) = \frac{c}{n}2\pi \frac{n}{\omega \mu_0^2} \int_{\omega \in \mathbb{R}} \left( \frac{\beta(\omega)}{\omega \mu_0} \right)^2 |\hat{A}(\omega)|^2d\omega, \quad (2.54) \]

and

\[ N^T_H(t) = -i \frac{c}{n}2\pi \int_{\omega \in \mathbb{R}} \left( \frac{-\beta}{\omega \mu_0} \right) \overline{Ae^{+i\omega t}[\partial_{\omega}\beta]}^{-1}\partial_{\omega} \left[ \hat{A}e^{-i\omega t}\left( \frac{-\beta}{\omega \mu_0} \right) \right] d\omega. \]

\[ = -i \frac{n}{\omega \mu_0^2}2\pi \int_{\omega \in \mathbb{R}} \overline{Ae^{+i\omega t}[\partial_{\omega}\beta]}^{-1}\partial_{\omega} \left( \hat{A}e^{-i\omega t} \right) d\omega. \quad (2.55) \]

Here, it has been used the fact that \( \frac{\beta}{\omega \mu_0} = \frac{n}{\omega \mu_0} \). Looking at this results it is immediate to see that \( D^T_H(t) \) (resp. \( N^T_H(t) \)) is equal, up to a multiplicative constant, to \( D^E_H(t) \) (resp. \( N^E_H(t) \)) in equation (2.35) (resp. (2.36)). Therefore, when taking the ratio of the position of Eq. (2.55) over Eq. (2.54), the position of the wave center for the magnetic field that propagates in transparent media is the same as for case of the electric field.
Magnetic wave center in gentle media

By using the same arguments for the invertibility of $\beta$ when dealing with the electric field, we have that the magnetic counterpart of Eq. (2.40) is expressed by the integral $M^G_t(t, \omega)$ (naturally, the $G$ stands one more time for gentle) which reads:

$$M^G_t(t, \omega) = -2\pi [\partial_\omega \beta]^{-1} \hat{A} e^{-i\omega t} \left( \frac{-\beta}{\omega \mu_0} \right).$$

(2.56)

Here and for the sequel we have omitted the $\omega$ dependence of $\hat{A}$ and $\beta$. Consequently, the functions $D^G_H(t)$ and $N^G_H(t)$ can be written as:

$$D^G_H(t) = -2\pi \int_{\omega \in \mathbb{R}} \left( \frac{-\beta}{\omega \mu_0} \right) |\hat{A}|^2 [\partial_\omega \beta]^{-1} d\omega,$$

(2.57)

$$N^G_H(t) = 2\pi i \int_{\omega \in \mathbb{R}} \hat{A} e^{i\omega t} [\partial_\omega \beta]^{-1} \partial_\omega \left[ \left( \frac{-\beta}{\omega \mu_0} \right) [\partial_\omega \beta]^{-1} \hat{A} e^{-i\omega t} \right] d\omega.$$  

(2.58)

Notice that in this case $\frac{\beta(\omega)}{\omega \mu_0} = \frac{n(\omega)}{c \mu_0}$, and contrary to the case of transparent media, $D^G_H(t)$ (resp. $N^G_H(t)$) is not proportional to $D^G_E(t)$ (resp. $N^G_E(t)$) in equation (2.41) (resp. (2.42)). This reflects the physical fact that for the case of transparent materials there is no dispersion whereas for the case of gentle materials the dispersion, albeit mild, exists. Nevertheless, the position of the magnetic wave center does obey an affine law:

$$Y^G_H(t) = Y^G_H + t V^G_H$$

(2.59)

where:

$$Y^G_H = -i \int_{\omega \in \mathbb{R}} \hat{A} [\partial_\omega \beta]^{-1} \partial_\omega \left[ \left( \frac{-\beta}{\omega \mu_0} \right) [\partial_\omega \beta]^{-1} \hat{A} \right] d\omega,$$

(2.60)

$$V^G_H = - \int_{\omega \in \mathbb{R}} \left( \frac{-\beta}{\omega \mu_0} \right) |\hat{A}|^2 [\partial_\omega \beta]^{-2} d\omega,$$

(2.61)

$$\frac{1}{\int_{\omega \in \mathbb{R}} \left( \frac{-\beta}{\omega \mu_0} \right) |\hat{A}|^2 [\partial_\omega \beta]^{-1} d\omega}.$$  

Notice that in principle the centrovelocity for the magnetic field is not the same for the electric one. However, after considering the same assumption that the one made for the electric field (that is $\beta$ does not vary too much with respect to $\omega$) we get again the same result as for the group velocity:

$$V^0_H = -[\partial_\omega \beta]^{-1} = -\partial_\beta \omega.$$  

(2.62)
2.5 Partial conclusion

In this chapter we studied the propagation of an EM pulse in transparent and in gentle material. This was made by considering the equations that describe the motion of the wave centers for the electric and magnetic fields. The result was that without exception of the field (electric or magnetic) and the medium in which they propagate, the equations of motion are always given by an affine law. Even more, under the extra assumption that the wave number does not change too much with respect to the frequency we were able to recover the group velocity definition as a particular case. Finally, two fundamental and underlying ideas deserve special attention: 1) The fact that the centrovelocity definition depends on the domain within the pulse propagates and 2) The centrovelocity of the magnetic wave center is in principle not the same as for the electric one when dealing with gentle materials. This second point makes think that the answer is in the fundamental definition of what is energy for a pulse that propagates in a medium. We will explore these ideas in the next chapter.
Chapter 3

Energy balance and velocities of an electromagnetic pulse in highly dispersive media

But not at the same rate. The dirt went first, cleanly separated from the roots. Then all the vegetable matter slid down, leaving only the grubs and the earthworm on the face of the barrier. At last they, too, slid down. This barrier is able to sort out what strikes it, thought Nafai.
—Orson Scott Card, The ships of Earth

3.1 Introduction

The study of the propagation of electromagnetic fields (such as optical pulses) through dielectric media, possibly exhibiting both dispersion and absorption, goes back to the early 1900’s papers by Sommerfeld and Brillouin [1]. A significant contribution to the study of this phenomenon has been done by Oughston [9, 10, 11], by using complex and asymptotic analysis techniques. Nevertheless some well established concepts in the case of non dispersive media need to be revisited.

In a non dispersive medium, an arbitrary pulse would propagate unaltered. In a frequency dispersive material, however, the pulse is modified as it propagates. Mathematically, a medium is called dispersive if the dielectric constant is a function of the frequencies of the field. In an absorbing material, the dielectric constant is a complex valued function and the traveling pulse will be attenuated as it travels with or without distortion [2]. In the case of the dielectric constant given as a complex valued rational function,
[2, 11, 52], it can be made a distinction between the gentle dispersive materials, which are those with poles far from the real axis, and highly dispersive materials whose poles are close to the real axis.

For the sake of simplicity in this chapter the case of a linearly polarized electric field with a central wavelength in the infra-red range is considered. This wave illuminates normally a slab embedded in vacuum. The homogeneous slab is considered as a non magnetic temporally dispersive absorbing material. The solution obtained will address to the analysis of two fundamental concepts in wave propagation: The very definition of energy for a leaky dispersive material and the propagation velocity of an electromagnetic wave in this kind of material. The study of a dispersive slab presents many advantages: i) It is more realistic in the sense that a semi-infinite dispersive medium does not exist. ii) The outgoing wave conditions are well defined for vacuum [53, 54] iii) In principle, it is possible to establish an energy balance capturing the whole phenomenon.

The problem of defining the energy for a propagating pulse in a dispersive material was already acknowledged by Brillouin in 1932 who wrote Since ε depends on frequency, it becomes very difficult to define an electrical energy. Even if the electric field is known at an instant t, still, the energy stored is completely unknown [1]. An adequate definition, in the frame of classical electrodynamics, of the energy density considering the field-medium system has been given in [9, 55] which is a particular case of a more general definition given by Nicolet et al. [15] by using the formalism of differential geometry and more general constitutive relations than temporal dispersion.

Regarding the velocity of light, for non dispersive materials it is possible to use the group velocity [14, 2]. The usual way to obtain such expression is by considering a Taylor’s expansion about the carrier frequency and then truncating up to first order [56, 57]. It can be thought that the more terms are added to the Taylor’s expansion the better the accuracy of the approximation to the velocity of light. Unfortunately, this is not the case as it is shown in [56]. Smith in his paper of 1970 [8] makes a review of the different theoretical concepts of light velocity. In this work he recognizes the mathematical nature of the group velocity which does not necessarily describe the velocity of any signal, mass, particle or energy; being this particularly
clear in the case of anomalous dispersion [14]. Ware et al [57] give a different context to the group velocity as a particular case of a group delay function that considers also a Taylor expansion and deals only with the real part of the wave number [57]. The question that arises naturally is: What happens with the imaginary part of the wave number? According to Oughstun in [58]: *The physical meaning of a complex-valued velocity remains to be given.* Anderson et al [59] make also a review on the different concepts of the velocity of light and via a recursive method propose a temporal pulse velocity as the velocity of propagation of the temporal maximum of the envelope function at a given distance. However as it was noticed in the case of signal velocity the maximum position can be shifted forward and backwards in the case of highly dispersive materials. In this same paper Smith proposes the so called centrovelocity defined as:

\[
v_c(r) = \left[ \nabla \left( \frac{\int_{t \in \mathbb{R}} t |E(r, t)|^2 dt}{\int_{t \in \mathbb{R}} |E(r, t)|^2 dt} \right) \right]^{-1} \tag{3.1}
\]

However, this definition is not suitable for our purposes because it only deals with the amplitude of the electric field and implicitly considers the equipartition of energy between the electric and magnetic fields. Bolda et al. [60] and Loudon [61] also proposed definitions of wave velocity by energy consideration. Nevertheless these definitions are made in the harmonic regime and are highly dependent of the particular model chosen for the permittivity. A modified version of the Smith’s centrovelocity was proposed by Peatross et al. [62]. This approach takes into account the energy propagation direction given by the Poynting vector and describes the expected arrival time at a certain position \( r \). Despite these advantages, this definition (as in the case of Eq. (3.1)) is made for a single propagation direction.

In this chapter will be used the approach given by Van Groesen and Maniardi [16] that uses a centrovelocity obtained by considering an energy density from a continuity equation. This point of view is a generalization of the definition given e.g. by Petit [13] for the centrovelocity. This definition is quite easy to evaluate numerically and some clarifying numerical results will be provided.
3.2 Mathematical Formulation

In this section we provide the standard derivation of an electromagnetic pulse that lights a dispersive slab. Notations for the rest of the chapter are introduced and all the physical considerations are established. Particularly important, is the discussion about the wave number (and consequently the optical index) when dealing with highly dispersive materials.

Preliminary settings

Starting by setting the spatial domain let \( l \) and \( L \) be two real number such that \( l > L \). Then, three spatial domains are defined: The slab \( U_{II} = \{(x,y,z) | L < y < l\} \), the superstratum \( U_{I} = \{(x,y,z) | y > l\} \) and the substratum \( U_{III} = \{(x,y,z) | y < L\} \). Let \( E_\xi(r,t) = E(r,t)|_\xi \) be the restrictions of the electric field to each sub-domain \( U_\xi \) where \( \xi = \{I, II, III\} \). A schematic version of this setup is shown in Figure 3.1.

![Figure 3.1. Setup of a slab of frequency dispersive material embedded in vacuum.](image-url)
Keeping in mind that this work is made in the framework of classical electrodynamics, Maxwell’s equations in source free regions provide the adequate way to describe the electromagnetic fields:

\[
\nabla \times E = -\frac{\partial B}{\partial t}, \quad (3.2)
\]

\[
\nabla \times H = \frac{\partial D}{\partial t}, \quad (3.3)
\]

\[
\nabla \cdot D = 0, \quad (3.4)
\]

\[
\nabla \cdot B = 0, \quad (3.5)
\]

with the boundary conditions given by taking these equations in the sense of distributions [42]. The constitutive relations for the substratum and superstratum, which in this case are considered as vacuum, are simply given by

\[
H_\psi = \frac{1}{\mu_0} B_\psi, \quad D_\psi = \epsilon_0 E_\psi, \quad \psi = \{I, III\}. \quad (3.6)
\]

Whereas the constitutive relations for the slab are [13] [2]

\[
H_{II} = \frac{1}{\mu_0} B_{II}, \quad (3.7) \quad D_{II} = \epsilon_0 E_{II} + P_e, \quad (3.8)
\]

with

\[
P_e(r, t) = \frac{\epsilon_0}{2\pi} \int_{-\infty}^{+\infty} \chi(\tau) E(r, t-\tau)d\tau. \quad (3.9)
\]

The negligible magnetization of the material is expressed in Eq. (3.7). On the other hand Eq. (3.8) states that the electrical displacement \( D \) is influenced not just by the electric field \( E \) but also by the electric polarization of the material given by vector \( P_e \). Finally the causal nature of this polarization is shown in Eq. (3.9) and has been explained in the previous chapter. It is important to remember that the susceptibility of the material \( \chi \) has positive support [9] and in particular for the case of non dispersive materials \( \chi(t) = 2\pi\epsilon_c\delta(t) \), where \( \epsilon_c \) is a real number.

In order to study the behavior of the electromagnetic pulse in terms of the angular frequency \( \omega \), Fourier Transform convention employed is the same as given in Appendix A:
\[ \nabla \times \hat{E} = +i\omega \hat{B}, \quad (3.10) \quad \nabla \times \hat{H} = -i\omega \hat{D}, \quad (3.11) \]

\[ \nabla \cdot \hat{D} = 0, \quad (3.12) \quad \nabla \cdot \hat{B} = 0, \quad (3.13) \]

with the transformed constitutive relations:

\[ \hat{H}_\xi = \frac{1}{\mu_0} \hat{B}_\xi, \quad \hat{D}_\xi = \varepsilon_0 \hat{e}_{r\xi}(\omega) \hat{E}_\xi, \quad \xi = \{I, II, III\}, \quad (3.14) \]

and depending on the region, the permittivity is:

\[ \hat{e}_{r\xi}(\omega) = \begin{cases} 1 & \text{if } \xi = \{I, III\}, \\ 1 + \hat{\chi}_c(\omega) & \text{if } \xi = II. \end{cases} \quad (3.15) \]

Notice that due to its reality, \( \hat{e}_{r\xi}(\omega) \) presents Hermitian symmetry (i.e. \( \hat{e}_{r\xi}(-\omega) = \hat{e}_{r\xi}(\omega) \)). Even more, for non dispersive materials the permittivity is a constant and represents the same response of material for any frequency, whereas for gentle dispersive materials \( \hat{e}_{r\xi}(\omega) \) is a real-valued function [13] and models dispersive non-lossy materials. Finally for dispersive materials the transformed permittivity is a complex-valued function. These properties will be studied with more detail later in the text.

Taking the curl of Faraday’s law in frequency domain and after some elementary substitutions it is obtained the vectorial Helmholtz equation for the electric field

\[ \nabla^2 \hat{E}_\xi = -\frac{\omega^2}{c^2} \hat{e}_{r\xi} \hat{E}_\xi, \quad \xi = \{I, II, III\}. \quad (3.16) \]

Once the electric field is given, the magnetic field can be calculated as:

\[ \hat{H}_\xi = \frac{1}{i\omega \mu_0} \nabla \times \hat{E}_\xi, \quad \xi = \{I, II, III\}. \quad (3.17) \]

**Solution of the problem**

In this section we focus our attention on an electric field which is linearly polarized along the z-axis and propagates along the y-direction (this implies...
normal incidence). In that case, the electric field writes:

$$\vec{E}_\xi = \hat{u}_\xi(y, \omega) \hat{e}_z, \quad \xi = \{I, \text{II}, \text{III}\}. \quad (3.18)$$

And as a consequence, the magnetic field expressed in Eq. (3.17) takes the form

$$\vec{H}_\xi = \hat{h}_\xi(y, \omega) \hat{e}_x, \quad \xi = \{I, \text{II}, \text{III}\},$$

with

$$\hat{h}_\xi(y, \omega) = \frac{1}{i\mu_0 \omega} \frac{\partial \hat{u}_\xi}{\partial y}, \quad \xi = \{I, \text{II}, \text{III}\}. \quad (3.19)$$

Upon substitution of Eq. (3.18) into Eq. (3.16) the vectorial Helmholtz equation is reduced to a second order ordinary differential equation

$$\frac{d^2 \hat{u}_\xi}{dy^2} = -\beta^2_\xi \hat{u}_\xi, \quad \xi = \{I, \text{II}, \text{III}\}, \quad (3.20)$$

with

$$\beta^2_\xi(\omega) = \frac{\omega^2_c}{\varepsilon_\xi(\omega)}, \quad \xi = \{I, \text{II}, \text{III}\}. \quad (3.21)$$

From this equation it is quite clear that the wave number $\beta_\xi(\omega)$ is the square root of $\omega^2_c \varepsilon_\xi(\omega)$. What it is not so clear is the meaning of square root. For instance, in references [63, 61, 53, 58, 62, 11], the wave number is defined as:

$$\beta_\xi(\omega) = \frac{\omega}{c n_\xi(\omega)}, \quad n_\xi(\omega) = \sqrt{\varepsilon_\xi(\omega)} \quad (3.22)$$

where $n_\xi(\omega)$ is the so called refractive (or optical) index. Albeit this concept is well established for the case of monochromatic light and non dispersive materials, it is necessary a more detailed study of what does the symbol $\sqrt{}$ means when the permittivity is a complex-valued function. Thinking about the square root as an inverse function, the first requisite is to define its domain. Keeping in mind that the solutions in time are real, the solutions in the frequency domain must show Hermitian symmetry:

$$\hat{u}_\xi(y, -\omega) = \bar{\hat{u}}_\xi(y, \omega). \quad (3.23)$$

One of the consequences of Eq. (3.23) is that $\beta_\xi(\omega)$ is anti hermitian i.e.

$$\beta_\xi(-\omega) = -\overline{\beta_\xi(\omega)}. \quad (3.24)$$
Therefore it is enough to find the square root of $\beta^2(\omega)$ either for $\omega \geq 0$ or $\omega \leq 0$ and then use Eq. (3.24). Given the fact that we are (in general) dealing with lossy materials we must require $\Im\{\beta(\omega)\}$ to have a defined sign, that is $\Im\{\beta(\omega)\} \leq 0$ or $\Im\{\beta(\omega)\} \geq 0$. In this chapter, the convention employed will be the latter one. Remembering that the sine function is non-negative when its argument lies in the interval $[0, \pi]$, the most natural way to choose the parameters of our specified complex logarithm, defined on Appendix C, is $\sigma = +$ and $\theta = \pi$. Then, following all these conventions one gets the wave number as per:

$$\beta(\omega) := \exp\left(\frac{1}{2} \log^+ \left[\frac{\omega^2}{c^2} \hat{\epsilon}_r(\omega)\right]\right), \quad \xi = \{I, II, III\}, \quad \omega \geq 0. \quad (3.25)$$

Regarding the refractive index, it is important to remember that in general $\log^+(ab) \neq \log^+(a) + \log^+(b)$ with $a, b \in \mathbb{C}$. This is because not always $\arg^+ (ab) = \arg^+ (a) + \arg^+ (b)$ due to the branch cut discontinuity [64, 65]. However, in this particular case of the wave number, $\arg^+(\frac{\omega^2}{c^2} \hat{\epsilon}_r(\omega)) = \arg^+(\hat{\epsilon}_r(\omega))$ for $\omega \geq 0$. This allows to redefine the refractive index as:

$$n(\omega) := \exp\left(\frac{1}{2} \log^+ \left[\hat{\epsilon}_r(\omega)\right]\right), \quad \xi = \{I, II, III\}, \quad \omega \geq 0. \quad (3.26)$$

It is worthy to remark that in order to preserve the anti hermitian symmetry of $\beta(\omega)$ the refractive index must be extended to negative frequencies in a Hermitian way, that is $n(\omega) = \pi(\omega)$ for $\omega \geq 0$.

Once $\beta(\omega)$ is well defined, the solution of (3.20) for each $U_\xi, \xi = \{I, II, III\}$ has the form:

$$\hat{u}_\xi = \hat{A}^+_\xi(\omega)e^{i\beta(\omega)} + \hat{A}^-_{\xi}(\omega)e^{-i\beta(\omega)}. \quad (3.27)$$

Here the Fresnel coefficients denoted by $\hat{A}^\phi_{\xi}(\omega)$ with $\xi = \{I, II, III\}$ and $\phi = \{+, -\}$ must be determined. Due to the Fourier transform convention (See Appendix A), the amplitude of the incident field is expressed by $\hat{A}^+_\xi(\omega)$. This amplitude represents the Fourier transform of a finite energy time dependent function $A(t)$ i.e. a square integrable function defined on the whole $\mathbb{R}$ and that decays, together with their derivatives, sufficiently fast at infinity [16]. By considering the outgoing wave condition (or Sommerfeld radiation condition) [53, 54, 13, 66] we set $\hat{A}^+_{III}(\omega) = 0$ and finally
by solving an algebraic system of equations given by the interface conditions [14, 13] the Fresnel coefficients are:

\[ \hat{A}^+_I(\omega) = \frac{1}{4aD} \left[ \frac{b}{d} (1 + p)(1 - q) + \frac{d}{b} (1 + q)(1 - p) \right] \hat{A}^-_I(\omega), \]  
(3.28)

\[ \hat{A}^+_{II}(\omega) = \frac{1}{2dD} (1 - q) \hat{A}^-_I(\omega), \]  
(3.29)

\[ \hat{A}^-_{II}(\omega) = \frac{d}{2D} (1 + q) \hat{A}^-_I(\omega), \]  
(3.30)

\[ \hat{A}^-_{III}(\omega) = \frac{f}{D} \hat{A}^-_I(\omega), \]  
(3.31)

where:

\[ D = \frac{a}{4} \left[ \frac{b}{d} (1 - p)(1 - q) + \frac{d}{b} (1 + p)(1 + q) \right], \]  
(3.32)

with:

\[ p = \frac{\beta_{II}(\omega)}{\beta_I(\omega)}, \quad q = \frac{\beta_{III}(\omega)}{\beta_{II}(\omega)}, \]  
(3.33)

and \( a = e^{i\beta_I}, b = e^{i\beta_{II}}, d = e^{i\beta_{III}}, f = e^{i\beta_{III}}. \)

The solutions in time domain can be retrieved as wave packets by taking the Inverse Fourier Transform defined in Eq. (A.2). Before going to the next section, we will show some results that are going to be needed later. By introducing the notation:

\[ \hat{u}^+_{\xi} = \hat{A}^+_{\xi}(\omega)e^{i\beta_{\xi}(\omega)y}, \quad \hat{u}^-_{\xi} = \hat{A}^-_{\xi}(\omega)e^{-i\beta_{\xi}(\omega)y}, \]  
(3.34)

equations (3.27) and (3.19) can be expressed, after some elementary manipulations, as:

\[ \hat{u}^+_{\xi} = \hat{u}^+_{\xi} + \hat{u}^-_{\xi}, \quad \hat{h}^+_{\xi} = \frac{n_{\xi}(\omega)}{\mu_0c} (\hat{u}^+_{\xi} - \hat{u}^-_{\xi}), \quad \xi = \{I, II, III\}, \]  
(3.35)

where according to our convention the minus sign denotes propagation in the direction of the incident field and the plus sign is to the opposite one. Notice that in the particular case of the substratum and superstratum \( n_{\psi}(\omega) \) \( \psi = \{I, III\} \). Then the electric and magnetic fields can be written as:

\[ E_\psi = E^+_{\psi} + E^-_{\psi}, \quad H_\psi = H^+_{\psi} + H^-_{\psi}, \]  
(3.36)

where

\[ H^+_{\psi} = \frac{1}{\mu_0c} E^+_{\psi}, \quad H^-_{\psi} = -\frac{1}{\mu_0c} E^-_{\psi}. \]  
(3.37)
CHAPTER 3. ENERGY AND VELOCITY OF AN EM PULSE

3.3 Energy Considerations

Energy Densities

This section strives to follow the spirit of what Richard Feynman said on the Volume I of his Lectures on Physics [67] concerning energy and its conservation: There is a fact, or if you wish, a law, governing all natural phenomena that are known to date. There is no known exception to this law—it is exact so far as we know. The law is called the conservation of energy. It states that there is a certain quantity, which we call energy, that does not change in the manifold changes which nature undergoes.(...)It is important to realize that in physics today, we have no knowledge of what energy is. We do not have a picture that energy comes in little blobs of a definite amount. It is not that way. However, there are formulas for calculating some numerical quantity, and when we add it all together it gives “28”—always the same number.

From this point of view and restricting our analysis to the framework of Classical Electrodynamics, the Poynting vector identity [2, 15, 61, 68, 20, 55] provides the starting point

\[ \nabla \cdot \mathbf{S} = \nabla \cdot (\mathbf{E} \times \mathbf{H}) = -\frac{\partial \mathbf{B}}{\partial t} \cdot \mathbf{H} - \frac{\partial \mathbf{D}}{\partial t} \cdot \mathbf{E}. \quad (3.38) \]

Using the differential geometry formalism Nicolet et al. [15] give a general approach for obtaining an electromagnetic energy density \( W \) by considering the very general equality:

\[ \frac{\partial W}{\partial t} = \frac{\partial \mathbf{B}}{\partial t} \cdot \mathbf{H} + \frac{\partial \mathbf{D}}{\partial t} \cdot \mathbf{E}. \quad (3.39) \]

This approach (like the Maxwell’s equations) does not involve explicitly any metric concept and is completely independent of any material relation (which is expressed in the constitutive relations) [15]. For the case of dispersive materials (in which the Hodge star operator that relates \( \mathbf{E} \) and \( \mathbf{D} \) is simply a convolution), this same equality can be found e.g. in [9, 68, 55, 69]. Then, plugging Eq. (3.39) into Eq. (3.38) the continuity equation for the electromagnetic pulse-slab system is:

\[ \nabla \cdot \mathbf{S} + \frac{\partial W}{\partial t} = 0, \quad (3.40) \]
Taking the integral with respect to a certain volume \( U \) and after applying the divergence theorem we get:

\[
\int_{\partial U} \mathbf{S} \cdot \mathbf{n} dA = - \int_{U} \frac{\partial W}{\partial t} dV, \tag{3.41}
\]

The term on the left hand side of Eq. (3.41) can be interpreted as the flow of electromagnetic energy through the boundary of the volume \( U \), that is the loss due to the propagation of the wave. Whereas the term on the right hand side is the total decrease of energy density–ohmic losses (Joule effect) within the volume \( U \) [55, 13].

In order to have a better insight of the energy density change, the constitutive relations for the different sub-domains must be considered. Plugging Eqs. (3.6), (3.7), and (3.8) into Eq. (3.39) the energy densities take the form:

\[
W_\psi = \frac{\mu_0}{2} |\mathbf{H}_\psi|^2 + \frac{\epsilon_0}{2} |\mathbf{E}_\psi|^2, \quad \psi = \{I, III\}, \tag{3.42}
\]

\[
W_{II} = \frac{\mu_0}{2} |\mathbf{H}_{II}|^2 + \frac{\epsilon_0}{2} |\mathbf{E}_{II}|^2 + \int_{-\infty}^{t} \mathbf{E}_{II} \cdot \frac{\partial \mathbf{P}_e}{\partial t'} dt'. \tag{3.43}
\]

Equation (3.42) and the first two terms of Eq. (3.43) can be read as the energy density associated to the propagating fields [9, 13, 70]. On the other hand, about the integral term in Eq. (3.43) it has to be said that this formulation only holds when the electric field vanishes as \( t \) goes to minus infinity [9]. Regarding the way in which this term must be interpreted different approaches has been proposed: Webb and Shivanand [68] consider the real and imaginary parts of the Fourier representation of the polarization vector \( \mathbf{P}_e \). The real part would play the role of the stored energy and the imaginary part of the lost energy. The problem with this approach is that each of these terms are not causal by themselves, it is only their sum that ensures causality. Nunes et al [55] try to go further and derive expressions for the energy transference between the electromagnetic field and the material. The main drawback for using this method is that they only consider harmonic electromagnetic fields and their results cannot been generalized (for instance, it is not possible to use the time-averaged Poynting vector). Barash et al [70] say that One cannot, in general, express the electromagnetic energy density and dissipation separately in terms of the dielectric permittivity, magnetic permeability and electric conductivity of a general causal, temporally dispersive medium.
This idea is followed by Oughstun [9] who adds *Consequently, in order to unambiguously determine these quantities, it may be necessary to employ a specific physical model of the dispersive medium, for example, the equation of motion at the microscopic level.* This final approach is the one that will be followed here but with a very important difference: We will only consider the constitutive relations given by Eqns. (3.8) and (3.9) and not an specific model (for instance Drude-Lorentz like models). Thus we can establish the convention that the integral term in Eq. (3.43) corresponds to the stored energy within the slab. The advantage of this convention relies in its generality. It is then not necessary to limit ourselves to simple models for the permittivity and look for perfect time differentials [61, 69] or to cut general expansion up to certain orders [9, 70].

**Energy balance**

With our definitions of energy density, it is possible to establish a balance equation for the energy. Recalling that in this case the Poynting vector $S$ just propagates in the $y$-direction, Eq (3.40) reads:

$$\frac{\partial S_y}{\partial y} + \frac{\partial W}{\partial t} = 0,$$

with

$$S_y = S \cdot e_y$$

(3.44)

which is the uniaxial continuity equation in the $y$ axis. Taking the spatial integral in $\mathbb{R}$, it follows that;

$$\frac{dE}{dt} = 0,$$

where

$$E = \int_{y \in \mathbb{R}} W(y, t) dy$$

(3.45)

This can be ensured by the fact that the amplitude of the incident field is of finite energy and decays, together with their derivatives, sufficiently fast at infinity. The main consequence of Eq. (3.45) is that the total energy of the electromagnetic pulse-slab system is a constant $E(t) = E_c$. Thus the conservation of energy has been proved. Next, we consider the energy density in the superstratum given by Eq. (3.42). Using equations (3.36) and (3.37) we obtain:

$$W_I = W_I^+ + W_I^-,$$

$$W_I^\phi = \frac{\mu_0}{2} |H_I^\phi|^2 + \frac{\varepsilon_0}{2} |E_I^\phi|^2,$$

$\phi = \{+,-\}.$

(3.46) (3.47)
That is, the total energy density in $U_I$ can be separated as the sum of the incident pulse energy density $W_I^-$ and the reflected pulse energy density $W_I^+$. Even more, considering now the first term on the right hand side of (3.47) and plugging it into Eq. (3.37) we see that:

$$\frac{\mu_0}{2} |H^I_\phi|^2 = \frac{\mu_0}{2} \left| \frac{1}{\mu_0 c} E^I_\phi \right|^2 = \epsilon_0 \frac{1}{2} |E^I_\phi|^2. \quad (3.48)$$

This shows the equipartition of the energy density between its electric and magnetic parts. The same results can be obtained, mutatis mutandis, for the energy density in the substratum $W_{III}$.

Finally, taking the integral with respect to $y$ for all the energy densities (3.42) and (3.43) the following equality holds

$$E^+_{II}(t) + E^-_{II}(t) + E^+_{III}(t) + E^-_{III}(t) = E_c, \quad (3.49)$$

(with $\int_{y \in \mathbb{R}} Wdy = E_c$) and establishes the energy balance between the incident pulse energy $E^+_{I}(t)$ and the sum of the reflected energy $E^-_{I}(t)$, the transmitted energy $E^-_{III}(t)$ and the energy stored within the slab $E_{II}(t)$.

### 3.4 Electromagnetic wave center and its velocity

As said in the introduction, there have been many ways to define the velocity of light. The seminal works of Leon Brillouin started to tackle this problem [1] and years later Smith [8] makes a recount of several definitions of this concept. The particular case of an electromagnetic pulse in a dispersive and possibly absorptive material and its associated propagation velocity has been treated in several references v.gr. [71, 59, 60, 62, 58]. In this section we will give a different (and hopefully more simple) way of defining the velocity of light, also we will show its adequacy when dealing with different spatial sub-domains (as is the case of the slab).

#### The centrovelocity in vacuo

Before starting, the following notation will be used: For any posible variable function $\mathcal{W}(y, t)$ of finite energy [16] which not necessarily denotes the energy density introduced above (i.e. $W \neq \mathcal{W}$) we write:

$$\langle \mathcal{W}(y, t) \rangle := \int_{y \in \mathbb{R}} \mathcal{W}(y, t)dy. \quad (3.50)$$
Making an analogy with the way in which is defined the center of gravity in mechanics, we define a wave center by using the electromagnetic energy density [13, 16] as follows:

$$ Y(t) = \frac{\langle yW(y,t) \rangle}{\langle W(y,t) \rangle}. \quad (3.51) $$

Taking the time derivative of (3.51) it is possible to obtain the velocity of the corresponding wave center. This velocity is called the centrovelocity of energy and is simply referred as the centrovelocity,

$$ V(t) = \frac{dY}{dt}. \quad (3.52) $$

It is important to mention the instantaneous nature of this definition (contrary to the one used by Peatross et al. [62]) and also remark that it differs from Eq. (3.1). Even more, it has been proved by Petit [13] that for materials with \( \epsilon_r(\omega) \) that depend on \( \omega \) as a real even function, the centrovelocity Eq. (3.52) is the weighted average of the group velocities corresponding to the superposition of the plane waves in a wave packet.

In order to obtain a more explicit form of Eq. (3.52) we start by multiplying Eq. (3.51) by \( \langle W(y,t) \rangle \):

$$ Y(t) \langle W(y,t) \rangle = \langle yW(y,t) \rangle. \quad (3.53) $$

Then, taking the time derivative on both sides one has:

$$ \frac{d}{dt}[Y(t) \langle W(y,t) \rangle] = Y(t) \langle \partial_t W \rangle + V(t) \langle W \rangle, $$

$$ \frac{d}{dt} \langle yW(y,t) \rangle = \langle y\partial_t W \rangle, $$

and after some elementary manipulations Eq. (3.52) reads:

$$ V(t) = \frac{\langle y\partial_t W \rangle}{\langle W \rangle} - Y(t) \frac{\langle \partial_t W \rangle}{\langle W \rangle}. \quad (3.54) $$

From the continuity equation given by Eq. (3.44), it is easy to see that for a system with constant energy in time (\( \langle W \rangle = E_c \)), we have:

$$ V(t) = \frac{\langle y\partial_t W \rangle}{E_c} = - \frac{\langle y\partial_y S_y \rangle}{E_c} = \frac{\langle S_y \rangle}{E_c} \quad (3.55) $$
The last equality is the so called energy-flux velocity and represents the mean velocity of the energy transport \[16\]. Therefore for conservative systems the centrovelocity and the energy-flux velocity of the wave are the same. This same conclusion for conservative linear waves has been shown by Broer \[72\] via the stationary phase method. The advantage of our approach is that we have used only the continuity equation and elementary manipulations.

The centrovelocity of the slab in vacuo

Superstratum and Substratum

Considering the energy densities obtained for each sub-domain given by equations (3.42) and (3.43), the total density \(W(y, t)\) can be written as:

\[
W(y, t) = \sum_{\xi} W_{\xi}^0 + W_{\xi}^p, \quad \xi = \{I, II, III\},
\]

with

\[
W_{\xi}^0 = \frac{\mu_0}{2} |H_\xi|^2 + \frac{\varepsilon_0}{2} |E_\xi|^2, \quad \xi = \{I, II, III\},
\]

\[
W_{\xi}^p = \int_{-\infty}^t E_{\xi} \cdot \frac{\partial P_\xi}{\partial t'} dt'.
\]

Notice that \(W_{\xi}^0(y, t), \xi = \{I, II, III\}\) are the energies restricted to each spatial domain \(\xi\) and can be seen as if they were the energy densities corresponding to an electromagnetic pulse that propagates in vacuo, whereas \(W_{\xi}^p\) represents the density of the energy stored within the slab due to the polarization of the material (Joule effect), this explains the choice of the superscript \(p\) in \(W_{\xi}^p\). Upon substitution of Eq. (3.56) into Eq. (3.51) we get:

\[
Y(t) = \sum_{\xi} \mathcal{Y}_{\xi}^0(t) C_{\xi}^0(t) + \mathcal{Y}_{\xi}^p(t) C_{\xi}^p(t), \quad \xi = \{I, II, III\},
\]

with

\[
\mathcal{Y}_{\xi}^p(t) = \frac{\langle W_{\xi}^p \rangle}{\mathcal{E}_c}, \quad \mathcal{Y}_{\xi}^0(t) = \frac{\langle W_{\xi}^0 \rangle}{\mathcal{E}_c}, \quad \xi = \{I, II, III\}
\]

and

\[
C_{\xi}^p(t) = \frac{\langle W_{\xi}^p \rangle}{\mathcal{E}_c}, \quad C_{\xi}^0(t) = \frac{\langle W_{\xi}^0 \rangle}{\mathcal{E}_c}, \quad \xi = \{I, II, III\}.
\]
Equation (3.59) establishes that the center of gravity considering the total energy density is given by the position of the centers of gravity defined for the different densities in each sub-domain (see Eq. (3.60)) and weighted by their respective energy ratios Eq. (3.61). However in general Eq. (3.59) does not represent the position (and consequently the centrovelocity) of any physical electromagnetic pulse besides the total incident one. It is then convenient to study the behavior of the velocities of the centers of gravity \( Y_0^0(t), \xi = \{I, II, III\} \). This is due to the fact that the associated energy densities are easy to obtain from the experimental point of view, whereas the density associated to \( Y^0_{I_1}(t) \) depends of the slab polarization. Moreover, it is very important to remember that the position of the center of gravity is obtained as a quotient and for the case of each domain \( U_\xi, \xi = \{I, II, III\} \) and it only makes sense for the times when the density of energy is different from zero. This is a problem already noticed by Smith in his discussion about the signal velocity [8].

We will now study the velocity of the center of gravity \( Y^0_I(t) \) in the superstratum \( U_I \), which is given by:

\[
V^0_I(t) = \partial_t Y^0_I(t) = \frac{\langle y \partial_t W^0_I \rangle}{\langle W^0_I \rangle} - Y^0_I(t) \frac{\langle \partial_t W^0_I \rangle}{\langle W^0_I \rangle},
\]

(3.62)

where \( W^0_I(t) \) satisfies the continuity equation restricted to \( \Omega_I \)

\[
\partial_y S^0_{1,y} + \partial_t W^0_I = 0,
\]

(3.63)

and \( S^0_{1,y} \) is the Poynting vector restricted to the superstratum projected on \( e_y \). Plugging Eq. (3.63) into Eq. (3.62) the velocity \( V^0_I(t) \) is written as

\[
V^0_I(t) = \frac{\langle y W^0_I \rangle \langle \partial_y S^0_{1,y} \rangle}{\langle W^0_I \rangle^2} - \frac{\langle W^0_I \rangle \langle y \partial_y S^0_{1,y} \rangle}{\langle W^0_I \rangle^2}.
\]

(3.64)

It is worthy to remark here that \( \langle \partial_y S^0_{1,y} \rangle \) doesn’t vanishes for all times. Therefore \( V^0_I(t) \) coincides with the energy-flux velocity, defined as Eq. (3.55), only for certain times such that \( S^0_{1,y}(l, t) = 0 \). In other words: The boundaries affect the centrovelocity. This obvious statement doesn’t appear in the usual definition of group velocity because it only considers the case of an infinite or semi-infinite medium. At this point, it is worthy to mention the importance of studying the wave propagation within a slab and not in a infinite
medium. Whereas the amplitude of a propagative electromagnetic pulse remains unaltered in a non dispersive (and absorptive) material, when we consider these two phenomena, we know that the wave is exponentially decreasing with time, but conversely, the wave is of infinite energy when \( t \) tends to \(-\infty\).

Following the ideas exposed by Van Groesen and Maniardi [16], Eq. (3.64) can be seen in a more illuminating way as:

\[
V^0_I(t) = \frac{1}{\langle W^0_I \rangle} \left[ \langle yW^0_I \rangle \langle \partial_y S^0_{I,y} \rangle - \langle y \partial_y S^0_{I,y} \rangle \right],
\]

\[
= \frac{1}{\langle W^0_I \rangle} \left[ y \left[ \langle \partial_y S^0_{I,y} \rangle \frac{W^0_I}{\langle W^0_I \rangle} - \partial_y S^0_{I,y} \right] \right],
\]

\[
= \frac{\langle yL^0_I \rangle}{\langle W^0_I \rangle}.
\]

That is, the centrovelocity is expressed through a new density \( L^0_I(y,t) \) which is defined as follows

\[
L^0_I(y,t) = \langle \partial_y S^0_{I,y} \rangle \frac{W^0_I}{\langle W^0_I \rangle} - \partial_y S^0_{I,y},
\]

i.e. is a difference between the weighted total flux density change (with weight \( \frac{W^0_I}{\langle W^0_I \rangle} \)) minus the instantaneous flux density change at \( y \), being clear that the procedure for obtaining the centrovelocity in the substratum \( U_{III} \) is analogous to the one described for the superstratum.

**The slab**

It would be natural to extend this procedure to the velocity in \( U_{II} \) by considering the continuity equation:

\[
\partial_y S_{II,y} + \partial_t W_{II} = 0,
\]

with \( W_{II} = W^0_{II} + W^p_{II} \). Nevertheless, as has been discussed for the center of gravity Eq. (3.59), the centrovelocity related to \( W_{II} \) will not be related to the center of gravity pulse propagating in the slab, is what is left of it since the slab is absorptive, but to the center of gravity for the electromagnetic pulse-slab system. For these reasons, the centrovelocity related to \( W^0_{II} \) will be studied in analogy to Eq. (3.64):

\[
V^0_{II}(t) = \frac{1}{\langle W^0_{II} \rangle^2} \left[ \langle W^0_{II} \rangle \langle y \partial_t W^0_{II} \rangle - \langle \partial_t W^0_{II} \rangle \langle y W^0_{II} \rangle \right].
\]
while considering the continuity equation:
\[ \partial_y S_{II,y}^0 + \partial_t W_{II}^0 = -\partial_t W_{II}^p. \] (3.69)

There is a very important difference between the perspectives of Eq. (3.67) and Eq. (3.69). Equation (3.67) takes the perspective of the electromagnetic pulse-slab system for which the change of the energy density of the system \( W_{II} \) is only related to the change in the flux density \( S_{II,y} \). On the other hand, Eq. (3.69) considers only the propagating electromagnetic pulse point of view. Here the change in the energy density \( W_{II}^0 \) of the pulse is not just related to the change in the energy flux \( S_{II,y} \) but also to a loss term represented by \( -\partial_t W_{II}^p \). Plugging Eq. (3.69) into Eq. (3.68) the centrovelocity is
\[ V_{II}^0(t) = \frac{\langle y L_{II}^0 \rangle}{\langle W_{II}^0 \rangle} + \frac{\langle y M_{II}^0 \rangle}{\langle W_{II}^0 \rangle}, \] (3.70)

with \( L_{II}^0(y, t) \) defined as in (3.66) and \( M_{II}^0(y, t) \) being
\[ M_{II}^0(y, t) = \frac{W_{II}^0}{\langle W_{II}^0 \rangle} \partial_t \langle W_{II}^p \rangle - \partial_t W_{II}^p, \] (3.71)

which is similar to Eq. (3.66) but in this case the important quantity is the energy density change with respect to time.

### 3.5 Numerical Results

In order to illustrate our discussion, we present the following numerical results obtained via a home made python code. The implementation of the Discrete Fourier Transform was made by following the approximations in [73, 74] and the numerical frequency/time domains were sampled keeping in mind the Nyquist sampling Theorem [75, 76]. For this example it is considered a susceptibility given by the data fitting model given in Chapter 1. The values for the parameters taken from Table 1.1 for Gold, with the best fitting corresponding to wavelengths in \( \lambda : 0.188 - 1.937 \mu m \).

As we said before, the incident field in time domain \( A_{I}^{-}(t) \) must be of finite energy. For this reason, a Gaussian envelope is considered as in [59, 60, 71]. Thus, the amplitude of the incident field is given by
\[ A_{I}^{-}(t) = \sin(\omega_c t)e^{-\frac{t^2}{2\sigma^2}}, \] (3.72)
where the used parameters corresponding to a femto-second pulse with
\( \sigma = 4.5 \text{ fs} \) centred on \( \omega_c = \frac{2\pi c}{\lambda_c} \) with \( \lambda_c = 1300\text{nm} \). Figure 3.2 shows a scaled
version of \( \hat{A}_I^-(\omega) \) with \( \beta_{II}(\omega) \) the wave number in the dispersive slab. It
is possible to see how for most of the frequencies windowed by \( \hat{A}_I^-(\omega) \) the
corresponding electromagnetic field will present relatively low absorption
(\( \text{Im}\{\beta_{II}(\omega)\} \)). This is because otherwise the energy balance fails due
the numerical Fourier transform which requires the numerical time and
frequency domains to be linked according the Nyquist sampling theorem
[75]. Thus frequency ranges that can studied is limited not by theoretical
reasons, but to the memory of our computer. The numerical spatial domain

\[ \Omega = [-200, 100] \mu m \]

with \( l = 4 \mu m \) and \( L = -4 \mu m \) (i.e. the thickness of the
slab is 8 \( \mu m \)). Notice that the length of the substratum is larger, this is be-
cause the transmitted electromagnetic pulse is wider after passing through
the dispersive slab. Figures 3.3 and 3.4 show a numerical simulation of
the electric and magnetic fields when they illuminate normally the golden
slab. It can be seen from these simulations how the pulse is absorbed but it
doesn’t show appreciable dispersion. This is due, as explained lines above,
to our choice of the frequency range in which the numerical simulation was
performed.

---

**Fig. 3.2.** Scaled amplitude of the Fourier transform of the incident field
compared with \( \beta_{II}(\omega) \) showing the frequencies included in the electro-
magnetic pulse.
Fig. 3.3. Numerical simulation of the electric field that illuminates normally the slab. The paper version shows a snapshot at \( t = 2902 \) fs, and the full animation can be seen at https://youtu.be/TuUMcORx9nk. The pdf version shows the full animation just by clicking in the figure. Upper left: all the sub-domains. Upper right: Zoom to the superstratum. Lower left: Zoom to the slab. Lower right: Zoom to the substratum.
Fig. 3.4. Numerical simulation of the magnetic field that illuminates normally the slab. The paper version shows a snapshot at $t = 2902$ fs, and the full animation can be seen at https://youtu.be/8t4Hh5yZCHc. The pdf version shows the full animation just by clicking in the figure. Upper left: all the sub-domains. Upper right: Zoom to the superstratum. Lower left: Zoom to the slab. Lower right: Zoom to the substratum.
Numerical energy balance

The next part in our analysis is to consider the energy balance given by Eq. (3.49). By means of Eq. (3.42) and Eq. (3.43) it is possible to split the total energy density into an electric and magnetic part. Figures 3.5 and 3.6 show the normalized energy balance of the electric and magnetic parts. Here, when dealing with the propagation in vacuo, it is possible to see a clear equipartition of energy between the electric and magnetic parts. However, contrary to the well known case of propagation in transparent media, there is no more equipartition of energy when the pulse travels within the dispersive slab. Thus, it is not enough to consider just the electric or magnetic field amplitudes in order to make a correct energy balance (and therefore to define a correct centrovelocity of light). Figure 3.7 shows the total energy balance which satisfies Eq. (3.49) as expected. Moreover, it is possible to see how the energy corresponding to each propagating pulse is increasing until it reaches a maximum which is maintained during a certain time and then starts to decrease until it vanishes. This implies that each one of the pulses enters into one numerical spatial domain $U_{\xi}$ until it is completely contained with in and then leaves this spatial domain. On the other hand, when dealing with $E_{II}$ the line doesn’t show a decreasing as the time passes, this is because this line represents the stored energy within the slab.

Wave center’s position and velocity

Once the numerical results have been tested via an energy balance, it is straightforward to compute the position of the centers of gravity for the electromagnetic field restricted to each domain. This is shown in Fig 3.8. Also, in the case of the superstratum and the substratum, the positions are compared with a particle that travels at the speed of light in vacuum $-c$ (for incident and transmitted fields) or $+c$ (for the reflected fields). As explained in Section 3.4, the position of the center of gravity was only taken for times for which the energy density $W_{0,\xi}$ is different from zero. Due to the fact that we perform numerical integrals, these times depend on the time and space grid resolution. Moreover, remembering our discussion in the previous section, we know that the position of the center of gravity is influenced by the
CHAPTER 3. ENERGY AND VELOCITY OF AN EM PULSE

Fig. 3.5. Electric energies corresponding to the incident $\mathcal{E}_{e,I}(t)$, reflected $\mathcal{E}_{e,I}^+(t)$, transmitted $\mathcal{E}_{e,III}(t)$ pulses and the electric energy of the electric field-slab system $\mathcal{E}_{e,II}(t)$. The energies are normalized to the total incident one.

Fig. 3.6. Normalized magnetic energies corresponding to the incident $\mathcal{E}_{m,I}(t)$, reflected $\mathcal{E}_{m,I}^+(t)$, transmitted $\mathcal{E}_{m,III}(t)$ pulses and the magnetic energy of the magnetic pulse within the slab $\mathcal{E}_{m,II}(t)$.
energy flux between the different sub-domains. Regarding the position of
the electromagnetic pulse within the slab the behavior appears to be linear
with an slope of $-0.66 \times 10^8 \text{m/s} \approx -0.22c$. This can be seen with more
detail in Fig 3.9.

Validation

In order to test the validity of the numerical results, it has been realized
a comparison between the results reported in section 6 of [58] by Ough-
stun and Cartwright, for a single resonance Lorentz permittivity. The pa-
rameters used correspond to the ones chosen by Brillouin [58]. In order
to emulate the semi-infinite dispersive media, the thickness of the slab is
chosen very large ($16 \mu \text{m}$) such that the transmission is negligible. This is
because the numerical experiments reported in [58] consider a semi infinite
medium. The initial pulse time structure used by us is given by Eq. (3.72)
with $\sigma = 2.8125\text{fs}$. The results for the centrovelocity at long propagating
distance with central frequencies $\omega_c = 0.5\omega_0$ and $\omega_c = 0.75\omega_0$ ($\omega_0$ being
the Lorentz resonance frequency) correspond to the ones reported in [58]
i.e. a speed of $0.65c$ is obtained in both cases.
Fig. 3.8. Position of the centers of gravity for the superstratum \( Y_1(t) \), substratum \( Y_{III}(t) \), within the slab \( Y_{II}(t) \) and their comparison with \( ct \) and \(-ct\).

Fig. 3.9. Position of the center of gravity for pulse propagating within the slab \( Y_{II}(t) \).
3.6 Partial conclusion

A semi analytical approach has been used to study the propagation of an electromagnetic pulse in a slab of leaky dispersive material. The concepts of electromagnetic energy, and pulse propagation velocity have been revisited and a general frame adapted to multi-domains has been developed. The numerical simulation that illustrates these results considers the case of a slab of gold with electric susceptibility given by the model developed in chapter 1. The solution obtained has been validated by a total time-domain energy balance. The position of the center of gravity of different electromagnetic pulses was computed. These results generally show a linear behavior and allow thus to derive the velocity of light in a dispersive leaky medium as the slope of these graphs.
Chapter 4

The QNM’s on a Fabry-Perot cavity

All her blocks looked as bright and new as the day there were bought, many years ago. The best thing about them was that with Lego she could construct any kind of object. And then she could separate the blocks and construct something new.
—Jostein Gaarder, Sophie’s world

In any wave-like phenomenon resonance is of uttermost importance. This can be seen when small modifications in the incident field produce significant changes in the diffracted field. Finding the resonant frequencies and consequently the resonant modes is therefore a well known problem in physics [67, 77]. In the context of optical cavities, a fundamental distinction can be made: 1) Close cavities, when it is considered that the fields are confined to a finite region in space, and 2) Open cavities, in which the fields are not strictly confined and can leak to the whole universe [30]. Closed cavities with perfect conducting walls have real resonant frequencies and normal modes, whereas for open electromagnetic systems, even for materials without losses, the resonant frequencies are in general complex [29]. The associated modes to these complex frequencies are called Quasi Normal Modes and exponentially diverge as $|r| \to \infty$.

In this chapter we are going to deal with the simple case of finding the resonant frequencies and QNMs associated to a slab. Although this problem has been already solved [30], we think that fundamental issue has been overlooked when solving this problem: The right definition of the branch cut for the complex logarithm which determines the wave number $\beta$. It is important to remark here that without a precise definition, the solutions of
the transcendental equation that provides the resonant frequencies could be erroneous. In addition, we solve how to deal with the problem of exponential divergence by making use of Perfectly Matched Layers (PMLs). Finally we provide a way to obtain a QNM expansion of a linearly polarized field by using bi-orthogonality.

4.1 Mathematical formulation

We directly start by taking the Fourier Transform of the Maxwell’s equations:

\[
\hat{\nabla} \times \hat{\mathbf{E}} = +i\omega \hat{\mathbf{B}} \tag{4.1}
\]
\[
\hat{\nabla} \times \hat{\mathbf{H}} = -i\omega \hat{\mathbf{D}} \tag{4.2}
\]
\[
\hat{\nabla} \cdot \hat{\mathbf{D}} = 0 \tag{4.3}
\]
\[
\hat{\nabla} \cdot \hat{\mathbf{B}} = 0 \tag{4.4}
\]

with constitutive relations given by:

\[
\hat{\mathbf{D}} = \varepsilon_0 \hat{\mathbf{\epsilon}}_r \hat{\mathbf{E}} \tag{4.5}
\]
\[
\hat{\mathbf{B}} = \mu_0 \hat{\mathbf{\mu}}_r \hat{\mathbf{H}} \tag{4.6}
\]

Where the tensors \( \hat{\mathbf{\epsilon}}_r \) and \( \hat{\mathbf{\mu}}_r \) have the form:

\[
\hat{\mathbf{\eta}} = \begin{pmatrix}
\eta_{xx} & \eta_a & 0 \\
\eta_a & \eta_{xx} & 0 \\
0 & 0 & \eta_{zz}
\end{pmatrix}, \quad \eta = \{\varepsilon, \mu\}. \tag{4.7}
\]

This is because we need anisotropy further when dealing with PML’s. Plugging (4.6) into the Faraday’s law, it is possible to obtain after some manipulations the following formulation for the electric field:

\[
\hat{\mathbf{\epsilon}}_r^{-1} \hat{\nabla} \times \left( \hat{\mathbf{\mu}}_r^{-1} \hat{\nabla} \times \hat{\mathbf{E}} \right) = \frac{\omega^2}{c^2} \hat{\mathbf{E}} \tag{4.8}
\]

We consider the case of a (possibly dispersive) slab of thickness \( l - L \) with \( l > L \) in vacuo, which is invariant along the z and x axes. With this configuration in mind, it is natural to define the following domains

- **superstratum** \( U_l = \{(x, y, z) | y > l\} \),
slab \( \mathcal{U}_{II} = \{(x, y, z)|L < y < l\}, \)

substratum \( \mathcal{U}_{III} = \{(x, y, z)|y < L\}. \)

Then, the electric and magnetic field must satisfy the interface conditions:

\[
\begin{align*}
[e_y \times \mathbf{E}]_{y=l} &= 0, & [e_y \times \mathbf{H}]_{y=L} &= 0, \quad (4.9) \\
[e_y \times \mathbf{H}]_{y=l} &= 0, & [e_y \times \mathbf{E}]_{y=L} &= 0, \quad (4.10)
\end{align*}
\]

by considering Faraday’s and Ampere’s law in the sense of distributions [42]. For the case of a Fabry-Perot cavity it is apropos to study the very simple case of a linearly polarized electric field along the \( z \)-axis, that is:

\[
\mathbf{E} = \hat{u}(x, y, \omega)\mathbf{e}_z. \quad (4.11)
\]

In this case the magnetic field \( \mathbf{H} \) is retrieved by Faraday’s law (4.1):

\[
\mathbf{H} = \frac{1}{i\Delta \omega \mu_0} \left( \begin{array}{ccc}
\mu_{yy} \frac{\partial \hat{u}}{\partial y} + \mu_{aa} \frac{\partial \hat{u}}{\partial \sigma} \\
-\mu_{a} \frac{\partial \hat{u}}{\partial y} - \mu_{xx} \frac{\partial \hat{u}}{\partial \sigma} \\
0
\end{array} \right), \quad \Delta = \mu_{xx} \mu_{yy} - |\mu_a|^2 \quad (4.12)
\]

which combined with the interface conditions imposes certain restrictions on the derivatives of \( \hat{u} \).

Then, equation (4.8) takes the form

\[
-\frac{1}{\Delta} \nabla \cdot \left( \begin{array}{ccc}
\mu_{xx} & \mu_a & 0 \\
\mu_a & \mu_{xx} & 0 \\
0 & 0 & \Delta / \mu_{zz}
\end{array} \right) \nabla \hat{u} = \frac{\omega^2}{c^2} \epsilon_{zz} \hat{u}, \quad (4.13)
\]

where

\[
\Delta = \mu_{xx} \mu_{yy} - |\mu_a|^2. \quad (4.14)
\]

4.2 Preliminary remarks: Plane wave at normal incidence

Making another simplifying assumption, we consider the case of normal incidence (\( i.e. \hat{u} = \hat{u}(y, \omega) \)). Moreover, we consider a material with no magnetization (\( \mu_{xx} = \mu_{yy} = \mu_{zz} = 1, \mu_a = \mu_{aa} = 0 \)) and electrically polarized just along the \( z \)-component (\( \epsilon_{zz} = \hat{\epsilon}_r(y, \omega), \epsilon_{xx} = \epsilon_{yy} = 1 \) and \( \epsilon_{aa} = \epsilon_{a} = 0 \)).
Thus, under all these assumptions, equation (4.13) is simplified in the following way:

\[
\frac{\partial^2 \hat{u}_\xi}{\partial y^2} = -\beta_\xi^2 \hat{u}_\xi, \quad \beta_\xi^2 = \frac{\omega^2}{c^2} \hat{\epsilon}_\xi(y, \omega)
\]  

(4.15)

where the sub index $\xi$ denotes the restriction of the function to each one of the sub-domains $U_\xi$, $\xi = \{I, II, III\}$. In addition, the magnetic field is simply given by:

\[
\hat{H} = \frac{1}{i\omega \mu_0} \frac{\partial \hat{u}_\xi}{\partial y} \mathbf{e}_x.
\]  

(4.16)

Keeping in mind the outgoing wave conditions [54], the solutions of (4.15) are:

\[
\hat{u}_I = \hat{A}_I^+ (\omega) e^{i(y-L)\beta_I} + \hat{A}_I^- (\omega) e^{-i(y-L)\beta_I},
\]  

(4.17)

\[
\hat{u}_{II} = \hat{A}_{II}^+ (\omega) e^{i(y-L)\beta_{II}} + \hat{A}_{II}^- (\omega) e^{-i(y-L)\beta_{II}},
\]  

(4.18)

\[
\hat{u}_{III} = \hat{A}_{III}^- (\omega) e^{-i(y-L)\beta_{III}}.
\]  

(4.19)

Here we remark one more time that in principle $\beta_\xi^2$ is a complex function and it is necessary to define a branch cut of the complex logarithm in order to define correctly the meaning of square root. However, for reasons that will be unveiled later, this definition must be postponed and we will carry on with the discussion with a non defined $\beta$. Proceeding in a different way as we did on chapter 3, where the $\hat{A}$’s coefficients were obtained by considering the amplitude of the incident field $\hat{A}_I^- (\omega)$ as given, here, it will be assumed that the transmitted field amplitude $\hat{A}_{III}^- (\omega)$ is the known data. In this way the Fresnel coefficients take the form:

\[
\hat{A}_I^- (\omega) = \frac{1}{4} \left[ (1-p)(1-q)e^{i(y-L)\beta_{II}} + (1+p)(1+q)e^{-i(y-L)\beta_{II}} \right] \hat{A}_{III}^- (\omega),
\]  

(4.20)

\[
\hat{A}_I^+ (\omega) = \frac{1}{4} \left[ (1+p)(1-q)e^{i(y-L)\beta_{II}} + (1-p)(1+q)e^{-i(y-L)\beta_{II}} \right] \hat{A}_{III}^- (\omega),
\]  

(4.21)

\[
\hat{A}_{II}^- (\omega) = \frac{1}{2} (1+q) \hat{A}_{III}^- (\omega),
\]  

(4.22)

\[
\hat{A}_{II}^+ (\omega) = \frac{1}{2} (1-q) \hat{A}_{III}^- (\omega),
\]  

(4.23)
with \( p = p(\omega) = \frac{\beta_{III}(\omega)}{\beta_{II}(\omega)} \) and \( q = q(\omega) = \frac{\beta_{III}(\omega)}{\beta_{II}(\omega)} \). Notice that it is easy to go back to the formulation when the incident amplitude is given, by just taking:

\[
\hat{A}_{III}(\omega) = 4 \left[ (1 - p)(1 - q)e^{i(l - L)\beta_{II}} + (1 + p)(1 + q)e^{-i(l - L)\beta_{II}} \right]^{-1} \hat{A}_I(\omega).
\]  

(4.24)

4.3 In absence of incident field: The resonant modes

As we know, the QNM’s are the natural resonance modes of an open cavity [30] and consequently are radiated by no sources. In order to find such fields we just set the incident field \( \hat{A}_I(\omega) = 0 \), which leads to the following transcendental equation:

\[
e^{i2(l - L)\beta_{II}} = G, \quad \text{where} \ G = -\frac{(1 + p)(1 + q)}{(1 - p)(1 - q)} = \frac{(\beta_{II} + \beta_{I})(\beta_{II} + \beta_{III})}{(\beta_{II} - \beta_{I})(\beta_{II} - \beta_{III})}.
\]  

(4.25)

Up to this point, one could be tempted to use his/her favorite appropriate numerical method in order to find the roots of this equation. However, it is important to say that, so far the meaning of \( \beta \) is not well defined, and proceeding without settling this issue or worse to leave it to the intern definition of some software could lead to pitfalls.

Recalling our definition of the complex logarithm in Eq. (C.1) of Appendix C, it is possible to set the parameters \( \theta \) and \( \sigma \) in order to define a specific complex logarithm. Then, equation (4.25) reads:

\[
\beta_{II} = \frac{1}{l - L} \left[ n\pi + \frac{1}{2} \text{Arg}_{\theta}^\sigma(G) - \frac{i}{2} \ln(|G|) \right], \quad n \in \mathbb{N}
\]  

(4.26)

Notice that this one is still a transcendental equation because \( G \) is in terms of \( \beta_{II} \). Nevertheless it is possible to see that the sign of the imaginary part of \( \beta_{II} \) is given by \(-\frac{1}{2} \ln(|G|)\). From the definition of \( G \) in Eq. (4.25) it is clear that when \( |G| > 1 \) we have \( \Im\{\beta_{II}\} < 0 \). With this in mind, the natural choice of parameters for the complex logarithm in Eq. (4.26) is \( \theta = \pi, \sigma = -\pi \). And finally, the resonant frequencies \( \Omega_n \) will be the roots of the well defined equation:

\[
\frac{1}{l - L} \left[ n\pi + \frac{1}{2} \text{Arg}_{\pi}^\pi(G(\Omega_n)) - \frac{i}{2} \ln(|G(\Omega_n)|) \right] - \beta_{II}(\Omega_n) = 0, \quad n \in \mathbb{N}.
\]  

(4.27)
It is important to remark here that Eq. (4.27) holds under the very general condition that \(|G| > 1\) which can satisfied by transparent, gentle and highly dispersive materials when \(\Im \{\beta_{II}\} < 0\). In practice, the complex roots \(\Omega_n\) can be found on the complex plane via the Tetrachotomy method [43].

Studying Eq. (4.27) two important consequences of the choice of the branch cut can immediately be observed:

- The resonant wave numbers \(\beta_{\xi}(\Omega_n)\), \(\xi = \{I, II, III\}\) are located in the lower-half complex plane.

- The eigenfunctions \(\hat{u}_n = \hat{u}(y, \Omega_n)\) are exponentially increasing at plus and minus infinity.

In the next section we will show how to modify these eigenfunctions of infinite energy \(\hat{u}_n\), via a change of variables in the complex plane.

### 4.4 The modified resonant modes

As we saw before, the solutions corresponding to resonant modes of a Fabry-Perot cavity diverge exponentially to infinity. One way to normalize these solutions is to considering the analytic continuation [31]:

\[
\tilde{x}(x) = x, \quad \tilde{z}(z) = z, \quad \tilde{y}(y) = y + if(y) \tag{4.28}
\]

with \(f\) an arbitrary function by the moment. Next, the derivatives are transformed as follows:

\[
\frac{\partial}{\partial \tilde{x}} = \frac{\partial}{\partial x'}, \quad \frac{\partial}{\partial \tilde{z}} = \frac{\partial}{\partial z'}, \quad \frac{\partial}{\partial \tilde{y}} = \frac{1}{1 + is(y)} \frac{\partial}{\partial y'} \quad s(y) = \frac{df}{dy} \tag{4.29}
\]

Setting \(s(y)\) as:

\[
s(y) = d(1 - \theta(y - M) + \theta(y - m)), \tag{4.30}
\]

where \(d\) is a free real parameter, \(\theta\) is the Heaviside step function \(m\) and \(M\) are two constants such that \(m > l\) and \(M < L\), we find that equation (4.15) can be read (omitting the tildes in Cartesian coordinates) as:

\[
\frac{\partial^2 \hat{u}_n}{\partial y^2} = -\frac{\Omega_n^2}{\varepsilon^2} \hat{c}_{r, \xi}(\Omega_n) \hat{u}_n, \quad \xi = \{0, 1, 2, 3, 4\} \tag{4.31}
\]
with a new permittivity defined as:

\[
\hat{\epsilon}_{r,\xi} := \begin{cases} 
\hat{\epsilon}_{r,0} = (1 + id)^2 \epsilon_I & \text{if } y > m, \\
\hat{\epsilon}_{r,1} = \epsilon_I & \text{if } m < y < l, \\
\hat{\epsilon}_{r,2} = \epsilon_{II}(\Omega_n) & \text{if } L < y < l, \\
\hat{\epsilon}_{r,3} = \epsilon_{III} & \text{if } M < y < L, \\
\hat{\epsilon}_{r,4} = (1 + id)^2 \epsilon_{III} & \text{if } y < M. 
\end{cases}
\] (4.32)

This defines new spatial subdomains:

- **PML-superstratum** \(U_0 = \{(x, y, z) | y > m\}\),
- **superstratum** \(U_1 = \{(x, y, z) | m < y < l\}\),
- **slab** \(U_2 = \{(x, y, z) | L < y < l\}\),
- **substratum** \(U_3 = \{(x, y, z) | M < y < L\}\),
- **PML-substratum** \(U_4 = \{(x, y, z) | y < M\}\).

The PML holds for *Perfectly Matched Layers* and it refers to a *reflectionless absorbing material* [31] in this case with permittivity \(\hat{\epsilon}_{r,\psi}\) where \(\psi = \{1, 4\}\). Notice that due to the definition of \(s(y)\) in Eq. (4.30), the equation (4.31), the interface conditions and consequently their solutions are the same as before. On the other hand, for the regions \(U_0\) and \(U_4\), the interfaces at \(y = m\) and \(y = M\) are:

\[
\hat{u}_n(m^+) = \hat{u}_n(m^-), \quad \frac{1}{1 + id} \frac{\partial \hat{u}_n}{\partial y} \bigg|_{m^+} = \frac{\partial \hat{u}_n}{\partial y} \bigg|_{m^-}, \quad (4.33)
\]

\[
\hat{u}_n(M^+) = \hat{u}_n(M^-), \quad \frac{\partial \hat{u}_n}{\partial y} \bigg|_{M^+} = \frac{1}{1 + id} \frac{\partial \hat{u}_n}{\partial y} \bigg|_{M^-}. \quad (4.34)
\]

Even more, because the solutions in \(U_0\) and \(U_4\) must decay at plus and minus infinity, it is necessary to use the complex logarithm C.1 with \(\theta = 0\), \(\sigma = +\).

Putting the pieces together, each one of the restrictions of \(\hat{u}_n\) is given as
follows:

\[
\hat{u}_{n1}(y) = \hat{A}^+_I(\Omega_n)e^{+i(y-L)\beta_I(\Omega_n)},
\]

\[
\hat{u}_{n2}(y) = \hat{A}^+_I(\Omega_n)e^{+i(y-L)\beta_{II}(\Omega_n)} + \hat{A}^-_{II}(\Omega_n)e^{-i(y-L)\beta_{II}(\Omega_n)},
\]

\[
\hat{u}_{n3}(y) = \hat{A}^-_{III}(\Omega_n)e^{-i(y-L)\beta_{III}(\Omega_n)},
\]

\[
\hat{u}_{n0}(y) = \hat{u}_{n1}(m)e^{+i(y-m)\beta_I(\Omega_n)(1+id)},
\]

\[
\hat{u}_{n4}(y) = \hat{u}_{n3}(M)e^{-i(y-M)\beta_{III}(\Omega_n)(1+id)}.
\]

Making use of the free parameter \(d\), we can ensure the exponential decay of \(\hat{u}_{n0}(y)\) at plus infinity by first focusing our attention on the product \(\beta_I(\Omega_n)(1+id)\), namely:

\[
\beta_I(\Omega_n)(1+id) = [\beta'_I(\Omega_n) - d\beta''_I(\Omega_n)] + i[d\beta'_I(\Omega_n) + \beta''_I(\Omega_n)].
\]

From this equation, it is clear that \(d\) must satisfy: \(d\beta'_I(\Omega_n) + \beta''_I(\Omega_n) > 0\), thus we consider as a first approach the quantity:

\[
d_I = \frac{\max\{|\beta''_I(\Omega_n)|\}}{\min\{|\beta'_I(\Omega_n)|\}}
\]

and \textit{mutatis mutandis} for \(\hat{u}_{n4}(y)\):

\[
d_{III} = \frac{\max\{|\beta''_{III}(\Omega_n)|\}}{\min\{|\beta'_{III}(\Omega_n)|\}}.
\]

The reasonable thing is to set \(d = D \max\{d_I, d_{III}\}\), where \(D\) is a positive constant greater than one, which will allows us to tune the decay rate.

### 4.5 Bi-orthogonal solutions: The case of a non dispersive slab

Once the problem with the divergence \textit{ad infinitum} has been solved, we would like to use this modified QNM’s as a basis to express a given \(z\)-polarized electric field \(\hat{E}^1 = \hat{u}^1 \mathbf{e}_z\), in other words:

\[
\hat{u}(y, \omega) = \sum_n P_n(\omega)\hat{u}_n(y, \Omega_n).
\]

Our goal now, is to determine the coefficients \(P_n(\omega)\) by considering the inner product:

\[
\langle f, g \rangle = \int_{\mathbb{R}} f(y)\overline{g}(y)dy,
\]
CHAPTER 4. THE QNM’S ON A FABRY-PEROT CAVITY

where the bar denotes complex conjugation. Then, we would like to find the functions \( v \) such that \( \langle \hat{u}_n, v \rangle = 0 \). However, as it is stated by Lalanne et al in [30] the QNM’s are orthogonal when dealing with non dispersive materials. For this reason we will work now under the assumption that \( \hat{\epsilon}_{r,2}(\Omega_n) = \epsilon_2 \) a complex constant.

Starting by the family of resonant modes \( \{ \hat{u}_n \}_n \) (here for simplicity we have dropped the underline), we know that these functions are solutions of Eq. (4.31) which can be rewritten in terms of the operator \( \mathcal{M}_{\xi}[\cdot] := \frac{1}{\hat{\epsilon}_{r,\xi}} \frac{\partial^2}{\partial y^2}[\cdot] \xi = \{0 \rightarrow 4\} \) as:

\[
\mathcal{M}_{\xi}[\hat{u}_n] = -\lambda_n \hat{u}_n \quad \text{where} \quad \lambda_n = \frac{\Omega_n^2}{c^2}
\]

(4.45)

Let us remark here that, the operator \( \mathcal{M}_{\xi} \) only depends on the sub-domain \( U_{\xi}, \xi = \{0 \rightarrow 4\} \) and not on the particular frequency \( \Omega_n \). It is a result from spectral theory that the eigenvectors \( \hat{u}_n \) are bi-orthogonal to their adjoint counterparts \( v_n \) [32]. Thus, the same way as in [29] we are going to look for the adjoint operator \( \mathcal{M}_{\xi}^{\dagger}[\cdot] \) which satisfies:

\[
\langle \mathcal{M}_{\xi}[\hat{u}_n,\xi], v \rangle = \langle \hat{u}_n,\xi, \mathcal{M}_{\xi}^{\dagger}[v] \rangle.
\]

(4.46)

Using the definition of inner product in Eq. (4.44), we have:

\[
\langle \mathcal{M}_{\xi}[\hat{u}_n,\xi], v \rangle = \int_{\mathbb{R}} \mathcal{M}_{\xi}[\hat{u}_n,\xi] \bar{v} dy = \sum_{\xi=0}^{4} \int_{U_{\xi}} \frac{1}{\hat{\epsilon}_{r,\xi}} \frac{\partial^2}{\partial y^2} \hat{u}_n,\xi d y,
\]

(4.47)

where in the last equality we have separated the integral according to each one of the spatial sub-domains. Now, we propose that depending on the sub-domain \( \bar{\sigma} = \bar{\sigma}_{\xi} = \hat{\epsilon}_{r,\xi} \bar{v} \) for \( \xi = \{0 \rightarrow 4\} \). This eliminates the \( \hat{\epsilon}_{r,\xi} \) in the integrand of Eq. (4.47) and then:

\[
\langle \mathcal{M}_{\xi}[\hat{u}_n,\xi], v \rangle = \sum_{\xi=0}^{4} \int_{U_{\xi}} \bar{w} \frac{\partial^2}{\partial y^2} \hat{u}_n,\xi d y,
\]

(4.48)

and:

\[
\langle \mathcal{M}_{\xi}[\hat{u}_n,\xi], v \rangle = \sum_{\xi=0}^{4} \mathcal{M}_{\xi}[\hat{u}_n,\xi] \bar{w} dy = \sum_{\xi=0}^{4} \int_{U_{\xi}} \hat{u}_n,\xi \bar{w} dy,
\]

(4.49)

where \( A_{\xi} \) and \( B_{\xi} \) are the endpoints of each interval. Due to the definition of the adjoint operator in Eq. (4.46) it is necessary for the first term on the right hand side of Eq. (4.49) to vanish. Fortunately we know that this is possible...
when \( \bar{\omega} \) and its derivative have the same behavior as \( \hat{u}_n \). **Notice that this could have not been possible without the assumption of non dispersion.**

Then:

\[
\langle M_\xi [\hat{u}_n, \xi], v \rangle = \frac{4}{\xi} \int_{\mathbb{R}} \hat{u}_n, \xi \partial_y^2 \bar{\omega}_\xi dy = \int_{\mathbb{R}} \hat{u}_n, \xi \left[ \frac{1}{\xi} \partial_y^2 \bar{\omega}_\xi \right] dy,
\]

and

\[
= \int_{\mathbb{R}} \hat{u}_n, \xi \left[ \frac{1}{\xi} \partial_y^2 \bar{\omega}_\xi \right] dy = \langle \hat{u}_n, \xi, M_\xi^*[v_\xi] \rangle.
\]

Therefore, the adjoint operator is:

\[
M_\xi^*[v_\xi] = \frac{1}{\xi} \partial_y^2 \bar{\omega}_\xi. \tag{4.50}
\]

Combining Eq. (4.45) and Eq. (4.46) one gets:

\[
\langle -\lambda_n \hat{u}_n, \xi, v_\xi \rangle = \langle M_\xi [\hat{u}_n, \xi], v_\xi \rangle = \langle \hat{u}_n, \xi, M_\xi^*[v_\xi] \rangle, \tag{4.51}
\]

then:

\[
\langle \hat{u}_n, \xi, -\lambda_m v_\xi \rangle = \langle \hat{u}_n, \xi, M_\xi^*[v_\xi] \rangle, \tag{4.52}
\]

and by the inner product properties [26] we arrive to the expression:

\[
-\lambda_n \bar{\omega}_\xi = \frac{1}{\xi} \partial_y^2 \bar{\omega}_\xi. \tag{4.53}
\]

By the existence and uniqueness theorem for ODE’s [78] we have that \( \bar{\omega}_\xi = \hat{u}_n, \xi \) and therefore the adjoint eigenvectors are \( v_n, \xi = \hat{\xi} \hat{u}_n, \xi \). After this work, the bi-orthogonality between \( \hat{u}_n \) and \( v_m \) can be proved in a straightforward fashion: Given the equalities

\[
M_\xi [\hat{u}_n] = -\lambda_n \hat{u}_n, \quad \text{and} \quad M_\xi^*[v_m] = -\lambda_m v_m, \tag{4.54}
\]

The following chain of equalities holds:

\[
-\lambda_n \langle \hat{u}_n, v_m \rangle = \langle -\lambda_n \hat{u}_n, v_m \rangle = \langle M_\xi [\hat{u}_n], v_m \rangle = \langle \hat{u}_n, M_\xi^*[v_m] \rangle \tag{4.55}
\]

\[
= \langle \hat{u}_n, -\lambda_m v_m \rangle = -\lambda_m \langle \hat{u}_n, v_m \rangle. \tag{4.56}
\]

It follows immediately that \( (\lambda_m - \lambda_n) \langle \hat{u}_n, v_m \rangle = 0 \) and because \( \lambda_n \neq \lambda_m \) one gets \( \langle \hat{u}_n, v_m \rangle = 0 \) i.e. \( \hat{u}_n \) and \( v_m \) are bi-orthogonal. Finally, the coefficients are:

\[
P_n(\omega) = \frac{\langle \hat{u}_n, v_m \rangle}{\langle \hat{u}_n, v_n \rangle}. \tag{4.57}
\]
An application of the modified resonant modes bi-orthogonality

For this last part, we are going to show an application for the QNM expansion. Let us assume the equivalent on 1D of the diffracted field formulation as in Eq. (5.213) of chapter, that is:

$$\frac{\partial^2 \hat{u}^1}{\partial y^2} + \hat{\epsilon}_r \omega^2 c^2 \hat{u}^1(y, \omega) = -\frac{\omega^2}{c^2} (\epsilon_2 - 1) \Pi_L^1(y) \hat{u}^0(y, \omega) \quad (4.58)$$

where $\hat{u}^0$ is a given function, $\Pi_L^1$ is the rectangle function in $[L, l]$ and $\hat{\epsilon}_r$ is as in (4.32) but with $\epsilon_2$ constant (non dispersive slab). This equation can be rewritten in terms of the operator $\mathcal{M}_{\xi}[\hat{u}^1]$ as:

$$\mathcal{M}_{\xi}[\hat{u}^1] + \frac{\omega^2}{c^2} \hat{u}^1 = -\frac{\omega^2 \epsilon_2 - 1}{\hat{\epsilon}_r} \Pi_L^1(y) \hat{u}^0. \quad (4.59)$$

Now, we propose that $\hat{u}^1$ can be written as a QNME, namely:

$$\hat{u}^1(y, \omega) = \sum_n P_n(\omega) \hat{u}_n(y, \Omega_n). \quad (4.60)$$

Plugging (4.60) into Eq. (4.59) and after some elementary manipulations:

$$\sum_n (\omega^2 - \Omega_n^2) P_n(\omega) \hat{u}_n = -\frac{\omega^2 \epsilon_2 - 1}{\hat{\epsilon}_r} \Pi_L^1(y) \hat{u}^0 \quad (4.61)$$

multiplying by $\bar{v}_m$ and taking the integral over the whole real line, one gets:

$$P_n(\omega) = -\frac{\omega^2 (\epsilon_2 - 1)}{(\omega^2 - \Omega_n^2) \langle \hat{u}_n, \bar{v}_n \rangle} \int_L^l \hat{u}^0(\omega, y) \hat{u}_{n,2}(y, \Omega_n) dy. \quad (4.62)$$

Thus our problem is solved.

4.6 Partial conclusion

In this chapter we have studied the problem of finding the QNM’s for a Fabry Perot cavity. The main results of our discussion are: 1) It has been possible to determine the right branch cut for the complex logarithm, which allows to determine the right resonant frequencies. 2) The exponential divergence of the QNM’s was eliminated by considering the use of PML’s. 3) A QNME for a linearly polarized electric field was made by obtaining the
bi-orthogonal vector to the QNMs. This was possible by finding the adjoint operator to the equivalent of Helmholtz equation in 1D. Finally, the next goal is to use this same procedure *mutatis mutandis* to determine the QNM’s of a spherical cavity (See Appendix G).
Chapter 5

Harmonic representation of the EM Field
generated by an oscillating particle and its interaction with a dispersive bulk

Everything that exists has a sound and has an order. This suppose that the movement of the celestial bodies must produce a sound, which is a result of the proportion between movement and distance; music of the spheres and harmony on the sky.

—Raúl Zambrano, *Minimal history of the western music.*

5.1 Introduction

This chapter consists in two main parts: In the first one we will address the problem of the electromagnetic field generated by an oscillating particle in *vacuo* and the second one is devoted to its interaction near to a bulk made of some dispersive material (See Fig 5.1 for a schematic representation). Albeit the apparently pure academic nature of this problem, many applications to this case of configurations can be found. Starting from the study of antennas made by Hertz and Sommerfeld [79, 80, 53] to the more recently study of quantum nanoemitters and its interaction with nano spheres [81, 82]. For this kind of phenomena, it is common to use an approximation to describe the field generated by an oscillating charged particle, the most common of these approximations for the far field is to use a *dipole approximation* as
described in [2, 20, 83, 80]. However, it is important to remark here that **the dipole approximation is only valid when dealing with the far field.**

It is then necessary to find a better way to describe the field generated by an oscillating charge, the immediate approach is to use the Liénard-Wiechert fields, which describe in quite a compact form the fields produced by a moving charge. The problem with this solution is that it is not tractable from the practical (**i.e.** numerical) point of view as we will show in Section 5.4. Other approaches have been to consider the moving charge as a delta distribution that can be approximated by a Taylor’s series [84] or a harmonic expansion [22]. Here we propose a different way for obtaining the harmonic representation of the fields which explicitly depends on time and space. Finally, once sources are obtained in harmonic form we use them as an incident field of the diffraction problem to obtain the diffracted field by a sphere by using a Finite Elements’ Method.

### 5.2 Mathematical formulation

For this, it is necessary to consider the Maxwell’s equations

\[
\nabla \times \mathbf{E}_\xi = -\frac{\partial}{\partial t} \mathbf{B}_\xi, \quad (5.1)
\]

\[
\nabla \times \mathbf{H}_\xi = \frac{\partial}{\partial t} \mathbf{D}_\xi + j, \quad (5.2)
\]

\[
\nabla \cdot \mathbf{D}_\xi = \rho, \quad (5.3)
\]

\[
\nabla \cdot \mathbf{B}_\xi = 0. \quad (5.4)
\]

where \(\xi = \{I, II\}\) represents the restriction of the fields, \(I\) corresponds to the total field **outside the bulk** and \(II\) to the field **inside the sphere**. The constitutive relations are then \(\mathbf{H}_\xi = \mu_0^{-1} \mathbf{B}_\xi\) and \(\mathbf{D} = \epsilon_0 (\epsilon_r, II \ast \mathbf{E}_\xi)\), where \(\chi\) is the electric susceptibility and its support is within the bulk. Thus, our new system of equations reads:

\[
\nabla \times \mathbf{E}_\xi = -\frac{\partial}{\partial t} \mathbf{B}_\xi, \quad (5.5)
\]

\[
\nabla \times \mathbf{B}_\xi = \frac{1}{c^2} \frac{\partial}{\partial t} (\epsilon_r, II \ast \mathbf{E}_\xi) + \mu_0 j, \quad (5.6)
\]

\[
\nabla \cdot (\epsilon_r, II \ast \mathbf{E}_\xi) = \frac{\rho}{\epsilon_0}, \quad (5.7)
\]

\[
\nabla \cdot \mathbf{B}_\xi = 0. \quad (5.8)
\]
Fig. 5.1. A charged particle oscillates close to dispersive bulk, in this case: a nano-sphere. The paper version shows a snapshot at $t = 0$ fs, and the full animation can be seen at https://youtu.be/KtI6nkfQyg0. The pdf version shows the full animation just by clicking in the figure.
The sources $\rho$ and $j$ represents the charge density and current corresponding to an oscillating particle and their explicit expression will be given later. The fields generated by these sources in vacuo are given by:

$$\nabla \times \mathbf{E}^0 = -\partial_t \mathbf{B}^0,$$

(5.9)

$$\nabla \times \mathbf{B}^0 = \frac{1}{c^2} \partial_t \mathbf{E}^0 + \mu_0 j,$$

(5.10)

$$\nabla \cdot \mathbf{E}^0 = \frac{\rho}{\varepsilon_0},$$

(5.11)

$$\nabla \cdot \mathbf{B}^0 = 0,$$

(5.12)

where the constitutive relations $\mathbf{D}^0 = \varepsilon_0 \mathbf{E}^0$ and $\mathbf{H}^0 = \mu_0^{-1} \mathbf{B}^0$ have been used. Let us remark here that $(\mathbf{E}^0, \mathbf{B}^0)$ is the incident field of our diffraction problem. The next step is to consider a new set of fields defined as: $\mathbf{E}_\xi^1 := \mathbf{E}_\xi - \mathbf{E}^0$, $\mathbf{B}_\xi^1 := \mathbf{B}_\xi - \mathbf{B}^0$ which satisfy the system of so called diffracted fields:

$$\nabla \times \mathbf{E}_\xi^1 = -\partial_t \mathbf{B}_\xi^1,$$

(5.13)

$$\nabla \times \mathbf{B}_\xi^1 = \frac{1}{c^2} \partial_t (\varepsilon_{r,II} * \mathbf{E}_\xi^1) + \mu_0 j^0_{II},$$

(5.14)

$$\nabla \cdot (\varepsilon_{r,II} * \mathbf{E}_\xi^1) = \frac{\rho^0_{II}}{\varepsilon_0},$$

(5.15)

$$\nabla \cdot \mathbf{B}_\xi^1 = 0,$$

(5.16)

where the new sources are defined as:

$$\rho^0_{II} := -\varepsilon_0 \nabla \cdot ([\varepsilon_{II} - 2\pi \delta] * \mathbf{E}^0), \quad \text{and} \quad j^0_{II} := \varepsilon_0 \partial_t ([\varepsilon_{II} - 2\pi \delta] * \mathbf{E}^0),$$

(5.17)

and from these definitions it is easy to see that they satisfy conservation of charge. Notice that the support of these new sources is within the bulk and depends on the electromagnetic field generated by the oscillating particle. However obtaining a handy expression of such field requires a very careful crafting as it will be shown in the next section.

### 5.3 The EM Field generated by an arbitrary charge distribution

The problem of obtaining the electromagnetic field generated by an oscillating particle is a very important problem per se. Usually, in order to obtain
such field, it is customary to use the so called dipole approximation. However this approximation is only valid for the radiated field and for particles that move at low speed.

Here we present a deduction without any magic steps, as far as our ability allows, starting from the Maxwell’s equations and continuing until to obtain expressions that allow the analysis for the electric and magnetic fields.

First, we consider the system of equations (5.9-5.12) (for the sequel the superscript 0 has been removed). From the magnetic divergence-less nature of the magnetic Gauss’ law in Eq. (5.12) and the second Helmholtz theorem for vector fields [20] we can see \( B \) as the curl of another potential field, \( i.e. \)

\[
B = \nabla \times A
\]  

(5.18)

Plugging this result into Eq. (5.9) we have:

\[
\nabla \times \left[ E + \partial_t A \right] = 0
\]  

(5.19)

Thus, the expression between square brackets in Eq. (5.19) is irrotational and, by virtue of the first Helmholtz theorem [20], it is possible to define it as the gradient of a certain potential \( \phi \):

\[
E + \partial_t A = - \nabla \phi,
\]  

(5.20)

and reordering the expression above we have:

\[
E = - \partial_t A - \nabla \phi.
\]  

(5.21)

On the other hand, substituting Eq. (5.18) into Eq. (5.10) and Eq. (5.19) into Eq. (5.11) one gets:

\[
\nabla \times \nabla \times A = \frac{1}{c^2} \partial_t \left[ - \partial_t A - \nabla \phi \right] + \mu_0 j,
\]  

(5.22)

\[
\nabla \cdot \left[ \nabla \phi + \partial_t A \right] = -\rho / \epsilon_0.
\]  

(5.23)

Using the identities \( \nabla \times \nabla \times A = \hat{\nabla} (\nabla \cdot A) - \nabla^2 A \), and \( \nabla \cdot \nabla \phi = \nabla^2 \phi \) and rearranging the terms

\[
\nabla^2 A - \frac{1}{c^2} \partial_t^2 A - \nabla \left[ \nabla \cdot A + \partial_t \phi \right] = - \mu_0 j,
\]  

(5.24)

\[
\nabla^2 \phi + \partial_t \left[ \nabla \cdot A \right] = -\rho / \epsilon_0.
\]  

(5.25)
Amongst the infinity of pair of potentials \((A, \phi)\) it exists a couple \((A_0, \phi_0)\) satisfying the so called Lorenz’s gauge \([20]\)

\[
\vec{\nabla} \cdot A_0 + \partial_t \phi_0 = 0
\]

it is possible to uncouple the system (5.9-5.12) as per:

\[
\vec{\nabla}^2 A - \frac{1}{c^2} \partial_t^2 A = -\mu_0 j,
\]

\[
\nabla^2 \phi - \frac{1}{c^2} \partial_t^2 \phi = -\rho / \epsilon_0.
\]

The solutions of these equations are obtained as retarded potentials:

\[
\phi = \frac{1}{4\pi\epsilon_0} \int_{\mathbb{R}^3} \frac{\rho(x', t_r)}{R} d^3 x',
\]

\[
A = \frac{\mu_0}{4\pi} \int_{\mathbb{R}^3} \frac{j(x', t_r)}{R} d^3 x',
\]

with the retarded time \(t_r = t - \frac{R}{c}\) and \(R = |\mathbf{R}|\) with \(\mathbf{R} = \mathbf{x} - \mathbf{x}'\). The next step is to plug equations (5.28) and (5.29) into Eq. (5.18) and Eq. (5.19) and then take their corresponding derivatives. Nevertheless, this implies to take time derivatives with respect to a function which is in terms of \(t_r\). In order to avoid this difficulty and carry our calculations further, we propose to use the Fourier transform and then consider just the spatial derivatives. Starting by transforming the potential \(\phi\) one has:

\[
\hat{\phi} = \frac{1}{4\pi\epsilon_0} \int_{\mathbb{R}^3} \frac{1}{R} \mathcal{F}_{t \rightarrow \omega} \{\rho(x', t - R/c)\} d^3 x',
\]

\[
= \frac{1}{4\pi\epsilon_0} \int_{\mathbb{R}^3} \frac{1}{R} e^{iRk_0} \hat{\rho}(x', \omega) d^3 x',
\]

where \(k_0 = \frac{\omega}{c}\). In a similar way the vector potential in the frequency domains reads:

\[
\hat{A} = \frac{\mu_0}{4\pi} \int_{\mathbb{R}^3} e^{iRK_0} \frac{j(x', \omega)}{R} d^3 x'.
\]

Before proceeding, the following identities are necessary:

\[
\vec{\nabla} \cdot \mathbf{R} = \frac{\mathbf{R}}{R},
\]

\[
\vec{\nabla} \frac{1}{R} = -\frac{1}{R^2} \vec{\nabla} R = \frac{\mathbf{R}}{R^3},
\]

\[
\vec{\nabla} e^{iRk_0} = ik_0 e^{iRk_0} \vec{\nabla} R = ik_0 e^{iRk_0} \frac{\mathbf{R}}{R},
\]

and combining Eq. (5.33) and Eq. (5.34) we get:

\[
\vec{\nabla} \left( \frac{e^{iRk_0}}{R} \right) = \left( ik_0 - \frac{1}{R} \right) \frac{e^{iRk_0}}{R^2} \mathbf{R}.
\]
Equipped with these tools, it is quite easy to obtain \( B \) by simply taking the curl of Eq. (5.31):

\[
\hat{\mathbf{B}} = \frac{\mu_0}{4\pi} \int_{\mathbb{R}^3} \vec{\nabla} \times \left( \frac{e^{iRk_0}}{R} \hat{j}(\mathbf{x}', \omega) \right) d\mathbf{x}'
\]

(5.36)

\[
= \frac{\mu_0}{4\pi} \int_{\mathbb{R}^3} \vec{\nabla} \left( \frac{e^{iRk_0}}{R} \right) \times \hat{j}(\mathbf{x}', \omega) d\mathbf{x}'
\]

(5.37)

\[
= \frac{\mu_0}{4\pi} \int_{\mathbb{R}^3} \left( ik_0 - \frac{1}{R} \right) \frac{e^{iRk_0}}{R^2} \mathbf{R} \times \hat{j}(\mathbf{x}', \omega) d\mathbf{x}'
\]

(5.38)

And by taking the inverse Fourier transform, we arrive to the expression:

\[
\mathbf{B} = \mathbf{B}_{\text{int}} + \mathbf{B}_{\text{rad}}
\]

(5.39)

where \( \mathbf{B}_{\text{int}} \) is the intermediate field and \( \mathbf{B}_{\text{rad}} \) is the radiated field which are given by the integrals:

\[
\mathbf{B}_{\text{int}} = \frac{\mu_0}{4\pi} \int_{\mathbb{R}^3} \hat{j}(\mathbf{x}', t_r) \times \frac{\mathbf{R}}{R^3} d\mathbf{x}'
\]

(5.40)

\[
\mathbf{B}_{\text{rad}} = \frac{\mu_0}{4\pi c} \int_{\mathbb{R}^3} \frac{\partial \hat{j}(\mathbf{x}', t_r)}{\partial t} \times \frac{\mathbf{R}}{R^2} d\mathbf{x}'.
\]

(5.41)

In order to obtain the electric field, it is necessary to consider the Fourier transform of Eq. (5.21):

\[
\hat{\mathbf{E}} = +i\omega \hat{\mathbf{A}} - \vec{\nabla} \hat{\phi}.
\]

(5.42)

The first term on the right hand side of Eq. (5.42) is quite easy to calculate,

\[
i\omega \hat{\mathbf{A}} = \frac{1}{4\pi \varepsilon_0 c} \int_{\mathbb{R}^3} ik_0 \hat{j}(\omega, \mathbf{x}') \frac{e^{iRk_0}}{R} d\mathbf{x}'.
\]

(5.43)

The second term is much more tricky and its derivation goes as follows:

\[
-\vec{\nabla} \hat{\phi} = -\frac{1}{4\pi \varepsilon_0} \int_{\mathbb{R}^3} \vec{\nabla} \left( \frac{e^{iRk_0}}{R} \right) \hat{\rho}(\mathbf{x}', \omega) d\mathbf{x}'
\]

\[
= -\frac{1}{4\pi \varepsilon_0} \int_{\mathbb{R}^3} \vec{\nabla} \left( \frac{e^{iRk_0}}{R} \right) \hat{\rho}(\mathbf{x}', \omega) d\mathbf{x}',
\]

\[
= -\frac{1}{4\pi \varepsilon_0} \int_{\mathbb{R}^3} ik_0 \hat{\rho}(\mathbf{x}', \omega) \frac{e^{iRk_0}}{R^2} \mathbf{R} d\mathbf{x}'
\]

\[
+ \frac{1}{4\pi \varepsilon_0} \int_{\mathbb{R}^3} \hat{\rho}(\mathbf{x}', \omega) \frac{e^{iRk_0}}{R^3} \mathbf{R} d\mathbf{x}'
\]

(5.44)
Up to this point most books [2, 20, 21] simply take the inverse Fourier transform of Eq. (5.44) and give the electric field in terms of the derivative of the density of charges and obtain the so called Jefimenko’s equations [21]. Despite the straightforward nature of this derivation, we are going to carry the calculations further. The interest of doing so will be shown later. For our purposes, the second integral in Eq. (5.44) is already in optimum form, and we will focus our attention on the integral defined within a bounded volume $\Omega$:

$$
I_\Omega := \int\limits_\Omega ik_0\hat{\rho}(x',\omega)e^{iRk_0}Rdx'.
$$

Notice that the integral we are looking for, is the limit case when $\Omega \to \mathbb{R}^3$. Next, we will make use of the continuity equation in the frequency domain:

$$
i\omega\hat{\rho}(x',\omega) = \vec{\nabla}' \cdot \hat{j} 
$$

and by defining the function:

$$
F(R) := \frac{e^{iRk_0}}{cR^2}
$$

the integral $I_\Omega$ Eq. (5.45) can be written in a more compact way (omitting the $x'$, $R$ and $\omega$ dependencies) as:

$$
I_\Omega := \int\limits_\Omega F\vec{\nabla}' \cdot \hat{j}Rdx'.
$$

It is very important to remark here that the divergence is being taken with respect to the primed coordinates. Due to the fact that we are working with Cartesian coordinates, it is possible to write

$$
R = x - x' = \sum_{\eta=x,y,z} (\eta - \eta')e_\eta
$$

and then:

$$
I_\Omega = \sum_{\eta=x,y,z} (\eta - \eta') F\vec{\nabla}' \cdot \hat{j}dx'e_\eta = \sum_{\eta=x,y,z} I_{\Omega,\eta}e_\eta.
$$

Each one of these $\eta$ integrals can be evaluated by means of the identity $(\eta - \eta') F\vec{\nabla}' \cdot \hat{j} = \vec{\nabla}' \cdot [(\eta - \eta')F\hat{j}] - \hat{j} \cdot \vec{\nabla}'[(\eta - \eta')F]$ and the Green-Ostrogradsky’s theorem [42, 50] as follows:

$$
I_{\Omega,\eta} = \int\limits_{\partial\Omega}(\eta - \eta')F\hat{j} \cdot n_{out}|_{\partial\Omega}dx' - \int\limits_{\Omega} \hat{j} \cdot \vec{\nabla}'[(\eta - \eta')F]dx'
$$
Taking the limit $\Omega \to \mathbb{R}^3$ and keeping in mind that the boundary term vanishes as $\frac{1}{R}$ we have:

$$I_{\mathbb{R}^3, \eta} = - \int_{\mathbb{R}^3} \hat{j} \cdot \vec{\nabla}'[(\eta - \eta') F] \, dx'. \quad (5.52)$$

The gradient (with respect to the primed coordinates) can be computed explicitly:

$$\vec{\nabla}'[(\eta - \eta') F] = F\vec{\nabla}'(\eta - \eta') + (\eta - \eta')\vec{\nabla}' F \quad (5.53)$$

and then

$$I_{\mathbb{R}^3, \eta} = \int_{\mathbb{R}^3} F\hat{j} \cdot e_\eta + (\eta - \eta')\hat{j} \cdot R\left(\frac{ik_0}{R} - \frac{2}{R^2}\right) F \, dx'. \quad (5.55)$$

Plugging Eq. (5.55) into Eq. (5.50) we get:

$$I_{\mathbb{R}^3} = \int_{\mathbb{R}^3} \left[\hat{j} + R(\hat{j} \cdot R)\left(\frac{ik_0}{R} - \frac{2}{R^2}\right)\right] F \, dx'. \quad (5.56)$$

Before taking the inverse Fourier transform, we will try to express the term between square brackets (which we will call $J$) in a more illuminating way. First, we rearrange $J$ in the following way:

$$J = \hat{j} - R(\hat{j} \cdot R)\frac{2}{R^2} + ik_0 R(\hat{j} \cdot R) \quad (5.57)$$

Now we consider the vector identity $(\hat{j} \times R) \times R = R(\hat{j} \cdot R) - R^2\hat{j}$ [50], and from this we have:

$$R(\hat{j} \cdot R) = (\hat{j} \times R) \times R + R\hat{j}, \quad (5.58)$$

$$\hat{j} - 2 \frac{R(\hat{j} \cdot R)}{R^2} = - \frac{(\hat{j} \times R) \times R}{R^2} - \frac{R(\hat{j} \cdot R)}{R^2}. \quad (5.59)$$

Then $J$ can be seen as:

$$J = - \left[\frac{(\hat{j} \times R) \times R}{R^2} + \frac{R(\hat{j} \cdot R)}{R^2}\right] + ik_0 \left[\frac{(\hat{j} \times R) \times R}{R} + R\hat{j}\right] \quad (5.60)$$
Substituting this result into Eq. (5.56) and then plugging that new integral into Eq. (5.44) we finally arrive to the expression:

\[
-\nabla \hat{\phi} = \frac{1}{4\pi\epsilon_0} \int_{\mathbb{R}^3} \rho(x', t_r) \frac{e^{ik_0 x'R}}{R^3} dx' \\
- \frac{1}{4\pi\epsilon_0 c} \int_{\mathbb{R}^3} ik_0 \left( \hat{j} \times \frac{R}{R^3} \right) e^{ik_0 x'R} dx' \\
+ \frac{1}{4\pi\epsilon_0 c} \int_{\mathbb{R}^3} \left[ \hat{j} \times \frac{R}{R^4} + \frac{R(\hat{j} \cdot R)}{R^4} \right] e^{ik_0 x'R} dx' \\
- \frac{1}{4\pi\epsilon_0 c} \int_{\mathbb{R}^3} ik_0 \hat{j} \left( \omega, x' \right) \frac{e^{ik_0 x'R}}{R^3} dx' 
\]

(5.61)

From Eq. (5.43) we recognize the last integral as \(-i\omega \hat{A}\) and then, after taking the inverse Fourier transform, we get:

\[
E = E_c + E_{int} + E_{rad} 
\]

(5.62)

where \(E_c\) is the Coulomb field, \(E_{int}\) the intermediate field and \(E_{rad}\) the radiated field given by the integrals:

\[
E_c = \frac{1}{4\pi\epsilon_0} \int_{\mathbb{R}^3} \frac{\rho(x', t_r)}{R^3} R dx' 
\]

(5.63)

\[
E_{int} = \frac{1}{4\pi\epsilon_0 c} \int_{\mathbb{R}^3} \left[ \hat{j}(x', t_r) \times \frac{R}{R^4} + \frac{R(\hat{j} \cdot R)}{R^4} \right] dx' 
\]

(5.64)

\[
E_{rad} = \frac{1}{4\pi\epsilon_0 c^2} \int_{\mathbb{R}^3} \frac{\partial_t \hat{j}(x', t_r) \times R}{R^3} dx' 
\]

(5.65)

At this point the reader may wonder the reason why we made all these extra steps when the Jefimenko’s equations already provide an explicit expression for the electric field. The reason is that in the case of the Jefimenko’s equations, the magnetic field is terms of the electric current \(j\) and the electric field is in terms of the distribution of charges \(\rho\) [21, 20]. This point of view albeit intuitively is very clear, makes difficult to compare the terms corresponding to the radiation field. By making the manipulations described above, we have ensured the fact that the intermediated and radiated electric and magnetic fields are all just in terms of the electric current. Thus utility of this approach will be shown later.
5.4 The Liénard-Wiechert’s Fields

The academic problem of describing the electric and magnetic induction fields generated by a particle that moves along a given trajectory \( u(t) \) which are called the Liénard-Wiechert fields, has been studied in many books [2, 20, 22, 23, 24, 25]. The basic idea is to consider a charge density and an electric current given by:

\[
\rho(x, t) = q\delta(x - u(t)), \quad (5.66)
\]
\[
j(x, t) = q\delta(x - u(t))v(t), \quad (5.67)
\]

where \( v(t) = \dot{u}(t) \). And from here there are many ways to tackle the problem of obtaining \( E \) and \( B \): Jackson [2] and Landau [22] consider an elegant formalism using quadrivector approach. Panofsky [25] and Heald [23] use the so called Liénard-Wiechert potentials which can be obtained by direct substitution on equations (5.28-5.29) and then carrying all the necessary derivatives. The deduction of the fields \( E \) and \( B \) following this procedure can be seen in [20]. For this section we have decided not to follow any of these approaches, but rather to proceed by direct substitution of the sources Eq. (5.66) and Eq. (5.67) into equations (5.40-5.41) and (5.63-5.65), that is:

\[
B_{\text{int}} = \frac{qc\mu_0}{4\pi} \int_{R^3} \delta(x' - u) \frac{\beta \times n}{R^2} dx', \quad (5.68)
\]
\[
B_{\text{rad}} = \frac{qc\mu_0}{4\pi} \frac{\partial}{\partial t} \int_{R^3} \delta(x' - u) \frac{\beta \times n}{cR} dx', \quad (5.69)
\]
\[
E_c = \frac{q}{4\pi\epsilon_0} \int_{R^3} \frac{\delta(x' - u)}{R^2} n dx', \quad (5.70)
\]
\[
E_{\text{int}} = \frac{q}{4\pi\epsilon_0} \int_{R^3} \frac{\delta(x' - u)}{R^2} [(\beta \times n) \times n + (\beta \cdot n) n] dx', \quad (5.71)
\]
\[
E_{\text{rad}} = \frac{q}{4\pi\epsilon_0} \frac{\partial}{\partial t} \int_{R^3} \frac{\delta(x' - u)}{cR} (\beta \times n) \times n dx', \quad (5.72)
\]

where we have introduced the following short hand conventions:

\[
\beta = \frac{v}{c}, \quad n = \frac{R}{R}. \quad (5.73)
\]

The procedure that we are going to show, follows the ideas expressed by Heald and Marion in [24], the main difference is that while Heald and Marion consider the Jefimenko’s equations, we are going to use equations (5.68-5.72). We have decided to put the full deduction of the Liénard-Wiechert
fields because as far as we have seen this result is quoted but the steps towards its obtention are not shown. Griffiths just states that the deduction is very difficult and Heald and Marion say that it is necessary to perform heroic algebra. Therefore, we believe that it is important to show, as best as we can, how to obtain one of the main results in classical electrodynamics.

In order to fix ideas, we are going to deal just with $B_{int}$ in Eq. (5.68). At first sight it would be tempting to just evaluate everything at $x' = u$. However, it is important to remember that $u$, and $n$ are functions of the retarded time $t_r$ which is defined as:

$$t_r = t - \frac{|x - u(t_r)|}{c} \quad (5.74)$$

A change of strategy is then necessary, instead of asking in Eq. (5.68) which $x'$ makes $x' - u = 0$ for each $t_r$, we ask which $t_r$ satisfies the transcendental equation (5.74) for each $t$, the present time, and the given trajectory $u$ [24]. Mathematically, the space integral in Eq. (5.68) is equivalent to:

$$B_{int} = \frac{c\mu_0}{4\pi} \int \delta \left(t_r - t + \frac{|x - u(t_r)|}{c}\right) \beta \times n \frac{R^2}{R} dt_r. \quad (5.75)$$

The next step to evaluate this integral, is to perform a change of variable with respect to the argument of the delta distribution:

$$\tau = t_r - t + \frac{|x - u(t_r)|}{c}. \quad (5.76)$$

Then, the differential $d\tau$ is given by:

$$d\tau = dt_r \left[1 + \frac{1}{c} \frac{d}{dt_r}|x - u(t_r)|\right]. \quad (5.77)$$

The derivative of $|x - u(t_r)|$ with respect to the retarded time, can be easily computed by remembering that:

$$\frac{d}{dt_r}|x - u(t_r)|^2 = \frac{d}{dt_r}(x - u(t_r)) \cdot (x - u(t_r)), \quad (5.78)$$

and taking the derivative from both sides we have:

$$2|x - u(t_r)| \frac{d}{dt_r}|x - u(t_r)| = -2v(t_r) \cdot (x - u(t_r)), \quad (5.79)$$
which after some elementary manipulations gives:
\[
\frac{d}{dt_r} |x - u(t_r)| = -v(t_r) \cdot n(t_r),
\]
(5.80)

and by defining \( K := 1 - \beta(t_r) \cdot n(t_r) \) we finally obtain:
\[
d\tau = dt_r [1 - \beta(t_r) \cdot n(t_r)] = dt_r K.
\]
(5.81)

Thus, the intermediate magnetic induction field is:
\[
B_{int} = \frac{qc\mu_0}{4\pi} \int_R \delta(\tau) \frac{\beta \times n}{KR^2} d\tau = \frac{qc\mu_0}{4\pi} \frac{\beta \times n}{KR^2} \bigg|_{\tau=0},
\]
(5.82)

where due to the fact that \( \tau = 0 \) we have the retarded time defined implicitly as in Eq. (5.75).

*Mutatis mutandis*, this procedure can be repeated for the other fields in equations (5.69-5.72). Then, the total electric and magnetic induction fields read:
\[
B = \frac{qc\mu_0}{4\pi} \left[ \left( \frac{\beta \times n}{KR^2} \right) \bigg|_{t_r} + \partial_t \left( \frac{\beta \times n}{cKR} \bigg|_{t_r} \right) \right],
\]
(5.83)
\[
E = \frac{q}{4\pi\varepsilon_0} \left[ \left( \frac{\beta \times n}{KR^2} \times n \right) \bigg|_{t_r} + \partial_t \left( \frac{\beta \times n}{cKR} \times n \bigg|_{t_r} \right) \right] + \frac{q}{4\pi\varepsilon_0} \left( \frac{1 + n \cdot \beta}{KR^2} \right) \bigg|_{t_r}.
\]
(5.84)

Now, it is necessary to compute the derivatives with respect to the present time \( t \). Assuming the convention that the doted quantities denote partial derivation with respect to time \( t \), the following identities will be useful:
\[
\dot{R} = \partial_t(x - u(t_r)) = -\frac{dt_r}{dt} v(t_r) = -c \frac{dt_r}{dt} \beta(t_r)
\]
(5.85)
\[
\dot{R} = \partial_t(\sqrt{R \cdot R}) = \frac{1}{R} R \cdot \dot{R} = -c(n \cdot \beta) \frac{dt_r}{dt}
\]
(5.86)
\[
= c \partial_t(t - t_r) = c \left( 1 - \frac{dt_r}{dt} \right)
\]
(5.87)

from Eq. (5.86) and Eq. (5.87) one can solve for:
\[
\frac{dt_r}{dt} = \frac{1}{1 - n \cdot \beta} = \frac{1}{K'}
\]
(5.88)
and upon substitution of Eq. (5.88) into Eq. (5.86) and Eq. (5.87) one gets:

\[
\dot{R} = \partial_t (x - u(t_r)) = -\frac{\partial t_r}{\partial t} v(t_r) = -\frac{c}{K} \beta \tag{5.89}
\]

\[
\dot{\mathbf{R}} = \partial_t (\sqrt{\mathbf{R} \cdot \mathbf{R}}) = \frac{1}{R} \mathbf{R} \cdot \dot{\mathbf{R}} = -\frac{c}{K} (\mathbf{n} \cdot \beta) \tag{5.90}
\]

\[
\dot{R} = c \partial_t (t - t_r) = c \left( 1 - \frac{1}{K} \right) \tag{5.91}
\]

From the expression \( \mathbf{R} \mathbf{n} = \mathbf{R} \) we can derive with respect to \( t \) and after some manipulations we obtain:

\[
\dot{\mathbf{n}} = \frac{1}{R} [\dot{\mathbf{R}} - \dot{\mathbf{R}} \mathbf{n}] = \frac{1}{R} \left[ -\frac{c}{K} \beta - c \left( 1 - \frac{1}{K} \right) \mathbf{n} \right] = -\frac{c}{KR} \left[ (K-1) \mathbf{n} + \beta \right]. \tag{5.92}
\]

In addition, we have:

\[
\dot{\beta} = \frac{a}{Kc} \tag{5.93}
\]

and

\[
\dot{K} = -\partial_t (\beta \cdot \mathbf{n}) = -\dot{\beta} \cdot \mathbf{n} - \beta \cdot \dot{\mathbf{n}}
\]

\[
= -\frac{a \cdot \mathbf{n}}{Kc} + \frac{c}{KR} \left[ (K-1) \beta \cdot \mathbf{n} + \beta^2 \right]
\]

\[
= -\frac{a \cdot \mathbf{n}}{Kc} + \frac{c}{KR} \left[ \beta^2 - (K-1)^2 \right] \tag{5.94}
\]

Using these identities, we will first deal with \( \mathbf{B} \) in Eq. (5.83):

\[
\mathbf{B} = \frac{qa \mu_0}{4\pi} \left[ \frac{\mathbf{M}}{R} + \frac{\dot{\mathbf{M}}}{c} \right], \tag{5.95}
\]

where we have defined:

\[
\mathbf{M} := \frac{\beta \times \mathbf{n}}{KR}. \tag{5.96}
\]

It is then necessary to calculate the derivative of \( \mathbf{M} \):

\[
\dot{\mathbf{M}} = \frac{1}{KR} \left[ \partial_t (\beta \times \mathbf{n}) - \mathbf{M} \partial_t (KR) \right]. \tag{5.97}
\]

The first derivative in the right hand side of Eq. (5.97) is:

\[
\partial_t (\beta \times \mathbf{n}) = \dot{\beta} \times \mathbf{n} + \beta \times \dot{\mathbf{n}},
\]

\[
= \frac{a \times \mathbf{n}}{Kc} - \frac{c}{KR} \left[ (K-1) \beta \times \mathbf{n} + \beta \times \beta \right],
\]

\[
= \frac{a \times \mathbf{n}}{Kc} - c(K-1) \mathbf{M}, \tag{5.98}
\]
and the second one is given by:

\[ \partial_t (K R) = \dot{K} R + \dot{R} K, \]

\[ = - a \cdot \frac{n}{K c} R + c \frac{1}{K} [\beta^2 - (K - 1)^2] + c(K - 1), \]

\[ - a \cdot \frac{n}{K c} R + c \frac{1}{K} [\beta^2 - 1] + c. \]  

(5.99)

Plugging Eq. (5.98) and Eq. (5.99) into Eq. (5.97) we obtain:

\[ \dot{M} = \left[ a \times \frac{n}{K^2 R c} - \frac{M}{R} + \frac{M a \cdot n}{c K^2} + c \frac{1}{K^2 R} [1 - \beta^2] M \right] + c(K - 1), \]  

(5.100)

and substituting Eq. (5.100) into Eq. (5.95) we obtain the Liénard-Wiechert magnetic induction field:

\[ B = \frac{q c \mu_0}{4 \pi} \left[ \frac{a \times n}{K^2 R c^2} + \frac{a \cdot n (\beta \times n)}{c^2 K^3 R} + \frac{(1 - \beta^2) (\beta \times n)}{K^3 R^2} \right] \times n. \]  

(5.101)

For the case of the electric field, we start again by expressing Eq. (5.84) in terms of Eq. (5.96):

\[ E = \frac{q}{4 \pi \varepsilon_0} \left[ \left( \frac{M}{R} + \frac{\dot{M}}{c} \right) \times n + \frac{M}{c} \times \hat{n} + \frac{2 - K}{K R^2} n \right] \times n. \]  

(5.102)

Then, we consider the second term in the right hand side of Eq. (5.102):

\[ \frac{M}{c} \times \hat{n} = - \frac{[(K - 1)(\beta \times n) \times n + (\beta \times n) \times \beta]}{K^2 R^2}, \]

\[ = - \frac{[(K - 1)(n(\beta \cdot n) - \beta) - (\beta(\beta \cdot n) - \beta^2 n)]}{K^2 R^2}, \]

and using \( 1 - K = \beta \cdot n \)

\[ \frac{M}{c} \times \hat{n} = - \frac{[(K - 1)(n - 1) - \beta) - (\beta(1 - K) - \beta^2 n)]}{K^2 R^2}, \]

\[ = - \frac{n}{K^2 R^2} (\beta^2 - (K - 1)^2), \]

\[ = - \frac{2 - K}{K R^2} n + \frac{n}{K^2 R^2} (1 - \beta^2). \]  

(5.103)

Notice that the first term in Eq. (5.103) is going to cancel with the third term in Eq. (5.102). Then, we can focus our attention in the first term of Eq. (5.102):

\[ \left( \frac{M}{R} + \frac{\dot{M}}{c} \right) \times n = \left[ \frac{a \times n}{K^2 R c^2} + \frac{a \cdot n (\beta \times n)}{c^2 K^3 R} + \frac{(1 - \beta^2) (\beta \times n)}{K^3 R^2} \right] \times n \]  

(5.104)
Let us work with the first two terms of Eq. (5.104):
\[
\left[ \frac{a \times n + a \cdot n (\beta \times n)}{K^2 R c^2} \right] \times n = \frac{[K(a \times n) + a \cdot n (\beta \times n)]}{c^2 K^3 R} \times n,
\]
\[
= \frac{[(1 - \beta \cdot n)(a \times n) + a \cdot n (\beta \times n)]}{c^2 K^3 R} \times n.
\]

Now, by means of the vector identity
\[
A \cdot (B \times C)D = (A \cdot D)(B \times C) + (B \cdot D)(C \times A) + (C \cdot D)(A \times D)
\]
and letting \(A = a, B = \beta, \) and \(C = D = n\) we have:
\[
\left[ \frac{a \times n + a \cdot n (\beta \times n)}{K^2 R c^2} \right] \times n = \frac{[a \times n - \beta \times n + a \cdot (\beta \times n)n]}{c^2 K^3 R} \times n,
\]
\[
= \frac{a \times (n - \beta) \times n}{c^2 K^3 R}.
\]

On the other hand, the third term on Eq. (5.104) can be seen as:
\[
\frac{(1 - \beta^2)(\beta \times n)}{K^3 R^2} \times n = \frac{(1 - \beta^2)(n(1 - K) - \beta)}{K^3 R^2},
\]
\[
= \frac{(1 - \beta^2)(n - \beta)}{K^3 R^2} - \frac{(1 - \beta^2)n}{K^2 R^2}
\]

Putting Eq. (5.105), and Eq. (5.106) into Eq. (5.104) and then plugging this result and Eq. (5.103) into Eq. (5.102), we finally obtain the electric Liénard-Wiechert field:
\[
E = \frac{q}{4 \pi \epsilon_0} \left[ \frac{(1 - \beta^2)(n - \beta)}{K^3 R^2} + \frac{a \times (n - \beta) \times n}{c^2 K^3 R} \right] t_r
\]

We can see that these are the same results as obtained by Griffiths [20] and Heald and Marion [24].

The case of an oscillating particle
Once the fields \(E\) and \(B\) are given by Eq. (5.107) and Eq. (5.101) respectively, it would be easy to think that the fields produced by an oscillating particle could be retrieved by considering the trajectory:
\[
u(t_r) = a \cos(\omega_0 t_r)e_z,
\]
where \(a\) and \(\omega_0\) are the oscillation amplitude and frequency respectively. Nevertheless, as pointed by Spohn in [23], the Liénard Wiechert fields are
less explicit than they appear to be. This is due to the fact that Eq. (5.107) and Eq. (5.101) depend on the retarded time which is still itself a solution of a (in general non trivial) transcendental equation, namely:

\[ t_r = t - \frac{|x - a \cos(\omega_0 t_r) e_z|}{c}. \] (5.109)

Let us notice here that if the particle is at constant speed with a straight trajectory, the Liénard Wiechert fields can be almost straightforwardly. However, the solution of this problem, when dealing with an oscillating charge, in this case the retarded time is a function of the present time and the position \( (t_r := t_r(t, x)) \). The solution of this problem is a matter of the next section.

### 5.5 Harmonic decomposition of the sources

As we saw in the previous section, the Liénard-Wiechert fields are not the best way to obtain the fields produced by an oscillating particle. The main problem is that the source terms depend on the trajectory that describes the charge. For this reason it will be convenient to find a way to decompose the source terms in a polyharmonic way. This idea has been previously considered by Landau [22]. However, by going from a continuous charge distribution to point charges, Landau repeats more or less the same arguments that were used when the Liénard-Wiechert fields were deduced. The only difference is that this deduction is done for each one of the multiples of the fundamental frequency \( \omega_0 \). The expected problem is the same as in previous section: the resolution of a transcendental equation for the retarded time.

In this section we propose another way inspired in quantum mechanics, which can be summarized as: The superposition of waves spread in a certain domain can be seen as a particle. Physically, this means that a very localized source can be seen as the interference of a certain kind of waves. Mathematically speaking, we are looking to find a sequence such that, we can have convergence in the sense of distributions to a Dirac delta [26, 27, 28].
Two Fourier expansions for the sources

Let us start our analysis by having the charge density $\rho$ and its current density $j$ simply given by:

$$\rho(x, t) = q \delta(x_\perp) \otimes \varrho(z, t),$$  \hspace{1cm} (5.110)

with $\varrho(z, t) := \delta(z - a \cos(\omega_0 t))$ and

$$j(x, t) = q \delta(x_\perp) \otimes j(z, t) e^z,$$  \hspace{1cm} (5.111)

with $j(z, t) := -a \omega_0 \sin(\omega_0 t) \varrho(z, t)$ out of charge conservation. Notice that $\varrho$ and $j$ are not multiplied by the charge. It then turns out that the charge density is not harmonic despite the harmonic motion of the particle. In other words, no complex function $\varrho(z)$ can be found in such a way that $\varrho(z, t) = \Re\{\varrho(z)e^{i\omega t}\}$. Nevertheless it is apropos to notice that the distribution $\varrho(z, \cdot)$ is a $2\pi/\omega_0$-periodic distribution. Thus, it can be written as a Fourier series:

$$\varrho(z, t) = \sum_{l \in \mathbb{Z}} c_l(z) e^{i\omega lt},$$  \hspace{1cm} (5.112)

It remains to compute the functions $c_l(z)$. For this, the distribution $\varrho(z, t)$ has to be considered as a $\delta$-distribution of a function $f(t) := z - a \cos(\omega_0 t)$. Using the expansion given in [85, 2], we obtain:

$$\varrho(z, t) = \delta(f(t)) = \sum_{l \in \mathbb{Z}} \frac{1}{f(t_l)} \delta(t - t_l),$$  \hspace{1cm} (5.113)

where $t_l$ are the zeros of the function $f(t)$, i.e.

$$\cos(\omega_0 t) = \frac{z}{a}.$$  \hspace{1cm} (5.114)

Given the fact that the absolute value of the cosine is bounded by 1, there are only two solutions within the range $[-a, a]$. Then, by considering the principal branch of the arc cosine function and denoting $t_0(z) := \frac{1}{\omega_0} \arccos\left(\frac{z}{a}\right)$, these zeros are

$$t_l^+(z) = t_0(z) + 2l\pi/\omega_0, \hspace{2cm} (5.115)$$
$$t_l^-(z) = -t_0(z) + 2l\pi/\omega_0.$$  \hspace{1cm} (5.116)
In addition, it turns out that for every \( t_l \) (\( t_l^+ \) or \( t_l^- \)) \( |\dot{f}(t)| = \omega_0 \sqrt{a^2 - z^2} \) and the \( \delta \)-distribution reads:

\[
\varrho(z, t) = \delta(f(t)) = \frac{1}{\omega_0 \sqrt{a^2 - z^2}} (W_+(t) + W_-(t)) \chi_{[-a,a]}(z), \tag{5.117}
\]

where \( W_\pm(t, z) = \sum_{l \in \mathbb{Z}} \delta(t - t^\pm(l)) \). These last two series of distributions (Dirac’s combs) are expandable in a Fourier series as follows [86]:

\[
W_\pm(t, z) = \sum_{l \in \mathbb{Z}} \delta\left(t \mp t_0(z) - \frac{2\pi l}{\omega_0}\right) = \sum_{m \in \mathbb{Z}} \Phi^\pm_m e^{im\Phi t_0}, \tag{5.118}
\]

with \( T_0 = \frac{\pi}{\omega_0} \). Making the change of variables \( t = \tau \pm t_0(z) \) one gets:

\[
\sum_{l \in \mathbb{Z}} \delta(\tau - 2lT_0) = \sum_{m \in \mathbb{Z}} \Phi^\pm_m e^{im\Phi T_0 (\tau \pm t_0(z))}. \tag{5.119}
\]

Multiplying this equation by \( e^{-i\frac{\Phi}{T_0}(\tau \pm t_0(z))} \), taking the integral from \(-T_0\) to \(T_0\) and performing the change of variables \( \sigma = \tau - 2lT_0 \), equation (5.119) can be rewritten as:

\[
\sum_{l \in \mathbb{Z}} \int_{-2l+1T_0}^{2l+1T_0} \delta(\sigma) e^{-im\Phi \frac{\sigma}{T_0}} e^{+im\frac{\Phi}{T_0}(\tau \pm t_0(z))} d\sigma = 2T_0 \Phi^\pm_m. \tag{5.120}
\]

or in a more illuminating way

\[
e^{+im\frac{\Phi}{T_0}(\tau \pm t_0(z))} \int_{-\infty}^{+\infty} \delta(\sigma) e^{-im\Phi \frac{\sigma}{T_0}} d\sigma = 2T_0 \Phi^\pm_m, \tag{5.121}
\]

which implies

\[
\Phi^\pm_m = \frac{1}{2T_0} e^{+im\frac{\Phi}{T_0}(\tau \pm t_0(z))} \frac{\omega_0}{2\pi} e^{+im\omega_0 t_0(z)}. \tag{5.122}
\]

Then

\[
W_\pm(t, z) = \frac{\omega_0}{2\pi} e^{+im\omega_0 t_0(z)} e^{im\omega_0 t}, \tag{5.123}
\]

and naturally (recovering the \( l \) index)

\[
W_+(t, z) + W_-(t, z) = \frac{\omega_0}{2\pi} \sum_{l \in \mathbb{Z}} \left[ e^{il\omega_0 t_0(z)} + e^{-il\omega_0 t_0(z)} \right] e^{im\omega_0 t}, \tag{5.124}
\]

\[
= \frac{\omega_0}{\pi} \sum_{l \in \mathbb{Z}} \cos(l\omega_0 t_0(z)) e^{il\omega_0 t}. \tag{5.125}
\]

Remembering the definition of \( t_0 \) one gets:

\[
\cos(l\omega_0 t_0) = \cos \left( l \arccos \left( \frac{z}{a} \right) \right) = T_l \left( \frac{z}{a} \right), \tag{5.126}
\]
where $T_l$ are the Chebyshev polynomials of first kind. Therefore

$$W_+(t,z) + W_-(t,z) = \sum_{l \in \mathbb{Z}} T_l\left(\frac{z}{a}\right) e^{i\omega_0 l t}$$  \hspace{1cm} (5.127)

Plugging this equation into Eq. (5.117) and defining the function

$$w(z) := \frac{1}{\pi \sqrt{a^2 - z^2}} X_{[-a,a]}(z),$$  \hspace{1cm} (5.128)

the function $\varrho$ reads

$$\varrho(z, t) = \sum_{l \in \mathbb{Z}} w(z) T_l\left(\frac{z}{a}\right) e^{i\omega_0 l t}. \hspace{1cm} (5.129)$$

As a consequence of this, the function $j$ is given by

$$j(z, t) = -a\omega_0 \sin(\omega_0 t) \sum_{l \in \mathbb{Z}} w(z) T_l\left(\frac{z}{a}\right) e^{i\omega_0 l t}. \hspace{1cm} (5.130)$$

In short, $\varrho$ and $j$ are in the following form

$$\varrho(z, t) = \sum_{l \in \mathbb{Z}} \varrho_l^F(z, t), \quad j(z, t) = \sum_{l \in \mathbb{Z}} j_l^F(z, t), \hspace{1cm} (5.131)$$

with

$$\varrho_l^F(z, t) = w(z) T_l\left(\frac{z}{a}\right) e^{i\omega_0 l t}, \hspace{1cm} (5.132)$$

$$j_l^F(z, t) = -a\omega_0 \sin(\omega_0 t) w(z) T_l\left(\frac{z}{a}\right) e^{i\omega_0 l t}. \hspace{1cm} (5.133)$$

On the other hand, the Fourier transform $\varrho(z, t) := \delta(z - a \cos(\omega_0 t))$ can be derived by considering the convention:

$$\hat{\varrho}(k, t) = \mathcal{F}_{z \rightarrow k}\{\delta(z - a \cos(\omega_0 t))\} = \frac{1}{2\pi} \int_{z \in \mathbb{R}} \delta(z - a \cos(\omega_0 t)) e^{izk} dz.$$  \hspace{1cm} (5.134)

After a suitable change of variable ($\sigma = z - a \cos(\omega_0 t)$) we obtain that:

$$\hat{\varrho}(k, t) = \frac{1}{2\pi} e^{ia\cos(\omega_0 t)k} = \frac{1}{2\pi} \sum_{l \in \mathbb{Z}} i^l f_l(ka) e^{i\omega_0 l t}, \hspace{1cm} (5.135)$$

where the last equality comes from the generating function of the Bessel's functions [87, 64, 76]. Taking the Fourier transform of Eq. (5.129) and keeping in mind that these two Fourier series are equal term by term we arrive to this beautiful and unexpected expression:

$$\mathcal{F}_{z \rightarrow k}\{w(z) T_l\left(\frac{z}{a}\right)\} = i^l \frac{1}{2\pi} f_l(ka) \hspace{1cm} (5.136)$$

which will be used later.
Continuity equation for the harmonic components of the sources

In the previous paragraph, an expansion for $\rho$ and $j$ are linked by the so-called charge conservation, namely: $\vec{\nabla} \cdot j + \dot{\rho} = 0$. Notice that for moving point particles this equation has to be understood in the sense of distributions $[42, 26, 27, 28]$. What about the different components $\rho_l$ and $j_l$? In other words, is there any transference of energy, between the different waves oscillating with the different frequencies at stake $\omega_0, 2\omega_0, \text{etc.}$? To answer this question, we have to care much more about the notation referring this $l$. While $\rho^T_F(z, t)$ oscillates with frequency $l\omega_0$, the $j^T_F(z, t)$ is a mix of two oscillations with different frequencies namely $(l-1)\omega_0$ and $(l+1)\omega_0$ due to the presence of $\sin(\omega_0 t)$ term in Eq. (5.133). Making use of the complex representation of $\sin(\omega_0 t)$ it follows:

$$j(z, t) = \sum_{l \in \mathbb{Z}} j^T_F(z, t) = \sum_{l \in \mathbb{Z}} \frac{d\omega_0}{2i} \omega(z) T_l(z) \frac{e^{i(l-1)\omega_0 t} - e^{i(l+1)\omega_0 t}}{a_0}. \quad (5.137)$$

The expected terms oscillating at the frequency $l\omega_0$ (where $l$ is a dummy index) are given by the Fourier series:

$$j(z, t) = \sum_{l \in \mathbb{Z}} j^T_F(z) e^{+il\omega_0 t}. \quad (5.138)$$

After renaming indices $(l-1 \to l$ and $l+1 \to l)$ we obtain:

$$j^T_F(z) := \frac{d\omega_0}{2i} \frac{\Xi_{l+1}(z) - \Xi_{l-1}(z)}{a_0}, \quad (5.139)$$

where $\Xi_l(z) = w(z) T_l(z)$. Analogously for $\rho$ we get:

$$\rho(z, t) = \sum_{l \in \mathbb{Z}} \rho^T_F(z, t) = \sum_{l \in \mathbb{Z}} \rho^T_F(z) e^{+il\omega_0 t} = \sum_{l \in \mathbb{Z}} \Xi_l(z) e^{+il\omega_0 t}. \quad (5.140)$$

The arcane meaning of the superscripts $T$ and $F$ is therefore clear: $T$ (resp. $F$) means true (resp. false) in the sense that each spatial coefficient corresponds to only one $l \in \mathbb{Z}$. Correspondingly the conservation of charge can be now formulated for each multiple of the frequency $\omega_0$. By the definition of $\rho(x, t)$ and $j(x, t)$ The conservation of charge implies:

$$\partial_t \rho(z, t) + \partial_z j(z, t) = 0, \quad (5.141)$$
and plugging the harmonic expansions of \( \varrho(z, t) \) and \( j(z, t) \)

\[
\sum_{l \in \mathbb{Z}} \left[ il\omega_0 \Xi_l(z) + \frac{a\omega_0}{2i} \partial_z (\Xi_{l+1}(z) - \Xi_{l-1}(z)) \right] e^{+il\omega_0 t} = 0. \tag{5.142}
\]

Given the fact that \( e^{+il\omega_0 t} \) with \( (l \in \mathbb{Z}) \) is a basis \([26, 27]\), all the terms between square brackets are equal to zero. Thus the following identity is obtained:

\[
l \Xi_l(z) = \frac{a}{2} \partial_z (\Xi_{l+1}(z) - \Xi_{l-1}(z)). \tag{5.143}
\]

And the conservation of charge for each \( l \) follows.

### 5.6 Polyharmonic computations

The main consequence of the harmonic decomposition of the sources and the conservation of charge term by term is that the electric and magnetic induction fields, respectively \( E \) and \( B \), can be also decomposed in terms of multiples of the fundamental frequency \( \omega_0 \). This section is devoted to this issue and before starting equations (5.40-5.41) and (5.63-5.65), with \( R = x - x' \), \( R = |R| \) and \( t_r = t - \frac{R}{c} \) the retarded time. It is important to remark here that \textbf{in this case the retarded time is not in terms of a transcendental equations but rather explicitly given in terms of the present time \( t \).}

After applying the delta distribution \( \delta(x') \) we get that \( E \) and \( B \) are given by:

\[
E(x, t) = \frac{1}{4\pi\epsilon_0} \int_{R} \frac{q}{cR^3} \left[ j(z', \tilde{t}_r) e_z \times \tilde{R} + \frac{\partial j(z', \tilde{t}_r)}{c} \right] (e_z \times \tilde{R}) \times \tilde{R} d\tilde{z}',
\]

\[
B(x, t) = \frac{\mu_0}{4\pi} \int_{R} \frac{q}{\tilde{R}^2} \left[ j(z', \tilde{t}_r) e_z + \frac{\partial j(z', \tilde{t}_r)}{c} \right] e_z \times \tilde{R} d\tilde{z}', \tag{5.145}
\]

where \( \tilde{R} = x - z'e_z \), \( \tilde{R} = |\tilde{R}| \) and \( \tilde{t}_r = t - \frac{\tilde{R}}{c} \). The next step is to define the functions:

\[
Q(z', \tilde{R}, \tilde{t}_r) := q(z', \tilde{t}_r) + j(z', \tilde{t}_r) \frac{e_z \cdot \tilde{R}}{\tilde{R}c}, \tag{5.146}
\]

\[
K(z', \tilde{R}, \tilde{t}_r) := \frac{j(z', \tilde{t}_r)}{\tilde{R}} + \frac{\partial j(z', \tilde{t}_r)}{c}. \tag{5.147}
\]
And then the electric and magnetic fields can be written in a more compact way as:

\[
E(x, t) = \frac{1}{4\pi\varepsilon_0} \int_{R} \frac{q}{c R^3} \left( cQ(z', \hat{R}, \hat{r})\hat{R} + K(z', \hat{R}, \hat{r})(e_z \times \hat{R}) \times \hat{R} \right) dz',
\]

(5.148)

\[
B(x, t) = \frac{\mu_0}{4\pi} \int_{R} \frac{q}{R^2} K(z', \hat{R}, \hat{r})e_z \times \hat{R} dz'.
\]

(5.149)

From the definitions of \(\varrho(z, t)\) in Eq. (5.135) and \(j(z, t)\) in Eq. (5.138) we have that equations (5.146) and (5.147) read:

\[
Q(z', \hat{R}, \hat{r}) = \sum_{l \in \mathbb{Z}} e^{+il\omega_0 t} Q_l(z', \hat{R}),
\]

(5.150)

\[
K(z', \hat{R}, \hat{r}) = \sum_{l \in \mathbb{Z}} e^{+il\omega_0 t} K_l(z', \hat{R}),
\]

(5.151)

where

\[
Q_l(z', \hat{R}) := \left[ q T_l(z') + j T_l(z') \frac{e_z \cdot \hat{R}}{R c} \right] e^{-ik_0 R},
\]

(5.152)

\[
K_l(z', \hat{R}) := \left[ \frac{1}{R} + \frac{il\omega_0}{c} \right] j T_l(z') e^{-ik_0 R}.
\]

(5.153)

Therefore \(E(x, t)\) and \(B(x, t)\) can be seen as a superposition of elementary harmonic terms, \textit{i.e.}:

\[
E(x, t) = \sum_{l \in \mathbb{Z}} e^{+il\omega_0 t} E_l(x),
\]

(5.154)

\[
B(x, t) = \sum_{l \in \mathbb{Z}} e^{+il\omega_0 t} B_l(x),
\]

(5.155)

with spatially dependent coefficients given by:

\[
E_l(x) = \frac{1}{4\pi\varepsilon_0} \int_{R} \frac{q}{c R^3} \left( cQ_l(z', \hat{R})\hat{R} + K_l(z', \hat{R})(e_z \times \hat{R}) \times \hat{R} \right) dz',
\]

(5.156)

\[
B_l(x) = \frac{\mu_0}{4\pi} \int_{R} \frac{q}{R^2} K_l(z', \hat{R})e_z \times \hat{R} dz'.
\]

(5.157)
A geometrical description of the fields

By using the vector identity \((\mathbf{e}_z \times \mathbf{R}) \times \mathbf{R} = (\mathbf{e}_z \cdot \mathbf{R})\mathbf{R} - \mathbf{R}^2 \mathbf{e}_z\) we can rewrite the spatial coefficients as per:

\[
\begin{align*}
E_l(x) &= \frac{1}{4\pi\varepsilon_0} \left\{ \int_{\mathbb{R}} \frac{q}{cR^3} \left[ cQ_l(z', R) + (z - z')K_l(z', R) \right] dz' \mathbf{x} \\
&\quad - \int_{\mathbb{R}} \frac{q}{cR^3} \left[ z' (cQ_l(z', R) + (z - z')K_l(z', R)) + K_l(z', R) R^2 \right] dz' \mathbf{e}_z \right\}, \\
&= \frac{\mu_0}{4\pi} \int_{\mathbb{R}} \frac{q}{R^2} K_l(z', R) \mathbf{e}_z \times \mathbf{x}_\perp dz',
\end{align*}
\]

(5.158)

\[
B_l(x) = \frac{\mu_0}{4\pi} \int_{\mathbb{R}} \frac{q}{R^2} K_l(z', R) \mathbf{e}_z \times \mathbf{x}_\perp dz',
\]

(5.159)

From this representation it is easy to see that the first integral term of \(E\), which will be called \(E_{sph}\), is a field with spherical symmetry. However due to the action of the second integral term, in the sequel \(E_{flat}\), the total field is flattened out in the direction perpendicular to the motion. On the other hand, the field lines of \(B\) circle around the \(z\)-axis and, as expected, are perpendicular to the field lines of the electric field. Figure 5.2 and (resp. 5.4) show imaginary (resp. real) part of the the harmonic field components \(E_l\) (resp. \(B_l\)) for \(l = 1, 2, 3, 4\). Whereas figure 5.6 represents the real part of the Poynting vector \(S_l = \frac{1}{2\mu_0} E_l\). Albeit the electric and magnetic fields seem to be more or less the same, the figures that show the fields at the canonical planes \(y = 0\) and \(x = 0\) reveal a quite different behavior, that is: the electric field shows the expected geometrical behavior (this is more evident for fig. 5.2d) and the magnetic field circles around the \(z\)-axis (see for instance fig. 5.4a ). Finally, the projection of the Poynting vector field on the canonical planes is shown in figure 5.7.
Fig. 5.2. Harmonic components of the electric field generated by an oscillating particle, $E_l$ for $l = 1, 2, 3, 4$
Fig. 5.3. Harmonic components of the electric field generated by an oscillating particle, $E_l$ for $l = 1, 2, 3, 4$ (cut in canonical planes view)
Fig. 5.4. Harmonic components of the real part of magnetic induction field generated by an oscillating particle, $B_l$, for $l = 1, 2, 3, 4$ (cut in canonical planes view)
Fig. 5.5. Harmonic components of the real part of magnetic induction field generated by an oscillating particle, $B_l$ for $l = 1, 2, 3, 4$ (cut in canonical planes view)
Fig. 5.6. Harmonic components of the real part of Poynting vector field generated by an oscillating particle, $S_l$, for $l = 1, 2, 3, 4$ (cut in canonical planes view)
Fig. 5.7. Harmonic components of the real part of Poynting vector field generated by an oscillating particle, $S_l$ for $l = 1, 2, 3, 4$ (cut in canonical planes view)
5.7 Far Field radiated power

As we know, the radiated electric and magnetic induction fields are given by:

\[
B_{\text{rad}} = q \frac{\mu_0}{4\pi c} \int_{R^3} \frac{\partial_t j(x', t_r)}{R} \times \frac{n}{R} d^3x',
\]

\[
E_{\text{rad}} = q \frac{1}{4\pi \epsilon_0 c^2} \int_{R^3} \frac{(\partial_t j(x', t_r) \times n)}{R} \times \frac{n}{R} d^3x',
\]

where \(n = \frac{R}{R'}\). Using the fact that the electric current is defined as \(j(x', t_r) := q\delta(x_\perp) \otimes j(z, t_r) e_z\), the fields read:

\[
B_{\text{rad}} \approx B_\infty = q \frac{\mu_0}{4\pi c} \int_{R} \frac{\partial_t j(z', \tau_r) e_z \times \hat{n}}{R} dz',
\]

\[
E_{\text{rad}} \approx E_\infty = q \frac{1}{4\pi \epsilon_0 c^2} \int_{R} \left( \frac{\partial_t j(z', \tau_r) \times \hat{n}}{R} \right) \times \hat{n} d^3z',
\]

and as we did before \(\vec{R} = x - z'e_z\), \(\vec{n} = \frac{\vec{R}}{R}\), and \(\tau_r = t - \frac{R}{c}\). Now, in order to compute the fields radiated at infinitum we make the following approximations for when \(|x'| \ll |x|\):

\[
\hat{n} \approx \frac{x}{|x|} = \nu,
\]

\[
\frac{1}{R} \approx \frac{1}{|x'|}
\]

\[
\tau_r \approx t - \frac{|x|}{c} + \left( \frac{z}{|x|} \right) \left( \frac{z'}{c} \right) = \tau_r.
\]

By plugging these approximations into equations (5.162) and (5.163), one arrives to the expressions:

\[
B_{\text{rad}} \approx B_\infty = q \frac{\mu_0}{4\pi c |x|} \int_{R} \partial_t j(z', \tau_r) dz' e_z \times \nu,
\]

\[
E_{\text{rad}} \approx E_\infty = q \frac{1}{4\pi \epsilon_0 c^2 |x|} \int_{R} \partial_t j(z', \tau_r) dz' (e_z \times \nu) \times \nu,
\]

\[
= c B_\infty \times \nu.
\]

From this last equation it is clear that we can focus our attention just in \(B_\infty\).

Remembering the definition of \(j(z', \tau_r)\) in Eq. (5.138) and \(\tau_r\) we have that

\[
B_\infty = \sum_{l \in \mathbb{Z}} e^{il\omega_0 t} B_l^\infty,
\]

(5.169)
with the spatial coefficient $B^l_{\infty}$ defined as:

$$B^l_{\infty} := i\omega_0 \frac{q}{4\pi c} \exp \left( -i k_0 |x| \right) \int_{R^3} j^T_l (z') \exp \left( i k_0 \frac{z}{|x|} z' \right) d'(e_z \times \nu), \quad (5.170)$$

Notice that the integral term resembles to a spatial Fourier transform that goes from $z' \rightarrow \eta_l$ with the new variable

$$\eta_l := l k_0 \frac{z}{|x|}. \quad (5.171)$$

Thus

$$B^l_{\infty} = i\omega_0 \frac{q}{4\pi c} \exp \left( -i k_0 |x| \right) 2\pi \mathcal{F}_{z' \rightarrow \eta_l} \{ j^T_l (z') \} (e_z \times \nu). \quad (5.172)$$

This Fourier transform can be easily computed by using the definition in Eq. (5.139):

$$2\pi \mathcal{F}_{z' \rightarrow \eta_l} \{ j^T_l (z') \} = 2\pi \left[ \mathcal{F}_{z' \rightarrow \eta_l} \{ \Xi_{l+1}(z') - \Xi_{l-1}(z') \} \right] \frac{\omega_0}{2i} \quad (5.173)$$

Fortunately, the Fourier transform of $\Xi_l$ is given in Eq. (5.136) and after using identity Eq. (D.2) one gets:

$$2\pi \mathcal{F}_{z' \rightarrow \eta_l} \{ j^T_l (z') \} = a l^l \omega_0 \frac{j_l(\eta l a)}{\eta l a}, \quad (5.174)$$

which implies that:

$$B^l_{\infty} = i^{l+1} \frac{q}{4\pi c} (l \omega_0)^2 \frac{a}{|x|} \exp \left( -i k_0 |x| \right) \frac{j_l(\eta l a)}{\eta l a} (e_z \times \nu). \quad (5.175)$$

Calling

$$A_l = i^{l+1} \frac{q}{4\pi c} (l \omega_0)^2 \frac{a}{|x|} \exp \left( -i k_0 |x| \right), \quad (5.176)$$

we get:

$$B^l_{\infty} = A_l \frac{j_l(\eta l a)}{\eta l a} (e_z \times \nu), \quad (5.177)$$

and its square norm is given by:

$$|B^l_{\infty}|^2 = |A_l|^2 \left[ \frac{j_l(\eta l a)}{\eta l a} \right]^2 \left[ 1 - \left( \frac{z}{|x|} \right)^2 \right], \quad (5.178)$$

where it has been used the fact that: $\eta_l = l k_0 \frac{z}{|x|}$
Radiated power

Relativistic case

We know from the definition of the Poynting vector and Eq. (5.168) that:
\[
S_\infty = E_\infty \times H_\infty = \frac{c}{\mu_0} (B_\infty \times \nu) \times B_\infty = \frac{c}{\mu} |B_\infty|^2 \nu. \tag{5.180}
\]

Remembering the Fourier expansion of \( B_\infty \) in Eq. (5.169) we have that:
\[
|B_\infty|^2 = \sum_{l \in \mathbb{Z}} \sum_{m \in \mathbb{Z}} e^{i(l-m)\omega_0 t} B_l^m B_m^l. \tag{5.181}
\]

Now, we consider the averaged Poynting vector, given the fact that \( B_\infty \) is \( \frac{2\pi}{\omega_0} \) we integrate from \(-\frac{\omega_0}{\pi}\) to \(\frac{\omega_0}{\pi}\) to have:
\[
\langle S_\infty \rangle = \frac{c}{\mu_0} \langle |B_\infty|^2 \rangle \nu, \tag{5.182}
\]

where the quantities between brackets are time averaged. For obtaining the power it is customary to calculate the flux of the averaged Poynting vector through a spherical surface (it could be any surface encompassing the EM sources, but the spherical surface is the one that allows the simplest calculations). That is:
\[
\int_0^{2\pi} \int_0^{\pi} \langle S_\infty \rangle \sin \theta d\theta d\phi = \frac{c}{\mu_0} \int_0^{2\pi} \int_0^{\pi} \langle |B_\infty|^2 \rangle \sin \theta d\theta d\phi. \tag{5.183}
\]

Next, we perform the change of variable:
\[
u = a\eta_l = a\eta_l \frac{z}{c} = alk_0 \cos \theta \tag{5.184}
\]
then the differential \( du \) reads
\[
du = -alk_0 \sin \theta d\theta. \tag{5.185}
\]

After these calculations, the flux of the averaged Poynting vector reads:
\[
\int_0^{2\pi} \int_0^{\pi} \langle S_\infty \rangle \sin \theta d\theta d\phi = \frac{c}{\mu_0 alk_0} \int_{-alk_0}^{alk_0} \langle |B_\infty|^2 \rangle \, du \tag{5.186}
\]

By the orthogonality of the complex exponential we have:
\[
\langle |B_\infty|^2 \rangle = \frac{2\pi}{\omega_0} \sum_{l \in \mathbb{Z}} |A_l|^2 \left( \frac{J_l(\eta_\lambda)}{\eta_\lambda} \right)^2 \left[ 1 - \left( \frac{a\eta_l}{alk_0} \right)^2 \right], \tag{5.187}
\]
\[
= \frac{2\pi}{\omega_0} \sum_{l \in \mathbb{Z}} |A_l|^2 \left( \frac{J_l(u)}{u} \right)^2 \left[ 1 - \left( \frac{u}{alk_0} \right)^2 \right]. \tag{5.188}
\]
Therefore:

\[
\int_0^{2\pi} \int_0^{\pi} \langle S_\infty \rangle \sin \theta \, d\theta \, d\phi = \sum_{l \in \mathbb{Z}} \frac{c(2\pi)^2}{\omega_0 \mu_0 \omega k_0} |A_l|^2 \int_{-\omega k_0}^{\omega k_0} \left( \frac{J_l(u)}{u} \right)^2 \left[ 1 - \left( \frac{u}{\omega k_0} \right)^2 \right] du.
\]  

(5.189)

Calling:

\[
D_l := \frac{c(2\pi)^2}{\omega_0 \mu_0 \omega k_0} |A_l|^2,
\]  

(5.190)

one has that the averaged energy flux can be seen as:

\[
\int_0^{2\pi} \int_0^{\pi} \langle S_\infty \rangle \sin \theta \, d\theta \, d\phi = \sum_{l \in \mathbb{Z}} P_l
\]  

(5.191)

with \(P_l\) the \(l\)-th contribution given by:

\[
P_l = 2D_l \int_{-\omega k_0}^{\omega k_0} \left( \frac{J_l(u)}{u} \right)^2 \left[ 1 - \left( \frac{u}{\omega k_0} \right)^2 \right] du.
\]  

(5.192)

This integral can be evaluated by means of the integrals obtained in Appendix D. Let us focus our attention in the case for \(l = 1\):

\[
P_1 = 2D_1 \int_{0}^{\omega k_0} \left( \frac{J_1(u)}{u} \right)^2 \left[ 1 - \left( \frac{u}{\omega k_0} \right)^2 \right] du
\]  

(5.193)

From the Appendix D we know that

\[
\int_{0}^{\omega k_0} \left( \frac{J_1(u)}{u} \right)^2 \, du = \frac{\omega k_0}{2} \left[ \frac{J_1^2}{3} - \frac{J_2 J_1'}{3} + J_1 J_0' - J_0 J_1' \right]_{\omega k_0},
\]  

(5.194)

\[
\int_{0}^{\omega k_0} J_1^2(u) \, du = \mathcal{I}_0^R(\omega k_0 - \omega k_0) \left[ J_1^2(\omega k_0) + J_0^2(\omega k_0) \right],
\]  

(5.195)

where the function \(\mathcal{I}_0^R\) is defined through an integral (see Eq. (D.21)). Thus

\[
P_1 = 2D_1 \left\{ \frac{\omega k_0}{2} \left[ \frac{J_1^2}{3} - \frac{J_2 J_1'}{3} + J_1 J_0' - J_0 J_1' \right]_{\omega k_0} + \frac{\mathcal{I}(\omega k_0)^R}{\omega k_0} \left[ \frac{J_1^2(\omega k_0) + J_0^2(\omega k_0)}{\omega k_0^2} \right]_{\omega k_0} \right\},
\]  

(5.196)

**Non-relativistic case**

We are then in the case of \(\omega k_0 \ll 1\). For \(l = 1\), we have \(0 < u < \omega k_0 \ll 1\). In that case, the behavior of \(J_1\) near the origin is well known namely \(J_1(u) \sim \frac{u}{2}\) and as a result:

\[
\frac{J_1^2(u)}{u^2} \sim \frac{1}{4}
\]  

(5.197)
and we obtain

\[ P_1 \sim 2D_1 \int_0^{a k_0} \left( 1 - \frac{u^2}{(a k_0)^2} \right) \frac{1}{4} du \]  
(5.198)

i.e.

\[ P_1 \sim \frac{D_1}{2} \frac{2}{3} a k_0 \]  
(5.199)

Finally, figure 5.8 shows a comparison between the power \( P_l \) (for \( l = 1, 2, 3 \)) obtained analytically by means of Eq. (5.192) when using the far field approximation and the power numerically computed by considering the Poynting vector flux across the surface of a pill box that encloses the trajectory of the charged particle. The Poynting vector is obtained via equations (5.156-5.157) and the numerical integrations is performed by using the solver GetDP [17]. As we can see, both approaches fit perfectly.

![Graph showing comparison of powers](image)

**Fig. 5.8.** Comparison of the powers \( P_l \) (\( l = 1, 2, 3 \)) obtained analytically and numerically.

**The particle cannot be supraluminal**

It is common sense that for the \( l \)-th component of the magnetic induction field in Eq. (5.167), namely \( B_{l\infty} \), the \( l \)-th averaged Poynting vector \( \langle S_{l\infty} \rangle := \frac{c}{\mu_0} |B_{l\infty}|^2 \) (see Eq. (5.168)) as well as for the power \( P_l \) (given by equations (5.189-5.192)) in the value converges with growing \( l \). A divergence would result in the total value of infinity. Due to the connection between \( B_{l\infty} \), \( \langle S_{l\infty} \rangle \) and \( P_l \) it follows, that if the magnetic field diverges, the two others diverge,
The \( l^{th} \) magnetic field depends on \( l \) only in
\[
B_l^\infty \sim l \cdot J_l(l \cdot ak_0 \cos \theta)
\] (5.200)

For large \( l \), \( J_l(l \beta) \) can be written as follows [88]:
\[
J_l(l \cdot ak_0 \cos \theta) \sim \frac{e^{l(tanh(a_0) - a_0)}}{\sqrt{\frac{1}{2} \pi l \cdot tanh(a_0)}}
\text{, with } a_0 = \text{arccosh}\left(\frac{1}{ak_0 \cos \theta}\right)
\] (5.201)

With this, \( B_l^\infty \) goes with
\[
B_l^\infty \sim \sqrt{\frac{2l}{\pi \sqrt{1 - (ak_0 \cos \theta)^2}}} e^{l\sqrt{1-(ak_0 \cos \theta)^2} - \text{arccosh}\left(\frac{1}{ak_0 \cos \theta}\right)}
\] (5.202)

This only converges with \( l \to \infty \) if the argument of the exponential function is negative. That leads in the form of Eq. 5.201 to the following inequalities:
\[
a_0 > \tanh(a_0)
\]
\[
\leftrightarrow a_0 > 0
\]
\[
0 < ak_0 \cos \theta < 1
\]
\[
\leftrightarrow ak_0 < 1
\]
\[
\leftrightarrow v := a\omega_0 < c
\] (5.203)

With \( v = a\omega_0 \) the maximum velocity of our point charge in his sinusoidal movement, the condition for convergence is matched in the physically sense of Albert Einstein’s postulate that nothing is faster than light [20, 2]. It is important to remark here the fact that this result holds irrespective of whether the particle has got a mass.

### 5.8 Obtaining the diffracted field

After all this work, we have that the fields \( E^0 \) and \( B^0 \) of the system of equations (5.9-5.12) can be seen as a superposition of waves in the form of Eq. (5.156) and Eq. (5.157). The second part of this chapter (which is going to be considerably shorter that the first one) can be tackled in a straightforward fashion. First, the sources in Eq. (5.17) can be easily retrieved by
noticing that:

\[ [\varepsilon_{r,II} - 2\pi\delta] \ast \mathbf{E}^0 = \frac{1}{2\pi} \int_{\tau \in \mathbb{R}} [\varepsilon_{r,II}(\tau) - 2\pi\delta] \sum_{l \in \mathbb{Z}} e^{+il\omega_0(t-\tau)} \mathbf{E}_l^0(x) d\tau, \]

\[ = \sum_{l \in \mathbb{Z}} e^{+il\omega_0} \mathbf{E}_l^0(x) \frac{1}{2\pi} \int_{\tau \in \mathbb{R}} [\varepsilon_{r,II}(\tau) - 2\pi\delta] e^{-il\omega_0\tau} d\tau, \]

\[ = \sum_{l \in \mathbb{Z}} e^{+il\omega_0} \mathbf{E}_l^0(x) [\varepsilon_{r,II}(l\omega_0) - 1]. \] (5.204)

Then:

\[ \rho^0_{II} = -\varepsilon_0 \sum_{l \in \mathbb{Z}} [\varepsilon_{r,II}(l\omega_0) - 1] e^{+il\omega_0 t} \mathbf{E}_l^0(x), \] (5.205)

\[ j^0_{II} = \varepsilon_0 \sum_{l \in \mathbb{Z}} il\omega_0 [\varepsilon_{r,II}(l\omega_0) - 1] e^{+il\omega_0 t} \mathbf{E}_l^0(x). \] (5.206)

It is then natural to propose as solutions of the system (5.9-5.12):

\[ \mathbf{E}_\xi(x, t) = \sum_{l \in \mathbb{Z}} e^{+il\omega_0 t} \mathbf{E}_{\xi,l}(x), \] (5.207)

\[ \mathbf{B}_\xi(x, t) = \sum_{l \in \mathbb{Z}} e^{+il\omega_0 t} \mathbf{B}_{\xi,l}(x), \] (5.208)

Plugging these solutions into equations (5.13-5.16) (and recalling that \( E_{\xi,l}^1 := E_{\xi,l}^0 - E^0 \)), we arrive to the following system which must be satisfied for each \( l \in \mathbb{Z} \).

\[ \nabla \times \mathbf{E}_{\xi,l}^1 = -il\omega_0 \mathbf{B}_{\xi,l}^1, \] (5.209)

\[ \nabla \times \mathbf{B}_{\xi,l}^1 = \frac{il\omega_0}{c^2} [\varepsilon_{r,II}(l\omega_0) - 1] \mathbf{E}_{\xi,l}^0(x) + \frac{il\omega_0}{c^2} [\varepsilon_{r,II}(l\omega_0) - 1] \mathbf{E}_l^0(x), \] (5.210)

\[ \nabla \cdot \mathbf{E}_{\xi,l}^1 = -\left[ \frac{[\varepsilon_{r,II}(l\omega_0) - 1]}{\varepsilon_{r,II}(l\omega_0)} \right] \nabla \cdot \mathbf{E}_l^0(x), \] (5.211)

\[ \nabla \cdot \mathbf{B}_{\xi,l}^1 = 0 \] (5.212)

Taking the curl on Faraday’s Law we get:

\[ \nabla \times \nabla \times \mathbf{E}_{\xi,l}^1 - \left( \frac{l\omega_0}{c} \right)^2 \nabla_{r,II}(l\omega_0) \mathbf{E}_{\xi,l}^1 = \left( \frac{l\omega_0}{c} \right)^2 \left[ \frac{[\varepsilon_{r,II}(l\omega_0) - 1]}{\varepsilon_{r,II}(l\omega_0)} \right] \mathbf{E}_{\xi,l}^0, \] (5.213)

where the ring hand side of this expression is a source term. Moreover equation can be solved for instance, by using Finite Elements Method as it is explained in [43].
5.9 Numerical results

In order to illustrate our discussion, we present the following numerical results for the case of an oscillating charged particle close to a sphere (albeit this method can be applied for more complicated geometries). For this example it is considered that the particle oscillates at a frequency $\omega_0 = \frac{2\pi c}{\lambda}$ with $\lambda = 900$ nm. The amplitude of oscillation is $2a$ with $a = \frac{\lambda}{7}$. The radius of the sphere is $\frac{a}{2}$ and its center is separated from the $z$-axis by a distance of $a$, in addition the permittivity of the sphere is $9+i$. The computed fields were obtained by using the FEM solver GetDP [17] (The incident field was hard-coded as well in GetDP), figure 5.9 illustrates the meshing of the spatial domain. Next, we present our results as follows:

- Figures 5.11 and 5.12 show the $E_0^l$ and $B_0^l$ fields respectively, for $l = 1, 2, 3, 4$. The computation of these fields has been made by means of equations (5.156) and (5.157). In order to compute these integrals numerically, the following change of variables is used: $z' = a \sin(\theta)$, this allows to eliminate the term $\frac{1}{\sqrt{a^2 - z'^2}}$ that comes from the definition of $w(z')$ (see Eq. (5.128)). Once the change of variable is made the formulae are coded into GetDP using a simple trapezoidal rule with 300 integration points. The only drawback we have encountered is that $E_0^l$ might be singular between $(0, 0, -a)$ and $(0, 0, +a)$. This is a problem that needs to be tackled in the future. The illustration of their Poynting vector $S_0^l = \frac{1}{2\mu_0} E_0^l \times B_0^l$ is shown in figure 5.13.

- Figure 5.14 shows the harmonic components of diffracted field $E_1^l$ for $l = 1, 2, 3, 4$. Notice that this field was obtained as a numerical solution of Eq. (5.213) by using FEM. Moreover, due to the fact that the support of source term on the right hand side of Eq. (5.213) is within the sphere, the possible singularity of $E_0^l$ does not affect our numerical results. PML’s were used to truncate the surrounding free space.

- Figure 5.15 shows the total electric field ($E_l = E_1^l + E_0^l$) and its interaction with the sphere, whereas the total Poynting vector has been computed as $S_l = \frac{1}{2\mu_0} E_l \times B_l$ and can be seen in Figure 5.16 for $l = 1, 2, 3, 4$. It is important to see in the case of the Poynting vector how this one is
kind of pulled by the sphere. This is due to the passivity of the material (remember that the permittivity of the sphere is $9+i$).

Finally, all our results have been corroborated by considering an energy balance that measures the total energy flux that crosses a pill-box that surrounds the sphere. This is shown in Figure 5.10.

(a) Mesh showing the different regions of integration  
(b) Zoom enclosing the sphere and the region where the particle oscillates.

Fig. 5.9. Mesh showing the regions where the different fields are obtained via FEM.
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(a) Integration box that shows the
(b) Zoom enclosing the sphere

Fig. 5.10. Pill-box surface enclosing the sphere. The tube below the sphere in Figure 5.10a is just there to refine the mesh around the trajectory of the particle (see figure 5.9b) and to represent the total field.

5.10 Partial conclusion

In this chapter we have studied the problem of an oscillating particle near to a nano-sphere by using the diffracted field formalism. The first problem to tackle was the description of the electromagnetic field generated by an oscillating particle in vacuo. Albeit this problem can be solved in principle by the Liénard-Wiechert fields, the resulting equations are not useful in practice. In order to overcome this difficulty we propose a harmonic decomposition of the sources $\rho$ and $j$ which will allow us to find the harmonic representation of the electromagnetic fields. Next, we make an analysis of the radiated fields for the relativistic and non-relativistic cases. Finally, by using the finite Elements Method, we solve the full problem that involves the interaction between the oscillating charge and the dispersive nano sphere. The solutions obtained have been validated by an energy balance.
Fig. 5.11. Harmonic components of the imaginary part of the incident electric field $E_0^l$ for $l = 1, 2, 3, 4$
Fig. 5.12. Harmonic components of the real part of the incident magnetic induction field $B_0^l$ for $l = 1, 2, 3, 4$.
Fig. 5.13. Harmonic components of the real part of the incident Poynting vector field $S_0^l$ for $l = 1, 2, 3, 4$
Fig. 5.14. Harmonic components of the real part of the diffracted electric field $E_l^1$ for $l = 1, 2, 3, 4$
Fig. 5.15. Harmonic components of the real part of the total electric field $E_l$ for $l = 1, 2, 3, 4$
Fig. 5.16. Harmonic components of the real part of the total Poynting vector field $S_l$ for $l = 1, 2, 3, 4$
General conclusions

La commedia è finita! (The comedy is over!)
—Ruggero Leoncavallo, Opera Pagliacci, end of the final act.

In this thesis we have provided different results when dealing with electromagnetic pulses that illuminate dispersive and lossy materials. The most important of them are:

- In chapter 1 we have proposed a simple yet systematic procedure for fitting experimental data of permittivities of resonant materials such as metals and semiconductors in the visible range. This procedure does not assume a priori any particular shape for the electric susceptibility $\hat{\chi}$. The final expression obtained for the permittivity preserves causality and stability. Tables with numerical parameters to fit different materials are provided along with the fitting error for infinity norm and energy norm.

- In chapter 2 we studied the propagation of an EM pulse in transparent in gentle material. This was made by considering the equations that describe the motion of the wave centers for the electric (Eq. (2.19)) and magnetic (Eq. (2.46)) fields. By considering propagation on an infinite medium we obtained that without exception of the field (electric or magnetic) and the medium in which they propagate (transparent or gentle) the equations of motion are always given by an affine law. Even more, under the extra assumption that the wave number does not change too much with respect to the frequency we were able to recover the group velocity definition as a particular case.
• Chapter 3 was devoted to generalize the ideas introduced in chapter 2. One of the main results is the precise definition of complex logarithm (Eq. (C.1)) that allows to obtain the complex-valued wave number. Moreover, the centrovelocity adapted to multi-domains has been generalized by considering an energy density that satisfies the continuity equation in each one of the domains under consideration. This energy density has been found by considering a more general frame as provided in [15]. The solution obtained has been validated by a total time-domain energy balance. The position of the center of gravity of different electromagnetic pulses was computed. These results generally show a linear behavior and allow thus to derive the velocity of light in a dispersive lossy medium as the slope of these graphs.

• In chapter 4 we have studied the problem of finding the QNM’s for a Fabry Perot cavity. By studying Eq. (4.27) it has been possible to determine the right branch cut for the complex logarithm (see Eq. (C.1)). With this definition, the right resonant frequencies \( \Omega_n \) can be obtained numerically via the Tetrachotomy method [43]. The exponential divergence of the QNM’s when \(|y| \to \infty\) was eliminated by considering the use of PML’s and modified resonant modes were obtained as it is shown in equations (4.35-4.39). Finally, a QNM expansion for a linearly polarized electric field (see Eq. (4.60)) was made by obtaining the bi-orthogonal vector to the QNMs.

• In the first part of chapter 5 we worked on the description of the electromagnetic field generated by an oscillating particle \textit{in vacuo}. First, we started by giving an alternative expression to the electric field given by Jefimenko’s equation [21] and instead we provided equations (5.63-5.65) in order to compare the terms corresponding to the electric and magnetic radiation fields. Next, we went through the full procedure to obtain the EM fields generated by a charged particle that moves along a given trajectory. The solution of this general problem are the so called \textit{Liénard-Wiechert} fields. However the resulting equations (Eq. (5.107) and Eq. (5.101)) are not useful in practice. In order to overcome this difficulty we propose a harmonic decomposition of
the sources $\rho$ and $j$ which will allow us to find the harmonic representation of the electromagnetic fields (Eq. (5.154) and Eq. (5.155)). Next, we made an analysis of the radiated fields for the relativistic and non-relativistic cases. Finally, by using the Finite Elements Method, we solved the full problem that involves the interaction between the oscillating charge and the dispersive nano sphere. The solutions obtained have been validated by an energy balance.
Appendix A

Fourier Transform convention and the Heaviside step function transform

In this appendix we set the Fourier transform convention (in the classical sense) for all the chapters in this thesis as:

\[ \hat{f}(\omega) := \frac{1}{2\pi} \int_{t \in \mathbb{R}} f(t)e^{+i\omega t} dt, \quad (A.1) \]

\[ f(t) := \int_{\omega \in \mathbb{R}} \hat{f}(\omega)e^{-i\omega t} d\omega. \quad (A.2) \]

If we want to extend these definitions to a wider family of mathematical objects (e.g. \( \delta \)'s, unit steps, ramps, sines, cosines), it is necessary to consider the definition of the Fourier transform in a more general way as per [89, 86, 76]:

\[ \langle \mathcal{F}_{t \to \omega} \{ f(t) \} (\omega), \varphi(\omega) \rangle_{\omega \in \mathbb{R}} := \langle f(t), \hat{\varphi}(t) \rangle_{t \in \mathbb{R}}, \quad (A.3) \]

accordingly the inverse is defined as:

\[ \langle \mathcal{F}^{-1}_{\omega \to t} \{ \hat{f}(\omega) \} (t), \varphi(t) \rangle_{t \in \mathbb{R}} := \langle \hat{f}(\omega), \varphi(\omega) \rangle_{\omega \in \mathbb{R}}, \quad (A.4) \]

where the brackets denote integration in the whole real line and \( \varphi(\omega) \) is a gaussian test function as it is explained in [89]. From this definition one can get the Fourier transform of a more general kind of objects like the delta distribution:

\[ \langle \mathcal{F}_{t \to \omega} \{ \delta(t) \} (\omega), \varphi(\omega) \rangle_{\omega \in \mathbb{R}} = \langle \delta(t), \varphi(t) \rangle_{t \in \mathbb{R}} = \varphi(0) = \langle (2\pi)^{-1} \mathbb{1}(\omega), \varphi(\omega) \rangle, \quad (A.5) \]

proceeding in a similar fashion, one gets:

\[ \mathcal{F}^{-1}_{\omega \to t} \{ \delta(\omega) \} = \mathbb{1}(t). \quad (A.6) \]
The derivative in time $d_t[*]$ can be computed in the following manner:

$$\langle \mathcal{F}_{t \to \omega} \{d_tf\}(\omega), \varphi(\omega) \rangle_{\omega \in \mathbb{R}} = \langle d_tf(t), \hat{\varphi}(t) \rangle_{t \in \mathbb{R}}, \quad (A.7)$$

$$= \langle -f(t), d_t \hat{\varphi}(t) \rangle_{t \in \mathbb{R}}, \quad (A.8)$$

$$= \langle -f(t), (2\pi)^{-1} d_t \langle \varphi(\omega)e^{+i\omega t} \rangle_{\omega \in \mathbb{R}} \rangle_{t \in \mathbb{R}}$$

$$= \langle f(t), (2\pi)^{-1} \langle -i\omega \varphi(\omega)e^{+i\omega t} \rangle_{\omega \in \mathbb{R}} \rangle_{t \in \mathbb{R}}$$

$$= \langle f(t), \mathcal{F}_{\omega \to t} \{-i\omega \varphi(\omega)\}(t) \rangle_{t \in \mathbb{R}}$$

$$= \langle \mathcal{F}_{t \to \omega} \{f(t)\}(\omega), -i\omega \varphi(\omega) \rangle_{\omega \in \mathbb{R}}$$

$$= \langle -i\omega \mathcal{F}_{t \to \omega} \{f(t)\}(\omega), \varphi(\omega) \rangle_{\omega \in \mathbb{R}}. \quad (A.9)$$

Notice that for going from Eq. (A.7) to Eq. (A.8) we have used the definition of derivative in the sense of distributions [76, 26, 89, 42, 28], and the rest follows from the fact that $\varphi$ is a test function and can be transformed in the usual sense as is Eq. (A.1).

With these tools, the Fourier transform of a Heaviside step function $\theta(t)$ can be obtained. First, we consider the equality given by Eq. (A.5):

$$\langle \mathcal{F}_{t \to \omega} \{2\pi \delta(t)\}(\omega), \varphi(\omega) \rangle_{\omega \in \mathbb{R}} = \langle 1(\omega), \varphi(\omega) \rangle_{\omega \in \mathbb{R}},$$

$$= \langle -i\omega, \varphi(\omega) \rangle_{\omega \in \mathbb{R}},$$

$$= \langle -i\omega \text{Vp}(\omega^{-1}), \varphi(\omega) \rangle_{\omega \in \mathbb{R}}, \quad (A.10)$$

$$= \langle id_t \mathcal{F}_{\omega \to t}^{-1} \{\text{Vp}(\omega^{-1})\}(t), \hat{\varphi}(t) \rangle_{t \in \mathbb{R}}, \quad (A.11)$$

where the Fourier transform of the derivative in Eq. (A.9) has been used for going from Eq. (A.10) to Eq. (A.11). Thus we arrive to the expression:

$$id_t \mathcal{F}_{\omega \to t}^{-1} \{\text{Vp}(\omega^{-1})\}(t) = 2\pi \delta(t), \quad (A.12)$$

and knowing that the derivative in the sense of distributions of a diract delta is $\theta(t)$ [76, 26, 89, 42, 28], one has:

$$i \mathcal{F}_{\omega \to t}^{-1} \{\text{Vp}(\omega^{-1})\}(t) = 2\pi [\theta(t) + C] \quad (A.13)$$

where $C$ is a constant to be determined, this can be accomplished by proving that $\mathcal{F}_{\omega \to t}^{-1} \{\text{Vp}(\omega^{-1})\}(t)$ is an odd function in $t$. Starting from the definition of the generalized inverse Fourier transform in Eq. (A.4) one has:

$$\langle \mathcal{F}_{\omega \to t}^{-1} \{\text{Vp}(\omega^{-1})\}(t), \hat{\varphi}(t) \rangle_{t \in \mathbb{R}} = \langle \omega^{-1}, \varphi(\omega) \rangle_{\omega \in \mathbb{R}} \quad (A.14)$$
and from this the following equalities hold:

\[
\langle \mathcal{F}_{\omega \to t}^{-1}\{Vp(\omega^{-1})\}(-t), \hat{\phi}(t) \rangle_{t \in \mathbb{R}} = \langle \mathcal{F}_{\omega \to t}^{-1}\{Vp(\omega^{-1})\}(t), \hat{\phi}(-t) \rangle_{t \in \mathbb{R}},
\]

\[
= \langle \omega^{-1}, \phi(-\omega) \rangle_{\omega \in \mathbb{R}},
\]

\[
= \langle -\omega^{-1}, \phi(\omega) \rangle_{\omega \in \mathbb{R}},
\]

\[
= \langle -\mathcal{F}_{\omega \to t}^{-1}\{Vp(\omega^{-1})\}(t), \hat{\phi}(t) \rangle_{t \in \mathbb{R}}.
\]

(A.15)

Thus, \( C \) can be retrieved by considering the equalities:

\[
2\pi[\theta(-t) + C] = \mathcal{F}_{\omega \to t}^{-1}\{Vp(\omega^{-1})\}(-t),
\]

(A.16)

\[
= -\mathcal{F}_{\omega \to t}^{-1}\{Vp(\omega^{-1})\}(t) = -2\pi[\theta(t) + C],
\]

(A.17)

and after some elementary algebra one gets:

\[
C = \frac{1}{2}.
\]

(A.18)

From this

\[
\mathcal{F}_{\omega \to t}^{-1}\left\{Vp\left(\frac{1}{\omega}\right)\right\}(t) = -i2\pi \left[\hat{\theta}(t) + \frac{1}{2}\right],
\]

(A.19)

then, taking the inverse Fourier transform:

\[
= -i2\pi \left[\hat{\theta}(\omega) + \frac{1}{2}\delta(\omega)\right],
\]

(A.20)

and finally:

\[
\hat{\theta}(\omega) = \frac{1}{2} \left[\frac{i}{\pi}Vp\left(\frac{1}{\omega}\right) - \delta(\omega)\right].
\]

(A.21)
Appendix B

Proof of the Titchmarsh’s theorem

The causality of the susceptibility, can be translated to the frequency domain via a Fourier Transform into a complex-valued function. The analytical properties of this function will be studied and summarized in the so called Titchmarsh’s theorem [90, 91, 92].

We start our study by considering that \( \chi(t) \) is causal and therefore has positive support, then it is possible to write

\[
\chi(t) = \chi(t)\theta(t),
\]

where \( \theta(t) \) is the Heaviside step function [28, 76]. Taking the Fourier Transform of this expression one gets:

\[
\hat{\chi}(\omega) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{i\omega t} \chi(t) dt = \frac{1}{2\pi} \int_{0}^{+\infty} \chi(t) e^{i\omega t} dt.
\]

Assuming that \( \hat{\chi}(\omega) \) exists, we can consider its analytical continuation [93, 94] by setting \( \omega = \omega' + i\omega'' \), which implies:

\[
\hat{\chi}(\omega' + i\omega'') = \frac{1}{2\pi} \int_{0}^{+\infty} e^{i\omega' t} e^{-\omega'' t} \chi(t) dt
\]

From this, one can see that in order to have a convergent integral it is necessary to have \( \omega'' \geq 0 \). Therefore, provided that \( \chi(t) \) is well behaved, we get that \( \hat{\chi} \) is holomorphic on \( \mathbb{C}^+ \) [42, 64]. However this is still not enough to guarantee causality, because we must have information about the behavior of \( \hat{\chi} \) when \( \omega \to \infty \) (the transparency zone).

First, we start by assuming that \( \hat{\chi} \) is square integrable

\[
\int_{-\infty}^{+\infty} |\hat{\chi}(\omega)|^2 d\omega < C
\]

(B.4)
for a certain constant $C$. Using Parseval-Plancherel’s theorem [76, 85] we get:

$$\int_{-\infty}^{+\infty} |\hat{\chi}(\omega)|^2 d\omega = \frac{1}{2\pi} \int_{-\infty}^{+\infty} |\chi(t)|^2 dt = \frac{1}{2\pi} \int_0^{+\infty} |\chi(t)|^2 dt$$  \hspace{1cm} (B.5)

where $|\cdot|$ denotes the complex modulus, and putting Eq. (B.4) into Eq. (B.5)

$$\int_0^{+\infty} |\chi(t)|^2 dt < 2\pi C. \hspace{1cm} (B.6)$$

If now we consider the analytical extension of $\hat{\chi}$ we get by integrating on the real axis and the Parseval-Plancherel’s theorem:

$$\int_{-\infty}^{+\infty} |\hat{\chi}(\omega + i\omega'')|^2 d\omega' = \frac{1}{2\pi} \int_{-\infty}^{+\infty} |\chi(t)|^2 e^{-2\omega'' t} dt$$  \hspace{1cm} (B.7)

Combining Eq. (B.4) and Eq. (B.7) we arrive to the following chain of inequalities:

$$2\pi \int_{-\infty}^{+\infty} |\hat{\chi}(\omega' + i\omega'')|^2 d\omega' = \int_{-\infty}^{+\infty} |\chi(t)|^2 e^{-2\omega'' t} dt, \hspace{1cm} (B.8)$$

$$\leq \int_{-\infty}^{+\infty} |\chi(t)|^2 dt, \hspace{1cm} (B.9)$$

$$< 2\pi C \hspace{1cm} (B.10)$$

and thus

$$\int_{-\infty}^{+\infty} |\hat{\chi}(\omega' + i\omega'')|^2 d\omega' < C \hspace{1cm} (B.11)$$

This implies that $\hat{\chi}$ is square integrable on the real axis and also on any straight line parallel to the real axis that lies on $\mathbb{C}^+$.

For the second part of our discussion, It is now necessary to prove the following Lemma [90]:

Let $\hat{\chi}$ be analytic and let

$$\int_{-\infty}^{+\infty} |\hat{\chi}(\omega' + i\omega'')|^p d\omega'$$  \hspace{1cm} (B.12)

exist and be bounded for $\omega'_1 \leq \omega'' \leq \omega''_2$. Then, as $\omega' \to \pm \infty$, $\hat{\chi}(\omega' + i\omega'') \to 0$ uniformly for $\omega''_1 + \delta \leq \omega'' \leq \omega''_2 - \delta$.

We start the proof by considering $\omega''$ in the band $[\omega''_1 + \delta, \omega''_2 - \delta]$, i.e. $\omega''_1 + \delta \leq \omega'' \leq \omega''_2 - \delta$ (See Fig. B.1). Then, if we consider Cauchy theorem’s [64, 42, 93] with a circular contour centered on a point $\omega$ and radius $\rho$
such that \(0 < \rho \leq \delta\), one gets:
\[
\hat{\chi}(\omega) = \frac{1}{2\pi i} \oint_{|\zeta - \omega| = \rho} \frac{\hat{\chi}(\zeta)}{\zeta - \omega} \, d\zeta.
\] (B.13)

Making the change of variables \(\zeta - \omega = \rho e^{i\phi}\) we get
\[
\hat{\chi}(\omega) = \frac{1}{2\pi} \int_{0}^{2\pi} \hat{\chi}(\omega + \rho e^{i\phi}) \, d\phi.
\] (B.14)

Multiplying by
\[
\frac{1}{2} \delta^{2} = \int_{0}^{\delta} \rho \, d\rho
\] (B.15)
we get after using Fubini’s theorem [50]
\[
\frac{1}{2} \delta^{2} \hat{\chi}(\omega) = \frac{1}{2\pi} \int_{0}^{\delta} \int_{0}^{2\pi} \hat{\chi}(\omega + \rho e^{i\phi}) \rho \, d\phi \, d\rho.
\] (B.16)

By triangle inequality [26, 93] one gets:
\[
\frac{1}{2} \delta^{2} |\hat{\chi}(\omega)| \leq \frac{1}{2\pi} \int_{0}^{\delta} \int_{0}^{2\pi} |\hat{\chi}(\omega + \rho e^{i\phi})| \rho \, d\phi \, d\rho.
\] (B.17)

For the next step we must recall that
\[
|\hat{\chi}(\omega + \rho e^{i\phi})| \rho = |\hat{\chi}(\omega + \rho e^{i\phi})| \rho^{\frac{1}{p}} \rho^{\frac{1}{q}}, \quad \text{with} \quad \frac{1}{p} + \frac{1}{q} = 1
\] (B.18)
then, by using Holder’s inequality [26, 93]
\[
\frac{1}{2} \delta^{2} |\hat{\chi}(\omega)| \leq \frac{1}{2\pi} \left\{ \int_{0}^{\delta} \int_{0}^{2\pi} |\hat{\chi}(\omega + \rho e^{i\phi})|^{p} \rho \, d\phi \, d\rho \right\}^{\frac{1}{p}} \left\{ \int_{0}^{\delta} \int_{0}^{2\pi} \rho^{q} \, d\phi \, d\rho \right\}^{\frac{1}{q}}.
\] (B.19)

Calling
\[
K(\delta) = \frac{1}{2\delta^{2} \pi} \left\{ \int_{0}^{\delta} \int_{0}^{2\pi} \rho^{q} \, d\phi \, d\rho \right\}^{\frac{1}{q}}
\] (B.20)
and after some elementary manipulations one arrives to:
\[
|\hat{\chi}(\omega)| \leq K(\delta) \left\{ \int_{0}^{\delta} \int_{0}^{2\pi} |\hat{\chi}(\omega + \rho e^{i\phi})|^{p} \rho \, d\phi \, d\rho \right\}^{\frac{1}{p}}.
\] (B.21)

Now, let us focus our attention on the integral
\[
\int_{0}^{\delta} \int_{0}^{2\pi} |\hat{\chi}(\omega + \rho e^{i\phi})|^{p} \rho \, d\phi \, d\rho.
\] (B.22)
Fig. B.1. The circle of radius $\delta$ is within the rectangle $[-\delta, \delta] \times [\omega''_1, \omega''_2]$ centered on $\omega$.

Notice that, this integral is taken considering the interior and boundary points [26, 93] of a circle of radius $\delta$ centered on $\omega$. Due to the fact that $|\hat{\chi}(\omega + \rho e^{i\theta})|^p > 0$ this integral is less than the integral taken on a rectangle $[-\delta, \delta] \times [\omega''_1, \omega''_2]$ centered on $\omega$ as it can be seen in Fig. B.1. Thus,

$$|\hat{\chi}(\omega)| < K(\delta) \left\{ \int_{\omega''_1}^{\omega''_2} \int_{\omega' - \delta}^{\omega' + \delta} |\hat{\chi}(\xi'' + i\xi''')|^p d\xi'' d\xi'''ight\}^{\frac{1}{p}}. \quad (B.23)$$

Now, the integral

$$\int_{\omega' - \delta}^{\omega' + \delta} |\hat{\chi}(\xi'' + i\xi'''')|^p d\xi''' \quad (B.24)$$

is bounded for $\omega''_1 \leq \xi''''' \leq \omega''_2$ and tends to 0 when $\omega' \to \pm \infty$. Hence, the right hand side of Eq. (B.23) also goes to 0 and the result follows. This completes the proof of our lemma.

Continuing with our study on the properties of $\hat{\chi}$, let us consider an arbitrary point on $\mathbb{C}^+ \omega_0 = \omega'_0 + i\omega''_0$ within a rectangular loop $\Gamma$ with corners at points $\pm U, \pm U + iV$ (See Fig B.2), where $U$ and $V$ will go eventually to $+\infty$. According to Cauchy’s theorem:

$$\hat{\chi}(\omega_0) = \frac{1}{2\pi i} \int_{\Gamma} \frac{\hat{\chi}(\sigma)}{\sigma - \omega_0} d\sigma. \quad (B.25)$$
If now we define:

\[ I_1 := \frac{1}{2\pi i} \int_{-U}^{+U} \frac{\hat{\chi}(\sigma)}{\sigma - \omega_0} d\sigma, \]

\[ I_2 := \frac{1}{2\pi i} \int_{0}^{V} \frac{\hat{\chi}(U + iv)}{U + iv - \omega_0} dv, \]

\[ I_3 := -\frac{1}{2\pi i} \int_{-U}^{+U} \frac{\hat{\chi}(u + iV)}{u + iV - \omega_0} du, \]

\[ I_4 := \frac{1}{2\pi i} \int_{0}^{V} \frac{\hat{\chi}(-U + i|V - v|)}{-U + i|V - v| - \omega_0} dv, \]

it is easy to see that \( \hat{\chi}(\omega_0) = I_1 + I_2 + I_3 + I_4 \). Starting by \( I_2 \) one gets:

\[ I_2 \leq \frac{\max_{0 \leq v \leq V} |\hat{\chi}(U + iv)|}{2\pi i} \int_{0}^{V} \frac{dv}{|U + iv - \omega_0|^2} \]

\[ = \frac{\max_{0 \leq v \leq V} |\hat{\chi}(U + iv)|}{2\pi i} \int_{0}^{V} \frac{dv}{\sqrt{(U - \omega_0')^2 + (v - \omega''_0)^2}} \]

\[ = \frac{\max_{0 \leq v \leq V} |\hat{\chi}(U + iv)|}{2\pi i} \ln \frac{V - \omega''_0 + \sqrt{(U - \omega_0')^2 + (v - \omega''_0)^2}}{\sqrt{(U - \omega_0')^2 + (v - \omega''_0)^2 - \omega''_0}} \]

and from this last inequality we obtain:

\[ \lim_{U \to +\infty} I_2 = 0. \]
Even more, following an analogous procedure for $I_4$ one gets also

$$\lim_{U \to +\infty} I_4 = 0. \quad (B.32)$$

Next, by taking this same limit for $\hat{\chi}(\omega_0)$ (which is a constant) we have:

$$\hat{\chi}(\omega_0) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{\hat{\chi}(\sigma)}{\sigma - \omega_0} d\sigma - \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{\hat{\chi}(u + iV)}{u + iV - \omega_0} du \quad (B.33)$$

The second integral can be bounded by means of the Schwartz inequality [93, 26]

$$\left| \int_{-\infty}^{\infty} \frac{\hat{\chi}(u + iV)}{(U - \omega_0') + i(V - \omega_0'')} du \right|^2 \leq \int_{-\infty}^{\infty} |\hat{\chi}(u + iV)|^2 du \times \int_{-\infty}^{\infty} \frac{du}{(u - \omega_0')^2 + (V - \omega_0'')^2} \leq \frac{C \pi}{V - \omega_0''} \quad (B.34)$$

where the last inequality comes from Eq. (B.11) and the integral [64]

$$\int_{-\infty}^{\infty} \frac{du}{(u - \omega_0')^2 + (V - \omega_0'')^2} = \frac{\pi}{V - \omega_0''} \quad (B.35)$$

Taking now the limit of this expression when $V \to \infty$ we have:

$$\hat{\chi}(\omega_0) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{\hat{\chi}(\sigma)}{\sigma - \omega_0} d\sigma, \quad \omega_0'' > 0, \quad (B.37)$$

which expresses the fact that $\hat{\chi}$ evaluated at $\omega_0$ on the upper half of the complex plane depends of its values on the real axis. Now, we consider the case when $\omega_0$ is on the real axis. In this case, the contour $\Gamma$ must avoid the real point $\omega_0$ by a semicircle of radius $\epsilon$ in $C^+$ as it is shown on Fig B.3. Thus

$$0 = \frac{1}{2\pi i} \lim_{\epsilon \to 0^+} \left[ \int_{-\infty}^{\omega_0 - \epsilon} \frac{\hat{\chi}(\sigma)}{\sigma - \omega_0} d\sigma + \int_{\omega_0 + \epsilon}^{\infty} \frac{\hat{\chi}(\sigma)}{\sigma - \omega_0} d\sigma ight] \\
- \int_{0}^{\pi} \hat{\chi}(\omega_0 + e^{i\theta}) d\theta, \quad (B.38)$$

$$= \int_{-\infty}^{\omega_0} \hat{\chi}(\sigma) d\sigma - i\pi \hat{\chi}(\omega_0), \quad (B.39)$$
APPENDIX B. APPENDIX B: PROOF OF THE TITCHMARSH’S THEOREM

Fig. B.3. Rectangular loop on the upper complex plane with a semicircle avoiding the point $\omega_0$ on the real axis.

where the second term on Eq. (B.39) comes from the shrinking path lemma [64]. After some elementary manipulations and remembering that $\omega_0$ was real and arbitrary we get:

$$\hat{\chi}(\omega) = \frac{i}{\pi} \int_{-\infty}^{+\infty} \frac{\hat{\chi}(\sigma)}{\omega - \sigma} d\sigma, \quad \text{(B.40)}$$

for every point $\omega$ on the real axis. Taking now the real and imaginary parts of Eq. (B.40) we retrieve the so called Kramers-Kronig relations [2, 9, 91]:

$$\mathfrak{R}\{\hat{\chi}(\omega)\} = -\frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{\mathfrak{I}\{\hat{\chi}(\sigma)\}}{\omega - \sigma} d\sigma, \quad \mathfrak{I}\{\hat{\chi}(\omega)\} = \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{\mathfrak{R}\{\hat{\chi}(\sigma)\}}{\omega - \sigma} d\sigma. \quad \text{(B.41)}$$

Another consequence of Eq. (B.40) (and equivalently of the Kramers-Kronig relations) is that:

$$\hat{\chi}(\omega) = \int_{-\infty}^{+\infty} \hat{\chi}(\sigma) \left[ \frac{1}{2} \delta(\omega - \sigma) + \frac{i}{\pi} \text{Vp}\left(\frac{1}{\omega - \sigma}\right) \right] d\sigma.$$

Remembering that the Fourier transform of the Heaviside step function (see Eq. (A.21) on Appendix A) is:

$$\hat{\theta}(\omega) = \frac{1}{2} \left[ \delta(\omega) + \frac{i}{\pi} \text{Vp}\left(\frac{1}{\omega}\right) \right], \quad \text{(B.42)}$$
it is possible to see that
\[ \hat{\chi}(\omega) = \int_{-\infty}^{+\infty} \hat{\chi}(\sigma) \theta(\omega - \sigma) d\sigma. \] (B.43)

and by taking the inverse Fourier transform one gets
\[ \chi(t) = \chi(t) \theta(t), \] (B.44)

which is the mathematical way to say that \( \chi(t) \) is causal.

These results can be formulated on the Titchmarsh’s theorem as follows:

If a square integrable function \( \hat{\chi}(\omega) \) fulfills one of the conditions below, then fulfills all of them:

i The inverse Fourier transform \( \chi(t) \) of \( \hat{\chi}(\omega) \) is causal, i.e.
\[ \chi(t) = \chi(t) \theta(t). \] (B.45)

ii \( \hat{\chi}(\omega') \) is, for almost all \( \omega' \), the limit as \( \omega'' \to 0^+ \) of an analytic function \( \hat{\chi}(\omega' + i\omega'') \) that is holomorphic in the upper half plane and square integrable over any line parallel to the real axis:
\[ \int_{-\infty}^{+\infty} |\hat{\chi}(\omega' + i\omega'')|^2 d\omega' < C, \quad \omega'' > 0. \] (B.46)

iii \( \hat{\chi}(\omega') \) satisfy the Kramers-Kronig relations.
Appendix C

Complex logarithm convention

As it is known, the complex logarithm, contrary to its real counterpart, has many ways to be determined \([42]\) (in many text books this is called a multiple-valued function \([64, 65]\)). In order to avoid this difficulty, it is necessary to consider the domain of definition for the complex logarithm as the whole complex plane minus a straight line that goes from zero, without including it, to infinitum, such line is called the branch-cut of the complex logarithm.

Let us now introduce notation for a single-valued complex logarithm as follows:

\[
\text{Log}_\sigma^\theta(z) = \ln |z| + i \text{Arg}_\sigma^\theta(z), \quad \sigma = \{+, -\}, \tag{C.1}
\]

The term on the left hand side of the equation denotes the principal branch of the complex logarithm, which is now single valued. The real part of this function (\(\ln |z|\)) is the natural logarithm of the complex modulus of \(z\) and it is defined in the usual sense for real-valued functions \([49]\). On the other hand, the imaginary part is given by \(\text{Arg}_\sigma^\theta(z)\), which represents the principal argument of \(z\) \([64, 93]\). This argument is taken counterclockwise from the positive real axis on the complex plane and depends on two parameters \(\sigma\) and \(\theta\) which will determine the image interval \([93]\) of \(\text{Arg}_\sigma^\theta(z)\). The first parameter \(\sigma\) says that if \(\sigma = +\) then \(\text{Arg}_\sigma^\theta(z) \in [\theta - \pi, \theta + \pi]\) and if \(\sigma = -\) then \(\text{Arg}_\sigma^\theta(z) \in ]-\theta - \pi, -\theta + \pi]\), whereas the second parameter \(\theta\) can take values on the interval \([0, \pi]\). In other words, \(\sigma\) tells us how to take the window of values that \(\text{Arg}_\sigma^\theta(z)\) can take, and \(\theta\) allows us to translate such windows. Notice that the branch cut is determined by the open extreme of the intervals given by \(\sigma\).

As an example of our convention, let us consider \(\text{Arg}_{\pi/2}^{-\pi}(z)\), then, by the
previous discussion we have that $\text{Arg}^+_{\pi}(z) \in [0, 2\pi[$ with a branch-cut on $2\pi$. On the other hand $\text{Arg}^-_{\pi}(z) \in ] - 2\pi, 0]$ with a branch-cut on $-2\pi$. 
Appendix D

Derivation of the integrals used to obtain $P_l$

Here the goal is to express $P_l$ with the minimum of *ad hoc* special functions. For this reason, we are going to derive the integrals used in Section 5.7. As we know, the Bessel functions of first kind are non diverging solutions at the origin of the differential equation [78, 87, 76]:

$$r^2 \frac{d^2}{dr^2} J_l(r) + r \frac{d}{dr} J_l(r) + J_l(r) \left( r^2 - l^2 \right) = 0 \quad (D.1)$$

which satisfy the identities [76, 85, 88]:

$$J_{l-1}(r) + J_{l+1}(r) = \frac{2l}{r} J_l(r), \quad (D.2)$$

$$J_{l-1}(r) - J_{l+1}(r) = 2 \frac{d}{dr} J_l(r), \quad (D.3)$$

Equipped with these tools, our first goal is to compute the integral

$$I^c_l(A) = \int_0^a \frac{J^2_l}{r^2} dr. \quad (D.4)$$

In order to do that, consider Eq. (D.1) and divide it over $r$, after some elementary manipulations this equation reads:

$$\frac{d}{dr} \left[ r \frac{dJ_l}{dr} \right] + J_l \left( r - \frac{l^2}{r} \right) = 0, \quad (D.5)$$

and analogously for $J_k$

$$\frac{d}{dr} \left[ r \frac{dJ_k}{dr} \right] + J_k \left( r - \frac{k^2}{r} \right) = 0. \quad (D.6)$$

Multiplying Eq. (D.5) by $J_k$, Eq. (D.6) by $J_l$ and taking its difference one gets:

$$J_k \frac{d}{dr} \left[ r \frac{dJ_l}{dr} \right] - J_l \frac{d}{dr} \left[ r \frac{dJ_k}{dr} \right] + \left( k^2 - l^2 \right) \frac{1}{r} J_k J_l = 0. \quad (D.7)$$
Next, we take the integral from 0 to $A$ to obtain:

$$J_k r \frac{d J_l}{d r} \bigg|_0^A - J_l r \frac{d J_k}{d r} \bigg|_0^A = (l^2 - k^2) \int_0^A \frac{1}{r} J_k J_l dr, \quad (D.8)$$

and then:

$$\int_0^A \frac{1}{r} J_k J_l dr = \frac{A}{(l^2 - k^2)} \left[ J_k \frac{d J_l}{d r} - J_l \frac{d J_k}{d r} \right]_A. \quad (D.9)$$

Now, by means of the identity in (D.2), it is easy to see Eq. (D.4) as:

$$\int_0^A \frac{1}{r^2} J_l^2 dr = \frac{1}{2l} \left[ \int_0^A \frac{1}{r} J_{l-1} J_l dr + \int_0^A \frac{1}{r} J_{l+1} J_l dr \right]. \quad (D.10)$$

These last two integrals in the right hand side of Eq. (D.10) can be easily obtained via (D.9) and finally

$$I_S^l(A) = \frac{A}{2l} \left[ J_l J_{l+1}^l - J_{l+1} J_l^l \frac{1}{1+2l} + J_l J_{l-1}^l - J_{l-1} J_l^l \frac{1}{1-2l} \right]_A. \quad (D.11)$$

The second goal, is to compute the integral

$$I_R^l(A) = \int_0^A J_l^2 dr. \quad (D.12)$$

Despite its harmless appearance, this integral is in general not easy to integrate and there is no analytical expression in the consulted references [78, 87, 76, 85, 88]. Thus, we propose here a semi analytical approach that give us a way to obtain this integral in a recursive manner.

Starting by assuming $l > 1$, taking the product of equations (D.2) and (D.3) and integrating this resulting equation from 0 to $A$ one gets:

$$\int_0^A J_{l-1}^2 dr - \int_0^A J_{l+1}^2 dr = 4l \int_0^A \frac{1}{r} J_l \frac{d J_l}{d r} dr, \quad (D.13)$$

and after performing integration by parts in the right hand side of this equation one arrives to the expression:

$$I_R^{l+1}(A) = I_R^l(A) - \frac{2l}{A} I_S^l(A) - 2I_S^l(A) dr. \quad (D.14)$$

Notice that the last integral in the right hand side of Eq. (D.14) is given by (D.11). This establishes a two step recurrence relation between the integrals.
\( I_{l+1}^R (A) \) and \( I_{l-1}^R (A) \) as defined in Eq. (D.12). Next, we are going to get an expression for \( I_{l-1}^R (A) \) by considering Eq. (D.5) with \( l = 0 \)

\[
\frac{d}{dr} \left[ r \frac{d}{dr} J_0 \right] + J_0 r = 0. \tag{D.15}
\]

Remembering that \( \frac{d}{dr} J_0 = -J_1 \) we get:

\[- \frac{d}{dr} \left[ r J_1 \right] + J_0 r = 0, \tag{D.16}\]

and multiplying by \( \frac{d J_0}{dr} = -J_1 \)

\[J_1 \frac{d}{dr} \left[ r J_1 \right] + \frac{d J_0}{dr} J_0 r = 0 \tag{D.17}\]

which implies

\[J_1^2 + \frac{1}{2} \frac{d}{dr} [J_1^2 + J_0^2] r = 0 \tag{D.18}\]

and after performing integration by parts

\[\int_0^A J_1^2 dr - \int_0^A J_0^2 dr + A [J_1^2 + J_0^2]_{A} = 0. \tag{D.19}\]

This expression can be arranged in a more illuminating way as per:

\[I_{l}^R (A) = I_{l}^R (A) - A [J_1^2 - J_0^2]_{A} \tag{D.20}\]

Therefore Eq. (D.12) depends at the end only of

\[I_{l}^R (A) = \int_0^A J_0^2 dr, \tag{D.21}\]

which can be evaluated numerically in a very precise way by the Periodisation method described for instance in [95].
Appendix E

Asymptotic representation of $J_n(n \sech \alpha)$ as it is expressed in Abramowitz and Stegun

This appendix is devoted to obtain the asymptotic expression in Eq. (5.201) in chapter 5. The first step is to consider the integral representation of a Bessel function with integer order $n$ [76, 87]:

$$J_n(z) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \exp[i(n\theta - z \sin \theta)]d\theta$$  \hspace{1cm} (E.1)

Now, let us assume that $z$ has the form $z = n \sech \alpha$ with $\alpha \in \mathbb{R}$. This implies

$$J_n(n \sech \alpha) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \exp[i(n\theta - \sech \alpha \sin \theta)]d\theta, \hspace{1cm} (E.2)$$

$$= \frac{1}{2\pi} \int_{-\pi}^{\pi} \exp[im\theta]d\theta \hspace{1cm} (E.3)$$

From this expression we can see that as $n$ grows, the number of oscillations in the integrand also increases. However, if there exists a stationary point $\theta_0$ such that $p'(\theta_0) = 0$ this would imply that most of the contribution to the integral comes from the part of the function in the vicinity of the stationary point. Away from the stationary point, the function oscillates and the areas cancel out. Thus

$$p'(\theta) = 1 - \sech \alpha \cos \theta\hspace{1cm} (E.4)$$

From this equation it is clear that the stationary point we are looking for is not on the real axis, even more $\theta_0 = i\alpha$. Then, we can approximate $p(\theta)$ via its Taylor’s expansion of up to second order to get:

$$p(\theta) \approx p(i\alpha) + p''(i\alpha)(\theta - i\alpha)^2,\hspace{1cm} (E.5)$$
because by construction \( p'(i\alpha) = 0 \). Then, this Bessel function approximation reads:

\[
J_n(n \sech \alpha) \approx \exp\left[\frac{\text{in}p(i\alpha)}{2\pi} \int_{-\pi}^{\pi} \exp\left[\frac{\text{in}p''(i\alpha)(\theta - i\alpha)^2}{2}\right] d\theta\right], \quad (E.6)
\]

\[
= \exp\left[\frac{\text{in}p(i\alpha)}{2\pi} \int_{-\pi}^{\pi} \exp\left[-n \tanh \frac{(\theta - i\alpha)^2}{2}\right] d\theta\right]. \quad (E.7)
\]

Defining \( A_n^2 := \frac{n \tanh \alpha}{2} \) and making the change of variables \( v_n = A_n \theta \) we have:

\[
J_n(n \sech \alpha) \approx \exp\left[\frac{\text{in}p(i\alpha)}{2\pi A_n} \int_{-A_n \pi}^{A_n \pi} \exp[-(v_n - iA_n \alpha)^2] dv_n\right] \quad (E.8)
\]

now, consider the loop in the complex plane \( \Gamma \) given by \( \Gamma = \gamma_1 \cup \gamma_2 \cup \gamma_3 \cup \gamma_4 \) with:

\[
\gamma_1 = \{z = -A_n \pi + t2A_n \pi | t \in [0, 1]\}, \quad \gamma_2 = \{z = A_n \pi + tiA_n \alpha | t \in [0, 1]\}, \quad \gamma_3 = \{z = A_n \pi + iA_n \alpha - t2A_n \pi | t \in [0, 1]\}, \quad \gamma_4 = \{z = -A_n \pi + iA_n \alpha - tiA_n \alpha | t \in [0, 1]\}
\]

as it is shown in Fig E.1. It is now convenient to call the following integrals

\[\text{Fig. E.1. Rectangular loop } \Gamma \text{ on the upper complex plane.}\]
\[ I_n^n = \int_{\gamma_l} \exp[-(z - iA_n\alpha)^2] dz, \quad (E.13) \]

\[ I^n = \int_{\Gamma} \exp[-(z - iA_n\alpha)^2] dz = \sum I_l^n. \quad (E.14) \]

Due to the fact that \( \exp[-(v_n - iA_n\alpha)^2] \) has no singularities inside \( \Gamma \), we have \( I = 0 \) and then \( I_n^n = -(I_3^n + I_2^n + I_4^n) \). This implies that our approximation to the Bessel function reads:

\[ J_n(n \text{ sech } \alpha) \approx -\frac{\exp[\text{inp}(i\alpha)]}{2\pi A_n} (I_3^n + I_2^n + I_4^n). \quad (E.15) \]

We are now in a position to study \( J_n(n \text{ sech } \alpha) \) for large values of \( n \)

\[ \lim_{n \to \infty} J_n(n \text{ sech } \alpha) \approx -\frac{\exp[\text{inp}(i\alpha)]}{2\pi A_n} (I_3^n + I_2^n + I_4^n). \quad (E.16) \]

We deal with these integrals one by one. First we consider the case \( I_3^n \)

\[ \lim_{n \to \infty} I_3^n = -\int_{-\infty}^{\infty} e^{-t^2} dt = -\sqrt{\pi}. \quad (E.17) \]

For the case of \( I_2^n \) we need to be more careful and consider the following bound to our integral

\[ I_2^n = \int_0^1 \exp[-(A_n\pi + iA_n(t - 1))^2] dt, \quad (E.18) \]

\[ = \exp[-(A_n\pi)^2] \int_0^1 e^{A_n^2(t-1)^2} e^{-2iA_n^2 \pi(t-1)} dt, \quad (E.19) \]

\[ \leq \exp[-(A_n\pi)^2] \left| \int_0^1 e^{A_n^2(t-1)^2} e^{-2iA_n^2 \pi(t-1)} dt \right|, \quad (E.20) \]

\[ \leq \exp[-(A_n\pi)^2] \left| \int_0^1 \left| e^{A_n^2(t-1)^2} \right| e^{-2iA_n^2 \pi(t-1)} dt \right|, \quad (E.21) \]

\[ \leq \exp[-(A_n\pi)^2]. \quad (E.22) \]

From this last equality it follows that:

\[ \lim_{n \to \infty} I_2^n \leq \lim_{n \to \infty} e^{-(A_n\pi)^2} = 0, \quad (E.23) \]

and proceeding in the same fashion for \( I_4^n \) one has finally:

\[ \lim_{n \to \infty} J_n(n \text{ sech } \alpha) \approx \frac{\exp[\text{inp}(i\alpha)]}{2\pi A_n} \sqrt{\pi}, \quad (E.24) \]

or in a more illuminating form:

\[ \lim_{n \to \infty} J_n(n \text{ sech } \alpha) \approx \frac{e^{n(tanh - \alpha)}}{\sqrt{2\pi n tanh}}, \quad (E.25) \]
On the redefinition of the spherical Bessel function

Consider the equation of the spherical Bessel function given by:

\[ r^2 R_n'' + 2r R_n' + R_n(r^2 \beta^2 - n(n + 1)) = 0. \quad (F.1) \]

Dividing by \( r \) and after some simple manipulations one gets:

\[ \frac{d^2}{dr^2}[r R_n] + R_n \left( r \beta^2 - \frac{n(n + 1)}{r} \right) = 0. \quad (F.2) \]

Now, we introduce a new unknown function \( S_n \)

\[ S_n := r^{n+1} R_n(r), \quad (F.3) \]

this implies that Eq. (F.1) reads:

\[ \frac{d^2}{dr^2}[r^{-n} S_n] + r^{-n} S_n \beta^2 - n(n + 1) S_n r^{n-2} = 0. \quad (F.4) \]

Using the fact that

\[ \frac{d^2}{dr^2}[r^{-n} S_n] = r^{-n} S_n'' - 2n r^{-n-1} S_n' + n(n + 1) r^{n-2} S_n = 0. \quad (F.5) \]

We have by plugging Eq. (F.5) into Eq. (F.4)

\[ S_n'' + \beta^2 S_n - 2n r^{-1} S_n' = 0. \quad (F.6) \]

This expression suggest some kind of oscillating behavior, so we propose:

\[ S_n := S_{n,\pm} = e^{\pm i \beta r} Q_{n,\pm}(r) \quad (F.7) \]

Again, we expand the derivatives

\[ S_n' = \frac{d}{dr}[e^{\pm i \beta r} Q_{n,\pm}] = e^{\pm i \beta r} Q_{n,\pm}' \pm i \beta e^{\pm i \beta r} Q_{n,\pm}, \quad (F.8) \]

\[ S_n'' = \frac{d^2}{dr^2}[e^{\pm i \beta r} Q_{n,\pm}] = -\beta^2 e^{\pm i \beta r} Q_{n,\pm} \pm 2i \beta e^{\pm i \beta r} Q_{n,\pm} + e^{\pm i \beta r} Q_{n,\pm}' \quad (F.9) \]
Thus, equation \((F.6)\) can be seen as:

\[
(Q''_{n,\pm} - 2nr^{-1}Q'_{n,\pm}) \pm 2i\beta(Q'_{n,\pm} - nr^{-1}Q_{n,\pm}) = 0
\]  \(\text{(F.10)}\)

This Ordinary Differential equation can be solved by the Frobenius method \([78, 76]\), so we propose:

\[
Q_{n,\pm}(r) = \sum_{m=0}^{\infty} a_{n,m}^\pm r^{k+m}
\]  \(\text{(F.11)}\)

and differentiating term by term

\[
Q'_{n,\pm}(r) = \sum_{m=0}^{\infty} a_{n,m}^\pm (m+k)r^{k+m-1},
\]  \(\text{(F.12)}\)

\[
Q''_{n,\pm}(r) = \sum_{m=0}^{\infty} a_{n,m}^\pm (m+k)(m+k-1)r^{k+m-2}.
\]  \(\text{(F.13)}\)

Upon substitution in Eq. \((F.10)\) we get

\[
\sum_{m=0}^{\infty} a_{n,m}^\pm (m+k) \{(m+k-1) - 2n\} r^{k+m-2} \pm 2i\beta \sum_{m=0}^{\infty} a_{n,m}^\pm \{m+k-n\} r^{k+m-1} = 0
\]  \(\text{(F.14)}\)

The lowest power that appears in \(r^{k-2}\) with coefficient \(a_0^\pm k\{k - (1 + 2n)\}\). Since \(a_0^\pm \neq 0\) we have that:

\[
k = 0 \quad \text{or} \quad k = 2n + 1.
\]  \(\text{(F.15)}\)

Given the fact that the distance between the indicial roots is an integer, their corresponding solutions are linearly dependent \([78, 76]\). Therefore, it is enough to focus our attention to just one root. In this work we are going to pick the case when \(k = 0\). This implies that equation \((F.14)\) reads

\[
\sum_{m=1}^{\infty} a_{n,m}^\pm m \{m - (1 + 2n)\} r^{m-2} \pm 2i\beta \sum_{m=0}^{\infty} a_{n,m}^\pm \{m - n\} r^{m-1} = 0
\]  \(\text{(F.16)}\)

Moving the index in the second sum \(m \rightarrow m - 1\) we get:

\[
\sum_{m=1}^{\infty} \left[ m \{m - (1 + 2n)\} a_{n,m}^\pm \pm 2i\beta \{m - (n + 1)\} a_{m-1}^\pm \right] r^{m-2} = 0
\]  \(\text{(F.17)}\)
And because this sum must be equal to zero for each power we get the following recurrence relation for the coefficients

\[ a_{n,m}^\pm = - (\pm 2i\beta) \frac{(m - (n + 1))}{m(m - (1 + 2n))} a_{m-1}^\pm = (\mp 2i\beta) \frac{(n + 1 - m)}{m(1 + 2n - m)} a_{n,m-1}^\pm. \]  

(F.18)

Then, \( a_{n,m}^\pm \) can be written:

\[ a_{n,m}^\pm = (\mp 2i\beta)^m \prod_{p=1}^m (n + 1 - p) \prod_{p=1}^m (1 + 2n - p) a_{n,0}^\pm, \quad m \geq 1. \]  

(F.19)

and \( Q_{n,\pm}(r) \):

\[ Q_{n,\pm}(r) = a_{n,0}^\pm \left[ 1 + \sum_{m=1}^{\infty} r^m (\mp 2i\beta)^m \prod_{p=1}^m (n + 1 - p) \prod_{p=1}^m (1 + 2n - p) \right] = a_{n,0}^\pm q_{n,\pm}(r). \]  

(F.20)

Noticing that \( a_{n,m}^\pm = 0 \) for \( m > n \) we get:

\[ q_{n,\pm}(r) = 1 + (1 - \delta_0^n) \sum_{m=1}^{n} r^m (\mp 2i\beta)^m \prod_{p=1}^m (n + 1 - p) \prod_{p=1}^m (1 + 2n - p), \]  

(F.21)

where \( \delta_0^n \) is a Kronecker’s delta. In addition calling

\[ \sigma_{n,m} := (1 - \delta_0^n) \frac{\prod_{p=1}^m (n + 1 - p)}{m! \prod_{p=1}^m (1 + 2n - p)}, \]  

(F.22)

allows to rewrite Eq. (F.21) in a more compact form as:

\[ q_{n,\pm}(r) = 1 + \sum_{m=1}^{n} r^m (\mp 2i\beta)^m \sigma_{n,m} \quad n \geq 0, \]  

(F.23)

and its derivative is then given by

\[ q'_{n,\pm}(r) = \sum_{m=1}^{n} m r^{m-1} (\mp 2i\beta)^m \sigma_{n,m} \quad n \geq 0, \]  

(F.24)

Combining Eq. (F.3), Eq. (F.7) and Eq. (F.20) we get that:

\[ R_{n,\pm} = \frac{e^{\pm i\beta r}}{r^{n+1}} Q_{n,\pm}(r) \]  

(F.25)

and then the complete solution of Eq. (F.1) is given by

\[ R_n = a_{n,0}^+ e^{+i\beta r} q_{n,\pm}(r) + a_{n,0}^- e^{-i\beta r} q_{n,\pm}^{-}(r) \]  

(F.26)
which represents a superposition of two traveling waves. As we can see, this solution is well defined for \( r \neq 0 \), however, for the case when \( r \) is near to zero, we must be more careful in our approach. First, we consider the case for when \( n = 0 \), then \( R_0 \) reads:

\[
R_0 = a_0^+ e^{i\beta r} + a_0^- e^{-i\beta r} \tag{F.27}
\]

Now, in order to remove the singularity in zero we set: \( a_0^- = -a_0^+ \) and \( a_0^+ = \frac{1}{2i\beta} \) to have

\[
R_0 = \sin(\beta r) \frac{\beta r}{\beta} . \tag{F.28}
\]

Consequently, we can redefine the spherical Bessel function of order zero as:

\[
j_R^0(r\beta) = \begin{cases} 
\sin(\beta r) \frac{\beta r}{\beta} & \text{if } r \neq 0, \\
1 & \text{if } r = 0,
\end{cases} \tag{F.29}
\]

where the super index \( R \) stands for \textit{Redefined}. For the case of \( n \geq 1 \) we set in a similar way we set: \( a_{n,0}^- = -a_{n,0}^+ \) and \( a_{n,0}^+ = \frac{1}{2i\beta^{n+1}} \), to have:

\[
R_n = \frac{\sin(\beta r)}{(\beta r)^{n+1}} + \sum_{m=1}^{n} \frac{(2i)^{m-1} \left\{ (-1)^m e^{i\beta r} - e^{-i\beta r} \right\}}{(\beta r)^{n+1-m}} \sigma_{n,m} \tag{F.30}
\]

From this expression, we can see that \((\beta r)^{n+1} R_n\) is analytical on \( r = 0 \) and equals the value zero [64]. Thus it is possible to redefine the spherical Bessel function of order \( n \geq 1 \) as:

\[
j_R^n(r\beta) = \begin{cases} 
\sin(\beta r) \frac{\beta r}{\beta} + \sum_{m=1}^{n} \frac{(2i)^{m-1} \left\{ (-1)^m e^{i\beta r} - e^{-i\beta r} \right\}}{(\beta r)^{n+1-m}} \sigma_{n,m} & \text{if } r \neq 0, \\
0 & \text{if } r = 0,
\end{cases} \tag{F.31}
\]

In the same fashion, the redefined Hankel functions for \( r \neq 0 \) are given by:

\[
h_R^{\pm,n}(\beta r) = \pm \frac{1}{2} \left[ \frac{e^{i\beta r}}{(\beta r)^{n+1}} \left( 1 + \sum_{m=1}^{n} r^m (\mp 2i\beta)^m \sigma_{n,m} \right) \right], \quad n \geq 0 . \tag{F.32}
\]

Notice that these definitions allow us to recover the well known identity [87]:

\[
h_R^{+,n}(\beta r) + h_R^{-,n}(\beta r) = 2j_R^n(r\beta) . \tag{F.33}
\]
Appendix G

The quasinormal modes on a sphere

G.1 Preliminary considerations

We know from Maxwell’s Equations that the Electric field is given by the equation

\[ \nabla \times \nabla \times \hat{E} = \beta^2(\omega) \hat{E}, \quad \beta^2(\omega) = \frac{\omega^2}{c^2} \epsilon(\omega), \quad \zeta = \{I, II\} \quad (G.1) \]

where \( U_I = \{r | r > a\} \) is the spatial domain corresponding to the exterior of the sphere and \( U_{II} = \{r | r < a\} \) corresponds to the interior of the sphere.

It is apropos to consider the spherical coordinates

\[ x = r \sin \vartheta \cos \phi \quad e_x = \sin \vartheta \cos \phi e_r + \cos \vartheta \sin \phi e_\vartheta \]
\[ y = r \sin \vartheta \sin \phi \quad e_y = \sin \vartheta \sin \phi e_r + \cos \vartheta \cos \phi e_\vartheta + \sin \phi e_\varphi \]
\[ z = r \cos \vartheta \quad e_z = \cos \vartheta e_r - \sin \vartheta e_r, \quad (G.2) \]

and for an arbitrary vector expressed in this basis \( v = v_\vartheta e_\vartheta + v_\phi e_\phi \) and an arbitrary scalar function \( \psi := \psi(r, \vartheta, \phi) \) the following identities hold:

\[ \nabla \times \psi := \frac{\partial \psi}{\partial r} e_r + \frac{1}{r} \frac{\partial \psi}{\partial \vartheta} e_\vartheta + \frac{1}{r \sin \vartheta} \frac{\partial \psi}{\partial \phi} e_\phi \quad (G.5) \]

\[ \nabla \times v := \frac{1}{r \sin \vartheta} \left[ \frac{\partial}{\partial \vartheta} (\sin \vartheta v_\phi) - \frac{\partial v_\phi}{\partial \vartheta} \right] e_r + \frac{1}{r} \left[ \frac{\partial v_\vartheta}{\partial r} - \frac{\partial}{\partial r} (r v_\phi) \right] e_\vartheta + \frac{1}{r} \left[ \frac{\partial v_r}{\partial \vartheta} - \frac{\partial}{\partial \vartheta} (r v_\vartheta) \right] e_\varphi, \quad (G.6) \]

\[ \nabla^2 \psi := \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2} \left[ \frac{1}{\sin \vartheta} \frac{\partial}{\partial \vartheta} \left( \sin \vartheta \frac{\partial \psi}{\partial \vartheta} \right) + \frac{1}{\sin^2 \vartheta} \frac{\partial^2 \psi}{\partial \phi^2} \right] \quad (G.7) \]
By defining the operator

\[\Delta_{\theta\varphi} := \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \]  

(G.8)

the spherical vectorial laplacian can be written in a more compact way as:

\[\nabla^2 \psi = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \psi}{\partial r} \right) + \frac{\Delta_{\theta\varphi} \psi}{r^2} \]  

(G.9)

We propose a TE polarized solution for Eq. (G.1)

\[\hat{E} = \vec{\nabla} \times (r \hat{u}(\omega, r, \theta, \varphi) \hat{e}_r) = \frac{1}{\sin \theta} \frac{\partial}{\partial \varphi} \hat{e}_\theta - \frac{\partial}{\partial \theta} \hat{e}_\varphi \]  

(G.10)

In order to see if this is a good choice, we take the curl of \(\hat{E}\) twice, then:

\[
\vec{\nabla} \times \vec{\nabla} \times \hat{E} = -\frac{1}{r \sin \theta} \left[ \frac{\partial}{\partial \varphi} \left( \frac{1}{\sin \theta} \frac{\partial \hat{u}}{\partial \varphi} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 \hat{u}}{\partial \varphi^2} \right] \hat{e}_r \\
+ \frac{1}{r} \frac{\partial}{\partial r} \left( \frac{1}{\sin \theta} \frac{\partial \hat{u}}{\partial \varphi} \right) \hat{e}_\theta + \frac{1}{r} \frac{\partial}{\partial r} \left( \frac{1}{\sin \theta} \frac{\partial \hat{u}}{\partial \varphi} \right) \hat{e}_\varphi,
\]

\[= -\frac{1}{r} \Delta_{\theta\varphi} u \hat{e}_r + \frac{\partial}{\partial \varphi} \left( \frac{1}{r} \frac{\partial}{\partial r} (r \hat{u}) \right) \hat{e}_\theta + \frac{1}{\sin \theta} \frac{\partial}{\partial \varphi} \left( \frac{1}{r} \frac{\partial}{\partial r} (r \hat{u}) \right) \hat{e}_\varphi \]  

(G.11)

and

\[
\vec{\nabla} \times \vec{\nabla} \times \hat{E} = \frac{1}{r \sin \theta} \left[ \frac{\partial}{\partial \varphi} \left\{ \frac{\partial}{\partial \varphi} \left( \frac{1}{r} \frac{\partial}{\partial r} (r \hat{u}) \right) \right\} \right] \hat{e}_r \\
+ \frac{1}{r} \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \varphi} \left\{ -\frac{1}{r} \Delta_{\theta\varphi} \hat{u} \right\} \right] \hat{e}_\theta \\
+ \frac{1}{r} \left[ \frac{\partial}{\partial r} \left\{ \frac{\partial}{\partial \varphi} (r \hat{u}) \right\} \right] \hat{e}_\varphi,
\]

\[= \frac{1}{\sin \theta} \frac{\partial}{\partial \varphi} \left( -\nabla^2 \hat{u} \right) \hat{e}_\theta - \frac{\partial}{\partial \theta} \left( -\nabla^2 \hat{u} \right) \hat{e}_\varphi \]  

(G.12)

Therefore \(\hat{u}(\omega, r, \theta, \varphi)\) must satisfy the scalar equation:

\[\nabla^2 \hat{u} = -\beta^2(\omega)\hat{u}. \]  

(G.13)

From the theory of PDE’s we know that there is a family of solutions \(u_{n,m}\) that satisfy Eq. (G.13), namely:

\[u_{nm} = R_n(\omega, r) Y_n^m(\theta, \varphi), \]  

(G.14)
where \( Y_{n,m}(\theta, \varphi) \) are the spherical harmonics defined as:

\[
Y_{n,m}(\theta, \varphi) = \sqrt{\frac{2n+1}{4\pi} \frac{(n-|m|)!}{(n+|m|)!}} P^m_n(\cos \theta) e^{im\varphi}, \quad n \geq 0, \quad -n \leq m \leq n,
\]

where \( P^m_n \) are the associated Legendre’s polynomials. The spherical harmonics are eigenfunctions of the equation:

\[
\Delta_{\theta\varphi} Y_{n,m}(\theta, \varphi) = -n(n+1). \quad (G.16)
\]

Thus the equation for \( R_n(\omega, r) \) is:

\[
r^2 \frac{\partial^2 R_n}{\partial r^2} + 2r \frac{\partial R_n}{\partial r} + R_n (r^2 \beta^2(\omega) - n(n+1)) = 0 \quad (G.17)
\]

In the standard literature the solution of this equation is given by a spherical Bessel function defined as:

\[
R_n(r) = j_n(\beta(\omega)r) = \sqrt{\frac{\pi}{2\beta(\omega)r}} J_{n+\frac{1}{2}}(\beta(\omega)r) \quad (G.18)
\]

where is the Bessel function of fractional order. The problem with this representation is evident: it requires to define a square root of \( \beta(\omega) \) which is already a square root of the complex permittivity \( \epsilon(\omega) \). In order to avoid such complications, we have taken in Appendix F a longer path to bypass the use of fractional Bessel functions. From this work, the new spherical Bessel functions are given by equations (F.29), (F.31 and the new Hankel functions by (F.32):

\[
\tilde{R}_{n,\xi} = \left[ \frac{1}{\sin \theta} \frac{\partial Y_{n,m}}{\partial \varphi} \mathbf{e}_\varphi - \frac{\partial Y_{n,m}}{\partial \theta} \mathbf{e}_\theta \right] \tilde{R}_{n,\xi}(r), \quad \xi = \{I, II\} \quad (G.22)
\]

Whereas the magnetic field is given by using Faraday’s law and Eq. (??):

\[
\tilde{H}_{n,\xi} = \frac{1}{\iota \omega \mu_0} \left[ \frac{1}{\sin \theta} \frac{\partial Y_{n,m}}{\partial \varphi} \mathbf{e}_\varphi + \frac{\partial Y_{n,m}}{\partial \theta} \mathbf{e}_\theta \right] \frac{1}{r} \frac{\partial}{\partial r} (r \tilde{R}_{n,\xi}) + \frac{1}{\iota \omega \mu_0} \frac{n(n+1)}{r} Y_{n,m} \tilde{R}_{n,\xi}(r) \mathbf{e}_r \quad \xi = \{I, II\} \quad (G.21)
\]

where:

\[
\tilde{R}_{n,I}(r) = A_{n,I}^+(\omega) h^+_R(\beta_1 r) + A_{n,I}^-(\omega) h^-_R(\beta_1 r), \quad (G.22)
\]

\[
\tilde{R}_{n,II}(r) = A_{n,II}(\omega) j^+_R(\beta_1 r) \quad (G.23)
\]
**G.2 The spherical resonant modes**

By considering the interface condition’s we arrive to the expressions (omitting the $\omega$ and $r$ dependencies):

\[
A_{n,II}R_{n,II}(a) = A_{n,II}^+R_{n,II}^+(a) + A_{n,II}^-R_{n,II}^-(a) \quad (G.24)
\]

\[
A_{n,II} \left( \frac{\partial}{\partial r} (rR_{n,II}) \right) \bigg|_{r=a} = A_{n,II}^+ \left( \frac{\partial}{\partial r} (rR_{n,II}^+) \right) \bigg|_{r=a} + A_{n,II}^- \left( \frac{\partial}{\partial r} (rR_{n,II}^-) \right) \bigg|_{r=a} \quad (G.25)
\]

Solving for $A_{n,II}^-$ and $A_{n,II}^+$ we have:

\[
A_{n,II}^\pm = \pm A_{n,II} \frac{R_{n,II} \left( \frac{\partial}{\partial r} (rR_{n,II}^+) \right) \bigg|_{r=a} - R_{n,II}^- \left( \frac{\partial}{\partial r} (rR_{n,II}^-) \right) \bigg|_{r=a}}{R_{n,II}^+ \left( \frac{\partial}{\partial r} (rR_{n,II}^-) \right) \bigg|_{r=a} - R_{n,II}^- \left( \frac{\partial}{\partial r} (rR_{n,II}^+) \right) \bigg|_{r=a}} \quad (G.26)
\]

Due to our Fourier transform convention we set the coefficients or $A_{n,II}^- = 0$ which correspond to incoming waves, this implies:

\[
R_{n,II} \left( \frac{\partial}{\partial r} (rR_{n,II}^+) \right) \bigg|_{r=a} - R_{n,II}^+ \left( \frac{\partial}{\partial r} (rR_{n,II}^-) \right) \bigg|_{r=a} = 0 \quad (G.27)
\]

this implies:

\[
R_{n,II} \left( \frac{\partial}{\partial r} R_{n,II}^+ \right) \bigg|_{r=a} - R_{n,II}^+ \left( \frac{\partial}{\partial r} R_{n,II}^- \right) \bigg|_{r=a} = 0 \quad (G.28)
\]

Notice that this solution does not imply the use of Ricatti-Bessel functions as in [83]. The roots of this equation are the frequencies $\Omega_{n,\nu}$ which satisfy:

\[
R_{n,II}(\Omega_{n,\nu},a)\partial_r R_{n,II}^+(\Omega_{n,\nu},a) - R_{n,II}^+(\Omega_{n,\nu},a)\partial_r R_{n,II}(\Omega_{n,\nu},a) = 0 \quad (G.29)
\]

From the solved example with the slab, we know that before trying to use a numerical method to obtain the roots of this equation, it is necessary to define a branch cut for the complex logarithm. This is an important point which is generally omitted. Nevertheless, the way that we have found for defining a branch cut is quite simple. By simple inspection of the spherical Bessel function differential equation in Eq. (G.17), it is clear that all the solutions $R_n$ for $n \geq 0$ share the same eigenvalue $\beta$ and consequently they share the same branch cut of the complex logarithm. Therefore, it is enough to define the branch cut for the simplest case when $n = 0$ and this same convention will hold for all the other orders.
From the definitions in Eq. (G.23) and Eq. (G.22) we have that

\[
R^+_{0,l}(\Omega_{0,v}, a) = e^{\pm i\beta_I(\Omega_{0,v})}, \quad (G.30)
\]

\[
\partial_r R^+_{0,l}(\Omega_{0,v}, a) = R^+_{0,l}(\Omega_{0,v}, a) \left[ i\beta_I(\Omega_{0,v}) - \frac{1}{r} \right], \quad (G.31)
\]

\[
R_{0,II}(\Omega_{0,v}, a) = \sin(\beta_{II}(\Omega_{0,v})a), \quad (G.32)
\]

\[
\partial_r R_{0,II}(\Omega_{0,v}, a) = \frac{\cos(\beta_{II}(\Omega_{0,v})a)}{r} - \frac{1}{r} R_{0,II}(\Omega_{0,v}, a). \quad (G.33)
\]

After some elementary algebra the transcendental equation that must be solved for \(n = 0\) is:

\[
e^{2ia\beta_{II}(\Omega_{0,v})} = G, \quad G = -\frac{\beta_{II}(\Omega_{0,v}) + \beta_I(\Omega_{0,v})}{\beta_{II}(\Omega_{0,v}) - \beta_I(\Omega_{0,v})} \quad (G.34)
\]

taking the complex logarithm as it is explained is Appendix C we have:

\[
\beta_{II}(\Omega_{0,v}) = \frac{1}{a} \left[ \pi v + \frac{1}{2} \text{Arg}_\theta(G) - \frac{i}{2} \ln|G| \right], v \in \mathbb{N}. \quad (G.35)
\]

In order to set the parameters \(\theta\) and \(\sigma\) for non dispersive materials we notice that \(\Im \{\beta_{II}\} < 0\) and then \(\theta = \pi\) and \(\sigma = -\).


