Optimization and Physical Bounds for Passive and Non-passive Systems
OPTIMIZATION AND PHYSICAL BOUNDS FOR PASSIVE AND NON-PASSIVE SYSTEMS

YEVHEN IVANENKO

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Abstract

Physical bounds in electromagnetic field theory have been of interest for more than a decade. Considering electromagnetic structures from the system theory perspective, as systems satisfying linearity, time-invariance, causality and passivity, it is possible to characterize their transfer functions via Herglotz functions. Herglotz functions are useful in modeling of passive systems with applications in mathematical physics, engineering, and modeling of wave phenomena in materials and scattering. Physical bounds on passive systems can be derived in the form of sum rules, which are based on low- and high-frequency asymptotics of the corresponding Herglotz functions. These bounds provide an insight into factors limiting the performance of a given system, as well as the knowledge about possibilities to improve a desired system from a design point of view. However, the asymptotics of the Herglotz functions do not always exist for a given system, and thus a new method for determination of physical bounds is required. In Papers I–II of this thesis, a rigorous mathematical framework for a convex optimization approach based on general weighted $L^p$-norms, $1 \leq p \leq \infty$, is introduced. The developed framework is used to approximate a desired system response, and to determine an optimal performance in realization of a system satisfying the target requirement. The approximation is carried out using Herglotz functions, B-splines, and convex optimization.

Papers III–IV of this thesis concern modeling and determination of optimal performance bounds for causal, but not passive systems. To model them, a new class of functions, the quasi-Herglotz functions, is introduced. The new functions are defined as differences of two Herglotz functions and preserve the majority of the properties of Herglotz functions useful for the mathematical framework based on convex optimization. We consider modeling of gain media with desired properties as a causal system, which can be active over certain frequencies or frequency intervals. Here, sum rules can also be used under certain assumptions. In Papers V–VII of this thesis, the optical theorem for scatterers immersed in lossy media is revisited. Two versions of the optical theorem are derived: one based on internal equivalent currents and the other based on external fields in terms of a T-matrix formalism, respectively. The theorems are exploited to derive fundamental bounds on absorption by using elementary optimization techniques. The theory has a potential impact in applications where the surrounding losses cannot be neglected, e.g., in medicine, plasmonic photothermal therapy, radio frequency absorption of gold nanoparticle suspensions, etc. In addition to this, a new method for detection of electrophoretic resonances in a material with Drude-type of dispersion, which is placed in a straight waveguide, is proposed.

Keywords: Convex optimization, physical bounds, Herglotz functions, quasi-Herglotz functions, passive systems, non-passive systems, approximation, absorption in lossy media
Sammanfattning
Fundamentala begränsningar inom elektromagnetisk fältteori har varit intressanta i mer än ett decennium. Om man betraktar elektromagnetiska strukturer ur systemteoriperspektiv, som linjära, tidsinvarianta, kausala och passiva system, är det möjligt att karakterisera deras överföringsfunktioner via Herglotzfunktioner. Herglotzfunktioner är användbara vid modellering av passiva system med tillämpningar inom matematisk fysik, teknik och modellering av vågfenomen i material och spridning. Begränsningarna för passiva system kan härledas i form av summationsregler som baseras på låg- och högfrekvensasymptoter för deras motsvarande Herglotzfunktioner. Dessa begränsningar ger en inblick i de faktorer som begränsar prestandan för ett givet system, såväl som kunskap om möjligheterna att förbättra ett önskat system ur en designsynpunkt. Det är dock inte alltid som Herglotzfunktionernas asymptoter existerar för ett givet system. Då kan summationsregler inte härledas, och därför krävs en ny metod för att bestämma de fysikaliska begränsningarna. I artiklarna I–II i denna avhandling introduceras ett rigoröst matematiskt ramverk för en konvex optimeringsmetod baserad på viktade $L^p$-normer, $1 \leq p \leq \infty$. Ramverket används för att approximera en önskad systemrespons och för att bestämma en optimal prestanda vid realiseringen av ett system som uppfyller givna specifikationer. Approximationen utförs med hjälp av Herglotzfunktioner, B-splines och konvex optimering.

Artiklarna III–IV i denna avhandling handlar om modellering och bestämning av optimala prestandagränser för kausala, men icke-passiva system. För att modellera dessa introduceras en ny funktionsklass, s.k. kvasi-Herglotzfunktioner. De nya funktionerna definieras som differensen mellan två Herglotzfunktioner och bevarar viktiga egenskaper för Herglotzfunktioner. Detta gör dem användbara i det matematiska ramverket baserat på konvex optimering. Förstärkande, eller s.k. aktiva media med vissa önskade egenskaper modelleras som ett kausalt system som kan vara aktivt för vissa frekvenser eller frekvensintervall. En summationsregel kan också användas under vissa antaganden.

Artiklarna V–VI i den här avhandlingen behandlar det optiska teoremet för spridare i förlustmedia. Två versioner av det optiska teoremet härleds fram. Den första versionen bygger på interna ekvivalenta strömmar medan den andra bygger på externa fält i termer av $T$-matriksformalism. Teoremen utnyttjas för att härleda fundamentala begränsningar för absorption med hjälp av optimeringstekniker. Denna teori är relevant för tillämpningar där de omgivande förlusterna inte kan försummas, t.ex. inom medicin, plasmonisk fototermisk terapi, radiofrekvensabsorption av guldnanopartikel-suspensioner, etc. Utöver detta, föreslås en ny metod för detektering av elektroforetiska resonanser i ett material med dispersion av Drude-typ, som placerats i en rak vågledare.
Dedicated to my family and friends, those who are alive and passed away...
Abstract

Physical bounds in electromagnetic field theory have been of interest for more than a decade. Considering electromagnetic structures from the system theory perspective, as systems satisfying linearity, time-invariance, causality and passivity, it is possible to characterize their transfer functions via Herglotz functions. Herglotz functions are useful in modeling of passive systems with applications in mathematical physics, engineering, and modeling of wave phenomena in materials and scattering. Physical bounds on passive systems can be derived in the form of sum rules, which are based on low- and high-frequency asymptotics of the corresponding Herglotz functions. These bounds provide an insight into factors limiting the performance of a given system, as well as the knowledge about possibilities to improve a desired system from a design point of view. However, the asymptotics of the Herglotz functions do not always exist for a given system, and thus a new method for determination of physical bounds is required. In Papers I–II of this thesis, a rigorous mathematical framework for a convex optimization approach based on general weighted $L^p$-norms, $1 \leq p \leq \infty$, is introduced. The developed framework is used to approximate a desired system response, and to determine an optimal performance in realization of a system satisfying the target requirement. The approximation is carried out using Herglotz functions, B-splines, and convex optimization.

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Acknowledgments

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Växjö, Sweden
2019
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<th>Symbol</th>
<th>Description</th>
</tr>
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<tbody>
<tr>
<td>(\mathbb{R}), (\mathbb{C})</td>
<td>the sets of real numbers and complex numbers, respectively</td>
</tr>
<tr>
<td>(\mathbb{C}^+)</td>
<td>the upper half-plane, (\mathbb{C}^+ = {z \in \mathbb{C} \mid \text{Im}(z) &gt; 0})</td>
</tr>
<tr>
<td>(\mathbb{C}_+)</td>
<td>the right half-plane, (\mathbb{C}_+ = {z \in \mathbb{C} \mid \text{Re}(z) &gt; 0})</td>
</tr>
<tr>
<td>(i)</td>
<td>imaginary unit, (i^2 = -1)</td>
</tr>
<tr>
<td>(z = x + iy)</td>
<td>complex number with (x = \text{Re}(z)) and (y = \text{Im}(z))</td>
</tr>
<tr>
<td>(z^*)</td>
<td>complex conjugate, ((x + iy)^* = x - iy)</td>
</tr>
<tr>
<td>(\hat{\rightarrow})</td>
<td>non-tangential limit</td>
</tr>
<tr>
<td>(\text{p.v.} \int(\cdot))</td>
<td>the Cauchy principal value integral</td>
</tr>
<tr>
<td>((\cdot)_+)</td>
<td>highlights the fact that parameters with the corresponding underscore represent a function with non-negative imaginary part</td>
</tr>
<tr>
<td>(\alpha)</td>
<td>Hölder exponent</td>
</tr>
<tr>
<td>(c_n)</td>
<td>B-spline expansion coefficient or optimization variable</td>
</tr>
<tr>
<td>(h)</td>
<td>a Herglotz function</td>
</tr>
<tr>
<td>(q)</td>
<td>a quasi-Herglotz function</td>
</tr>
<tr>
<td>(F)</td>
<td>the target function</td>
</tr>
<tr>
<td>(p_n)</td>
<td>B-spline basis function</td>
</tr>
<tr>
<td>(\hat{p}_n)</td>
<td>the (negative) Hilbert transform of B-spline basis function</td>
</tr>
<tr>
<td>(p_i)</td>
<td>magnitude of a point-mass</td>
</tr>
<tr>
<td>(w)</td>
<td>weight function</td>
</tr>
<tr>
<td>(w(t))</td>
<td>the impulse response</td>
</tr>
<tr>
<td>(C)</td>
<td>space of continuous functions</td>
</tr>
<tr>
<td>(C^k)</td>
<td>space of (k) times continuously differentiable functions</td>
</tr>
<tr>
<td>(C^{0,\alpha})</td>
<td>space of Hölder continuous functions, (0 &lt; \alpha &lt; 1)</td>
</tr>
<tr>
<td>(C^\infty)</td>
<td>space of smooth functions with compact support</td>
</tr>
<tr>
<td>(| \cdot |_{L^p(w)})</td>
<td>the norm corresponding to the weighted Lebesgue (L^p) space, (w &gt; 0), (1 \leq p \leq \infty)</td>
</tr>
<tr>
<td>(\Omega)</td>
<td>the approximation domain</td>
</tr>
<tr>
<td>(\mathcal{O})</td>
<td>open neighborhood of (\Omega)</td>
</tr>
<tr>
<td>(Q)</td>
<td>set of all quasi-Herglotz functions</td>
</tr>
<tr>
<td>(Q_{\text{sym}})</td>
<td>set of all symmetric quasi-Herglotz functions, (Q_{\text{sym}} \subseteq Q)</td>
</tr>
</tbody>
</table>
Preface

This doctoral dissertation summarizes the research I have carried out at the Department of Physics and Electrical Engineering at Linnaeus University during the last five years. The first introductory part provides a review on causal and passive systems, their integral representations, electromagnetic models, as well as approximation and optimization tools for the determination of optimal realizations and physical bounds used in Papers I–VII. The second part presents the Papers I–VII, which have been published or are submitted to peer reviewed scientific journals and conference proceedings. The papers are the outcome of collaboration within the project Complex analysis and convex optimization for EM design supported by the Swedish Foundation for Strategic Research (SSF), grant no. AM13-0011 under the program Applied Mathematics.

List of Included Papers


Contributions of the author: The author of this thesis has been leading the writing of this paper, which has been conducted as a subproject within the larger SSF project mentioned above. The first author has collected information, comments and suggestions from the co-authors and has been responsible for the numerical examples.


Contributions of the author: The author of this thesis has been responsible for all of the analysis, numerical examples and writing of this paper.


Contributions of the author: The author of this thesis has been leading the writing of this paper, which has been conducted as a subproject within the
larger SSF project mentioned above. The first author has been responsible for the parts concerning convex optimization whereas the second author has been responsible for the mathematical analysis and theorems. The first author has collected information, comments and suggestions from the co-authors, and has been responsible for the numerical examples.


Contributions of the author: The author of this thesis has been responsible for all of the analysis, numerical examples and writing of this paper.


Contributions of the author: The author of this thesis has contributed with comments and suggestions on theory as well as on writing, and numerical experiments.


Contributions of the author: The author of this thesis has been responsible for all of the analysis, numerical examples and writing of this paper.


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*Awarded with the URSI Young Scientist Award at 2019 URSI Commission B International Symposium on Electromagnetic Theory (EMTS) in San Diego CA, United States.
Other Publications by the Author

The author of this dissertation is also the author or co-author of the following publications which are related to but not part of the dissertation:


Part I

Introduction and Research Overview

Yevhen Ivanenko
1 Background, Motivation, and Goals

Holomorphic mappings between certain half planes have taken an important place in modeling electromagnetic structures from a system viewpoint in the last decades. Such mappings are characteristic for passive systems [95,98–100], which intuitively can be defined as systems that do not produce energy. However, for a physical system to be passive from a system point of view, it has to be single-valued, linear, continuous, time-translationally invariant, and have an input-output relation in convolution form. An important property implied by passivity is causality [100]. Causality associates the real and imaginary parts of a signal in the frequency domain in the form of the Hilbert transform [3,48]. The corresponding relations are also known as Kramers-Kronig relations [45,48,52,62], which play an important role in Titchmarsh's theorem [48,72]. However, passivity adds more severe constraints on bandwidth of a signal than causality [100]. The impulse response of a passive system in the frequency domain is given by a Herglotz function. Herglotz functions (also known as Nevanlinna and R-functions) or Positive Real (PR) functions [1,4,5,30,47,72,100] are analytic functions mapping complex half planes to their corresponding closures, and provide a complete information about a passive system via their integral representation formula. The low- and/or high-frequency asymptotic properties of Herglotz functions are used in the derivation of sum rules, which are related to physical bounds for given passive systems [13].

Sum rules are useful in the determination of physical bounds in many physical and engineering branches such as dielectric constants [52], matching networks [28], antennas [34,37,38,46], high-impedance surfaces [36], absorbers [76], periodic structures [39], extraordinary transmission [56], reflection coefficients [33], broadband metamaterials [35], as well as for interaction between the waves and scatterers [11,83]. They relate dynamic parameter values of a passive system to its asymptotics, and provide theoretical insight on improvement of a designed system. Also, several other limitations, such as speed-of-light limitations in passive linear media, have been derived by using general Herglotz function theory [94]. However, in some cases, the presence of losses in a considered system affects the small- and large-argument asymptotic expansions of a representing Herglotz function. An example of such a system is the reflection coefficient from a passive metal-backed dielectric slab, where the metal is finitely conductive; see e.g., [69]. This results in an impossibility to derive the physical bound based on sum rules, and hence for systems that inhibit asymptotic properties of Herglotz functions, an alternative approach is required.

To derive a physical bound on a given system, the problem has to be reformulated with respect to the following question: “What is a best/optimal realization of a linear system with a desired target response over a finite frequency band subject to given system constraints?” Existing methods for solving such a problem are related to
boundary values of analytic functions on the real axis, where linear systems can be approximated via the Routh approximation method, i.e., by linear systems of lower order [42], using minimum energy functions [49], Laguerre and Kautz functions [91], or Hardy approximations [8]. However, for approximation theory, a different route is followed, where passive approximation based on convex optimization is employed [69].

The first goal of this thesis is to develop a rigorous mathematical tool for studying physical bounds on given passive systems, which is supported by constructive proofs. This framework is supposed to be equipped with weighted $L^p$-norms, and involves the convex cone of approximating Herglotz functions, which are Hölder continuously extended to an open neighborhood of the real axis and have a measure given as a finite B-spline expansion of a fixed arbitrary order. In Papers I–II of this thesis, we incorporate this framework with convex optimization approach, which allows us to add a priori knowledge about a desired system, such as measurement data or asymptotic properties in the form of a sum rule, as a constraint in the optimization problem to be considered.

Papers III–IV of this thesis are focused on modeling of causal systems, which do not satisfy the passivity requirement. Such systems can e.g., be associated with the use of gain media. One well known example of gain media are fluorescent dyes. The fluorescent dye is a causal non-linear material which can be linearized as a four-level system for pumping energy [19], and its corresponding dispersion relation is given by the Lorentz model for non-passive materials [19,53,78,93,96]. Gain media are used for light localization in plasmonics, extraordinary transmission, nanoantennas, plasmon waveguides, cloaking, and other applications; see e.g., [6,19,20,31,53,55,58,81] with references. These causal systems can be treated on the real axis via Kramers-Kronig relations in the Hilbert space [48, 72], or in the sense of distributions [10, 100]. The bounds on dispersion relations for causal systems over a finite frequency intervals has been proposed in [62], where the method is based on finite Kramers-Kronig relations. There exist several studies and methods for approximation of given causal systems using Hardy approximants [7] for $L^p$-functions, and solving bounded external problems with pointwise constraints [9]. However, these methods do not relate the dynamic parameters of causal systems to their low- and/or high-frequency asymptotics, and the causal systems cannot be described by Herglotz functions.

The problem we would like to solve in Papers III–IV of this thesis is based on the question: “What is an optimal realization of a causal system with a given target response over a finite frequency band, which may have amplification properties over certain frequencies or frequency intervals, and is passively constrained outside of these intervals?” Hereby, the second goal of this thesis is to extend the existing class of admittance passive systems, which will involve a subclass of non-passive systems characterized by a certain set of analytic functions in the frequency domain. As a result, a new set of functions, the quasi-Herglotz functions, is proposed. These
functions are defined as differences of two Herglotz functions, and preserve most of the properties of Herglotz functions: the integral representation formula, the boundary-value representation, and for some cases admit the sum-rule identities. We restrict the set of functions to those, which have a Hölder continuous extension to an open neighborhood of the approximation domain on the real axis, and where the generating measure is defined as a finite-order B-spline expansion. The proposed approximants are suitable for incorporation with the convex optimization approach formulated in Papers I–II of this thesis. In some cases, it is also possible to correlate a priori known asymptotic properties of a desired causal system with its dynamic parameters using sum-rule constraints in the optimization problem under consideration.

Papers V–VII of this thesis are focused on physical bounds on absorption of power by scatterers immersed in lossy media. The bounds on scattering and absorption have been derived for many physical and engineering applications such as small dipole scatterers [88], radar absorbers [76], high-impedance surfaces [36], passive metamaterials [81,84], absorption and scattering [61,65,80], etc. The Herglotz function theory has been used in [83] to derive the physical bound on the extinction cross section, which depends on the geometry of a considered scatterer. However, these bounds have been derived under condition that the medium surrounding the scattering object is lossless. It has been shown in [14,27,29,54,63,64,70,71,85,86,97] that these bounds will be nullified in the presence of losses, and thus, the power absorbed by the surrounding medium should be included in the power balance for the optical theorem [15].

Physical bounds on absorption in lossy media will bring new insight on the scattering properties of objects both from the theoretical and from the design perspective in application areas, where losses cannot be neglected. One such example from medicine, is shown in Figure 1. Figure 1 shows the uptake of gold nanoparticles by cancer cells. This can enable the cancer cells to be heated in the radio frequency and microwave frequency ranges, without damaging the surrounding normal tissue; see the references [21–23,68,79]. The cancer cell with inserted gold nanoparticles is henceforth referred to in this thesis as a gold nanoparticle suspension. The phenomenon of heating of gold nanoparticle suspensions is not completely understood [68,79] and requires additional studies from the physical and design perspectives. In the optical frequency range, the applications include the use of gold nanoparticles in plasmonic photothermal therapy for cancer treatment [41], and are concerned with light penetration in biological tissue [26]. Beyond cancer, scattering and absorption parameters are important in medical telemetry [60,82], where the objective is to reduce the amount of absorbed power, and to design a reliable communication link for transmission of power from an antenna implanted in the human body to a receiver. Yet other applications include photonics with z-dotted PMMA materials [2], and
in short-wave communications at 60GHz [40,59,74,90,92], where the absorption band of oxygen is.

Figure 1: Uptake of 5nm glutathione coated gold nanoparticles in colorectal cancer cells: a) after 90 minutes; b) after 15 hours. Reprinted from Biomaterials, 32, T. Lund, M. F. Callaghan, P. Williams, M. Turmaine, C. Bachmann, T. Rademacher, I. M. Roitt, and R. Bayford, The influence of ligand organization on the rate of uptake of gold nanoparticles by colorectal cancer cells, 9776–9784, 2011, with permission from Elsevier.

Physical bounds on absorption in lossy media cannot be determined in the form of a sum rule due to the presence of losses in the considered system, which has been discussed in Papers I–II of this thesis described above. Hence, a different approach based on optimization techniques is proposed. We present two versions of an optical theorem in lossy media. The first version is formulated in terms of the internal fields, i.e., it is based on equivalent currents and serves as an extension of the work in [61]. The second version is based on external fields, where the T-matrix method [52, Eq. (7.34)] is used, and generalizes the results in [70]. The two versions are incorporated then with the Method of Lagrange Multipliers [17,57], which is an elementary optimization technique used to determine the physical bounds on absorption in lossy media for arbitrary scatterers made of arbitrary materials.

1.1 Thesis Outline

This thesis consists of two parts and is organized as follows. Section 2 provides an overview on one-port causal and passive systems, and the corresponding integral representations of these systems are discussed in Section 3. Section 4 introduces optimization techniques used in Part II for determination of optimal realizations and physical bounds for passive and a subclass of non-passive systems. Section 5 contains theory for the developed approximation framework incorporated with the numerical convex optimization approach described in Section 4.1. Section 6 reviews the dispersion models characterizing linear passive and non-passive materials, and the corresponding constructed Herglotz and
quasi-Herglotz functions, respectively, describing the systems based on these models. Section 7 presents physical bounds on absorption in lossy media derived using the analytical optimization technique discussed in Section 4.2. Section 8 gives an overview on the contributions included in Part II of this thesis and highlights the results achieved in this manuscript. Part I ends with conclusions and discussions on future work in Sections 9 and 10, respectively. Part II includes the scientific papers, as listed in the Preface.

1.2 Notation and Conventions

The electric and magnetic field intensities E and H are given in SI-units [45] and the time convention for time harmonic fields (phasors) is given by $e^{-j\omega t}$, where $\omega$ is the angular frequency and $t$ the time. Let $\mu_0$, $\varepsilon_0$, $\eta_0$ and $c_0$ denote the permeability, the permittivity, the wave impedance and the speed of light in vacuum, respectively, and where $\eta_0 = \sqrt{\mu_0/\varepsilon_0}$ and $c_0 = 1/\sqrt{\mu_0\varepsilon_0}$. The wave number of vacuum is given by $k_0 = \omega\sqrt{\mu_0\varepsilon_0}$, and hence $\omega\mu_0 = k_0\eta_0$ and $\omega\varepsilon_0 = k_0\eta_0^{-1}$. The definition of spherical vector waves [3, 15, 16, 45, 52, 67] is summarized in Appendix B of Paper VII. The field expansions based on the spherical vector waves [3, 15, 16, 45, 52, 67] are presented in Section 7. In particular, the regular spherical Bessel functions, the Neumann functions, the spherical Hankel functions of the first kind and the corresponding Riccati-Bessel functions [52] are denoted by $j_l(z)$, $y_l(z)$, $h_l^{(1)}(z) = j_l(z) + iy_l(z)$, $\psi_l(z) = zj_l(z)$ and $\xi_l(z) = zh_l^{(1)}(z)$, respectively, all of order $l$, where the complex-valued argument $z \in \mathbb{C}$ is written $z = x + iy$ with $x, y \in \mathbb{R}$. The real and imaginary parts and the complex conjugate of a complex number $\zeta$ are denoted by $\text{Re}\{\zeta\}$, $\text{Im}\{\zeta\}$ and $\zeta^*$, respectively. For dyadics, the notation $()^\dagger$ denotes the Hermitian transpose.

2 Passive and Causal Systems

In this section, we give an overview on the basic properties of passive and causal systems, which are within the scope of this thesis.

Passive systems can intuitively be thought of as physical objects that do not produce energy. However, from a system point of view, the mathematical issue is with definition of such a system and its corresponding input-output relation. Here, we consider systems from macroscopic point of view, i.e., a system considered as a “black box” having one input and one corresponding output, where the signals can be measured, see Figure 2(a), and all its dynamic properties can be described mathematically by the representation formula in integral form. To define passive and causal systems, we restrict the systems under consideration to satisfy the criteria of linearity, time-invariance, continuity and having input-output relation in convolution form.
Figure 2: Illustration of a one-port system: a) Structural representation; b) Mathematical representation.

For the definitions given below, let $\mathcal{R}$ denote the system’s operator as shown in Figure 2(b).

**Definition 2.1** A system with input $u(t)$ and output $v(t)$ in the time domain is linear if
\[ \mathcal{R}\{\alpha_1 u_1(t) + \alpha_2 u_2(t)\} = \alpha_1 \mathcal{R}\{u_1(t)\} + \alpha_2 \mathcal{R}\{u_2(t)\} \] (1)
for $\alpha_1, \alpha_2 \in \mathbb{R}$ or $\mathbb{C}$, implying that the output is given as a linear function of the input [100, Sec. 5.8].

**Definition 2.2** A system with input $u(t)$ and output $v(t)$ in the time domain is time-translationally invariant if
\[ v(t) = \mathcal{R}\{u(\cdot)\} \Rightarrow v(t + t') = \mathcal{R}\{u(\cdot + t')\} \] (2)
for all $t'$, implying that the system does not explicitly depend on time, by producing a shifted output $v(t + t')$ for a given shifted input $u(t + t')$ [100, Sec. 5.8].

**Definition 2.3** A system with input $u(t)$ and output $v(t)$ in the time domain is continuous if [100, Sec. 5.8]
\[ u_n \to u \Rightarrow \mathcal{R}\{u_n\} \to \mathcal{R}\{u\}. \] (3)

Intuitively, this can be interpreted as a small perturbation in the input signal to a continuous system only leads to a small perturbation in the output signal [12].

The properties given in Definitions 2.1 through 2.3 characterize systems in convolution form [100, Sec. 5.8].

**Definition 2.4** A system with input $u(t)$ and output $v(t)$ in the time domain is in convolution form if
\[ v(t) = (w * u)(t) := \int_{\mathbb{R}} w(\tau) u(t - \tau) d\tau, \] (4)
where $w(t)$ is the impulse response [66].
Systems satisfying the criteria given in Definitions 2.1 through 2.4 are called one-ports. In this thesis, we restrict ourselves to real-valued one-port systems.

To define a causal system, a one-port system should be restricted as follows.

**Definition 2.5** A one-port system with convolution operator $\mathcal{R}\{\cdot\}$ in the time domain is causal if

$$w(t) = 0 \quad \text{for} \quad t < 0,$$

where $w$ is the impulse response of the one-port system [100, Sec. 10.3].

The Definition 2.5 implies that the output of a one-port causal system cannot precede the given input. It is also applicable to the input signals $u(t)$, which can be causal as well. The corresponding holomorphic Fourier transform of a causal signal is given by

$$U(\omega) = \int_{\mathbb{R}} u(t)e^{i\omega t} \, dt$$

for $\text{Im}\{\omega\} > 0$. Note that if the function $U(v)$, $v \in \mathbb{R}$, is square integrable, i.e., that $U(v)$ is in the Hilbert space (or $L^2$-space) [3], and has its inverse Fourier transform $u(t)$ vanishing for $t < 0$, i.e., $u(t) = 0$ for $t < 0$ as in (5), then by Titchmarsh's theorem [72, Thm. 1.6.1], it can be shown that the function is also square integrable on any straight line parallel to the real axis as

$$\int_{\mathbb{R}} |U(\omega)|^2 \, d\nu < C,$$

where $\omega = v + i\text{Im}\{\omega\}$, $U(\omega)$ is holomorphic for $\text{Im}\{\omega\} > 0$, and $U(v) = \lim_{\text{Im}\{\omega\} \to 0^+} U(v + i\text{Im}\{\omega\})$ for almost all $v \in \mathbb{R}$, and $C$ is a constant. Further, from Titchmarsh's theorem [72, Thm. 1.6.1], the real and imaginary parts of a causal signal $U$ in the Hilbert space can be determined by employing Sokhotski-Plemelj formulas [72] as

$$\text{Re}\{U(v)\} = \frac{1}{\pi} \text{p.v.} \int_{\mathbb{R}} \frac{\text{Im}\{U(\xi)\}}{\xi - v} \, d\xi,$$

and

$$\text{Im}\{U(v)\} = -\frac{1}{\pi} \text{p.v.} \int_{\mathbb{R}} \frac{\text{Re}\{U(\xi)\}}{\xi - v} \, d\xi,$$

respectively, for $v \in \mathbb{R}$. The relations (8) and (9) are well known as Kramers-Kronig relations [45,52]. The symmetry property of these relations implies that they are the Hilbert transforms [48] of each other, which allows reconstruction of the whole signal when either its real or imaginary part is given, such as $U = \text{Re}\{U\} - i\mathcal{H}\text{Re}\{U\}$ or $U = \mathcal{H}\text{Im}\{U\} + i\text{Im}\{U\}$, respectively, where $\mathcal{H}$ denotes the Hilbert transform operator.

Passive systems can be considered as a subclass of causal systems additionally satisfying certain requirements. There exist two ways to define passivity for
different types of systems: admittance passivity developed by Zemanian [99, 100] and scattering passivity developed by Youla et al. [98]. Note that it is possible to construct a new admittance passive system from a given scattering passive via the Cayley transform, and vice versa; see [95, Thm. 5], as well as [89,98,99].

**Definition 2.6** Consider a convolution system with input signal $u(t)$ and output signal $v(t)$, both of which in general can be complex valued. The system is called admittance-passive if

$$W_{\text{adm}}(T) := \text{Re} \int_{-\infty}^{T} v(t)u(t)^* \, dt \geq 0$$

for all $T \in \mathbb{R}$ and all $u \in C^\infty_0$ (i.e., smooth functions with compact support).

Here, $W_{\text{adm}}(T)$ denotes the energy absorbed by the system until the time $T$. By requiring this quantity to be non-negative, we say that the system absorbs more energy than it emits, and hereby, it does not produce energy. Passivity also implies that the system is causal [100].

Consider an example of an admittance-passive system in electromagnetics.

**Example 2.7** Passive material models

Consider a linear, isotropic and time-translationally invariant material having the response to an applied electric field intensity $E(t)$ in terms of a time domain constitutive relation

$$D(t) = \varepsilon_0 \varepsilon_r(t) * E(t) = \varepsilon_0 \varepsilon_\infty E(t) + \varepsilon_0 \int_{\mathbb{R}} \chi(t - \tau) E(\tau) \, d\tau,$$

(11)

where $D(t)$ is the electric flux density, $\varepsilon_r(t)$ the real-valued relative permittivity convolution kernel, $\varepsilon_0$ the permittivity of free space, $\varepsilon_\infty > 0$ the instantaneous response, and the susceptibility $\chi = 0$ for $t < 0$; see, e.g., [45,52]. Based on Poynting’s theorem [45,52] and according to the Definition 2.6, the material (or more precisely, the convolution operator $\varepsilon_r(t)$) is passive if

$$\int_{-\infty}^{T} E(t) \cdot \frac{\partial D}{\partial t} \, dt = \varepsilon_0 \int_{-\infty}^{T} \int_{\mathbb{R}} E(t) \cdot \frac{\partial}{\partial t} (\varepsilon_\infty \delta(t - \tau) + \chi(t - \tau)) E(\tau) \, d\tau \, dt \geq 0,$$

(12)

for all $T$, and for all electric fields $E(t)$ given as testing functions with compact support. If the passive convolution operator is an operator of slow growth, then the energy expression (12) is valid also for the testing functions of rapid descent [100]. It can be shown that this passivity condition is equivalent to the condition

$$h(\omega) = \omega \varepsilon(\omega),$$

(13)

where $h(\omega)$ is a function characterizing passive systems in the frequency domain, known as a Herglotz function; see details in Section 3. Here, $\varepsilon(\omega)$ is the holomorphic Fourier transform of the convolution kernel $\varepsilon_r(t)$

$$\varepsilon(\omega) = \int_{\mathbb{R}^+} \varepsilon_r(t)e^{i\omega t} \, dt$$

(14)
in the upper complex half plane for \( \text{Im}\{\omega\} > 0 \); see e.g., \([35,100]\).

Let us now consider the second definition of passivity, scattering passivity.

**Definition 2.8** Consider a convolution system with input signal \( u(t) \) and output signal \( v(t) \). The system is called scattering-passive if

\[
W_{scat}(T) := \int_{-\infty}^{T} (|u(t)|^2 - |v(t)|^2) \, dt \geq 0
\]

for all \( T \in \mathbb{R} \) and all \( u \in \mathbb{C}_0^\infty \).

Here, \( W_{scat}(T) \) corresponds to the energy balance of a given system until the time \( T \). \( W_{scat} \) is non-negative if the system is passive, implying that the energy of its output signal is always less than that of its input signal. It can be shown that the transfer function \( W_{scat}(s) \) of a scattering-passive system satisfies the relation \( |W_{scat}(s)| \leq 1 \) for \( s \in \mathbb{C}_+ \), i.e., \( s \in \mathbb{C} \) for \( \text{Re}\{s\} > 0 \) \([13,100]\). Then a suitable rational (Cayley) transformation of the transfer function, namely the function \( s \mapsto i(1 + W_{scat}(-is))/(1 - W_{scat}(-is)) \) where the Laplace parameter \( s = -i\omega \) for \( \text{Im}\{\omega\} > 0 \), is a Herglotz function, described in Section 3.

Consider an example of a scattering-passive system in electromagnetics.

**Example 2.9** Reflection from an isotropic slab placed above a ground plane

Consider the reflection coefficient \( \Gamma \) from an isotropic non-magnetic slab of thickness \( d \) characterized by passive permittivity \( \varepsilon \), and placed above a perfect electric conducting plane (PEC), see Figure 3. The reflection coefficient can be used for describing the given system as a scattering-passive system. Let the incident wave \( E_i \) be the input signal and the reflected wave \( E_r \) the output signal of the system. Assume the reference plane is placed in front of the slab, i.e., \( x \leq 0 \).

The reflection coefficient for an isotropic slab corresponds to the reflected wave \( E_r = \Gamma E_i \) and is calculated as

\[
\Gamma(k) = \frac{\Gamma_0 - e^{2iknd}}{1 - \Gamma_0 e^{2iknd}},
\]
where \( \Gamma_0 = (\eta - 1)/(\eta + 1) \) is the reflection coefficient at the air-slab interface, \( k \) the wavenumber, \( n = \sqrt{\varepsilon} \) the refractive index of the slab, and \( \eta = \sqrt{1/\varepsilon} \) the relative wave impedance of the slab. This function can be shown to map the open upper half of complex plane to the closed unit disk.

### 3 Integral Representation of Passive and Causal Systems

The impulse response of a passive real-valued one-port system [95, 100] can be represented in the time domain as [100]:

\[
w(t) = b \delta'(t) + H(t) \int_{\mathbb{R}} \cos(\xi t) d\beta_+(\xi),
\]

where \( b \geq 0 \), \( \delta' \) denotes the first derivative of the Dirac delta distribution, \( H \) the Heaviside step function, and \( \beta_+ \) the positive Borel measure satisfying the growth condition \( \int_{\mathbb{R}} d\beta_+(\xi)/(1 + \xi^2) < \infty \); see also [66].

Borel measures can be defined as follows; see for details [87, Chs. 8.2 and 8.4].

**Definition 3.1** A measure \( \beta \) defined on all open sets of a topological space is called a Borel measure, if \( \beta(K) < \infty \) for every compact set \( K \).

By application of the Fourier–Laplace transform [77] to \( iw(t) \), where \( w(t) \) is given by (17), the impulse response of the passive system in the frequency domain gets the representation similar to the integral representation of Herglotz functions [13, 30] satisfying the symmetry property to be described in this section. This result demonstrates a crucial connection between passive systems and Herglotz functions, which have properties useful for determination of physical bounds.

In this section, we give a review information about Herglotz functions and their properties related to bounds on passive systems. Further, a class of quasi-Herglotz functions is introduced, which is useful for modelling a subclass of causal systems that do not fulfil admittance-passivity requirement (10) (see Definition 2.6), but still preserving the integral representation typical for passive systems.

#### 3.1 Herglotz Functions

Throughout of this section and till the end of Part I, let the following open half planes be defined as:

\[
\mathbb{C}^+ = \{ z \in \mathbb{C} \mid \text{Im}(z) > 0 \},
\]

\[
\mathbb{C}_+ = \{ z \in \mathbb{C} \mid \text{Re}(z) > 0 \},
\]

where \( \mathbb{C}^+ \) and \( \mathbb{C}_+ \) denote the open upper and right half planes, respectively.
Definition 3.2 A function \( h : \mathbb{C}^+ \to \mathbb{C} \) is called a Herglotz function if it is holomorphic with \( \text{Im}\{h(z)\} \geq 0 \) for any \( z \in \mathbb{C}^+ \).

One of the properties of Herglotz functions is their integral representation formula, given by

\[
h(z) = a_+ + b_+z + \int_{\mathbb{R}} \frac{1 + \xi z}{\xi - z} \, d\sigma_+(\xi)
\]

for \( z \in \mathbb{C}^+ \), where \( a_+ \in \mathbb{R}, \ b_+ \geq 0, \) and \( \sigma_+ \) is a finite positive Borel measure; see, e.g., [1, 5, 10, 30, 47, 72]. Let \( \beta_+ \) denote the positive Borel measure satisfying the growth condition \( \int_{\mathbb{R}} d\beta_+(\xi)/(1 + \xi^2) < \infty \); then the integral representation of Herglotz functions becomes

\[
h(z) = a_+ + b_+z + \int_{\mathbb{R}} \left( \frac{1}{\xi - z} - \frac{\xi}{1 + \xi^2} \right) d\beta_+(\xi).
\]

In the representations (20) and (21), the real-valued parameter \( a_+ \) is given by \( a_+ = \text{Re}\{h(i)\} \), and \( b_+ \) can be obtained as \( b_+ = \lim_{z \to \infty} h(z)/z \), where \( \to \) denotes a non-tangential limit, and hence \( z \to \infty \) means that \( |z| \to \infty \) in the Stolz cone

\[
\phi \leq \text{arg} \ z \leq \pi - \phi
\]

for any \( \phi \in (0, \pi/2) \).

\[
\text{Im}\{z\} > 0 \quad \text{Re} \quad \text{Im} \quad h(z) \quad \text{Re} \quad \text{Im}\{h(z)\} \geq 0
\]

**Figure 4:** Illustration of a Herglotz function \( h \) mapping the open upper half of complex plane \( \mathbb{C}^+ \) to the closed upper half of complex plane \( \mathbb{C}^+ \cup \mathbb{R} \).

As mentioned in this section above, the crucial property of symmetric Herglotz functions satisfying the symmetry condition

\[
h(z) = -h(-z^*)^*\]

is that they are related to real-valued one-port passive systems and used in determination of physical bounds.

Definition 3.3 A Herglotz function \( h \) satisfying the additional condition (23) is called symmetric.

\[
\text{Definition 3.2 A function } h : \mathbb{C}^+ \to \mathbb{C} \text{ is called a Herglotz function if it is holomorphic with } \text{Im}\{h(z)\} \geq 0 \text{ for any } z \in \mathbb{C}^+. \]
The symmetric Herglotz function can be represented as

\[ h(z) = b_+ z + \text{p.v.} \int_{\mathbb{R}} \frac{1 + \xi^2}{\xi - z} d\sigma_+(\xi), \]

(24)

for \( z \in \mathbb{C}^+ \), and where the measure \( \sigma_+ \) is symmetric, and the integral is the Cauchy principal value (p.v.) integral at infinity. Consequently, symmetric Herglotz functions have integral representation in terms of the measure \( \beta_+ \):

\[ h(z) = b_+ z + \text{p.v.} \int_{\mathbb{R}} \frac{1}{\xi - z} d\beta_+(\xi), \]

(25)

where the measure \( \beta_+ \) is symmetric, i.e., \( d\beta_+(\xi) = d\beta_+(-\xi) \). Note that the measure \( \beta_+ \) can be uniquely determined by the Herglotz function \( h \) from the Stieltjes inversion formula [47] as

\[ \beta_+((x_1,x_2)) + \frac{1}{2} \beta_+(\{x_1\}) + \frac{1}{2} \beta_+(\{x_2\}) = \lim_{y \to 0^+} \frac{1}{\pi} \int_{x_1}^{x_2} \text{Im}\{h(\xi + iy)\} d\xi, \]

(26)

including a possibility of having point masses \( x_i \) on the real axis, i.e., \( x_i \in \mathbb{R} \). For absolutely continuous measures on \( \mathbb{R} \), the following notation can be introduced:

\[ d\beta_+(\xi) = \beta_+(\xi) d\xi = \frac{1}{\pi} \text{Im}\{h(\xi + i0)\} d\xi, \]

(27)

implying the relation between the imaginary part of the Herglotz function and its corresponding measure \( \text{Im}\{h\} = \pi \beta'_+ \); see [30,47].

Assume that a symmetric Herglotz function admits the following small- and large-argument asymptotic expansions:

\[ h(z) = \begin{cases} a_{-1} z^{-1} + a_1 z + \cdots + a_{2N_0-1} z^{2N_0-1} + o(z^{2N_0-1}) & \text{as } z \to 0, \\ b_1 z + b_{-1} z^{-1} + \cdots + b_{1-2N_\infty} z^{1-2N_\infty} + o(z^{1-2N_\infty}) & \text{as } z \to \infty, \end{cases} \]

(28)

respectively, for all real-valued expansion coefficients, where \( \to \) denotes the non-tangential limit such that \( z \to 0 \) and \( z \to \infty \) denote \( |z| \to 0 \) and \( |z| \to \infty \) in the Stoltz cone (22), respectively. Here, \( a_{-1} \leq 0, b_1 \geq 0 \) and coincides with \( b_+ \) in the integral representation (25), \( N_0 \) and \( N_\infty \) are non-negative such that \( 1 - N_\infty \leq N_0 \).

By employing the integral representation (25), the following integral identities, known as sum rules, can be derived:

\[ \frac{2}{\pi} \int_{0^+}^{\infty} \frac{\text{Im}\{h(x)\}}{x^{2k}} dx \overset{\text{def}}{=} \lim_{\varepsilon \to 0^+} \lim_{y \to 0^+} \frac{2}{\pi} \int_{\varepsilon}^{1/\varepsilon} \frac{\text{Im}\{h(x + iy)\}}{x^{2k}} dx = a_{2k-1} - b_{2k-1} \]

(29)

for \( k = 1 - N_\infty, \ldots, N_0 \); see e.g., [1,13].
3. INTEGRAL REPRESENTATION OF PASSIVE AND CAUSAL SYSTEMS

3.2 Quasi-Herglotz Functions

Here, a class of analytic functions on the upper half of complex plane useful for modeling a subclass of non-passive systems is introduced.

**Definition 3.4** An analytic function \( q : \mathbb{C}^+ \to \mathbb{C} \) is called a quasi-Herglotz function if there exist two Herglotz functions \( h_1 \) and \( h_2 \) such that

\[
q(z) = h_1(z) - h_2(z)
\]  

for any \( z \in \mathbb{C}^+ \). The set of all quasi-Herglotz functions is denoted by \( Q \).

Any quasi-Herglotz function \( q \in Q \) admits the following integral representation

\[
q(z) = a + bz + \int_{\mathbb{R}} \frac{1 + \xi z}{\xi - z} \, d\sigma(\xi)
\]

for \( z \in \mathbb{C}^+ \), which is inherited from the properties of Herglotz functions. Here, the parameters \( a, b \in \mathbb{R} \) are defined as \( a = a_{+1} - a_{+2} \) and \( b = b_{+1} - b_{+2} \), respectively, and \( \sigma = \sigma_{+1} - \sigma_{+2} \) is the signed measure, where for \( j = 1, 2 \), the triple of parameters \( (a_{+j}, b_{+j}, \sigma_{+j}) \) represents the corresponding Herglotz function \( h_j \) in the sense of representation (20).

**Figure 5:** Illustration of a quasi-Herglotz function \( q \) mapping the upper half of complex plane \( \mathbb{C}^+ \) to the entire complex plane \( \mathbb{C} \).

Symmetric quasi-Herglotz functions can be defined in a similar way as follows.

**Definition 3.5** An analytic function \( q : \mathbb{C}^+ \to \mathbb{C} \) is called a symmetric quasi-Herglotz function if there exist two symmetric Herglotz functions \( h_1 \) and \( h_2 \) satisfying (23) such that equality (30) holds for any \( z \in \mathbb{C}^+ \). The set of all symmetric quasi-Herglotz functions is denoted by \( Q_{\text{sym}} \). 

\( \square \)
Any symmetric quasi-Herglotz function \( q \in \mathcal{Q}_{\text{sym}} \) admits the following integral representation:

\[
q(z) = bz + \text{p.v.} \int_{\mathbb{R}} \frac{1 + \xi^2}{\xi - z} \, d\sigma(\xi)
\]  

(32)

for \( z \in \mathbb{C}^+ \), and where the signed measure \( \sigma \) is symmetric. In representations (31) and (32), the parameter \( b \) can be defined as \( b = \lim_{z \to \infty} q(z)/z \), where \( z \to \infty \) denotes that \( |z| \to \infty \) in the Stolz cone (22) for any \( q \in (0, \phi/2] \).

Further, it has to be noted that any Herglotz or symmetric Herglotz function can be considered as a quasi-Herglotz or symmetric quasi-Herglotz function, respectively, assuming that \( h_2(z) = 0 \) in equality (30). There is also an issue of non-uniqueness in Definition 3.4: for any Herglotz (symmetric Herglotz) functions \( h_1 \) and \( h_2 \) in (30), the corresponding quasi-Herglotz (symmetric quasi-Herglotz, respectively) function can also be defined

\[
q(z) = (h_1 + h_3)(z) - (h_2 + h_3)(z)
\]  

(33)

in terms of other Herglotz (symmetric Herglotz, respectively) function \( h_3 \).

The representation of quasi-Herglotz functions (31) can be also written in terms of the measure \( \beta \) as

\[
q(z) = a + bz + \int_{\mathbb{R}} \left( \frac{1}{\xi - z} - \frac{\xi}{1 + \xi^2} \right) \, d\beta(\xi),
\]  

(34)

for example, when the measure \( \sigma \) from representation (31) has compact support. Then the measure \( \beta \) may be defined as \( d\beta(\xi) = (1 + \xi^2) \, d\sigma(\xi) \). Similarly, symmetric quasi-Herglotz functions may be given in terms of the symmetric measure \( \beta \) as

\[
q(z) = bz + \text{p.v.} \int_{\mathbb{R}} \frac{1}{\xi - z} \, d\beta(\xi),
\]  

(35)

such that \( d\beta(\xi) = d\beta(-\xi) \).

Suppose that a symmetric quasi-Herglotz function admits the following asymptotic expansions:

\[
q(z) = \begin{cases} 
  a_{-1}z^{-1} + a_1z + \cdots + a_{2N_0-1}z^{2N_0-1} + o(z^{2N_0-1}) & \text{as } z \to 0, \\
  b_1z + b_{-1}z^{-1} + \cdots + b_{1-2N_\infty}z^{1-2N_\infty} + o(z^{1-2N_\infty}) & \text{as } z \to \infty,
\end{cases}
\]  

(36)

for all real-valued expansion coefficients at \( z = 0 \) and \( z = \infty \), respectively, and that at least one of the symmetric Herglotz functions \( h_1 \) and \( h_2 \) admits the corresponding asymptotic expansion there, respectively. Here, \( b_1 \) coincides with \( b \) given in the integral representation (35), \( N_0 \) and \( N_\infty \) are non-negative such that \( 1 - N_\infty \leq N_0 \), and similarly as for Herglotz functions, \( \to \) means the non-tangential limit. Then, it can be shown that the following sum-rule identities hold:

\[
\frac{2}{\pi} \int_{\epsilon}^{\infty} \frac{\text{Im}\{q(x)\}}{x^{2k}} \, dx \overset{\text{def}}{=} \lim_{\epsilon \to 0^+} \lim_{y \to 0^+} \frac{2}{\pi} \int_{\epsilon}^{1/\epsilon} \frac{\text{Im}\{q(x + iy)\}}{x^{2k}} \, dx = a_{2k-1} - b_{2k-1}
\]  

(37)

for \( k = 1 - N_\infty, \ldots, N_0 \); see e.g., [44, Sec. 3].
4 Optimization Techniques

In this section, we describe the optimization techniques used Papers I–V and VII to determine physical bounds and optimal realizations of given properties of passive and non-passive systems. In Section 4.1, we give a summary on convex optimization and on the framework, where the optimization procedure is involved. Section 4.2 is focused on analytical optimization techniques, which has been used for determination of physical bounds described in Paper VII.

4.1 Convex Optimization

Convex optimization has been employed as a part of mathematical framework developed in Papers I and III for modeling and determination of optimal performance bounds for passive and non-passive systems, respectively. In this section, we introduce the central concepts in convex optimization, as well as the properties used in formulation of convex optimization problems. For complete information on convex optimization and related algorithms, see [17].

Definition 4.1 A set $S \subset \mathbb{R}^n$ is convex if

$$x_1, x_2 \in S \Rightarrow (1-t)x_1 + tx_2 \in S,$$

for all $0 < t < 1$ [17, p. 23].

Geometrically this means that the straight line between any two points in a convex set remains in the set, see Figure 6 for an illustration of the two-dimensional case.

![Figure 6: Illustration of sets in $\mathbb{R}^2$: a) a convex set; b) a non-convex set.](image)

Theorem 4.2 The intersection $\cap_{\alpha} S_\alpha$ of convex sets $S_\alpha$ is a convex set [17, p. 36].

Definition 4.3 Let $f$ be a function defined on the convex set $S \subset \mathbb{R}^n$. The function $f$ is said to be a convex function if

$$x_1, x_2 \in S \Rightarrow f((1-t)x_1 + tx_2) \leq (1-t)f(x_1) + tf(x_2),$$

for all $0 < t < 1$ [17, p. 67].
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Geometrically this means that a convex function $f$ is always less then or equal to a corresponding linear (or affine) function passing through the values $f(x_1)$ and $f(x_2)$ where $x_1$ and $x_2$ are any two points in the convex set $S$, see Figure 7 for an illustration of the one-dimensional case.

**Definition 4.4** If the function $f$ satisfies a strict inequality in (39), it is said to be a strictly convex function [17, p. 67].

**Definition 4.5** A function $f$ is said to be concave if $-f$ is convex [17, p. 67].

**Theorem 4.6** Let $f_1$ and $f_2$ be convex functions defined on a convex set $S$. Then the positive linear combination

$$f = \alpha_1 f_1 + \alpha_2 f_2$$

(with $\alpha_1 > 0$ and $\alpha_2 > 0$) is a convex function. If any one of $f_1$ and $f_2$ is strictly convex, then the function $f$ is strictly convex [17, p. 79].

**Theorem 4.7** Let $f$ be a two times differentiable continuous function defined on the open convex set $S \subset \mathbb{R}^n$ ($f \in C^2(S)$). It can then be shown that $f$ is a convex function if and only if the Hessian $H_{ij}(x) = \nabla x_i \nabla x_j f(x)$ is a positively semidefinite matrix for all $x \in S$, i.e.,

$$H(x) \succeq 0 \quad \forall x \in S \Leftrightarrow f \text{ convex}.$$  

If the Hessian $H(x)$ is positively definite for all $x \in S$, then $f$ is strictly convex, i.e.,

$$H(x) > 0 \quad \forall x \in S \Rightarrow f \text{ strictly convex;}$$

see e.g., [17, p. 71].

The converse for positive definite case is not true: take e.g., $f(x) = x^4$, see e.g., [17].
Theorem 4.8 Let \( f(x) = \frac{1}{2}x^T Ax + b^T x + c \) be a quadratic form where \( A \) is an \( n \times n \) matrix, \( x \) and \( b \) are \( n \times 1 \) vectors, \( c \) a scalar and \( \cdot^T \) denotes the transpose. The function \( f \) is convex if and only if the Hessian matrix \( A \) is positively semidefinite, i.e.,

\[
A \geq 0 \iff f \text{ convex.} \tag{41}
\]

The quadratic form \( f \) is strictly convex if and only if the Hessian matrix \( A \) is positively definite, i.e.,

\[
A > 0 \iff f \text{ strictly convex;} \tag{42}
\]

see [17, p. 71].

Theorem 4.9 Let \( f \) be a convex function defined on the convex set \( S \subset \mathbb{R}^n \). Then \( f \) is a continuous function on the interior of \( S \) [17, p. 68].

Definition 4.10 A convex optimization problem, in general, is a problem of the form

\[
\begin{align*}
\text{minimize} & \quad f(x) \\
\text{subject to} & \quad x \in S,
\end{align*}
\]

where \( f \) is a convex function defined on the convex set \( S \). It is common that the convex set \( S \) is given in the form \( S = \{ x \in \mathbb{R}^n | g_i(x) \leq 0 \} \) where \( \{g_i(x)\}_{i=1}^M \) is a set of convex functions representing the convex constraints [17, p. 127].

Definition 4.11 A point \( x^* \in \Omega \) is said to be a local minimum point of \( f \) over \( \Omega \) if there is an \( \varepsilon > 0 \) such that \( f(x) \geq f(x^*) \) for all \( x \in \Omega \) within a distance \( |x - x^*| < \varepsilon \) [57, p. 184].

Definition 4.12 A point \( x \in \Omega \) is said to be a global minimum point of \( f \) over \( \Omega \) if \( f(x) \geq f(x^*) \) for all \( x \in \Omega \) [57, p. 184].

One of the most important properties of a convex optimization problem is the following.

Theorem 4.13 Any local minimum in convex set \( S \) is also a global minimum\(^1\) [57, p. 197].

Theorem 4.14 Any norm \( f(x) = \|x\| \) is a convex function on \( \mathbb{R}^n \) since by the triangle inequality we have

\[
f((1 - t)x_1 + tx_2) = \|(1 - t)x_1 + tx_2\| \leq (1 - t)\|x_1\| + t\|x_2\| = (1 - t)f(x_1) + tf(x_2), \tag{44}
\]

where \( 0 < t < 1 \) [17, pp. 72–73].

\(^1\)Here the term “minimum” refer to the minimizing point \( x \) and the term “minimum value” to the corresponding minimum value \( f(x) \).
Theorem 4.15 The norm of a linear (or affine) form is a convex function on \( \mathbb{R}^n \) [17, pp. 72–73].

Example 4.16 Consider the function \( f(x) = \|Ax - b\| \), where \( A \) is an \( M \times N \) matrix, \( x \) an \( N \times 1 \) vector and \( b \) an \( M \times 1 \) vector. The function \( f(x) \) is convex since by the triangle inequality

\[
 f((1-t)x_1 + tx_2) = \|A((1-t)x_1 + tx_2) - b\| \\
 = \|(1-t)(Ax_1 - b) + t(Ax_2 - b)\| \\
 \leq (1-t)\|Ax_1 - b\| + t\|Ax_2 - b\| \\
 = (1-t)f(x_1) + tf(x_2); 
\]

see also Definitions 4.1 and 4.3.

The following example is related to the quasi-Herglotz function theory introduced in Section 3.2. In this example, the associated approximation theory to be discussed in Section 5 is used in the applications described in Papers III–IV.

Example 4.17 Consider the following convex optimization problem:

\[
\begin{align*}
\text{minimize} & \quad \|q - F\|_{L^p(w,\Omega)} \\
\text{subject to} & \quad c_n \leq 0, \\
& \quad b_1 \geq 0, \\
\end{align*}
\]

where \( \| \cdot \|_{L^p(w,\Omega)} \), \( 1 \leq p \leq \infty \), denotes a suitable weighted Lebesgue norm [51] on the approximation domain \( \Omega \subset \mathbb{R} \), where \( w \) is a positive continuous weight function on \( \Omega \), \( q \) the approximating symmetric quasi-Herglotz function, which has a representation on \( \Omega \) to be discussed in Section 5, and \( F \) the symmetric target function. The convex optimization formulation (45) can be represented in matrix form as

\[
\begin{align*}
\text{minimize} & \quad \|b_1x + Hc + iPc - f\|_{L^p(w,\Omega)} \\
\text{subject to} & \quad c \leq 0, \\
& \quad b_1 \geq 0, \\
\end{align*}
\]

where \( \| \cdot \|_{L^p(w,\Omega)} \) denotes the norm of a weighted sequence space [51]. Here, \( w \) and \( \Omega \) are sampled versions of the weight function and the approximation domain, respectively, corresponding to (45), \( c \) is the \( N \times 1 \) vector of optimization variables \( c_n \) for \( n = 1, \ldots, N \), and \( f \) the corresponding column vector representing the target function \( F \). The imaginary and real parts of \( q \) can be expressed in a semi-infinite matrix notation as \( \text{Im}\{q\} = Pc \) and \( \text{Re}\{q\} = b_1x + Hc \), where \( x \) is a column vector corresponding to the approximation domain, \( x_i \in \Omega \), and the columns of the matrices \( P \) and \( H \) are similarly given by the B-spline basis functions \( p_n(x) \) and their corresponding Hilbert transform \( \hat{p}_n(x) \), respectively. The corresponding numerical problem (45) can be solved efficiently by using the CVX MATLAB software for disciplined convex programming [32].
4.2 Method of Lagrange Multipliers

In this section, we introduce some general definitions and conditions necessary for solving problems with the described method. A more detailed description can be found in [17,57].

The method of Lagrange multipliers is an optimization technique used to determine extreme points of function $f$ subject to the constrained vector-valued functions $g$ and $h$ and is applied to the problems of the form:

$$\begin{align*}
\text{minimize} & \quad f(x) \\
\text{subject to} & \quad g_i(x) \leq 0, \\
& \quad h_j(x) = 0,
\end{align*}$$

where $x \in \mathbb{R}^n$, $\{g_i(x)\}_{i=1}^m$ and $\{h_j(x)\}_{j=1}^p$ are sets of inequality and equality constraint functions representing the convex and active constraints, respectively, and $m, p \leq n$. Note that if functions $g_i(x)$, $i = 1, \ldots, m$, are convex, and functions $h_j(x)$, $i = 1, \ldots, p$, are affine, then (47) is a convex optimization problem [17, Eq. (4.15)].

Definition 4.18 Let $x^*$ be the point satisfying the constraints

$$g(x^*) \leq 0, \quad h(x^*) = 0,$$

and let $I$ be the set of indices $i$ for which $g_i(x^*) = 0$. Then $x^*$ is said to be a regular point of the constraints (48) if the gradient vectors $\nabla g_i(x)$, $i \in I$, and $\nabla h_j(x)$, $j = 1, \ldots, p$, are linearly independent [57, p. 342].

Karush-Kuhn-Tucker conditions [57, p. 342]: Let $\{f, g, h\} \in C^1$, where $g$ and $h$ are the $m$- and $p$-dimensional ($m, p \leq n$) vector-valued functions, respectively, and let $x^*$ be a local minimum point for the problem

$$\begin{align*}
\text{minimize} & \quad f(x) \\
\text{subject to} & \quad g(x) \leq 0, \\
& \quad h(x) = 0, \\
& \quad x \in \Omega \subset \mathbb{R}^n,
\end{align*}$$

where $\Omega$ denotes the constrained set, and suppose that $x^*$ is a regular point for the constraints. Then, there is a vector $\lambda \in \mathbb{R}^m$ with $\lambda \geq 0$ and vector $v \in \mathbb{R}^p$ such that

$$\nabla f(x^*) + \sum_{i=1}^m \lambda_i \nabla g_i(x^*) + \sum_{j=1}^p v_j \nabla h_j(x^*) = 0,$$

$$\sum_{i=1}^m \lambda_i g_i(x^*) = 0.$$
The corresponding Lagrangian associated with the problem (49) is

\[ L(x, \lambda, \nu) = f(x) + \sum_{i=1}^{m} \lambda_i g_i(x) + \sum_{j=1}^{p} \nu_j h_j(x), \tag{52} \]

where \( \lambda \) and \( \nu \) are the Lagrange multiplier vectors associated with the inequality and equality constraints, respectively, and for which the Karush-Kuhn-Tucker conditions (48), (50) and (51) for \( \lambda \geq 0 \) are necessary. Note that if the problem (49) is convex, then the Karush-Kuhn-Tucker conditions for \( \lambda \geq 0 \) are not only necessary, but also sufficient [17, p. 244].

5 Approximation of Passive and Non-passive Systems

In this section, we describe the mathematical framework developed for approximation and identification of passive and a subclass of non-passive systems which can be characterized, in general, by the class of quasi-Herglotz functions described in Section 3.2. The framework is based on the integral representation of quasi-Herglotz functions (31) used for approximation of causal and passive one-port systems in convolution form; see Definition 2.4 in Section 2. Note that the theory and formulation given in this section are applicable to passive systems given in terms of Herglotz functions, because a Herglotz function can be considered as a quasi-Herglotz function as in (30), with \( h_2 = 0 \); see Section 3.2 for details.

To facilitate the formulation of a convex optimization problem, it is necessary to first put a priori constraints on the class of quasi-Herglotz functions to be used as approximants, as well as on the target function characterizing the system of interest. In particular, the interest is in approximating functions having continuous real and imaginary parts. Thus, quasi-Herglotz functions are restricted to have a local Hölder continuous extension to some given intervals on the real axis. In addition, the target response of the system of interest \( F \in C(\Omega) \) can be given by an arbitrary complex-valued continuous function over the approximation domain \( \Omega \subset \mathbb{R} \) consisting of a finite union of closed and bounded intervals on the real axis. The norms used in approximation problems are weighted \( L^p \)-norms [77], where \( 1 \leq p \leq \infty \), and are denoted by \( \| \cdot \|_{L^p(w, \Omega)} \), where the weight \( w \) is a positive continuous function on \( \Omega \).

Let \( O \) denote some open neighborhood of the approximation domain \( \Omega \) such that \( \Omega \subset O \subset \mathbb{R} \), as illustrated in Figure 8. Further, let \( q \) denote the approximating function which is Hölder continuous on \( \Omega \) and which coincides with a quasi-Herglotz function having a Hölder continuous extension to the closure of \( O \). Thus, the approximating quasi-Herglotz function can be generated by an absolutely continuous measure \( \beta \) having a Hölder continuous density \( \beta' \) on the closure...
\( O \supset \Omega \). This implies that the function \( \beta' \) belongs to the Hölder space \( C^{0,\alpha}(\overline{O}) \) with Hölder exponent \( \alpha \), meaning that \( |\beta'(\zeta_1) - \beta'(\zeta_2)| \leq C|\zeta_1 - \zeta_2|^\alpha \) for all \( \zeta_1, \zeta_2 \in \overline{O} \) and fixed \( 0 < \alpha < 1 \), and where \( C > 0 \) is an arbitrary constant; see e.g., [50, pp. 94-104]. The Hölder continuity requirement is necessary in order to show that the Hilbert transform operator \( \mathcal{H} \) is a bounded operator \( \mathcal{H} : C^{0,\alpha}(\overline{O}) \rightarrow C^{0,\alpha}(\Omega) \); cf., [50, Thm. 7.6 and Cor. 7.7] and [48]. Since the imaginary part of the approximating quasi-Herglotz function is related to the measure \( \{\Im q\} \overset{\star}{\approx} \mathcal{C} \) on \( \overline{O} \) (cf., [47, p. 7]) and, thus the Hölder continuity of the density \( \beta' \) on \( \overline{O} \) implies that the real part of \( q \) given by the associated Hilbert transform [50] is continuous.

**Figure 8**: Illustration of the approximation domain \( \Omega \) and the closure of some open neighborhood \( \mathcal{O} \) of the approximation domain, such that \( \Omega \subset \mathcal{O} \subset \mathbb{R} \) for \( x \in \Omega \).

Let us formulate an approximation problem of interest. The greatest lower bound on the approximation error can be defined by

\[
d := \inf_{q} \|q - F\|_{L^p(w,\Omega)},
\]

where the infimum is taken over all quasi-Herglotz functions \( q \) generated by a measure having a Hölder continuous density on \( \overline{O} \), and where where the norms are well-defined for \( 1 \leq p \leq \infty \) due to continuity of \( q \).

A best approximation in problem (53) can be achieved by solving a finite-dimensional approximation problem. This approach is suitable to incorporate with numerical optimization algorithms [32], where B-spline expansions [25] of an arbitrary order can be utilized for discretization of approximating functions.

B-spline basis functions of a fixed polynomial order \( m \geq 2 \) are compactly supported positive basis functions that are \( m - 2 \) times continuously differentiable [24,25], and have \( m + 1 \) break points and a continuous (negative) Hilbert transform [43]. Here, the B-spline basis functions are defined as \( p_n(x) \), where \( n = 1, \ldots, N \) is the number of spline functions used for a finite-dimensional discretization of the function \( \beta' \), and \( \tilde{p}_n(x) \) denotes their corresponding (negative) Hilbert transform. The explicit formulas on B-splines functions and their Hilbert transforms are given in [43].
Let the approximating function \( q \) can be represented on the closure \( \overline{\Omega} \) as:

\[
q(x) = a + bx + \sum_{i=1}^{M} \frac{p_i}{\xi_i - x} + \text{p.v.} \int_{\mathbb{R}} \left( \frac{1}{\xi - x} - \frac{\xi}{1 + \xi^2} \right) \beta'(\xi) d\xi + i\pi \beta'(x)
\]  

(54)

\[
= \tilde{a} + bx + \sum_{i=1}^{M} \frac{p_i}{\xi_i - x} + \text{p.v.} \int_{\mathbb{R}} \frac{1}{\xi - x} \beta'(\xi) d\xi + i\pi \beta'(x)
\]  

(55)

for \( x \in \Omega \), and where \( \tilde{a} = a - \text{p.v.} \int_{\mathbb{R}} \frac{\xi}{1 + \xi^2} \beta'(\xi) d\xi \). In (54) and (55) the density \( \beta' \) is assumed to be given by a finite uniform B-spline expansion of a fixed order, and a finite number of point masses at \( \xi_i \notin \Omega \) with real-valued amplitudes \( p_i \), \( i = 1, \ldots, M \), have also been included.

A discretization problem of (53) on the finite partition of \( \Omega \) can be formulated as follows. Let \( q_N \) denote approximating functions represented as in (55), and hence

\[
\text{Im}\{q_N(x)\} = \pi \beta'(x) = \sum_{n=1}^{N} c_n p_n(x),
\]  

(56)

and

\[
\text{Re}\{q_N(x)\} = \tilde{a} + bx + \sum_{i=1}^{M} \frac{p_i}{\xi_i - x} + \sum_{n=1}^{N} c_n \tilde{p}_n(x),
\]  

(57)

for \( x \in \Omega \), and where \( c_n \) are the corresponding B-spline expansion coefficients. Note that all the parameters \( \tilde{a}, b, \{p_i\}_{i=1}^{M} \) and \( \{c_n\}_{n=1}^{N} \), as well as the break-points of the B-splines defined above depend on \( N \).

Consider the following optimization problem

\[
\begin{align*}
\text{minimize} & \quad \|q - F\|_{L^p(w,\Omega)} \\
\text{subject to} & \quad b_{\text{lower}}(x) \leq \beta'(x) \leq b_{\text{upper}}(x),
\end{align*}
\]  

(58)

where the upper and lower bounds on density \( \beta' \) are included to regularize the physical properties of a given system inside and outside of the approximation domain \( \Omega \). Further, these constraints are useful for prevention of non-physical oscillatory behavior and for regularization of small- and large-argument properties of a given system. In practice, we solve the following discretized problem

\[
\begin{align*}
\text{minimize} & \quad \|q_N - F\|_{L^p(w,\Omega)} \\
\text{subject to} & \quad \theta_{\text{lower},j} \leq \theta_j \leq \theta_{\text{upper},j}, \quad j \in J,
\end{align*}
\]  

(59)

for fixed \( N \) and finite index set \( J \), and where the minimization is over the vectors \( \theta_j \), each of them consisting of the parameters \( \theta_j \in \{\tilde{a}, b, p_1, \ldots, p_M, c_1, \ldots, c_N\} \), for \( j \in J \). Further, it should be noted that the sum-rule identities (29) and (37) can be discretized and used as convex constraints for a given optimization problem.

Finally, numerical implementations of convex optimization problems given by (59) can be obtained by using, e.g., the CVX MATLAB software for disciplined
convex programming [32], where the calculation of the norm above must be approximated based on a finite set of sample points in $\Omega$. However, due to the uniform continuity of all functions involved, this can, in principle, be done within arbitrary numerical accuracy.

6 Material Models

In this section, we describe the dielectric permittivity models used in Papers I–VII included in this thesis. The corresponding Herglotz and quasi-Herglotz functions are constructed and their asymptotic expansions are derived. Note that these functions do have an analytic extension to some open neighborhood of the real axis; however, this is not true for all physical systems in general. Here, for convenient representation, the complex-valued frequency $\omega$ (in rad/s) is used as an argument of Herglotz and quasi-Herglotz functions, respectively. Furthermore, the time convention $e^{-i\omega t}$ for time harmonic fields (phasors) is used, as stated in Section 1.2.

6.1 Debye Model

The Debye model is used in modeling of dielectric responses of dispersive materials and has the following representation in the frequency domain:

$$
\varepsilon(\omega) = \varepsilon_\infty + \frac{\varepsilon_s - \varepsilon_\infty}{1 - i\omega\tau},
$$

(60)

where $\varepsilon_\infty$, $\varepsilon_s$, and $\tau > 0$ denote the instantaneous response (at $\omega = \infty$), the static response (at $\omega = 0$), and the relaxation time, respectively. The corresponding response of the Debye model in the time domain is given by

$$
e(t) = \varepsilon_\infty \delta(t) + \frac{\varepsilon_s - \varepsilon_\infty}{\tau} e^{-t/\tau} H(t),
$$

(61)

where $\delta(t)$ is the Dirac delta function, and $H(t)$ the Heaviside unit step function. Using (60), the corresponding Herglotz function $h(\omega) = \omega \varepsilon(\omega)$ can be constructed, which has the following small- and large-argument asymptotics:

$$
h(\omega) = \omega \varepsilon_\infty + \omega \frac{\varepsilon_s - \varepsilon_\infty}{1 - i\omega\tau} = \left\{
\begin{array}{ll}
\omega \varepsilon_s + o(\omega), & \omega \to 0, \\
\omega \varepsilon_\infty + o(\omega), & \omega \to \infty.
\end{array}
\right.
$$

(62)

The function (62) can be extended to the meromorphic function in $\mathbb{C}\setminus\{-i/\tau\}$ with a pole at $\omega = -i/\tau$. From (62), the spectral measure $\operatorname{Im}\{h(\xi)\} = \pi \beta^*_s(\xi)$ is given by

$$
\operatorname{Im}\{h(\xi)\} = \frac{\xi^2 \tau (\varepsilon_s - \varepsilon_\infty)}{1 + \xi^2 \tau^2}
$$

(63)

for $\xi = \operatorname{Re}\{\omega\} \in \mathbb{R}$. Note that for $\varepsilon_s = \varepsilon_\infty$, the spectral measure $\operatorname{Im}\{h(\xi)\} = 0$ over all $\xi \in \mathbb{R}$, and hence the material is lossless.
For this model, there exists a sum rule given as
\[
\frac{2}{\pi} \int_{0^+}^{\infty} \frac{\text{Im}\{h(\xi)\}}{\xi^2} \, d\xi = \frac{2}{\pi} \int_{0^+}^{\infty} \frac{\text{Im}\{e(\xi)\}}{\xi} \, d\xi = \epsilon_s - \epsilon_\infty
\]  \hspace{1cm} (64)
for \( k = 1 \), and where \( a_1 = \epsilon_s \), and \( b_1 = \epsilon_\infty \), respectively. Note that the sum rule (64) is valid for all the passive materials having the same asymptotic expansions as in (62).

### 6.2 Conductivity Model

The conductivity model is used for materials with an electric conductivity satisfying the Ohm’s law
\[
J = \sigma E,
\]  \hspace{1cm} (65)
and is given in the frequency domain as
\[
\epsilon(\omega) = \epsilon_\infty + i \frac{\sigma}{\omega \epsilon_0},
\]  \hspace{1cm} (66)
where \( \epsilon_\infty \), \( \epsilon_0 \approx 8.854 \times 10^{-12} \text{F/m} \), and \( \sigma > 0 \) denote the instantaneous response, the permittivity of free space, and the static conductivity, respectively. The corresponding time-domain representation of this model is
\[
\epsilon_s(t) = \epsilon_\infty \delta(t) + \frac{\sigma}{\epsilon_0} H(t),
\]  \hspace{1cm} (67)
where \( H(t) \) is the Heaviside unit step function. Note that the Fourier transform of (67) is a distribution [100]
\[
\epsilon(\xi) = \epsilon_\infty + \frac{\sigma}{\epsilon_0} \left[ \frac{1}{\xi} + \pi \delta(\xi) \right], \quad \text{as} \quad \text{Im}\{\omega\} \to 0^+,
\]  \hspace{1cm} (68)
and \( \xi = \text{Re}\{\omega\} \in \mathbb{R} \). The corresponding Herglotz function is constructed as \( h(\omega) = \omega \epsilon(\omega) \) and has the following small- and large-argument asymptotics:
\[
h(\omega) = \omega \epsilon_\infty + i \frac{\sigma}{\epsilon_0} = \begin{cases} o(\omega^{-1}), & \omega \to 0, \\ \omega \epsilon_\infty + o(\omega), & \omega \to \infty. \end{cases}
\]  \hspace{1cm} (69)
The Herglotz function (69) can be extended to an entire function, i.e., the function is analytic in the entire complex plane. For this function, the spectral measure \( \text{Im}\{h(\xi)\} = \pi \beta_\epsilon' (\xi) \) is given by
\[
\text{Im}\{h(\xi)\} = \frac{\sigma}{\epsilon_0}.
\]  \hspace{1cm} (70)
Note that for such a Herglotz function (69), no sum rule can be constructed.

In practice, the conductivity model can be combined with the Debye model described in Section 6.1 to characterize materials with conductive characteristics.
such as saline water, metals, etc. The resulting permittivity function for this case is known as the modified Debye model, which is given by

$$e(\omega) = e_\infty + \frac{\varepsilon_s - e_\infty}{1 - i\omega \tau} + i \frac{\sigma}{\omega \varepsilon_0}.$$  \hspace{1cm} (71)

The resulting Herglotz function $h(\omega) = \omega e(\omega)$ has the same asymptotic properties as in (62).

### 6.3 Havriliak–Negami Model

The Havriliak-Negami model is an empirical relaxation model that is used to characterize conductive materials with non-Debye dispersive behavior. The frequency-domain representation of this model is given by

$$e(\omega) = e_\infty + \frac{\varepsilon_s - e_\infty}{1 + (-i\omega \tau)^\alpha} + i \frac{\sigma}{\varepsilon_0}$$  \hspace{1cm} (72)

for $0 < \alpha \leq 1$ and $0 < \beta \leq 1$, and where $\varepsilon_s$ and $e_\infty$ denote the static and the instantaneous responses, respectively, $\tau > 0$ the relaxation time, $e_0 \approx 8.854 \cdot 10^{-12}$ F/m the permittivity of free space, and $\sigma > 0$ the static conductivity. Using De Moivre's formula \[3\], the real and imaginary parts of the Havriliak-Negami model can be determined as:

$$\text{Re}\{e(\omega)\} = e_\infty + \frac{(\varepsilon_s - e_\infty)\cos(\gamma \phi)}{[1 + 2(\omega \tau)^\alpha \sin\left(\frac{\pi}{2}(1 + \alpha)\right) + (\omega \tau)^{2\alpha}]^{\gamma/2}}$$  \hspace{1cm} (73)

and

$$\text{Im}\{e(\omega)\} = \frac{(\varepsilon_s - e_\infty)\sin(\gamma \phi)}{[1 + 2(\omega \tau)^\alpha \sin\left(\frac{\pi}{2}(1 + \alpha)\right) + (\omega \tau)^{2\alpha}]^{\gamma/2}} + i \frac{\sigma}{\omega \varepsilon_0},$$  \hspace{1cm} (74)

respectively, where

$$\phi = \arctan\left\{\frac{(\omega \tau)^\alpha \cos\left(\frac{\pi}{2}(1 + \alpha)\right)}{1 + (\omega \tau)^\alpha \sin\left(\frac{\pi}{2}(1 + \alpha)\right)}\right\}$$  \hspace{1cm} (75)

for $\omega \in \mathbb{C}^+$. The corresponding Herglotz function can be constructed as:

$$h(\omega) = \omega e(\omega) = \omega e_\infty + \frac{\omega(\varepsilon_s - e_\infty)}{1 + (-i\omega \tau)^\alpha} + i \frac{\sigma}{\omega \varepsilon_0}$$  \hspace{1cm} (76)

for $\omega \in \mathbb{C}^+$, and which can be used e.g., in the approximation problem with high-order B-splines described in Paper II.

### 6.4 Lorentz’ Model

The Lorentz’ model is used to model the response of a plasma and is given by

$$e(\omega) = e_\infty - \frac{\omega_p^2}{\omega^2 + i\omega\nu - \omega_0^2},$$  \hspace{1cm} (77)
where \( \varepsilon_\infty \) is the optical response, \( \omega_p > 0 \) the plasma frequency, \( \omega_0 > 0 \) the resonance frequency, and \( \nu > 0 \) the collision frequency. The corresponding time-domain response is given by

\[
e_r(t) = \varepsilon_\infty \delta(t) + \frac{\omega_p^2}{\nu_0} e^{-vt/2} \sin(\nu_0 t) H(t),
\]

(78)

where \( \nu_0 = \sqrt{\omega_p^2 - \nu^2/4} \) and \( \omega_0 \geq 2 \). The corresponding Herglotz function \( h(\omega) = \omega \varepsilon(\omega) \) can be constructed and has the following asymptotic expansions:

\[
h(\omega) = \omega \varepsilon_\infty - \frac{\omega \omega_p^2}{\omega^2 + 1\omega \nu - \omega_0^2} = \begin{cases} \omega \varepsilon_s + o(\omega), & \omega \to 0, \\ \omega \varepsilon_\infty - \omega^{-1} \omega_p^2 + o(\omega^{-1}), & \omega \to \infty, \end{cases}
\]

(79)

where the static permittivity \( \varepsilon_s = \varepsilon_\infty + \omega_p^2/\omega_0^2 \) and \( \omega \neq 0 \). The Herglotz function (79) can be extended to a function meromorphic in \( \mathbb{C} \setminus \{\omega_1, \omega_2\} \) with two poles at \( \omega_{1,2} = -i\nu/2 \pm \sqrt{\nu^2/4 + \omega_0^2} \). The spectral measure \( \text{Im}\{h(\xi)\} = \pi \beta_\nu^\nu(\xi) \) is given by

\[
\text{Im}\{h(\xi)\} = \frac{\xi^2 \omega_p^2 \nu}{(\xi^2 - \omega_0^2)^2 + \xi^2 \nu^2}
\]

(80)

for \( \xi = \text{Re}\{\omega\} \in \mathbb{R} \). For \( \omega_0 \neq 0 \), there exists a sum rule for \( k = 1 \), the same as in (64). However, for \( \omega_0 = 0 \), there is another sum rule derived for \( k = 0 \), which is given by:

\[
\frac{2}{\pi} \int_{0^+}^{\infty} \text{Im}\{h(\xi)\} \, d\xi = \omega_p^2,
\]

(81)

which is also valid for the Drude model; see Section 6.5.

The Lorentz’ model is also useful in modeling of linear non-passive gain media, i.e., the media having \( \text{Im}\{\varepsilon\} < 0 \) over some frequency intervals. Note that the representation of Lorentz’ model for gain media is different in comparison with the model for passive media (77), and is given by

\[
\varepsilon(\omega) = \varepsilon_\infty + \frac{\omega_p^2}{\omega^2 + 1\omega \nu - \omega_0^2}.
\]

(82)

The corresponding representation of this model in the time domain can be obtained as:

\[
e_r(t) = \varepsilon_\infty \delta(t) - \frac{\omega_p^2}{\nu_0} e^{-vt/2} \sin(\nu_0 t) H(t),
\]

(83)

where \( \nu_0 = \sqrt{\omega_p^2 - \nu^2/4} \). The corresponding quasi-Herglotz function \( q(\omega) = \omega \varepsilon(\omega) \) can be constructed and has the following asymptotic expansions:

\[
q(\omega) = \omega \varepsilon_\infty + \frac{\omega \omega_p^2}{\omega^2 + 1\omega \nu - \omega_0^2} \begin{cases} \omega \varepsilon_s + o(\omega), & \omega \to 0, \\ \omega \varepsilon_\infty + \omega^{-1} \omega_p^2 + o(\omega^{-1}), & \omega \to \infty, \end{cases}
\]

(84)
where the static permittivity \( \varepsilon_s = \varepsilon_\infty - \omega_p^2/\omega_0^2 \) and \( \omega \neq 0 \). Consequently, the quasi-Herglotz function based on the negative Lorentz’ model (82) admits the sum rules for \( k = 1 \) as in (64) for passive media characterized by the Debye model when \( \omega_0 \neq 0 \). However for \( k = 0 \), the sum rule based on the quasi-Herglotz function (84) is

\[
\frac{2}{\pi} \int_{\omega_0}^{\infty} \text{Im}\{q(\xi)\} \, d\xi = -\omega_p^2,
\]

which is valid when \( \omega_0 = 0 \).

In practical examples, such as modeling of laser dyes (e.g., Rhodamine 6G and Rhodamine R800 laser dye molecules [19]) considered as a four-level atomic system, the Lorentz model for linear gain media is given by:

\[
\varepsilon(\omega) = \varepsilon_\infty + \frac{1}{\varepsilon_0 \omega^2 + i\omega \Delta \omega_a - \omega_a^2} \frac{(\tau_{21} - \tau_{10})\Gamma_{\text{pump}}}{1 + (\tau_{32} + \tau_{21} + \tau_{10})\Gamma_{\text{pump}}} - \overline{N}_0,
\]

where \( \sigma_a \) is the coupling strength of the polarization density at the emission frequency band to the electric field, \( \Delta \omega_a \) the bandwidth of the dye transition at the emitting angular frequency \( \omega_a \), \( \tau_{ij} \) the lifetime for transition from state \( i \) to state \( j \), \( \Gamma_{\text{pump}} \) the pumping rate from level 0 to level 3, and \( \overline{N}_0 \) the total dye concentration [19].

### 6.5 Drude Model

The Drude model is used to model the condition of charges in metals and is a special case of the Lorentz’ model with \( \omega_0 = 0 \):

\[
\varepsilon(\omega) = \varepsilon_\infty - \frac{\omega_p^2}{\omega(\omega + i\nu)} = \varepsilon_\infty + \frac{1}{\varepsilon_0 \omega^2} \frac{1}{1 - i\omega/\nu},
\]

where \( \varepsilon_\infty \) denotes the instantaneous response, \( \omega_p > 0 \) the plasma frequency, \( \nu > 0 \) the collision frequency, \( \varepsilon_0 \approx 8.854 \cdot 10^{-12} \text{F/m} \) the permittivity of free space, and \( \sigma_0 = \omega_p^2 \varepsilon_0/\nu \) the static conductivity. The corresponding representation in the time domain is given as:

\[
\varepsilon_t(t) = \varepsilon_\infty \delta(t) + \frac{\sigma_0}{\varepsilon_0} (1 - e^{-\nu t}) H(t).
\]

The corresponding Herglotz function \( h(\omega) = \omega \varepsilon(\omega) \) can be constructed, which has the following asymptotic expansions:

\[
h(\omega) = \omega \varepsilon_\infty + i \frac{\sigma}{\varepsilon_0} \frac{1}{1 - i\omega/\tau} = \begin{cases} 
  i\sigma_0/\varepsilon_0 + o(1) = o(\omega^{-1}), & \omega \to 0, \\
  \omega \varepsilon_\infty - \omega^{-1} \omega_p^2 + o(\omega^{-1}), & \omega \to \infty,
\end{cases}
\]

where \( \omega_p^2 = \sigma_0 \nu/\varepsilon_0 \). The Herglotz function (89) can be extended to a function meromorphic in \( \mathbb{C} \setminus \{-i\nu\} \) with a single pole at \( \omega = -i\nu \). The spectral measure \( \text{Im}\{h(\xi)\} = \pi \beta'_+(\xi) \) is given by

\[
\text{Im}\{h(\xi)\} = \frac{\sigma_0}{\varepsilon_0} \frac{1}{1 + \xi^2/\nu^2}
\]
for $\xi = \Re\{\omega\} \in \mathbb{R}$. There exists a sum rule for $k = 0$ given as

$$
\frac{2}{\pi} \int_{0+}^{\infty} \Im\{h(\xi)\} \, d\xi = \frac{2}{\pi} \int_{0+}^{\infty} \xi \Im\{e(\xi)\} \, d\xi = \omega_p^2.
$$

It can be concluded that a priori knowledge of the static conductivity as well as the mean value (the first moment) of $\Im\{e(\xi)\}$ gives us a possibility to determine the modified Debye model via (91); the collision frequency can be determined as $\nu = \omega_p^2 \varepsilon_0 / \sigma_0$. Note that the sum rule for $k = 1$ as in (64) does not exist.

The Drude model is related to the modified Debye model (71) described in Section 6.2. To show this relation, first we have apply the partial fraction decomposition to (87), and thus, the representation of the Drude model becomes

$$
e(\omega) = \varepsilon_{\infty} - \frac{\omega_p^2 / \nu^2}{1 - i\omega / \nu} + 1 - \frac{\omega_p^2 / \nu}{\omega}.
$$

Now, the Drude model can be considered as a partial case of the modified Debye model, where

$$
\begin{cases}
    \varepsilon_s = \varepsilon_{\infty} - \frac{\omega_p^2 / \nu^2}{1 - i\omega / \nu}, \\
    \tau = 1 / \nu, \\
    \sigma = \varepsilon_0 \omega_p^2 / \nu.
\end{cases}
$$

Note that the parameters of the Debye model can be given in terms of the parameters of the Drude model as in (93) if the condition

$$
\varepsilon_s - \varepsilon_{\infty} + \frac{\sigma \tau}{\varepsilon_0} = 0
$$

is satisfied [52]. Further note that the standard conductivity model

$$
e(\omega) = \tilde{\varepsilon}(\omega) + i \frac{\sigma}{\omega \varepsilon_0}
$$

is a special case of the Drude and the modified Debye models, respectively, where $\tilde{\varepsilon}(\omega)$ is regular at the origin [52].

One of the practical applications of the Drude model is within characterization of gold nanoparticle suspensions, where the electric current is governed by an electrophoretic mechanism. A realistic electrophoretic Drude model depends on the physical and chemical properties of nanoparticle’s components. The mass of one gold nanoparticle can be obtained as $m = \rho_{\text{Au}} \left( 4\pi a_{\text{Au}}^3 / 3 \right) + \rho_{\text{L}} \left( 4\pi (a^3 - a_{\text{Au}}^3) / 3 \right)$, where $\rho_{\text{Au}}$ and $\rho_{\text{L}}$ are the mass densities of gold and ligands, respectively, $a$ and $a_{\text{Au}}$ are the radii of one nanoparticle and its core, respectively. Additionally to the discussed parameters, the net charge of a gold nanoparticle, the friction constant, and the number of particles per unit volume have to be taken into account. The net charge of the gold nanoparticle depends on the radius of core $a_{\text{Au}}$ as well as on the electron count $n_{\text{L}}$, and can be determined as $q = \left( 3a_{\text{Au}} + 0.5a_{\text{Au}}^2 \right) e_0 + n_{\text{L}} e_0$, where
where $e_0 = 1.6 \cdot 10^{-19}$ C denotes the electron charge [68,79]. The friction constant $\beta = 6\pi \mu_0 a$ is obtained from Stoke's law, where $\mu_i$ is the dynamic shear viscosity of the host medium [68,79]. The number of particles per unit volume can be obtained as $N = \phi/(4\pi a^3/3)$, where $\phi$ is the volume fraction of gold nanoparticles in the spherical suspension [68,79]. Finally, the corresponding static conductivity and the relaxation time of electrophoretic Drude model can be determined as $\sigma_0 = Nq^2/\beta$ and $\tau = m/\beta$, respectively.

### 6.6 Brendel–Bormann Model

The Brendel–Bormann model is used for modeling dielectric properties of materials, especially metals, in the optical frequency range, and has the following representation in the frequency domain as:

$$
\epsilon(\omega) = \epsilon_\infty - \frac{\Omega_p^2}{\omega(\omega - i\Gamma_0)} + \sum_{j=1}^{k} \chi_j(\omega),
$$

(96)

where $\epsilon_\infty$ is the instantaneous response, $\Omega_p = \sqrt{f_0\omega_p}$ the plasma frequency associated with interband transitions with oscillator strength $f_0$ and damping constant $\Gamma_0$ [75]. Here, $k$ is the number of Gaussian-line-shape oscillators $\chi_j(\omega)$ defined as:

$$
\chi_j(\omega) = \frac{1}{\sqrt{2\pi}\sigma_j} \int_{-\infty}^{\infty} \exp\left(-\frac{(x - \omega_j)^2}{2\sigma_j^2}\right) \frac{f_j a_p^2}{(x^2 - \omega^2) + i\omega\Gamma_j} \, dx,
$$

(97)

where $\sigma_j$ is the Gaussian broadening parameter. The analytical solution of (97) is given by

$$
\chi_j(\omega) = \frac{i\sqrt{\pi}f_j a_p^2}{2\sqrt{2}\sigma_j a_j} \left[ w\left(\frac{a_j - \omega_j}{\sqrt{2}\sigma_j}\right) + w\left(\frac{a_j + \omega_j}{\sqrt{2}\sigma_j}\right) \right]
$$

(98)

for $a_j = \sqrt{\omega^2 - i\omega\Gamma_j}$ and $\text{Im}\{a_j\} > 0$; see [75] for details. Here, $w(z)$ denotes the error function integral

$$
w(z) = e^{-z^2} \left( 1 + \frac{12}{\pi} \int_{0}^{z} e^{t^2} \, dt \right) = e^{-z^2} \text{erfc}(iz)
$$

(99)

for $\text{Im}\{z\} > 0$.

In [75], an alternative solution of (97) based on confluent hypergeometric functions, the Kummer functions of the second kind $U(a, b, z)$, is proposed. As a result, the Gaussian oscillators $\chi_j(\omega)$ can be represented as:

$$
\chi_j(\omega) = \frac{i f_j a_p^2}{2\sqrt{2}\sigma_j a_j} \left\{ U\left(1, \frac{1}{2}, \frac{(a_j - \omega_j)^2}{2\sigma_j^2}\right) + U\left(1, \frac{1}{2}, \frac{(a_j + \omega_j)^2}{2\sigma_j^2}\right) \right\},
$$

(100)
where the relation between the Kummer and error functions

\[
U\left(\frac{1}{2}, \frac{1}{2}, z^2\right) = \sqrt{\pi} e^{z^2} \text{erfc}(z)
\]

has been employed [75].

The Brendel–Bormann model has demonstrated more accurate results in fitting the experimental data of materials in the optical frequency range in comparison with the Drude–Lorentz model, which is based on the Lorentz-line-shape oscillator [18]. In Paper IV, the Brendel–Bormann model of gold [75] is used to determine the optimal plasmonic singularity in terms of the non-passive gain surrounding medium. In Paper VII, the same model of gold is used to characterize the dielectric properties of homogeneous and core-shell spheres. However in 2018, it turned out that this model does not satisfy the Kramers-Kronig relations (8) and (9), and thus, it is impossible to achieve an impulse response in the time domain of a dielectric material characterized by this model in the frequency domain; see [73]. To satisfy the symmetry requirement of the Kramers-Kronig relations, a singularity cancellation procedure at the origin in the Gaussian-line-shape oscillator is required, which is described in [73].

7 Optical Theorem in Lossy Media

In this section, we review optical theorems for scatterers immersed in surrounding absorptive media described in Paper VII.

Consider a scatterer of a volume \( V \) made of a linear general bianisotropic material and immersed in a linear isotropic passive background medium, as shown in Figure 9. The incident and scattered fields in the exterior region \( \mathbb{R}^3 \setminus V \) are given by Maxwell’s equations

\[
\left\{ \begin{array}{l}
\nabla \times E_{(i,s)} = ik_0 \eta_0 \mu_b H_{(i,s)}, \\
\nabla \times H_{(i,s)} = -ik_0 \eta_0^{-1} \epsilon_b E_{(i,s)},
\end{array} \right.
\]

where \( E \) and \( H \) are electric and magnetic field intensities, the subscripts “i” and “s” correspond to the incident and scattered fields, respectively, \( \mu_b \) with \( \text{Im}\{\mu_b\} \geq 0 \) and \( \epsilon_b \) with \( \text{Im}\{\epsilon_b\} \geq 0 \) denote the permeability and permittivity of the passive background medium, respectively, and the total fields are given by \( E = E_i + E_s \) and \( H = H_i + H_s \). Note that the incident fields \( E_i \) and \( H_i \) are valid in the whole \( \mathbb{R}^3 \).

The power balance at the external boundary surface \( \partial V \) surrounding the scatterer in a lossy medium can be obtained by employment of the Poynting’s theorem

\[
P_a = -P_s + P_t + P_l,
\]
Figure 9: Problem setup. Here, $\varepsilon_b$ and $\mu_b$ denote the relative permittivity and permeability of the background medium, respectively, $\varepsilon$ and $\mu$ the permittivity and permeability dyadics, respectively, $\chi_{em}$ and $\chi_{me}$ the dimensionless susceptibility dyadics, and $\hat{n}$ the outward unit vector.

where $P_a$ denotes the absorbed power, $P_s$ the scattered power, $P_t$ the total (extinct) power, and $P_i$ the incident power absorbed by the surrounding medium. Here, the powers are given by

$$P_a = -\frac{1}{2} \text{Re} \left\{ \int_{\partial V} E \times H^* \cdot \hat{n} \, dS \right\},$$  \hfill (104)

$$P_s = \frac{1}{2} \text{Re} \left\{ \int_{\partial V} E_s \times H_{s}^* \cdot \hat{n} \, dS \right\},$$  \hfill (105)

$$P_t = -\frac{1}{2} \text{Re} \left\{ \int_{\partial V} (E_1 \times H_{s}^* + E_s \times H_{i}^*) \cdot \hat{n} \, dS \right\},$$  \hfill (106)

and

$$P_i = -\frac{1}{2} \text{Re} \left\{ \int_{\partial V} E_1 \times H_{i}^* \cdot \hat{n} \, dS \right\},$$  \hfill (107)

where the integrals are defined with the outward unit normal $\hat{n}$, see also [15, Eq. (3.19)].

7.1 Physical bound on absorption based on interior-field formulation

Let the interior scattering region $V$ be characterized by the following constitutive relations for a general bianisotropic material:

$$\begin{align*}
D &= \varepsilon_0 \varepsilon \cdot E + \frac{1}{c_0} \chi_{em} \cdot H, \\
B &= \frac{1}{c_0} \chi_{me} \cdot E + \mu_0 \mu \cdot H,
\end{align*}$$  \hfill (108)
where \( D \) is the electric flux density, \( B \) the magnetic flux density, \( \varepsilon = \varepsilon_0 I + \chi_{ee} \) and \( \mu = \mu_0 I + \chi_{mm} \) are the permittivity and permeability dyadics, where \( \chi_{ee}, \chi_{em}, \chi_{me}, \) and \( \chi_{mm} \) are the dimensionless susceptibility dyadics. Then, the Maxwell’s equations for the interior region \( V \)

\[
\begin{align*}
\nabla \times E &= ik_0 \chi_{me} \cdot E + ik_0 \eta_0 \mu \cdot H, \\
\nabla \times H &= -ik_0 \eta_0^{-1} \varepsilon_0 E - ik_0 \chi_{em} \cdot H,
\end{align*}
\]

(109)
can be reformulated in terms of the background medium by using the volume equivalent principle as:

\[
\begin{align*}
\nabla \times E &= ik_0 \eta_0 \mu_b H - J_m, \\
\nabla \times H &= -ik_0 \eta_0^{-1} \varepsilon_0 E + J_e,
\end{align*}
\]

(110)
where

\[
\begin{align*}
J_e &= -ik_0 \eta_0^{-1} \chi_{ee} \cdot E - ik_0 \chi_{em} \cdot H, \\
J_m &= -ik_0 \chi_{me} \cdot E - ik_0 \eta_0 \chi_{mm} \cdot H.
\end{align*}
\]

(111)
are the equivalent electric and magnetic contrast currents.

By employing the boundary conditions at the surface \( \partial V \)

\[
\begin{align*}
\hat{n} \times (E_i + E_a) &= \hat{n} \times E, \\
\hat{n} \times (H_i + H_a) &= \hat{n} \times H,
\end{align*}
\]

(112)
together with the divergence theorem and the vector identity \( \hat{n} \cdot (X \times Y) = \hat{n} \times (X \cdot Y) \), it is possible to show that the absorbed, total, and incident powers involved in the optical theorem for the lossy background (103) can be given in the form based on the interior fields

\[
\begin{align*}
P_a &= \frac{k_0}{2 \eta_0} \text{Im} \left\{ \int_V F^* \cdot M_a \cdot F \, dv \right\}, \\
P_t &= \frac{k_0}{2 \eta_0} \text{Im} \left\{ \int_V F_i^* \cdot M_t \cdot F \, dv \right\} - 2P_i, \\
P_i &= \frac{k_0}{2 \eta_0} \text{Im} \left\{ \int_V F_i^* \cdot M_b \cdot F_i \, dv \right\},
\end{align*}
\]

(113–115)
where the field vectors are

\[
F = \left( \begin{array}{c} E \\ \eta_0 H \end{array} \right) \quad \text{and} \quad F_i = \left( \begin{array}{c} E_i \\ \eta_0 H_i \end{array} \right).
\]

(116)
Here, the material dyadics are given by

\[
M_a = \left( \begin{array}{cc} \varepsilon & \chi_{em} \\ \chi_{me} & \mu \end{array} \right) = \chi + M_b,
\]

(117)
where
\[ \chi = \begin{pmatrix} \chi_{ee} & \chi_{em} \\ \chi_{me} & \chi_{mm} \end{pmatrix}, \quad M_b = \begin{pmatrix} \varepsilon_b I & 0 \\ 0 & \mu_b I \end{pmatrix}, \] (118)

and
\[ M_t = \begin{pmatrix} \varepsilon - \varepsilon^*_b I & \chi_{em} \\ \chi_{me} & \mu - \mu^*_b I \end{pmatrix} = \chi + i2\text{Im}\{M_b\}. \] (119)

Note that the absorbed power \( P_a \) in (113) is given by a positive definite (strictly convex) quadratic form, and the total power \( P_t \) is given by an affine form in the field quantities.

The optimization problem of interest can now be formulated as:
\[
\begin{align*}
\text{maximize} & \quad P_a \\
\text{subject to} & \quad P_s = -P_a + P_t + P_i \geq 0,
\end{align*}
\] (120)

which is a convex maximization problem formulated in terms of the interior fields \( \mathbf{F} \) and constrained with a non-negative scattered power. The Lagrangian for this optimization problem is given by
\[
\mathcal{L}(\mathbf{F}, \lambda) = (1 - \lambda)\text{Im} \left\{ \int_V \mathbf{F}^* \cdot M_a \cdot \mathbf{F} \, d\mathbf{v} \right\} + \lambda \text{Im} \left\{ \int_V \mathbf{F}_i^* \cdot M_t \cdot \mathbf{F}_i \, d\mathbf{v} \right\} - \lambda \text{Im} \left\{ \int_V \mathbf{F}_i^* \cdot M_b \cdot \mathbf{F}_i \, d\mathbf{v} \right\},
\] (121)

where \( \lambda \) is the Lagrange multiplier. Taking the first variation of (121)
\[
\delta \mathcal{L}(\mathbf{F}, \lambda) = \text{Im} \left\{ \int_V \delta \mathbf{F}^* \cdot \left[ (1 - \lambda) \left( M_a - M_a^\dagger \right) \right] \cdot \mathbf{F} - \lambda M_t^\dagger \cdot \mathbf{F}_i \, d\mathbf{v} \right\},
\] (122)

a stationary solution \( (\delta \mathcal{L}(\mathbf{F}, \lambda) = 0) \) for the field quantity \( \mathbf{F} \) can be found as
\[
\mathbf{F} = \frac{\alpha}{2i} (\text{Im}\{M_a\})^{-1} \cdot M_t^\dagger \cdot \mathbf{F}_i,
\] (123)

where \( (\cdot)^\dagger \) denotes the Hermitian transpose, \( \alpha = \lambda/(1 - \lambda), \) and \( \text{Im}\{M_a\} = \left( M_a - M_a^\dagger \right)/2i. \)

The optimal absorbed power can be determined by inserting the stationary solution into the expression for absorbed power (113), which results as
\[
P_a^{\text{opt}} = \frac{k_0\alpha^2}{8\eta_0} \int_V \mathbf{F}_i^* \cdot M_t \cdot (\text{Im}\{M_a\})^{-1} \cdot M_t^\dagger \cdot \mathbf{F}_i \, d\mathbf{v}.
\] (124)

The parameter \( \alpha \) can be determined by putting the solution (123) into the active constraint in optimization (120) and resulting from the equation
\[
\alpha^2 + 2\alpha = q,
\] (125)
with the maximizing root determined as

\[ \alpha = -1 - \sqrt{1 - q}, \]  

(126)

where

\[ q = \frac{4 \int_V F'_i \cdot \text{Im}\{M_b\} \cdot F_1 \, dv}{\int_V F'_i \cdot M_t \cdot (\text{Im}\{M_a\})^{-1} \cdot M'_i \cdot F_1 \, dv} \]  

(127)

in the range \( 0 \leq q \leq 1 \). The lower bound of this range can be approached for \( \text{Im}\{M_b\} = 0 \), i.e., in the case when the surrounding medium is lossless. To determine the upper bound of \( q \), observe that its denominator is convex in \( M_a \) for \( \text{Im}\{M_a\} > 0 \). By minimization of denominator, it can be proved that \( \max\{q\} = 1 \) for \( M_a = M_b \).

### 7.2 Physical bound on absorption based on exterior-field formulation

Let the electromagnetic field be expanded in spherical vector waves as:

\[
\begin{align*}
E(r) &= \sum_{\tau,m,l} a_{\tau ml} \mathbf{v}_{\tau ml}(kr) + f_{\tau ml} \mathbf{u}_{\tau ml}(kr), \\
H(r) &= \frac{1}{\ii \eta} \sum_{\tau,m,l} a_{\tau ml} \mathbf{v}_{\tau ml}(kr) + f_{\tau ml} \mathbf{u}_{\tau ml}(kr),
\end{align*}
\]

(128)

where \( \mathbf{v}_{\tau ml}(kr) \) and \( \mathbf{u}_{\tau ml}(kr) \) are the incident (regular) and the scattered (outgoing) spherical vector waves, respectively, having the properties described in Appendix B of Paper VII, and \( a_{\tau ml} \) and \( f_{\tau ml} \) the corresponding multipole coefficients, \( l = 1, 2, \ldots \), is the multipole order, \( m = -l, \ldots, l \), the azimuthal index, and \( \tau = 1, 2 \) corresponds to a transverse electric (TE) magnetic multipole (with \( \tau = 1 \)) and a transverse magnetic (TM) electric multipole (with \( \tau = 2 \)); see e.g., [3,15,16,45,52,67]. Here, \( \tilde{\tau} \) is the dual index, i.e., \( \tilde{1} = 2 \) and \( \tilde{2} = 1 \).

Let us consider an arbitrary linear scatterer, which may consist of a general bianisotropic linear material. The scatterer is circumscribed by a spherical volume of radius \( a \), which is surrounded by a linear isotropic lossy medium; see Figure 9. The power balance to be used for this problem is the same as in (103), and involves the absorbed, scattered, total, and the incident powers defined by (104) through
(107), respectively. By employing the orthogonality properties of spherical vector waves

\[
\int_{\partial V_a} \mathbf{w}_{\tau ml}(kr) \times \mathbf{z}^*_{\tau ml'}(kr) \cdot \hat{r} \, dS \\
= a^2 \delta_{mm'} \delta_{ll'} \begin{cases} \\
  w_1(ka) \left( \frac{(kaz_1(ka))^\tau}{ka} \right)^*, & \tau = 1, \\
  -\left( \frac{(kaw_1(ka))^\tau}{ka} \right) z_1^*(ka), & \tau = 2,
\end{cases}
\]

(129)

and

\[
\int_{\partial V_a} \mathbf{w}_{\tau ml}(kr) \times \mathbf{z}^*_{\tau ml'}(kr) \cdot \hat{r} \, dS = 0,
\]

(130)

for \( \tau = 1, 2 \) on the spherical surface \( \partial V_a \), the scattered, total, and incident powers can be given by

\[
P_s = \frac{\text{Re}\{\sqrt{\varepsilon_b}\}}{2|k_b|^2 \eta_0} \sum_{\tau,m,l} A_{\tau l} |f_{\tau ml}|^2,
\]

(131)

\[
P_t = \frac{\text{Re}\{\sqrt{\varepsilon_b}\}}{2|k_b|^2 \eta_0} \sum_{\tau,m,l} 2\text{Re}\{B_{\tau l} a_{\tau ml}^* f_{\tau ml}\},
\]

(132)

and

\[
P_i = \frac{\text{Re}\{\sqrt{\varepsilon_b}\}}{2|k_b|^2 \eta_0} \sum_{\tau,m,l} C_{\tau l} |a_{\tau ml}^i|^2,
\]

(133)

respectively, where

\[
A_{\tau l} = \frac{1}{\text{Re}\{k_b\}} \begin{cases} \\
 -\text{Im}\{k_b^* \xi_1 \xi_l^*\}, & \tau = 1, \\
 \text{Im}\{k_b^* \xi_1^* \xi_l^*\}, & \tau = 2,
\end{cases}
\]

(134)

\[
B_{\tau l} = \frac{1}{2\text{Re}\{k_b\}} \begin{cases} \\
 k_b^* \xi_1 \psi_l^* - k_b \psi_l^* \xi_1^*, & \tau = 1, \\
 -k_b^* \xi_1^* \psi_l^* + k_b \psi_l \xi_1, & \tau = 2,
\end{cases}
\]

(135)

\[
C_{\tau l} = \frac{1}{\text{Re}\{k_b\}} \begin{cases} \\
 \text{Im}\{k_b^* \psi_l \psi_l^*\}, & \tau = 1, \\
 -\text{Im}\{k_b^* \psi_l^* \psi_l^*\}, & \tau = 2,
\end{cases}
\]

(136)

for \( \tau = 1, 2 \) and \( l = 1, \ldots, \infty \), and the arguments of the Ricatti-Bessel (\( \psi_l \)) and Ricatti-Hankel functions (\( \xi_l \)) are \( z = k_b a \). The coefficients \( A_{\tau l} > 0 \) and \( C_{\tau l} \geq 0 \), which follows from the application of the divergence theorem to (105) and (107) in the case when the surrounding medium is passive implying that \( P_s \geq 0 \) and \( P_i \geq 0 \), respectively. The coefficient \( B_{\tau l} \) is complex-valued.
The physical bound on absorption in terms of the exterior fields can be derived as follows. First, consider the contribution to the absorbed power from a single partial wave obtained from the power balance relation (103)

$$P_{a, \tau ml} = \frac{\text{Re}\{\sqrt{\varepsilon_b}\}}{2|k_b|^2 \eta_0} \left[ -A_{\tau l} |f_{\tau ml}|^2 + 2 \text{Re}\{B_{\tau l} a_{\tau ml}^* f_{\tau ml}\} + C_{\tau l} |a_{\tau ml}^1|^2 \right],$$  \hspace{1cm} (137)

for a given multi-index $(\tau, m, l)$, which is based on the expressions for the scattered, total, and incident powers (131) through (133), respectively. Then, we define the scattering coefficients $f_{\tau ml}$ in terms of T-matrix for an arbitrary linear scatterer, which is circumscribed by a spherical volume $V_a$, as

$$f_n = \sum_{n'} T_{n,n'} a_{n'}^1,$$  \hspace{1cm} (138)

where the multi-index notation $n = (\tau, m, l)$ has been introduced. It is observed that (137) is a concave function of the complex-valued variables $T_{n,n'}$ with respect to the primed index $n'$. This allows to derive the stationary condition

$$A_{\tau l} a_{n'}^1 \sum_{n''} a_{n''}^* T_{n,n''} = B_{\tau l} a_{n}^* a_{n'}^1,$$  \hspace{1cm} (139)

by differentiating (137) with respect to $T_{n,n'}$ for fixed $n$, from which the pseudo-inverse solution to the T-matrix can be obtained as

$$T_{n,n'} = \frac{B_{\tau l}^*}{A_{\tau l} g} a_{n} a_{n'}^*,$$  \hspace{1cm} (140)

where $g = \sum_{\tau, m, l} |a_{\tau ml}^1|^2$ is the corresponding matrix norm. Using the results (137) and (140), and by completing the squares, the contribution from a single wave to the absorbed power can be given by

$$P_{a, \tau ml} = \frac{\text{Re}\{\sqrt{\varepsilon_b}\}}{2|k_b|^2 \eta_0} \left[ -A_{\tau l} \sum_{\tau', m', l'} \left| T_{\tau ml, \tau' m'l'} - \frac{B_{\tau l}^* a_{\tau ml}^1 a_{\tau ml}^1}{A_{\tau l} g} \right| a_{\tau' m'l'}^1 \right]^2 + \left( \frac{|B_{\tau l}|^2}{A_{\tau l}} + C_{\tau l} \right) |a_{\tau ml}^1|^2,$$  \hspace{1cm} (141)

which is concave since $A_{\tau l} > 0$. It is observed that (141) reaches its maximum when the first term equals to 0. Hereby, summing over all the indices $(\tau, m, l)$, the physical bound on absorption formulated in terms of exterior fields is given by

$$P_{a}^{\text{opt}} = \frac{\text{Re}\{\sqrt{\varepsilon_b}\}}{2|k_b|^2 \eta_0} \sum_{\tau, m, l} \left( \frac{|B_{\tau l}|^2}{A_{\tau l}} + C_{\tau l} \right) |a_{\tau ml}^1|^2,$$  \hspace{1cm} (142)

which is independent of the T-matrix, and thus is valid for scatterers of an arbitrary shape circumscribed by a spherical surface $\partial V_a$ and made of arbitrary
linear materials (including general bianisotropic). It should be noted that the
infinite dimensional matrix equation in (139) in general is related to an unbounded
operator, where the series given by \( g \) in (140) does not converge because the
corresponding matrix norm does not exist. However, this is merely a mathematical
subtlety that does not pose any real problem here because in presence of a lossy
background, the T-matrix (138) can be truncated to a finite size \( L \) with \( l, l' \leq L \),
for which the solution converges. Hereby, the obtained physical bound (142) can
also be interpreted as the optimal absorption with respect to all incident and
scattered fields up to multipole order \( L \), as \( L \to \infty \).

8 Research Contribution

Paper I. Passive approximation and optimization using B-splines

Paper I provides a method for approximation of linear, time-translationally
invariant passive systems. The proposed method is based on Herglotz functions
with Hölder continuous extension to the real axis, finite B-spline expansion of
an arbitrary order, and convex optimization. Here, the objective is to develop a
mathematical framework that allows determination of an optimal realization of
a passive system, characterized by a given continuous target function over the
approximation domain. Such a system must satisfy the Kramers-Kronig relations,
and thus the real and imaginary parts of the system function are related to each
other via the Hilbert transform. The method exploits the fact that the Hilbert
transform is a bounded operator on Hölder spaces.

In this paper, one of the main results is that we have proved that the convex
cone consisting of approximating functions, whose measure is given by a finite
uniform B-spline expansion of a fixed arbitrary order, is dense in the convex cone
of Herglotz functions which are Hölder continuous in an open neighborhood
of the approximation domain, as mentioned above; see Theorem 3.4 in Paper I.
We have also proved that the greatest lower bound can be approached within
arbitrary accuracy by using a finite B-spline expansion of an arbitrary order
as a generating measure for the approximating function; see Theorem 3.7 in
Paper I. We have also derived a new physical bound on realization of passive
lossy metamaterials with constant permittivity over a finite frequency interval. In
the numerical examples, we treat the passive realization of lossy metamaterials
with a fixed negative-permittivity property over various frequency bandwidths,
including the passive realization of an optimal plasmonic resonance (pole
singularity) of a dielectric sphere immersed in vacuum. Here, the resulting
approximating Herglotz functions have been generated by a linear B-spline
expansion.
Part I. Introduction and Research Overview

Paper II. Passive Approximation with High-Order B-Splines

Paper II is focused on application of the mathematical framework developed in Paper I. Here, we summarize the explicit results concerning the Hilbert transform of general B-splines and the sum rule, which can be expanded with B-spline basis functions of an arbitrary order. The developed framework is applied to a system with a non-trivial response over a large frequency bandwidth. A numerical example of a power-engineering application is presented. The example concerns the estimation of the static conductivity of power-cable insulation material. The obtained approximation results show that high-order, cubic, B-splines are efficient in solving convex optimization problems for given systems with non-trivial response and non-uniform measurement data.

Paper III. Quasi-Herglotz functions and convex optimization

In Paper III, we introduce the class of quasi-Herglotz functions suitable for modeling a subclass of non-passive systems. The new class of functions is a straightforward extension of the convex cone of Herglotz functions. We define quasi-Herglotz functions as differences of two Herglotz functions, and thus, the new functions preserve the integral representation similar to the representation of Herglotz functions. However, not all the quasi-Herglotz functions admit the sum-rule identities, which are based on the small- and large-argument asymptotic properties of these functions; see Section 3 in Paper III.

The new functions can also be restricted to be Hölder continuous on the open neighborhood of the subset of the real axis, which is suitable for the approximation theory developed in Paper I. We also prove that the subspace of quasi-Herglotz functions generated by finite B-spline expansions of an arbitrary order is dense in the space of quasi-Herglotz functions, which are Hölder continuous on the open neighborhood of the approximation interval on the real axis; see Theorem 4.5 in Paper III. It is also proved that we can approach the greatest lower bound with an arbitrary accuracy by using a fixed-order B-spline expansion and point masses as generating measures for the approximating function; see Theorem 4.7 and Corollary 4.8 in Paper III. In the numerical examples, we employ the non-passive approximation framework to determine optimal realizations of non-passive metamaterials with a fixed negative-permittivity property over a finite frequency interval. Interestingly, the support of the measure of the optimized permittivity function is concentrated at the outermost points of frequency sets, where the measure is restricted to be non-positive. Using this observation, it has been discovered that the desired permittivity property can be similarly realized by a function, which has a measure generated only by point masses inside the active (gain) frequency regions. Also in these examples, it is noted that the approximating measure is
typically zero inside the approximation interval itself. We have also shown that by using the sum rules, it is possible to construct the optimization problem for realization of both the negative-permittivity and asymptotic properties of the desired material.

**Paper IV. Non-passive approximation as a tool to study the realizability of amplifying media**

Paper IV presents an application of the non-passive approximation framework as a tool for realization of amplifying media. As a physical application problem, we study the dipole absorption of a dielectric sphere immersed in a hypothetical gain medium. Hereby, we formulate Mie theory for amplifying media and derive the plasmonic singularity of sphere with a given dielectric property in terms of amplifying background medium; see Sections 2 and 3 in Paper IV, respectively. In the numerical example, we study an optimal realization of a background medium with the desired amplifying properties over a given finite frequency interval. It has been investigated that for accurate realizations of such materials, it is necessary to restrict the density of the measure to be non-negative over finite frequency intervals surrounding the approximation domain. Note that the accuracy of realization depends on the width of these intervals. Finally, we have studied the electric-dipole absorption of a gold sphere immersed in an amplifying background medium. We have observed that when the sphere is embedded in the optimal amplifying medium, the electric-dipole absorption level of the sphere is three orders of magnitude higher than the physical bound on electric-dipole absorption for sphere in vacuum.

**Paper V. On the physical limitations for radio frequency absorption in gold nanoparticle suspensions**

Paper V focuses on determination of physical limitations on absorption in gold nanoparticle (GNP) suspensions in the MHz and GHz frequency ranges. In this paper, as a problem setup, a spherical geometry consisting of GNP suspension immersed in a weak electrolyte solution is considered. The suspension is characterized by electrophoretic Drude model, and the electrolyte solution is represented via the Debye model with parameters relatively close to the ones that are used in the model of saline water [52]. For study of absorption properties, a generalized Mie theory in lossy media has been used. In this generalization, one needs to take into account the power absorbed by a surrounding lossy medium. It has been investigated that maximal absorption in GNP suspensions can be achieved when the permittivity characterizing the suspension is a conjugate match with respect to the permittivity of the surrounding medium. Hereby, we have studied narrowband and wideband realizabilities of the conjugate match.
The narrowband optimization has been achieved by "tuning" the Drude model by using the suitable parameters with respect to the desired frequency. The wideband realization is with the metamaterial problem, i.e., with the achievement of the desired property over a given frequency bandwidth. Hereby, we employ the passive approximation framework developed in Paper I to determine an optimal realization of the desired property.

Paper VI. On the plasmonic resonances in a layered waveguide structure

Paper VI presents an investigation on transmission and reflection coefficients though a thin layer made of a composite material and which is placed in a rectangular straight waveguide working in TM-mode. The material of the layer has a Drude type of dispersion, which is suitable for study of electrophoretic microwave heating of gold nanoparticles described in Paper V and for obtaining plasmonic resonances. Through the asymptotic analysis of expressions for the transmission and reflection coefficients, we show that it is possible to obtain a resonance in a plasmonic thin layer when the permittivity of the layer tends to zero, while the layer’s thickness is fixed. Furthermore, we derive the Fröhlich resonance condition, which indicates the resonance frequency of a thin layer under certain assumptions. The numerical example presented in this paper illustrates the derived theoretical results.

Paper VII. Optical theorems and physical bounds on absorption in lossy media

Paper VII introduces two versions of an optical theorem for scatterers immersed in a lossy surrounding medium. The corresponding upper bounds on absorption are derived using conventional analytical optimization techniques. The two versions are based on interior and exterior fields, respectively: the first version of the optical theorem is derived in terms of equivalent currents inside a scattering object, while the second version is formulated in terms of T-matrix parameters of a linear scatterer circumscribed by a spherical volume. The first upper bound on absorption is valid for scattering objects of an arbitrary shape with a given material property. The second upper bound on absorption corresponds to the absorption inside a given spherical inclusion for a given material property of surrounding lossy medium. This bound is valid for linear scatterers that can be placed inside the spherical inclusion. The shape of such a scatterer can be arbitrary, as well as its material properties (including general bianisotropic). Numerical examples with homogeneous and core-shell spheres immersed in lossy surrounding media demonstrate that the corresponding upper bounds on absorption provide complementary information in given scattering problems.
9 Conclusions

This thesis has presented an overview on the determination of physical limitations of linear, time-translationally invariant, causal passive and non-passive systems based on their integral representation properties, as well as numerical and analytical optimization techniques for passive and non-passive approximation. The following results have been achieved:

- The mathematical and numerical frameworks for determination of physical bounds for passive systems based on Herglotz functions, convex optimization, and B-splines has been developed.

- The new class of functions, i.e., the quasi-Herglotz functions, based on differences of two Herglotz functions, has been introduced for modeling admittance non-passive systems.

- The mathematical and numerical frameworks for determination of optimal realizations of admittance non-passive systems based on the set of approximating quasi-Herglotz functions, convex optimization, point masses and B-splines has been developed.

- A method for detection of electrophoretic resonances in sub-wavelength particles placed in straight waveguides through measurements of the reflection coefficient has been proposed.

- The optical theorem for scattering objects immersed in lossy media has been revisited. Physical bounds on absorption of an arbitrary scatterer made of arbitrary materials, which is immersed in a lossy isotropic medium, have been derived by employing the method of Lagrange multipliers. The two physical bounds on absorption derived in terms of internal and external fields, respectively, provide complementary information, and serve as a tool for understanding the limits of power that can be absorbed by homogeneous, composed, or homogenized scatterers immersed in lossy media in a given frequency range.

10 Future Work

The developed theory for mathematical frameworks presented in Papers I and III is quite general and leaves possibilities to consider other electromagnetic and engineering applications. Several tracks remain for future work.

The first track is to extend the developed theory to matrix-valued operators, i.e., to involve the matrix-valued Herglotz and quasi-Herglotz functions for characterization of multiport passive and non-passive systems. The second track is to apply the theory developed in Paper III to studying bounds on optimal
realization of non-passive electric-circuit components with desired properties, which is of interest in antenna and communication systems. The third track is to determine physical bounds on scattering and extinction in lossy media based on the methods employed in Paper VII, which is of interest in antenna design and telemetry applications. The last track is to utilize the physical bounds on absorption derived in Paper VII for understanding the electrophoretic heating of gold nanoparticle suspensions, and improving their corresponding design with respect to the desired characteristics and properties.
Bibliography


[83] C. Sohl, M. Gustafsson, and G. Kristensson. Physical limitations on broad-

[84] C. Sohl, M. Gustafsson, and G. Kristensson. Physical limitations on meta-


[86] I. W. Sudiarta and P. Chylek. Mie scattering by a spherical particle in an


[89] V. S. Vladimirov. *Equations of Mathematical Physics*. Mir Publishers, Moscow,
1984.


[95] M. Wohlers and E. Beltrami. Distribution theory as the basis of generalized

and plasmon dynamics in active negative-index metamaterials. *Philos. Trans.

