Quasi-Herglotz functions and convex optimization

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Abstract. We introduce the set of quasi-Herglotz functions and demonstrate that it has properties useful in the modeling of non-passive systems. The linear space of quasi-Herglotz functions constitutes a natural extension of the convex cone of Herglotz functions. It consists of differences of Herglotz functions, and we show that several of the important properties and modeling perspectives of Herglotz functions are inherited by the new set of quasi-Herglotz functions. In particular, this applies to their integral representations, the associated integral identities or sum rules (with adequate additional assumptions), their boundary values on the real axis and the associated approximation theory. Numerical examples are included to demonstrate the modeling of a non-passive gain media formulated as a convex optimization problem, where the generating measure is modeled by using a finite expansion of B-splines and point masses.

1. Introduction

It is well known that an admittance passive system (admittances, impedances, electromagnetic constitutive relations, etc.) can be represented mathematically by a symmetric Herglotz function (or Positive Real (PR) function), see *e.g.*, [1,5,12,24,33,42]. The condition of passivity implies, among other things, that the system has also to be causal [41]. Furthermore, the integral representation formula of symmetric Herglotz functions leads to integral identities or sum rules [1, 5] that are useful to derive physical bounds in a variety of technical applications such as *e.g.*, radar absorbers [34], passive metamaterials [16], high-impedance surfaces [17], antennas [18, 23], reflection coefficients [15], waveguides [38], and periodic structures [19], only to mention a few. The integral representation formula can also be utilized in a convex optimization setting to construct an optimal approximating passive realization of a desired target response [22, 32], which typically is given on a finite closed interval of the real (frequency) axis. Optimal realizations of passive metamaterials are typical examples, where it *e.g.*, is desired to synthesize low loss materials with negative refractive index over a frequency interval [16, 22, 32]. It is emphasized that the term *realizability* is employed here in the sense of realizability theory as in [43]. This means that a given system response is realizable, not as a physical system, but rather as a function possessing mathematically well defined properties of physical significance, such as causality and passivity [43], and also as in our case, having some a priori assumed regularity properties regarding its boundary values on the real (frequency) axis.

The boundary values of analytic functions representing causal systems are treated classically in L^2 spaces as in Titchmarsh's theorem [25, 33] or in the sense of tempered distributions as in [4, 42]. There are a few results concerned with approximation theory or interpolation problems associated with partial information on the real axis (or on the unit circle). For example in [2] an approximation theory is given with density results for Hardy space approximants targeted for L^p functions defined on subsets of the circle. Furthermore, a related bounded extremal problem is examined in [3] with point-wise constraints on the complementary part of the circle.

In this paper, we are interested in extending the class of admittance passive systems to include certain causal, non-passive systems. This extension is aimed to preserve the integral representation formula for the system, as well as, in certain cases a sum rule. However, the class of Herglotz functions is not characterized by these sum-rule identities, as there exist other functions which also satisfy the same identities. As a characterization of the full class of functions that satisfy the sum-rule identities seems out of reach, we use a class of functions, that includes all Herglotz functions, and for which the sum-rule identities still hold under some appropriate additional assumptions regarding their asymptotic expansions. Moreover, it is also desirable that the new class of functions can be incorporated in an approximation theory, similar to the Herglotz functions [22]. It turns out that differences of Herglotz functions are suitable in this sense. We denote the (real) vector space generated by Herglotz functions as the space of *quasi-Herglotz functions*. As for the approximation theory, we follow a slightly different route than [2,3] and consider as approximants some certain subspaces of quasi-Herglotz functions which are Hölder continuously extendable to a neighborhood of a given approximation interval on the real line, and equipped with a topology from a larger L^p space. This is a formulation that will imply that even smaller subspaces generated by finite B-spline expansions (useful in convex optimization) will be dense in the larger set of approximants.

As a motivation for studying the new class of functions from a physical point of view, we refer to the use of gain media which has been proposed to improve the light localization effects in plasmonics, with applications such as plasmon waveguides, extraordinary transmission, perfect lenses, artificial magnetism, negative refractive index, cloaking, tunneling, high directivity radiators, optical nanocircuits, nanowires etc., see *e.g.*, [7,8,13,27,28,30,37] with references. Here, the use of gain media refers to the use of fluorescent dyes through optical pumping for which there exist explicit Lorentz type of resonance models in the standard laser literature, see *e.g.*, [7, 27, 36, 39, 40] with references. Hence, laser pumping is a physical mechanism that allows for a linearized description of the medium in terms of an electric permittivity that can have a negative imaginary part over some frequency intervals. Naturally, it has been recognized that such models must satisfy causality and the associated Kramers-Kronig relations. However, our purpose of employing quasi-Herglotz functions in this context is to add the restrictions imposed by passivity outside the (non-passive) emitting frequency range.

Numerical examples are included to demonstrate the modeling of a non-passive (gain) metamaterial formulated as a convex optimization problem, where the generating measure is modeled by using a finite expansion of B-splines and point-masses. In particular, we are interested here to investigate how well a fixed negative value of permittivity can be approximated over a given approximation interval as a causal, non-passive system and where the amplifying properties are restricted to a finite bandwidth and compare with the passive case.

The rest of the paper is organized as follows: In Section 2, we introduce the new set of quasi-Herglotz functions and discuss their basic properties, integral representations and boundary values. In Section 3, the sum-rules are formulated and proved. In Section 4, the mathematical approximation theory and related convex optimization is formulated. It is based on certain assumptions regarding the Hölder continuity of the approximating quasi-Herglotz functions extended to the real line. In Section 5, the theory is illustrated by numerical examples.

2. Quasi-Herglotz functions

2.1. Background

An important function class in applied mathematics is the class of so-called *Herglotz functions*. Known also under a variety of different names, such as Herglotz-Nevanlinna functions, Pick functions and R-function, these are analytic functions on the upper half-plane

$$\mathbb{C}^+ := \{z := x + \mathrm{i}\, y \in \mathbb{C} \mid y > 0\} \tag{1}$$

having non-negative imaginary part [1, 24]. The major significance of this class of functions lies in the fact that the subclass of all symmetric Herglotz functions, *i.e.*, Herglotz functions which, in addition, satisfy the property

$$h(z) = -h(-z^*)^* \tag{2}$$

for all $z \in \mathbb{C}^+$, is closely connected with passive systems [42]. Above, the superscript $(\,\cdot\,)^*$ denotes complex conjugation.

One of the most powerful tools in the theory of Herglotz functions is the existence of an integral representation formula [1,24]. This well-known formula states that a function $h\colon \mathbb{C}^+ \to \mathbb{C}$ is a Herglotz function if and only if it can be written, for any $z \in \mathbb{C}^+$, as

$$h(z) = a_+ + b_+ z + \int_{\mathbb{R}} \frac{1 + \xi\, z}{\xi - z} \mathrm{d}\sigma_+(\xi), \tag{3}$$

where $a_+ \in \mathbb{R}$, $b_+ \geq 0$ and σ_+ is a finite positive Borel measure on $\mathbb{R}$, and the subscrpit $(\,\cdot\,)_+$ is used to highlight the fact that these parameters represent a function with *non-negative* imaginary part. Furthermore, the correspondence between the function h and the triple of its representing parameters (a_+, b_+, σ_+) is unique.

If we are, instead, considering a symmetric Herglotz function, condition (2) implies first that the function must take purely imaginary values along the imaginary axis, yielding that the coefficient a_+ from representation (3) must be zero. Furthermore, the Stieltjes inversion formula [24] implies that the measure σ_+ from representation (3) must be even, *i.e.*, $\sigma_+(U) = \sigma_+(-U)$ for any Borel measurable set $U \subseteq \mathbb{R}$, where $-U := \{x \in \mathbb{R} \mid -x \in U\}$.

As such, all symmetric Herglotz functions h admit, for $z \in \mathbb{C}^+$, an integral representation of the form

$$h(z) = b_+ z + \mathrm{p.v.} \int_{\mathbb{R}} \frac{1 + \xi^2}{\xi - z} \mathrm{d}\sigma_+(\xi), \tag{4}$$

where b_+ and σ_+ are as in representation (3), with the additional constraint that the measure σ_+ is symmetric, *cf.*, [1, 12, 24, 33, 42] and p.v. denotes that the integral in representation (4) is taken as the Cauchy principal value at infinity.

2.2. Basic properties

We now introduce the following class of analytic functions on the upper half-plane.

Definition 2.1 *An analytic function $q\colon \mathbb{C}^+ \to \mathbb{C}$ is called a* quasi-Herglotz function *if there exist two Herglotz functions h_1 and h_2, such that*

$$q(z) = h_1(z) - h_2(z) \tag{5}$$

for any $z \in \mathbb{C}^+$. Analogously, an analytic function $q\colon \mathbb{C}^+ \to \mathbb{C}$ is called a symmetric quasi-Herglotz function *if there exist two symmetric Herglotz functions h_1 and h_2, such that equality (5) holds for all $z \in \mathbb{C}^+$. The set of all quasi-Herglotz functions will be denoted by $\mathcal{Q}$, while the set of all symmetric quasi-Herglotz functions will be denoted by $\mathcal{Q}_{\mathrm{sym}}$.*

We mention two trivial observations. First, any Herglotz (resp. symmetric Herglotz) function is also a quasi-Herglotz (resp. symmetric quasi-Herglotz) function, as we only need to take the function h_2 in Definition 2.1 to be identically equal to zero. Second, there is an element of non-uniqueness in Definition 2.1. If an analytic function q can be written as in formula (5) for some Herglotz (resp. symmetric Herglotz) functions h_1 and h_2, then it can also be written as

$$q(z) = (h_1 + h_3)(z) - (h_2 + h_3)(z), \tag{6}$$

where $z \in \mathbb{C}^+$, for any other Herglotz (resp. symmetric Herglotz) function h_3.

2.3. Integral representations

It is an immediate consequence of the integral representation formulas (3) and (4) that quasi-Herglotz functions in the sets $\mathcal{Q}$ and $\mathcal{Q}_{\mathrm{sym}}$ admit similar integral representations. Any function $q \in \mathcal{Q}$ can be written, for $z \in \mathbb{C}^+$, as

$$q(z) = a + b\,z + \int_{\mathbb{R}} \frac{1 + \xi\,z}{\xi - z}\mathrm{d}\sigma(\xi), \tag{7}$$

where a and b are real numbers and σ is a signed Borel measure. In particular, if q is given as $q = h_1 - h_2$, then $a = a_{+,1} - a_{+,2}$, $b = b_{+,1} - b_{+,2}$ and $\sigma = \sigma_{+,1} - \sigma_{+,2}$ where, for $j = 1, 2$, the parameters $a_{+,j}, b_{+,j}$ and $\sigma_{+,j}$ are the representing parameter for the Herglotz function h_j in the sense of representation (3).

Similarly, any function $q = h_1 - h_2$ in the class $\mathcal{Q}_{\mathrm{sym}}$ can be written, for $z \in \mathbb{C}^+$, as

$$q(z) = b\,z + \mathrm{p.v.}\int_{\mathbb{R}} \frac{1 + \xi^2}{\xi - z}\mathrm{d}\sigma(\xi), \tag{8}$$

where b and σ are as in the previous case.

Note that, despite the element of non-uniqueness in Definition 2.1 discussed in Section 2.2, the triple of representing parameter (a, b, σ) corresponding to a quasi-Herglotz function q in the sense of representation (7) is determined uniquely by the function q.

The integral representation formula (3) for ordinary Herglotz functions may also be written in terms of a non-finite measure β_+. Indeed, on may show that the right-hand side of representation (3) may equivalently be written as

$$a_+ + b_+\, z + \int_{\mathbb{R}} \left(\frac{1}{\xi - z} - \frac{\xi}{1+\xi^2} \right) \mathrm{d}\beta_+(\xi), \tag{9}$$

where a_+ and b_+ are as before and β_+ is a positive Borel measure on $\mathbb{R}$ satisfying the growth condition

$$\int_{\mathbb{R}} \frac{1}{1+\xi^2} \mathrm{d}\beta_+(\xi) < \infty. \tag{10}$$

However, an integral representation of this form cannot yield an integral representation for all quasi-Herglotz functions, as the difference of two measures satisfying the growth condition (10) is not-necessarily well-defined. Nevertheless, some quasi-Herglotz function q do admit an integral representation of the form

$$q(z) = a + b\, z + \int_{\mathbb{R}} \left(\frac{1}{\xi - z} - \frac{\xi}{1+\xi^2} \right) \mathrm{d}\beta(\xi), \tag{11}$$

and one case where this happens, which will appear later in Sections 4 and 5, is when the measure σ from representation (7) has compact support. Then, the measure β in representation (11) may be defined via $\mathrm{d}\beta(\xi) = (1+\xi^2)\mathrm{d}\sigma(\xi)$.

2.4. Boundary values

In general, Herglotz, as well as quasi-Herglotz functions, and in particular their imaginary parts, have boundary values (on the real line) only in the distributional sense, see *e.g.*, [4, 5, 22, 42]. In what follows, however, we will be interested in complex-valued functions on some interval $\Omega \subset \mathbb{R}$ which appear as continuous extensions of suitable quasi-Herglotz functions. Recall that the property that assures the existence of such boundary values (of both the real and the imaginary part) is Hölder continuity of the density of the measure. More precisely, the following theorem holds, see *e.g.*, [22, Thm. 2.2] for the argument.

Theorem 2.1 *Let q be a quasi-Herglotz function with representing parameters (a, b, σ) and let $\Omega \subseteq \mathbb{R}$ be a compact interval. Then the function q can be Hölder continuously (with Hölder exponent α) extended to $\Omega \cup \mathbb{C}^+$ if and only if the measure σ is absolutely continuous on the closure of some open neighborhood $\mathcal{O}$ of Ω and the corresponding restriction $\sigma|_{\overline{\mathcal{O}}}$ has a Hölder continuous density σ'_Ω (with Hölder exponent α), i.e., it belongs to the space $C^{0,\alpha}(\overline{\mathcal{O}})$. In this case, for every $x \in \Omega$, this extension is given by*

$$q(x) = a + b\, x + \mathrm{p.v.} \int_{\mathbb{R}} \frac{1 + \xi\, x}{\xi - x} \mathrm{d}\sigma(\xi) + \mathrm{i}\pi(1+x^2)\sigma'_\Omega(x), \tag{12}$$

where the integral is taken as a Cauchy principal value both at infinity and at the singularity $x \in \mathbb{R}$.

We also want to mention certain inclusions of function spaces, which will be very useful in Section 4. As usual, we let $C(\Omega)$ denote the Banach space consisting of all complex-valued continuous functions defined on Ω with max-norm denoted $\|\cdot\|_\infty$. The Hölder space with exponent $0 < \alpha < 1$ is denoted $C^{0,\alpha}(\Omega)$ and the corresponding norm is denoted $\|\cdot\|_\alpha$, *cf.*, [26, pp. 94-104]. Further, let $\mathrm{L}^p(w,\Omega)$ denote the Banach space with norm $\|f\|_{\mathrm{L}^p(w,\Omega)} = \left(\int_\Omega w(x)|f(x)|^p \mathrm{d}x\right)^{1/p}$, where $1 \le p < \infty$ and $w > 0$ denotes a positive continuous weight function on Ω, *cf.*, [35]. The Banach space $\mathrm{L}^\infty(w,\Omega)$ is similarly equipped with the norm $\|f\|_{\mathrm{L}^\infty(w,\Omega)}$ defined by taking the essential supremum [35] of the function $w|f|$. Then, the spaces defined above satisfy the following inclusions

$$C^{0,\alpha}(\Omega) \subset C(\Omega) \subset \mathrm{L}^p(w,\Omega), \tag{13}$$

where $0 < \alpha < 1$ and $1 \le p \le \infty$.

3. Sum rules

One of the most important properties satisfied by the class of Herglotz functions are the, so-called, *sum-rule identities* [5, Thm. 4.1] and [1]. These identities relate weighted integrals of the imaginary part of a Herglotz function, via the moments of its representing measure, to the coefficients of the asymptotic expansion of the function at the points zero and infinity.

The asymptotic expansions we are interested in are always taken with respect to non-tangential limits in a Stoltz domain. A Stoltz domain with parameter $\theta \in (0, \frac{\pi}{2}]$ is the angular domain

$$\{z \in \mathbb{C}^+ \mid \theta < \mathrm{Arg}(z) < \pi - \theta\}. \tag{14}$$

As such, the limits $z \hat{\to} 0$ (resp. $z \hat{\to} \infty$) denotes that the limit $z \to 0$ (resp. $|z| \to \infty$) is taken in any Stoltz domain as above.

Consider now the following definitions.

Definition 3.1 *Let q be a quasi-Herglotz function. We say that q admits, at $z = 0$, an* asymptotic expansion of order $M \ge -1$ *if there exist real numbers $a_{-1}, a_0, a_1, \ldots, a_M$ such that q can be written as*

$$q(z) = \frac{a_{-1}}{z} + a_0 + a_1 z + \ldots + a_M z^M + o(z^M) \qquad \text{as} \quad z \hat{\to} 0. \tag{15}$$

Definition 3.2 *Let q be a quasi-Herglotz function. We say that q admits, at $z = \infty$, an* asymptotic expansion of order $K \ge -1$ *if there exist real numbers $b_1, b_0, b_{-1}, \ldots, b_{-K}$ such that q can be written as*

$$q(z) = b_1 z + b_0 + \frac{b_{-1}}{z} + \ldots + \frac{b_{-K}}{z^K} + o\left(\frac{1}{z^K}\right) \qquad \text{as} \quad z \hat{\to} \infty. \tag{16}$$

At $z = 0$, an expansion of order $M = -1$ always exists for any quasi-Herglotz function q, as it always exists for any two Herglotz functions h_1 and h_2, *cf.*, [5, 24], yielding that

$$\lim_{z \hat{\to} 0} z\, q(z) = -\sigma(\{0\}), \tag{17}$$

where the measure σ is as in representation (7). Similarly, at $z = \infty$, an expansion of order $K = -1$ always exists for any quasi-Herglotz function q, as it always exists for any two Herglotz functions h_1 and h_2, *cf.*, [5, 24], yielding that

$$\lim_{z \hat{\to} \infty} \frac{q(z)}{z} = b, \tag{18}$$

where the number b is as in representation (7). Furthermore, the number b equals the number b_1 appearing in Definition 3.2.

We may now derive the following sum-rule theorem.

Theorem 3.1 *The following two statements hold.*

(i) Let $q = h_1 - h_2$ be a quasi-Herglotz function, such that at least one of the functions h_1 and h_2 admits, at $z = 0$, an asymptotic expansion (15) of some order $M \geq -1$. Then, for some integer $N_0 \geq 1$, the limit

$$\lim_{\varepsilon \to 0^+} \lim_{y \to 0^+} \int\limits_{\varepsilon < |x| < \frac{1}{\varepsilon}} x^{-2N_0} \mathrm{Im}\{q(x + \mathrm{i}y)\}\mathrm{d}x \tag{19}$$

exists as a finite number if and only if the function q admits, at $z = 0$, an asymptotic expansion (15) of order $2N_0 - 1 \leq M$.

(ii) Let $q = h_1 - h_2$ be a quasi-Herglotz function, such that at least one of the functions h_1 and h_2 admits, at $z = \infty$, an asymptotic expansion (16) of some order $K \geq -1$. Then, for some integer $N_\infty \geq 0$, the limit

$$\lim_{\varepsilon \to 0^+} \lim_{y \to 0^+} \int\limits_{\varepsilon < |x| < \frac{1}{\varepsilon}} x^{2N_\infty} \mathrm{Im}\{q(x + \mathrm{i}y)\}\mathrm{d}x \tag{20}$$

exists as a finite number if and only if the function q admits, at $z = \infty$, an asymptotic expansion (16) of order $2N_\infty + 1 \leq K$.

Furthermore, the identities

$$\lim_{\varepsilon \to 0^+} \lim_{y \to 0^+} \frac{1}{\pi} \int_{\varepsilon < |x| < \frac{1}{\varepsilon}} x^k \mathrm{Im}\{q(x + \mathrm{i}y)\}\mathrm{d}x = \begin{cases} a_{-k-1}, & -2N_0 \leq k \leq -3, \\ a_{-k-1} - b_{-k-1}, & -2 \leq k \leq 0, \\ -b_{-k-1}, & 1 \leq k \leq 2N_\infty \end{cases} \tag{21}$$

are valid

- *for $k = -2N_0, -2N_0 + 1, \ldots, -2$ if there exists an integer N_0 satisfying statement (i),*
- *for $k = 0, 1, \ldots, 2N_\infty$ if there exists an integer N_∞ satisfying statement (ii),*
- *for $k = -1$ if there exist integers N_0 and N_∞ satisfying statements (i) and (ii), respectively.*

In formula (21), the numbers $a_{-1}, a_0, a_1, \ldots, a_{2N_0-1}$ are as in Definition 3.1 and the numbers $b_{-1}, b_{-2}, \ldots, b_{-(2N_\infty+1)}$ are as in Definition 3.2.

Proof 3.1 *In the case of statement (i), we may, without loss of generality, assume that, if we write $q = h_1 - h_2$, it is the function h_2 that admits, at $z = 0$, an asymptotic expansion (15) of some order $M \geq -1$.*

Then, it follows from e.g., [5, Thm. 4.1], that the limit (19) exists and, moreover, that the sum rules identities (21) hold for the function h_2 for all k between $-M-1$ and -2. Thus, the existence of the limit (19) is equivalent to the existence of the limit

$$\lim_{\varepsilon \to 0^+} \lim_{y \to 0^+} \int\limits_{\varepsilon < |x| < \frac{1}{\varepsilon}} x^{-2N_0} \mathrm{Im}\{h_1(x + \mathrm{i}y)\} \mathrm{d}x. \tag{22}$$

and the existence of an asymptotic expansion of the function q of the form (15) is equivalent to the existence of an analogous expansion of the function h_1. Statement (i) is then established by applying the sum-rule for the function h_1, namely [5, Thm. 4.1].

The proof of statement (ii) follows an analogous reasoning.

Remark 3.3 *For $q = h_1 - h_2$, the requirement of statement (i) in Theorem 3.1 will certainly be satisfied if the representing measure of at least one of the functions h_1 or h_2 has support that does not include the point zero. Similarly, the requirement of statement (ii) in Theorem 3.1 will certainly be satisfied if the representing measure of at least one of the functions h_1 or h_2 has compact support.*

Remark 3.4 *If, in Theorem 3.1, we have a function $q \in \mathcal{Q}_{\mathrm{sym}}$, all integrals with odd powers k on the left-hand side of identity (21) are zero due to the symmetry of the measure. Furthermore, for even powers k, these integrals may be written as*

$$\lim_{\varepsilon \to 0^+} \lim_{y \to 0^+} \frac{2}{\pi} \int_{\varepsilon}^{\varepsilon^{-1}} x^k \mathrm{Im}\{q(x + \mathrm{i}y)\} \mathrm{d}x. \tag{23}$$

Remark 3.5 *Theorem 3.1 cannot be formulated for arbitray quasi-Herglotz functions. Examples show that it even does not hold for all meromorphic quasi-Herglotz functions, e.g., it can be shown that the quasi-Herglotz function $q(z) := \tan(z) - \mathrm{i}$ admits, at $z = \infty$, an asymptotic expansion of order $K = 0$, but there exists no integer N_∞ that would fulfill statement (ii) of Theorem 3.1.*

4. Approximation and optimization based on quasi-Herglotz functions

In this section, we derive the rationale for employing convex optimization as a tool to approximate a given continuous function defined on a compact approximation domain by certain quasi-Herglotz functions. The approximating quasi-Herglotz functions are first restricted to a certain subspace characterized by a particular requirement regarding their Hölder continuity on the approximation domain. Then it is shown that a smaller set of quasi-Herglotz functions generated by finite B-spline expansions (suitable for convex optimization) is dense in the larger space of Hölder continuous quasi-Herglotz functions in the topology induced by any L^p-norm. In essence, this development constitutes a straightforward, but very important extension of previous results derived for Herglotz functions [22].

4.1. Approximation theory based on quasi-Herglotz functions

To make the statements given above precise, we fix the approximation domain $\Omega \subset \mathbb{R}$ as a finite union of closed and bounded intervals on the real axis.

With a finite B-spline expansion we refer to a finite linear combination of B-splines of any order $m \geq 2$. A B-spline of order m is a compactly supported positive basis spline function which is piecewise polynomial of order $m-1$, *i.e.*, linear, quadratic, cubic, etc., and which is defined by $m+1$ break-points as described in *e.g.*, [10, 11]. With a finite uniform B-spline expansion we refer to a finite B-spline expansion with equidistant break-points.

The following definitions and theorems are similar as in [22] but extended to the current situation with quasi-Herglotz functions. Let Ω be given as above and let $w > 0$ denote a positive continuous weight function, and let $0 < \alpha < 1$, $1 \leq p \leq \infty$ and $m \geq 2$.

Definition 4.1 *Let $W^{\alpha,p}(w,\Omega) \subset L^p(w,\Omega)$ denote the subspace of all complex-valued functions $q \in C^{0,\alpha}(\Omega)$ with the following property: There exists a quasi-Herglotz function that has a Hölder continuous (with exponent α) extension to the closure of some neighboorhood $\mathcal{O}$ of Ω which coincides with q on Ω.* □

Note that we consider $W^{\alpha,p}(w,\Omega)$ as a subspace of $L^p(w,\Omega)$ and hence equipped with the topology from $L^p(w,\Omega)$.

Remark 4.2 *If it is clear from the context, in the following, we denote by q the quasi-Herglotz function as well as the extension to $\mathbb{C}^+ \cup \mathcal{O}$ and its restriction to Ω.*

Definition 4.3 *Let $W^{m,p}(w,\Omega) \subset W^{\alpha,p}(w,\Omega)$ denote the subspace of those functions for which the measure β (in (11)) of the quasi-Herglotz function q in Definition 4.1 is absolutely continuous with density β' that is a finite uniform B-spline expansion of order m.* □

Note that the sets $W^{\alpha,p}(w,\Omega)$ and $W^{m,p}(w,\Omega)$ are independent of p and w, but are equipped with the topology of $L^p(w,\Omega)$.

Remark 4.4 *The measure β is a non-finite Borel measure and can be represented in terms of the finite measure σ as described in Section 2.3.*

The following Theorem is a straightforward generalization of [22, Theorem 3.2] to the situation of quasi-Herglotz functions instead of Herglotz functions.

Theorem 4.5 *The subspace $W^{m,p}(w,\Omega)$ is dense in $W^{\alpha,p}(w,\Omega)$ with respect to the topology of $L^p(w,\Omega)$.* ■

Proof 4.1 *Let $\varepsilon > 0$ and let a function $q \in W^{\alpha,p}(w,\Omega)$ be given. Since both the positive and the negative part of a real valued Hölder continuous function are again Hölder continuous it follows that q can be written as $q = h_1 - h_2$ with functions h_1 and h_2 belonging to the convex cone $V^{\alpha,p}(w,\Omega)$, similar to $W^{\alpha,p}(w,\Omega)$ but generated by extensions of* Herglotz functions *rather than quasi-Herglotz functions. Then Theorem 3.2 in [22, pp. 11-14] implies that there exist functions $\widetilde{h}_1$ and $\widetilde{h}_2$ belonging to the convex cone $W^{m,p}(w,\Omega)$ such that $\|\widetilde{h}_i - h_i\|_{\mathrm{L}^p(w,\Omega)} < \frac{\varepsilon}{2}$ for $i = 1,2$. Hence for $\widetilde{q} := \widetilde{h}_1 - \widetilde{h}_2 \in W^{m,p}(w,\Omega)$ it holds $\|\widetilde{q} - q\|_{\mathrm{L}^p(w,\Omega)} < \varepsilon$, which finishes the proof.*

Definition 4.6 *Let $F \in C(\Omega)$ and consider the problem to approximate F based on the set of functions $q \in W^{\alpha,p}(w,\Omega)$. The greatest lower bound on the approximation error over the subspace $W^{\alpha,p}(w,\Omega)$ is defined by*

$$d := \inf_{q \in W^{\alpha,p}(w,\Omega)} \|q - F\|_{\mathrm{L}^p(w,\Omega)}. \tag{24}$$

□

Note that the distance d depends on the chosen topology of $\mathrm{L}^p(w,\Omega)$, but is independent of the Hölder exponent α, *cf.*, [22]. The following theorem demonstrates the usefulness of employing finite B-spline expansions in the associated approximation problem.

Theorem 4.7 *The greatest lower bound on the approximation error defined in (24) is given by*

$$d = \inf_{q \in W^{m,p}(w,\Omega)} \|q - F\|_{\mathrm{L}^p(w,\Omega)}. \tag{25}$$

■

The theorem is a straightforward consequence of Theorem 4.5 together with an application of the triangle inequality. It is noted that the distance d is independent of the Hölder exponent α as well as of the spline order m, *cf.*, [22]. The following obvious corollary can be used when the measure of the approximating quasi-Herglotz function contains a set of point masses. Such cases will be discussed in Sections 44.2 and 5.

Corollary 4.8 *Let $W(w,\Omega) \subset W^{\alpha,p}(w,\Omega)$ be a set which contains $W^{m,p}(w,\Omega)$. Then, $W(w,\Omega)$ is dense in $W^{\alpha,p}(w,\Omega)$ and it holds that*

$$d = \inf_{q \in W(w,\Omega)} \|q - F\|_{\mathrm{L}^p(w,\Omega)}. \tag{26}$$

4.2. Convex optimization with B-splines

The significance of the Theorems 4.5 and 4.7 is that B-spline expansions [9–11], which are well suited for numerical optimization [6, 14, 22], can be used to approximate a given continuous function F with arbitrary small deviation from the greatest lower bound defined in (24). A detailed description of the associated convex optimization problem is given as follows.

Let the approximation domain Ω, the taget function $F \in C(\Omega)$ and the weight function $w \in C(\Omega)$ be given as above, and let $0 < \alpha < 1$, $1 \leq p \leq \infty$ and $m \geq 2$. As approximating functions we can use functions q from a set $W(w,\Omega)$ defined by the following representations

$$q(x) = a + bx + \sum_{i=1}^{M} \frac{p_i}{\xi_i - x} + \text{p.v.} \int_{-\infty}^{\infty} \left(\frac{1}{\xi - x} - \frac{\xi}{1+\xi^2} \right) \beta'(\xi) \mathrm{d}\xi + \mathrm{i}\pi\beta'(x) \tag{27}$$

$$= \breve{a} + bx + \sum_{i=1}^{M} \frac{p_i}{\xi_i - x} + \text{p.v.} \int_{-\infty}^{\infty} \frac{1}{\xi - x} \beta'(\xi) \mathrm{d}\xi + \mathrm{i}\pi\beta'(x) \tag{28}$$

for $x \in \Omega$, and where the second part of the integral in (27) has been absorbed into the constant $\breve{a}$ in (28). In (27) and (28) the density β' is a finite uniform B-spline expansion as in Definition 4.3, 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. It is noted that the set $W(w,\Omega)$ satisfies the condition $W^{m,p}(w,\Omega) \subset W(w,\Omega) \subset W^{\alpha,p}(w,\Omega)$ of Corollary 4.8.

In particular, we employ here B-spline basis functions $p_n(x)$ of fixed polynomial order $m-1$ for $n = 1, \ldots, N$, where N is the number of B-splines, and $\hat{p}_n(x)$ the (negative) Hilbert transform [25] of the B-spline functions. Explicit formulas for general uniform as well as non-uniform B-splines and their Hilbert transforms are given in [21, Section 3.1]. Let $q_N \in W$ denote approximating functions represented as in (28), and hence

$$\mathrm{Im}\{q_N(x)\} = \pi\beta'(x) = \sum_{n=1}^{N} c_n p_n(x), \tag{29}$$

and

$$\mathrm{Re}\{q_N(x)\} = \breve{a} + bx + \sum_{i=1}^{M} \frac{p_i}{\xi_i - x} + \sum_{n=1}^{N} c_n \hat{p}_n(x), \tag{30}$$

for $x \in \Omega$, and where c_n are the corresponding B-spline expansion coefficients. Note that all the parameters $\breve{a}$, 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. It is further assumed that the support of q_N grows with N at the same time as the distance δ between breakpoints decreases, *e.g.*, as $|\mathrm{supp}\{q_N\}| = \sqrt{N}$ and $\delta = |\mathrm{supp}\{q_N\}|/N = 1/\sqrt{N}$. For a fixed N, the minimization of the norm of the approximation error $\|q_N - F\|_{\mathrm{L}^p(w,\Omega)}$ is a finite-dimensional convex optimization problem over the real parameters $\breve{a}$, b, p_i and c_n, and we denote the optimal value d_N. The important implication of Theorem 4.7 and Corollary 4.8 is that $d_N \to d$ as $N \to \infty$. Finally, it is noted that for a numerical implementation using *e.g.*, the CVX Matlab software for disciplined convex programming [14] the calculation of the norm above must be approximated based on a finite set of sample points in Ω. However, due to the uniform continuity of all functions involved, this can, in principle, be done within arbitrary numerical accuracy.

Now that we have established the rationale for using numerical convex optimization as a tool for approximating a given continuous function based on the set of quasi-Herglotz functions, we can also expand the setting by incorporating any additional convex constraints of interest, see also [20, 31, 32]. For example we can incorporate upper and lower bounds on the density β' stated as

$$\begin{aligned} &\text{minimize} && \|q - F\|_{\mathrm{L}^p(w,\Omega)} \\ &\text{subject to} && b_{\text{lower}}(x) \leq \beta'(x) \leq b_{\text{upper}}(x), \end{aligned} \tag{31}$$

where the optimization is over $q \in W(w,\Omega)$ and b_{lower} and b_{upper} are suitable functions. Note that these functions can be used for constraining the density $\beta'(x)$ outside of Ω to prevent non-physical oscillatory behavior of the resulting function outside of the approximation domain. Also, these constraints are useful in regularization of the low-frequency behavior of materials, see the numerical examples in Section 5.2. In practice, this might for instance amount to solving for $q_N \in W(w,\Omega)$

$$\begin{aligned} &\text{minimize} && \|q_N - F\|_{\mathrm{L}^p(w,\Omega)} \\ &\text{subject to} && \theta_{\text{lower},j} \leq \theta_j \leq \theta_{\text{upper},j}, \quad j \in J, \end{aligned} \tag{32}$$

where N is fixed, J is a finite index set, and the vector θ may consist of any of the parameters $\theta_j \in \{\check{a}, b,\ p_1, \ldots, p_M, c_1, \ldots, c_N\}$, for $j \in J$.

When a priori information is available about the asymptotic properties of a given non-passive system to be approximated and which admits the sum rules discussed in Section 3, the identities (21) can be involved in an optimization (31) as an additional convex constraint. Due to the finite-dimensional approximation (29), the left-hand side of (21) becomes

$$\lim_{\varepsilon\to 0^+}\lim_{y\to 0^+}\frac{1}{\pi}\int_{\varepsilon<|x|<\frac{1}{\varepsilon}} x^k \mathrm{Im}\{q(x+\mathrm{i}y)\}\mathrm{d}x = \lim_{\varepsilon\to 0^+}\frac{1}{\pi}\sum_{n=1}^{N} c_n \int_{\varepsilon<|x|<\frac{1}{\varepsilon}} x^k p_n(x)\mathrm{d}x, \tag{33}$$

for even $k = -2N_0, \ldots, 2N_\infty$, see Theorem 3.1, and which can be employed as an additional constraint in the optimization formulation (32).

5. Numerical examples

In the numerical examples presented below, non-passive approximation is employed as a tool to determine optimal realizations (in the sense of a mathematical representaion) of non-passive metamaterials with dielectric permittivity ϵ, where $\mathrm{Im}\{\epsilon\}$ can be negative over some frequency intervals. The target functions to be approximated are symmetric, and hence, we employ symmetric quasi-Herglotz functions to solve the convex optimization problems.

The symmetry property affects the representation (28), and hence the term $\check{a} = 0$, and we can take into account the contribution from the negative part of the real axis in an explicit manner. Consequently, the real and the imaginary parts of the approximating functions q_N become

$$\mathrm{Re}\{q_N(x)\} = bx + \frac{p_0}{-x} + \sum_{i=1}^{M} p_i\left(\frac{1}{\xi_i - x} - \frac{1}{\xi_i + x}\right) + \sum_{n=1}^{N} c_n\left[\hat{p}_n(x) - \hat{p}_n(-x)\right], \tag{34}$$

and

$$\operatorname{Im}\{q_N(x)\} = \sum_{n=1}^{N} c_n \left[p_n(x) + p_n(-x)\right], \tag{35}$$

respectively, where p_0 denotes the amplitude of the point mass located at 0.

In the following numerical examples, the dielectric permittivity functions ϵ are considered as functions of a dimensionless real-valued normalized frequency x corresponding to an angular frequency ω in rad/s. For simplicity and since the approximants $q(x)$ and $q_N(x)$ in (31) and (32) are conjugate symmetric on $\mathbb{R}$ we will consider only a "right-sided" approximation domain $\Omega \subset \mathbb{R}^+$.

5.1. Passive and non-passive approximation of metamaterials

A typical application example of the present non-passive approximation formulation (26) concerns physical bounds on passive or non-passive metamaterials. In this first example, we consider both passive and non-passive approximations of the same target function (which is not a Herglotz function) and compare the obtained results.

First, consider the case with passive approximation of metamaterials (which are described in [16]), and note that the case with passive systems and passive approximation based on Herglotz functions as in [22] constitutes a special case of the present non-passive approximation based on the representations (34) and (35), with $b_{\text{lower}} = 0$ in (31), this is $\beta'(x) \geq 0$ for all x. Hence, an interesting canonical example for which (24) gives a non-trivial lower bound is with the passive approximation of a negative symmetric Herglotz function $F = -h_0$, which can be Hölder continuously extended to $\mathbb{C}^+ \cup \Omega$, and which has the large-argument asymptotics $h_0(z) = b_1^0 z + o(z)$ as $z \hat{\to} \infty$. Based on the theory of Herglotz functions and associated sum rules [5], it can be shown that

$$\|h - F\|_\infty \geq (b_1 + b_1^0)\frac{1}{2}|\Omega|, \tag{36}$$

for all Herglotz functions h with large-argument asymptotics $h(z) = b_1 z + o(z)$ as $z \hat{\to} \infty$, see [16, 22]. Here, $|\Omega|$ is the length of the interval Ω.

For a passive metamaterial, a dielectric permittivity function $\epsilon(z)$ is considered, where $h(z) = z\epsilon(z)$ is the associated symmetric Herglotz function [16]. The high-frequency permittivity of the metamaterial is assumed to be given by ϵ_∞, and hence $b_1 = \epsilon_\infty$. A real-valued and constant target permittivity $\epsilon_{\text{t}} < 0$ is given over the approximation interval Ω with $\Omega = [1 - B/2, 1 + B/2]$, where the center frequency of Ω is equal to 1, B the relative bandwidth, $0 < B < 2$, and hence $F(x) = x\epsilon_{\text{t}}$ with $h_0(z) = -z\epsilon_{\text{t}}$, and $b_1^0 = -\epsilon_{\text{t}}$. Now, by using (36) the resulting physical bound can thus be obtained as

$$\|\epsilon - \epsilon_{\text{t}}\|_\infty = \|h - F\|_{\mathrm{L}^\infty(w,\Omega)} \geq \frac{\|h - F\|_\infty}{1 + B/2} \geq \frac{(\epsilon_\infty - \epsilon_{\text{t}})B}{2 + B} =: \Delta, \tag{37}$$

see also [16, 22]. Note that here $\|\epsilon - \epsilon_{\text{t}}\|_\infty = \|h - F\|_{\mathrm{L}^\infty(w,\Omega)}$, where the weight function is $w(x) = 1/x$ for $x \in \Omega$, with $0 \notin \Omega$, and where Δ is the resulting physical bound.

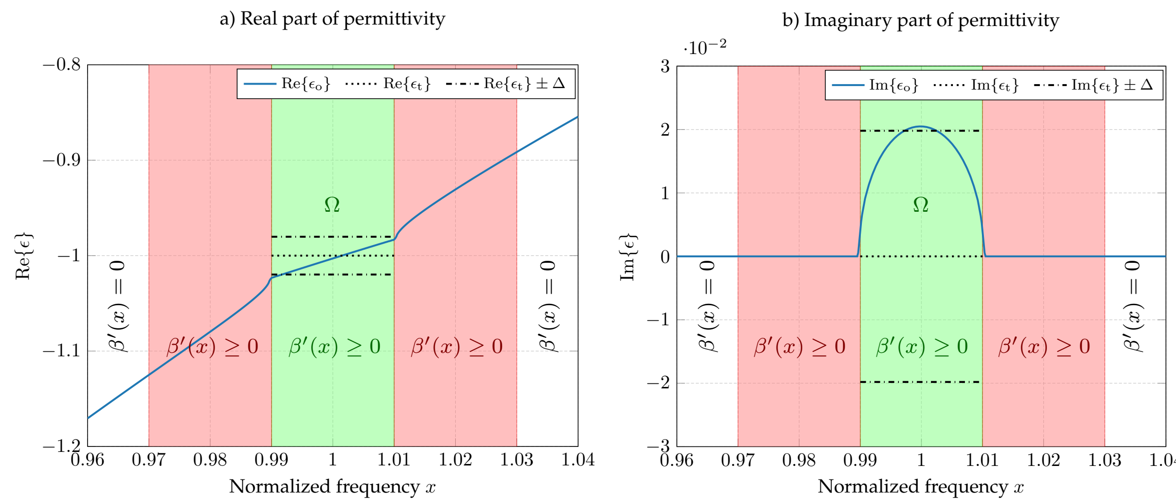

Figure 1. Real and imaginary part of the optimal passive permittivity function approximating a metamaterial with $\epsilon_{\mathrm{t}} = -1$.

Figure 1 shows the result of an optimization (32) for the target function F defined as for (37) over the approximation domain $\Omega = [1 - B/2, 1 + B/2]$, $B = 0.02$, $\epsilon_{\mathrm{t}} = -1$, and $\epsilon_\infty = 1$. In this passive approximation problem, the support of the generating measure $\mathrm{supp}\{\beta\} \cap \mathbb{R}^+$ is contained in $\{0\} \cup [0.97, 1.03]$ including one positive point mass with amplitude p_0 at the origin, and the lower bound for the density β' is constrained to be zero, *i.e.*, $\beta'(x) \geq 0$. The optimization is carried out using $N = 100$ uniform linear B-splines (of order $m = 2$). The real and imaginary parts of the resulting optimal permittivity function ϵ_{o} are shown in Figures 1a and 1b, respectively, together with a comparison with the fundamental sum-rule-bound limits $\epsilon_{\mathrm{t}} \pm \Delta$, where Δ is given in (37). Note that the resulting optimal solution ϵ_{o} intersects these limits because the target function ϵ_{t} cannot be approximated by Herglotz functions with error less than Δ as shown in (37). Interestingly, the optimal permittivity is, in principal, supported only on $\Omega = [0.99, 1.01]$, *i.e.*, the optimal solution for β' is approximately zero outside of the approximation domain Ω, except for the point mass $p_0 \approx 79.1$ at 0. It should be noted that the point mass at the origin contributes with a response at frequencies $x \neq 0$, which is very similar to that of a Drude model with sufficiently large relaxation time τ so that $x\tau \gg 1$.

Secondly, we consider an optimization problem, where the approximating functions are not restricted to Herglotz functions, but to quasi-Herglotz functions. For such a non-passive case, Figure 2 shows the corresponding optimization results for the constrained $\beta'(x) = 0$ over $\Omega = [0.99, 1.01]$ (letting $\beta'(x) \geq 0$ over Ω gives negligible deviation from the optimal solution shown in Figure 2), $\beta'(x) \geq 0$ on the frequency set $I_1 = \{0\}$ that includes only a positive point mass with amplitude p_0 at 0, and $\beta(x) \leq 0$ on the frequency set $I_2 = [0.97, 0.99) \cup (1.01, 1.03]$. In this optimization, we used $N = 100$ linear B-splines which is sufficient to achieve an approximation error in the order of magnitude 10^{-6}. In this case, the resulting point mass at the origin is essentially the

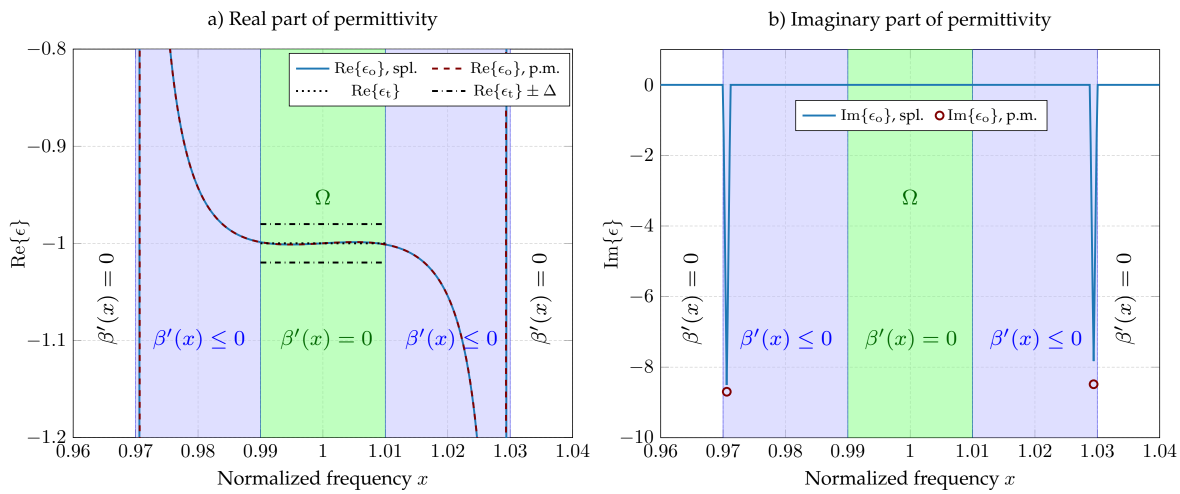

Figure 2. Real and imaginary parts of the optimal non-passive permittivity function approximating a metamaterial with $\epsilon_{\mathrm{t}} = -1$.

same as before with $p_0 \approx 79.1$, but the support of q_N over I_2 becomes concentrated to the outermost endpoints of the set. This seems to suggest that two point masses with amplitudes p_1 and p_2 located at the two outermost end points $\xi_1 = x_{\mathrm{l}}$ (lower endpoint) and $\xi_2 = x_{\mathrm{u}}$ (upper endpoint) of I_2 should be sufficient for the optimization. Hence, Figure 2, also includes optimization results where the measure β consists solely of these two point masses with positive amplitudes p_1 and p_2, together with the original point mass at 0 with amplitude p_0. Note that the corresponding two curves in Figure 2a (blue solid line and dark-red dashed lines) coincide and are hardly distinguishable. Note as well that the optimal solution ϵ_{o} does not intersect the sum-rule-bound limits $\epsilon_{\mathrm{t}} \pm \Delta$ as it fits well the target permittivity ϵ_{t} over the approximation domain. Figure 2b also shows the optimized point masses $p_1 \approx -8.7$ and $p_2 \approx -8.48$ (indicated by the dark-red "o") normalized to the same area as the corresponding linear B-spline basis functions. The example illustrates that by using quasi-Herglotz functions, it is possible under certain circumstances to obtain a much better realization of the target permittivity ϵ_{t} over the approximation interval with smaller approximation error, than by using only Herglotz functions compare the results in Figures 2a and 1a, respectively. This phenomenon is further investigated below.

Finally, Figure 3 shows how the optimal approximation error $\|\epsilon - \epsilon_{\mathrm{t}}\|_\infty$ depends on the assumed a priori point mass at normalized frequency x_{u} where the lower point mass at normalized frequency x_{l} is mirrored accordingly as $x_{\mathrm{l}} = 1 - (x_{\mathrm{u}} - 1)$, and the optimization is done solely over the three point masses with amplitudes p_0 (which is located at 0), p_1 and p_2. It can be concluded that the passive approximation is more restrictive in comparison with the non-passive approximation. The non-passive approximation provides a good agreement between the target and the optimal solution based on a sequence of quasi-Herglotz functions, in particular when the placement of the point masses p_1 and p_2 is located more than 2% away from the center normalized

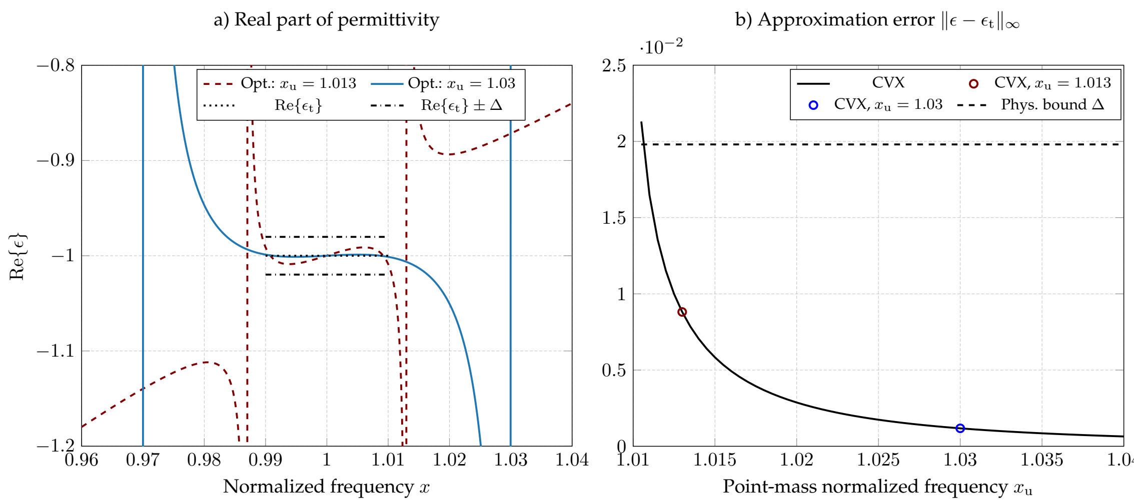

Figure 3. a) Real part of the non-passive permittivity function optimized with point masses only; b) Approximation error as a function of upper point mass normalized frequency x_u (the normalized frequency of lower point mass is $x_l = 1 - (x_u - 1)$).

frequency of the approximation domain Ω at $x = 1$, see the approximation error in Figure 3b.

5.2. Non-passive approximation of metamaterials with a priori known low-frequency behavior

In the following numerical examples, a constriction of the optimization (31) is studied with application to non-passive approximation of metamaterials. Here, we are interested in determination of optimal permittivities with controlled low- and high-frequency behavior. To achieve such realizations, we can put additional information about low- and high-frequency limits of the desired permittivity function $\epsilon(x)$ to the optimization problem (31) in the form of sum rule (21).

Given the continuous symmetric target function F, a convex optimization problem [6] related to the constriction of (32) is now formulated with an additional convex constraint obtained from (33) for $k = -2$ as

$$\lim_{\varepsilon\to 0^+} \frac{1}{\pi} \int_{\varepsilon<|x|<\frac{1}{\varepsilon}} \frac{\mathrm{Im}\{q(x)\}}{x^2} \mathrm{d}x = a_1 - b_1 = \epsilon_s - \epsilon_\infty, \tag{38}$$

where $a_1 = \epsilon_s$ and $b_1 = \epsilon_\infty$ denote the a priori static and instantaneous responses of the dielectric material, respectively. Here, F is the same as in Section 5.1, which is given to be a real constant over the finite interval $\Omega = [1 - B/2, 1 + B/2]$, $0 < B < 2$. Note that $b_1 = \epsilon_\infty$ coincides with b in the representation (28) of the approximating quasi-Herglotz function.

Figures 4a-b show the corresponding optimization results for $p_0 = 0$, and when the density $\beta'(x) = 0$ over the approximation domain $\Omega = [0.9, 1.1]$ (the results for $\beta'(x) \geq 0$ have negligible deviation), $\beta'(x) \geq 0$ on the set I_1 consisting of $[0.01, 0.9) \cup (1.5, 2]$, and $\beta'(x) \leq 0$ on the set $I_2 = (1.1, 1.5]$, with no a priori point masses. For this optimization,

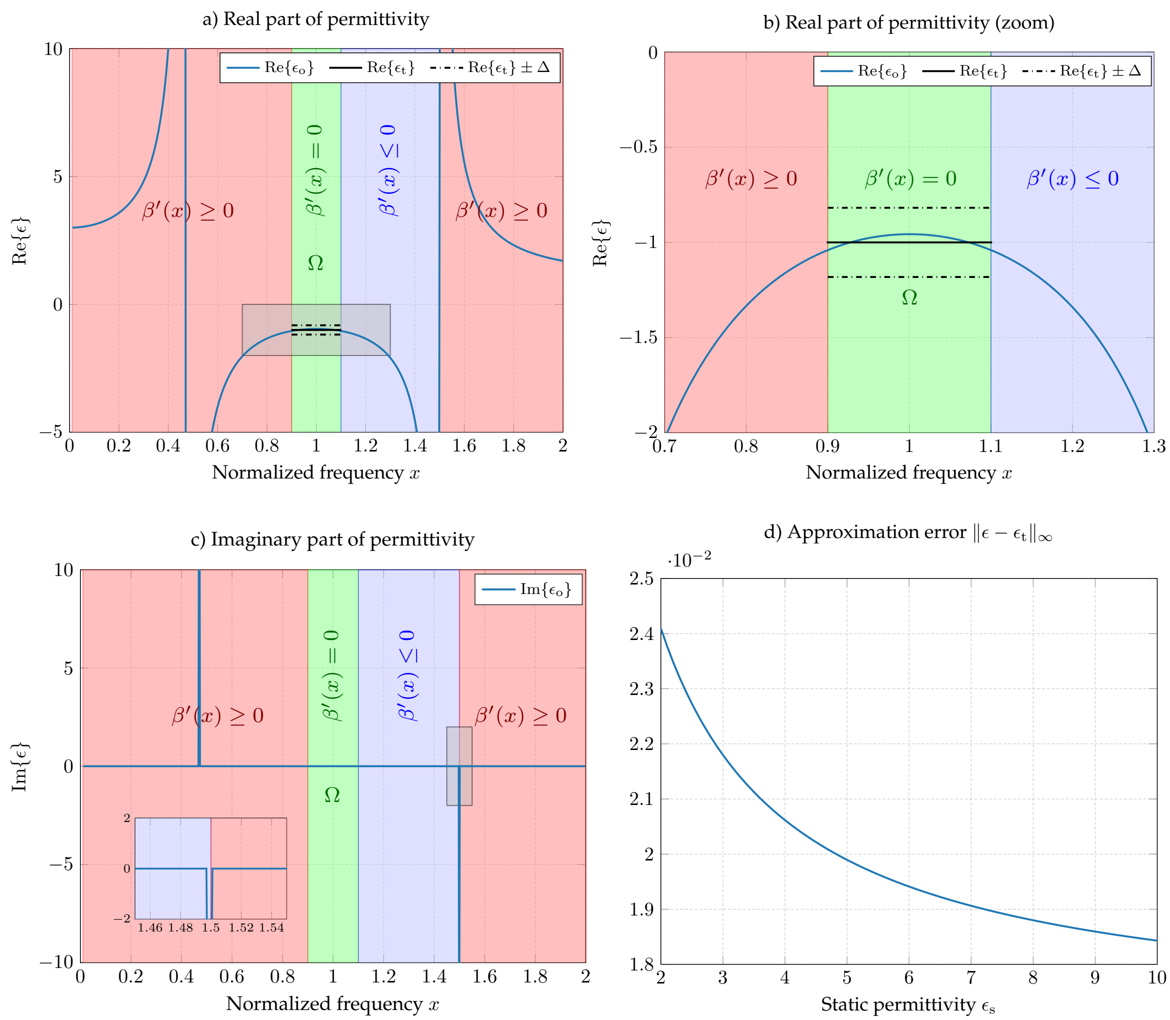

Figure 4. a-c) Real and imaginary parts of the optimal non-passive permittivity function approximating a metamaterial with $\epsilon_{\mathrm{t}} = -1$, $\epsilon_{\mathrm{s}} = 3$, and $\epsilon_{\infty} = 1$. The zoomed-in region in a) is depicted in b); d) Approximation error plotted as a function of the static permittivity ϵ_{s}.

$B = 0.2$, and $N = 1000$ linear B-splines were used due to increased optimization domain (for regularity of low-frequency behavior of the desired function), which is sufficient for an accurate solution.

The obtained optimization result shows a good realization of the target function $\epsilon_{\mathrm{t}} = -1$ over the approximation domain Ω, see Figure 4b. The approximation error $\|\epsilon - \epsilon_{\mathrm{t}}\|_{\infty} = 4.3 \cdot 10^{-2}$ is much less than the sum-rule bound for passive case (37) $\Delta = 0.182$, and hence the optimal solution ϵ_{o} fits the target permittivity over Ω. Also, it is interesting to note that the approximation of the permittivity function $\epsilon(x)$ satisfies the low-frequency limit $\epsilon_{\mathrm{s}} = 3$, see Figure 4a. Note that the same result can be achieved when the measure β consists of two point masses with amplitudes $p_1 \approx 989.9$ and $p_2 \approx -790.8$ placed at $\xi_1 = x_1 \approx 0.469$ and $\xi_2 = x_2 \approx 1.499$, respectively. In Figure 4d, the approximation error is shown as a function of the static permittivity

ϵ_s. It is interesting to note that the approximation error decreases as ϵ_s increases, and meanwhile, the location of the positive point mass p_1 moves towards 0. Hence, in the limit, when the point mass reaches 0, we obtain the non-passive case described in Section 5.1.

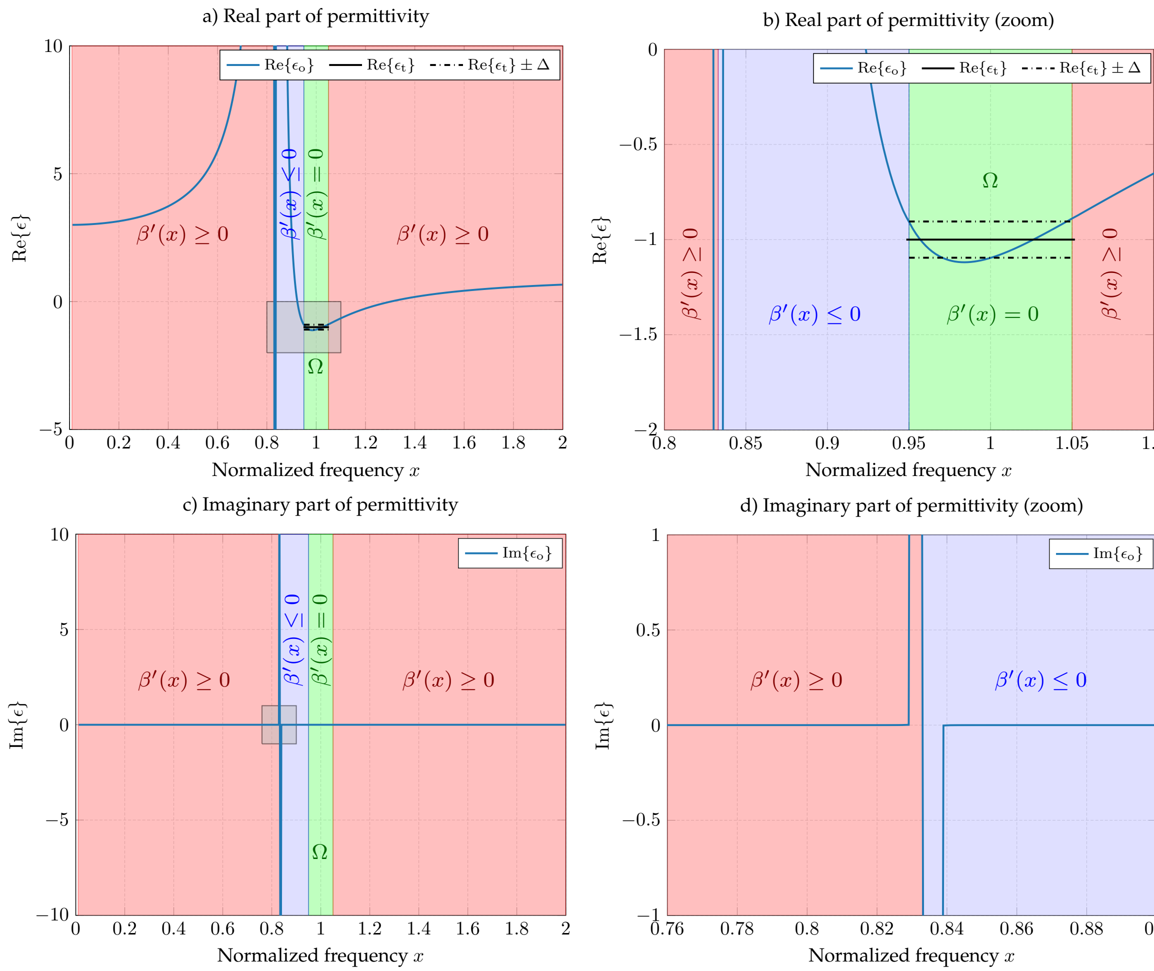

Figure 5. a-d) Real and imaginary parts of the optimal non-passive permittivity function approximating a metamaterial with $\epsilon_t = -1$, $\epsilon_s = 3$, and $\epsilon_\infty = 1$. The zoomed-in region in a) and c) are depicted in b) and d), respectively.

A variation of the last minimization problem is depicted in Figure 5. In this approximation problem, the constraint for the density $\beta'(x)$ over $\Omega = [0.95, 1.05]$ is the same as in the example given above, $\beta'(x) \geq 0$ on the set $I_1 = [0.01, 0.833) \cup (1.05, 2]$, and $\beta'(x) \leq 0$ on the set $I_2 = [0.833, 0.95)$, with no a priori point masses. We used $B = 0.1$, $N = 1000$ linear B-splines, and predefined the static and the instantaneous responses as $\epsilon_s = 3$ and $\epsilon_\infty = 1$ for this optimization. Interestingly, the approximation error $\|\epsilon - \epsilon_t\|_\infty = 0.24$ is larger than the sum-rule bound for passive case (37) is $\Delta = 0.095$. As a result, the resulting optimized permittivity ϵ_o intersects the sum-rule-bound limits $\epsilon_t \pm \Delta$, see Figure 5b. Such approximation result can also be obtained when the measure β consists of two point masses with amplitudes $p_1 \approx 4.69 \cdot 10^4$ and $p_2 \approx -4.57 \cdot 10^4$

placed at $\xi_1 = x_1 \approx 0.831$ and $\xi_2 = x_2 \approx 0.835$, respectively. Nevertheless, the interest of this example is in the double resonance observable around the normalized frequency $x = 0.833$, see Figures 5b and 5d. Such phenomenon takes place in non-linear optics and is called as dynamic Stark effect [29, Figure 5.2 on p. 63]. Hence, it can be concluded that for some cases we can achieve better approximation results with the passive approximation than with the non-passive one, that are sign restricted on certain intervals.

6. Conclusions

In this paper, the non-passive framework for a certain class of non-passive causal systems has been formulated. This has been done by introducing the class of quasi-Herglotz functions. We have showed that these functions can be described by an integral representation formula, similar to the one describing Herglotz functions, and we have examined some of its properties. Furthermore, we show that quasi-Herglotz functions admit, under certain additional constraints, sum-rule identities that generalize the known identities for Herglotz functions.

We also demonstrate that a family of B-splines can be used in the representation of approximating quasi-Herglotz functions, which is utilized in a number of numerical examples. It has been concluded that a very efficient mathematical representation of a non-passive metamaterial with $\epsilon_{\rm t} \approx -1$ (which is typical in plasmonic applications) can be achieved by choosing point masses representing the power excitation at certain frequencies outside of the approximation domain. A constricted problem for non-passive metamaterials with controlled low- and high-frequency responses shows that the sum-rule identities can be efficiently utilized in the realization of such permittivities with desired properties as a constraint for convex optimization problem (31).

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Appendix A. Notation

$\mathbb{R}$, $\mathbb{C}$	the sets of real numbers and complex numbers, respectively
$\mathbb{C}^+$	the upper half-plane, $\mathbb{C}^+ = \{z \in \mathbb{C} \mid \mathrm{Im}\{z\} > 0\}$
i	imaginary unit, $\mathrm{i}^2 = -1$
$z = x + \mathrm{i}y$	complex number with $x = \mathrm{Re}\{z\}$ and $y = \mathrm{Im}\{z\}$
z^*	complex conjugate, $(x + \mathrm{i}y)^* = x - \mathrm{i}y$
$\hat{\to}$	non-tangential limit
$(\cdot)_+$	highlights the fact that parameters with the corresponding underscore represent a function with non-negative imaginary part
α	Hölder exponent
m	the order of B-spline function, $m \geq 2$
c_n	B-spline expansion coefficient or optimization variable
h	a Herglotz function
q	a quasi-Herglotz function, or in $W^{\alpha,p}$ below
d	the distance function, the greatest lower bound
F	the target function
p_n	B-spline basis function
$\hat{p}_n$	the (negative) Hilbert transform of B-spline basis function
p_i	magnitude of a point-mass
w	weighting function
C	space of continuous functions
$C^{0,\alpha}$	space of Hölder continuous functions, $0 < \alpha < 1$
$\\| \cdot \\|_{\mathrm{L}^p(w)}$	the norm corresponding to the weighted Lebesgue L^p space, $w > 0$, $1 \leq p \leq \infty$
σ	finite positive Borel measure on $\mathbb{R}$, $\mathrm{d}\sigma(\xi) < \infty$
β	non-finite positive Borel measure, $\mathrm{d}\beta(\xi) = (1 + \xi^2)\mathrm{d}\sigma(\xi)$
β'	the Hölder continuous density of β on Ω, $\beta' \in C^{0,\alpha}$, $0 < \alpha < 1$
Ω	the approximation domain
$\mathcal{O}$	open neighborhood of Ω
$\mathcal{Q}$	set of all quasi-Herglotz functions
$\mathcal{Q}_{\mathrm{sym}}$	set of all symmetric quasi-Herglotz functions, $\mathcal{Q}_{\mathrm{sym}} \subseteq \mathcal{Q}$
$V^{\alpha,p}(w, \Omega)$	the set/convex cone of all complex-valued functions $h \in \mathrm{L}^p(w)$ that have a Hölder continuous (with exponent α) extension to the closure of some neighboorhood $\mathcal{O}$ of Ω such that h coincides on Ω with this extension, $0 < \alpha < 1$, $1 \leq p \leq \infty$
$W^{\alpha,p}(w, \Omega)$	the subspace of all complex-valued functions $q \in C^{0,\alpha}(\Omega)$ that have a Hölder continuous (with exponent α) extension to the closure of some neighboorhood $\mathcal{O}$ of Ω such that q coincides on Ω with this extension, $0 < \alpha < 1$

$W^{m,p}(w,\Omega)$	the subspace of those functions for which the measure β of the quasi-Herglotz function $q \in W^{\alpha,p}(w,\Omega)$ is absolutely continuous with density β' that is a finite uniform B-spline expansion of order m, $m \geq 2$
$W(w,\Omega)$	is defined analogously as $W^{m,p}$ with additional assumption that the measure of q contains a set of point masses, $W^{m,p}(w,\Omega) \subset W(w,\Omega) \subset W^{\alpha,p}(w,\Omega)$

Table A1: Table with the used notation.