Sum rules and physical bounds on passive metamaterials

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Abstract

Frequency dependence of the permittivity and permeability is inevitable in metamaterial applications such as cloaking and perfect lenses. In this paper, Herglotz functions are used as a tool to construct sum rules from which we derive physical bounds suited for metamaterial applications, where the material parameters are often designed to be negative or near zero in the frequency band of interest. Several sum rules are presented that relate the temporal dispersion of the material parameters with the difference between the static and instantaneous parameter values, which are used to give upper bounds on the bandwidth of the application. This substantially advances the understanding of the behavior of metamaterials with extraordinary material parameters, and reveals a beautiful connection between properties in the design band (finite frequencies) and the low- and high-frequency limit.

1 Introduction

The intriguing physics based on negative index of refraction [28] and \( \epsilon \)-near-zero materials [26] with applications such as the perfect lens [33] and cloaking [2, 24] has created a renewed interest in the fundamental properties of the interaction between electromagnetic fields and materials [14, 20, 32]. The ideal behavior of, e.g., the (relative) permittivity is that \( \epsilon(\omega) \approx \epsilon_m \) over a range of angular frequencies, where \( \epsilon_m \) is a real-valued number, e.g., \( \epsilon_m \approx -1 \) or \( \epsilon_m \approx 0 \), depending on the application [2, 26, 28, 33]. It is well known that the electromagnetic response of materials is temporally dispersive, i.e., it depends on frequency. The classical Kramers-Kronig relations [10, 13, 16] relate the frequency dependence of the real- and imaginary parts of the permittivity and the permeability for causal material models.

In metamaterial applications it is essential to consider realistic material models to obtain reliable and physically realizable results. Since engineered materials with very complex frequency dependence are often considered, it is not sufficient to analyze only Drude and Lorentz models if all potentials and restrictions of future metamaterials applications are to be evaluated.

Approaches based on the Hilbert transform or equivalently the Kramers-Kronig relations [10] are commonly used to derive bounds for causal material models. The investigation in [32] is one attempt to understand the constraints that causality puts on negative index of refraction materials. However, as illustrated in [18], it is difficult to derive absolute bounds from this approach due to the high sensitivity to losses at the evaluation frequency [14]. In [20, 27], it is also shown that there are no severe restrictions if just the condition of causality is employed. The results in [17] show that \( |\epsilon(\omega) - \epsilon_m| \geq B \), where \( \epsilon_m = -1 \) and \( B \) denotes the fractional bandwidth, if the additional assumption of passivity is used [13, 34].

In this paper, constraints on the constitutive relations based on the assumptions of causality and passivity are further analyzed. The analysis is for simplicity restricted to isotropic constitutive relations (with some extensions to bi-anisotropic media given in Sec. 4), that are characterized by their (relative) permittivity \( \epsilon \) and (relative) permeability \( \mu \). The results are given in Sec. 3 as several sum rules that
relate the instantaneous and static response of the material model with weighted integrals of the constitutive parameter over all spectrum. The integrals typically measure how close a material parameter \( \epsilon(\omega) \) can be to a target value \( \epsilon_m \) over a frequency interval. The sum rules can be expressed as bounds on the variation around the target value, and are somewhat different depending on the value of \( \epsilon_m \). Let \( \epsilon_s \) and \( \epsilon_\infty \) denote the limiting values of \( \epsilon(\omega) \) as \( \omega \to 0 \) and \( \omega \to \infty \), respectively. If \( \epsilon_\infty \leq \epsilon_m \leq \epsilon_s \), there is in principle no bandwidth limitation, but if \( \epsilon_m < \epsilon_\infty \), we derive the following bounds in sections 3.1 and 3.2 (where \( B = [\omega_1, \omega_2] \) is the frequency band, and \( B = (\omega_2 - \omega_1)/\omega_0 \) is the fractional bandwidth, writing \( \omega_0 = (\omega_2 + \omega_1)/2 \) for the center frequency):

\[
\max_{\omega \in B} |\epsilon(\omega) - \epsilon_m| \geq \frac{B/2}{1 + B/2} (\epsilon_\infty - \epsilon_m) \quad \text{(with or without static conductivity)} \quad (1.1)
\]

\[
\max_{\omega \in B} \frac{|\epsilon(\omega) - \epsilon_m|}{|\epsilon(\omega) - \epsilon_\infty|} \geq \frac{B/2}{1 + B/2} \frac{\epsilon_s - \epsilon_m}{\epsilon_s - \epsilon_\infty} \quad \text{(no static conductivity, i.e., an insulator)} \quad (1.2)
\]

If instead the target value is larger than the static value, i.e., \( \epsilon_m \geq \epsilon_s \), we derive the following bound in Sec. 3.3:

\[
\max_{\omega \in B} |\epsilon(\omega) - \epsilon_m| \geq \frac{B/2}{1 + B/2} \frac{\epsilon_m - \epsilon_s}{\epsilon_s - \epsilon_\infty} \quad (1.3)
\]

If the material is lossless in the frequency band of interest \( B = [\omega_1, \omega_2] \), the right hand sides should be multiplied by 2. The bounds can be tightened if a priori knowledge of the plasma frequency is added, see Sec. 3.4.

# 2 Theoretical background

## 2.1 Constitutive relations and Herglotz functions

We assume that the Maxwell equations in the time-domain can be used to model the interaction between the electromagnetic field and the material. The linear, causal, time translational invariant, continuous, and isotropic constitutive relations are [12]

\[
D(t) = \epsilon_0 \epsilon_\infty E(t) + \epsilon_0 \int_{\mathbb{R}} \chi_{ee}(t - t') E(t') \, dt'
\]

and

\[
B(t) = \mu_0 \mu_\infty H(t) + \mu_0 \int_{\mathbb{R}} \chi_{mm}(t - t') H(t') \, dt',
\]

where \( \chi_{ee}(t) = 0 \) and \( \chi_{mm}(t) = 0 \) for \( t < 0 \), the dependence of the spatial coordinates is suppressed, and \( \epsilon_0 \) and \( \mu_0 \) denote the free space permittivity and permeability, respectively. The material model is passive if

\[
0 \leq \int_{-\infty}^{T} E(t) \cdot \frac{\partial D(t)}{\partial t} \, dt = \epsilon_0 \int_{-\infty}^{T} \int_{\mathbb{R}} E(t) \cdot \frac{\partial}{\partial t} (\epsilon_\infty \delta(t - t') + \chi_{ee}(t - t')) E(t') \, dt' \, dt
\]

(2.3)
and

\[ 0 \leq \int_{-\infty}^{T} \mathbf{H}(t) \cdot \frac{\partial \mathbf{B}(t)}{\partial t} \, dt = \mu_0 \int_{-\infty}^{T} \int_{\mathbb{R}} \mathbf{H}(t) \cdot \frac{\partial}{\partial t} \left( \mu_{\infty}\delta(t-t') + \chi_{\text{mm}}(t-t') \right) \mathbf{H}(t') \, dt' \, dt \]

for all times \( T \) and fields \( \mathbf{E} \) and \( \mathbf{H} \). This classifies

\[ \frac{\partial}{\partial t} \left( \epsilon_0 \delta(t) + \chi_{\text{ee}}(t) \right) \quad \text{and} \quad \frac{\partial}{\partial t} \left( \mu_{\infty}\delta(t) + \chi_{\text{mm}}(t) \right) \]

as a passive convolution kernel [34], where \( \delta(t) \) is the Dirac delta distribution. It also restricts the instantaneous responses \( \epsilon_\infty \) and \( \mu_\infty \) to be non-negative. Moreover, the Maxwell equations together with the constitutive relations (2.1) and (2.2) and standard initial and boundary conditions are well posed if \( \epsilon_\infty > \alpha \) and \( \mu_\infty > \alpha \) for some \( \alpha > 0 \). This means that this requirement is sufficient to guarantee that a solution exists, is unique, and depends continuously on data [15]. This is e.g., required for numerical solutions in the time domain such as with finite differences [15]. Here, we analyze the constraints that passivity (2.3) and (2.4) enforces on the temporal dispersion of the models (2.1) and (2.2).

The wave-front speed limits the speed of the electromagnetic waves and is given by \( c_0/n_\infty \), where \( n_\infty = \sqrt{\epsilon_\infty \mu_\infty} \) is the instantaneous refractive index. It is often assumed that materials reduce to free space in the high-frequency limit, implying that \( n_\infty = \epsilon_\infty = \mu_\infty = 1 \). This is possible, but it is not necessary for the results presented in this paper. Moreover, it is not obvious that \( \epsilon_\infty = \mu_\infty = 1 \) apply for all engineered materials. Instead, a modeling approach is used where the high-frequency limit is obtained by analytic continuation from the frequency interval of interest [7].

The Fourier transform (using time dependence \( e^{-i\omega t} \)) of the constitutive relations (2.1) and (2.2) gives the frequency domain model

\[ \mathbf{D}(\omega) = \epsilon_0 \epsilon(\omega) \mathbf{E}(\omega) \quad \text{and} \quad \mathbf{B}(\omega) = \mu_0 \mu(\omega) \mathbf{H}(\omega), \]

where the symbols \( \mathbf{D}, \mathbf{E}, \mathbf{B} \) and \( \mathbf{H} \) are reused to denote the electromagnetic fields as functions of the angular frequency \( \omega \). The permittivity, \( \epsilon(\omega) \), and permeability, \( \mu(\omega) \), are also functions of \( \omega \), with frequency dependencies restricted by the Kramers-Kronig relations [10, 13]. This relation follows from the analytic properties of \( \epsilon(\omega) \) in \( \text{Im} \omega > 0 \) (using time dependence \( e^{-i\omega t} \)) together with basic assumptions on the asymptotic properties of \( \epsilon \) for low- and high frequencies. Here, an alternative approach is considered that is based on the additional assumption of passivity (2.3) and (2.4). This restricts \( \epsilon \) such that \( h_\epsilon = \omega \epsilon(\omega) \) is a Herglotz function [13, 21], i.e., \( h_\epsilon(\omega) \) is holomorphic and \( \text{Im} h_\epsilon(\omega) \geq 0 \) in the upper halfplane \( \text{Im} \omega > 0 \). The time-domain origin (2.1) imply the symmetry \( h_\epsilon(\omega) = -h_\epsilon^*(-\omega^*) \), where a star denotes the complex conjugate. The permeability defines a similar Herglotz function \( h_\mu(\omega) = \omega \mu(\omega) \). Note that the high-frequency asymptotic is consistent with the properties of Herglotz functions as a Herglotz function can not increase more than linearly for large \( \omega \), i.e., \( h(\omega) = O(\omega) \) as \( \omega \rightarrow \infty \) [21], where the symbol \( \rightarrow \) is a short hand notation for limits in \( \alpha < \arg \omega < \pi - \alpha \) for some \( \alpha > 0 \).
Herglotz functions can be represented as

$$h(z) = Az + \int_{\mathbb{R}} \left( \frac{1}{\xi - z} - \frac{\xi}{1 + \xi^2} \right) d\beta(\xi) = Az + \int_{\mathbb{R}} \frac{z}{\xi^2 - z^2} d\beta(\xi),$$

(2.7)

where $\int (1 + \xi^2)^{-1} d\beta(\xi) < \infty$, $z = x + iy$, $y > 0$, the symmetry is used in the second equality, and $\lim_{y \to 0} \text{Im} \ h(\xi + iy) d\xi = \pi d\beta(\xi)$ if $\text{Im} \ h(\xi)$ is regular [11], cf., the Kramers-Kronig relations [13].

2.2 A classical bound for lossless media

In this paper, we analyze how the basic assumptions (2.1) to (2.4) constrain the frequency dependence of the constitutive parameters. To start, consider a permittivity $\epsilon(\omega)$ with the low- and high-frequency asymptotes $\epsilon(0) = \epsilon_s$ and $\epsilon(\infty) = \epsilon_\infty$, respectively. Simple examples show that the variation around $\epsilon_m \in [\epsilon_\infty, \epsilon_s]$ is not restricted by passivity, e.g., the two-term Lorentz model

$$\epsilon(\omega) = \epsilon_\infty + \frac{\epsilon_s - \epsilon_m}{1 - (\omega/\omega_1)^2 - i\nu\omega/\omega_1} + \frac{\epsilon_m - \epsilon_\infty}{1 - (\omega/\omega_2)^2 - i\nu\omega/\omega_2}$$

(2.8)

with $\omega_1 \ll \omega_0 \ll \omega_2$ and $\nu \ll 1$ has $\epsilon(\omega) \approx \epsilon_m$ for a large bandwidth, see Fig. 1.
The example shows that the temporal dispersion does not restrict the frequency dependence for values \( \epsilon_m \in [\epsilon_\infty, \epsilon_s] \). However, the example also shows that the temporal dispersion severely limits the bandwidth for \( \epsilon(\omega) \approx \epsilon_m = -1 \). This is in general true and basic restrictions on the dispersion for lossless models of \( \epsilon(\omega) \) and \( \mu(\omega) \) can be obtained from the Kramers-Kronig relations \([10, 13, 16]\) (Hilbert transform) or here by the representation (2.7). Consider an interval \([\omega_1, \omega_2]\) with \( d\beta(\xi) = 0 \) (or equivalently \( \text{Im} \epsilon = 0 \)), then differentiation of \( h(\omega) \) gives

\[
\frac{\partial h(\omega)}{\partial \omega}(\omega_0) = \epsilon_\infty + \int_{R} \frac{1}{(\xi - \omega_0)^2} d\beta(\xi) \geq \epsilon_\infty \tag{2.9}
\]

for \( \omega_1 < \omega_0 < \omega_2 \). With \( h(\omega) = \omega \epsilon(\omega) \), it shows that

\[
\omega_0 \frac{\partial \epsilon}{\partial \omega}(\omega_0) \geq \epsilon_\infty - \epsilon(\omega_0). \tag{2.10}
\]

The derivative of \( \epsilon(\omega_0) \) is hence positive in intervals where \( \text{Im} \epsilon(\omega) = 0 \) and \( \epsilon(\omega_0) < \epsilon_\infty \). A sharper bound follows from \([16]\)

\[
\frac{\partial \omega h(\omega)}{\partial \omega}(\omega_0) = 2\omega_0 \epsilon_\infty + \int_{R} \frac{\xi}{(\xi - \omega_0)^2} d\beta(\xi) \geq 2\omega_0 \epsilon_\infty \tag{2.11}
\]

for \( \omega_1 < \omega_0 < \omega_2 \). With \( h(\omega) = \omega \epsilon(\omega) \), it shows that

\[
\omega_0 \frac{\partial \epsilon}{\partial \omega}(\omega_0) \geq 2(\epsilon_\infty - \epsilon(\omega_0)). \tag{2.12}
\]

In particular, the restrictions on \( \frac{\partial \epsilon}{\partial \omega} \) increases as \( \epsilon(\omega_0) \) decreases. The constraint (2.12) is transformed into a bound on the variation around \( \epsilon_m \) over a fractional bandwidth \( B = (\omega_2 - \omega_1)/\omega_0 \) around the center frequency \( \omega_0 = (\omega_2 + \omega_1)/2 \) by observing that

\[
\frac{\partial \epsilon(\omega)}{\partial \omega} \geq \frac{\partial \epsilon(\omega_0)}{\partial \omega} \quad \text{for} \quad \omega_1 < \omega \leq \omega_0 \quad \text{and hence, with} \quad \epsilon(\omega_0) = \epsilon_m
\]

\[
\epsilon_m - \epsilon(\omega_1) = \int_{\omega_1}^{\omega_0} \frac{\partial \epsilon(\omega)}{\partial \omega} d\omega \geq 2\frac{\omega_1 - \omega_0}{\omega_0} (\epsilon_\infty - \epsilon_m). \tag{2.13}
\]

This can be rewritten as

\[
\max_{\omega \in B} |\epsilon(\omega) - \epsilon_m| \geq B(\epsilon_\infty - \epsilon_m) \tag{2.14}
\]

which demonstrates that the deviation of \( \epsilon(\omega) \) around \( \epsilon_m \) is proportional to the fractional bandwidth, \( B \), in the interval \( B = [\omega_1, \omega_2] \) where the material model is lossless.

The pointwise bound on the derivative (2.12) is not true when losses are present, even if the loss (\( i.e. \), the imaginary part \( \text{Im} h(\omega) \)) is arbitrarily small. Consider, \( e.g. \), the Lorentz model

\[
h(\omega) = \epsilon_\infty \omega + \frac{\omega \nu^{3/2}}{1 - \omega^2 - i\nu \omega}, \tag{2.15}
\]

where \( \epsilon_\infty > 0 \) and \( \nu \geq 0 \). It has \( h(1) = \epsilon_\infty + i\nu^{1/2} \approx \epsilon_\infty \) for \( \nu \ll 1 \) but

\[
\frac{\partial h}{\partial \omega}(1) = \epsilon_\infty + i\nu^{1/2} - \frac{2 + i\nu}{\nu^{1/2}} = \epsilon_\infty - \frac{2}{\nu^{1/2}} \to -\infty \quad \text{as} \quad \nu \to 0. \tag{2.16}
\]
This simple example shows that it is very difficult to bound the derivative of Herglotz functions (and hence $\epsilon$ and $\mu$) pointwise. The requirements of lossless material models are removed in [17], where it is shown that $|\epsilon(\omega) + 1| \geq B$ for all square integrable susceptibilities $\epsilon(\omega) - 1$.

### 2.3 Construction of sum rules

Here, it is shown that bounds similar to (2.14) are valid for all passive constitutive relations of the form (2.6). It is also shown that the difference $\epsilon_s - \epsilon_\infty$ further restricts the bandwidth. The results are based on sum rules obtained by considering weighted integrals applied to Herglotz functions under the assumption of the following asymptotic expansions at low frequencies: $h(\omega) = \sum_n a_{2n-1} \omega^{2n-1} + o(\omega^{2N_0-1})$ as $k \to 0$, and at high frequencies, $h(\omega) = \sum_n b_{2n-1} \omega^{1-2n} + o(\omega^{-2N_\infty+1})$ as $k \to \infty$. The results are restricted to Herglotz functions satisfying the cross symmetry $h(\omega) = -h^*(-\omega^*)$, where a star denotes the complex conjugate, and hence to real valued $a_n$ and $b_n$ for odd $n$, giving the following family of integral identities:

$$\frac{2}{\pi} \int_0^\infty \frac{\text{Im} h(\omega)}{\omega^{2n}} \, d\omega = a_{2n-1} - b_{1-2n}, \quad (2.17)$$

for $1 - N_\infty \leq n \leq N_0$. Physical bounds are obtained by bounding the integral from below by restricting it to a finite interval [3–6, 8, 9, 23, 30, 31].

The sum rules generated by $h_\epsilon$ and $h_\mu$ with no static conductivity are identical to the ones obtained from the Kramers-Kronig relations [10, 13, 16], e.g.,

$$\frac{2}{\pi} \int_0^\infty \frac{\text{Im} h_\epsilon(\omega)}{\omega^2} \, d\omega = \frac{2}{\pi} \int_0^\infty \frac{\text{Im} \epsilon(\omega)}{\omega} \, d\omega = \epsilon_s - \epsilon_\infty. \quad (2.18)$$

This sum rule relates the losses to the asymptotic values and it shows that $\epsilon_s \geq \epsilon_\infty$.

Compositions of Herglotz functions are used to create new Herglotz functions that instead relate the variation around a fixed value, e.g., $\epsilon_m$, to the corresponding asymptotes.

As the Herglotz identities (2.17) relate the imaginary part of the function with its asymptotic values, it is necessary to transform the Herglotz function such that the imaginary part is of primary interest. Construct a Herglotz function, $h_\Delta(z)$, with an imaginary part given by $\text{Im} h_\Delta(x) = 1$ for $|x| < \Delta$ and $\text{Im} h_\Delta(x) = 0$ for $|x| > \Delta$, where $z = x + iy$ with $y > 0$. Analytic continuation using the representation (2.7) gives

$$h_\Delta(z) = \frac{1}{\pi} \int_{-\Delta}^\Delta \frac{1}{\xi - z} \, d\xi = \frac{1}{\pi} \ln \frac{z - \Delta}{z + \Delta} \quad \text{for } \text{Im} z > 0 \quad (2.19)$$

Here, the logarithm has its branch cut along the negative real axis. The imaginary part is bounded by unity and the region with $1 \geq \text{Im} h_\Delta(z) \geq \zeta \geq 1/2$ is given by the union of the circle

$$x^2 + \left( y - \frac{\Delta}{\tan(\pi \zeta)} \right)^2 \leq \Delta^2 \left( 1 + \frac{1}{\tan^2(\pi \zeta)} \right) \quad (2.20)$$
Figure 2: Illustrations of the Herglotz function $h_{\Delta}(z)$ in (2.19) with $\Delta = 1$. a) real and imaginary parts for $\text{Im } z = 0$. b) contour plot of $\text{Im } h_{\Delta}(x + iy)$.

and the plane $y > 0$, see Fig. 2. Note that the circle intersects the points $z = \pm \Delta$ and $z = i\Delta 2\sin^2(\pi \zeta/2)/\sin(\pi \zeta)$ and in particular $\text{Im } h_{\Delta}(z) \geq 1/2$ for $|z| \leq \Delta$. The asymptotes of (2.19) are

$$h_{\Delta}(z) \sim \begin{cases} 
1, & \text{as } z \to 0 \\
-2\Delta/\pi z, & \text{as } z \to \infty
\end{cases}$$

where $\sim$ denotes asymptotic similar, defined as $h(\omega) \sim h_1(\omega)$ as $\omega \to \infty$ if $h(\omega) = h_1(\omega) + o(|h_1(\omega)|)$ as $\omega \to \infty$. The function (2.19) is useful to restrict the interval where the amplitude of a Herglotz function is small, as compositions of $h_{\Delta}$ with e.g., $h_\epsilon$ maps regions where $|h_\epsilon| < \Delta$ to imaginary values between 1/2 and 1.

3 Sum rules for metamaterials

In this section, four sum rules are used to derive bounds for different a priori knowledge of the low- and high-frequency asymptotes. In Sec. 3.1 sum rules independent of the low-frequency asymptote are derived which gives a bound expressed in the difference between the target value and the high-frequency asymptote. Sum rules valid for models without a static conductivity are derived in Sec. 3.2 which produces
a bound proportional to the difference between the high- and low-frequency asymptotes. The third sum rule in Sec. 3.3 constrains parameter values larger than the static limit and is particular interesting for artificial magnets. The final sum rules derived in Sec. 3.4 are identities expressed in the plasma frequency.

3.1 Bounds expressed in the instantaneous response

Consider a permittivity $\epsilon(\omega)$ with the high-frequency asymptotes $\epsilon_{\infty}$ obtained from (2.1) and construct the Herglotz function

$$h_1(\omega) = \frac{\omega}{\omega_0} (\epsilon(\omega) - \epsilon_m) \sim \begin{cases} \mathcal{O}(1), & \text{as } z \to 0 \\ \frac{\omega(\epsilon_{\infty} - \epsilon_m)}{\omega_0}, & \text{as } z \to \infty \end{cases} \quad (3.1)$$

where $\epsilon_m < \epsilon_{\infty}$ is the desired value of $\epsilon(\omega)$ around $\omega = \omega_0$. It has the property $h_1(\omega) \approx 0$ if $\epsilon(\omega) \approx \epsilon_m$. Compose $h_\Delta$ with $h_1$ to construct a new Herglotz function, i.e.,

$$h_{1\Delta}(\omega) = h_\Delta(h_1(\omega)) \sim \begin{cases} \mathcal{O}(1), & \text{as } z \to 0 \\ -\frac{2\omega_0}{\pi(\epsilon_{\infty} - \epsilon_m)}, & \text{as } z \to \infty \end{cases} \quad (3.2)$$

These asymptotes show that $h_{1\Delta}$ has an $n = 0$ sum rule in (2.17), i.e.,

$$\int_0^\infty \text{Im} \, h_{1\Delta}(\omega) \, d\omega = \int_0^\infty \frac{1}{\pi} \arg \left( \frac{\omega(\epsilon(\omega) - \epsilon_m) - \omega_0\Delta}{\omega(\epsilon(\omega) - \epsilon_m) + \omega_0\Delta} \right) d\omega = \frac{\omega_0\Delta}{\epsilon_{\infty} - \epsilon_m}. \quad (3.3)$$

The properties of this sum rule are easiest to understand for intervals with Im $\epsilon(\omega) \approx 0$, where it is seen that the integrand is approximately one or zero depending on whether $|h_1(\omega)|$ is smaller or larger than $\Delta$, respectively. This is made more precise by consideration of a function $h_1(\omega)$ that is restricted to the region defined by $\zeta$ in (2.20) over the interval $\omega \in B = [\omega_1, \omega_2]$ with $\omega_0 = (\omega_2 + \omega_1)/2$ and $B = (\omega_2 - \omega_1)/\omega_0$. The integral (3.3) is then bounded as

$$B \min_{\omega \in B} \text{Im} \, h_\Delta(h_1(\omega)) \leq \frac{1}{\omega_0} \int_{\omega_1}^{\omega_2} \text{Im} \, h_{1\Delta}(\omega) \, d\omega \leq \frac{\Delta}{\epsilon_{\infty} - \epsilon_m} \quad (3.4)$$

and in particular in lossy and lossless cases

$$\min_{\omega \in B} \text{Im} \, h_\Delta(h_1(\omega)) \geq \begin{cases} 1/2 & \text{for max}_{\omega \in B} |h_1(\omega)| = \Delta \\ 1 & \text{for max}_{\omega \in B} |h_1(\omega)| = \Delta \text{ and max}_{\omega \in B} |\text{Im} \, h_1(\omega)| = 0 \end{cases} \quad (3.5)$$

giving

$$\max_{\omega \in B} |h_1(\omega)| \geq B(\epsilon_{\infty} - \epsilon_m) \begin{cases} 1/2 & \text{lossy case} \\ 1 & \text{lossless case} \end{cases} \quad (3.6)$$

The bound (3.6) on $h_1 = \omega(\epsilon - \epsilon_m)/\omega_0$ is transformed into a bound on $\epsilon - \epsilon_m$ as

$$\max_{\omega \in B} |\epsilon(\omega) - \epsilon_m| \geq \frac{B}{1 + B/2}(\epsilon_{\infty} - \epsilon_m) \begin{cases} 1/2 & \text{lossy case} \\ 1 & \text{lossless case} \end{cases} \quad (3.7)$$
Figure 3: Illustrations of the Drude model (3.8) with the sum rule (3.3) and bound (3.7). a) the permittivity $\varepsilon(\omega)$. b) the integrand in the sum rule (3.3), $\text{Im} \, h_{\Delta 1} = \text{Im} \, h_{\Delta}(h_1)$, the function $|h_1|$, the difference $|\varepsilon - \varepsilon_m|$, and the bandwidth bound (3.4) with $\varepsilon_m = -1$ and $\Delta = 0.4$.

where the bound in lossy media is identical to the bound in [17] for $B \ll 1$, $\varepsilon_{\infty} = 1$, and $\varepsilon_m = -1$.

As an example consider the Drude model

$$
\varepsilon(\omega) = 1 + \frac{1}{-i\omega(0.01 - i\omega)},
$$

where $\omega$ is a dimensionless frequency variable and the plasma frequency is $\omega_p = 1$, see Fig. 3a. It has a negative real part for $\omega < 1$. The sum rule (3.3) is evaluated for $\varepsilon_m = -1$ and $\Delta = 0.4$. The integrand in (3.3) is depicted in Fig. 3b, where it is observed that it has most of its area in the region around $\omega_0 \approx 0.7$, i.e., in the region where $|\varepsilon(\omega) - \varepsilon_m| \approx \text{Re} \, \varepsilon(\omega) - \varepsilon_m \leq \Delta$. The amplitudes $|h_1(\omega)|$ and $|\varepsilon(\omega) - \varepsilon_m|$ together with the bandwidth bound (3.4) are also included in the figure. The bound states that $\varepsilon(\omega)$ can not be designed such that its bandwidth is wider than the bound depicted in Fig. 3b.

The sum rule (3.3) and bounds (3.7) are valid with or without a static conductivity. The corresponding results for the permeability $\mu$ are obtained by substitution of $\mu$ for $\varepsilon$ in (3.1) to (3.7). They are also valid for the refractive index $n(\omega)$ defined by the square-root composition of $\omega \varepsilon$ and $\omega \mu$, i.e., the Herglotz function $h_n = \omega n = i\sqrt{-h_\varepsilon h_\mu} = i\sqrt{-\omega^2 \varepsilon \mu}$. Here, the square root has its branch cut along the negative real axis and the minus sign inside the square root and multiplication with the imaginary unit are essential steps to preserve the symmetry and the Her-
Figure 4: Illustrations of the model (3.9) with $n_m = -1$. a) the refractive index $n(\omega)$. b) integrand (solid curved) of the sum rule (3.3), $|h_1(\omega)|$, $|n(\omega) - n_m|$, and bandwidth bound (3.7).

Let $n_\infty$ denote the instantaneous response of the refractive index, i.e., $n(\omega) \sim n_\infty$ as $\omega \to \infty$. It is often assumed that $n_\infty \geq 1$ to ensure consistency with the speed of light in free space [10, 16]. The corresponding instantaneous permittivity, $\epsilon_\infty > 0$, and permeability, $\mu_\infty > 0$, are related through $\epsilon_\infty \mu_\infty = n_\infty^2$.

A numerical example with negative index of refraction and low losses over a broad frequency range is suggested in [18]. It is generated by the Kramers-Kronig relations [10, 13] using the imaginary parts

$$\text{Im} \epsilon(\omega) = 0.9 \frac{\omega(\omega^2 - 25)^2}{\omega^8 + 5.5}, \quad \text{and} \quad \text{Im} \mu(\omega) = 0.7 \frac{\omega(\omega^2 - 25)^2}{\omega^8 + 4.2}. \quad (3.9)$$

The index of refraction $n = i\sqrt{-\epsilon_\mu}$ is depicted in 4a and it has $n(0) \approx 79$, $n_\infty = 1$, $\omega_p \approx 6.7$, and $n(\omega_0) \approx -1$, where $\omega_0 \approx 4.9$. The integrand in the sum rules (3.3) for $n(\omega) \approx -1$ and $\Delta = 0.25$ is depicted in Fig. 4. It is observed that the area is concentrated around $\omega_0$.

3.2 Metamaterials without a static conductivity

The low-frequency asymptotes of $\epsilon$, $\mu$, and $n$ depend on the presence of static conductivity. In the case with no static conductivity, the linear response of $h_\epsilon(\omega) =$
\( \epsilon_0 \omega + o(\omega) \) as \( \omega \to 0 \) results in sum rules expressed in the static permittivity \( \epsilon_s \). Consider a permittivity with high-frequency limit \( \epsilon_\infty \geq 0 \) and a desired permittivity \( \epsilon_m \leq \epsilon_\infty \). The corresponding results for the permeability and index of refraction are obtained from the corresponding permittivity sum rules with the substitution of \( \mu \) or \( n \) for \( \epsilon \).

A sum rule that incorporates the static permittivity \( \epsilon_s \) in the bound on \( |\epsilon(\omega) - \epsilon_m| \) is constructed from the Herglotz function

\[
h_2(\omega) = -\frac{\omega_0}{\omega} \frac{\epsilon_\infty - \epsilon_m}{\epsilon(\omega) - \epsilon_\infty} - \frac{\omega_0}{\omega} \frac{\epsilon(\omega) - \epsilon_m}{\epsilon(\omega) - \epsilon_\infty} \sim \begin{cases} \frac{-\omega_0}{\omega} \frac{\epsilon_s - \epsilon_m}{\epsilon_s - \epsilon_\infty} & \text{as } \omega \to 0 \\ O(\omega) & \text{as } \omega \to \infty \end{cases} \quad (3.10)
\]

that has the property \( |h_2(\omega)| \approx 0 \) if \( \epsilon(\omega) \approx \epsilon_m \). Compose (3.10) with (2.19) to get the Herglotz function

\[
h_\Delta h_2(\omega) = h_\Delta(h_2(\omega)) \sim \begin{cases} \frac{2\omega_0}{\omega_0^2} \frac{\epsilon_s - \epsilon_\infty}{\epsilon_s - \epsilon_m} & \text{as } \omega \to 0 \\ 0(\omega) & \text{as } \omega \to \infty \end{cases} \quad (3.11)
\]

It has the \( n = 1 \) sum rule

\[
\int_0^\infty \frac{\omega_0^2}{\omega^2 \pi} \arg \left( \frac{\omega_0 (\epsilon(\omega) - \epsilon_m) + \omega \Delta (\epsilon(\omega) - \epsilon_\infty)}{\omega_0 (\epsilon(\omega) - \epsilon_m) - \omega \Delta (\epsilon(\omega) - \epsilon_\infty)} \right) d\omega = \omega_0 \Delta \frac{\epsilon_s - \epsilon_\infty}{\epsilon_s - \epsilon_m} \quad (3.12)
\]

Bound the integral as in (3.4) to get

\[
B \min_{\omega \in B} \text{Im} h_\Delta(h_2(\omega)) \leq \Delta \frac{\epsilon_s - \epsilon_\infty}{\epsilon_s - \epsilon_m} \quad (3.13)
\]

and finally

\[
\max_{\omega \in B} \frac{|\epsilon(\omega) - \epsilon_m|}{|\epsilon(\omega) - \epsilon_\infty|} \geq \frac{B}{1 + B/2} \frac{\epsilon_s - \epsilon_m}{\epsilon_s - \epsilon_\infty} \begin{cases} 1/2 & \text{lossy case} \\ 1 & \text{lossless case} \end{cases} \quad (3.14)
\]

The sum rule (3.12) and bound (3.14) show that the constraints on the variation of \( \epsilon \) around \( \epsilon_m \) is proportional to the difference \( \epsilon_s - \epsilon_\infty \). It is hence necessary to have a static permittivity \( \epsilon_s > 1 \) or a small instantaneous response \( \epsilon_\infty < 1 \) for broadband performance. Note that these results are valid for the case \( \epsilon_\infty = 0 \), although it is in general very difficult to show that the time-domain Maxwell equations are well posed in this case.

As an example, the classical Lorentz model is considered for the permittivity

\[
\epsilon(\omega) = 1 + \frac{0.2}{1 - \omega^2 - 0.001 i \omega} \quad (3.15)
\]

that has \( \epsilon_\infty = 1 \) and \( \epsilon_s = 1.2 \). It is not a particularly good candidate for \( \epsilon_m = -1 \) materials but it has a narrow frequency range around \( \omega = 1.05 \omega_0 \) where \( \text{Re} \epsilon \approx -1 \). The integrand of the sum rules (3.10) is depicted in Fig. 5. for \( \epsilon_m = -1 \) and \( \Delta = 0.2 \).
Figure 5: Illustrations of a Lorentz model (3.15) and sum rules. a) the permittivity $\varepsilon(\omega)$. b) imaginary part of the integrand of the sum rule (3.12).

Although an effective small-signal magnetic conductivity can theoretically be created in suitably biased ferromagnetic material [22], we exclude the possibility of a static magnetic conductivity in linear, passive materials as considered in this paper. Thus, the corresponding sum rules and bounds for permeability are given by simply replacing $\varepsilon$ by $\mu$ in the preceding equations.

If a static electric conductivity is present, the low-frequency asymptote of $n$ is $h_n(\omega) = \mathcal{O}(\omega^{1/2})$ as $\omega \to 0$. The sum rules and bounds for the refractive index are then given by replacing $\varepsilon$ by $n$ and replacing the static value by infinity, $n_s = \infty$. It is seen that in the sum rules and bounds, the right hand side is maximized if the static material properties are large. This implies that the bounds are generally tighter for permeability than for permittivity and refractive index if an electrical conductivity is present.

3.3 Artificial permeability

In applications with artificial magnetics, it is desired to design materials with a permeability, Re $\mu(\omega)$ larger than its static value $\mu_s$, i.e., $\mu(\omega_0) \approx \mu_m > \mu_s$. Consider the Herglotz function

$$h_3(\omega) = -\frac{\omega_0(\mu_m - \mu_\infty)}{\omega(\mu(\omega) - \mu_\infty)} - \frac{\omega_0}{\omega} \frac{\mu(\omega) - \mu_m}{\mu_m - \mu_\infty} \sim \begin{cases} \frac{-\omega_0}{\omega} \frac{\mu_m - \mu_s}{\mu_m - \mu_\infty} \text{ as } \omega \to 0 \\ \mathcal{O}(\omega) \text{ as } \omega \to \infty \end{cases}$$ (3.16)
where \( \mu_m > \mu_s \). Compose with \( h_\Delta \) to get the Herglotz function \( h_{\Delta 3} \) with the asymptotes

\[
h_{\Delta 3}(\omega) = h_\Delta(h_3(\omega)) \sim \begin{cases} 
\frac{2\omega \Delta}{\pi \omega_0} \frac{\mu_s - \mu_\infty}{\mu_m - \mu_s} & \text{as } \omega \to 0 \\
O(\omega^{-1}) & \text{as } \omega \to \infty
\end{cases}
\]

and the sum rule

\[
\int_0^\infty \frac{\omega_0^2}{\omega^2 \pi} \arg \left( \frac{h_3(\omega) + \Delta}{h_3(\omega) - \Delta} \right) d\omega = \omega_0 \Delta \left( \frac{\mu_s - \mu_\infty}{\mu_m - \mu_s} \right)
\]

with the bound

\[
\max_{\omega \in B} \left| \frac{\mu(\omega) - \mu_m}{\mu(\omega) - \mu_\infty} \right| \geq \frac{B}{1 + B/2} \frac{\mu_m - \mu_s}{\mu_s - \mu_\infty} \begin{cases} 
1/2 & \text{lossy case} \\
1 & \text{lossless case}
\end{cases}
\]

The Lorentz model is a common resonance model that has a narrow frequency range with values larger than its static value. Here, it used to illustrate the sum rule (3.18) and bound (3.19) on artificial permeability. Consider a permeability

\[
\mu(\omega) = 1 + \frac{2}{1 - \omega^2 - 0.01i\omega}
\]

that has \( \mu_\infty = 1 \) and \( \mu_s = 3 \). It is has a narrow frequency range around \( \omega = 0.9 \) where \( \Re \mu \approx \mu_m = 10 \). The integrand of the sum rules (3.18) is depicted in Fig. 5. for \( \epsilon_m = 10 \) and \( \Delta = 0.5 \).

### 3.4 Bounds expressed in the plasma frequency

A priori information about the plasma frequency can be used to derive additional sum rules and constraints on metamaterials. It is often assumed that, e.g., \( \epsilon(\omega) \sim \epsilon_\infty - \omega_p^2/\omega^2 \) as \( \omega \to \infty \), where \( \omega_p \) is the plasma frequency [10].

A sum rule involving the plasma frequency \( \omega_p \) is constructed from the Herglotz function \( h_2 \) in (3.10) with the high-frequency asymptote \( h_2(\omega) \sim \frac{\omega \omega_0}{\omega_p^2} (\epsilon_\infty - \epsilon_m) \) as \( \omega \to \infty \) and

\[
h_\Delta(h_2(\omega)) \sim \begin{cases} 
O(\omega) & \text{as } \omega \to 0 \\
-\frac{2\omega_0^2 \Delta}{\pi \omega_0 (\epsilon_\infty - \epsilon_m)} & \text{as } \omega \to \infty
\end{cases}
\]

It has an \( n = 0 \) sum rule, viz.,

\[
\int_0^\infty \frac{1}{\pi} \arg \left( \frac{\omega_0 (\epsilon(\omega) - \epsilon_m) + \Delta \omega (\epsilon(\omega) - \epsilon_\infty)}{\omega_0 (\epsilon(\omega) - \epsilon_m) - \Delta \omega (\epsilon(\omega) - \epsilon_\infty)} \right) d\omega = \frac{\omega_p^2 \Delta}{\omega_0 (\epsilon_\infty - \epsilon_m)}
\]

and the associate physical bound

\[
\max_{\omega \in B} \left| \frac{\epsilon(\omega) - \epsilon_m}{\epsilon(\omega) - \epsilon_\infty} \right| \geq \frac{B}{1 + B/2} \frac{\omega_0^2 (\epsilon_\infty - \epsilon_m)}{\omega_p^2 (\epsilon_\infty - \epsilon_m)} \begin{cases} 
1/2 & \text{lossy case} \\
1 & \text{lossless case}
\end{cases}
\]
Figure 6: Illustrations of the Lorentz model (3.20) and sum rule (3.18) for artificial permeability. a) the permeability $\mu(\omega)$. b) imaginary part of the integrand of the sum rule (3.18).

The Herglotz function $h_3$ in (3.16) with $\mu(\omega) \sim \mu_\infty - \omega_p^2/\omega^2$ as $\omega \to \infty$ has the high-frequency asymptote $h_3(\omega) \sim (\mu_m - \mu_\infty)\omega_0/\omega_p^2$ giving

$$h_\Delta(h_3(\omega)) \sim \begin{cases} O(\omega) & \text{as } \omega \to 0 \\ -2\omega_p^2\Delta & \pi\omega_0(\mu_m - \mu_\infty) & \text{as } \omega \to \infty \end{cases}$$

(3.24)

for $\mu_m > \mu_s$ giving the sum rule

$$\int_0^\infty \frac{1}{\pi} \arg \left( \frac{h_3(\omega) + \Delta}{h_3(\omega) - \Delta} \right) d\omega = \frac{\omega_p^2\Delta}{\omega_0(\mu_m - \mu_\infty)}$$

(3.25)

with the bound

$$\max_{\omega \in B} \frac{|\mu(\omega) - \mu_m|}{|\mu(\omega) - \mu_\infty|} \geq \frac{B}{1 + B/2} \frac{\omega_0^2}{\omega_p^2} (\mu_m - \mu_\infty) \begin{cases} 1/2 & \text{lossy case} \\ 1 & \text{lossless case} \end{cases}$$

(3.26)

The bounds show that it is advantageous to have $\omega_0 < \omega_p$ for good performance.

4 Bi-anisotropic constitutive relations

The constitutive relations treated in this paper can be augmented to include so-called bi-anisotropic materials. These are materials where the relation between the
\[ [E, H] \text{ and } [D, B] \text{ fields is written in the frequency domain as} \]
\[
\begin{pmatrix}
D(\omega) \\
B(\omega)
\end{pmatrix} = \begin{pmatrix}
\epsilon_0 \epsilon(\omega) & c_0^{-1} \xi(\omega) \\
\xi(\omega) & \mu_0 \mu(\omega)
\end{pmatrix} \begin{pmatrix}
E(\omega) \\
H(\omega)
\end{pmatrix} \tag{4.1}
\]

where the dimensionless \( \epsilon, \xi, \zeta, \mu \) are now matrix-valued functions of \( \omega \). The material is passive if the total dissipated power is non-negative \( [12] \), i.e., the imaginary part of all hermitian quadratic forms over the \( 6 \times 6 \) material matrix weighted by \( \omega \) are non-negative,

\[
\text{Im} \left\{ \omega \begin{pmatrix}
E(\omega)^* \\
H(\omega)^*
\end{pmatrix} \cdot \begin{pmatrix}
\epsilon_0 \epsilon(\omega) & c_0^{-1} \xi(\omega) \\
\xi(\omega) & \mu_0 \mu(\omega)
\end{pmatrix} \begin{pmatrix}
E(\omega) \\
H(\omega)
\end{pmatrix} \right\} \geq 0 \text{ for all } E \text{ and } H \tag{4.2}
\]

Choosing \([E(\omega), H(\omega)] = E_0[e_0, \eta_0^{-1} h_0]\) where \( E_0 \) is a normalization constant and \( e_0 \) and \( h_0 \) are dimensionless, constant and real-valued vectors, the dimensionless quadratic form

\[
q(\omega) = \begin{pmatrix}
e_0 \\
h_0
\end{pmatrix} \cdot \begin{pmatrix}
\epsilon(\omega) & \xi(\omega) \\
\zeta(\omega) & \mu(\omega)
\end{pmatrix} \begin{pmatrix}
e_0 \\
h_0
\end{pmatrix} \tag{4.3}
\]

then defines a Herglotz function \( h_q(\omega) = \omega q(\omega) \) for each fixed vector pair \([e_0, h_0]\), and all the previous sum rules apply to \( q(\omega) \). The vectors \( e_0 \) and \( h_0 \) need to be real-valued in order to keep the symmetry \( h_q(\omega) = -h_q^*(-\omega^*) \). The quadratic form \( q(\omega) \) is a linear combination of different components of the material matrices \( \epsilon(\omega), \xi(\omega), \zeta(\omega), \mu(\omega) \), but not all linear combinations are possible, only those corresponding to diagonal elements of the \( 6 \times 6 \) material matrix. Note in particular that we cannot find a Herglotz function \( h_q(\omega) \) involving only the matrices \( \xi(\omega) \) or \( \zeta(\omega) \), they are always mixed with \( \epsilon(\omega) \) or \( \mu(\omega) \). We must also take into account that for reciprocal media, the static limit of \( \xi(\omega) \) and \( \zeta(\omega) \) is zero, since the coupling between electric and magnetic fields disappears in the static limit \([25, p. 36]\), so that

\[
q(0) = \begin{pmatrix}
e_0 \\
h_0
\end{pmatrix} \cdot \begin{pmatrix}
\epsilon(0) & 0 \\
0 & \mu(0)
\end{pmatrix} \begin{pmatrix}
e_0 \\
h_0
\end{pmatrix} = e_0 \cdot \epsilon(0)e_0 + h_0 \cdot \mu(0)h_0 \tag{4.4}
\]

For instance, this means that the bound \((3.7)\) for bi-anisotropic materials becomes

\[
\max_{\omega \in B} |q(\omega) - q_m| \geq \frac{B}{1 + B/2} (q_\infty - q_m) \begin{cases} 1/2 & \text{lossy case} \\ 1 & \text{lossless case} \end{cases} \tag{4.5}
\]

The simplest example of a material with coupling between electric and magnetic fields is a chiral material, which is a bi-isotropic material where all material matrices are proportional to the identity matrix \( I \),

\[
\begin{pmatrix}
\epsilon(\omega) & \xi(\omega) \\
\zeta(\omega) & \mu(\omega)
\end{pmatrix} = \begin{pmatrix}
\epsilon(\omega)I & i\chi(\omega)I \\
-i\chi(\omega)I & \mu(\omega)I
\end{pmatrix} \tag{4.6}
\]

The quadratic form \( q(\omega) \) then only contains information on \( \epsilon(\omega) \) and \( \mu(\omega) \),

\[
q(\omega) = \begin{pmatrix}
e_0 \\
h_0
\end{pmatrix} \cdot \begin{pmatrix}
\epsilon(\omega)I & i\chi(\omega)I \\
-i\chi(\omega)I & \mu(\omega)I
\end{pmatrix} \begin{pmatrix}
e_0 \\
h_0
\end{pmatrix} = |e_0|^2 \epsilon(\omega) + |h_0|^2 \mu(\omega) \tag{4.7}
\]
This means the sum rules in this paper can be used to bound a linear combination of \( \varepsilon(\omega) \) and \( \mu(\omega) \), but provide no information on \( \chi(\omega) \). This is due to the requirement of \( e_0 \) and \( h_0 \) to be real-valued vectors. The physical importance of the chirality parameter \( \chi \) is that it is proportional to the rotation of the polarization direction of a linearly polarized wave as it propagates through the chiral material. Denoting the real and imaginary parts with primes as \( \chi = \chi' + i\chi'' \), the angle of rotation is [29]

\[
\phi(\omega) = \frac{\omega}{c_0} \chi'(\omega) = \frac{2\pi}{\lambda} \chi'(\omega)
\]

per unit length of propagation. The following sum rule is proposed in [29]

\[
\int_0^\infty \omega \chi'(\omega) \, d\omega = 0 \iff \int_0^\infty \phi(\omega) \, d\omega = 0
\]

i.e., the total rotation of the polarization direction for all frequencies is zero. If the material is also an insulator at zero frequency (no static conductivity), the additional sum rule

\[
\int_0^\infty \omega^{-1} \chi'(\omega) \, d\omega = 0 \iff \int_0^\infty \phi(\lambda) \, d\lambda = 0
\]

also applies. Thus, for an insulating chiral material, the total rotation for all frequencies and all wavelengths is zero [29].

5 Conclusions

In conclusion, sum rules are presented that constrain the bandwidth of passive metamaterials. The bandwidth limitations on \( \varepsilon(\omega) \approx \varepsilon_m < \varepsilon_{\infty} \) are expressed in either the differences between the low- and high-frequency permittivity or the plasma frequency. The corresponding expressions for permeability or refractive index are given by replacing \( \varepsilon \) by \( \mu \) or \( n \). The static permittivity and permeability are well defined and can be determined by homogenization techniques for heterogeneous materials; it is then well known that the effective material parameter is bounded by the parameters of the included materials [19]. This demonstrates that for instance a high static permeability cannot be created by a composite material unless one of its component materials already has a high static permeability [1]. Many proposed metamaterial designs for negative refractive index utilize only dielectrics and metal structures, and since the static permeability of some good conductors such as copper is very close to unity, the bandwidth is penalized by (3.10) and (3.14). We have also demonstrated how a priori information about the plasma frequency can be used to derive additional sum rules. Finally, we have shown that the sum rules can be applied to bi-anisotropic material models, but only for the diagonal elements of the \( 6 \times 6 \) material matrix.

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References


