Causality and passivity properties of effective parameters of electromagnetic multilayered structures

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Effective properties of periodic structures are investigated at all frequencies. It is shown that a simple dielectric multilayer with arbitrary low contrast can display artificial magnetoelectric coupling and magnetism. Effective parameters, as functions of the complex frequency, possess all the analytic properties required by the causality principle. The theoretical expression of the effective index and surface impedance are numerically tested; the former is shown to reduce to the mean refractive index at infinite frequency, just like the refractive index in the x-ray regime. We stress that periodic multilayers, with frequency-independent (noncausal) dielectric constants, make effective media with artificial causality.

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I. INTRODUCTION

There is currently a renewed interest in photonic crystals and metamaterials,^{1,2} i.e., periodic structures exhibiting new phenomena such as anomalous dispersion³⁻⁵ and negative refraction,⁶⁻⁸ and optical activity.⁹ The former composites are known to possess ranges of frequencies (band gaps) for which waves are disallowed to propagate within the structure for wavelengths on the order of the period,¹ while the latter composites exhibit a magnetic response associated with local RLC circuit type¹⁰ or Mie¹¹ resonances, at low frequencies. However, it seems that there is no effective medium description which encapsulates all the physics of periodic structures from low frequencies to stop band frequencies and beyond. Thus, the extension of classical homogenization theory¹² to higher orders of approximation^{13,14} and high frequencies^{15,16} appears to be of pressing importance for physicists working in the field of photonic crystals and metamaterials. A challenge is to understand extraordinary properties such as artificial optical activity.⁹ To achieve this goal, effective parameters ought to make sense for sufficiently high frequencies including the resonances of the structure. Applied mathematicians from the wave community also show a keen interest in this topic,^{16–21} since periodic structures with small inductive and capacitive elements structured at subwavelength length scales can often be regarded as almost homogeneous.

In this paper, we propose a notion of all frequency homogenization (AFH) based on effective parameters satisfying causality principle and passivity.^{22,23} This necessitates one to go beyond the graphical retrieval method²⁴ and Fresnel inversion²⁵ which, for each fixed frequency and wave vector, directly translates reflectivity, transmission into effective permittivity, permeability, and chirality. At low frequencies, we use a frequency power expansion to derive analytic expressions of effective homogeneous parameters such as the permittivity $\varepsilon_{\rm eff}$, the permeability $\mu_{\rm eff}$ corresponding to artificial magnetism, and a bianisotropy coefficient $\xi_{\rm eff}$, the hallmark of magnetoelectric coupling. At higher frequencies, we turn to another set of effective parameters: The propagation index $n_{\rm eff}$ and the surface impedance $\zeta_{\rm eff}$. It is shown that these parameters are analytic functions in the upper half-plane of complex frequencies z and that they have a well-defined limit at infinite frequencies. According to passivity, the imaginary part of $zn_{\text{eff}}(z)$ and real part of $\zeta_{\text{eff}}(z)$ are both positive. As the central result of this paper, it follows that both effective index and impedance satisfy causality and passivity requirements. This leads us to conclude that a periodic multilayered stack can be replaced by a frequency- and spatially dispersive²⁶ homogeneous effective medium for the entire spectrum of frequencies and wave vectors. The tool of choice for our one-dimensional model is the transfer matrix method, as it allows for analytical formulas. However, arguments are provided to stress that ideas contained therein might be extended to frequency dispersive and three-dimensional periodic structures.

II. ANALYTIC PROPERTIES OF THE TRANSFER MATRIX

We start with a periodic multilayer with a unit cell made of two homogeneous layers \mathcal{L}_1 and \mathcal{L}_2 of thicknesses h_1 and h_2 [see Fig. 1 ($h = h_1 + h_2$ is the thickness of the unit cell)]. The frequency ω and the wave vector $\mathbf{k} = (k_1, k_2)$ are the conserved quantities of the system which is homogeneous with respect to time and space variables (x_1, x_2) [an orthogonal set of coordinates (x_1, x_2, x_3) is considered such that the layers are stacked in the x_3 direction; see Fig. 1]. At the oscillating frequency ω , the electric and magnetic fields \mathbf{E} and \mathbf{H} are related to the electric and magnetic inductions \mathbf{D} and \mathbf{B} through the time-harmonic Maxwell's equations,

$$-i\omega \boldsymbol{D}(\boldsymbol{x}) = \boldsymbol{\nabla} \times \boldsymbol{H}(\boldsymbol{x}), \quad i\omega \boldsymbol{B}(\boldsymbol{x}) = \boldsymbol{\nabla} \times \boldsymbol{E}(\boldsymbol{x}), \quad (1)$$

and the phenomenological constitutive relations for nonmagnetic isotropic dielectric media:

$$\boldsymbol{D}(\boldsymbol{x}) = \varepsilon_m \boldsymbol{E}(\boldsymbol{x}), \quad \boldsymbol{B}(\boldsymbol{x}) = \mu_0 \boldsymbol{H}(\boldsymbol{x}), \quad \boldsymbol{x} \in \mathcal{L}_m, \quad (2)$$

where μ_0 is the vacuum permeability, and ε_m is the permittivity in the homogeneous layer \mathcal{L}_m , m = 1,2. Note that, at this stage, the frequency dependence of the permittivity is omitted. However, as will be discussed later on, all the results of this paper remain valid when frequency dispersion is considered. In order to take advantage of invariance under translations in (x_1, x_2) , the Fourier decomposition from (x_1, x_2) to $\mathbf{k} = (k_1, k_2)$, defined for a vector field $\mathbf{U}(\mathbf{x})$ by

$$\widehat{U}(k_1, k_2, x_3) = \frac{1}{2\pi} \int_{\mathbb{R}^2} U(x_1, x_2, x_3) \exp[-ik_1 x_1] \\ \times \exp[-ik_2 x_2] dx_1 dx_2,$$
(3)

is introduced. This decomposition is applied to Eqs. (1) and (2), and next the components \widehat{E}_3 and \widehat{H}_3 are eliminated to



FIG. 1. (Color online) Example of a periodic multilayered stack of identical unit cells made of two dielectric homogeneous layers. The system is invariant under translations in the space directions x_1 and x_2 and the corresponding electric permittivity $\varepsilon(x_3)$ is a periodic function of variable x_3 .

derive a first order differential equation:

$$\frac{\partial F}{\partial x_3}(\omega, \boldsymbol{k}, x_3) = -i M_m(\omega, \boldsymbol{k}) F(\omega, \boldsymbol{k}, x_3), \qquad (4)$$

where F is a column vector containing the tangential components of the Fourier-transformed electromagnetic field $(\widehat{E}, \widehat{H})$, and $M_m(\omega, k)$ is a matrix independent of x_3 in each homogeneous layer \mathcal{L}_m . Also, a coordinate rotation of the (x_1, x_2) plane is introduced in order to obtain two independent systems for s and p polarizations. For all vector \mathbf{x} , the couple of coordinates (x_1, x_2) is replaced by $(x_{\parallel}, x_{\perp})$, where x_{\parallel} denotes the component along the wave vector $\mathbf{k} = (k_1, k_2)$ and x_{\perp} the component along $(-k_2, k_1)$. Then, omitting the (ω, \mathbf{k}) dependence, one has for s polarization

$$F = \begin{bmatrix} \widehat{E}_{\perp} \\ \omega \widehat{H}_{\parallel} \end{bmatrix}, \quad M_m = \begin{bmatrix} 0 & \mu_0 \\ \omega^2 \varepsilon_m - \mathbf{k}^2 / \mu_0 & 0 \end{bmatrix}, \quad (5)$$

and for p polarization

$$F = \begin{bmatrix} \widehat{H}_{\perp} \\ \omega \widehat{E}_{\parallel} \end{bmatrix}, \quad M_m = \begin{bmatrix} 0 & -\varepsilon_m \\ \mathbf{k}^2 / \varepsilon_m - \omega^2 \mu_0 & 0 \end{bmatrix}. \quad (6)$$

Since the matrices M_m are x_3 independent, the solution of (4) in each layer \mathcal{L}_m is simply

$$F(x_3 + h_m) = \exp[-iM_m h_m]F(x_3).$$
 (7)

The exponential above is well defined as a power series of the matrix M_m :

$$\exp[-iM_m h_m] = I + \sum_{p=1}^{\infty} \frac{(-iM_m h_m)^p}{p!},$$
 (8)

where *I* is the identity matrix. This power series defines the transfer matrix in the medium *m* over the distance h_m . Since this power series has infinite radius of convergence, the transfer matrix is analytic with respect to the three independent variables ω , k_1 , and k_2 describing the whole complex plane (more precisely, the transfer matrix is an entire function²⁷ of the three variables ω , k_1 , and k_2). From now on, we focus on the complex frequency denoted by $z = \omega + i\eta$, where ω remains the real frequency and η is the imaginary part. The transfer matrix associated with the unit cell,

$$T(z, \mathbf{k}) = \exp[-iM_2(z, \mathbf{k})h_2] \exp[-iM_1(z, \mathbf{k})h_1], \quad (9)$$

is also an analytic function over the whole complex plane of variables z, k_1 , and k_2 . We stress that, for an arbitrary one-dimensional permittivity profile bounded by a constant *C* [i.e., $|\varepsilon(x_3)| \leq C$ for all x_3], a Dyson expansion²⁷ can be used to prove that the analyticity property of the transfer matrix remains valid.

The analyticity property opens the possibility to define effective parameters which are valid throughout the whole frequency spectrum. Indeed, suppose that effective parameters can be extracted from the transfer matrix in a finite range of frequencies, for instance, in the classical homogenization regime $\omega = 0$. If the analytic property of the transfer matrix can be allocated to effective parameters, then a unique continuation of the latter can be defined in the whole frequency spectrum: such analytic continuation may be the foundation for a notion of AFH. Moreover, it has to be noted that the analyticity property may be used to show that effective parameters satisfy the causality principle and that they have a physical meaning.

III. HIGH-ORDER HOMOGENIZATION

The infinite radius of convergence of the power series expansion of $T(z, \mathbf{k})$ suggests introducing a notion of highorder homogenization (HOH), which extends the standard homogenization (corresponding to the limit $z \rightarrow 0$) by expanding the effective permittivity and permeability as the power series of z. To carry out the asymptotic analysis, we use the Baker-Campbell-Hausdorff formula (BCH formula, an extension of the S. Lie theorem; see Ref. 28):

$$\exp[A] \exp[B] = \exp[X], X = A + B + [[A, B]] + [[A - B, [[A, B]]]]/3 + \cdots,$$
(10)

where A + B is defined as the zeroth-order approximation (standard homogenization), the commutator of A and B: [[A,B]] = (AB - BA)/2 is the first-order correction, [[A - B, [[A,B]]]]/3 is the second-order correction, and so forth. The BCH formula (10) shows that the transfer matrix (9) can be written as that of a frequency- and spatially dispersive homogeneous medium characterized by $-iM_{\text{eff}}(z, k)h \equiv X$, i.e.,

$$\exp[-iM_{\text{eff}}(z,\boldsymbol{k})h] = T_{\text{eff}}(z,\boldsymbol{k}).$$
(11)

The resulting matrix $M_{\text{eff}}(z, \mathbf{k})$ is found to correspond to the constitutive equations of a homogeneous medium:

$$\widehat{\boldsymbol{D}}(\boldsymbol{k}, x_3) = \varepsilon_{\text{eff}}(z, \boldsymbol{k}) \ \widehat{\boldsymbol{E}}(\boldsymbol{k}, x_3) + i \, \boldsymbol{K}_{\text{eff}}(z, \boldsymbol{k}) \boldsymbol{J} \ \widehat{\boldsymbol{H}}(\boldsymbol{k}, x_3),$$

$$\widehat{\boldsymbol{B}}(\boldsymbol{k}, x_3) = \mu_{\text{eff}}(z, \boldsymbol{k}) \ \widehat{\boldsymbol{H}}(\boldsymbol{k}, x_3) + i \, \boldsymbol{J} \, \boldsymbol{K}_{\text{eff}}(z, \boldsymbol{k}) \widehat{\boldsymbol{E}}(\boldsymbol{k}, x_3).$$
(12)

Here, matrix *J* represents the 90° rotation around the x_3 axis and, in the coordinate system $(x_{\parallel}, x_{\perp}, x_3)$, the effective permittivity and permeability are

$$\varepsilon_{\text{eff}} = \text{diag}(\varepsilon_{\parallel}, \varepsilon_{\perp}, \varepsilon_{3}), \quad \mu_{\text{eff}} = \text{diag}(\mu_{\parallel}, \mu_{\perp}, \mu_{3}), \quad (13)$$

while the bianisotropic parameter measuring the magnetoelectric coupling effect^{9,29} is given by

$$K_{\rm eff} = {\rm diag}(K_{\parallel}, K_{\perp}, 0). \tag{14}$$

Although the system is isotropic in the plane (x_1, x_2) , the spatial dispersion induced by the k dependence introduces a difference between the coefficients ε_{\parallel} and ε_{\perp} , μ_{\parallel} and μ_{\perp} , and K_{\parallel} and K_{\perp} .³⁰ At k = 0, equalities $\varepsilon_{\parallel}(z, 0) = \varepsilon_{\perp}(z, 0)$, and so forth, are retrieved.

After some elementary algebra, collecting terms up to the second-order correction in (10) with $A = -iM_2h_2$ and $B = -iM_1h_1$, we obtain the following homogenized coefficients for k = 0:

$$\begin{aligned} \varepsilon_{\parallel}(\hat{z}) &= \varepsilon_{1}f_{1} + \varepsilon_{2}f_{2} + \hat{z}^{2}f_{1}f_{2}(\varepsilon_{1} - \varepsilon_{2})(\varepsilon_{1}f_{1} - \varepsilon_{2}f_{2})/(6\varepsilon_{0}), \\ \mu_{\parallel}(\hat{z}) &= \mu_{0} - \hat{z}^{2}f_{1}f_{2}\mu_{0}(\varepsilon_{1} - \varepsilon_{2})(f_{1} - f_{2})/(6\varepsilon_{0}), \\ K_{\parallel}(\hat{z}) &= \hat{z}(\varepsilon_{1} - \varepsilon_{2})f_{1}f_{2}/(2\sqrt{\varepsilon_{0}/\mu_{0}}), \end{aligned}$$
(15)

with $\hat{z} = zh\sqrt{\varepsilon_0\mu_0}$ the normalized complex frequency and $f_m = h_m/h$. Note that, in the static limit $\hat{z} \to 0$, $\mu_{\parallel}(\hat{z})$ and $K_{\parallel}(\hat{z})$ tend to μ_0 and 0, respectively. It is also stressed that magnetoelectric coupling comes from the odd order approximation in (10), while artificial magnetism and high-order corrections to permittivity emerge from even order approximation. These results are fully consistent with descriptions in terms of spatial dispersion^{30,31} wherein, expanding the permittivity in power series of the wave vector, first order yields optical activity and second-order magnetic response. The equivalence of these two descriptions (frequency and wave vector power series) is confirmed by considering a unit cell with a center of symmetry, for example, a stack of three homogeneous layers (permittivity ε_m and thickness h_m , m = 1, 2, 3) with $\varepsilon_3 = \varepsilon_1$ and $h_3 = h_1$. Extending (10) to the case $\exp[A] \exp[B] \exp[A] = \exp[X]$ (see Ref. 32), it is found that $K_{\text{eff}} = 0$, and thus it is retrieved that both magnetoelectric coupling and optical activity vanish in a medium with a center of symmetry.

Expansion in power series of frequency provides a new explanation for artificial magnetism and optical activity. Analytic expressions (15) of effective parameters can be used to analyze artificial properties (expressions for higher orders in normal and conical incidence are provided in Ref. 32). In particular, we obtain from (15) that artificial magnetism, previously proposed with high contrast,^{11,18,19} can be obtained with arbitrarily low contrast; and magnetoelectric coupling, previously achieved in Ω composites,⁹ can be present in simple one-dimensional multilayers.

Nevertheless, this frequency expansion of effective parameters cannot be used for frequencies higher than the frequency ω_1 at the first band-gap edge.³² To show this limitation, we consider for the sake of simplicity a three-layer unit cell with a center of symmetry and purely real dielectric constants $\varepsilon_1 = \varepsilon_3$ and ε_2 : Effective parameters ε_{eff} and μ_{eff} derived from (10) and (11) are then purely real for real frequencies, and $K_{\text{eff}} = 0$. Under normal incidence, $\mathbf{k} = \mathbf{0}$, the Bloch wave number reduces to

$$k_B(\omega) = \omega \sqrt{\varepsilon_{\text{eff}}(\omega)} \mu_{\text{eff}}(\omega), \qquad (16)$$

where the right-hand side of (16) is the wave number of the homogeneous effective medium. Since ε_{eff} and μ_{eff} derived from the power expansion take purely real values, the Bloch wave number must be either purely real or purely imaginary. If the definition of ε_{eff} and μ_{eff} is valid in the neighborhood of the first band-gap edge ω_1 , then the Bloch wave vector is purely real for $\omega \leq \omega_1$ in the first band and purely imaginary for $\omega \geq \omega_1$ in the first gap. Also, if the definition of ε_{eff} and μ_{eff} is valid, then these parameters, as well as $k_B(\omega)$, are continuous functions of ω . Thus, under these conditions, the Bloch wave number must vanish at the first band-gap edge ω_1 : This is clearly in contradistinction with the requirement



FIG. 2. (a) Representation of the dispersion law in the periodic multilayer: ω_1 is the frequency at the first band-gap edge. (b) Domains of analyticity (striped areas) of effective parameters ε_{eff} , μ_{eff} , K_{eff} , n_{eff} , and ζ_{eff} : The dashed circle defines the disk within which the power expansion converges.

 $k_B(\omega_1) = \pi/h$ (see Fig. 2). Thus we can conclude at this stage that the frequency power expansion of the effective ε_{eff} and μ_{eff} cannot be valid in both sides of the first band-gap edge ω_1 . Now, we assume that the power expansion is valid only for frequencies in the first band, i.e., $\omega \leq \omega_1$. At the first band-gap edge, $k_B(\omega_1) = \pi/h$ and thus

$$\varepsilon_{\rm eff}(\omega_1)\mu_{\rm eff}(\omega_1) = \frac{\pi^2}{h^2\omega_1^2}.$$
 (17)

Since the product $\varepsilon_{\text{eff}}(\omega)\mu_{\text{eff}}(\omega)$ cannot be positive within the band gap, either $\varepsilon_{\text{eff}}(\omega_1)$ or $\mu_{\text{eff}}(\omega_1)$ must vanish to allow for sign shifting at ω_1 , say $\mu_{\text{eff}}(\omega_1) = 0$. Consequently, it is found that the other parameter is bound to take an infinite value at ω_1 :

$$\varepsilon_{\rm eff}(\omega) \sim_{\omega_1} \frac{\pi^2}{h^2 \omega_1^2 \mu_{\rm eff}(\omega)} \xrightarrow[\omega \to \omega_1]{\infty} \infty.$$
 (18)

These arguments show that the power series expansion of $X = -i M_{\text{eff}} h$ in (10) diverges at ω_1 . Indeed, from the expression of M_{eff} , formally equivalent to (11),

$$M_{\rm eff}(z, \boldsymbol{k}) = (i/h) \log[T(z, \boldsymbol{k})], \tag{19}$$

it appears that the function log is not analytic when its argument "vanishes," which introduces a branch point at ω_1 (see Fig. 2): This branch point implies that the radius of convergence of the power expansion of effective parameters is certainly bounded by ω_1 (Fig. 2).

Hence we obtain that the HOH is only valid for complex frequencies inside a disk with radius ω_1 . However, it is possible to choose the branch cut of the complex logarithm from the branch point ω_1 in the lower half complex plane (Fig. 2). This choice makes it possible to use analytic continuation to define effective parameters in the upper half plane of the complex frequency *z*.

IV. ALL FREQUENCY HOMOGENIZATION

An analytic continuation of the matrix $M_{\text{eff}}(z, \mathbf{k}) = (i/h) \log[T(z, \mathbf{k})]$ can be defined outside the disk with radius ω_1 in the upper half plane of complex frequencies z by choosing the branch cuts of the complex logarithm from the branch points in the lower half plane (see Fig. 2). From this analytic continuation of $M_{\text{eff}}(z, \mathbf{k})$, effective parameters $\varepsilon_{\text{eff}}(z, \mathbf{k})$, $\mu_{\text{eff}}(z, \mathbf{k})$, and $K_{\text{eff}}(z, \mathbf{k})$ can be defined for complex frequencies z in the upper half plane (i.e., $z = \omega + i\eta$ with $\eta > 0$). These effective parameters are, by construction, analytic in the upper half plane of complex frequencies as required by the causality principle.^{30,33} Nevertheless, it appears that the pair of effective parameters $\varepsilon_{\text{eff}}(z, \mathbf{k})$ and $\mu_{\text{eff}}(z, \mathbf{k})$ is not appropriate to describe the effective homogeneous medium of a multilayered stack because they cannot satisfy simultaneously the passivity requirement, as shown hereafter.

Passivity requires that electromagnetic energy must be a decreasing function of time. From the calculation of electromagnetic energy, it shows²² that the permittivity and permeability have positive imaginary part^{22,30} or, more precisely, that $\omega \operatorname{Im}[\varepsilon(\omega)] \ge 0$ and $\omega \operatorname{Im}[\mu(\omega)] \ge 0$. Taking into account the causality principle and generalized Kramers and Kronig relations,²² this passivity property can be extended to complex frequencies with positive imaginary parts:

$$\operatorname{Im}[z\varepsilon(z)] \ge \operatorname{Im}(z)\varepsilon_0, \quad \operatorname{Im}[z\mu(z)] \ge \operatorname{Im}(z)\mu_0.$$
(20)

Now, let us assume that the permittivity and permeability are purely real in a frequency range of the real axis. Then, for $z = \omega + i\eta$ with $1 \gg \eta > 0$, we have

$$z\varepsilon(z) \approx \omega\varepsilon(\omega) + i\eta \frac{dz\,\varepsilon}{dz}(\omega),$$
 (21)

and thus (20) implies that the derivative of $\omega \varepsilon(\omega)$ is positive. Thus $\varepsilon(\omega)$ and $\mu(\omega)$ must be increasing functions in a frequency range without absorption.

However, for the effective parameters $\varepsilon_{\rm eff}(\omega)$ and $\mu_{\rm eff}(\omega)$, the analysis realized in the previous section reveals that one of them has to be a decreasing function. Indeed, in the limit $\omega \rightarrow 0$, standard homogenization (12) provides $\mu_{\rm eff}(0) = \mu_0$ and $\varepsilon_{\rm eff}(0) = f_1 \varepsilon_1 + f_2 \varepsilon_2 \ge \varepsilon_0$ (for a stack of transparent dielectrics in normal incidence); and, at the first band-gap edge, we have either $\varepsilon_{\rm eff}(\omega_1) = 0$ or $\mu_{\rm eff}(\omega_1) = 0$. Hence we conclude that the effective parameters $\varepsilon_{\rm eff}(\omega)$ and $\mu_{\rm eff}(\omega)$ cannot both be increasing functions, and they cannot simultaneously satisfy the passivity requirement. Similar remarks have already been reported in the literature. In particular, it has been found that the effective permeability has a negative imaginary part in periodic multilayered stacks³⁴ and metamaterials.³⁵ Also, it has been proposed that the Kramers-Kronig relations be modified³⁶ in order to allow for a negative imaginary part for the permeability.³

Thus, an alternative set of effective parameters is considered: the effective index, impedance, and magnetoelectric coupling coefficient. We start with a unit cell with a center of symmetry to keep things simple (see the Appendix for the general case with magnetoelectric coupling). The general expression of the transfer matrix is³⁴

$$T(z, \mathbf{k}) = \begin{bmatrix} a(z, \mathbf{k}) & b(z, \mathbf{k}) \\ d(z, \mathbf{k}) & a(z, \mathbf{k}) \end{bmatrix}, \quad a^2 - bd = 1.$$
(22)

TABLE I. Passivity properties in a standard homogeneous medium of permittivity $\varepsilon(z)$, permeability $\mu(z)$, propagating index n(z), and surface impedance $\zeta(z)$ for complex frequency z with a positive imaginary part.

ReImArg $z = \omega + i\eta$ >0 $\in]0, \pi[$ $z\varepsilon(z)$ >0 $\in]0, \pi[$ $z\mu(z)$ >0 $\in]0, \pi[$ $z\mu(z)$ >0 $\in]0, \pi[$ $z^{n^2}(z) = z\mu(z)z\varepsilon(z)$ $\in]0, 2\pi[$ $zn(z) = z\sqrt{\mu(z)\varepsilon(z)}$ >0 $\in]0, \pi[$ $z'^2(z) = z\mu(z)/[z\varepsilon(z)]$ $\in]-\pi, \pi[$ $z'(z) = \sqrt{\mu(z)/\varepsilon(z)}$ >0 $\in]-\pi/2, \pi/2[$				
$z = \omega + i\eta \qquad >0 \qquad \in]0,\pi[$ $z\varepsilon(z) \qquad >0 \qquad \in]0,\pi[$ $z\mu(z) \qquad >0 \qquad \in]0,\pi[$ $z^{n^{2}}(z) = z\mu(z)z\varepsilon(z) \qquad \qquad \in]0,\pi[$ $z^{n^{2}}(z) = z\mu(z)z\varepsilon(z) \qquad \qquad \in]0,\pi[$ $z^{n^{2}}(z) = z\sqrt{\mu(z)\varepsilon(z)} \qquad >0 \qquad \in]0,\pi[$ $z^{n^{2}}(z) = z\mu(z)/[z\varepsilon(z)] \qquad \qquad \in]-\pi,\pi[$ $z^{n^{2}}(z) = \sqrt{\mu(z)/\varepsilon(z)} \qquad >0 \qquad \in]-\pi/2,\pi/2[$		Re	Im	Arg
$z\varepsilon(z) > 0 \in]0,\pi[$ $z\mu(z) > 0 \in]0,\pi[$ $z^2n^2(z) = z\mu(z)z\varepsilon(z) e]0,\pi[$ $zn(z) = z\sqrt{\mu(z)\varepsilon(z)} > 0 e]0,\pi[$ $\zeta^2(z) = z\mu(z)/[z\varepsilon(z)] e]-\pi,\pi[$ $\zeta(z) = \sqrt{\mu(z)/\varepsilon(z)} > 0 e]-\pi/2,\pi/2[$	$z = \omega + i\eta$		>0	$\in]0,\pi[$
$z\mu(z) > 0 \in]0,\pi[$ $z^{2}n^{2}(z) = z\mu(z)z\varepsilon(z) \in [0,\pi[$ $zn(z) = z\sqrt{\mu(z)\varepsilon(z)} > 0 \in]0,\pi[$ $z^{2}(z) = z\mu(z)/[z\varepsilon(z)] \in [-\pi,\pi[$ $\zeta(z) = \sqrt{\mu(z)/\varepsilon(z)} > 0 \in]-\pi/2,\pi/2[$	$z\varepsilon(z)$		>0	$\in]0,\pi[$
$z^{2}n^{2}(z) = z\mu(z)z\varepsilon(z) \qquad \qquad \in]0,2\pi[$ $zn(z) = z\sqrt{\mu(z)\varepsilon(z)} \qquad >0 \qquad \in]0,\pi[$ $\zeta^{2}(z) = z\mu(z)/[z\varepsilon(z)] \qquad \qquad \in]-\pi,\pi[$ $\zeta(z) = \sqrt{\mu(z)/\varepsilon(z)} \qquad >0 \qquad \qquad \in]-\pi/2,\pi/2[$	$z\mu(z)$		>0	$\in]0,\pi[$
$zn(z) = z\sqrt{\mu(z)\varepsilon(z)} > 0 \in]0,\pi[$ $\zeta^{2}(z) = z\mu(z)/[z\varepsilon(z)] \in]-\pi,\pi[$ $\zeta(z) = \sqrt{\mu(z)/\varepsilon(z)} > 0 \in]-\pi/2,\pi/2[$	$z^2 n^2(z) = z \mu(z) z \varepsilon(z)$			$\in]0,2\pi[$
$\begin{aligned} \zeta^2(z) &= z\mu(z)/[z\varepsilon(z)] \\ \zeta(z) &= \sqrt{\mu(z)/\varepsilon(z)} \end{aligned} > 0 \qquad \qquad$	$zn(z) = z\sqrt{\mu(z)\varepsilon(z)}$		>0	$\in]0,\pi[$
$\zeta(z) = \sqrt{\mu(z)/\varepsilon(z)} > 0 \qquad \in \left] -\pi/2, \pi/2\right[$	$\zeta^2(z) = z\mu(z)/[z\varepsilon(z)]$			\in]- π , π [
	$\zeta(z) = \sqrt{\mu(z)/\varepsilon(z)}$	>0		\in]- $\pi/2,\pi/2[$

This matrix is compared with $T_{\text{eff}}(z, \mathbf{k})$, the transfer matrix corresponding to the constitutive equations (12) with $K_{\text{eff}} = 0$: Omitting the (z, \mathbf{k}) dependence, we have

$$T_{\rm eff} = \begin{bmatrix} \cos[zn_{\rm eff}h] & -i(\zeta_{\rm eff}/z)\sin[zn_{\rm eff}h] \\ -i(z/\zeta_{\rm eff})\sin[zn_{\rm eff}h] & \cos[zn_{\rm eff}h] \end{bmatrix},$$
(23)

where for *s* polarization, $z^2 n_{\text{eff}}^2 = z^2 \varepsilon_{\perp} \mu_{\parallel} - k^2 \mu_{\parallel} / \mu_3$ and $\zeta_{\text{eff}} = \mu_{\parallel} / n_{\text{eff}}$ (similar formulas for *p* polarization can be derived). By inspection of (22) and (23), the propagation index n_{eff} along the x_3 axis is defined by

$$\cos[zn_{\rm eff}(z,\boldsymbol{k})h] = a(z,\boldsymbol{k}), \tag{24}$$

and surface impedance by

$$\zeta_{\rm eff}(z, \boldsymbol{k}) = z \sqrt{\frac{b(z, \boldsymbol{k})}{d(z, \boldsymbol{k})}}.$$
(25)

Here, notice that $zn_{\text{eff}}(z, k)$ is just the Bloch wave number k_B given by (16).

As the central result of this paper, we show that the effective index $n_{\text{eff}}(z, \mathbf{k})$ and surface impedance $\zeta_{\text{eff}}(z, \mathbf{k})$ have all the properties required by causality principle and passivity. According to Table I and Kramers and Kronig relations, it is necessary to prove the following statements on the sign properties, analytic properties, and asymptotic behavior. In the upper half plane of z, i.e., for Im(z) > 0:

(i) imaginary part of $zn_{\text{eff}}(z, k)$ and real part of $\zeta_{\text{eff}}(z, k)$ are positive;

(ii) $n_{\text{eff}}(z, \mathbf{k})$ and $\zeta_{\text{eff}}(z, \mathbf{k})$ are analytic functions of z; and

(iii) $n_{\text{eff}}(z, \mathbf{k})$ and $\zeta_{\text{eff}}(z, \mathbf{k})$ have limits n_{∞} and ζ_{∞} when $|z| \rightarrow \infty$, wherein $n_{\infty} = \langle \sqrt{\epsilon \mu_0} \rangle$ corresponds to the mean index.

To prove these claims, we first use the theorem stating that no Bloch mode exists for z in the upper half plane.³⁸ As a consequence, the function $zn_{\text{eff}}(z, \mathbf{k})$ cannot be purely real and its imaginary part $\text{Im}(zn_{\text{eff}})$ cannot vanish. This proves assertion (i) for n_{eff} . Next, it is stressed that the coefficient $a(z, \mathbf{k})$ is z analytic in all the complex plane of z, and that (24) can be written

$$\exp[izn_{\rm eff}(z, k)h] = a(z, k) + i\sqrt{1 - a^2(z, k)}.$$
 (26)

Since $\text{Im}(zn_{\text{eff}})$ cannot vanish if Im(z) > 0, we have $\cos[zn_{\text{eff}}(z, \mathbf{k})h] = a(z, \mathbf{k}) \neq \pm 1$, and thus the square root in (26) is z analytic in the upper half plane. The function on

the left-hand side of (26) is then analytic and, in addition, cannot vanish. The complex logarithm can be applied to (26)without alteration of the analyticity property: This proves (ii) for n_{eff} . Next, combining the two equations $a^2 - bd = 1$ and $a \neq \pm 1$ for Im(z) > 0, it is found that neither of the two analytic functions b(z, k) and d(z, k) vanishes, thus the ratio $b(z, \mathbf{k})/d(z, \mathbf{k}) \neq 0$ is analytic. The square root in (26) preserves the analyticity property, which proves assertion (ii) for ζ_{eff} . The proof of (i) for ζ_{eff} is based on the local density of states.³⁹ The Green's function of the multilayer is calculated⁴⁰ with a point source located in the plane $x_3 = 0$: The value of the electric field in the same plane is found to be $i\pi \zeta_{\text{eff}}$. Since the imaginary part of the Green's function is positive (it corresponds to the local density of states), it follows that ζ_{eff} has a positive real part $\text{Re}(\zeta_{\text{eff}}) \ge 0$. Finally, (iii) is established by writing the complex frequency $z = |z| \exp[i\phi]$ and then taking the limit of the modulus $|z| \to \infty$. In each layer \mathcal{L}_m , let n_m and ζ_m be defined by $n_m^2 = \varepsilon_m \mu_0 - k^2/z^2$ and $\zeta_m = \mu_0/n_m$ (s polarization). Then, the expression of elementary transfer matrix (8) becomes

$$T_m = \exp[-iM_m h_m] = \begin{bmatrix} \cos[zn_m h_m] & -i(\zeta_m/z)\sin[zn_m h_m] \\ -i(z/\zeta_m)\sin[zn_m h_m] & \cos[zn_m h_m] \end{bmatrix}.$$
(27)

Using that the imaginary part of zn_m is strictly positive, the following estimate is obtained in the limit $|z| \rightarrow \infty$:

$$T_m \sim \frac{1}{|z| \to \infty} \frac{1}{2} \exp[-izn_m h_m] \begin{bmatrix} 1 & \zeta_m/z \\ z/\zeta_m & 1 \end{bmatrix}.$$
(28)

And for the transfer matrix T of a symmetric stack

$$T = T_p \cdots T_1 \underset{|z| \to \infty}{\sim} \frac{\alpha}{2} \exp[-iz\langle n \rangle h] \begin{bmatrix} 1 & \beta/z \\ z/\beta & 1 \end{bmatrix}, \quad (29)$$

where α and β are complex numbers depending on the different n_m and ζ_m , and $\langle n \rangle$ is

$$\langle n \rangle = n_1 f_1 + n_2 f_2 + \dots + n_p f_p.$$
 (30)

The expression (29) is compared to the estimate of the effective transfer matrix derived from (23):

$$T_{\rm eff} \sim \frac{1}{|z| \to \infty} \frac{1}{2} \exp[-izn_{\rm eff}h] \begin{bmatrix} 1 & \zeta_{\rm eff}/z \\ z/\zeta_{\rm eff} & 1 \end{bmatrix}.$$
 (31)

Hence the effective index and impedance have the limits

$$n_{\text{eff}} \underset{|z| \to \infty}{\sim} \langle n \rangle + i \frac{\ln(\alpha)}{zh} \underset{|z| \to \infty}{\longrightarrow} n_{\infty} = \langle n \rangle$$
(32)

and

$$\zeta_{\text{eff}} \xrightarrow[|z| \to \infty]{} \zeta_{\infty} = \beta.$$
(33)

To conclude the proof, notice that, if the wave vector \mathbf{k} is fixed and independent of the frequency z, then the numbers n_m tend to the optical indices $\sqrt{\varepsilon_m \mu_0}$ and the limit n_∞ corresponds to the mean index:

$$n_{\infty} = \sqrt{\varepsilon_1 \mu_0} f_1 + \sqrt{\varepsilon_2 \mu_0} f_2 + \dots + \sqrt{\varepsilon_p \mu_0} f_p = \langle \sqrt{\varepsilon \mu_0} \rangle.$$
(34)

For more details on these limits, see the discussion Sec. V C.



FIG. 3. (Color online) Real (left axis) and imaginary (right axis) parts of effective refractive index $n_{\text{eff}}(z)$ for $z = \omega + 0.001 \times i$, deduced from (24); Kramers-Kronig formula (35) unveils Re(n_{eff}) in plus markers; $\varepsilon_1/\varepsilon_0 = \varepsilon_3/\varepsilon_0 = 2$, $\varepsilon_2/\varepsilon_0 = 12$, $f_1 = f_3 = 0.4$, $f_2 = 0.2$, $\sqrt{\langle \varepsilon/\varepsilon_0 \rangle} = \sqrt{f_1\varepsilon_1/\varepsilon_0 + f_2\varepsilon_2/\varepsilon_0 + f_3\varepsilon_3/\varepsilon_0} = 2$, and $\langle \sqrt{\varepsilon/\varepsilon_0} \rangle = \sqrt{\varepsilon_1/\varepsilon_0} f_1 + \sqrt{\varepsilon_2/\varepsilon_0} f_2 + \sqrt{\varepsilon_3/\varepsilon_0} f_3 \approx 1.82$. The vertical dotted lines highlight the location of the first stop band.

The main result tells us that artificial frequency dispersion, i.e., z dependence (of effective parameters) generated by periodic spatial modulation, has the same properties as the natural frequency dispersion in usual media. Part (i) ensures passivity, while parts (ii) and (iii) imply that the effective parameters fulfill causality principle.³⁰ Indeed, from (ii) and (iii), the Cauchy integral formula can be applied to the function $g(z, \mathbf{k}) = n_{\text{eff}}(z, \mathbf{k}) - n_{\infty}$ to obtain Kramers and Kronig relations and their generalization:²²

$$n_{\rm eff}(z,\boldsymbol{k}) = n_{\infty} - \frac{1}{\pi} \int_{\mathbb{R}} d \, \frac{\nu \, \mathrm{Im}[n_{\rm eff}(\nu,\boldsymbol{k}) - n_{\infty}]}{z^2 - \nu^2}.$$
 (35)

Here, we used the fact that the real and imaginary parts of $n_{\text{eff}}(v, \mathbf{k})$ are, respectively, even and odd functions with respect to the real variable v (see Sec. V D).

An illustrative example in Fig. 3 confirms that this generalization of the Kramers-Kronig relations is satisfied by $n_{\text{eff}}(z, \mathbf{k})$, since the solid curve and plus markers of $\text{Re}(n_{\text{eff}})$ fit each other. Also, Fig. 3 confirms that, at the infinite frequency limit, the effective index tends to the mean refractive index $\langle \sqrt{\varepsilon} \rangle$.

For the effective surface impedance, a relation similar to the Kramers-Kronig formula is obtained applying the Cauchy formula to the function $g(z, \mathbf{k}) = \zeta_{\text{eff}}(z, \mathbf{k}) - \zeta_{\infty}$:

$$\zeta_{\rm eff}(z,\boldsymbol{k}) = \zeta_{\infty} - \frac{1}{i\pi} \int_{\mathbb{R}} d\nu \frac{\operatorname{Re}\left[\zeta_{\rm eff}(\nu,\boldsymbol{k}) - \zeta_{\infty}\right]}{z - \nu}.$$
 (36)

Figure 4 shows that the real and imaginary parts of $\zeta_{\text{eff}}(z, \mathbf{k})$ can be retrieved from the above formula, which confirms the causality property of the effective impedance. Also, it reveals that the support of the real part of $\zeta_{\text{eff}}(z, \mathbf{k})$ is reduced to the propagation bands, while the support of the imaginary part is reduced to the band gaps. Note the differences in (36) with the effective index (35) resulting from the presence of the real part (instead of the imaginary part) under the integral since it is the positive quantity. In particular, the difference of parity of the real and imaginary parts does not yield to an expression with resonances in $1/(z^2 - v^2)$ like in the Drude-Lorentz model. However, multiplying both the denominator and numerator in the integral in (36) by z + v, it is obtained that a standard



FIG. 4. (Color online) Real and imaginary parts (respectively, solid and dashed curves) of effective surface impedance $\zeta_{\text{eff}}(z)$ for $z = \omega + 0.001 \times i$, deduced from (25); while Cauchy integral formula (36) unveils Re [F(z)] in plus markers; here $\varepsilon_1 = \varepsilon_3 = (2 + 0.1 \times i)\varepsilon_0, \varepsilon_2 = (12 + 0.1 \times i)\varepsilon_0, f_1 = f_3 = 0.4$, and $f_2 = 0.2$. The vertical dotted lines highlight the location of the first stop band.

Kramers-Kronig relation holds for the ratio $\{\zeta_{\text{eff}}(z, \mathbf{k}) - \zeta_{\infty}\}/z$:

$$\frac{\zeta_{\rm eff}(z,\boldsymbol{k})-\zeta_{\infty}}{z} = -\frac{1}{i\pi} \int_{\mathbb{R}} d\nu \, \frac{\nu \operatorname{Re}\left[\{\zeta_{\rm eff}(\nu,\boldsymbol{k})-\zeta_{\infty}\}/\nu\right]}{z^2-\nu^2}.$$
(37)

The real and imaginary parts of this ratio are shown in Fig. 5. The structure of the real and imaginary parts of this quantity is similar to that of the effective index, except that the imaginary part of $\{\zeta_{\text{eff}}(z, \mathbf{k}) - \zeta_{\infty}\}/z$ can be positive and negative. Indeed, within the band gaps, the real part of function $\{\zeta_{\text{eff}}(\omega, \mathbf{k}) - \zeta_{\infty}\}/\omega$ takes the values of $-\zeta_{\infty}/\omega$ and thus behaves like $-1/\omega$, as evidenced in Fig. 5. As for the effective index, in the *p*th band gap, the real part of $\omega n_{\text{eff}}(\omega)h$ is equal to the constant $p\pi$, and thus

$$\operatorname{Re}[n_{\rm eff}(\omega)] = \frac{p\pi}{\omega h},\tag{38}$$

which behaves like $1/\omega$ (see Fig. 3).



FIG. 5. (Color online) Quantity $\{\zeta_{\text{eff}}(z) - \zeta_{\infty}\}/z$ as a function of the frequency $z = \omega + 0.001 \times i$. The parameters defining the multilayer are given in the caption of Fig. 3. The vertical dotted lines highlight the location of the first stop band.

V. DISCUSSION

A. Frequency dispersion of the materials

The main result remains valid when (natural) frequency dispersion is considered in the dielectric permittivity [e.g., dielectric constants $\varepsilon_m(z)$]. Indeed, permittivity is analytic in the upper half plane of z and theorems on the existence of Bloch modes and the imaginary part of the Green's function can be applied to the most general cases.^{22,38} A difference is that the analytic properties of transfer matrix become the same as those of the dielectric permittivity. Hence, with frequency dispersion, the transfer matrix is analytic in the upper half plane of z, and the radius of the convergence disk of effective parameters in Fig. 2 might be reduced by the frequency resonances of the materials. Also, when natural frequency dispersion is considered, all the dielectric constants $\varepsilon_m(z)$ tend to the vacuum permittivity ε_0 when $|z| \to \infty$. In that case, getting the limits n_{∞} and ζ_{∞} is straightforward, for they take the values of index and impedance in vacuum, i.e., $\sqrt{\varepsilon_0\mu_0}$ and $\sqrt{\mu_0/\varepsilon_0}$, respectively.

B. Homogenization at infinite frequency

It has been shown that the effective index and impedance have a limit when the modulus |z| of the complex frequency tends to infinity. This property is sufficient to close the integration path in the Cauchy integral formula by a semicircle with infinite radius, and to obtain Kramers-Kronig relations like (35) and (36). The same result can be obtained for purely real frequency ω tending to infinity. In this case, it is necessary to add an arbitrarily small absorption to all dielectric constants $\varepsilon_m(z)$. After passing to the limit $\omega \to \infty$, the arbitrarily small absorption can be canceled (low absorption limit). Figure 6 shows an example in which the effective impedance tends to $\zeta_{\infty} = \zeta_1 = \sqrt{\mu_0/\varepsilon_1}$ when $\omega \to \infty$ in the complex frequency $z = \omega + 0.001 \times i$: A small absorption has been introduced in the permittivities of the dielectrics to enforce the convergence of the effective surface impedance.

The limits n_{∞} and ζ_{∞} , given by (34) and (33), have been obtained for a fixed wave vector \mathbf{k} which is independent of the frequency z. The limits can also be identified for a fixed angle of incidence θ ($\theta = 0$ at normal incidence). Let \mathbf{u} be the vector defined by $\mathbf{k} = z\mathbf{u}$: It is related to the angle of incidence



FIG. 6. (Color online) Effective impedance $\zeta_{\text{eff}}(z)$ for $z = \omega + 0.001 \times i$ at large frequency ω . The parameters defining the multilayer are given in the caption of Fig. 4.

by $u^2 = \varepsilon_0 \mu_0 \sin^2 \theta$. Then all the calculations of the limits n_∞ and ζ_∞ (see Sec. IV) remain valid for $n_m^2 = \varepsilon_m \mu_0 - u^2$ and $\zeta_m = \mu_0/n_m$. In particular, the limit of the effective index is

$$n_{\infty} = \sqrt{\varepsilon_1 \mu_0 - \boldsymbol{u}^2} f_1 + \dots + \sqrt{\varepsilon_p \mu_0 - \boldsymbol{u}^2} f_p. \quad (39)$$

Specifically, for small angles $\theta \ll 1$, the square roots $\sqrt{\varepsilon_m \mu_0 - u^2}$ can be approached by $\sqrt{\varepsilon_m \mu_0} - u^2/(2\sqrt{\varepsilon_m \mu_0})$ and the multilayered stack becomes an anisotropic homogeneous medium with the dispersion law

$$\frac{k_B^2}{\langle\sqrt{\varepsilon\mu_0}\,\rangle^2} + \frac{\boldsymbol{k}^2}{\langle\sqrt{\varepsilon\mu_0}\,\rangle/\langle 1/\sqrt{\varepsilon\mu_0}\,\rangle} = z^2,\tag{40}$$

where $k_B = z n_{\text{eff}}(z)$ is the Bloch wave number, $\langle \sqrt{\varepsilon \mu_0} \rangle$ is the mean index (34), and

$$\langle 1/\sqrt{\varepsilon\mu_0} \rangle = \frac{f_1}{\sqrt{\varepsilon_1\mu_0}} + \frac{f_2}{\sqrt{\varepsilon_2\mu_0}} + \dots + \frac{f_p}{\sqrt{\varepsilon_p\mu_0}}.$$
 (41)

Here, it is found that the homogenization of periodic layered media proposed by Rytov⁴¹ can be extended to infinite frequency. In particular, the dispersion law (40) shows that, for a binary grating in grazing angle (i.e., $\theta \ll 1$ with the present notations), the components of the anisotropic effective index are related to the mean refractive index $\langle \sqrt{\varepsilon \mu_0} \rangle$, as in usual media for very high frequencies of neutrons.⁴²

Finally, from the expression (38), we note that for high frequency the *p*th band gap is centered around the frequency

$$\nu_p = \frac{p\pi}{n_\infty h}.\tag{42}$$

This estimate of the frequency center ω_p of the *p*th band gap had already been discovered⁴³ in the particular case of a periodic multilayer made of two alternative layers with identical optical thickness.

C. Extension of results to two dimensions and three dimensions

The possibility to extend our results to frequency dispersive three-dimensional periodic structures is discussed. Using the auxiliary field formalism,^{22,38} Maxwell's equations can be written as the unitary time evolution equation $[\partial F/\partial t](t) =$ $-i\mathbf{K}F(t)$, where K is selfadjoint and time independent (see also the frame of extension of dissipative operators⁴⁴). Consequently the resolvent $[z - \mathbf{K}]^{-1}$ is analytic if $\mathrm{Im}(z) > 0$, which prevents the existence of Bloch modes in the upper half-plane of z. Moreover the imaginary part of the Green's function is always positive for $\mathrm{Im}(z) > 0$ since the operator

$$-\frac{1}{2i}\left[\frac{1}{z-\mathsf{K}}-\frac{1}{\overline{z}-\mathsf{K}}\right] = \operatorname{Im}(z)\frac{1}{z-\mathsf{K}}\frac{1}{\overline{z}-\mathsf{K}} \ge 0 \qquad (43)$$

is positive. Assuming that appropriate effective parameters can be defined (see general notions of impedance in Refs. 45–47), these two properties on Bloch modes and the imaginary part of the Green's function can be used to prove causality principle and passivity. It is, however, stressed that such a generalization remains a challenging task: In particular, special attention should be paid to situations where single-mode Bloch approximation does not apply,⁴⁷ and to analytic continuations of Bloch wave number and impedance for complex *z*.

D. Artificial causality

The results presented in Sec. IV are established from a system with frequency-independent dielectric constants. Thus the different materials in the multilayer are not subject to the causality principle. Yet it has been shown that effective parameters $n_{\text{eff}}(z, k)$ and $\zeta_{\text{eff}}(z, k)$ possess all the properties required by causality principle. Thus, the artificial dispersion resulting from the mixing of different media has similar properties to natural dispersion generated at the atomic scale. In particular, let us assume that the dielectric constants ε_m become their complex conjugated $\overline{\varepsilon_m}$ when the complex frequency z passes across the imaginary axis (i.e., $z \rightarrow -\overline{z}$). Then it is found that the real and imaginary parts of the functions $n_{\rm eff}(\omega, \mathbf{k})$ and $\zeta_{\rm eff}(\omega, \mathbf{k})$ are, respectively, even and odd functions with respect to the real variable ω . Hence the effective parameters $n_{\rm eff}(z)$ and $\zeta_{\rm eff}(z)$ can be derived from real functions $\chi_n(t)$ and $\chi_{\zeta}(t)$ which vanish for negative times. As pointed out in Sec. VA, all these results remain valid when natural dispersion is taken into account. In this case both natural and artificial dispersions are superimposed (see Ref. 43 for a representation of such superimposition).

As a final remark, it is stressed that our investigations on artificial dispersion have shown that the effective index $n_{\rm eff}(z)$ and impedance $\zeta_{\rm eff}(z)$ are better suited than the effective permittivity $\varepsilon_{\rm eff}(z)$ and permeability $\mu_{\rm eff}(z)$ to describe the effective medium of multilayered stacks at higher frequencies. A similar conclusion is drawn in Ref. 30, §87, where it is indicated: "As the frequency increases, the spatial nonuniformity of the field renders impossible a macroscopic description of it in terms of the permittivity ε ; however, a boundary condition" expressed with the impedance "still holds at such frequencies."

VI. CONCLUSION

In summary, we have shown it is possible to replace a periodic multilayered stack at all frequencies by a homogeneous effective medium. At low frequencies, analytic expressions of effective permittivity, permeability, and magnetoelectric coupling have been derived. At higher frequencies, we find it is more appropriate to consider instead effective propagation index and surface impedance. Artificial frequency dispersion is then shown to possess the same properties as natural dispersion in terms of passivity and causality: Remarkably it follows that a periodic arrangement of frequency-independent (and thus noncausal) dielectric materials makes artificial causality. These results, based on general properties of existence of Bloch modes and the sign of the imaginary part of the Green's function, open new avenues toward AFH for frequency dispersive and three-dimensional periodic structures. The AHF theory which we proposed can also be applied to phononic^{21,48} and platonic⁴⁹ crystals, as well as other wave or diffusion equations.

APPENDIX: ALL FREQUENCY HOMOGENIZATION WITH MAGNETOELECTRIC COUPLING

The main result of this paper is extended to the general case: A multilayered stack with nonsymmetric unit cells,

where artificial magnetoelectric coupling ensues. The general expression of the transfer matrix is³⁴

$$T(z, \mathbf{k}) = \begin{bmatrix} a(z, \mathbf{k}) & b(z, \mathbf{k}) \\ c(z, \mathbf{k}) & d(z, \mathbf{k}) \end{bmatrix}, \quad ad - bc = 1.$$
(A1)

This matrix is compared to $T_{\text{eff}}(z, \mathbf{k})$, the transfer matrix corresponding to the constitutive equations (12): Its expression is

$$T_{\rm eff}(z, \boldsymbol{k}) = \begin{bmatrix} a_{\rm eff}(z, \boldsymbol{k}) & b_{\rm eff}(z, \boldsymbol{k}) \\ c_{\rm eff}(z, \boldsymbol{k}) & d_{\rm eff}(z, \boldsymbol{k}) \end{bmatrix},$$
(A2)

where, omitting the (z, k) dependence,

$$a_{\rm eff} = \cos[zn_{\rm eff}h] - \frac{K_{\rm eff}}{n_{\rm eff}} \sin[zn_{\rm eff}h],$$

$$b_{\rm eff} = -i\frac{\zeta_{\rm eff}}{z} \sin[zn_{\rm eff}h],$$

$$c_{\rm eff} = -i\frac{z}{\zeta_{\rm eff}} \frac{n_{\rm eff}^2 + K_{\rm eff}^2}{n_{\rm eff}^2} \sin[zn_{\rm eff}h],$$

$$d_{\rm eff} = \cos[zn_{\rm eff}h] + \frac{K_{\rm eff}}{n_{\rm eff}} \sin[zn_{\rm eff}h].$$
 (A3)

First the effective index is defined by

$$\cos[zn_{\rm eff}(z,\boldsymbol{k})h] = \frac{a(z,\boldsymbol{k}) + d(z,\boldsymbol{k})}{2}, \qquad (A4)$$

and then the effective impedance and magnetoelectric coupling are defined via $n_{\text{eff}}(z, \mathbf{k})$ by

$$\zeta_{\rm eff}(z, \mathbf{k}) = \frac{iz}{\sin[zn_{\rm eff}(z, \mathbf{k})h]} b(z, \mathbf{k}),$$
$$K_{\rm eff}(z, \mathbf{k}) = \frac{n_{\rm eff}(z, \mathbf{k})}{\sin[zn_{\rm eff}(z, \mathbf{k})h]} \frac{d(z, \mathbf{k}) - a(z, \mathbf{k})}{2}.$$
 (A5)

The arguments to show the properties of the effective index $n_{\text{eff}}(z, \mathbf{k})$ are exactly the same as in Sec. IV. Next note that, for Im(z) > 0, the imaginary part of $zn_{\text{eff}}(z, \mathbf{k})$ is strictly positive. Therefore the function $\sin[zn_{\text{eff}}(z, \mathbf{k})h]$ cannot vanish, which



FIG. 7. (Color online) Effective magnetoelectric coupling $K_{\rm eff}(z)$ for $z = \omega + 0.001 \times i$. The curve depicted by red crosses indicates the value of Re[$K_{\rm eff}(z)$] deduced by the Kramers and Kronig relation. The parameters defining the multilayer are given in the caption of Fig. 3.

implies that the parameters $\zeta_{\text{eff}}(z, k)$ and $K_{\text{eff}}(z, k)$ are analytic functions in the upper half-plane of complex frequencies.

In the limit of infinite frequency, the transfer matrix T of a stack takes the form

$$T \sim_{|z| \to \infty} \frac{1}{2} \exp[-iz\langle n \rangle h] \begin{bmatrix} \alpha & \beta/z \\ z/\gamma & \delta \end{bmatrix},$$
 (A6)

where α , β , γ , and δ are complex numbers depending on the different n_m and ζ_m . Hence the effective parameters have the limits

$$n_{\text{eff}} \xrightarrow{|z| \to \infty} n_{\infty} = \langle n \rangle,$$

$$\zeta_{\text{eff}} \xrightarrow{|z| \to \infty} \zeta_{\infty} = \beta,$$

$$K_{\text{eff}} \xrightarrow{|z| \to \infty} K_{\infty} = i \langle n \rangle \frac{\alpha - \delta}{\alpha + \delta}.$$
(A7)

Again, the Cauchy integral formula can be applied to the function $K(z, \mathbf{k}) = K_{\text{eff}} - K_{\infty}$, and the general Kramers-Kronig relations are evidenced in Fig. 7.

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