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A fundamental relation between phase and group velocity, and application to the failure of perfectly matched layers in backward-wave structures

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We demonstrate that the ratio of group to phase velocity has a simple relationship to the orientation of the electromagnetic field. In non-dispersive materials, opposite group and phase velocity corresponds to fields that are mostly oriented in the propagation direction. More generally, this relationship (including the case of dispersive and negative-index materials) offers a perspective on the phenomena of backward waves and left-handed media. As an application of this relationship, we demonstrate and explain an irrecoverable failure of perfectly matched layer absorbing boundaries in computer simulations, for constant cross-section waveguides with backward-wave modes, and suggest an alternative in the form of adiabatic isotropic absorbers.

PACS numbers: 41.20.Jb, 42.25.Bs, 42.79.Gn, 02.70.-c

I. INTRODUCTION

Recent years have seen a renewed interest in “left-handed” media in which the phase velocity (v_p) and group velocity (v_g) of waves are anti-parallel. Such media include theoretical negative-index ($\epsilon, \mu < 0$) media and their metamaterial realizations [1, 2], wavelength-scale periodic media that mimic some qualitative features of negative-index media [3–5] while not having a strictly well-defined v_p [6], and certain uniform cross-section positive-index waveguides with “backward-wave” modes [7, 8]. In this Rapid Communication, we derive a fundamental relationship between v_p , v_g , and the orientation of the fields, for any medium $\{\epsilon(x, y), \mu(x, y)\}$, where z -invariance ensures that the phase velocity in the z direction is unambiguously defined. In particular, we prove that, for non-dispersive materials:

$$v_g = v_p(f_t - f_z), \quad (1)$$

where f_t and f_z are the fractions of the electromagnetic (EM) field energy in the transverse (xy) and longitudinal (z) directions, respectively. Thus, the appearance of backward-wave modes ($v_p v_g < 0$) in non-dispersive media coincides with the fields being mostly oriented in the longitudinal direction (that is, $f_z > f_t$). The situation of negative-index media involves material dispersion and requires a modified equation discussed below. As an application of eq. (1), we identify and explain a fundamental failure of perfectly matched layers (PML), widely used as absorbing boundaries in simulating wave equations [9], for backward-wave structures. In particular, the stretched-coordinate derivation of PML suggests that such waves should be exponentially growing in the PML,

and we explain this physically by pointing out that PML is an anisotropic “absorber” with *gain* in the longitudinal direction, which dominates for backward-wave modes due to eq. (1). In inhomogeneous backward-wave media, unlike homogeneous negative-index media [10, 11], we argue that the only recourse is to abandon PML completely in favor of adiabatic non-PML absorption tapers [12] (unrelated to the failure of PML in periodic media described in our previous work [12]).

In what follows, we first review the fixed-frequency eigenproblem formulation of Maxwell’s equations [13, 14] and then use this to derive eq. (1) (an immediate precursor of which can also be found in our book [14]). We discuss the case of dispersive and negative-index media. Then, we review important cases of positive-index non-dispersive geometries with backward-wave modes, and argue that PML irredeemably fails in such geometries. This failure can be physically understood in light of eq. (1). We close by proposing a non-PML alternative for such cases.

II. RELATING GROUP AND PHASE VELOCITIES

A. Notation and review of the generalized Hermitian eigenproblem

Employing Dirac notation, Maxwell’s equations with time-harmonic fields of frequency ω can be cast (exactly) in the following form [13, 14]:

$$\hat{A}|\psi\rangle = -i\frac{\partial}{\partial z}\hat{B}|\psi\rangle, \quad (2)$$

where $|\psi\rangle$ is the four-component state vector

$$|\psi\rangle \equiv \begin{pmatrix} \mathbf{E}_t(x, y, z) \\ \mathbf{H}_t(x, y, z) \end{pmatrix} e^{-i\omega t} \quad (3)$$

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containing the transverse fields E_x, E_y, H_x, H_y , and the operators \hat{A} and \hat{B} are given by

$$\hat{A} \equiv \begin{pmatrix} \omega\varepsilon/c - \frac{c}{\omega}\nabla_t \times \frac{1}{\mu}\nabla_t \times & 0 \\ 0 & \omega\mu/c - \frac{c}{\omega}\nabla_t \times \frac{1}{\varepsilon}\nabla_t \times \end{pmatrix} \quad (4)$$

(where ε and μ are the relative permittivity and permeability) and

$$\hat{B} \equiv \begin{pmatrix} 0 & -\hat{\mathbf{z}} \times \\ \hat{\mathbf{z}} \times & 0 \end{pmatrix} = \begin{pmatrix} & & 1 \\ & -1 & \\ 1 & & \end{pmatrix} = \hat{B}^{-1}. \quad (5)$$

Moreover, under the inner product

$$\langle \psi | \psi' \rangle \equiv \int \mathbf{E}_t^* \cdot \mathbf{E}_t' + \mathbf{H}_t^* \cdot \mathbf{H}_t', \quad (6)$$

both \hat{A} and \hat{B} are Hermitian.

Specializing to the case of a z -uniform material allows us to choose modes with fixed propagation constant β , i.e.,

$$|\psi\rangle = e^{i(\beta z - \omega t)} |\beta\rangle \quad (7)$$

where $|\beta\rangle$ is z -uniform [6]. In this case eq. (2) immediately reduces to

$$\hat{A}|\beta\rangle = \beta \hat{B}|\beta\rangle, \quad (8)$$

which is a generalized Hermitian eigenproblem in β .

B. Case of continuous z -translational symmetry

The group velocity v_g can be derived from eq. (8). Viewing \hat{A} as an operator parametrized by ω , we know by the Hellmann-Feynman theorem [6] that the eigenvalues β of eq. (8) vary with ω according to

$$\frac{1}{v_g} = \frac{\partial \beta}{\partial \omega} = \frac{\langle \beta | \frac{\partial \hat{A}}{\partial \omega} | \beta \rangle}{\langle \beta | \hat{B} | \beta \rangle} = \frac{\langle \beta | \frac{\partial \hat{A}}{\partial \omega} | \beta \rangle}{\frac{1}{\beta} \langle \beta | \hat{A} | \beta \rangle}. \quad (9)$$

Plugging in eqs. (4) and (6)—assuming that the material is non-dispersive, so that \hat{A} has only the explicit ω -dependence and $\frac{\partial \hat{A}}{\partial \omega}$ simplifies—the numerator of eq. (9) evaluates to

$$\begin{aligned} & \frac{1}{c} \int \mathbf{E}_t^* \cdot \left(\varepsilon \mathbf{E}_t + \frac{c^2}{\omega^2} \nabla_t \times \frac{1}{\mu} \nabla_t \times \mathbf{E}_t \right) + \\ & \frac{1}{c} \int \mathbf{H}_t^* \cdot \left(\mu \mathbf{H}_t + \frac{c^2}{\omega^2} \nabla_t \times \frac{1}{\varepsilon} \nabla_t \times \mathbf{H}_t \right). \end{aligned} \quad (10)$$

Splitting the first integral into two summands, we obtain an $\int \varepsilon |\mathbf{E}_t|^2$ contribution from the first term; as for the second, integrating by parts gives

$$\int \frac{c^2}{\omega^2} (\nabla_t \times \mathbf{E}_t)^* \cdot \frac{1}{\mu} (\nabla_t \times \mathbf{E}_t) = \int \mu |H_z|^2, \quad (11)$$

where we used the relation $\nabla_t \times \mathbf{E}_t = i \frac{\omega}{c} \mu H_z \hat{\mathbf{z}}$ in the last step. Simplifying the second integral in an analogous manner and putting everything together, we find

$$\left\langle \beta \left| \frac{\partial \hat{A}}{\partial \omega} \right| \beta \right\rangle = \frac{1}{c} \int \varepsilon |\mathbf{E}_t|^2 + \mu |\mathbf{H}_t|^2 + \varepsilon |E_z|^2 + \mu |H_z|^2. \quad (12)$$

By a similar computation, we may rewrite the denominator of eq. (9) as

$$\frac{1}{\beta} \langle \beta | \hat{A} | \beta \rangle = \frac{\omega}{c\beta} \int \varepsilon |\mathbf{E}_t|^2 + \mu |\mathbf{H}_t|^2 - \varepsilon |E_z|^2 - \mu |H_z|^2. \quad (13)$$

Thus,

$$v_g = \frac{\omega}{\beta} \cdot \frac{\int \varepsilon |\mathbf{E}_t|^2 + \mu |\mathbf{H}_t|^2 - \varepsilon |E_z|^2 - \mu |H_z|^2}{\int \varepsilon |\mathbf{E}_t|^2 + \mu |\mathbf{H}_t|^2 + \varepsilon |E_z|^2 + \mu |H_z|^2}, \quad (14)$$

from which eq. (1) follows.

C. Subtleties with dispersive media and negative index materials

In deriving eqs. (14) and (1), we assumed that the constituent materials were non-dispersive. If ε and μ are ω -dependent, but we assume that absorption loss is negligible (so that the problem is still Hermitian), then $\partial \hat{A} / \partial \omega$ in eq. (9) has additional terms that change the denominator of eq. (14) to

$$\int \frac{d\omega \varepsilon}{d\omega} |\mathbf{E}|^2 + \frac{d\omega \mu}{d\omega} |\mathbf{H}|^2, \quad (15)$$

which is precisely the energy density of the EM field in a dispersive medium with negligible loss [15, 16]. Because the denominator has changed while the numerator is unchanged, one can no longer interpret the ratio as $f_t - f_z$. An interesting example of such a case is a negative-index metamaterial, in which ε and μ are negative in some frequency range with low loss [1, 2]. In this case, the numerator of eq. (14) flips sign, while the new denominator, eq. (15), is still positive (leading to a positive energy density [2, 16]). Hence in a dispersive negative-index medium a purely transverse field ($E_z = H_z = 0$) has opposite phase and group velocity. A non-dispersive negative-index medium is not physical (it violates the Kramers-Kronig relations [15, 16]); the definition of v_g in such a case is subtle and somewhat artificial (naively, the energy density is negative) and is not discussed here.

An interesting application of eq. (1) is to backward-wave waveguides made of positive-index materials. For example, a hollow metallic waveguide containing a concentric dielectric cylinder was shown to support backward-wave modes [7]. More recently, the same phenomenon was demonstrated in all-dielectric (positive-index, non-dispersive) photonic-crystal Bragg and holey fibers, and in general can be explained as an avoided eigenvalue crossing from a forced degeneracy at $\beta = 0$ [8].

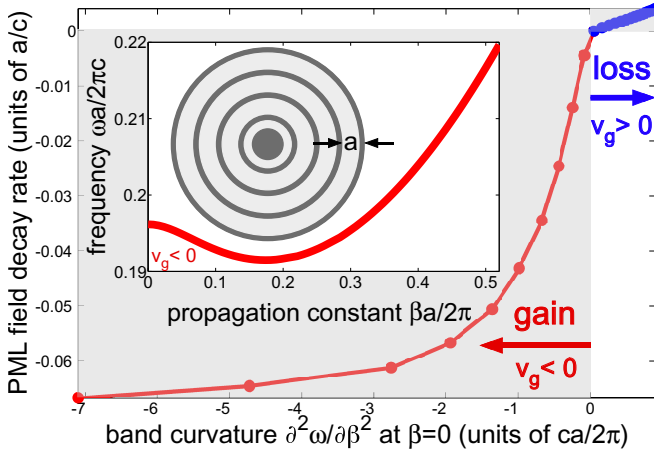


FIG. 1: Field decay rate within the PML vs. curvature of the dispersion relation at $\beta = 0$, showing onset of gain for $v_g < 0$ and loss for $v_g > 0$. *Inset.* Dispersion relation (of the first TE band) with $v_g < 0$ region at $\beta = 0$, and cross-section of the Bragg fiber.

An example of such a structure is shown in the inset of Fig. 1, which shows the cross-section of a Bragg fiber formed by alternating layers of refractive indices $n_{hi} = 4.6$ (thickness $0.25a$) and $n_{lo} = 1.4$ (thickness $0.75a$) with period a . The central high-index core has radius $0.45a$ and the first low-index ring has thickness $0.32a$. For this geometry, one of the guided modes (with angular dependence $e^{im\phi}$ and $m = 1$) has the dispersion relation $\omega(\beta)$ shown in the inset of Fig. 1: at $\beta = 0$, $d^2\omega/d\beta^2 < 0$, resulting in a downward-sloping backward-wave region with $v_g v_p < 0$. As the index of the core cylinder is varied, this curvature can be changed from negative to positive in order to eliminate the backward-wave region. Equation (1) tells us that the backward-wave region coincides with fields that are mostly oriented in the z (axial) direction.

A further consequence of eq. (1) appears if we consider the problem of terminating a waveguide like the one in Fig. 1(inset) in a computer simulation. A standard approach is to terminate the waveguide with a perfectly matched absorbing layer, which is an artificial absorbing material constructed so as to be theoretically reflectionless [9]. PML is reflectionless because it corresponds merely to a complex coordinate stretching $z \rightarrow (1 + \frac{i\sigma}{\omega})z$, so that propagating waves $e^{i\beta z}$ are transformed into exponentially decaying waves $e^{i\beta z - \sigma z/v_p}$ for some PML strength σ . From this perspective, an obvious problem occurs for backward waves: if $v_p < 0$ for $v_g > 0$, then a $+z$ -propagating wave ($v_g > 0$) will undergo exponential growth for $\sigma > 0$. (This is entirely distinct from the failure of PML in a medium periodic in the z direction, which in that case is due to the nonanalyticity of Maxwell's equations [12] and leads to reflections but not instability.) In a homogeneous backward-wave medium, this problem can be solved merely by making $\sigma < 0$ in the negative-index frequency ranges [10, 11]. This solu-

tion is impossible in the case of Fig. 1(inset), however, because at the same ω one has both forward and backward waves—no matter what sign is chosen for σ , one of these waves will experience exponential growth in the PML.

Precisely this exponential growth is observed in Fig. 1. We simulated the backward-wave structure of Fig. 1(inset) with a finite-difference time-domain (FDTD) simulation in cylindrical coordinates [9, 17], terminated in the z direction with PML layers. Both the forward- and backward-wave modes were excited with a short-pulse current source, and the fields in the PML region after a long time were fit to an exponential in order to determine the decay rate. Figure 1 plots this decay rate as a function of the curvature $d^2\omega/d\beta^2|_{\beta=0}$ as the core-cylinder index is varied from 2.6 to 5.0. The appearance of negative curvature, which indicates the appearance of a backward-wave region, precisely coincides with the decay rate changing sign to exponential growth.

This exponential growth is fully explained by the coordinate-stretching viewpoint of PML, but physically it may still seem somewhat mysterious: PML can also be viewed as an artificial anisotropic absorbing medium [9], so how can an absorbing medium lead to gain? The answer lies in the anisotropy of PML: as we review below, PML is actually a gain medium in the z direction, and in fact eq. (1) precisely explains how backward waves cause the z principal axis of the PML to dominate and produce a net gain. In particular, we look at the case where σ is small, so that we can analyze the effect of the PML with perturbation theory.

Using the $e^{-i\omega t}$ time convention as above, a z -absorbing PML for an isotropic material is obtained by multiplying ϵ and μ by the (anisotropic) tensor [9]

$$\begin{pmatrix} 1 + \frac{i\sigma}{\omega} & & \\ & 1 + \frac{i\sigma}{\omega} & \\ & & (1 + \frac{i\sigma}{\omega})^{-1} \end{pmatrix} \quad (16)$$

To first order in σ , this changes ϵ and μ by

$$\Delta\epsilon \approx \frac{i\sigma\epsilon}{\omega} \begin{pmatrix} 1 & & \\ & 1 & \\ & & -1 \end{pmatrix}, \quad \Delta\mu \approx \frac{i\sigma\mu}{\omega} \begin{pmatrix} 1 & & \\ & 1 & \\ & & -1 \end{pmatrix}. \quad (17)$$

Note the -1 in the z axis, which flips the sign of the imaginary part and hence corresponds to gain if the xy axes are loss. From standard perturbation theory, the first-order change in ω resulting from perturbations $\Delta\epsilon$ and $\Delta\mu$ is given by [18]:

$$\frac{\Delta\omega}{\omega} \approx -\frac{\int \mathbf{E}^* \Delta\epsilon \mathbf{E} + \mathbf{H}^* \Delta\mu \mathbf{H}}{\int \epsilon |\mathbf{E}|^2 + \mu |\mathbf{H}|^2}. \quad (18)$$

Substituting eq. (17), we find that

$$\begin{aligned} \Delta\omega &\approx -i\sigma \cdot \frac{\int \epsilon |\mathbf{E}_t|^2 + \mu |\mathbf{H}_t|^2 - \epsilon |E_z|^2 - \mu |H_z|^2}{\int \epsilon |\mathbf{E}_t|^2 + \mu |\mathbf{H}_t|^2 + \epsilon |E_z|^2 + \mu |H_z|^2} \\ &= -i\sigma(f_t - f_z) = -i\sigma \cdot \frac{v_g}{v_p} \end{aligned} \quad (19)$$

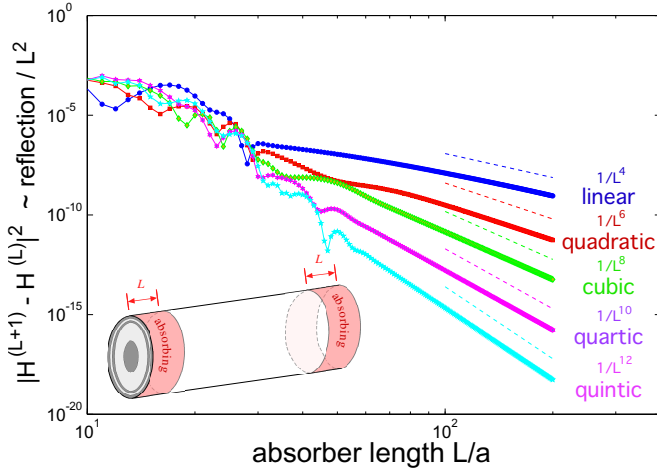


FIG. 2: Field convergence ($\sim \text{reflection}/L^2$) vs. absorber length for various σ ranging from linear [$\sigma(z/L) \sim (z/L)$] to quintic [$\sigma(z/L) \sim (z/L)^5$]. For reference, the corresponding asymptotic power laws are shown as dashed lines. *Inset*: Bragg-fiber structure in cylindrical computational cell with absorbing regions used in simulation.

upon applying our identity eq. (1).

The ramifications for PML behavior are now immediately apparent: turning on a small σ leads to an additional time-dependent exponential factor

$$\exp\left(-\frac{v_g}{v_p} \cdot \sigma t\right). \quad (20)$$

In the usual case in which group and phase velocities are oriented in the same direction, the overall rate constant is negative and this causes absorptive loss in the PML. In the case of backward waves, however, the ratio v_g/v_p is negative, and thus the overall rate constant is positive, i.e., PML produces gain. Physically, we can now understand the ratio v_g/v_p as determining whether the fields are mostly transverse or mostly longitudinal and hence whether the PML loss (xy axes) or gain (z axis) dominates. Forward waves are mostly transverse and hence ordinary PML is lossy. (Waveguides with backwards waves also possess complex- β evanescent waves [8], and we believe that these may also have gain in the PML, but as their appearance always coincides with the appearance of backwards-wave modes we focus on the instabilities due to the latter.)

D. Numerical results, modifications and alternatives to PML

With the understanding that the standard formulation of PML fails for backward waves, we now turn to a discussion of what can be done instead. As pointed out above, previous corrections for left-handed media [10, 11]

are inapplicable here because one has forward and backward waves at the same ω . Since the reflectionless property of PML fundamentally arises from the coordinate-stretching viewpoint, and gain is predicted by coordinate-stretching above, we are led to the conclusion that PML must be abandoned entirely for such backward-wave structures. The alternative is to use a scalar absorbing material, e.g. a scalar conductivity σ , which is absorbing for all field orientations and therefore cannot lead to gain (unlike our previous work where an anisotropic “pseudo-PML” could still be employed [12]). At the interface of such a material, however, there will be reflections. Such reflections can be made arbitrarily small, however, by turning on the absorption by a sufficiently gradual taper transition, similar to our approach for an unrelated failure of PML [12]. Even for PML, numerical reflections due to discretization require a similar gradual σ taper. In both cases, the reflection $R(L)$ goes to zero as the absorber thickness L is made longer (and more gradual), and the impact of PML (when it works) is merely to multiply $R(L)$ by a smaller constant coefficient [12]. Even without PML, the rate at which $R(L)$ goes to zero can be made more rapid by reducing the discontinuity in σ : for example, if $\sigma \sim (z/L)^2$ (for $z > 0$) then its second derivative is discontinuous at the transition $z = 0$ and $R(L)$ consequently scales as $1/L^4$, while if $\sigma \sim (z/L)^3$ then $R(L) \sim 1/L^6$. Figure 2 shows how a scalar conductivity σ can be used as a last-resort replacement for PML in the backward-wave structure of Fig. 1(inset). The plot shows the difference-squared of the magnetic field at a test point for absorber lengths L and $L+1$ (which scales as $R(L)/L^2$) [12] versus L for various conductivity profiles σ . Even with both forward and backward waves excited, the reflection can indeed be made small for a sufficiently thick absorber (albeit thicker than a PML for purely forward-wave modes) and displays the expected scaling $1/L^{2d+2}$ for $\sigma \sim (z/L)^d$ [12].

Colloquially, the term “left-handed medium” is sometimes applied to photonic-crystal structures with periodicity on the same scale as the wavelength that mimic some qualitative feature of negative-index media, such as negative refraction [3, 4]. In such media, however, the phase velocity v_p is not uniquely defined (any reciprocal lattice vector can be added to β) [6], so eq. (1) is not directly applicable. It may be interesting, however, to use eq. (1) as the *definition* of v_p in periodic media, in which case it turns out that one obtains a result similar in spirit to previous work that defined v_p as a weighted average of the phase velocity of each Fourier component [5].

This work was supported in part by the National Defense Science and Engineering Council, the MRSEC Program of the National Science Foundation under award number DMR-0819762, and the Army Research Office through the Institute for Soldier Nanotechnologies under Contract No. DAAD-19-02-D0002.

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