Folded bands in metamaterial photonic crystals

P Y Chen¹, C G Poulton², A A Asatryan², M J Steel³, L C Botten², C Martijn de Sterke¹ and R C McPhedran¹, ⁴

¹ Institute of Photonics and Optical Science (IPOS) and Centre for Ultrahigh bandwidth Devices for Optical Systems (CUDOS), School of Physics, University of Sydney, NSW 2006, Australia
² CUDOS, School of Mathematical Sciences, University of Technology, Sydney, NSW 2007, Australia
³ MQ Photonics Research Centre, CUDOS and Department of Physics and Astronomy, Macquarie University, Sydney, NSW 2109, Australia
E-mail: ross@physics.usyd.edu.au

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Abstract. The dispersion relation of periodic structures that include metamaterials or materials with large anomalous dispersion can give bands with infinite group velocity points. These bands do not span the entire first Brillouin zone but are instead localized in k-space. We show that these points arise when both positive and negative elements are present, with the group index rather than the refractive index being the controlling quantity. A rigorous condition and two approximations are derived, each showing that an appropriate weighted average of group index being zero leads to infinite group velocity points.

⁴ Author to whom any correspondence should be addressed.
Metamaterials have attracted significant research interest recently because they can be tailored to produce material parameters not found in nature, in particular allowing for a negative refractive index. These new material parameters can lead to novel physical phenomena in otherwise familiar physical systems. In the field of photonic crystals, metamaterials enable previously unobserved band structures. For example, Li et al [1] found that combinations of positive and negative refractive index $n$ media in a one-dimensional (1D) photonic crystal create band gaps that do not rely on Bragg reflection; instead, the gaps occur when the average refractive index is zero and thus the net phase accumulation through the structure is zero. These band gaps consequently have properties different from those of usual Bragg band gaps: for example, insensitivity to incidence angle [2]. Whereas these band gaps have been extensively discussed in the literature [3]–[7], much less attention has been focused on unusual in-band dispersion relations that arise when metamaterials are included in periodic structures. In this paper, we investigate these dispersion relations and discuss the physical origins of their unusual features.

In ordinary all-dielectric photonic crystals, there exists for each band a propagating mode for every value of the Bloch vector $\mathbf{k}$. In contrast, photonic crystals featuring metamaterials can exhibit bands that intersect with only one of the high-symmetry points in $\mathbf{k}$-space and so are localized in $\mathbf{k}$-space, leaving some values of $\mathbf{k}$ without a propagating mode. We refer to this as band folding, where fold refers to the topology of the band itself, rather than the folding of $\mathbf{k}$-space into the first Brillouin zone. An example is shown in figure 1, which shows the band structure of a square array of negative index rods in vacuum. Here, folding is enabled by points in the band where the group velocity $v_g \equiv \nabla_k \omega$ is infinite in magnitude. These critical points can also be found in continuous systems, such as the dispersion relations of propagating surface plasmon polariton modes [8].

Previous authors have already predicted the existence of these folded bands in calculations of metamaterial photonic crystals. Panoiu et al [4] have found similar band folding in a 1D analog of our figure 1. But such folded band topologies are not limited to photonic crystals containing negative $n$ media. Toader and John [9] have found folded bands in 2D photonic crystals containing media with exclusively positive $n$. The material dispersion relations were chosen to be sinusoidal functions of frequency and consequently were anomalously dispersive.
Figure 1. Band diagram of a 2D square array of dispersionless $\epsilon = -1.8$ and $\mu = -5$ rods of radius $r = 0.3d$ in vacuum. The TM ($E_z$) polarization is shown, where $E$ is always parallel to any interface between two media.

in certain frequency ranges. The appearance of folded bands coincided with these frequency ranges. Many folded bands were observed, with different bands localized around different high-symmetry points.

The previous examples considered negative $n$ or highly dispersive materials in the absence of loss and thus do not conform to the Kramers–Kronig relations [10]. Satisfying Kramers–Kronig enforces causality in the material response and is a necessary criterion for obtaining physical results. In particular, for folded bands where $v_g = |v_g| > c$ is observed, losses provide the pulse reshaping necessary to ensure that transmission of information remains subluminal [9, 11]. Hermann et al [12] later demonstrated folded bands in media satisfying the Kramers–Kronig relations. They considered a 2D photonic crystal incorporating a lossy anomalously dispersive positive $n$ metamaterial where the anomalous dispersion results from a resonance provided by quantum dots. These authors therefore demonstrate that folded bands can be observed in physically realizable systems rather than being curiosities that arise when one is considering artificial material dispersion relations.

Although folded bands have thus been predicted in physical systems, insights into their physical origins are still lacking. The main aim of this paper is to examine the physical origins, providing a unified understanding of the seemingly disparate examples found by other authors and in our own calculations. We derive a necessary and sufficient condition for points of infinite slope, where $v_g$ is infinite, which must occur within folded bands. These also provide quantitative tools to guide numerical searches for folded band topologies.

We show that, rather than a combination of positive and negative $n$, a combination of positive and negative group index $n_g(\omega, x) \equiv \partial(n(\omega))/\partial \omega$ media is required. Infinite $v_g$ is found to occur at the frequency where the appropriate weighted spatial average of $n_g(\omega, x) = 0$. The form of this weighting function varies: for the lossless long-wavelength regime, the filling fractions of the constituents suffice. For shorter wavelengths, field distributions are required,
with the weights appearing as field intensities in the lossless case and combinations of counter-propagating modes in the most general case.

This understanding of the physical origins informs the range of material parameters that are capable of producing folded bands, which we demonstrate in section 2. Furthermore, we demonstrate band topologies that exhibit anisotropy effects that cannot be observed in non-folded band topologies.

The effects of loss must be carefully considered in dispersive media, as loss is a necessary criterion for satisfying the Kramers–Kronig relations and hence causality. We provide numerical examples and derive the conditions that are consistent with these requirements. Nevertheless, we demonstrate that there is utility in considering systems where losses have been artificially ignored. In certain instances, the dispersion relation obtained in a lossless calculation can approximate, in the frequency range of interest, the dispersion relation obtained in a system that obeys the Kramers–Kronig relations. In particular, the key topological feature of the infinite \( v_g \) point is reproduced. This behavior is helpful as lossless calculations may be easier to perform and the lossless conditions are easier to handle.

This paper is structured as follows. Section 2 provides numerical examples that introduce folded bands and the types of structures that exhibit them. Section 3 provides the conditions for the existence of folded bands, and section 3.4 provides numerical confirmation of these conditions. In section 4, we provide the discussion and conclusions.

2. Examples of folded bands

In this section, we provide numerical examples to introduce folded band structures, surveying the range of physical structures that exhibit them. We show three examples, labelled A–C, of both positive and negative refractive index \( n \) media. These examples demonstrate some of the typical behavior of systems with folded bands. The impact of losses on the behavior of folded bands is carefully considered.

In the following, 1D numerical calculations were performed using transfer matrix methods [13]. 2D calculations were performed first using multipole modal expansions to simulate constituent grating layers of the 2D crystal [14] and then using the transfer matrix method between these gratings to construct the entire 2D structure [15]. These calculations were reproduced using finite element [16] and finite-difference time-domain methods, representing both frequency domain and time domain methods.

Example A consists of a 2D photonic crystal of lossless, dispersionless negative \( n \) rods in vacuum for \( E_z \) polarization. This represents an extension of Panoiu et al’s system [4] from 1D to 2D. Figure 1 shows the presence of many bands with infinite \( v_g \) folds. These bands begin at high-symmetry points, \( \Gamma \) and \( Y \), and return to the same points at a different frequency, rather than spanning the Brillouin zone. Through the infinite \( v_g \) fold, the band undergoes a transition from positive to negative values of \( v_g \).

Example A shows that in 2D, infinite \( v_g \) points can lead to dispersion relations that are impossible to obtain in all-dielectric photonic crystals. In the band at \( \omega d/(2\pi c) \approx 0.45 \) (labelled A1 in figure 1), \( v_g \) points towards and away from the \( Y \) point along the \( Y\Gamma \) and \( YM \) segments, respectively. This leads to anisotropy where \( v_g \cdot \hat{k} \) changes sign as \( \hat{k} \) changes. Furthermore, at frequencies near A1, only a single propagating mode exists at each frequency for each band edge segment. Such anisotropy can be obtained without infinite \( v_g \) folds, but two intersecting bands are then required, and hence there would be two or more propagating modes at each frequency.
Figure 2. (a) $E_z$ band surface and (b) band diagram showing Re($k$). The band surface is overlaid with band diagram segments. The structure is identical to figure 1, but with the effective material dispersion relation of the rods shown in (c), which shows Re($n$) (blue solid) and Im($n$) (red dash dot). (d) Real (solid) and imaginary (dash-dot) parts of $\epsilon$ (blue) and $\mu$ (red).

Although commonly used in the metamaterials literature as simulation parameters, the material parameters $\epsilon$ and $\mu$ considered in example A are not physical, as they violate the Kramers–Kronig relations. Our next example shows that the folded band topologies seen in example A can be exhibited in metamaterials with physical dispersion relations.

Example B demonstrates that folded bands also exist for $\epsilon$ and $\mu$ extracted from simulated transmission and reflection spectra of a physical fishnet structure [17]. In particular, the $v_g \cdot \hat{k}$ sign-change anisotropy seen in example A can be replicated. Figure 2(a) shows the calculated dispersion relation for one band of a square array of metamaterial rods in vacuum, where the rods are described by the extracted parameters shown in figure 2(c). The band folds along the $\Gamma$–Y segment but not along the $\Gamma$–M, and thus achieving $v_g \cdot \hat{k}$ sign-change anisotropy at the larger $\omega$ values (labeled B1) in figure 2.

We chose to use fishnet structure parameters because they were the first fabricated structures to achieve negative $\epsilon$ and $\mu$ at optical frequencies [34]. However, their response is not isotropic [35], which we implicitly assume in our simulation in figure 2. We note that metamaterial design is still an evolving materials science, and more isotropic designs for infrared frequencies based on the resonances of spherical dielectric inclusions have already been proposed [36] and fabricated [37]. Since metamaterial design is not the main focus of this paper, we have chosen to use parameters from the more familiar fishnet design.
Figure 3. The Γ–X band diagram of a 1D photonic crystal, consisting of Si and a polymer with a suspension of quantum dots with $\epsilon_{\text{Si}} = 12$ and $\epsilon_{\text{poly}} = 2.56$, and layer lengths $l_{\text{Si}} = l_{\text{poly}} = 0.5$. Shown are $\omega(k)$ calculated with loss (red–yellow line) and without loss (blue line). Where applicable, Im$(k)$ is represented by the red–yellow color gradient. The quantum dots are modeled by the Lorentz oscillator parameters $\omega_0 = 0.22d/\lambda$, $\omega_p = 0.8\omega_0$, and $\gamma = 0.01\omega_0$. The volume fractions of quantum dots are (a, b) $\eta = 0.05$ and (c) $\eta = 0.02$. (b) is the magnified version of (a), focusing on the folded band. (d) Re$(\epsilon_{\text{poly}})$ (blue solid) and Im$(\epsilon_{\text{poly}})$ (red dash dot) for $\eta = 0.05$, calculated using the Maxwell–Garnett model.

As discussed in section 1, folded bands are not solely the domain of negative $n$ media. Example C is a 1D photonic crystal of two exclusively positive $n$ media, adapted from the 2D simulation of Hermann et al [12]. The parameters of the Lorentz oscillator have also been changed to demonstrate new behavior. In one of the constituents, $n_g$ is negative due to a strong absorption resonance provided by embedded quantum dots, with a material dispersion relation shown in figure 3(d). As seen in figure 3, a folded band appears as the concentration of the quantum dots is increased and hence the strength of the anomalous dispersion increases. This new propagating band appears in the band gap between the first and second bands of the original $\eta = 0$ structure. The band remains localized around $k = \pi/d$, but its extent in $k$-space can be controlled by adjusting the strength of the anomalous dispersion.

Unlike the example given by Hermann et al, this folded band remains isolated from the lower band edge of the original ($\eta = 0$) second band, even as the quantum dot concentration is reduced. This allows the creation of an isolated band that can be engineered to be arbitrarily small in extent in both frequency and $k$-space. This is reminiscent of the prediction of discrete states in metamaterial photonic crystals, where a dispersion relation that was otherwise purely imaginary intersects the real axis at a single frequency [18].
Figure 3 shows the dispersion relation as calculated both with and without loss. In both cases, the infinite $v_g$ point is present, and for some parameter ranges, the lossless dispersion relation closely approximates the real part of the lossy dispersion relation. The deviation between the dispersion relations appears to be controlled by two factors: deviation increases at frequencies where the intrinsic material losses increase and when the fractional concentration of the modal field within the lossy medium increases. The effect of these factors can be observed in figure 3 for frequencies above the infinite $v_g$ point where deviation becomes increasingly large. Not only is the metamaterial becoming increasingly lossy, but also the field concentration changes from being localized within the lossless dielectric for frequencies below the infinite $v_g$ point to being localized within the lossy metamaterial for frequencies above the infinite $v_g$ point. We will demonstrate the change in field concentration and its significance to infinite $v_g$ in section 3. Deviation also increases near the band edges. This phenomenon is well known in the photonic crystal literature [19], and can be understood as the increase in the effective loss with increasing interaction time between the electromagnetic field and the medium.

Examples B and C feature lossy constituent media, and thus the dispersion relations $\omega(k)$ are necessarily complex. However, there is considerable freedom to choose whether $\omega$ or $k$ becomes complex and, furthermore, which component of $k$ becomes complex. In figures 2 and 3, we have chosen one particular component of $k$ to be complex, leaving the remaining parameters real, since we believe this to be the most physically useful representation when considering coupling into a finite photonic crystal from free space [20]. Boundary conditions dictate that the frequency and components of $k$ parallel to the interface be conserved; assuming plane wave input defined by real $\omega$ and $k$, only the component of $k$ perpendicular to the interface may be complex within the photonic crystal [21]. Where $k$ has two or more components, as in example B, this lifts the degeneracy between $k_x$ and $k_y$, and between the $\Gamma$–X and $\Gamma$–Y segments of the band diagram. Here, we have chosen $k_y$ to be complex. Nevertheless, band diagrams where instead $\omega$ becomes complex can be considered [22]. The most notable difference between $\omega$-complex and $k$-complex band diagrams is at band edges: in $k$-complex band diagrams, $\omega(k)$ remains real but deviates strongly from the lossless dispersion relation at band edges, as already discussed, and joins smoothly onto the highly spatially attenuating modes of the band gap region, as seen in figure 3; however, in $\omega$-complex band diagrams, $\text{Im}(\omega(k))$ deviates from the lossless dispersion relation but the deviation in $\text{Re}(\omega(k))$ is less pronounced, and no mode exists within the band gap frequencies [22].

We have shown a variety of physical structures where folded bands arise. The signs of $n$ of the constituent media are apparently irrelevant, and indeed $n$ can be everywhere positive, as in example D. However, each of the examples features negative $n_g$ media in combination with positive $n_g$ media. Section 3 demonstrates the critical role played by $n_g$. Conversely, combinations of positive and negative $n$ where $n_g$ is always positive do not lead to folded bands in our experience.

In these strongly dispersive systems, loss is of importance to satisfying causality. However, since the lossless dispersion relation can sometimes approximate the true dispersion relation for the frequency range of interest, there is utility in considering the lossless case. Section 3 provides conditions that treat both the lossy and lossless cases.

3. Conditions for infinite group velocity

In this section, we derive a rigorous necessary and sufficient mathematical condition for the appearance of infinite group velocity points, expressed in terms of a weighted average of $n_g(x)$.
across the unit cell. We follow this derivation with two approximations, finding the appropriate weighted average of $n_g(x)$ in the simpler lossless case and the long wavelength regime.

3.1. A condition based on the adjoint field velocity

We derive our rigorous condition by quantitatively linking the band structure to the material parameters of the structure and the electromagnetic field. In lossless periodic media, the energy velocity $v_E$ provides this link, as it is equal to the derivative of the dispersion relation $v_g$, but can also be calculated from an integral over the modal field and material parameters. However, it is well known that in lossy systems, $v_E$ is no longer equal to the group velocity, as $v_E$ now accounts for energy transfer between the electromagnetic field and the medium. Therefore, the $v_E$ of a lossy medium is not useful for our purposes.

We turn instead to the adjoint field velocity $v_a$ [21], which, as we have previously shown, provides a means of calculating the now complex $v_g$ from the modal fields of a periodic system even if these modes experience temporal or spatial attenuation. Thus, it does not reproduce $v_E$ within lossy media but instead retains its mathematical equality to $v_g$ even in lossy media. The adjoint field velocity only requires knowledge of the modal field and material parameters $\epsilon(\omega, x)$ and $\mu(\omega, x)$, and it can be applied to any structure that is periodic in at least one dimension or has infinite translational symmetry in at least one dimension. The treatment of loss is not perturbative, so $v_a$ can handle any degree of loss. The attenuation of the modal fields may be due to intrinsic material losses or due to propagation within band gap frequencies.

The adjoint field velocity is defined as

$$ v_a = \frac{\langle \mathcal{F} \rangle}{\langle \mathcal{U} \rangle}, \tag{1} $$

where

$$ \mathcal{F} = \frac{1}{4} (E^\dagger \times H - E \times H^\dagger), \tag{2} $$

$$ \mathcal{U} = \frac{1}{4} \left( \frac{\partial(\epsilon \omega)}{\partial \omega} E \cdot E^\dagger - \frac{\partial(\mu \omega)}{\partial \omega} H \cdot H^\dagger \right). \tag{3} $$

Here, $E^\dagger$ and $H^\dagger$ are the spatial fields of modes counter-propagating with respect to $E$ and $H$, given by $k \rightarrow -k$, and the angle brackets denote spatial averaging over the unit cell. This definition has been shown to satisfy [21]

$$ v_a = v_g. \tag{4} $$

Note the apparent similarity to the energy velocity in a dispersive but lossless medium,

$$ v_E = \frac{\langle S \rangle}{\langle U \rangle}, \tag{5} $$

where

$$ S = \frac{1}{2} \text{Re}(E \times \tilde{H}), \tag{6} $$

$$ U = \frac{1}{4} \left( \frac{\partial(\epsilon \omega)}{\partial \omega} |E|^2 + \frac{\partial(\mu \omega)}{\partial \omega} |H|^2 \right). \tag{7} $$

and the bar indicates complex conjugation. Whereas $v_a$ features modes counter-propagating with respect to each other, $v_E$ features modes $E$ and $\tilde{E}$ that are reversed in time with respect to each other. Indeed, it can be shown that $v_a$ reduces to $v_E$ in the case of a lossless system, where
spatial and temporal reversal can be considered equivalent [21], i.e. \( E^\dagger \rightarrow \bar{E} \) and \( H^\dagger \rightarrow -\bar{H} \). But when losses are introduced, counter-propagating solutions are the natural modes to consider instead of complex conjugate modes. This is because the complex conjugate modes now satisfy different boundary conditions given by \( \bar{\epsilon} \) and \( \bar{\mu} \), where loss has been replaced with gain, and so the complex conjugate modes are solutions to a different electromagnetic problem.

This similarity between \( v_a \) and \( v_E \) also extends to their derivations. Both can be obtained by considering a combination of the appropriate forward and backward modes. In the case of \( v_E \) for lossless systems, the modes conserve energy; therefore (5) is a statement of both reciprocity and energy conservation, where \( S \) and \( U \) can be interpreted as energy flux and energy density, respectively. In the case of \( v_a \) for the lossy case, the modes no longer conserve energy, and so the formulation is only a statement of reciprocity.

From a mathematical perspective, the adjoint field velocity utilizes a bi-orthogonal dual basis rather than the self-adjoint space of \( v_E \) [23]. The quantities \( \mathcal{F} \) and \( \mathcal{U} \) of \( v_a \) require the dual space of the adjoint modes because modal fields of a lossy system are no longer generated by a Hermitian linear operator and hence no longer belong to a self-adjoint function space [24].

We also compare \( v_a \) to \( v_E \) for a lossy system, where the two definitions now differ markedly. This is because \( v_E \) includes terms that describe the transformation of energy from electromagnetic waves into energy that is subsequently dissipated by the medium. This energy can be explicitly expressed in terms of damped mechanical oscillators that describe the medium. In comparison, the contribution to \( v_a \) of the damped mechanical oscillators is contained implicitly in \( \epsilon(\omega) \) and \( \mu(\omega) \). This difference means that energy lost from the modes to the medium is not tracked, and consequently \( v_a \) is not linked to energy conservation. However, the identity with \( v_g \) instead is maintained.

We now apply \( v_a \) to explain infinite \( v_g \) points. As shown in the appendix, we can express the derivatives in \( \mathcal{U} \) defined in (3) in terms of the bulk \( n_g \) of each constituent medium. Furthermore, \( H \) can be eliminated if \( \mu \) is assumed to be frequency invariant. We also show in the appendix that this assumption is not necessary to express \( \mathcal{U} \) in terms of \( n_g \) but a more complicated expression arises, involving terms inessential to the physical interpretation. Assuming frequency-independent \( \mu \) leads to

\[
\langle \mathcal{U} \rangle = \frac{1}{2c} \int_{\text{UC}} [Z^{-1}(x)E(x) \cdot E^\dagger(x)]n_g(x) \, dx,
\]

where \( Z = \sqrt{\mu/\epsilon} \) is the impedance, and UC denotes integration over a unit cell. The expression in the square brackets has units of intensity, and serves as the weighting factor for the average of \( n_g(x) \).

For dispersion relations where \( k \) is complex, folded bands require \( d\omega/d\text{Re}(k) \rightarrow \pm\infty \) or \( d\text{Re}(k)/d\omega = 0 \), and so

\[
\text{Re} \langle \mathcal{U} \rangle = 0
\]

is the necessary and sufficient condition. This follows from (1) and (4), assuming that \( \langle \mathcal{F} \rangle \) has been normalized to unity. This normalization is always possible unless \( \langle \mathcal{F} \rangle = 0 \), which occurs to our knowledge only at band edges. The terms in (8) are complex, and thus both the real and imaginary parts of material parameters contribute to the condition (9).

We apply (9) to show the consequences for \( n_g(x) \). In the special limiting case where the imaginary parts are zero, opposite signs of \( n_g \) are required for satisfying (8) as all other quantities...
in (8) are real and positive definite. This can be demonstrated more explicitly for a periodic structure containing only two constituents labeled $a$ and $b$ by expressing (8) as

$$\langle U \rangle = \frac{1}{2c} (Z_a^{-1} \Phi_a n_g^a + Z_b^{-1} \Phi_b n_g^b),$$

(10)

where the subscripts on parameters denote association with either medium $a$ or $b$, and $\Phi = \int E \cdot E^\dagger \, dx$ over the respective domains. If medium $a$ has positive non-dispersive $n$, the first term of (10) is positive and real, and so $n_g^b$ must be negative.

As losses are introduced, condition (9) remains. However, the condition of Re$(n_g)$ of opposing signs becomes weaker, as arg$(n_g)$ and arg$(Z)$ both become important in (10). The condition on $n_g^b$ is still relatively simple in the examples of section 2, where medium $a$ always had $n$ positive and non-dispersive. The first term in (10) is still positive and real, and satisfying (9) usually requires that Re$(n_g^b) < 0$, since Re$(Z)$ must always be positive [25]. When both media $a$ and $b$ are dispersive and lossy, other routes to satisfying (9) exist. In the opposite limiting case of imaginary parts of opposing signs, folded bands can also appear and have been observed in structures with a periodic modulation of loss and gain [26]–[28].

The condition (9), expressed in terms of $U$, is connected to field distributions and material parameters, but has no immediately apparent physical interpretation as an energy density. Since $v_a$ is based on reciprocity rather than energy conservation, the interpretations of $U$ and $F$ as energy density and flux are obvious only in the limit as loss goes to zero.

3.2. A condition based on the energy velocity

As found in section 2, the dispersion relation calculated from neglecting loss can approximate, over the frequency range of interest, the real part of a dispersion relation consistent with the Kramers–Kronig relations. Critically, the key topological feature of the infinite $v_g$ point persists. Therefore, there is utility in a condition for infinite $v_g$ points in lossless media that parallels the rigorous condition derived in the preceding section but does not rely on $v_a$. We derive such a condition in this section.

In the absence of losses, we can use the more familiar energy velocity rather than the adjoint field velocity. However, we emphasize that the terms within the energy velocity do not necessarily hold their usual interpretations, as $v_E$ is now being applied to describe a medium where loss is artificially neglected. Nevertheless, the mathematical equivalence between $v_E$ and $v_g$ remains, which is a result that we exploit in this section.

We follow the derivation of (9), beginning with $v_E$ as defined in (5)–(7) rather than $v_a$. As in the previous section, we express $U$ in terms of $n_g(x)$. Again using the simplifying assumption that $\mu$ is frequency invariant, we can eliminate $H$ to obtain

$$\langle U \rangle = \frac{1}{2c} \int_{\mathcal{U}} [Z^{-1}(x)|E(x)|^2] n_g(x) \, dx,$$

(11)

where again the expression in square brackets has units of intensity and serves as the weight for the spatial average of $n_g(x)$.

Since the condition for infinite group velocity is $d k / d \omega = 0$ and since $v_E = v_g$, we require that

$$\langle U \rangle = 0.$$

(12)

From (11), negative $n_g$ results in negative $U$, enabling the possibility of zero $\langle U \rangle$ when positive $n_g$ materials are also present. While the possibility of negative energy is startling and would
clearly be unphysical, the term $U$ no longer has the interpretation of energy density when $v_E$ is applied to dispersion relations where loss has been artificially ignored and hence no longer satisfy Kramers–Kronig. The true energy density of an anomalously dispersive medium when losses are accounted for is never negative, and the condition that $\langle U \rangle = 0$ is not a physical statement that infinite $v_g$ requires negative energy. Despite the inability to relate $\langle U \rangle$ itself to energy density, $\langle U \rangle$ can still be understood in terms of a weighted average of $n_g(x)$, with modal field intensity providing the weighting factor.

If the system contains only two constituents, condition (12) can be expressed in a form that highlights the required balance between positive and negative group index constituents,

$$\frac{n_{gb}}{n_{ga}} = -\frac{\Phi_a Z_b}{\Phi_b Z_a},\quad (13)$$

where $\Phi = \int |E|^2 \, dx$ over the respective domains. Since the impedance $Z$ must be positive $[29]$, $n_g$ of opposite signs is required. Losses and gains now do not feature, so there is no possibility of obtaining infinite $v_g$ points using the imaginary parts of the material parameters. Infinite $v_g$ points can be interpreted as the balance of modal field density in both the positive and negative $n_g$ media. Bragg scattering dictates the redistribution of fields as a function of $\omega$, enabling this balance to be satisfied at particular $\omega$. Above and below these $\omega$, $\langle U \rangle$ changes sign, inducing $v_g$ to also change sign, as the field becomes more localized in either the positive or the negative $n_g$ constituent.

Although (12) is not a rigorous condition for lossy systems, it exactly reproduces band structure calculations where loss has been artificially ignored, such as in figures 1 and 3. In cases like figure 3, where a degree of loss consistent with the Kramers–Kronig relations does not markedly alter the band structure, (12) and (13) represent a useful and simpler mathematical condition to guide the search for infinite $v_g$ points in a lossy medium, even if its validity does not rigorously extend to lossy systems.

There is a different situation where a lossless condition for infinite $v_g$ points holds without approximation: the specific case where the constituent negative index media of the photonic crystal has been engineered to be lossless at specific frequencies through the inclusion of gain resonances. This type of lossless negative index medium satisfies the Kramers–Kronig relations and therefore is possible in principle $[30]$, and has also been experimentally realized $[31]$. At these specific frequencies, $v_E$ is also appropriate to use, and its application is a special case of the rigorous condition (9) derived from $v_a$.

The condition for infinite $v_g$ remains that $U$ of the metamaterial is negative so that $\langle U \rangle = 0$ when positive $n_g$ media are also present in the unit cell. Here, negative $U$ also does not imply negative total energy, but for a different reason. While the identity between lossless $v_E$ and $v_g$ holds at the specific frequencies where $\text{Im}(n_g(x)) = 0$, this $v_E$ does not contain terms from energy flows to and from the medium due to the loss and gain resonances and so is not representative of the total energy. A negative contribution from electromagnetic fields to the total energy, but where total energy remains positive, has been previously observed and discussed in the literature $[32]$.

3.3. Long wavelength limit

In the long wavelength limit, the periodic structure may be treated as a homogeneous medium. The band structure can be calculated directly from material parameters, avoiding the need for
either $v_a$ or $v_E$. In this section, we use this approach to reproduce the long wave equivalent to (13)

$$n_{gb} = \frac{f_a Z_b}{f_b Z_a},$$ (14)

where $f$ represents filling fractions of media $a$ and $b$ within the periodic structure instead of field intensities. This is derived using the average refractive index,

$$k(\omega) = \bar{n}(\omega)\omega/c.$$ (15)

For non-magnetic $E_z$ modes of 1D or 2D photonic crystals with only two constituent media, denoted $a$ and $b$, $n$ is given by [33]

$$\bar{n}^2(\omega) = \bar{\epsilon}(\omega) = f_a \epsilon_a(\omega) + f_b \epsilon_b(\omega).$$ (16)

As $\epsilon_a$ and $\epsilon_b$ change, the slope of $k(\omega)$ changes, with infinite or negative values being possible. It is straightforward to show that (14) is satisfied when $v_g$ is infinite or $dk/d\omega = 0$. A similar condition may be derived for $H_z$ modes. Once again, since the Rhs quantities are positive definite, we find that $n_g$ of media $a$ and $b$ must have opposite signs to obtain infinite $v_g$. Specifically, a combination of media, such that the space averaged $n_g(x)$ is approximately zero, is required.

### 3.4. Numerical confirmation of the mathematical conditions

In this section, we provide numerical confirmation of conditions (9) and (12), derived in sections 3.1 and 3.2, respectively. The conditions state that the respective field integrals $\langle U \rangle$ or Re($\langle U \rangle$) over a unit cell be zero. Figure 4 shows field integrals for the modes corresponding to the lossless and lossy band structures of example D given in section 2, as shown in figure 3(a). In both cases, the values change from positive to negative, passing through zero at the $\omega$ corresponding to the infinite $v_g$ point in the respective dispersion relations. The similarity of the values produced by the two integrals is reflected in the similarity of the dispersion relations at this range of frequencies.

This numerically confirms the accuracy of (8) and (9) as conditions for infinite $v_g$. Greater field concentration in the negative $n_g$ parts of the unit cell weights the field integrals towards more negative values; these may be interpreted as a weighted average $n_g(x)$ of the medium changing from positive to negative. This corresponds to a change in sign of $v_g$ in the dispersion relation. It also confirms the numerical equivalence between $v_g$ and $v_a$ and between $v_g$ and $v_E$, which form the bases for deriving (9) and (12).

![Figure 4](http://www.njp.org/)
4. Discussion and conclusions

We have provided a necessary and sufficient mathematical condition for the appearance of vertical infinite \( v_g \) points in dispersion relations, which are topological necessities within folded bands. We have also derived approximations to this condition in the lossless and long wavelength limits. All three are stated as weighted spatial averages of \( n_g(x) \). These conditions unify previous numerical observations, demonstrating that infinite \( v_g \) arise when negative \( n_g \) materials are placed into a periodic structure in combination with positive \( n_g \) materials. These conditions were tested numerically. We have also demonstrated that folded bands allow for unique band topologies. Since folded bands do not span the entire Brillouin zone, we have demonstrated bands that are localized in \( k \)-space in addition to being localized in frequency. We have also used folded bands to demonstrate an anisotropic medium where \( v_g \cdot \hat{k} \) changes sign as the propagation direction \( \hat{k} \) changes.

We draw on the conclusions of the conditions derived to provide a heuristic understanding of the link between negative \( n_g \) and folded bands. The behavior of the dispersion relations is given by \( n(x) \) as a function of \( \omega \), but the relevant quantity to consider when describing the slope of dispersion relations is \( n_g(x) \) rather than \( n(x) \). In a homogeneous medium, there is no distinction between the material parameter \( n_g(x) \) and the modal group index. Infinite \( v_g \) occurs when \( n_g \) is zero. As shown by (14), this interpretation persists in the long wavelength regime, where homogenization relations are available for \( n_g \). For shorter wavelengths, infinite \( v_g \) occurs when the appropriate spatial average of \( n_g(x) \) is zero. Bragg scattering redistributes the field between the different constituents of the periodic structure as a function of frequency. As shown by (11), when the modal field is largely concentrated in the positive \( n_g \) constituent the mode has positive \( v_g \), whereas when the modal field is largely concentrated in the negative \( n_g \) constituent the mode has negative \( v_g \). At the specific frequency where the modal field is balanced between positive and negative \( n_g \) constituents, infinite \( v_g \) results. This balance is not necessarily difficult to achieve, considering the large field redistributions that are possible due to Bragg scattering, especially near the band edges. Thus, folded bands are a natural consequence of having sufficient field concentration in a sufficiently negative \( n_g \) constituent of a periodic structure.

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The general condition (9) depends non-trivially on the real and imaginary parts of $\epsilon(\omega)$ and $\mu(\omega)$ and on the residual phase information, so many routes to infinite $v_g$ points are possible. Besides negative $n_g$ media, other routes include plasmonic systems, such as surface modes on an interface between metal and dielectric, and media with a spatially periodic distribution of both loss and gain. We note that $v_a$ can be applied to any system with periodicity in at least one dimension, or with infinite translational symmetry in at least one dimension. Furthermore, we have not imposed any further constraints in our derivation of the condition (9). In principle, this condition should also hold for all systems with infinite $v_g$ points. However, we have not explicitly verified (9) in other systems, and a discussion of mechanisms that yield infinite $v_g$ beyond negative $n_g$ is outside the scope of this paper. So while (9) unites these systems under a single mathematical condition, the physical connections between these systems will remain unclear until better interpretations of $\mathcal{U}$ or $Z^{-1}\mathbf{E} \cdot \mathbf{E}^\dagger$ are available.

The sufficient condition (9), and its lossless approximation (12), can be used for predicting structural parameters required for folded bands, reducing the need to perform brute force numerical searches through parameter space. The conditions are stated in terms of the material dispersions of the constituent bulk media, and the way the field is distributed between these media in the periodic structure. At a chosen frequency $\omega_0$, the field can be shifted between the constituents by changing the structural parameters, for example changing the lattice constant to move a band edge with respect to $\omega_0$. The required change can be estimated from modal field calculations in which the material parameters have been fixed to those at $\omega_0$, or even by considering the refractive index contrast between the two constituent media. The search for folded bands has thus been reduced to the manipulation of the $n_g(x)$ and the field distribution, such that $\langle U \rangle = 0$ or $\Re\langle U \rangle = 0$. Furthermore, it is often sufficient to use the lossless approximation (12), rather than the rigorous condition (9), since we have found that many simulated folded bands survive the introduction of an amount of loss consistent with Kramers–Kronig.

In deriving our conditions in sections 3.1 and 3.2, we utilized the mathematical equivalence between $v_g$ and $v_a$ and between $v_g$ and $v_E$, for lossy and lossless materials, respectively. The velocities $v_a$ and $v_E$ clearly link $v_g$ to physical quantities such as $n_g$ and field distributions; however, there is no link between these velocities and concepts such as energy density or energy flux. In the case of $v_a$, it is only related to reciprocity and not to energy conservation when the medium being described is lossy. In the case of $v_E$ in section 3.2, we have applied $v_E$ to dispersion relations where loss has been neglected, which are only approximations to the true Kramers–Kronig obeying dispersion relations. When used in this manner, $v_E$ cannot be expected to be related to the usual concepts of energy flux or energy density. So while these conditions provide conclusions as to the weighted average of $n_g(x)$ required, these conditions do not provide any conclusions as to the energy flows required for achieving infinite $v_g$.

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Appendix

We provide a more detailed derivation of the conditions (9) and (12). We will also lift the restriction that $\mu$ is frequency independent, and show that $\langle U \rangle$ and $\langle U \rangle$ can still be expressed in terms of $n_g$. In this case, the $H$ cannot be eliminated and $\langle U \rangle$ and $\langle U \rangle$ must be expressed as an admixture of $E$ and $H$. In this section, we only give the derivation using complex conjugate fields, as the derivations using adjoint fields are very similar. We will specify the modifications necessary and quote the relevant results for adjoint fields.

We begin by providing the derivation of (11) from (7), which is for frequency-independent $\mu$,

$$\langle U \rangle = \frac{1}{4} \int_{UC} \frac{\partial (\epsilon \omega)}{\partial \omega} |E|^2 \, dx + \int_{UC} \mu |H|^2 \, dx,$$

$$= \frac{1}{4} \int_{UC} \left[ \frac{\partial (\epsilon \omega)}{\partial \omega} + \epsilon \right] |E|^2 \, dx,$n_g |E|^2 \, dx, \quad (A.1)$$

where in the second equality, we have used the identity

$$\int_{UC} \epsilon |E|^2 \, dx = \int_{UC} \mu |H|^2 \, dx. \quad (A.2)$$

Lifting the restriction on $\mu$ requires a more general version of (A.2), which we derive now. We begin with the vector identity

$$\nabla \cdot [(f E) \times \tilde{H}] = \tilde{H} \cdot [\nabla \times (f E)] - (f E) \cdot [\nabla \times \tilde{H}], \quad (A.3)$$

where $f(\omega, x)$ will be used later to describe material parameters and so has the same periodicity as the lattice. Then, integrating the identity over the unit cell provides

$$\oint_{UC} [(f E) \times \tilde{H}] \cdot ds = \int_{UC} \tilde{H} \cdot [\nabla \times (f E)] - (f E) \cdot [\nabla \times \tilde{H}] \, dx. \quad (A.4)$$

Due to periodicity, the lhs of (A.4) can be shown to be zero, as follows. The modal fields $E$ and $\tilde{H}$ are only quasi-periodic, i.e. varying from unit cell to unit cell by the Bloch factor; however, the multiplication of these quasi-periodic fields is fully periodic. This applies to modal fields that do not experience any spatial attenuation. Meanwhile, $f$ was assumed to be periodic and so the integrand of the lhs of (A.4) is periodic with the lattice. The surface integral of this periodic integrand is zero.

If spatial attenuation is present due to material loss, for example, a combination of fields and complex conjugate fields is no longer sufficient to produce periodicity and a combination of fields and adjoint fields is now required. This represents the principal difference between $v_a$ and $v_e$ of sections 3.1 and 3.2. The rest of the derivation then follows in an identical fashion, but the result leads to the condition for lossy media (9) instead of the condition for lossless media (12).
Now, manipulating the rhs of (A.4) using vector identities and Maxwell’s equations gives the result

\[ \int_{\text{UC}} f [\mu |\mathbf{H}|^2 - \epsilon |\mathbf{E}|^2] + (\nabla f) \cdot (\mathbf{E} \times \bar{\mathbf{H}}) \, dx = 0. \]  

(A.5)

Note that setting \( f = 1 \) gives (A.2). Instead, setting \( f = f_\epsilon \equiv \frac{1}{\epsilon} \frac{\partial (\epsilon \omega)}{\partial \omega} \) and \( f = f_\mu \equiv \frac{1}{\mu} \frac{\partial (\mu \omega)}{\partial \omega} \) produces the two identities

\[ \int_{\text{UC}} \frac{\partial (\epsilon \omega)}{\partial \omega} |\mathbf{E}|^2 \, dx = \int_{\text{UC}} \frac{\mu}{\epsilon} \frac{\partial (\epsilon \omega)}{\partial \omega} |\mathbf{H}|^2 \, dx + \int_{\text{UC}} \nabla \left( \frac{1}{\epsilon} \frac{\partial (\epsilon \omega)}{\partial \omega} \right) \cdot (\mathbf{E} \times \bar{\mathbf{H}}) \, dx, \]  

(A.6)

\[ \int_{\text{UC}} \frac{\partial (\mu \omega)}{\partial \omega} |\mathbf{H}|^2 \, dx = \int_{\text{UC}} \frac{\epsilon}{\mu} \frac{\partial (\mu \omega)}{\partial \omega} |\mathbf{E}|^2 \, dx - \int_{\text{UC}} \nabla \left( \frac{1}{\mu} \frac{\partial (\mu \omega)}{\partial \omega} \right) \cdot (\mathbf{E} \times \bar{\mathbf{H}}) \, dx. \]  

(A.7)

We are now ready to express \( \langle U \rangle \) in terms of \( n_g \). A mixture of \( \mathbf{E} \) and \( \mathbf{H} \) fields is now required, so we first partition \( \langle U \rangle \) into two parts,

\[ \langle U \rangle = \frac{1}{4} \, (p + q) \left[ \int_{\text{UC}} \frac{\partial (\epsilon \omega)}{\partial \omega} |\mathbf{E}|^2 \, dx + \int_{\text{UC}} \frac{\partial (\mu \omega)}{\partial \omega} |\mathbf{H}|^2 \, dx \right], \]  

subject to the condition \( p + q = 1 \). Inserting (A.6) and (A.7) into (A.8),

\[ \langle U \rangle = \frac{p}{4} \int \left[ \frac{\partial (\epsilon \omega)}{\partial \omega} + \frac{\epsilon}{\mu} \frac{\partial (\mu \omega)}{\partial \omega} \right] |\mathbf{E}|^2 \, dx + \frac{q}{4} \int \left[ \frac{\mu}{\epsilon} \frac{\partial (\epsilon \omega)}{\partial \omega} + \frac{\partial (\mu \omega)}{\partial \omega} \right] |\mathbf{H}|^2 \, dx 

+ \frac{1}{4} \int \nabla \left( q \frac{1}{\epsilon} \frac{\partial (\epsilon \omega)}{\partial \omega} - p \frac{1}{\mu} \frac{\partial (\mu \omega)}{\partial \omega} \right) \cdot (\mathbf{E} \times \bar{\mathbf{H}}) \, dx. \]  

(A.9)

With an appropriate choice of \( p \) and \( q \), the final term in (A.9) can be eliminated. For a piecewise uniform medium with two constituents, the following ratio of \( p \) and \( q \) is necessary,

\[ \frac{p}{q} = \frac{\Delta f_\epsilon}{\Delta f_\mu}, \]  

(A.10)

where \( \Delta f \) describes the change in \( f \) at the interface between the two constituents. This defines the specific mixture of \( \mathbf{E} \) and \( \mathbf{H} \) required for expressing \( \langle U \rangle \) in terms of \( n_g \). Note that the ratio required depends only on the material parameters and not on the properties of the modal field.

The final result can be obtained by manipulating (A.9) in a manner similar to (A.1), yielding

\[ \langle U \rangle = \frac{1}{4c} \int_{\text{UC}} n_g (p Z^{-1} |\mathbf{E}|^2 + q Z |\mathbf{H}|^2) \, dx. \]  

(A.11)

Following a very similar derivation but using adjoint fields rather than complex conjugate fields, we obtain a result relevant to \( v_a \) in section 3.1,

\[ \langle U \rangle = \frac{1}{4c} \int_{\text{UC}} n_g (p Z^{-1} \mathbf{E} \cdot \mathbf{E}^\dagger - q Z \mathbf{H} \cdot \mathbf{H}^\dagger) \, dx. \]  

(A.12)

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