



Origin of folded bands in metamaterial crystals



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ABSTRACT

Recently it has been found numerically that the spectra of metamaterial crystals may contain pairs of bands which disappear inside the Brillouin zone. We observe that the wave equations for such systems are essentially non-Hermitian, but \mathcal{PT} -symmetric. We show that the real-frequency spectra correspond to \mathcal{PT} -symmetric solutions of the wave equation. At those momenta in the Brillouin zone where apparently no solutions exist, there appear pairs of complex-frequency solutions with spontaneously broken \mathcal{PT} symmetry.

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1. Introduction

One of the basic characteristics of waves propagating in material media is their frequency spectrum. In periodic systems, for instance in photonic crystals, the frequency ω is a function of the wave vector \vec{q} , $\omega = \omega_s(\vec{q})$, where \vec{q} is restricted to an elementary tile of the reciprocal space, the so-called first Brillouin zone. The discrete index s numerates distinct branches of the dispersion, which correspond to different distributions of the wave field within the unit cell of the periodic system. Since in macroscopic systems the wave vector \vec{q} changes quasi-continuously, each branch s leads in general to a finite interval of allowed frequencies, the so-called bands, which may be divided by band gaps in-between them [1].

In most systems studied so far, either in the solid-state or photonic context, for each of the branches the function $\omega = \omega_s(\vec{q})$ stretches throughout the whole Brillouin zone. This is a simple consequence of Hermiticity. In fact, the plane wave $e^{i\vec{q}\cdot\vec{x}}$ may experience Bragg scattering to any of the plane waves of the form $e^{i(\vec{q}+\vec{K})\cdot\vec{x}}$, where \vec{K} is a reciprocal lattice vector. In the basis of such states, the Schrödinger or wave equation takes the form of an eigenvalue problem $H_{\vec{K}\vec{K}'}(\vec{q})c_{\vec{K}'} = \lambda(\vec{q})c_{\vec{K}}$. For a fixed cut-off we are then dealing with an $N \times N$ matrix which, if it is Hermitian, is guaranteed to have N real eigenvalues, independently of the value of \vec{q} . Smooth changes of $H_{\vec{K}\vec{K}'}(\vec{q})$ lead then to smooth changes of $\lambda(\vec{q})$, resulting in bands which cannot disappear inside the Brillouin zone. In other words, the number of eigenfrequencies cannot be reduced in a certain interval of wave vectors.

However, in numerical simulations it has recently been found that in certain systems the bands may disappear inside the Brillouin zone, forming the so-called folded bands [2]. In particular, such behavior has been observed in photonic crystals in the form of a square array of metamaterial cylinders immersed in vacuum. As an example, in Fig. 1 we show the two lowest-frequency bands for such a metamaterial photonic crystal calculated numerically from transmission spectra [3]. Folded bands appear when the radius of cylinders R increases above the critical value $R_c \approx 0.275a$, where a is the spatial period of the crystal. This surprising result indicates that the wave equation for electromagnetic field in a metamaterial photonic crystal has to be non-Hermitian.¹

Actually, it is well known that if both, permittivity ε and permeability μ , are non-constant functions of the spatial coordinate, then the wave equation for the magnetic field \vec{H} reads

$$\mathcal{M}\vec{H} \equiv \mu^{-1} \text{rot} \left[\varepsilon^{-1} \text{rot} \vec{H} \right] = \omega^2 \vec{H}, \quad (1)$$

where the operator \mathcal{M} is non-Hermitian even in ordinary photonic crystals made from dissipationless components [6,1]. Note that we set the speed of light $c = 1$.

So how can it be that folded bands have not been observed in ordinary photonic crystals? The reason is that the non-Hermitian character of (1) is often not essential, since it can be avoided by a reformulation of the problem. For instance, if the permeability μ

¹ Folded bands have been observed also earlier, see, e.g., [4] and [5]. However, in those papers systems with frequency-dependent material parameters were studied. Therefore, from the mathematical point of view, those authors did not study eigenvalue problems, and the presence of folded bands in spectra did not lead to the sort of questions which we address in this paper.

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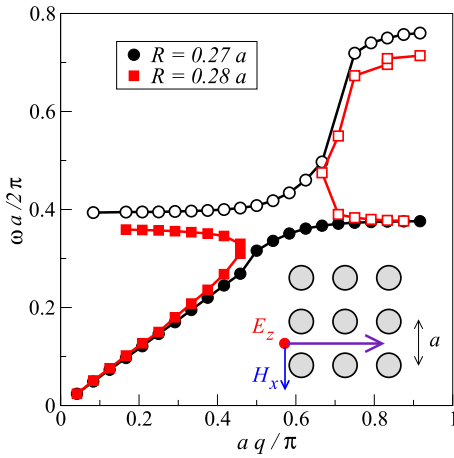


Fig. 1. Dispersion relation $\omega = \omega(\vec{q})$ in the ΓX direction for a two-dimensional photonic crystal made of metamaterial cylinders with real and dispersionless permittivity $\varepsilon = -1.8$ and permeability $\mu = -5$, see inset. Electric field is taken to be parallel to the cylinders. The two sets of curves correspond to cylinder radii slightly above and below the critical radius $R_c \approx 0.275a$ [3].

is real and positive definite, one can redefine the magnetic field by $\vec{H} = \vec{h}/\sqrt{\mu}$, thereby transforming (1) to the form

$$\mathcal{O}\vec{h} \equiv \mu^{-1/2} \text{rot} \left[\varepsilon^{-1} \text{rot} \left(\mu^{-1/2} \vec{h} \right) \right] = \omega^2 \vec{h} \quad (2)$$

with an explicitly Hermitian operator \mathcal{O} [1].

The observation of folded bands in metamaterial photonic crystals therefore suggests that their non-Hermitian character should be *essential*, i.e. not avoidable by any reformulation. In particular, it will be shown later that, in presence of interfaces between ordinary dielectric regions where $\sqrt{\mu}$ is purely real and metamaterial regions with purely imaginary $\sqrt{\mu}$, the operator \mathcal{O} remains non-Hermitian. We would like to point out that, since we are dealing with a metamaterial crystal, the alternative Hermitization of the wave equation for \vec{E} in terms of the substitution $\vec{E} = \vec{e}/\sqrt{\varepsilon}$ is plagued by the same problem.

The goal of the present paper is to demonstrate that the appearance of folded bands in metamaterial photonic crystals is a direct consequence of their essential non-Hermiticity. To this end, we will start by studying the simplest possible crystal structure, namely a one-dimensional (1D) periodic stack of right- and left-handed materials. Several anomalous features of electromagnetic wave propagation have already been observed in this model [7–10]. Here we observe that the 1D model exhibits the so-called \mathcal{PT} symmetry (for a review, see [11]) and, making use of this recently developed concept, we will explain the presence of folded bands in the spectrum of this model. Similar reasoning will be later applied to two-dimensional (2D) metamaterial crystals studied in [2,3].

2. One-dimensional toy model

We assume that the 1D stack consists of materials a and b characterized by ε_i , μ_i , refractive indices $n_i = \sqrt{\varepsilon_i \mu_i}$, impedances $Z_i = \sqrt{\mu_i / \varepsilon_i}$, and thicknesses ℓ_i , where $i = a, b$. All material parameters are assumed to be real and frequency-independent. The frequency spectrum of transverse electromagnetic waves, which propagate perpendicularly to the slabs with wave vector q , can be determined from the implicit equation [12]

$$f(\omega) \equiv \frac{1}{2}(A+1) \cos \omega \tau_+ - \frac{1}{2}(A-1) \cos \omega \tau_- = \cos q \ell, \quad (3)$$

where $\ell = \ell_a + \ell_b$ is the length of the unit cell, $\tau_{\pm} = \tau_a \pm \tau_b$ with $\tau_i = n_i \ell_i$, and $A = (Z_a/Z_b + Z_b/Z_a)/2 > 1$ is the impedance mismatch between the slabs a and b .

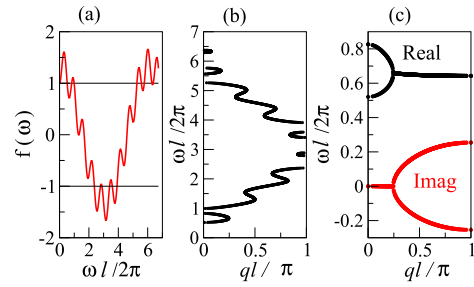


Fig. 2. 1D model with $\varepsilon_a = 1$, $\mu_a = 1$, $\ell_a = 1$, and $\varepsilon_b = -9$, $\mu_b = -1$, $\ell_b = 0.41$. (a) Function $f(\omega)$. (b) Frequency spectrum. (c) Real and imaginary parts of frequency in the lowest folded band.

In ordinary photonic crystals with $\varepsilon_i > 0$ and $\mu_i > 0$ we have $\tau_+ > |\tau_-| \geq 0$. Therefore the larger-amplitude first term of $f(\omega)$ oscillates faster than the smaller-amplitude second term. Let us denote the positions of local extrema of the function $f(\omega)$ as ω^* . In order to proceed, let us note that for frequencies $\omega_n = n\pi/\tau_+$, where n is an integer, we have $|f(\omega_n)| \geq 1$. Moreover, $f(\omega_n)$ exhibits even-odd oscillations with n . But since the second term in $f(\omega)$ oscillates with a longer period, in-between ω_n and ω_{n+1} there will be at most one extreme of $f(\omega)$, and therefore $|f(\omega^*)| \geq |f(\omega_n)| \geq 1$. From $|f(\omega^*)| \geq 1$ it follows that no folded bands can be present in the spectrum. This was of course to be expected, since the wave equation of an ordinary photonic crystal can be Hermitized.

Now let us assume that the slab a is an ordinary dielectric with $\varepsilon_a > 0$ and $\mu_a > 0$, whereas the slab b is made from a metamaterial with $\varepsilon_b < 0$, $\mu_b < 0$, and $n_b < 0$. In this case $\tau_- > |\tau_+| \geq 0$ and it is the smaller-amplitude second term of $f(\omega)$ which oscillates faster than the larger-amplitude first term. As shown explicitly in Fig. 2(a), then the values of $f(\omega^*)$ may lie within the interval $(-1, 1)$, and as a result folded bands can form in the spectrum. Such folded bands have been observed previously for oblique wave propagation [10]. Similarly as in the case of 2D metamaterial photonic crystals [3], also in the 1D case folded bands form only in a subset of the parameter space ($A, \beta = \tau_-/\tau_+$) of (3). It is worth pointing out that also the much debated zero- \bar{n} gaps [8] are associated with a special case of folded bands. In fact, the zero- \bar{n} condition is equivalent to $\tau_+ = 0$ and in this case (3) has solutions only for $q = 0$ and $\omega \tau_- = 2m\pi$, where m is an integer.

Since (3) does not shed light on the mathematical structure of the 1D problem, in what follows we shall restate its basic equations. Let us first observe that the wave equation (1) for the 1D problem reads piecewise

$$-n_i^{-2} H'' = \omega^2 H \quad (4)$$

with different refractive indices n_i in materials a and b . If we take the center of the slab a as the origin, then the boundary conditions at the interfaces $\xi = \pm \ell_a/2$ between the slabs require

$$H(\xi_-) = H(\xi_+), \quad E(\xi_-) = E(\xi_+), \quad (5)$$

where ξ_- and ξ_+ are infinitesimally shifted from ξ to the left and right, respectively, and $E(\xi_{\pm}) = H'(\xi_{\pm})/\varepsilon(\xi_{\pm})$. Moreover, from the Bloch theorem follows an additional boundary condition

$$H(\ell/2) = e^{iq\ell} H(-\ell/2). \quad (6)$$

To summarize, the boundary-value problem which we have to solve is defined by (4), (5), (6).

Let us prove now that the standard Hermitization procedure by means of a redefinition of fields $h(x) = H(x)\sqrt{\mu(x)}$ does not work for the 1D metamaterial photonic crystal. In other words, let us show that the operator \mathcal{O} for the boundary-value problem (4), (5), (6) is not Hermitian. To this end, let us calculate

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