

## Photonic Band Structure of Dispersive Metamaterials Formulated as a Hermitian Eigenvalue Problem

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We formulate the photonic band structure calculation of any lossless dispersive photonic crystal and optical metamaterial as a Hermitian eigenvalue problem. We further show that the eigenmodes of such lossless systems provide an orthonormal basis, which can be used to rigorously describe the behavior of lossy dispersive systems in general.

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Remarkable progress has been made over the past two decades in the study of nanoscale periodic photonic structures such as photonic crystals and metamaterials. The ability to accurately calculate the eigenmodes and band structures of such periodic structures has proven essential to continued progress in identifying novel optical phenomena and developing devices that exploit them. While early work in band structure computation focused on frequency-independent dielectric materials, there is now significant interest in computing the photonic band structures of material systems with frequency-dependent permittivities, for applications in optical metamaterials and dispersive photonic crystals [1–7].

In general, the photonic band structure for any periodic material system can be determined by solving the following equation [8]:

$$\nabla \times \frac{1}{\varepsilon} \nabla \times \mathbf{H} = \left(\frac{\omega}{c}\right)^2 \mathbf{H}, \quad (1)$$

where  $\varepsilon$  is the material permittivity,  $\mathbf{H}$  is the magnetic field, and  $\omega$  is the frequency of the photonic mode. When  $\varepsilon$  is independent of frequency, Eq. (1) becomes a Hermitian eigenvalue problem [8]. Such a Hermitian formalism greatly facilitates numerical calculations [9]. Moreover, it ensures mode orthogonality across different bands, which permits a global view of the band structure across the entire frequency spectrum [8], and enables advanced simulation techniques such as the Wannier function approach that greatly speed up the calculation of complex circuit elements [10,11].

Ideally one would like to perform a similar band structure calculation for material systems with arbitrary frequency-dependent dielectric functions,  $\varepsilon(\omega)$ . The difficulty here is that with the  $\omega$  dependence in  $\varepsilon$ , Eq. (1) no longer defines a standard eigenvalue problem. While the photonic band structures for such dispersive systems have been obtained by a variety of techniques that solve Maxwell's equations in either the frequency or time domain [5,12–18], in all these formalisms there are no apparent constraints between solutions at different frequencies. The resulting band structures are therefore of less

utility compared to the standard dielectric band structure, since many important calculations, including, for example, the calculations of local density of states [19], rely critically on the capabilities of expanding the fields on an orthonormal basis formed by the eigenmodes of the system.

In this Letter we demonstrate that the band structure of dispersive photonic crystals and optical metamaterials, in general, can be obtained by solving a standard matrix eigenvalue problem. In the case where the material can be approximated as lossless, the eigenvalue problem is Hermitian, which directly leads to an orthogonality condition for modes at different frequencies. For a lossy structure, the modal loss can be directly solved by a non-Hermitian eigenvalue problem. Moreover, we show that modal loss can alternatively be calculated by a perturbation approach starting from the lossless structure. Thus, the modes for lossless structures provide an important orthonormal basis for understanding dispersive metamaterial structures in general.

To illustrate this approach we, as an example, consider photonic crystals made of materials whose permittivities are described by a Lorentz pole [20]:

$$\varepsilon(\omega) = \varepsilon_\infty \left( 1 + \frac{\omega_p^2}{\omega_0^2 - \omega^2 + i\omega\Gamma} \right). \quad (2)$$

The method we present is, however, generalizable for systems with arbitrary number of poles, as we will explicitly show towards the end of the Letter.

The dielectric response of Eq. (2) arises from the coupling of the electric field  $\mathbf{E}$  to local mechanical oscillators. Thus, we explicitly introduce auxiliary fields for such local oscillators, and couple such auxiliary mechanical fields with the standard Maxwell's equations that describe the  $\mathbf{E}$  and  $\mathbf{H}$  fields. To develop this, we begin with the equations of motion for an electron with mass  $m$ , located at a position  $\mathbf{r}$ , bounded by a harmonic oscillator potential with a characteristic frequency  $\omega_0$ , and subject to an electric field  $\mathbf{E}$  and damping loss rate  $\Gamma$ :

$$\frac{d^2\mathbf{r}}{dt^2} + \Gamma \frac{d\mathbf{r}}{dt} + \omega_0^2 \mathbf{r} = \frac{e\mathbf{E}}{m}. \quad (3)$$

Defining the polarization field  $\mathbf{P} = Ne\mathbf{r}$ , where  $N$  is the electron density, and plasma frequency,  $\omega_p^2 = Ne^2/m\epsilon_\infty$ , we find an expression for  $\mathbf{P}$ :

$$\frac{d^2\mathbf{P}}{dt^2} + \Gamma\frac{d\mathbf{P}}{dt} + \omega_0^2\mathbf{P} = \omega_p^2\epsilon_\infty\mathbf{E}. \quad (4)$$

Equation (4) is exactly equivalent to the Lorentz model in Eq. (2). Consistent with the original form of the Maxwell's equations, which has a first-order differentiation in time, we introduce an additional polarization velocity field  $\mathbf{V}$  defined by  $\mathbf{V} = \frac{d\mathbf{P}}{dt}$ . We can now present the basic equations of motion for the electromagnetic field in a dispersive medium:

$$\frac{\partial\mathbf{H}}{\partial t} = -\frac{1}{\mu_0}\nabla\times\mathbf{E}, \quad (5)$$

$$\frac{\partial\mathbf{E}}{\partial t} = \frac{1}{\epsilon_\infty}(\nabla\times\mathbf{H} - \mathbf{V}), \quad (6)$$

$$\frac{\partial\mathbf{P}}{\partial t} = \mathbf{V}, \quad (7)$$

$$\frac{\partial\mathbf{V}}{\partial t} = \omega_p^2\epsilon_\infty\mathbf{E} - \omega_0^2\mathbf{P} - \Gamma\mathbf{V}. \quad (8)$$

With this established, and further assuming a steady state with all fields varying as  $\exp(i\omega t)$ , this system can be written as a matrix equation for  $\omega$ :

$$\omega \begin{pmatrix} \mathbf{H} \\ \mathbf{E} \\ \mathbf{P} \\ \mathbf{V} \end{pmatrix} = \begin{pmatrix} 0 & \frac{i}{\mu_0}\nabla\times & 0 & 0 \\ -\frac{i}{\epsilon_\infty}\nabla\times & 0 & 0 & \frac{i}{\epsilon_\infty} \\ 0 & 0 & 0 & -i \\ 0 & -i\omega_p^2\epsilon_\infty & i\omega_0^2 & i\Gamma \end{pmatrix} \begin{pmatrix} \mathbf{H} \\ \mathbf{E} \\ \mathbf{P} \\ \mathbf{V} \end{pmatrix}. \quad (9)$$

We emphasize that all coefficients in Eq. (9) are frequency independent. The entire effect of material dispersion has been taken into account through the use of the auxiliary fields. Moreover, both the  $\mathbf{E}$  and  $\mathbf{H}$  fields in this equation are identical to the physical  $\mathbf{E}$  and  $\mathbf{H}$  fields in the original form of Maxwell's equations.

Closely related to this approach, we note that similar auxiliary fields have been employed in standard finite-difference time-domain simulations for dispersive media [21], and have been used as a starting point for field quantization in dispersive media [22]. The original contribution in this Letter is to explicitly demonstrate the use of such auxiliary mechanical fields for band structure simulation and analysis.

We now apply Eq. (9) towards defining and solving the band structure for dispersive metamaterials in general. We consider first the lossless case, by setting  $\Gamma = 0$ . In this case, Eq. (9) can in fact be reformulated in terms of a Hermitian eigenvalue problem. To see this, defining  $\mathbf{x} = (\mathbf{H}, \mathbf{E}, \mathbf{P}, \mathbf{V})^T$ , we can rewrite Eq. (9) as  $\omega\mathbf{A}\mathbf{x} = \mathbf{B}\mathbf{x}$  where

$$\mathbf{A} = \text{diag}(\mu_0, \epsilon_\infty, \omega_0^2/\omega_p^2\epsilon_\infty, 1/\omega_p^2\epsilon_\infty), \quad (10)$$

$$\mathbf{B} = \begin{pmatrix} 0 & i\nabla\times & 0 & 0 \\ -i\nabla\times & 0 & 0 & \frac{i}{\omega_p^2\epsilon_\infty} \\ 0 & 0 & 0 & -i\frac{\omega_0^2}{\omega_p^2\epsilon_\infty} \\ 0 & -i & i\frac{\omega_0^2}{\omega_p^2\epsilon_\infty} & 0 \end{pmatrix}. \quad (11)$$

Here, both  $\mathbf{A}$  and  $\mathbf{B}$  are Hermitian matrices. Moreover,  $\mathbf{A}$  is positive definite. Defining  $\mathbf{y} = \sqrt{\mathbf{A}}\mathbf{x}$ , we get

$$\omega\mathbf{y} = (\sqrt{\mathbf{A}})^{-1}\mathbf{B}(\sqrt{\mathbf{A}})^{-1}\mathbf{y} \quad (12)$$

where  $(\sqrt{\mathbf{A}})^{-1}\mathbf{B}(\sqrt{\mathbf{A}})^{-1}$  is Hermitian.

The Hermitian formulation of Eq. (12) immediately leads to an orthogonality condition for the modes. For two modes at different frequencies  $\omega_m$  and  $\omega_n$ , the corresponding eigenmodes  $\mathbf{y}_m$  and  $\mathbf{y}_n$  should be orthogonal, i.e.,  $\int d\mathbf{r}\mathbf{y}_m \cdot \mathbf{y}_n = \delta_{mn}$ . Using the relation  $\mathbf{x} = (\sqrt{\mathbf{A}})^{-1}\mathbf{y}$ , we find the following orthogonality condition in terms of the physical fields:

$$\int d\mathbf{r} \left[ \frac{1}{2}(\epsilon_\infty\mathbf{E}_m^* \cdot \mathbf{E}_n + \mu_0\mathbf{H}_m^* \cdot \mathbf{H}_n) + \frac{1}{2\epsilon_\infty\omega_p^2}(\mathbf{V}_m^* \cdot \mathbf{V}_n + \omega_0^2\mathbf{P}_m^* \cdot \mathbf{P}_n) \right] = \delta_{mn}. \quad (13)$$

Such an orthogonality relation is essential for understanding various features of the band structure across the entire frequency spectrum. This result also connects directly with the energy density:

$$W = \frac{1}{2}(\epsilon_\infty|\mathbf{E}|^2 + \mu_0|\mathbf{H}|^2) + \frac{1}{2\epsilon_\infty\omega_p^2}(|\mathbf{V}|^2 + \omega_0^2|\mathbf{P}|^2), \quad (14)$$

where the last two terms correspond to the mechanical kinetic and potential energy of the electrons. We note further that the Hermitian nature of our operator ensures that the eigenfunctions of Eq. (12) form a complete, orthonormal basis [23].

The lossy version of Eq. (9) has  $\Gamma \neq 0$  which renders it non-Hermitian. To solve for the band structure of a lossy metamaterial, we directly diagonalize Eq. (9) to find the exact eigenmodes. The imaginary parts of these eigenvalues  $\omega = \omega' + i\omega''$  are the inverse lifetimes of the modes.

Furthermore, the orthonormal mode basis for the lossless system, as defined in Eq. (13), provides a basis for understanding lossy systems in general. To see this, we first define  $\mathbf{B}' = \mathbf{B} + \mathbf{D}$  where, in the same notation of Eq. (10),  $\mathbf{D} = \text{diag}(0, 0, 0, i\Gamma/\epsilon_\infty\omega_p^2)$ . Then, we treat the effect of  $\mathbf{D}$  with first-order perturbation theory: given solutions  $\omega_0$  and  $\mathbf{x}_0 = (\mathbf{H}_0, \mathbf{E}_0, \mathbf{P}_0, \mathbf{V}_0)^T$  that satisfy  $\omega_0\mathbf{A}\mathbf{x}_0 = \mathbf{B}\mathbf{x}_0$ , we find a first-order perturbative solution to the equation  $\omega\mathbf{A}\mathbf{x} = (\mathbf{B} + \mathbf{D})\mathbf{x}$ , where  $\omega = \omega_0 + \omega_1$  with

$$\omega_1 = \frac{\langle \mathbf{x}_0 | \mathbf{D} | \mathbf{x}_0 \rangle}{\langle \mathbf{x}_0 | \mathbf{A} | \mathbf{x}_0 \rangle} = \frac{i\Gamma/2\epsilon_\infty\omega_p^2 \int d\mathbf{r} |\mathbf{V}_0|^2}{\int d\mathbf{r} W_0}, \quad (15)$$

where  $W_0$  is the total energy density for the lossless mode as defined in Eq. (14).  $\omega_1$  is thus purely imaginary and defines the loss rate of the modes. Moreover, the form of

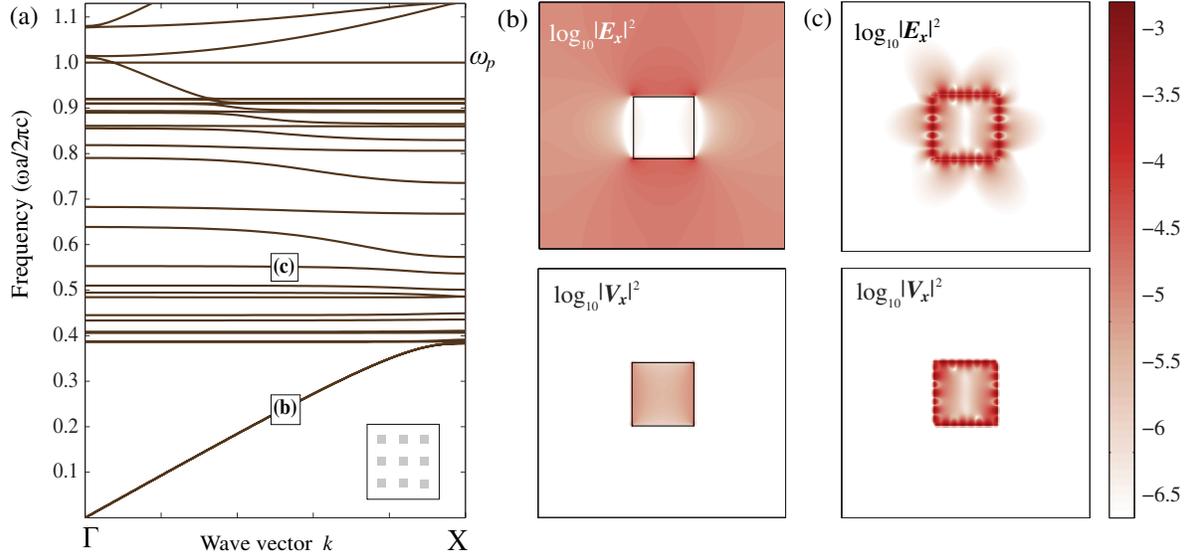


FIG. 1 (color online). (a) Computed band structure for 2D square plasmonic rods ( $r = 0.125a$ ) in air for the TE polarization. The band structure is shown between the  $\Gamma$  point wave vector ( $k = 0$ ), and the  $X$  point, ( $k = \pi/a$  along the  $x$  direction). (b) and (c) are visualizations of two field components at highlighted points in (a). Specifically, these are the electric and auxiliary polarization velocity field intensities for the modes.

Eq. (15) indicates that the modal loss is directly proportional to the kinetic energy of the electrons.

As a demonstration of this formalism, we consider a periodic array of plasmonic metal rods in air. This material, described by the Drude model, is treated in our formalism by setting  $\omega_0 = 0$ . In this case, Eq. (4) can be expressed entirely in terms of the  $\mathbf{V}$  field, while the  $\mathbf{P}$  fields are not present, reducing the size of our matrix equation. We set  $\omega_0 \rightarrow \infty$  and  $\omega_p \rightarrow 0$  for the air regions. This ensures that the  $\mathbf{V}$  field is not present in the air regions. The systems considered are two dimensional and are uniform along the third  $z$  dimension. For 2D systems we can completely separate the problem into calculations for TE and TM modes, with either the magnetic or the electric field entirely polarized along the  $z$  direction, respectively. To compute the band structure, we implement a finite-difference spatial discretization of the  $\mathbf{E}$  and  $\mathbf{H}$  fields with a Yee grid [24]. The use of Yee's grid ensures divergence-free behavior for the electromagnetic fields [25]. The equations are written for every cell in the Yee grid, with the spatial derivatives represented using finite-difference matrix operators [25]. The resultant matrix is very sparse and can be efficiently stored for computation purposes. We note here that our method is not constrained to 2D periodicity, and can be used for 3D periodic systems.

We start with the lossless case. The Hermitian eigenvalue problem of (12) can be solved efficiently using the well-known implicitly restarted Lanczos method [26]. The TE band structure of square metallic rods in air, where each side of the square has length  $s = 0.25a$  is presented in Fig. 1(a). The material used is defined by  $\epsilon_\infty = 1$ ,  $\omega_0 = 0$ ,  $\omega_p = 1$  for  $a = 137.6$  nm. These calculations are verified against the band structure calculated by analyzing the

spectrum from a finite-difference frequency domain (FDFD) simulation of the same structure [27]. We briefly highlight that the TE band structure presents numerous flat bands that correspond to surface plasmon modes, one of which is presented in Fig. 1(c).

For the plot shown in Fig. 1 we used a resolution of  $20 \times 20$  grid points. To test the convergence of the method we have also solved the band structure for higher resolutions. The band structure in Fig. 1 has a large number of flat bands, in particular frequency ranges [14]. Increasing the resolution increases the number of flat bands [16]. The frequency ranges where the flat bands occur, as well as the bands outside these ranges, are unchanged at higher resolutions.

To demonstrate the lossy version of the formalism, we consider the same plasmonic system with  $\Gamma = 0.01\omega_p$ . (As a comparison, silver has  $\Gamma = 0.0024\omega_p$  [28]. Here we have intentionally chosen a higher damping rate to demonstrate the utility of our formalism even in the presence of strong metal loss). We plot in Fig. 2 the inverse lifetime of the mode,  $\text{Im}[\omega] = \omega''$ , against the real frequency  $\omega'$ . Strong modal loss is observed in the frequency range where the flat surface plasmon bands are present.

We now demonstrate the connection between the lossless and the lossy band structures using first-order perturbation theory. For our example, we compare the perturbative solutions  $\omega_1$  against the exact solutions  $\omega''$  in Fig. 2 for  $\Gamma = 0.01\omega_p$  and find excellent agreement. The formalism here further enables us to quantitatively compare modes at different frequencies. We note that the two modal profiles in Fig. 1 are plotted with the same normalization such that the total energy inside a unit cell is set to unity. Examining these modal profiles, we note that the

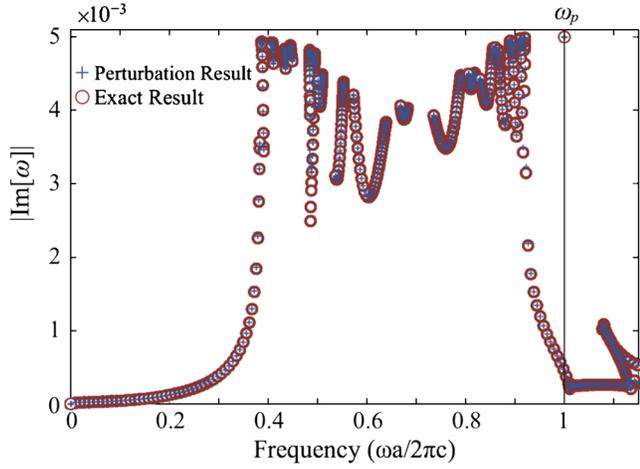


FIG. 2 (color online). Imaginary  $\omega$  ( $\omega''$ ) for the TE case, with loss term  $\Gamma = 0.01\omega_p$ . We compare the exact result to a perturbation theory result, and note excellent agreement.

mode calculated to have a higher loss [Fig. 1(c)] indeed has a much stronger mechanical field compared with a mode with lower loss [Fig. 1(b)]. The lossless Hermitian formalism thus provides important insights into understanding loss in such periodic material systems for realistic  $\Gamma$ .

Our method is easily extended to any linear material system by recognizing that the permittivity of any dispersive material can be modeled with several Lorentz poles, with increasing accuracy as the number of poles  $N$  increases:

$$\varepsilon(\omega) = \varepsilon_\infty + \varepsilon_\infty \sum_{n=1}^N \frac{\omega_{p,n}^2}{\omega_{0,n}^2 - \omega^2 + i\omega\Gamma_n}. \quad (16)$$

To model such a medium, for each Lorentz pole in Eq. (16) we introduce separate mechanical fields  $\mathbf{P}_n$  and  $\mathbf{V}_n$ . Equation (9) is then modified to

$$\omega \mathbf{E} = \frac{-i}{\varepsilon_\infty} \left( \nabla \times \mathbf{H} - \sum_{n=1}^N \mathbf{V}_n \right). \quad (17)$$

All of the discussion above on the formalism then follows in exactly the same way. In conclusion, we provide a direct, rigorous way of solving for the photonic band structure of any linear, lossy, dispersive periodic system. We also establish an orthonormal basis set, as obtained by considering a corresponding lossless case, for understanding lossy systems in general.

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