First principles calculation of topological invariants of non-Hermitian photonic crystals

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Topological photonic systems have recently emerged as an exciting new paradigm to guide light without back-reflections. The Chern topological numbers of a photonic platform are usually written in terms of the Berry curvature, which depends on the normal modes of the system. Here, we use a gauge invariant Green’s function method to determine from first principles the topological invariants of photonic crystals. The proposed formalism does not require the calculation of the photonic band-structure, and can be easily implemented using the operators obtained with a standard plane-wave expansion. Furthermore, it is shown that the theory can be readily applied to the classification of topological phases of non-Hermitian photonic crystals with lossy or gainy materials, e.g., parity-time symmetric photonic crystals.
Topological systems have fascinating and intriguing properties that can lead to unique physical effects and phenomena. Topological methods became part of mainstream condensed matter physics with the discovery of the quantum Hall effect. About one decade ago, the research of topological systems was extended to photonics and does not require any detailed knowledge of the topological band theory, the Green's function approach is based on references to calculate the Chern invariants of photonic platforms. Furthermore, we study the impact of material loss and gain on the topological invariants.

**Results and discussion**

**Topological band theory.** It is instructive to present a brief overview of the standard topological band theory in order to contrast it with the Green’s function theory used by us. In the topological band theory formalism, the gap Chern number of a (Hermitian) material system is obtained from the Berry curvature $F_{k}$ as

$$C_{\text{gap}} = \frac{1}{2\pi} \int \frac{d^{2}k}{BZ} F_{k}.$$  

(1)

The integral is over the first Brillouin zone (BZ) and $F_{k} = \sum_{n \in BZ} F_{nk}$ is the Berry curvature; the summation in $n$ is over all the “filled” photonic bands (FB) below the gap, i.e., modes with $\omega_{nk} < \omega_{\text{gap}}$, with $\omega_{\text{gap}}$ some frequency in the band gap. The Berry curvature of the $n$th band $F_{nk}$ is written in terms of the system eigenmodes $(H_{k}|nk\rangle = \omega_{nk}|nk\rangle)$ as

$$F_{nk} = \sum_{m \neq n} \frac{1}{\omega_{nk} - \omega_{nm}} \left[ \langle mk|\partial_{k}H_{k}|nk\rangle \langle nk|\partial_{k}H_{k}|mk\rangle - 1 \leftrightarrow 2 \right],$$

(2)

where $\partial_{i} = \partial/\partial k_{i}$ ($i = 1, 2$) with $k_{1} = k_{x}$ and $k_{2} = k_{y}$. The term $1 \leftrightarrow 2$ is obtained from the first term enclosed in rectangular brackets by exchanging the indices 1 and 2. Thus, from a computational point of view, the numerical calculation of the Chern invariants is a rather formidable problem: it generally requires finding the photonic band structure and all the Bloch states in the Brillouin zone. Moreover, Eq. (2) is ill-defined due to a 0/0 removable singularity when the Bloch eigenstates are degenerate, i.e., when there are band crossings. In such cases, the scalar products need to be replaced by the determinant of an overlap matrix which further increases the complexity of the problem. For further details a reader is referred to ref. 35.

The situation is even more complex for non-Hermitian systems, where the Chern number is found from a bi-orthogonal basis of left and right eigenstates of the non-Hermitian operator, i.e., from the eigenstates of $H_{k}$ and of $(H_{k})^\dagger$. The spectra of $H_{k}$ and of $(H_{k})^\dagger$ are not independent; their calculation requires the diagonalization of a non-Hermitian matrix which may be computationally demanding. The problem is especially complex for periodic structures, e.g., lossy non-reciprocal photonic crystals, where the relevant operator $H_{k}$ is isomorphic to a non-Hermitian matrix of finite dimension.

**Photonic Green’s function formalism.** In this Section, we describe the general Green’s function formalism introduced in references to calculate the Chern invariants of photonic platforms. The starting point is the generalized eigenvalue problem

$$\hat{L}_{k} \cdot Q_{nk} = \omega_{nk} M_{k} \cdot Q_{nk} \quad (n = 1, 2, \ldots)$$

(3)

with $\hat{L}_{k}$ a generic differential operator and $M_{k}$ a multiplication (matrix) operator. The operator $L_{k}$ is parameterized by the real wave vector $k = k_{x}\hat{\mathbf{x}} + k_{y}\hat{\mathbf{y}}$. The operator $M_{k}$ is independent of $k$. Here, $Q_{nk}$ are the generalized eigenstates of $\hat{L}_{k}$ and $\omega_{nk}$ are the generalized eigenvalues. The objective is to determine the interesting case of photonic crystals. We show how by using the operators obtained from the well-known plane wave method it is possible to find in a relatively simple and computationally inexpensive way the gap Chern number of topological photonic platforms.
topological phases of $\hat{\mathbf{I}}_k$, or equivalently the topological phases of $\hat{H}_k = \mathbf{M}_g \cdot \hat{\mathbf{I}}_k$.

To this end, we introduce the system Green’s function $\mathcal{G}_k$, defined by

$$\mathcal{G}_k(\omega) = i (\hat{\mathbf{I}}_k - \mathbf{M}_g \omega)^{-1}. \quad (4)$$

The Green’s function has poles at the eigenfrequencies $\omega = \omega_{\text{ek}}$, but otherwise is an analytic function of frequency. Let us first consider that $\hat{\mathbf{I}}_k$ and $\mathbf{M}_g$ are Hermitian operators. In that case, the eigenfrequencies $\omega_{\text{ek}}$ are real-valued numbers. Hence, the projection of the system band structure into the complex-frequency plane $\omega = \omega' + i \omega''$ consists of line segments contained in the real-frequency axis (see Fig. 1a). The band gaps are the regions of the complex frequency plane that separate disconnected sets of eigenfrequencies. For example, with reference to Fig. 1a the region $\omega_1 < \omega' < \omega_2$ is a band gap (vertical strip shaded in yellow in Fig. 1a), as it separates two sets eigenfrequencies, i.e., two bands. It should be noted that two non-touching bands do not in general yield a gap in the complex plane. The gap formation requires that the projections of the bands in the complex-frequency plane are disconnected.

The band-gap definition can be readily extended to non-Hermitian systems, with the difference that for non-Hermitian platforms the projected band structure is not restricted to the real-frequency axis. Hence, in the non-Hermitian case the projected band-structure can populate parts of the lower-half (for lossy systems) or upper-half (for gainy systems) complex-frequency plane. In general, the band gaps are vertical strips in the complex plane, i.e., of the form $\omega_1 < \omega' < \omega_2$, where the Green’s function is analytic (the vertical strip does not need to be rectangular and can have an arbitrary shape provided the initial and end points have $\xi = \pm \infty$, respectively).

Each band-gap is associated with a topological invariant, the gap Chern number, given by24,28

$$C_{\text{gap}} = \frac{1}{(2\pi)^2} \int \int_{\text{B.Z.}} \frac{d^2k}{i\omega_{\text{gap}} + \text{i}\omega} \text{Tr}[\partial_\omega \mathcal{G}_k^{-1} \cdot \mathcal{G}_k \cdot \partial_\omega \mathcal{G}_k^{-1} \cdot \partial_\omega \mathcal{G}_k], \quad (5)$$

where Tr[...] stands for the trace operator, $\partial_\omega = \partial / \partial \omega$ and $\partial_\omega \mathcal{G}_k^{-1} = \partial \mathcal{G}_k^{-1} / \partial k_j$ (j = 1, 2) with $k_1 = k_x$ and $k_2 = k_y$. The integral in $\omega$ is over a contour completely contained in the band gap that joins the points $-i\omega_{\text{gap}}$ and $+i\omega_{\text{gap}}$. For simplicity, throughout the article it is assumed that the contour is a straight line of the form $\text{Re} [\omega] = \omega_{\text{gap}}$ with $\omega_{\text{gap}}$ some (real valued) frequency in the gap (see Fig. 1a).

The derivatives in frequency and wave vector can be explicitly evaluated as $\partial_\omega \mathcal{G}_k = -i \mathbf{g}_k \cdot \mathbf{M}_g \mathcal{G}_k$ and $\partial_\mathbf{r} \mathcal{G}_k^{-1} = -i \partial \mathbf{l}_k / \partial k_j$. Hence, the gap Chern number can be expressed as

$$C_{\text{gap}} = \frac{i}{(2\pi)^2} \int \int_{\text{B.Z.}} \frac{d^2k}{i\omega_{\text{gap}} + \text{i}\omega} \text{Tr}[\partial_\omega \mathcal{G}_k^{-1} \cdot \mathbf{M}_g \cdot \partial_\omega \mathcal{G}_k \cdot \mathbf{M}_g \cdot \mathcal{G}_k \cdot \mathbf{M}_g \cdot \mathcal{G}_k]. \quad (6)$$

In order to numerically calculate the integral it is convenient to use the coordinates $\omega = \omega_{\text{gap}} + i \xi$ and $\mathbf{k} = \beta_1 \mathbf{b}_1 + \beta_2 \mathbf{b}_2$, where $\mathbf{b}_j$ are the reciprocal lattice primitive vectors of the photonic crystal and $-1/2 \leq \beta_j \leq 1/2$ (j = 1, 2). With these coordinate transformations we finally get

$$C_{\text{gap}} = \frac{1}{(2\pi)^2} \int \int_{\text{B.Z.}} \frac{d\beta_1 d\beta_2}{\omega_{\text{gap}} + i \xi} \text{Tr}[\partial_\omega \mathcal{G}_k^{-1} \cdot \mathbf{M}_g \cdot \partial_\omega \mathcal{G}_k \cdot \mathbf{M}_g \cdot \mathcal{G}_k]. \quad (7)$$

$$g(\xi, \beta_1, \beta_2) = \frac{-1}{(2\pi)^2} [\mathbf{b}_1 \times \mathbf{b}_2]^2 \times \left[ \text{Tr}[\partial_\omega \mathcal{G}_k^{-1} \cdot \partial_\mathbf{r} \mathcal{G}_k \cdot \mathbf{M}_g \cdot \mathcal{G}_k] \bigg| \omega = \omega_{\text{gap}} + i \xi, \mathbf{k} = \beta_1 \mathbf{b}_1 + \beta_2 \mathbf{b}_2 \right] + \text{Tr}[\partial_\mathbf{r} \mathcal{G}_k^{-1} \cdot \partial_\mathbf{r} \mathcal{G}_k \cdot \mathbf{M}_g \cdot \mathcal{G}_k] \bigg| \omega = \omega_{\text{gap}} - i \xi, \mathbf{k} = \beta_1 \mathbf{b}_1 + \beta_2 \mathbf{b}_2 \right]. \quad (8)$$

In practice, the upper-limit of the integral in $\xi$ needs to be truncated: $\int_0^\infty d\xi \rightarrow \int_0^{\xi_{\text{max}}} d\xi$, where $\xi_{\text{max}}$ should be on the order of $c/a$ with $c$ being the speed of light and $a$ the lattice constant. Typically, $g$ decays exponentially fast with $\xi$ and hence the integration in $\xi$ is quite efficient.24,28 The integrals in $\beta_1, \beta_2, \xi$ are done using a numerical quadrature rule, e.g., using the trapezoidal or the Simpson rules.

**Magnetic-gyrotropic photonic crystal.** To illustrate the ideas, we consider a photonic crystal formed by a hexagonal array of cylindrical rods with radius $R$ embedded in air as illustrated in Fig. 1b. The periodic structure contains two rods per unit cell, i.e., it is formed by two sub-lattices (honeycomb lattice). The direct lattice primitive vectors are taken equal to:

$$a_1 = \frac{a}{2} \left( 3x - \sqrt{3}y \right), \quad a_2 = \frac{a}{2} \left( 3x + \sqrt{3}y \right). \quad (9)$$
where $a$ is the distance between nearest neighbors (circles with different colors in Fig. 1b). The relative permittivity and permeability tensors of the photonic crystal are of the form:

$$\tau = i\mathbf{1}_{3 \times 3}, \quad \hat{\mu} = \begin{pmatrix} \mu & i\kappa & 0 \\ -i\kappa & \mu & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

(10)

with $\epsilon = \epsilon(x, y)$, $\mu_{11} = \mu_{22} = \mu(x, y)$, and $\mu_{12} = -\mu_{21} = i\kappa(x, y)$. The nonreciprocity parameter $\kappa$ vanishes in the air region and is equal to $\kappa_i$ ($i = 1, 2$) in the $i$th sub-lattice of the hexagonal array. Hence, the rods material response is nonreciprocal ($\mu \neq \mu^T$) and gyrotropic. This type of material response occurs in natural ferromagnetic materials (e.g., ferrites) biased with a magnetic field directed along the $z$-direction. The parameters $\epsilon$ and $\mu$ are identical to $\epsilon = \mu = 1$ in the air region and to $\epsilon_i$ and $\mu_i$ in the $i$th sub-lattice ($i = 1, 2$) of the crystal. For simplicity, here we neglect material dispersion so that $\mu_i$ and $\kappa_i$ are frequency independent. The generalized eigenvalue problem can be generalized to include the effects of material dispersion$^{34,28}$, but since there are a few nontrivial technicalities we leave that study for future work.

We consider waves with transverse electric (TE) polarization ($\mathbf{E} = E_z \mathbf{e}_z$) and propagation in the $xoy$ plane, so that $\mathbf{E} = E_z(\mathbf{x}, \mathbf{y})$. Here, the nomenclature transverse electric refers to the orientation of the electric field with respect to the direction of propagation of the wave (in the $xoy$ plane). From the Maxwell equations, $\nabla \times \mathbf{E} = i\omega \mu \hat{\mu} \cdot \mathbf{H}$ and $\nabla \times \mathbf{H} = -i\omega \epsilon \hat{\epsilon} \cdot \mathbf{E}$, it readily follows that

$$\nabla \times \left( \mu_e^{-1} \nabla E_z - i\chi \partial_x E_z \right) + \nabla \cdot \left( \mu_e^{-1} \partial_x E_z + i\chi \partial_x E_z \right) = \left( \frac{\omega^2}{c^2} \right) E_z,$$

(11)

with $\mu_e = (\mu^2 - \kappa^2)/\mu$ and $\chi = \kappa(\mu^2 - \kappa^2)$. The secular equation can be written in the form:

$$\hat{L}(-i\mathbf{\nabla}) \cdot \mathbf{E}_z = \mathcal{E} \mathbf{M}_g \cdot \mathbf{E}_z,$$

(12)

with $\mathcal{E} = (\omega/c)^2$ and

$$\mathbf{M}_g \cdot \mathbf{E}_z \equiv \epsilon \mathbf{E}_z.$$

$$\hat{L} \cdot \mathbf{E}_z \equiv -\partial_x \left( \mu_e^{-1} \partial_x E_z - i\chi \partial_x E_z \right) - \partial_y \left( \mu_e^{-1} \partial_y E_z + i\chi \partial_y E_z \right).$$

(13)

As seen, $\mathbf{M}_g$ is a multiplication operator (multiplication by the material permittivity) and $\hat{L} = \hat{L}(-i\mathbf{\nabla})$ is a differential operator. The Bloch modes associated with the wave vector $\mathbf{k} = k_x \mathbf{\hat{x}} + k_y \mathbf{\hat{y}}$ are of the form $E_z = e_z(\mathbf{x}, \mathbf{y}) e^{i\mathbf{r} \cdot \mathbf{k}}$, with the envelope $e_z(x, y)$ being a periodic function that satisfies the generalized eigenvalue problem:

$$\hat{L}_k \cdot e_z = \mathcal{E} \mathbf{M}_g \cdot e_z,$$

(14)

with $\hat{L}_k \equiv \hat{L}(-i\mathbf{\nabla} + \mathbf{k})$.

The operator $\hat{L}_k$ is obtained from $\hat{L}$ with the substitutions $\partial_j \to \partial_j + ik_j (j = x, y)$. Evidently, the generalized eigenvalue problem is of the same type as in Eq. (3), and hence the topological phases of $\hat{L}_k$ can be found using the Green’s function formalism. Note that here the eigenvalues are $\mathcal{E} = (\omega/c)^2$, i.e., they are the squared eigenfrequencies of the photonic crystal (apart from a normalization factor). Thus, the gap Chern number can be found using Eq. (7) with the substitution $\omega \to \mathcal{E}$. For example, the Green’s function is defined as $G_k(E) = i(\hat{L}_k - \mathbf{M}_g \mathcal{E})^{-1}$ and the integration in $\xi$ is associated with the contour $\mathcal{E} = \mathcal{E}_{gap} + i\epsilon$, where $\mathcal{E}_{gap} = (\omega_{gap}/c)^2$.

The band structure of the photonic crystal can be found with the plane wave method$^{32}$. To this end, the electric field envelope $e_z$ is expanded into plane waves as $e_z = \sum \xi_j e^{|\mathbf{J}_j| \mathbf{r}}$, with the envelope $e_{\xi}(\mathbf{x}, \mathbf{y})$. The plane wave expansion is truncated enforcing that $\xi_j \leq \xi_{\text{max}}$ for $i = 1, 2$. In these circumstances, $\mathbf{M}_g$ and $\hat{L}_k$ are given by matrices with dimension $(2\xi_{\text{max}} + 1)^2 \times (2\xi_{\text{max}} + 1)^2$ and Eq. (14) is reduced to a generalized matrix eigenvalue problem [Eq. (21)].

The calculated band structure is plotted in Fig. 2a for a nonreciprocal photonic crystal ($\kappa = 0.9$, solid lines) and for a reciprocal photonic crystal ($\kappa = 0.9$, dashed lines). A sketch of the Brillouin zone and the definition of the relevant high-symmetry points can be found in Fig. 1c. The radius of the scattering centers is $R = 0.346a$ and the gyrotropic material constitutive parameters are taken equal to $\epsilon_1 = \epsilon_2 = 12$ and $\mu_1 = \mu_2 = 1$. As seen in Fig. 2a, for the reciprocal case, the bands touch at the Dirac point ($\mathbf{K}$) due to the asymmetry of the hexagonal lattice ($\epsilon_1 = \epsilon_2$). Indeed, the reciprocal photonic crystal is a photonic analog of graphene$^{37}$. When a static magnetic field is applied to the system, so that $\kappa \neq 0$, the topological phases are shaded with different colors. The boundaries between the different regions are obtained with an interpolation of the numerically calculated pairs ($\kappa, \delta$) for which the band-gap closes (discrete black points).
0, the degeneracy around the Dirac points is lifted, leading to a complete photonic band-gap. For \( \kappa = 0.9 \), the band gap is determined by 1.12/\( a^2 \) < \( E < 1.53/\( a^2 \). The plane wave expansion was truncated with \( |j| \leq j_{\text{max}} = 3 \).

Analogous to the Haldane model\(^2,12,38 \), a band-gap between the first and second bands can be opened either by breaking the time-reversal symmetry \( (\kappa \neq 0, \text{as illustrated in Fig. 2a}) \) or, alternatively, by introducing some structural asymmetry between the two sub-lattices of the hexagonal array so that the inversion symmetry is broken. To model the latter situation, we introduce a spatial-asymmetry parameter \( (\delta) \) that controls the permittivity of the cylindrical rods as \( \varepsilon_1 = 12 + \delta \) and \( \varepsilon_2 = 12 - \delta \). For \( \delta \neq 0 \) the inversion symmetry of the system is broken. We numerically checked that for specific combinations of the parameters \( (\kappa, \delta) \) the band-gap between the first and second bands is closed. These pairs of \( (\kappa, \delta) \) are represented by the continuous black lines in Fig. 2b.

**Topological phases.** The gap Chern number can be found by feeding the matrices that represent \( M_k \) and \( L_k \) in the plane wave basis [Eq. (20)] into the integral (7). Thus, the Chern number is calculated as an integral along the imaginary axis \( \int_{\mathbb{C}} \) in a matrix. All the matrices have dimensions \( 2 \times 2 \) and we take \( \varepsilon_{\text{max}} = 5/\( a^2 \) \). The Brillouin zone is uniformly sampled with \( N_1 \times N_2 \) points in the \((\beta_1, \beta_2)\) coordinates. The integral along the imaginary axis \( \langle \varepsilon = \varepsilon_{\text{gap}} + i\lambda \rangle \) is truncated at \( \varepsilon_{\text{gap}} = 5/\( a^2 \) \) and the integrand is sampled with \( N_1 \) points. The parameter \( \varepsilon_{\text{gap}} \) is taken as the mid-point of the gap and we use \( j_{\text{max}} = 3 \).

The phase diagram of the ferrite photonic crystal is plotted in Fig. 3a. The diagram shows the gap Chern number for different combinations of the nonreciprocity and spatial-asymmetry parameters \( (\kappa, \delta) \). The different topological phases are shaded with different colors and the corresponding gap Chern numbers are shown in the insets. As previously mentioned, the two black curves show the combinations of \( (\kappa, \delta) \) for which the band gap closes. As seen, when the inversion symmetry breaking dominates (large values of \( |\delta| \)) the photonic crystal is topologically trivial.

In our numerical code, the integral (7) is evaluated using the trapezoidal quadrature rule. The Brillouin zone is uniformly sampled with \( N_1 \times N_2 \) points in the \((\beta_1, \beta_2)\) coordinates. The integral along the imaginary axis \( \langle \varepsilon = \varepsilon_{\text{gap}} + i\lambda \rangle \) is truncated at \( \varepsilon_{\text{gap}} = 5/\( a^2 \) \) and the integrand is sampled with \( N_1 \) points. The parameter \( \varepsilon_{\text{gap}} \) is taken as the mid-point of the gap and we use \( j_{\text{max}} = 3 \).

Figure 3a depicts the integrand of Eq. (7) as a function of \( \beta_1 \) for \( \xi = 0 \) and \( \beta_2 = 1/3 \) (solid line) and \( \beta_2 = -1/3 \) (dashed line). The photonic crystal parameters are the same as in Fig. 2a with \((\kappa, \delta) = (0.9, 0)\) and we take \( \varepsilon_{\text{gap}} = 1.325/\( a^2 \). As seen, the integrand is peaked near \( \beta_1 = 1/3 \), which correspond to the coordinates of the \( K \) and \( K' \) points, respectively. This reveals that the topological charge is concentrated near the two Dirac points.

Figure 3b–d shows the numerically calculated gap Chern number as a function of \( N \equiv N_1 = N_2, N_1 \) and \( \xi_{\text{max}} \) respectively. As seen, for modestly large values of \( N, N_1 \), and \( \xi_{\text{max}} \) the numerical result converges to \( C_{\text{gap}} = 1 \), consistent with the topological nature of the Chern number. The computation time of each Chern number is on the order of minutes in a standard personal computer with high-level language programming (Wolfram Mathematica).

The formalism can be applied with no modifications to take into account the effect of material dissipation in the cylindrical rods. Non-energy conserving (non-Hermitian) platforms have recently raised a lot of interest due to the exotic physics of systems with exceptional points\(^44 \). For simplicity, here we model the material loss by considering that \( \mu \) is complex valued: \( \mu = \mu' + i\mu'' \). As in the previous subsection, we take \( \mu' = 1 \).

Figure 4 shows the band structure of the non-Hermitian photonic crystal projected on the \( \varepsilon \)-plane for two different values of loss parameter: \( \mu'' = 0.1 \) [Fig. 4a] and \( \mu'' = 0.5 \) [Fig. 4b]. The projected band structure represents the locus of \( \varepsilon = \varepsilon' + i\varepsilon'' \) as a function of the real-valued wave vector of the Bloch modes with \( \varepsilon = (a/c)^2 \). For a lossy system the projected band structure lies in the lower-half frequency plane, different from the lossless case [Fig. 2a] where \( \varepsilon \) is real valued. As seen in Fig. 4, for both examples there is a vertical strip of the \( \varepsilon \)-plane (shaded light-blue region) free of natural modes. This vertical strip represents the band gap. The two projected bands remain disconnected even in case of relatively strong material dissipation. In other words, typically the material dissipation does not close the band gap.

Figure 5 reports a study analogous to that of Fig. 3, but for a lossy photonic crystal with \( \mu_1 = \mu_2 = 1 + 0.1 \). As in the lossless case, the integrand \( g \) is peaked at the Dirac points \( K' \) and \( K \) (see Fig. 5a), but now the topological charge is distributed more evenly through the wave vector space. The convergence rate and the computational effort to find the gap Chern number of the non-Hermitian system are similar to the lossless case (see Fig. 5b–d). Furthermore, the numerical results confirm that the band gap of the projected band structure [Fig. 4a] is topologically nontrivial.

The formalism can also be applied with no modifications to gainy systems. To illustrate this we consider a parity-time (PT) symmetric\(^45,46 \) gyrotropic photonic crystal. PT-symmetric systems have rather unique features and can be implemented in optics through a judicious inclusion of gain/loss regions\(^47–50 \) or with moving media\(^51,52 \). The spectrum of PT-symmetric systems is real valued when the eigenfunctions simultaneously diagonalize the system Hamiltonian and the PT operator. Otherwise, the spectrum can be complex valued, which corresponds to a spontaneously broken PT-symmetry.

In our case, the PT-symmetry can be enforced by imposing that \( \mu_1 = 1 + i\mu'' \) and \( \mu_2 = 1 - i\mu'' \) with \( \mu'' > 0 \), so that the first sub-lattice of cylinders is formed by dissipative elements and the second sub-lattice by gainy elements. The rest of the structural parameters are as in Fig. 2a. The parity operator is \( \mathcal{P} : (x, y, z) \to (-x, y, z) \). The operator \( \mathcal{P} \) interchanges the role of the two sub-lattices and flips the sign of the nonreciprocity parameter \( \kappa \). The time-reversal operator also flips the sign of (the real valued) \( \kappa \) and transforms loss into gain and vice versa. Thus, the photonic crystal of Fig. 1b is indeed PT-symmetric.

Figure 6 shows the band structure of the PT-symmetric gyrotropic photonic crystal projected on the \( \varepsilon \)-plane for four different cases: \( \mu'' = 0.1 \) [Fig. 6a], \( \mu'' = 2 \) [Fig. 6b], \( \mu'' = 2.1 \) [Fig. 6c], and \( \mu'' = 2.2 \) [Fig. 6d]. As seen in Fig. 6, for a lossy-gainy system the projected band structure lies both in the lower and upper-half frequency planes, different from the lossy case [Fig. 4] where \( \varepsilon'' \) is always negative. Because of the PT-symmetry the projected band structure exhibits a mirror-symmetry with respect to the real-frequency axis. Analogous to Fig. 4, the bands are projected onto the regions filled in dark-blue color. Figure 6 was obtained under the simplifying hypothesis that the boundary of the projected band structure is determined by the path \( \Gamma - M - K - \Gamma' - K' - \Gamma \). We numerically checked that such approximation...
leads to results almost coincident with the exact projected band structure. For small values of $\mu''$ [Fig. 6a], the first two projected bands are disconnected. The gap topological number is numerically calculated in the same manner as in the previous examples and is equal to $C_{\text{gap}} = \text{sgn}(\kappa)$, consistent with Figs. 3 and 5. Therefore, as could be expected, moderate values of $\mu''$ do not affect the topological properties of the system. For larger values of $\mu''$ [Fig. 6b], the band gap between the first two projected bands becomes very narrow. The band-gap closes approximately for $\mu'' = 2.1$, when the two bands touch at two distinct points [Fig. 6c]. For larger values of $\mu''$ [Fig. 6d], the two bands remain connected and the topological classification is not feasible.

**Conclusion**

We used a Green’s function method to calculate from first principles the topological invariants of Hermitian and non-Hermitian photonic crystals with a broken time-reversal symmetry. The main advantage of our formalism is that it does not require any detailed knowledge of the photonic band structure or of the Bloch modes. In particular, different from the topological band theory, the Green’s function approach can be applied with no modifications when the different photonic bands cross at one or more points of the Brillouin zone. The computational effort for the non-Hermitian case is essentially the same as for the Hermitian case. The Green’s function is numerically calculated using the standard plane wave method. We applied the formalism to magnetic-gyrotropic photonic crystals. It was shown that the topological phases of a photonic crystal are strongly robust to non-Hermitian perturbations (dissipation and/or gain). We expect that our work will find widespread application in the characterization of emergent topological photonic platforms.
Fig. 5 Convergence analysis of the Chern number of a non-Hermitian photonic crystal. The photonic crystal is formed by inclusions of a lossy gyrotropic material with $\varepsilon_1 = \varepsilon_2 = 12$, $\kappa = 0.9$ and $\mu_1 = \mu_2 = 1 + i\mu''$ with $\mu'' = 0.1$. a Integrands of Chern number integral $g$ [Eq. (7)] (in arbitrary units) as a function of $\beta_1$ for $\beta_2 = 1/3$ (solid line) and $\beta_2 = -1/3$ (dashed line). b-d The numerically calculated gap Chern number $C_{\text{gap}}$ as a function of b $N$, c $N_\xi$, and d $\xi_{\text{max}}$. The values of $N$, $N_\xi$, and $\xi_{\text{max}}$ are 10, 50, and $5/a^2$, respectively, except for the parameter shown in the horizontal axis of a plot.

Fig. 6 Projected band structures of $\mathcal{PT}$-symmetric gyrotropic photonic crystals. The band structures are projected onto the regions filled in dark-blue color of the complex $\varepsilon = \varepsilon' + i\varepsilon''$ plane. The photonic crystal parameters are $\varepsilon_1 = \varepsilon_2 = 12$, $\mu_1 = 1 + i\mu''$, $\mu_2 = 1 - i\mu''$, and $\kappa = 0.9$. The loss-gain parameter $\mu''$ is a $\mu'' = 0.1$, b $\mu'' = 2$, c $\mu'' = 2.1$, and d $\mu'' = 2.2$. 
Methods

Plane wave representation of the operators $\mathbf{M}_\alpha$ and $\hat{L}_k$. Here, we obtain the representations of the operators $\mathbf{M}_\alpha$ and $\hat{L}_k$ [see Eqs. (13) and (14)] in a plane wave basis:\footnote{Note that $\delta_{\alpha \beta}$ is Kronecker’s symbol, $I_1$ is the cylindrical Bessel function of first kind and first order, $R$ is the radius of the rods of the rh unit cell, and $\Phi_{\alpha \beta} = \pi R^2 / \Lambda_{\alpha \beta}$ with $\Lambda_{\alpha \beta} = [ b \times b ]$ the area of the unit cell.}

To begin with, we expand the periodic functions $\mu_\alpha^{-1}$, $\chi$, and $\epsilon$ in a Fourier series:

$$
\mu_\alpha^{-1} = \sum_r P_{\alpha r} e^{i \mathbf{k} \cdot \mathbf{r}}, \quad \chi = \sum_r P_{1 r} e^{i \mathbf{k} \cdot \mathbf{r}}, \quad \text{and} \quad \epsilon = \sum_r P_{2 r} e^{i \mathbf{k} \cdot \mathbf{r}}. 
$$

(15)

The Fourier coefficients are $P_{\alpha r} = \int_0^1 \int_0^1 \int_0^1 \mu_{\alpha r} e^{-i \mathbf{k} \cdot \mathbf{r}} d^3 r$. For a generic function $g$ the Fourier coefficients are $g_{\alpha r} = \int_0^1 \int_0^1 \int_0^1 g e^{-i \mathbf{k} \cdot \mathbf{r}} d^3 r$. The geometry of Fig. 1b, the function $g$ (where $g$ can stand either for $\mu_\alpha^{-1}$, $\chi$ or $\epsilon$) is sectorially constant. Let us suppose that $g = g_0$ in the (air) background region and $g = g_1$ in the first and second sub-lattices of the hexagonal array, respectively. A straightforward calculation shows that:\footnote{It is important to note that $\mathbf{G}$ is a matrix with element $G_{IJ}$ stands for a matrix with element $G_{IJ} = \epsilon [ \mathbf{M}_\alpha | \mathbf{M}_\beta ]$ in line I and column J. The generalized eigensystem (14) is equivalent to $[ G_{IJ} ] | J \rangle = \epsilon [ M_{IJ} ] | I \rangle$.

Finally, the operators $\hat{L}_k\hat{L}_k^\dagger$ are represented by

$$
\hat{L}_k \hat{L}_k^\dagger \rightarrow \begin{pmatrix} \mathbf{u} \times (2 \mathbf{G}_1 + \mathbf{G}_3) \\ \mathbf{u} \times (\mathbf{G}_3 - \mathbf{G}_1) \end{pmatrix} + \frac{i}{2} \left[ (\mathbf{G}_1 - \mathbf{G}_1) \times \mathbf{G}_1 \right]. 
$$

(22)

in the plane wave basis, where $\mathbf{u}_x = \hat{\mathbf{x}}$ and $\mathbf{u}_y = \hat{\mathbf{y}}$ are unit vectors along the coordinates axes.

Data availability

The data that support the findings of this study are available from the corresponding author upon reasonable request.

Received: 4 March 2020; Accepted: 16 October 2020; Published online: 03 December 2020

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**Acknowledgements**

This work was supported by the IET under the A F Harvey Engineering Research Prize and by Fundação para Ciência e a Tecnologia (FCT) under project UIDB/50008/2020. F. R.P. acknowledges financial support by FCT under the Post-Doctoral fellowship SFRH/BPD/108823/2015.

**Author contributions**

F.R.P. developed the formalism to calculate the topological invariants using the plane wave method and the Green’s function theory, did the numerical calculations and produced all the figures. F.R.P and M.G.S. discussed the theoretical and numerical results and wrote the manuscript.

**Competing interests**

The authors declare no competing interests.

**Additional information**

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