First Principles Calculation of Topological Invariants by Means of the Photonic Green's Function

Filipa R. Prudêncio[1,2], and Mário G. Silveirinha[1]

[1]University of Lisbon – Instituto Superior Técnico and Instituto de Telecomunicações, Avenida Rovisco Pais 1, 1049-001 Lisbon, Portugal
[2]Instituto Universitário de Lisboa (ISCTE-IUL), Avenida das Forças Armadas 376, 1600-077 Lisbon, Portugal
*corresponding author, E-mail: filipa.prudencio@lx.it.pt

Abstract

The Chern topological numbers of a material 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.

1. Introduction

Topological systems have fascinating and intriguing properties, which can lead to novel physical effects and phenomena [1-8]. The Chern topological numbers of a material system are usually written in terms of the Bloch eigenmodes. Thus, from a computational point of view, the numerical calculation of the Chern invariants is a rather complex problem: it generally requires finding the photonic band structure and all the Bloch states in the Brillouin zone. The problem is specially challenging in the case of periodic systems, e.g., nonreciprocal photonic crystals. In a few recent articles [6, 7] it was shown that the gap Chern numbers can alternatively be written in terms of the system Green's function. The theory is gauge invariant and does not require any detailed knowledge of the band structure or of the Bloch eigenstates. The method applies to both fermionic and bosonic platforms (even in case of material dispersion) and to non-Hermitian systems [6, 7]. Here, we illustrate the application of the formalism to ferrite photonic crystals. Specifically, we determine from first principles (i.e., without a tight-binding approximation) the gap Chern numbers of the photonic crystal relying on a plane wave expansion.

2. General formalism

Next, we briefly review the general Green's function formalism reported in [6, 7] to characterize the Chern invariants of photonic platforms. Consider a generalized eigenvalue problem of the form $\hat{L}_{\mathbf{k}} \cdot \mathbf{Q}_{n\mathbf{k}} = \mathcal{E}_{n\mathbf{k}} \mathbf{M}_g \cdot \mathbf{Q}_{n\mathbf{k}}$ (n=1,2,…), where $\hat{L}_{\mathbf{k}}$ and $\mathbf{M}_g$ are operators (possibly non-Hermitian). The operator $\hat{L}_{\mathbf{k}}$ is parameterized by the real wave vector $\mathbf{k} = k_x \hat{\mathbf{x}} + k_y \hat{\mathbf{y}}$ and the operator $\mathbf{M}_g$ is independent of $\mathbf{k}$. Here, $\mathbf{Q}_{n\mathbf{k}}$ are the generalized eigenstates of $\hat{L}_{\mathbf{k}}$ and $\mathcal{E}_{n\mathbf{k}}$ are the generalized eigenvalues. The system Green's function is defined by $\mathcal{G}_{\mathbf{k}}(\mathcal{E}) = i\left(\hat{L}_{\mathbf{k}} - \mathbf{M}_g \mathcal{E}\right)^{-1}$ [7]. The Green's function has poles at the eigenfrequencies $\mathcal{E} = \mathcal{E}_{n\mathbf{k}}$, but otherwise is an analytic function of frequency. The band gaps are vertical strips of the complex plane ($\mathcal{E}_L < \mathrm{Re}\{\mathcal{E}\} < \mathcal{E}_U$) where the Green's function is analytic. The gap Chern number is determined by [6, 7]:

$$\mathcal{C} = \frac{1}{(2\pi)^2} \iint_{B.Z.} d^2\mathbf{k} \int_{\mathcal{E}_{\mathrm{gap}}-i\infty}^{\mathcal{E}_{\mathrm{gap}}+i\infty} d\mathcal{E}\, \mathrm{Tr}\left\{\partial_1 \mathcal{G}_{\mathbf{k}}^{-1} \cdot \mathcal{G}_{\mathbf{k}} \cdot \partial_2 \mathcal{G}_{\mathbf{k}}^{-1} \cdot \partial_{\mathcal{E}} \mathcal{G}_{\mathbf{k}}\right\} \quad (1)$$

where $\partial_{\mathcal{E}} = \partial / \partial \mathcal{E}$ and $\mathcal{E}_{\mathrm{gap}}$ is some "frequency" in the gap. We denote $\partial_j \mathcal{G}_{\mathbf{k}}^{-1} = \partial \mathcal{G}_{\mathbf{k}}^{-1} / \partial k_j = -i\partial \hat{L}_{\mathbf{k}} / \partial k_j$ (j=1,2) with $k_1 = k_x$ and $k_2 = k_y$. The integral in $\mathcal{E}$ is over the line $\mathrm{Re}\{\mathcal{E}\} = \mathcal{E}_{\mathrm{gap}}$ and $\mathrm{Tr}\{...\}$ stands for the trace operator.

3. Ferrite photonic crystal

Consider a ferrite photonic crystal formed by a hexagonal array of ferrites embedded in air [9], as illustrated in Fig.1. Assuming transverse electric (TE) polarization ($\mathbf{E} = E_z \hat{\mathbf{z}}$) and propagation in the *xoy* plane it can be shown that the secular wave equation is of the form $\hat{L}(-i\nabla) \cdot E_z = \mathcal{E} \mathbf{M}_g \cdot E_z$ with $\mathcal{E} = (\omega / c)^2$, $\mathbf{M}_g \cdot E_z \equiv \varepsilon E_z$ and

$$\hat{L} \cdot E_z \equiv -\partial_x \left[\frac{1}{\mu_{ef}} \partial_x E_z + \frac{-i\kappa}{\mu_{ef}\mu} \partial_y E_z\right] - \partial_y \left[\frac{1}{\mu_{ef}} \partial_y E_z + \frac{i\kappa}{\mu_{ef}\mu} \partial_x E_z\right]. \quad (2)$$

Thus, $\mathbf{M}_g$ is a multiplication operator and $\hat{L}(-i\nabla)$ is a differential operator. In the above, $\varepsilon = \varepsilon(x, y)$ is the permittivity, $\mu = \mu_{11}(x, y)$ and $\kappa = -i\mu_{12}(x, y)$ are the diagonal and anti-diagonal elements of the permeability tensor, respectively, and $\mu_{ef} = (\mu^2 - \kappa^2)/\mu$. For simplicity,

in this work we ignore material dispersion and take $\varepsilon = 12$, $\mu = 1$ and $\kappa = 0.9$. The Bloch modes associated with the wave vector $\mathbf{k}$ are of the form $E_z = e_z(x,y)e^{i\mathbf{k}\cdot\mathbf{r}}$ with $e_z(x,y)$ a periodic function that satisfies $\hat{L}_\mathbf{k}\cdot e_z = \mathcal{E}\mathbf{M}_g \cdot e_z$, with $\hat{L}_\mathbf{k} \equiv \hat{L}(-i\nabla + \mathbf{k})$. The band structure can be found using the plane wave method by expanding e_z into plane waves, $e_z = \sum_\mathbf{J} c_\mathbf{J}^E e^{i\mathbf{G}_\mathbf{J}\cdot\mathbf{r}}$ ($\mathbf{G}_\mathbf{J} \equiv j_1\mathbf{b}_1 + j_2\mathbf{b}_2$ is a generic reciprocal lattice primitive vector) [10]. Thus, the operators $\mathbf{M}_g$ and $\hat{L}_\mathbf{k}$ can be represented by matrices (in the simulations the plane wave expansion was truncated with $|j_i| \le N_{\max} = 3$). The Chern topological number can be calculated by feeding the matrices that are used in the plane wave method into the integral (1). The band structure of a photonic crystal formed by ferrite cylinders with radius $r = 0.2\sqrt{3}a$ is shown in Fig.2. As seen, there is a complete band-gap delimited by $1.13/a^2 < \mathcal{E} < 1.53/a^2$. The Chern number $\mathcal{C}$ is found through the numerical integration of Eq. (1) taking $\mathcal{E}_{\text{gap}} = 1.3257/a^2$ the mid-point in the gap. A generic wave vector in the Brillouin zone is of the form $\mathbf{k} \equiv \beta_1\mathbf{b}_1 + \beta_2\mathbf{b}_2$ with $|\beta_i| \le 1/2$ and generic $\mathcal{E}$ is of the form $\mathcal{E} = \mathcal{E}_{\text{gap}} + i\xi$. Figure 3a depicts the integrand of Eq. (1) as a function of β_1 for $\xi = 0$ and $\beta_2 = 1/3$ (solid line) and $\beta_2 = -1/3$ (dashed line). As seen, the integrand is peaked near $\beta_1 = \mp 2/3$, which corresponds to the coordinates of the K and K' points, respectively. This reveals that the topological charge is concentrated near the two Dirac points. The integral is numerically evaluated using the trapezoidal rule. The Brillouin zone is sampled with $N_1 = N_2 = N$ points. The integral along the imaginary axis is truncated at $|\xi| \le \xi_{\max} = 5/a^2$ and is sampled with $N_w = 2\times 50$ points. Figure 3b shows that for sufficiently large N the numerical result approaches $\mathcal{C} \approx 1$, consistent with the topological nature of the Chern number.

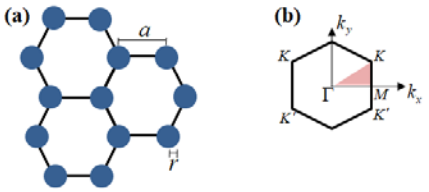

Figure 1: **(a)** Hexagonal array of ferrite cylinders. The distance between nearest neighbors is *a*. **(b)** First Brillouin zone of the 2D lattice.

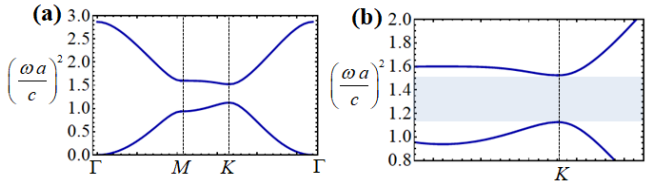

Figure 2: **(a)** Photonic band structure of the ferrite photonic crystal. **(b)** Zoom in of panel (a) around the K point.

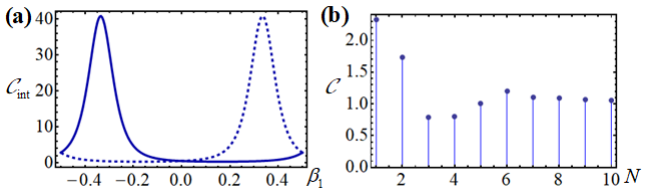

Figure 3: **(a)** Integrand of Eq. (1) [in arbitrary units] as a function of β_1. **(b)** The numerically calculated Chern number $\mathcal{C}$ as a function of N.

The computation time is on the order of a few minutes in a standard personal computer. At the conference, we will present additional examples and in particular we will discuss how the effect of loss impacts the topological properties of the material.

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