Topological insights into tight-binding descriptions of three-dimensional photonic crystals

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***Abstract*—Unlike their influential role in solid-state physics, tight-binding models have historically played a relatively modest role in photonic crystal research. This is especially so for three-dimensional photonic crystals, where efforts to apply Wannierization techniques have been hindered by the transverse polarization of light. I will discuss how insights from symmetry analysis and topology inform a new approach.**

***Index Terms*—symmetry, topology, photonic crystals, tight-binding.**

I. Introduction

Despite substantial efforts in method development [1], [2], tight-binding models have not seen wide use in photonic crystals research, except in 1D and 2D settings. This stands in sharp contrast to the popularity of tight-binding models and Wannierization techniques not only in solid-state physics [3], [4] but also for e.g., phononic crystals [5], [6]. Since the majority of archetypal models in topological band theory are underlied by a tight-binding perspective, their absence in 3D photonic crystals has been especially felt in the field of topological photonics.

The failure of tight-binding modeling efforts for 3D photonic crystals is directly tied to the polarization of light. Two facts conspire in this spoiling: (1) solutions to the Maxwell equations must be transverse, i.e., divergence free $\boldsymbol{\nabla} \cdot \mathbf{B} = 0$, and (2) solutions near zero frequency, $\omega \to 0$, solutions must necessarily be plane-wave-like, since the effective-medium limit is realized exactly at zero frequency. Since the two lowest bands of any 3D photonic crystal necessarily connect to $\omega = 0$ at zero wave-vector $\mathbf{k} = \mathbf{0} \equiv \Gamma$ (Fig. 1a), their polarization state is necessarily ill-defined at this point. This is clear since a transverse plane-wave $\hat{\mathbf{e}}_\mathbf{k} e^{i\mathbf{k}\cdot\mathbf{r}}$ must have its polarization vector $\hat{\mathbf{e}}_\mathbf{k}$ orthogonal to $\mathbf{k}$: consequently, if we attempt to determine $\hat{\mathbf{e}}_\mathbf{k}$ precisely at Γ, we find that it depends on the $\mathbf{k}$-space angle with which Γ is approached (Fig. 1b). Effectively, the Bloch state basis exhibits a vortex with an associated non-analytic singularity at $(\mathbf{k} = \mathbf{0}, \omega = 0)$. Since any tight-binding model must be founded in a set of Wannier orbitals—which are nothing but a Fourier transform of the Bloch states—this singularity implies that the Wannier orbitals cannot be localized, spoiling the outlook for effective tight-binding modeling of these bands [1], [7].

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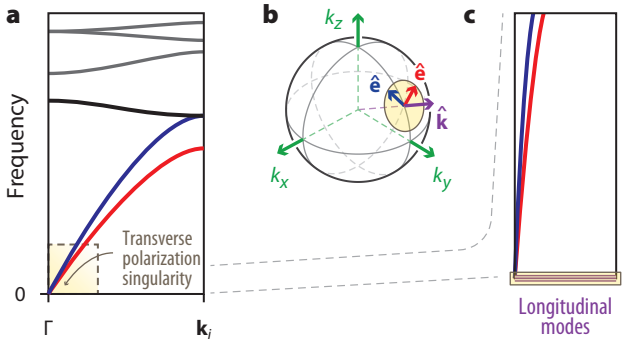

Fig. 1. **Transverse polarization singularity at zero frequency. a**, The lowest two bands (red and blue) of a 3D photonic crystal necessarily connect to zero frequency at Γ. **b**, There, they exhibit a polarization singularity because their polarization vectors $\hat{\mathbf{e}}$ must be orthogonal to the direction of the wave-vector $\mathbf{k}$, whose direction is ill-defined at $\mathbf{k} = \mathbf{0}$. **c**, An infinite set of longitudinal modes exist at zero frequency. By incorporating a subset of them as auxiliary bands, the singularity can be side-stepped because the space spanned by the sum of longitudinal and transverse polarization vectors is independent of the directionality of $\mathbf{k}$.

II. Regularization through auxiliary modes

This singularity also appears in a seemingly unrelated context, namely when attempting to adapt recent symmetry-based frameworks of topological band analysis to 3D photonic crystals [7], where the singularity prevents a regular assignment of band symmetry at zero frequency. In Ref. 7, we recently demonstrated that the problem can be effectively regularized by viewing the situation as the *difference* of two auxiliary problems. The key idea is the incorporation of a set of auxiliary longitudinal modes (Fig. 1c). Such longitudinal modes are unphysical since they are not divergence-free—but are nevertheless valid solutions of the photonic wave equation. However, by incorporating an appropriately chosen longitudinal band alongside the two singular transverse bands, the space spanned by their sum becomes well-defined at $(\mathbf{k} = \mathbf{0}, \omega = 0)$. By solving this regularized problem—a sum of transverse and longitudinal bands, which we call the *apolar* problem—and suitably "subtracting" the added longitudinal bands afterwards, the singularity is overcome, enabling use of symmetry-based topological frameworks. The singularity, in turn, endows photonic crystals with special band symmetry properties that translate to unique band connectivities, different

from those of other quasiparticles [7].

III. Symmetry and photonic tight-binding models

Building on this insight, Morales-Pérez et al. [8] recently proposed a new approach to the photonic tight-binding problem, building a tight-binding model for the set of apolar bands rather than just the transverse bands. With outset in this approach, we have developed a fully general software implementation [9] by interfacing with another set of software packages previously developed for symmetry-based topological analysis [10], [11].

The implementation involves three technical elements:

(1) Determine the band symmetry content (i.e., irreps at high-symmetry $\mathbf{k}$-points) of the photonic bands of interest.
(2) Convert this information from reciprocal space to real space, adding longitudinal bands as necessary, to extract a decomposition in so-called band representations. This gives the orbital character (s-like, p-like, etc.) and orbital locations of sites in the associated tight-binding model.
(3) Determine the possible tight-binding terms compatible with these orbitals.

Point 3 is perhaps the most broadly interesting, owing to the familiarity of manual tight-binding model building in simple contexts. To move from manual to automatic and from simple to general, recall that the Bloch Hamiltonian $h_{\mathbf{k}}$ must be invariant under each symmetry g of the space group G in the sense that $gh_{\mathbf{k}}g^{-1} = h_{g\mathbf{k}}$ for all $g \in G$. For the matrix form of Bloch Hamiltonian, $\mathbf{h}_{\mathbf{k}}$, implicitly formulated relative to an orbital basis, the action of g is represented by a matrix as well. In the language of space group theory, g is represented by $\mathbf{D}_{\mathbf{k}}(g)$: (a Fourier transform of) the space group representation induced by the orbitals of the tight-binding sites (equivalently, it is a band representation). The operator constraints then reduce to simple linear constraints $\mathbf{D}_{\mathbf{k}}(g)\mathbf{h}_{\mathbf{k}}\mathbf{D}_{\mathbf{k}}^{\dagger}(g) = \mathbf{h}_{\mathbf{k}}$. Aggregated over all $g \in G$ (and solved simultaneously for all $\mathbf{k}$), these symmetry constraints can be encoded as a homogeneous linear system, whose kernel defines the allowed Hamiltonian terms. By this approach, we obtain a general tool for determining all possible tight-binding terms consistent with a set of orbitals.

Figure 2 illustrates an application of the approach for an inverse opal design in space group 225 ($Fm\bar{3}m$). An apolar tight-binding model is built from 3-fold degenerate orbitals with T_2 symmetry (Mulliken notation) placed at the $8c$ Wyckoff positions (i.e., at $\frac{a}{4}(\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}})$ and $\frac{3a}{4}(\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}})$ in the cubic unit cell of side length a) and subsequently fitted to the spectrum of the lowest 5 bands, obtained from full-wave calculations in MPB. Excellent agreement between full-wave calculations and tight-binding fit is evident.

IV. Outlook

While our current implementation requires spectral fitting to obtain hopping amplitudes, the conceptual approach involving auxiliary longitudinal modes is general. This suggests that a general application of Wannierization techniques—long assumed unworkable for 3D photonic crystals due to their polarization singularity—might be within reach, provided a suitable scheme for incorporating the auxiliary longitudinal bands can be found.

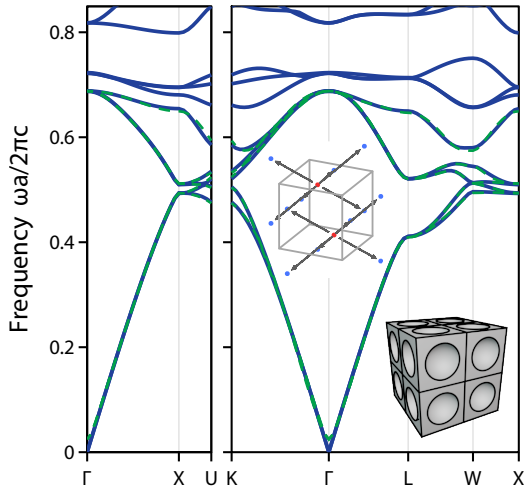

Fig. 2. **Full-wave and tight-binding band structure of inverse opal photonic crystal.** The tight-binding fit (dashed green; full-wave calculations in solid blue) is constructed using 31 hopping terms and restricted to the lowest five transverse bands (including one auxiliary longitudinal band, whose frequencies are imaginary and not shown); the dominant type of hopping term is shown in the central inset. The photonic crystal is a face-centered cubic inverse opal, in a touching void configuration (radius $a/\sqrt{8}$) with permittivity $\varepsilon = 13$; the lower left inset shows a 2×2 tiling of the cubic unit cell (side length a).

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