


Berry bands and pseudo-spin of topological photonic phases

Samuel J. Palmer^{1,*} and Vincenzo Giannini^{2,3,†}

¹The Blackett Laboratory, Imperial College London, London SW7 2AZ, United Kingdom

²Instituto de Estructura de la Materia (IEM), Consejo Superior de Investigaciones Científicas (CSIC), Serrano 121, 28006 Madrid, Spain

³Technology Innovation Institute, Masdar City, Abu Dhabi, United Arab Emirates

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Realizing photonic analogs of the robust, unidirectional edge states of electronic topological insulators would improve our control of light on the nanoscale and revolutionize the performance of photonic devices. Here, we show that new symmetry-protected topological phases can be detected by reformulating energy eigenproblems as Berry curvature eigenproblems. The “Berry bands” span the same eigenspace as the original valence energy bands, but separate into pseudo-spinful and pseudo-spinless subspaces in $C_2\mathcal{T}$ -symmetric crystals. We demonstrate the method on the well-known case of Wu and Hu [Phys. Rev. Lett. **114**, 223901 (2015)] and a recently discovered fragile topological crystal, and show that both crystals belong to the same photonic analog of the quantum spin-Hall effect. This work helps unite theory and numerics, and is useful in defining and identifying new symmetry-protected phases in photonics and electronics.

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Introduction. When guiding light on the nanoscale, impurities, imperfections, and sharp corners can scatter light in unintended ways and limit the performance of photonic devices. This unintended scattering could be reduced if light can be guided using the robust, unidirectional states that arise at the surfaces of crystals with nontrivial band topologies. This is the one of the principal goals of topological nanophotonics [1]. Although nontrivial topological phases were first observed in the electronic bands of atomic crystals [2–7], photonic analogs of topological phases such as the quantum Hall effect (QHE) [8,9] and symmetry-protected phases such as the quantum spin-Hall effect (QSHE) [2–4] have been built using photonic crystals: periodic nanostructures with tunable photonic bands [10,11].

The photonic QHE has robust surface states, but requires time-reversal symmetry to be broken [12–15]. This can also be achieved in photonics using, for example, an external magnetic field [16], but in practice the time-reversal breaking responses of common materials are weak in the visible spectrum [1,17]. As such, there is a particular interest in photonic analogs of topological phases that are time-reversal symmetric, such as the QSHE.

The QSHE can be considered as two counterpropagating instances of the QHE, one for each spin and with opposite magnetic fields to maintain time-reversal symmetry. In general, the surface states are not robust as

crossings between the counterpropagating surface states can be gapped by non-spin-preserving perturbations [18,19]. However, with fermionic time-reversal symmetry, $\mathcal{T}^2 = -1$, there are protected Kramers’ degeneracies at time-reversal invariant momenta and the number of topological surface states propagating in each direction can only change by an even number [20]. The QSHE is therefore a \mathbb{Z}_2 topological phase, with either an even (trivial) or odd (nontrivial) number of edge states propagating in each direction [3].

An elegant photonic analog of the QSHE was proposed by Wu and Hu [21] where the angular momentum of light mimics the spin space of the electrons, and crystalline symmetries produce a fermionic pseudo-time-reversal symmetry that protects the edge states at Γ . The design consists of hexagonal rings of cylinders arranged on a triangular lattice, as shown in Fig. 1(a). When the cylinders are circular ($d_1 = d_2$) there is a certain ring radius ($a_0/R = 3$) where the cylinders form a honeycomb lattice and the transverse magnetic modes meet at a double Dirac point between p (dipolar) and d (quadrupolar) modes at Γ . Breaking the Dirac point by expanding the rings of cylinders produces an effective Hamiltonian that is equivalent (in the vicinity of Γ) to the Bernevig-Hughes-Zhang model of the QSHE [4]. Owing to its simplicity, this model has been widely studied recently [22–28] and has been used to show the importance of finite-size effects in topological photonics and the emergence of topological particle resonances or topological whispering gallery modes [29,30].

It has been shown that in some cases [31,32], identifying topological photonic phases requires proper consideration of long-range interactions and retardation. However, to our knowledge the expected topological indices have not been determined from full-wave calculations over the full Brillouin zone for the structures proposed by Wu and Hu, but only with approximations near the Γ point [21,23,24,26]. This has led to

*samuel.palmer12@imperial.ac.uk

†<http://www.GianniniLab.com>

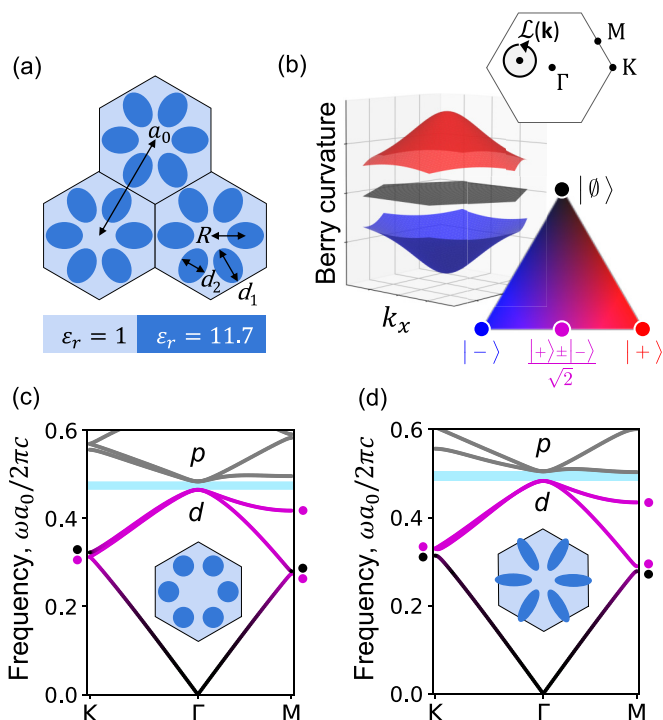


FIG. 1. (a) A topological photonic crystal consisting of dielectric cylinders ($\epsilon_r = 11.7$) in air ($\epsilon_r = 1$). The ellipsoidal cylinders have axes of lengths d_1 and d_2 and are arranged in rings of radius R on a triangular lattice of site-to-site separation a_0 . (b) In $C_2\mathcal{T}$ symmetric crystals, the Berry curvature of the valence bands comes in zero (pseudo-spinless) or positive/negative (pseudo-spinful) pairs. (c) Transverse magnetic (TM) polarized bands of a topological photonic crystal with $a_0/R = 2.9$, $d_1 = d_2 = 2R/3$ and (d) a similar crystal with $a_0/R = 3$, $d_1 = 0.4$, $d_2 = 0.13$. There is a complete band gap between the third and fourth bands, as shown in light blue. We show that there is a nontrivial \mathbb{Z}_2 topological phase for both crystals that can be observed in the Wilson loops of the pseudo-spinful subspace. Previous works had shown that Wilson loops through the full valence band spaces fail to detect a nontrivial topological phase [22,33]. By coloring the bands according to their pseudo-spin composition, we see that this is because the valence band spaces contain a mixture of pseudo-spinful and pseudo-spinless states.

the belief that the bulk topology of this crystal is not analogous to the QSHE [22,27].

In this Letter we show how the bands of Berry curvature, which we call the “Berry bands,” form a natural basis for the pseudo-spin of a crystal, as shown in Fig. 1(b), and how symmetry-protected phases can be identified using Wilson loops [20,34] through the pseudo-spin subspaces. The calculations are performed with Peacock.jl, a freely available JULIA package for studying topological photonics using the plane-wave expansion method and Wilson loops [35]. Taking, for example, the well-known crystal of Wu and Hu shown in Fig. 1(c) where the spectra of Wilson loops applied directly to the energy bands imply the existence of corner states but not necessarily helical edge states [36,37], we show that taking Wilson loops of the Berry bands reveals the photonic analogy to the QSHE. We also show that a related photonic crystal whose energy bands have fragile topology [22,33], shown in Fig. 1(d), belongs to the same symmetry-protected phase

as the crystal of Wu and Hu [21]. By coloring the energy bands of Figs. 1(c) and 1(d) according to their pseudo-spin composition, we see that the fragile topology arises when the energy bands are gapped in such a way as to separate the pseudo-spinful and pseudo-spinless spaces. These results help unite theory and numerics, and may be useful in defining and identifying new symmetry-protected phases.

Gapped topological phases. Two gapped Hamiltonians are in different topological phases when it is impossible to adiabatically deform from one to the other without closing the energy gap. In two dimensions (2D), the topological index of each phase is the total Chern number [13] of the valence band space, \mathcal{H}_{val} . Later, we will discuss how C_{val} can be calculated using Wilson loops. In the QHE, unidirectional surface states are observed at the interface between two different topological phases. The net number of edge states traveling in a certain direction is the difference in Chern number of the two phases, ΔC_{val} .

Moreover, two Hamiltonians belong to different *symmetry-protected* phases when we may adiabatically deform from one to the other without closing the energy gap, but only if the protecting symmetry is necessarily broken during the deformation. Systems in different symmetry-protected phases must belong to the same general topological phase and cannot be distinguished by C_{val} . For example, both the trivial and nontrivial phases in the QSHE have $C_{\text{val}} = 0$. Instead, the valence band space must be decomposed into subspaces, $\mathcal{H}_{\text{val}}(\mathbf{k}) = \bigoplus_{n=1}^N \mathcal{H}_n(\mathbf{k})$. If the projectors onto each subspace are smooth and periodic throughout the Brillouin zone, then each subspace has a well-defined Chern number [38], $C_{\text{val}} = \sum_{n=1}^N C_n$.

While there are many ways of decomposing \mathcal{H}_{val} into subspaces, leading to different $\{C_n\}$, the topological indices of a symmetry-protected phase must be robust against perturbations unless the protecting symmetry is broken or the valence-conduction band gap is closed. One approach is to decompose the band space according to symmetries that (block) diagonalize the Hamiltonian [38]. In the following sections we introduce “bands of Berry curvature,” which we call the Berry bands, and explain how decomposing \mathcal{H}_{val} according to these Berry bands reveals topological phases in $C_2\mathcal{T}$ -symmetric photonic crystals that emulate spin using the angular momentum of light.

Wilson loops. We use operators known as Wilson loops for two purposes: first, to decompose \mathcal{H}_{val} into subspaces according to the local Berry curvature, and then to calculate the corresponding topological indices of each subspace. The Wilson loop of a closed path, \mathcal{L} , is

$$\hat{W}_{\mathcal{L}}^{\{n\}} = \hat{P}(\mathbf{k}_1)\hat{P}(\mathbf{k}_N)\cdots\hat{P}(\mathbf{k}_2)\hat{P}(\mathbf{k}_1), \quad (1)$$

where $\hat{P}(\mathbf{k}_i) = \sum_{n \in \{n\}} |u_n(\mathbf{k}_i)\rangle\langle u_n(\mathbf{k}_i)|$ are projectors onto the subspace of interest, and \mathbf{k}_i are closely spaced points along \mathcal{L} . The action of the Wilson loop is to parallel transport a mode through this subspace. In general this produces a unitary mixing,

$$\hat{W}_{\mathcal{L}}^{\{n\}} |u_i(\mathbf{k}_1)\rangle = \sum_j U_{ij} |u_j(\mathbf{k}_1)\rangle, \quad (2)$$

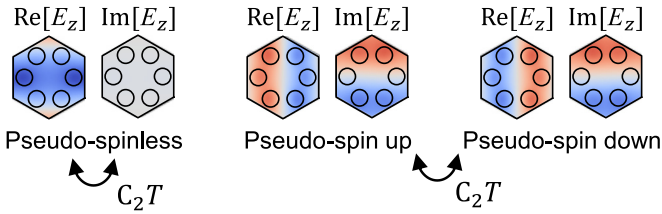


FIG. 2. Pseudo-spin modes at M for the topological crystal of Wu and Hu ($a_0/R = 2.9, d_1 = d_2 = 2R/3$). In $C_2\mathcal{T}$ -symmetric crystals the Berry curvature $\mathcal{F}(\mathbf{k})$ comes in positive/negative pairs or is zero. The pseudo-spinless mode $\mathcal{F}(\mathbf{k}) = 0$ is mapped to itself by $C_2\mathcal{T}$ symmetry, whereas the pseudo-spin-up and pseudo-spin-down modes $\pm\mathcal{F}(\mathbf{k})$ are mapped to each other by $C_2\mathcal{T}$ symmetry.

but there exist eigenmodes for each Wilson loop that will each accumulate a gauge-invariant geometric phase known as a Berry phase γ_i without mixing [34],

$$\hat{W}_{\mathcal{L}}^{[n]}|\tilde{u}_i(\mathbf{k}_1)\rangle = \exp(i\gamma_i)|\tilde{u}_i(\mathbf{k}_1)\rangle, \quad (3)$$

where $|\tilde{u}_i(\mathbf{k}_1)\rangle = \sum_j V_{ij}|u_j(\mathbf{k}_1)\rangle$ and \mathbf{V} is a unitary matrix that diagonalizes \mathbf{U} as $(\mathbf{V}^\dagger\mathbf{U}\mathbf{V})_{ij} = \delta_{ij}\exp(i\gamma_i)$.

Berry bands and pseudo-spin. We generate a pseudo-spin basis for $C_2\mathcal{T}$ -symmetric crystals using Wilson loops around infinitesimally small paths $\mathcal{L}(\mathbf{k})$ enclosing \mathbf{k} , as shown in the inset of Fig. 1(b). We want the decomposition to be unaffected by perturbations that open or close energy gaps within the valence bands, so we build these Wilson loops using projectors onto the full valence band space,

$$\hat{W}_{\mathcal{L}}^{\text{val}} = \hat{P}_{\text{val}}(\mathbf{k}_1)\hat{P}_{\text{val}}(\mathbf{k}_N)\cdots\hat{P}_{\text{val}}(\mathbf{k}_2)\hat{P}_{\text{val}}(\mathbf{k}_1),$$

thereby ensuring that different realizations of the same symmetry-protected phase, such as those in Figs. 1(c) and 1(d), are treated equally.

Because the Wilson loops are unitary operators, we can form a Hermitian eigenvalue problem for the non-Abelian Berry curvature $\mathcal{F}_i(\mathbf{k})$,

$$\hat{H}_{\mathcal{F}}(\mathbf{k})|\tilde{u}_i(\mathbf{k})\rangle = \mathcal{F}_i(\mathbf{k})|\tilde{u}_i(\mathbf{k})\rangle, \quad (4)$$

where $\hat{H}_{\mathcal{F}}(\mathbf{k}) = \lim_{A\rightarrow 0}[-i\log\hat{W}_{\mathcal{L}}^{\text{val}}/A]$ and $\mathcal{F}_i(\mathbf{k}) = \lim_{A\rightarrow 0}[\gamma_i(\mathbf{k})/A]$ for a vanishingly small loop \mathcal{L} of area A enclosing \mathbf{k} . This transforms the original energy eigenvalue problem $E(\mathbf{k})$ to a ‘‘Berry band’’ eigenvalue problem $\mathcal{F}(\mathbf{k})$ where the Berry bands span the valence band space and, as the Wilson loops are vanishingly small, inherit the spatial symmetries of the original energy bands, as shown in Fig. 2.

The combined C_2 and \mathcal{T} symmetries act on the Berry bands as [39,40]

$$C_2\mathcal{T}\hat{H}_{\mathcal{F}}(\mathbf{k})(C_2\mathcal{T})^{-1} = -\hat{H}_{\mathcal{F}}(\mathbf{k}), \quad (5)$$

and therefore each Berry band in a $C_2\mathcal{T}$ -symmetric crystal either has a value of zero (pseudo-spinless) or is part of a positive/negative pair (pseudo-spinful). The pseudo-spinful Berry bands have opposite angular momentum,

$$|\tilde{u}_{\pm}(\mathbf{k})\rangle = \frac{1}{\sqrt{2}}|u_1(\mathbf{k})\rangle \pm \frac{i}{\sqrt{2}}|u_2(\mathbf{k})\rangle, \quad (6)$$

where $C_2\mathcal{T}|\tilde{u}_{\pm}(\mathbf{k})\rangle = |\tilde{u}_{\mp}(\mathbf{k})\rangle$, and $|u_1(\mathbf{k})\rangle$ and $|u_2(\mathbf{k})\rangle$ are invariant under $C_2\mathcal{T}$.

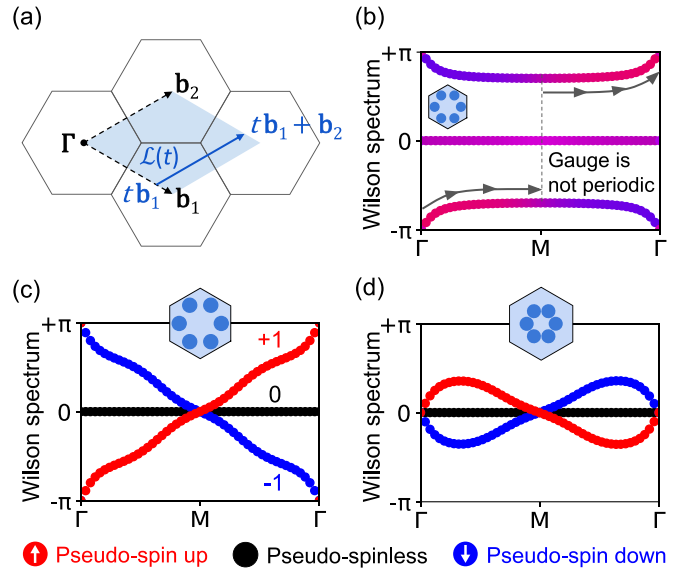


FIG. 3. (a) The Chern number of a space can be observed as a winding in the spectrum of Wilson loops made on a series of paths $\mathcal{L}(t)$. These paths sweep the Brillouin zone (shaded blue region) as $t \rightarrow t + 1$. (b) For the topological crystal of Wu and Hu ($a_0/R = 2.9, d_1 = d_2 = 2R/3$) the Wilson loop spectrum of the total valence band space has zero total winding, as expected from time-reversal symmetry. By coloring the spectrum according to the pseudo-spin composition, we see that the individual windings are not well defined as the resultant gauge is not smooth and periodic. No spin-Chern numbers are observed. (c) In contrast, Wilson loops made through the pseudo-spinful subspace (Berry bands) present well-defined nontrivial windings. The corresponding \mathbb{Z}_2 index is shown to be protected by $C_2\mathcal{T}$ symmetry. (d) Similarly, the pseudo-spin winding of a crystal without band inversion, $a_0/R = 3.125, d_1 = d_2 = 2R/3$, has a trivial winding protected by $C_2\mathcal{T}$ symmetry.

$C_2\mathcal{T}$ -protected \mathbb{Z}_2 phase. The total Chern number of the valence bands is equivalent [33] to the total spectral winding of Wilson loops built from projectors onto the valence bands. These Wilson loops are made along a series of parallel paths $\mathcal{L}(t)$, shown in Fig. 3(a), where the paths sweep the Brillouin zone as $t \rightarrow t + 1$. Figure 3(b) shows the Wilson loop spectra of the three-dimensional valence band space for the topological crystal introduced by Wu and Hu [21]. The total winding and therefore C_{val} are both zero, as expected for the valence bands of a time-reversal symmetric system [34]. However, coloring the Wilson loop spectra according to their pseudo-spin composition reveals that the windings of the individual eigenvalues are not smooth and periodic, and the individual spin-Chern numbers cannot be determined from this analysis.

One way of proceeding is to consider the two eigenvalues of Fig. 3(b) that cross $\pm\pi$ an odd number of times, indicating a nontrivial 2D Stiefel-Whitney insulating phase expected to host corner states [37]. This is also known as an obstructed atomic limit (OAL) [22] because the pair Wilson loop eigenvalues averaging around $\pm\pi$ indicate that two of the maximally localized Wannier functions of this crystal are localized at the edges of the unit cell [22,38]. Alternatively, this can be determined from the symmetry eigenvalues of

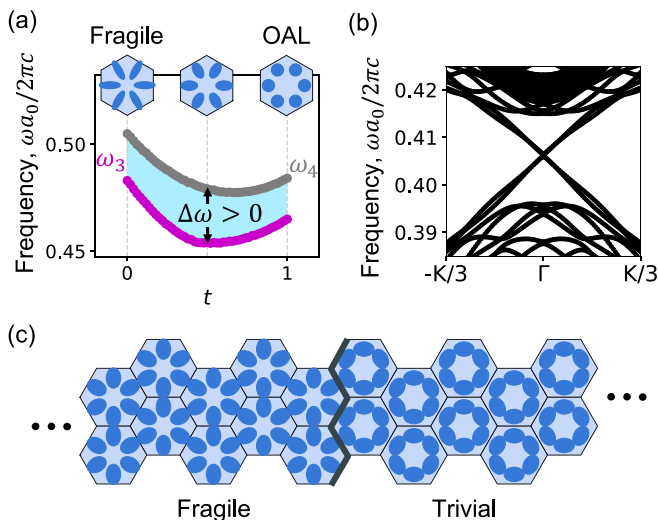


FIG. 4. (a) Band gap for a continuously deformed crystal. It is possible to adiabatically deform between the obstructed atomic limit ($a_0/R = 2.9$, $d_1 = d_2 = 2R/3$) and fragilely topological ($a_0/R = 3$, $d_1 = 0.4a_0$, $d_2 = 0.13a_0$) crystals without breaking $C_2\mathcal{T}$ symmetry or closing the topological band gap, $\Delta\omega = \omega_4 - \omega_3 > 0$ (shown in light blue). This means both crystals must belong to the same $C_2\mathcal{T}$ -protected phase. (b), (c) Edge states are observed at the interface between a fragilely topological ($a_0/R = 3$, $d_1 = 0.35a_0$, $d_2 = 0.25a_0$) and a trivial ($a_0/R = 3$, $d_1 = 0.25a_0$, $d_2 = 0.35a_0$) crystal. The parameters were chosen so the two crystals had an overlapping band gap at $\omega a_0/2\pi c \approx 0.4$. The emergence of these edge states agrees with the measured $C_2\mathcal{T}$ -protected \mathbb{Z}_2 indices of the pseudo-spin subspaces.

the bands at the time-reversal invariant momenta [41]. The Stiefel-Whitney insulator/OAL is expected to host topological corner states [36,37], but the observation of helical edge states [21,25–27] remains unexplained by this analysis.

Alternatively, we may use the Berry bands introduced in the previous section to decompose the valence band space into a pseudo-spinless subspace and a pseudo-spinful subspace,

$$\mathcal{H}_{\text{val}} = \mathcal{H}_\emptyset \oplus \mathcal{H}_\pm. \quad (7)$$

Figure 3(c) shows the spectra of Wilson loops made separately through \mathcal{H}_\emptyset and \mathcal{H}_\pm for the same crystal as in Fig. 3(b). There is no mixing of the pseudo-spinful states for Wilson loops through a two-band pseudo-spinful space [42]. The individual spectra are smooth and periodic, and so the corresponding spin-Chern numbers, $\{C_-, C_\emptyset, C_+\} = \{-1, 0, +1\}$, are well defined. In other words, the valence bands consist of two QHE related to each other by $C_2\mathcal{T}$ symmetry and an additional trivial subspace that is separable via the Berry bands. With pseudo-Kramers degeneracy enforced at Γ by C_6 symmetry [21], we conclude that the crystal is a photonic analog of the QSHE, with the parity of C_+ and C_- as the \mathbb{Z}_2 topological index. For the corresponding trivial phase, the spin-Chern numbers are $\{C_n\} = \{0, 0, 0\}$, as indicated by the lack of winding in Fig. 3(d). These windings can also be expressed in terms of the C_2 eigenvalues at the time-reversal invariant momenta [22], but the smooth, periodic multiband gauge of the Berry bands provide a convenient basis to calculate the corresponding Wannier functions.

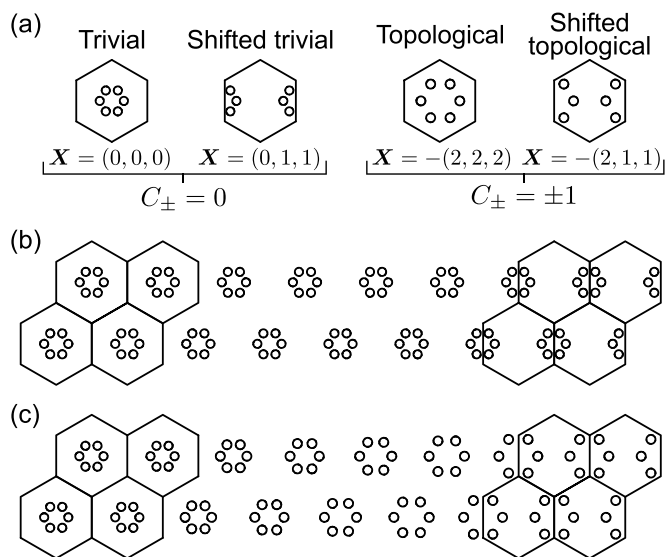


FIG. 5. (a) Schematics of shifted and unshifted cells. Although it is impossible to adiabatically deform between any of these unit cells without either closing the topological gap or breaking $C_2\mathcal{T}$ symmetry *about the origin of the unit cell*, some of the cells have equal spin-Chern numbers. (b), (c) Schematics of adiabatically graded (locally $C_2\mathcal{T}$ -symmetric) interface regions between different bulk regions. (b) An example of an adiabatically graded interface between shifted and unshifted cells with trivial spin-Chern numbers for which the topological band gap does not close. There are no helical edge states at this interface. (c) The topological band gap closes at all adiabatically graded interfaces between cells with different spin-Chern numbers, such as the one depicted here, resulting in helical edge states. The edge states of the adiabatically graded interface will survive as the interface is made increasingly sharp so long as the interface remains a relatively weak C_6 breaking perturbation.

We also studied the “fragilely topological” crystal introduced by Blanco de Paz *et al.* [22], and found the same spectral winding as seen in Fig. 3(c), indicating that both crystals are photonic analogs of the QSHE. This is supported by Fig. 4(a) which shows that it is possible to adiabatically deform between the crystals without closing the topological band gap or breaking $C_2\mathcal{T}$ symmetry, meaning the two crystals are in the same $C_2\mathcal{T}$ -protected phase [42], and also by Figs. 4(b) and 4(c) which show topological edge states at the interface between the trivial and fragilely topological crystals. Here, as in other works [21,27,28], there is a small gap in the edge modes (around 3% of the bulk valence-conduction gap) as the presence of the interface is a C_6 breaking perturbation that lifts the pseudo-Kramers degeneracy.

Interpreting the pseudo-spin Chern numbers. Let us now compare the spin-Chern numbers of the Berry bands to a different method of classifying symmetry-protected topological phases. Figure 5(a) shows four unit cells: the regular trivial and nontrivial unit cells, as well as a shifted copy of each. Each shifted cell has the same spin-Chern numbers as the corresponding unshifted cell, whereas all four cells are classified as different $C_2\mathcal{T}$ -protected phases labeled with vectors \mathbf{X} by the approach of Benalcazar *et al.* [41], where $\mathbf{X} \neq (0, 0, 0)$ indicates a fragilely topological or obstructed atomic limit phase [42].

The apparent contradiction of the two methods occurs because the classification of [41] is based on the absolute positions of Wannier centers within the cell, whereas the spin-Chern numbers are constructed from the relative flow of the Wannier centers in the gauge of the Berry bands and are independent of our choice of origin. It is impossible to deform between two bulks with different values of C_{\pm} without breaking $C_2\mathcal{T}$ symmetry or closing the band gap, but the origin of the $C_2\mathcal{T}$ symmetry is not fixed. On the other hand, it is impossible to deform between two bulks with different values of X without breaking $C_2\mathcal{T}$ symmetry *about the origin of the unit cell* or closing the band gap. We shall demonstrate that the origin-independent spin-Chern numbers are more relevant to predicting the existence of helical edge states.

Let us consider whether edge states exist at adiabatically graded (locally C_2 -symmetric) interface regions between shifted and unshifted bulks with the same spin-Chern numbers. Despite the bulks having different values of X , there exists a choice of slowly graded interface between the two bulks for which the band gap does not close, such as Fig. 5(b). There are no helical edge states along this interface. On the other hand, the topological band gap must close at *all* adiabatically graded interfaces between bulks with different spin-Chern numbers, such as the interface region shown in Fig. 5(c), resulting in helical edge states. As was seen in Figs. 4(b) and 4(c), these edge states survive as the interface region is made increasingly sharp if the interface can be considered as a relatively weak C_6 breaking perturbation.

Conclusion. We show that new symmetry-protected topological phases can be identified by reformulating the energy eigenvalue problem as a Berry curvature eigenproblem. In $C_2\mathcal{T}$ -symmetric crystals the “Berry bands” separate into pseudo-spinless (no angular momentum) and pseudo-spinful (opposite angular momentum) subspaces. Using straight Wilson loops through the pseudo-spinful subspaces of crystals with three valence bands detects topological phases where Wilson loops through the energy valence bands fail to do so. We demonstrate the method on the well-known photonic crystal of Wu and Hu and a recently discovered “fragile topological” crystal and show that both crystals belong to the same $C_2\mathcal{T}$ -protected \mathbb{Z}_2 topological phase that emulates the quantum spin-Hall effect in photonics. Studying the topology of photonic crystals with larger valence band spaces may be possible using bent Wilson loops [39,40] through the pseudo-spinful subspaces. The method presented here helps unite the numerics and theory of photonic topological insulators, and could also be applied to find new symmetry-protected phases in electronic systems [43].

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