Gapless surface states in a lattice of coupled cavities: a photonic analog of topological crystalline insulators

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Abstract

We show that a tetragonal lattice of weakly interacting cavities with uniaxial electromagnetic response is the photonic counterpart of topological crystalline insulators, a new topological phase of atomic band insulators. Namely, the frequency band structure stemming from the interaction of resonant modes of the individual cavities exhibits an omnidirectional band gap within which gapless surface states emerge for finite slabs of the lattice. Due to the equivalence of a topological crystalline insulator with its photonic-crystal analog, the frequency band structure of the latter can be characterized by a \( Z_2 \) topological invariant. Such a topological photonic crystal can be realized in the microwave regime as a three-dimensional lattice of dielectric particles embedded within a continuous network of thin metallic wires.

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I. INTRODUCTION

The frequency band structure of artificial periodic dielectrics formally known as photonic
crystals is the electromagnetic (EM) counterpart of the electronic band structure in ordi-
nary atomic solids. Recently, a new analogy between electron and photon states in periodic
structures has been proposed by Raghu and Haldane, namely the one-way chiral edge states
in two-dimensional (2D) photonic-crystal slabs which are similar to the corresponding edge
states in the quantum Hall effect. The photonic chiral edge states are a result of time-
reversal (TR) symmetry breaking which comes about with the inclusion of gyroelectric/
gyromagnetic material components; these states are robust to disorder and structural im-
perfections as long as the corresponding topological invariant (Chern number in this case)
remains constant.

In certain atomic solids, TR symmetry breaking is not prerequisite for the appearance
of topological electron states as it is the case in the quantum Hall effect. Namely, when
spin-orbit interactions are included in a TR symmetric graphene sheet, a bulk excitation
gap and spin-filtered edge states emerge without the presence of an external magnetic field,
a phenomenon which is known in literature as quantum spin Hall effect. Its generalization
to three-dimensional (3D) atomic solids lead to a new class of solids, namely, topological
insulators. The latter possess a spin-orbit-induced energy gap and gapless surface states
exhibiting insulating behavior in bulk and metallic behavior at their surfaces.

Apart from topological insulators where the spin-orbit band structure with TR symmetry
defines the topological class of the corresponding electron states, other topological phases
have been proposed such as topological superconductors (band structure with particle-hole
symmetry), magnetic insulators (band structure with magnetic translation symmetry), and, very recently, topological crystalline insulators. In the latter case the band structure
respects TR symmetry as well as a certain point-group symmetry leading to bulk energy
gap and gapless surface states.

In this work, we propose a photonic analog of a topological crystalline insulator. Our
model photonic system is a 3D crystal of weakly interacting resonators respecting TR sym-
metry and the point-symmetry group associated with a given crystal surface. As a result,
the system possesses an omnidirectional band gap within which gapless surface states of
the EM field are supported. It is shown that the corresponding photonic band structure is
equivalent to the energy band structure of an atomic topological crystalline insulator and, as such, the corresponding states are topological states of the EM field classified by a $Z_2$ topological invariant.

The frequency band structure of photonic crystals whose (periodically repeated) constituent scattering elements interact weakly with each other can be calculated by a means which is similar to the tight-binding method employed for atomic insulators and semiconductors. Photonic bands amenable to a tight-binding-like description are e.g., the bands stemming from the whispering-gallery modes of a lattice of high-index scatterers, the defect bands of a sublattice of point defects, within a photonic crystal with an absolute band gap, the plasmonic bands of a lattice of metallic spheres or of a lattice of dielectric cavities within a metallic host. In the latter case, the frequency band structure stems from the weak interaction of the surface plasmons of each individual cavity wherein light propagates within the crystal volume by a hopping mechanism. Such type of lattice constitutes the photonic analog of a topological crystalline insulator presented in this work whose frequency band structure will be revealed based on a photonic tight-binding treatment within the framework of the coupled-dipole method. The latter is an exact means of solving Maxwell’s equations in the presence of nonmagnetic scatterers.

II. TIGHT-BINDING DESCRIPTION OF DIELECTRIC CAVITIES IN A PLASMONIC HOST

We consider a lattice of dielectric cavities within a lossless metallic host. The $i$-th cavity is represented by a dipole of moment $P_i = (P_{ix}, P_{iy}, P_{iz})$ which stems from an incident electric field $E^{inc}$ and the field which is scattered by all the other cavities of the lattice. This way the dipole moments of all the cavities are coupled to each other and to the external field leading to the coupled-dipole equation

$$P_i = \alpha_i(\omega)[E^{inc} + \sum_{i' \neq i} G_{ii'}(\omega)P_{i'}].$$  \hspace{1cm} (1)

$G_{ii'}(\omega)$ is the electric part of the free-space Green’s tensor and $\alpha_i(\omega)$ is the $3 \times 3$ polarizability tensor of the $i$-th cavity. Eq. (1) is a $3N \times 3N$ linear system of equations where $N$ is the number of cavities of the system. We assume that the cavities exhibit a uniaxial EM response, i.e., the corresponding polarizability tensor is diagonal with $\alpha_x = \alpha_y = \alpha_\parallel$ and
For strong anisotropy, the cavity resonances within the $xy$-plane and along the $z$-axis can be spectrally distinct; thus, around the region of e.g., the cavity resonance $\omega_{\parallel}$ within the $xy$-plane, $\alpha_{\perp} \ll \alpha_{\parallel}$ (see appendix). In this case, one can separate the EM response within the $xy$-plane from that along the $z$-axis and Eq. (1) becomes a $2N \times 2N$ system of equations,

$$P_i = \alpha_{\parallel}(\omega)[\sum_{i' \neq i} G_{ii'}(\omega)P_{i'}].$$

where we have set $E^{inc} = 0$ since we are seeking the eigenmodes of the system of cavities. Also, now, $P_i = (P_{ix}, P_{iy})$.

For a particle/cavity of electric permittivity $\epsilon_{\parallel}$ embedded within a material host of permittivity $\epsilon_h$, the polarizability $\alpha_{\parallel}$ is given by the Clausius-Mossotti formula

$$\alpha_{\parallel} = \frac{3V}{4\pi} \frac{\epsilon_{\parallel} - \epsilon_h}{\epsilon_{\parallel} + 2\epsilon_h}$$

where $V$ is the volume of the particle/cavity. For a lossless plasmonic (metallic) host in which case the electric permittivity can be taken as Drude-type, i.e., $\epsilon_h = 1 - \omega_p^2/\omega^2$ (where $\omega_p$ is the bulk plasma frequency), the polarizability $\alpha_{\parallel}$ exhibits a pole at $\omega_{\parallel} = \omega_p \sqrt{2/(\epsilon_{\parallel} + 2)}$ (surface plasmon resonance). By making a Laurent expansion of $\alpha_{\parallel}$ around $\omega_{\parallel}$ and keeping the leading term, we may write

$$\alpha_{\parallel} = \frac{F}{\omega - \omega_{\parallel}} \equiv \frac{1}{\Omega}$$

where $F = (\omega_{\parallel}/2)(\epsilon_{\parallel} - \epsilon_h)/(\epsilon_{\parallel} + 2)$. For sufficiently high value of the permittivity of the dielectric cavity, i.e., $\epsilon_{\parallel} > 10$, the electric field of the surface plasmon is much localized at the surface of the cavity. As a result, in a periodic lattice of cavities, the interaction of neighboring surface plasmons is very weak leading to much narrow frequency bands. By treating such a lattice in a tight binding-like framework, we may assume that the Green’s tensor $G_{ii'}(\omega)$ does not vary much with frequency and therefore, $G_{ii'}(\omega) \simeq G_{ii'}(\omega_{\parallel})$. In this case, Eq. (2) becomes an eigenvalue problem

$$\sum_{i' \neq i} G_{ii'}(\omega_{\parallel})P_{i'} = \Omega P_i$$

where

$$G_{ii'}(\omega_{\parallel}) = q_{\parallel}^3 \left[ C(q_{\parallel}|r_{ii'}|)I_2 + J(q_{\parallel}|r_{ii'}|) \begin{pmatrix} \frac{x_i^2}{r_{ii'}^2} & \frac{x_i y_{i'} y_{ii'}}{r_{ii'}^2} \\
\frac{x_i y_{i'} x_{ii'}}{r_{ii'}^2} & \frac{y_{i'}^2}{r_{ii'}^2} \end{pmatrix} \right].$$

(6)
with $r_{ii'} = r_i - r_{i'}$, $q_\parallel = \sqrt{\epsilon \omega / c}$ and $I_2$ is the $2 \times 2$ unit matrix. The form of functions $C(q_\parallel | r_{ii'})$, $J(q_\parallel | r_{ii'})$ generally depends on the type of medium hosting the cavities (isotropic, gyrotropic, bi-anisotropic, etc). The Green’s tensor of Eq. (6) describes the electric interactions between two point dipoles $P_i$ and $P_{i'}$ each of which corresponds to a single cavity. The first term of $G_{ii'}$ describes an interaction which does not depend on the orientation of the two dipoles whilst the second one is orientation dependent.

\[ \Gamma \equiv \begin{pmatrix} \Xi_1 & \Xi_2 \\ \Xi_2^* & \Xi_3 \end{pmatrix} \]

\[ \mathbf{G} \equiv \begin{pmatrix} G_{II} & G_{II'} \\ G_{II'}^* & G_{II''} \end{pmatrix} \]

\[ \mathbf{I}_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \]

\[ \mathbf{q}_\parallel = \sqrt{\epsilon \omega / c} \]

\[ \mathbf{J} = \begin{pmatrix} J_{II} & J_{II'} \\ J_{II'}^* & J_{II''} \end{pmatrix} \]

\[ \mathbf{C} = \begin{pmatrix} C_{II} & C_{II'} \\ C_{II'}^* & C_{II''} \end{pmatrix} \]

The cavity index $i$ becomes composite, $i \equiv n_\beta$, where $n$ enumerates the unit cell and $\beta$ the positions of inequivalent cavities in the unit cell. Also, $R_n$ denotes the lattice vectors and $k = (k_x, k_y, k_z)$ is the Bloch wavevector. By substituting Eq. (7) into Eq. (5) we finally obtain

\[ \sum_{\beta'} \tilde{G}_{\beta\beta'}(q_\parallel, k)P_{0\beta'} = \Omega P_{0\beta} \quad (8) \]

where

\[ \tilde{G}_{\beta\beta'}(q_\parallel, k) = \sum_{n'} \exp[i k \cdot (R_n - R_{n'})]G_{n_\beta'n_\beta'}(q_\parallel). \quad (9) \]

Solution of Eq. (8) provides the frequency band structure of a periodic system of cavities.

\[ \text{III. TOPOLOGICAL FREQUENCY BANDS} \]

Since Eq. (8) is equivalent to a Hamiltonian eigenvalue problem, we adopt the crystal structure of Ref. \[4\]. Namely, a tetragonal lattice with a unit cell consisting of two same

FIG. 1: (Color online) (a) Tetragonal crystal with two cavities within the unit cell. (b) The bulk Brillouin zone and (c) the surface Brillouin zone corresponding to the (001) surface.

For an infinitely periodic system, i.e., a crystal of cavities, we assume the Bloch ansatz for the polarization field, i.e.,

\[ P_i = P_{n\beta} = \exp(i k \cdot R_n)P_{0\beta} \quad (7) \]

The cavity index $i$ becomes composite, $i \equiv n_\beta$, where $n$ enumerates the unit cell and $\beta$ the positions of inequivalent cavities in the unit cell. Also, $R_n$ denotes the lattice vectors and $k = (k_x, k_y, k_z)$ is the Bloch wavevector. By substituting Eq. (7) into Eq. (5) we finally obtain

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FIG. 2: Frequency band structure for tetragonal lattice of resonant cavities within a plasmonic host (see Fig. 1) corresponding to the Green’s tensor of Eq. (11) with $s^A_1 = -s^B_2 = 1.2, s^A_2 = -s^B_2 = 0.5, s'_1 = 2.5, s'_2 = 0.5, s_z = 2$.

cavities at inequivalent positions $A$ and $B$ [see Fig. 1(a)] along the $c$-axis. In this case, the index $\beta$ in Eq. (8) assumes the values $\beta = A, B$ for each sublattice (layer) of the crystal. The above lattice is characterized by the $C_4$ point-symmetry group. In order to preserve the $C_4$ symmetry in the Green’s tensor matrix of Eq. (8) we assume that the interaction between two cavities within the same layer (either $A$ or $B$) depends on the relative orientation of the point dipole in each cavity whilst the interaction between cavities belonging to adjacent layers is orientation independent. Also, we take into account interactions up to second neighbors in both inter- and intra-layer interactions. Taking the above into account, the lattice Green’s tensor assumes the form

$$\tilde{\mathbf{G}}(\mathbf{k}) = \begin{pmatrix} \tilde{G}^{AA}(\mathbf{k}) & \tilde{G}^{AB}(\mathbf{k}) \\ \tilde{G}^{AB\dagger}(\mathbf{k}) & \tilde{G}^{BB}(\mathbf{k}) \end{pmatrix}$$

(10)

where

$$\tilde{G}^{\beta\beta}(\mathbf{k}) = 2s_1^\beta \begin{pmatrix} \cos(k_x\alpha) & 0 \\ 0 & \cos(k_y\alpha) \end{pmatrix} + 2s_2^\beta \begin{pmatrix} \cos(k_x\alpha) \cos(k_y\alpha) & -\sin(k_x\alpha) \sin(k_y\alpha) \\ -\sin(k_x\alpha) \sin(k_y\alpha) & \cos(k_x\alpha) \cos(k_y\alpha) \end{pmatrix},$$

$$\tilde{G}^{AB}(\mathbf{k}) = [s'_1 + 2s'_2(\cos(k_x\alpha) + \cos(k_y\alpha)) + s'_2 \exp(i k_z\alpha)]I_2.$$

(11)
FIG. 3: Frequency band structure for a finite slab $ABAB \cdots ABB$ of the crystal of Fig. 1 made from 80 bilayers.

The lattice Green’s tensor of Eq. (11) is completely equivalent to the lattice Hamiltonian of Ref. 7. $s_1^\beta, s_2^\beta, s_1', s_2', s_z$ in Eq. (11) generally depend on $q_\parallel$, the lattice constant $a$ and the interlayer distance $c$ but hereafter will be used as independent parameters. Namely we choose $s_1^A = -s_2^B = 1.2, s_2^A = -s_2^B = 0.5, s_1' = 2.5, s_2' = 0.5, s_z = 2$. In Fig. 2 we show the (normalized) frequency band structure corresponding to Eq. (11) along the symmetry lines of the Brillouin zone shown in Fig. 1(b). It is evident that an omnidirectional frequency band gap exists around $\Omega = 0$ which is prerequisite for the emergence of surface states.

In order to inquire the occurrence of surface states we find the eigenvalues of the Green’s tensor of Eq. (11) in a form appropriate for a slab geometry. The emergence of surface states depends critically on the surface termination of the finite slab, i.e., for different slab terminations different surface-state dispersions occur (if occur at all). Namely, we assume a finite slab parallel to the (001) surface (characterized by the $C_4$ symmetry group) consisting of 80 alternating $AB$ layers except the last bilayer which is $BB$, i.e., the layer sequence is $ABAB \cdots ABB$. The corresponding frequency band structure along the symmetry lines of the surface Brillouin zone of the (001) surface [see Fig. 1(c)] is shown in Fig. 3. It is evident that there exist gapless surface states within the band gap exhibiting a quadratic degeneracy at the $\bar{M}$-point. In this case, the corresponding doublet of surface states can be described by an effective theory similarly to the doublet states at a point of linear degeneracy (Dirac point).

We note that the equivalence of the Green’s tensor $G$ with the atomic Hamiltonian of Ref. 7 as well as the form of the time-reversal $T$ and (geometric) $C_4$-rotation $U$ operators
for the EM problem\footnote{1} which are the same as for spinless electrons, allows to describe the photonic band structure with the $Z_2$ topological invariant $\nu_0$

\[
(-1)^{\nu_0} = (-1)^{\nu_{TM}} (-1)^{\nu_{AZ}}
\]  

(12)

where for real eigenvectors of $\tilde{G}(k)$ we have\footnote{7}

\[
(-1)^{k_1 \cdot k_2} = \text{Pf}[w(k_2)]/\text{Pf}[w(k_1)]
\]  

(13)

and

\[
w_{mn}(k_i) = \langle u_m(k_i) | U | u_n(k_i) \rangle.
\]  

(14)

Pf stands for the Pfaffian of a skew-symmetric matrix, i.e., $\text{Pf}[w]^2 = \det(w)$. Due to the double degeneracy of the band structure at the four special momenta points $\Gamma, M, A, Z$ the frequency bands come in doublets. Since frequency eigenvectors with different eigenfrequencies are orthogonal, all the inter-pair elements of the $w$-matrix are zero and the latter is written as:

\[
w(k_i) = \begin{pmatrix}
  w^1(k_i) & 0 & 0 & 0 \\
  0 & w^2(k_i) & 0 & 0 \\
  0 & 0 & \ddots & 0 \\
  0 & 0 & 0 & w^N(k_i)
\end{pmatrix}
\]  

(15)

where $w^j(k_i)$ are anti-symmetric $SU(2)$ matrices,\footnote{8} i.e., $w^j(k_i) = A_1$ or $A_2$, where

\[
A_1 = \begin{pmatrix}
  0 & 1 \\
  -1 & 0
\end{pmatrix},
A_2 = \begin{pmatrix}
  0 & -1 \\
  1 & 0
\end{pmatrix}.
\]  

(16)

In this case, $\text{Pf}[w(k_i)] = w^1_{12} w^2_{12} \cdots w^N_{12} = \pm 1$. Therefore, $(-1)^{k_1 \cdot k_2} = \pm 1$ and $\nu_0 = 1$ which ensures the presence of gapless surface states.

We note that the above analysis relies on the assumption of real frequency bands. The presence of losses in the constituent materials renders the frequency bands complex, i.e., the Bloch wavevector possesses both a real and an imaginary part. However, even in this case, one can still speak of real frequency bands if the imaginary part of the Bloch wavevector is at least \textit{hundred} times smaller than the corresponding real part. This a common criterion used in calculations of the complex frequency band structure by on-shell electromagnetic solvers such as the layer-multiple scattering method\footnote{19} or the transfer-matrix method.\footnote{20}
IV. BLUEPRINT FOR A PHOTONIC TOPOLOGICAL INSULATOR

A possible realization of the photonic analogue of topological insulator in the laboratory is depicted in Fig. 4. Since our model system requires dielectric cavities within a homogeneous plasma, a lattice of nano-cavities formed within a homogeneous Drude-type metal, e.g., a noble metal (Au, Ag, Cu), would be the obvious answer. However, the plasmon bands are extremely lossy due to the intrinsic absorption of noble metals in the visible regime. A solution to this would be the use of an artificial plasmonic medium operating in the microwave regime where metals are perfect conductors and losses are minimal. Artificial plasma can be created by a 3D network of thin metallic wires of a few tens of µm in diameter and spaced by a few mm. A lattice of dielectric particles within an artificial plasma can be modelled with the presented tight-binding Green’s tensor. Since the interaction among first and second neighbors within the same bilayer (A or B) should depend on the dipole orientation (in order to preserve the C4 symmetry), the dielectric particles in each layer are connected with cylindrical waveguiding elements (different in each layer A or B - see Fig. 4). In contrast, between two successive bilayers there are no such elements since interactions between dipoles belonging to different layers should be independent of the dipole orientations (s orbital-like). Another advantage of realizing the photonic analog in the microwave regime is the absence of nonlinearities in the EM response of the constituent materials since photon-photon interactions may destroy the quadratic degeneracy of the surface bands in analogy
Finally, we must stress that a photonic topological crystalline insulator can be also realized with purely dielectric materials if the host medium surrounding the cavities is not a plasmonic medium but a photonic crystal with an absolute band gap: the cavities would be point defects within the otherwise periodic photonic crystal and the tight-binding description would be still appropriate. In this case, Maxwell’s equations lack of any kind of characteristic length and the proposed analog would be realized in any length scale.

V. CONCLUSIONS

In conclusion, a 3D lattice of weakly interacting cavities respecting TR symmetry and a certain point-group symmetry constitutes a photonic analog of a topological crystalline insulator by demonstrating a spectrum of gapless surface states. A possible experimental realization would be a 3D lattice of dielectric particles within a continuous network of thin metallic wires with a plasma frequency in the GHz regime.

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Appendix

The $z$-component of the polarizability need not be zero but can assume finite values as far as the frequency band stemming from the surface-plasmon resonance corresponding to the $z$-component is spectrally distinct (no overlap) with the bands stemming from the $xy$-components of the polarizability. In this case, one can treat separately the two frequency bands (doublet) stemming from the $xy$-resonance from the band coming from the $z$-resonance (singlet). The above requirements can be quantified as follows,

$$C_{\parallel} \ll \frac{\omega_{\parallel} - \omega_{\perp}}{\omega_p}$$

(A.1)

where $C_{\parallel}$ is the width of the $xy$-frequency bands (in dimensionless frequency units). $C_{\parallel}$ is obtained from the first term of the right-hand side of Eq. [3] of the paper. To a first
approximation, it is given by\textsuperscript{12}

\[ C_\parallel \sim \frac{\exp(-q_\parallel a_\parallel)}{q_\parallel a_\parallel} \]  \hspace{1cm} (A.2)

where \( q_\parallel = \sqrt{\epsilon_h \omega_\parallel / c} \). Therefore, the condition (A.1) is written as

\[ \frac{\exp(-q_\parallel a_\parallel)}{q_\parallel a_\parallel} \ll \frac{\omega_\parallel - \omega_\perp}{\omega_p} \]  \hspace{1cm} (A.3)

where \( a_\parallel \) is the lattice constant in the \( xy \)-plane. Given that \( \omega_\parallel = \omega_p \sqrt{2/(\epsilon_\parallel + 2)} \), Eq. (A.3) becomes

\[ \frac{\exp(-\sqrt{\epsilon_h \omega_\parallel a_\parallel / c})}{\sqrt{\epsilon_h \omega_\parallel a_\parallel / c}} \ll \sqrt{\frac{2(\epsilon_\perp - \epsilon_\parallel)}{(\epsilon_\parallel + 2)(\epsilon_\perp + 2)}} \]  \hspace{1cm} (A.4)

From the above equation it is evident that for a given value of the dielectric anisotropy \( \epsilon_\perp - \epsilon_\parallel \), one can always find a suitably large lattice constant \( a_\parallel \) such that Eq. (A.4) is fulfilled. The latter allows the easy engineering of the photonic analog of a crystalline topological insulator since there is practically no restriction on the choice of the (uniaxial) material the cavities are made from. It can also be easily understood that if Eq. (6) holds, the same equation is true for the width \( C_\perp \) of the singlet frequency band (resulting from the \( z \)-resonance).

Numerical example. Suppose that the cavities are made from a nematic liquid crystal which is a uniaxial material. Typical values of the permittivity tensor \( \epsilon \) are e.g., \( \epsilon_\parallel = 1.5, \epsilon_\perp = 1.8 \). In this case, \( \omega_\parallel \approx 0.75 \omega_p \) and \( \epsilon_h = 1 - \omega_p^2 / \omega_\parallel^2 \approx -0.777 \). By choosing a large lattice constant, i.e., \( a_\parallel = 4c / \omega_p \), Eq. (A.4) is clearly fulfilled

\[ \frac{\exp(-\sqrt{\epsilon_h \omega_\parallel a_\parallel / c})}{\sqrt{\epsilon_h \omega_\parallel a_\parallel / c}} \approx 0.026866 \ll 0.2213 \approx \sqrt{\frac{2(\epsilon_\perp - \epsilon_\parallel)}{(\epsilon_\parallel + 2)(\epsilon_\perp + 2)}}. \]  \hspace{1cm} (A.5)

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