

Type-II Dirac Photons: Supplementary Materials

Hai-Xiao Wang,^{1,*} Yige Chen,^{2,*} Zhi Hong
Hang,¹ Hae-Young Kee,^{2,3,†} and Jian-Hua Jiang^{1,‡}

¹*College of Physics, Optoelectronics and Energy,
& Collaborative Innovation Center of Suzhou Nano Science and Technology,
Soochow University, 1 Shizi Street, Suzhou 215006, China*

²*Department of Physics, University of Toronto, Toronto, M5S 1A7, Canada*

³*Canadian Institute for Advanced Research,
Toronto, Ontario, M5G 1Z8, Canada*

(Dated: July 4, 2017)

* These authors contributed equally to this work

† hykee@physics.utoronto.ca

‡ jianhua.jiang@suda.edu.cn

Sec. SI Other symmetries and their consequences

In addition to the symmetries listed in the main text, there are also two glide symmetries, $G_x \equiv S_x * \mathcal{P}$ and $G_y \equiv S_y * \mathcal{P}$, which are irrelevant to the Dirac points and Weyl points studied in this work. Nevertheless these two glide symmetries can lead to Kramers double degeneracy on several high symmetry lines: the RZ line ($k_y = 0, k_z = \pi$) and the MY line ($k_y = \pi, k_z = 0$) (as shown in Fig. 2c in the main text). This is because $G_x * \mathcal{T}$ is an invariant operator on both these lines and $(G_x * \mathcal{T})^2 = T_{011} = -1$ for both lines.

Sec. SII Robustness of Kramers double degeneracy and parity inversion through screw symmetries

Here we show that the realization of Kramers double degeneracy and the emergence of parity inversion are robust to the material and geometry of the photonic crystals (PhCs). We calculate the photonic bands for the $k_x = \pi$ plane with four different geometric/material parameter sets. The results of the photonic bands are shown in Figure S1 where we also show the parity inversion on the MA line. We find that the synthetic Kramers double degeneracy on the $k_x = \pi$ plane holds for all parameters. This is because such double degeneracy are guaranteed by the screw symmetry S_x . In addition, the parity of the photonic bands are well-defined on the MA line. For all four sets of parameters in Figure S1, we observe parity inversion and emergence of DPs in the first six photonic bands. In these parameters, we adopted the permittivity of the blocks as $\varepsilon_b = 12$ (silicon) or 10 (e.g., GaAs) and the permittivity of the background medium as $\varepsilon_m = 2$ (polymer). The geometric parameters of the blocks are also varied. The robustness of the method on the realization of Dirac points on the MA line is thus robust to material parameters. This also indicates the stableness of the Dirac points and implies that such a symmetry-guided method can also be effective in other classical/bosonic systems.

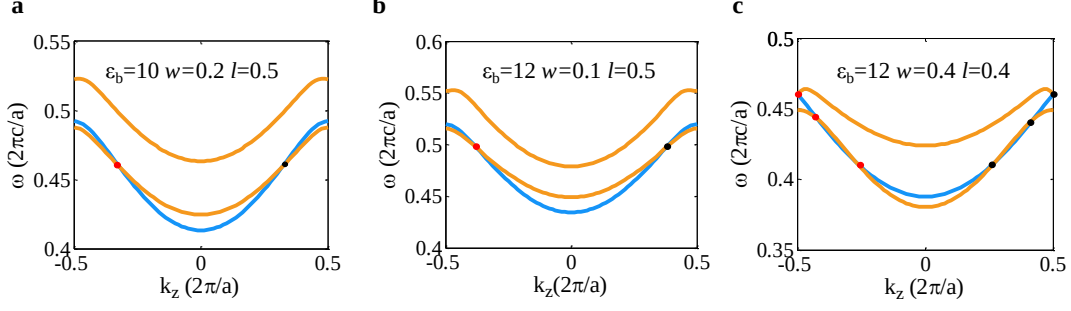


Figure S1: Photonic bands on the MA line for various geometry/material

parameters. **a**, Permittivity of the blocks $\varepsilon_b = 10$ (e.g., GaAs), the width of the blocks $w = 0.2$, and the height of the blocks $h = 0.5$. **b**, $\varepsilon_b = 12$ (silicon), $w = 0.1$, and $h = 0.5$. **c**, $\varepsilon_b = 12$, $w = 0.3$, and $h = 0.2$. **d**, $\varepsilon_b = 12$, $w = 0.3$, and $h = 0.5$. The figures show the first six bands of different parities (red: odd-parity, blue: even-parity) on the MA line. A crossing between bands of different color gives a Dirac point. Common parameters: permittivity of the background medium $\varepsilon_m = 2$ (polymer) and the length of the blocks $l = 0.5$.

Sec. SIII $\vec{k} \cdot \vec{P}$ theory for the Dirac points

Around a Dirac point, there are four states interacting with each other. According to the field profiles shown in Figure S3 in the main text, there are two p -wave states of which the spatial symmetry coincide with x_1 and x_2 where $x_1 = (x+y)/\sqrt{2}$ and $x_2 = (-x+y)/\sqrt{2}$. We shall denote them as $|p_1\rangle$ and $|p_2\rangle$, respectively. The other two states are d -waves which have the same spatial symmetry as x_1x_2 and $x_1x_2(x_1^2 - x_2^2)$, respectively. They shall be labeled as $|d_1\rangle$ and $|d_2\rangle$, respectively. According to the field profiles, we observe that $\langle p_i | S_x | p_i \rangle = 0$ for $i = 1, 2$, and $\langle p_1 | S_x | p_2 \rangle = -i = -\langle p_2 | S_x | p_1 \rangle$. Thus S_x is manifested as σ_y between the two degenerate p -states. This is also true for the d -states: $\langle d_i | S_x | d_i \rangle = 0$ for $i = 1, 2$, and $\langle d_1 | S_x | d_2 \rangle = -i = -\langle d_2 | S_x | d_1 \rangle$. The Θ_x operation is then simply $\Theta_x = \sigma_y \mathcal{K}$ where $\mathcal{K}$ is complex conjugation. Here the Pauli matrices σ_i ($i = x, y, z$) act on the “spin” space within each doublet of a given parity. The Kramers double degeneracy is due to $\Theta_x^2 = -1$. A better choice of “spin” is to construct the four states as $|p_{\pm}\rangle = \frac{1}{\sqrt{2}}(|p_1\rangle \pm i|p_2\rangle)$ and $|d_{\pm}\rangle = \frac{1}{\sqrt{2}}(|d_1\rangle \pm i|d_2\rangle)$. These four states carry total angular momentum (see Figure S2) which can be leveraged to emulate “spin”. Though we will eventually switch to such a representation, we stay for the p_1, p_2, d_1 and d_2 basis for now for simplicity.

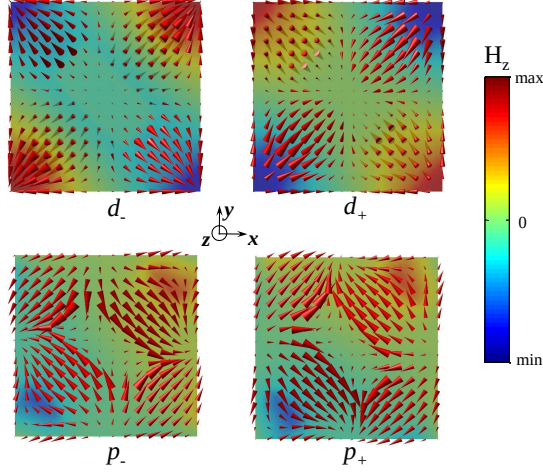


Figure S2: Magnetic field H_z and Poynting vector profiles of the $d_{\pm}$ and $p_{\pm}$ states at a slice of the unit cell. Profiles on this slice (with a fixed z coordinate) indicate that the Poynting vectors have a nontrivial winding approximately along the z axis. Such winding indicates that these states carry finite total angular momenta along the z direction. The opposite winding between p_+ and p_- (d_+ and d_-) states reflects that they carry opposite total angular momenta.

The aim of this section is to construct a $\vec{k} \cdot \vec{P}$ theory for the Dirac points to understand the dispersions around the Dirac points, particularly in the k_x - k_y plane. The photonic bands are solutions of the following eigenvalue equations

$$\nabla \times \frac{1}{\varepsilon(\vec{r})} \nabla \times \vec{h}_{n,\vec{k}}(\vec{r}) = \frac{\omega_{n,\vec{k}}^2}{c^2} \vec{h}_{n,\vec{k}}(\vec{r}), \quad (1)$$

where n is the band index and $\vec{h}_{n,\vec{k}}(\vec{r})$ is the Bloch function for the magnetic field of the electromagnetic wave. It is normalized as $\int_{u.c.} d\vec{r} \vec{h}_{n',\vec{k}}^*(\vec{r}) \vec{h}_{n,\vec{k}}(\vec{r}) = \delta_{nn'}$ with $u.c.$ denoting the unit cell (i.e., integration within a unit cell). The Hermitian operator $\nabla \times \frac{1}{\varepsilon(\vec{r})} \nabla \times$ is then regarded as the “photonic Hamiltonian” [1].

The $\vec{k} \cdot \vec{P}$ theory is constructed by expanding the Bloch functions of photonic bands near the DP with the Bloch functions at the DP. Direct calculation yields, the following $\vec{k} \cdot \vec{P}$ Hamiltonian,

$$\mathcal{H}_{nn'}(\vec{k}) = \frac{\omega_{n,0}^2}{c^2} \delta_{nn'} + \vec{q} \cdot \vec{P}_{nn'} - \int_{u.c.} \frac{d\vec{r}}{\varepsilon(\vec{r})} \vec{h}_{n,0}^*(\vec{r}) \cdot [\vec{q} \times (\vec{q} \times \vec{h}_{n',0}(\vec{r}))], \quad (2)$$

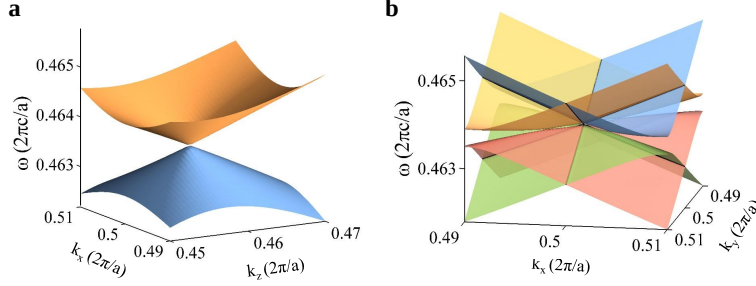


Figure S3: Dispersion of the type-I Dirac points. 3D dispersion of the type-I Dirac point at $k_z > 0$ for $h = 0.5$, $w = 0.2$, $l = 0.5$, $\varepsilon_b = 16$, and $\varepsilon_m = 1.9$. **a**, Dispersion on the k_z - k_x plane. **b**, Dispersion on the k_x - k_y plane around the DP.

where $\omega_{n,0}$ is the eigen-frequency of the n^{th} band at the DP. The matrix element of $\vec{P}$ is given by

$$\vec{P}_{nn'} = \int_{u.c.} \frac{d\vec{r}}{\varepsilon(\vec{r})} [\vec{h}_{n',0}(\vec{r}) \times (i\nabla \times \vec{h}_{n,0}^*(\vec{r})) + (i\nabla \times \vec{h}_{n',0}(\vec{r})) \times \vec{h}_{n,0}^*(\vec{r})]. \quad (3)$$

A crucial fact is that the matrix element $\vec{P}_{nn'}$ is nonzero only when the n and n' bands are of different parity. In our system the mirror planes are the (110) and $(1\bar{1}0)$ planes. Therefore, we shall calculate the two momentum matrix elements, $\hat{P}_1 = (\hat{P}_x + \hat{P}_y)/\sqrt{2}$ and $\hat{P}_2 = (-\hat{P}_x + \hat{P}_y)/\sqrt{2}$. According to the symmetry of the p and d states, we find that $\vec{q}$ -linear terms in the basis of $(|d_1\rangle, |d_2\rangle, |p_1\rangle, |p_2\rangle)^T$ is

$$q_1 P_1 + q_2 P_2 = \begin{pmatrix} 0 & 0 & a_1 q_2 & a_2 q_1 \\ 0 & 0 & b_1 q_2 & b_2 q_1 \\ a_1^* q_2 & b_1^* q_2 & 0 & 0 \\ a_2^* q_1 & b_2^* q_1 & 0 & 0 \end{pmatrix}, \quad (4)$$

$$q_z P_z = \frac{2\omega_0 v}{c^2} (q_z \tau_z + \eta q_z \tau_0),$$

where $q_1 = q_x + q_y$, $q_2 = q_y - q_x$, ω_0 is the frequency of the Dirac point, v is the group velocity along the z direction, η measures the deformation of the Dirac cone along the z direction. The Pauli matrix τ_i ($i = 0, z$) is defined in such a way that τ_z gives the parity of the photonic states. Here we consider the Dirac point with $k_z > 0$.

The invariance of the Hamiltonian under Θ_x implies that

$$\Theta_x \mathcal{H}(\vec{k}) \Theta_x^{-1} = \mathcal{H}(\Theta_x \vec{k}) \quad (5)$$

Note that $\Theta_x \vec{k} = S_x \mathcal{T} \vec{k} = -S_x \vec{k} = (-k_x, k_y, k_z)$. Because $q_1 = q_x + q_y$ and $q_2 = q_y - q_x$, we find $\Theta_x q_1 = q_2$ and $\Theta_x q_2 = q_1$. We thus find that

$$a_1 = -b_2^*, \quad a_2 = b_1^*. \quad (6)$$

We then define $i\alpha \equiv \frac{c^2}{2\omega_0 v} a_1$ and $i\beta \equiv \frac{c^2}{2\omega_0 v} a_2$ and find

$$q_1 P_1 + q_2 P_2 = \frac{2\omega_0 v}{c^2} \begin{pmatrix} 0 & 0 & \alpha q_2 & \beta q_1 \\ 0 & 0 & \beta^* q_2 & -\alpha^* q_1 \\ \alpha^* q_2 & \beta q_2 & 0 & 0 \\ \beta^* q_1 & -\alpha q_1 & 0 & 0 \end{pmatrix}. \quad (7)$$

Due to the $\mathcal{PT}$ symmetry, one can show that α and β are real numbers. Up to the $\vec{q}$ linear order, the Hamiltonian $\mathcal{H}$ gives a spectrum without degeneracy, except for $q_1 = \pm q_2$ (i.e., on the $k_x = \pi$ and $k_y = \pi$ planes). Therefore, the spectrum in the k_x - k_y plane has four branches for a generic direction. Only for the $q_1 = \pm q_2$ case the spectrum is double degenerate and has only two branches. Physically, the double degeneracy on the $k_x = \pi$ and $k_y = \pi$ planes is induced by the screw symmetries S_x and S_y . Specific dispersions around the type-I and type-II Dirac points on the k_x - k_y plane are shown in Figure S3b in the Supplementary Materials and Fig. 3b in the main text, respectively.

A more physical representation of the Dirac Hamiltonian is given in the basis of the states with finite angular momenta,

$$|p_{\pm}\rangle = \frac{|p_1\rangle \pm i|p_2\rangle}{\sqrt{2}}, \quad |d_{\pm}\rangle = \frac{|d_1\rangle \pm i|d_2\rangle}{\sqrt{2}}. \quad (8)$$

Here the doublet $|p_{\pm}\rangle$ ($|d_{\pm}\rangle$) are time-reversal partners of each other. They carry opposite total angular momenta (including both spin and orbital angular momenta). The photonic TAM precisely emulates the electron spin in the Dirac equation. In the basis of the above four states, the Hamiltonian is given by Eq. (??) in the main text.

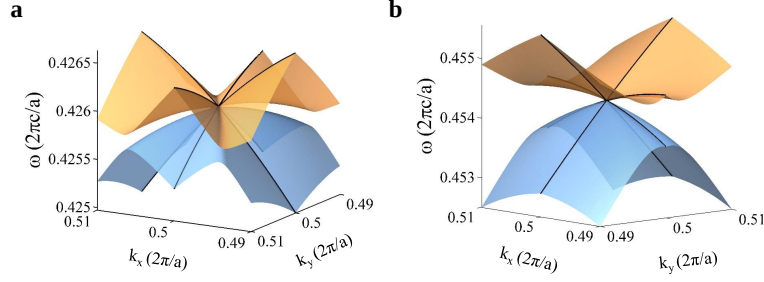


Figure S4: Dispersion of Weyl points on the k_x - k_y plane. **a**, 3D dispersion around the first type-II Weyl point at $k_z > 0$ on the k_x - k_y plane. **b**, 3D photonic spectrum around the first type-I Weyl point at $k_z > 0$.

Sec. SIV Weyl points on MA line for symmetry-broken photonic crystals

The photonic spectra of type-I and type-II Weyl points on the k_x - k_y plane around the Weyl points are shown in Figure S4, confirming the linear dispersion around the Weyl point on the k_x - k_y plane.

The distributions of the magnetic field H_z for the first six photonic bands on the MA line are shown in Fig. 4. The spatial distributions of H_z indicates two kinds of states: odd-parity states and even-parity states. All the odd-parity states are of p -wave nature, while all the even-parity states are of d -wave nature. There are four p -wave bands and two d -wave bands.

Due to the chiral structure, the photonic bands carry angular momenta. This is indicated by the rotation of the Poynting vector in each unit cell. According to such rotations, we can label the d state with angular momentum along z direction as d_+ , while the d state with opposite angular momentum as d_- . Similarly for the p -waves, we have p_+ and p_- states. According to the $\vec{k} \cdot \vec{P}$ analysis in Ref. [1], only the crossings between p_- and d_- or between p_+ and d_+ can lead to Weyl points, whereas the coupling between p_+ and d_- and other combinations cannot lead to $\vec{k}$ -linear spectrum with nonzero Chern number. In our PhCs, counting in frequency-ascending order, the first Weyl point is due to the crossing between the p_- and d_- state, as indicated by the field profiles near the Weyl point. The second Weyl point is due to the crossing between another p_- state and the d_- state. The third Weyl point is due to the crossing between the p_+ and d_+ states.

We shall now apply the $\vec{k} \cdot \vec{P}$ theory to show that the crossing between p_- and d_- states

at $k_z > 0$ leads to a Weyl point with Chern number -1. The two states can be represented according to their spatial symmetry as

$$|p_-\rangle = |c_1x - ic_2y\rangle, \quad |d_-\rangle = |f_1(x^2 - y^2) - 2if_2xy\rangle. \quad (9)$$

The coefficients $c_i > 0$ and $d_i > 0$ ($i = 1, 2$) characterizes the anisotropy of the p_- and d_- states, which can be determined numerically via the field distributions from ab initio simulation. However, the analysis here is already sufficient to determine the Chern number of the Weyl points, which is a topological quantity that does not depend on the specific numbers of the coefficients. The $\vec{k} \cdot \vec{P}$ Hamiltonian between the two states in the basis of $(|d_-\rangle, |p_-\rangle)^T$ is then

$$\begin{aligned} \mathcal{H} &= q_x P_x + q_y P_y + q_z P_z, \\ q_x P_x + q_y P_y &= \mathcal{B}[(c_1 f_1 + c_2 f_2) q_x \sigma_x - i(c_1 f_2 + c_2 f_1) q_y \sigma_y], \\ q_z P_z &= \frac{2\omega'_0 v'}{c^2} (q_z \sigma_z + \eta' q_z \sigma_0), \end{aligned} \quad (10)$$

a where $\mathcal{B} = \langle x | i\partial_x | (x^2 - y^2) \rangle = -\langle y | i\partial_y | (x^2 - y^2) \rangle = \langle x | i\partial_y | 2xy \rangle = \langle y | i\partial_x | 2xy \rangle$ is the $\vec{k} \cdot \vec{P}$ coefficient and can be set as a real number via a universal $U(1)$ transformation, ω'_0 is the frequency of the Weyl point and the coefficient η' describes the deformation of the Weyl point along the k_z direction. σ_i ($i = x, y, z$) are the Pauli matrices, and σ_0 is the 2×2 identity matrix. The above Hamiltonian gives a Weyl point with Chern number $-\text{sgn}(v')$. For the photonic spectrum given in Fig. 5 in the main text, $v' > 0$, and the Chern number is thus -1 .

In the $k_z < 0$ region, there is another Weyl point linked by time-reversal operation, which is hence a crossing between the $|p_+\rangle$ and $|d_+\rangle$ states. This Weyl point has Chern number $\text{sgn}(v')$. However, the velocity also switches sign, leading to a Chern number of -1 , as well. The crossing between the $|p_+\rangle$ and $|d_+\rangle$ states in the $k_z > 0$ region is then a Weyl point with a Chern number of $+1$. The time-reversal partner of this Weyl point also has Chern number of $+1$.

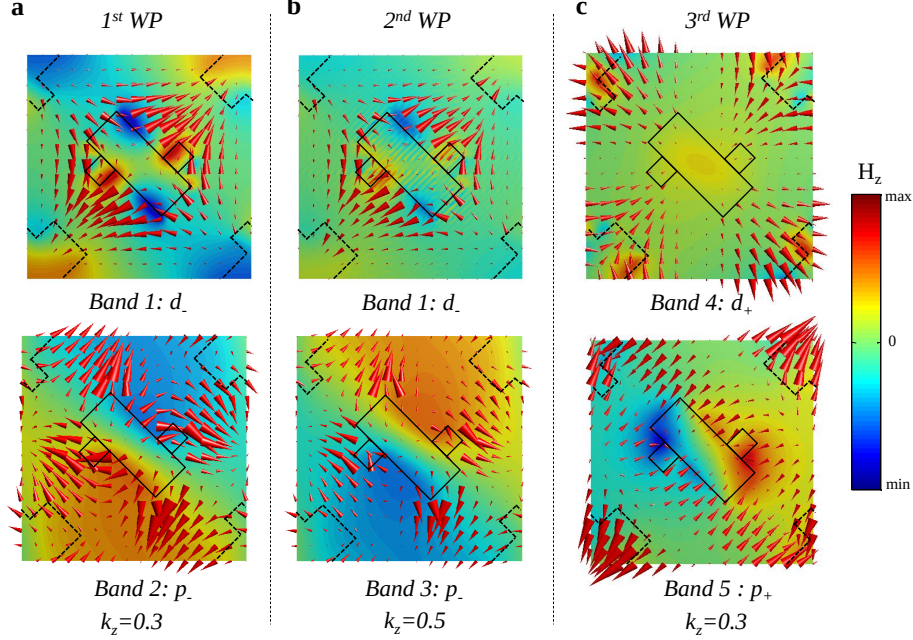


Figure S5: Field profiles of the upper and lower branches of the first three Weyl points with $k_z > 0$. **a—c:** Distributions of the magnetic field H_z (real part) for the first, second, and third WP, separately. Upper panels: the lower branch of each WP, lower panels: the upper branch of each WP. The Poynting vectors (red arrows, only the x - y plane components are indicated in the figures) have rotating distributions around the unit cell center, which indicates finite angular momentum along the z direction. According to their angular momenta, these bands can be labeled as p_+ or d_+ states (if the angular momentum is along z direction), or p_- or d_- state (if the angular momentum is along the $-z$ direction).

Sec. SVI Refraction angles for generic $\vec{q}$

To consider the refraction angles for generic $\vec{q}$ (i.e., away from the x - z or y - z plane), we shall consider the following dispersion

$$\omega = \omega_0 + v(\eta q_z + \rho \sqrt{\gamma^2 q_\tau^2 + q_z^2}) + \gamma' \frac{v^2(q_1^2 + q_2^2)}{\omega_0}, \quad \rho = \pm 1, \quad \tau = 1, 2. \quad (11)$$

Here $q_1 = \frac{q_x + q_y}{\sqrt{2}}$ and $q_2 = \frac{-q_x + q_y}{\sqrt{2}}$. The dimensionless constant γ' determines the quadratic dispersion which is important for $\vec{q}$ along the q_1 or q_2 direction. The displacement of wavevector from the DP $\vec{q} = \vec{k} - \vec{K}_0$ [$\vec{K}_0 = (\frac{\pi}{a}, \frac{\pi}{a}, k_0)$] is determined by

$$q_x = q_{\parallel} \cos(\phi_i), \quad q_y = q_{\parallel} \sin(\phi_i). \quad (12)$$

The parameter $q_{\parallel}$ is fixed, but the angle ϕ_i is varied. Other parameters are also taken from the photonic band calculation, e.g., $v \simeq 0.02c$, $\omega_0 \simeq 0.4 \frac{2\pi c}{a}$, $\eta \simeq -2$, $\gamma \simeq 1$ and $\gamma' \simeq -0.5$. $q_{\parallel} = 0.05 \frac{2\pi}{a}$ or $0.1 \frac{2\pi}{a}$.

We now define

$$\delta = \frac{1}{v}(\omega - \omega_0 - \gamma' \frac{v^2(q_1^2 + q_2^2)}{\omega_0}). \quad (13)$$

One then finds

$$(\delta - \eta q_z)^2 = \gamma^2 q_{\tau}^2 + q_z^2. \quad (14)$$

Here $q_1 = (q_x + q_y)/\sqrt{2}$ and $q_2 = (-q_x + q_y)/\sqrt{2}$ which vary with the angle ϕ_i according to Eq. (12). However, the wavevector perpendicular to the interface, q_z , is not conserved. q_z is in fact determined by the solutions of the above equation. We find that

$$q_z^{\pm, \tau} = \frac{\eta \delta \pm \sqrt{\eta^2 \delta^2 - (\eta^2 - 1)(\delta^2 - \gamma^2 q_{\tau}^2)}}{\eta^2 - 1}, \quad \tau = 1, 2. \quad (15)$$

For $\eta < -1$ ($\eta > 1$) the isofrequency contour always give larger q_z for the upper (smaller) branch (a case with $\eta > 1$ is shown in Figs. 3b and 3c in the main text). Therefore, q_z^{ρ} is the solution for the ρ branch. There are four solutions since there are four nondegenerate bands that intersect with the isofrequency plane. The group velocity is given by

$$v_1|_{\tau=1} = \left. \frac{\partial \omega}{\partial q_1} \right|_{\tau=1} = \rho v \frac{\gamma^2 q_1}{\sqrt{\gamma^2 q_1^2 + q_z^2}} + \frac{2\gamma' v^2 q_1}{\omega_0}, \quad (16a)$$

$$v_2|_{\tau=1} = \left. \frac{\partial \omega}{\partial q_2} \right|_{\tau=1} = \frac{2\gamma' v^2 q_2}{\omega_0}, \quad (16b)$$

$$v_z|_{\tau=1} = \left. \frac{\partial \omega}{\partial q_z} \right|_{\tau=1} = v \left(\eta \pm \frac{q_z}{\sqrt{\gamma^2 q_1^2 + q_z^2}} \right). \quad (16c)$$

For light injected from the medium above the PhC only beams with $v_z < 0$ yield refraction. Therefore, for $\eta > 2$, there is no solution, for $|\eta| < 1$ there is one solution, for $\eta < -2$, there are two solutions (see Figure S6).

For the $\tau = 2$ branches, we have

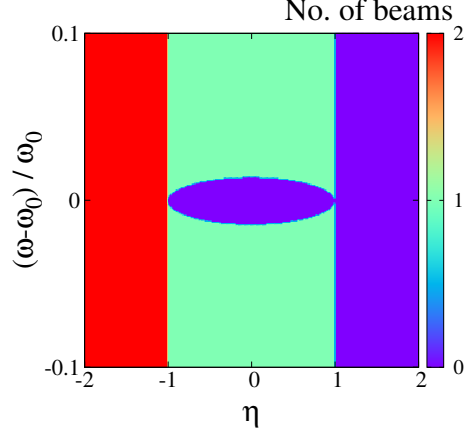


Figure S6: Number of refraction beams as a function of η and frequency. There are two refraction beams for $\eta < -1$, whereas there is no refraction beam for $\eta > 1$. For $|\eta| \leq 1$ the number of refraction beams depends on the frequency and the parameter η .

$$v_1|_{\tau=2} = \frac{2\gamma'v^2q_1}{\omega_0}, \quad (17a)$$

$$v_2|_{\tau=2} = \rho v \frac{\gamma^2 q_2}{\sqrt{\gamma^2 q_2^2 + q_z^2}} + \frac{2\gamma'v^2q_2}{\omega_0}, \quad (17b)$$

$$v_z|_{\tau=2} = v \left(\eta \pm \frac{q_z}{\sqrt{\gamma^2 q_2^2 + q_z^2}} \right). \quad (17c)$$

The refraction angles are obtained as

$$\theta_r = -\arctan\left(\frac{v_{\parallel}}{v_z}\right) \quad (18)$$

where $v_{\parallel}$ is the projection of the group velocity on the parallel wavevector direction,

$$v_{\parallel} = \vec{v} \cdot \vec{e}_{k_{\parallel}}, \quad \vec{e}_{k_{\parallel}} = \frac{1}{\sqrt{k_x^2 + k_y^2}}(k_x, k_y, 0), \quad k_i = \pi + q_i, \quad (i = x, y). \quad (19)$$

References

-
- [1] H.-X. Wang, L. Xu, H.Y. Chen, and J.-H. Jiang, *Three-dimensional photonic Dirac points stabilized by point group symmetry*, Phys. Rev. B **93**, 235155 (2016).