

Supplemental Material to “Topological Polaritons in a Quantum Spin Hall Cavity”

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In our main work we presented a symmetry argument that the Chern number of energy eigenstates has to be zero for the effective model. Here, we provide an argument that this result holds for the microscopic model, too. Furthermore, we verify that the Chern numbers of time reversed partners has to vanish for the effective model. Then, we show how a pseudo fermionic time-reversal operator for excitons can be constructed and present the embedding of the polariton Hilbert space into an enlarged Hilbert space of artificial electron-hole pair combinations. Finally, we consider a system with boundaries, evaluate analytically the polaritonic edge state wave function, and present details of the effective edge-state model.

Chern numbers

Microscopic model – We found that the eigenstates of polaritons in a QSH cavity transform under time reversal (TR) according to $T|\Phi(\vec{q})\rangle = \pm|\Phi(-\vec{q})\rangle$. By symmetry arguments we will show that for any state which satisfies this behavior the corresponding Chern number defined via

$$C = -\frac{i}{2\pi} \int_{\vec{q} \in \text{BZ}} \varepsilon_{ij} \langle \partial_i \Phi | \partial_j \Phi \rangle, \quad (\text{S.1})$$

has to vanish. We decompose the integrand into $(\langle \partial_i \Phi(\vec{q}) | \partial_j \Phi(\vec{q}) \rangle + \langle \partial_i \Phi(-\vec{q}) | \partial_j \Phi(-\vec{q}) \rangle)/2$, which is valid because the integration over the Brillouin zone is invariant under inversion of momentum. Then, the second summand is recast: $\langle \partial_i \Phi(-\vec{q}) | \partial_j \Phi(-\vec{q}) \rangle = \langle \partial_i T \Phi(\vec{q}) | \partial_j T \Phi(\vec{q}) \rangle = \langle \partial_j \Phi(\vec{q}) | \partial_i \Phi(\vec{q}) \rangle$. We used that the TR-operator and partial derivative commute, and that T is anti-unitary. Now, Eq. (S.1) takes the form $C \sim \varepsilon_{ij} (\langle \partial_i \Phi(\vec{q}) | \partial_j \Phi(\vec{q}) \rangle + \langle \partial_j \Phi(\vec{q}) | \partial_i \Phi(\vec{q}) \rangle) = 0$.

Effective model – In our main work we have used symmetry arguments to show that the Chern number

$$C = \frac{1}{4\pi} \int_{\text{BZ}} d^2q \vec{n} \cdot (\partial_{q_x} \vec{n} \times \partial_{q_y} \vec{n}). \quad (\text{S.2})$$

of the energy eigenstate $|\chi_{1,2}\rangle$ of the TR invariant Hamiltonian

$$H_{\text{LP}} = \epsilon_{\text{LP}} + \vec{\sigma} \cdot \vec{h}, \quad (\text{S.3})$$

has to be zero. In Eq. (S.2) the polarization vector of the eigenstate $|\chi_{1,2}\rangle$ is $\vec{n}_{1,2} = \mp \hat{h}$ with $\hat{h} = \vec{h}/|\vec{h}|$. We note that Eq. (S.2) and Eq. (S.1) are equivalent for 2×2 Hamiltonians. For the QSH model studied in the main manuscript, $\vec{n}_{1,2}$ winds twice around the z -axis if \vec{q} encircles the Γ -point, and the effective magnetic field has to vanish at the Γ -point in order to obtain a continuous Hamiltonian (S.3), which results in an ill-defined polarization vector $\vec{n}_{1,2}$. Thus, the Chern number Eq. (S.2) is formally not well defined. This raises the question of the validity of our previously presented argument. Although the limit $\vec{q} \rightarrow \vec{\Gamma}$ is not unique, we have verified that there

are no singular contributions from a neighbourhood of the Γ -point. Then, we can remove the Γ -point from the Brillouin zone integral, Eq. (S.2) is applicable, and our argument for $C_{1,2} = 0$ remains valid.

The Chern numbers C_{\pm} of the TR-partners $|\chi_{\pm}\rangle = (|\chi_2\rangle \pm |\chi_1\rangle)/\sqrt{2}$ are defined according to Eq. (S.2) with polarization vector $\vec{n}_{\pm} = \langle \chi_{\pm} | \vec{\sigma} | \chi_{\pm} \rangle$. Now, we will show that $C_{\pm} = 0$ for the effective model (S.3). To this end we calculate explicitly \vec{n}_{\pm} . For convenience we parametrize the effective magnetic field of Eq. (S.3) by $\vec{h} = (h_{\perp} \cos 2\varphi, h_{\perp} \sin 2\varphi, h_z)^T$ with $h_{\perp}(-\vec{q}) = h_{\perp}(\vec{q})$, $\varphi(-\vec{q}) = \varphi(\vec{q}) + \pi$ and $h_z(-\vec{q}) = -h_z(\vec{q})$. Then, the energy eigenstates take the form

$$\chi_{1,2} = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{1 \mp \hat{h}_z} e^{-i\varphi} \\ \mp \sqrt{1 \pm \hat{h}_z} e^{i\varphi} \end{pmatrix}, \quad (\text{S.4})$$

with normalized effective magnetic field $\hat{h} = \vec{h}/|\vec{h}|$. Using Eq. (S.4), \vec{n}_{\pm} can be calculated in a straightforward manner,

$$\vec{n}_{\pm} = \pm \begin{pmatrix} -\hat{h}_z \cos 2\varphi \\ -\hat{h}_z \sin 2\varphi \\ \sqrt{1 - \hat{h}_z^2} \end{pmatrix}. \quad (\text{S.5})$$

It cannot cover the Bloch sphere, since the z -component is always positive (negative). Therefore, the Chern numbers of the TR-partners have to vanish, $C_{\pm} = 0$.

Pseudo fermionic TR operator for excitons

The exciton spectrum is degenerate with respect to the pseudospin $\alpha \in \{+, -\}$, such that $[H_x, \sigma_z] = 0$. Furthermore, H_x is invariant under TR. In a basis $\{|b_+\rangle, |b_-\rangle\}$ with $\sigma_z |b_{\pm}\rangle = \pm |b_{\pm}\rangle$ the excitonic TR-operator is $T = \sigma_x \mathcal{K}$, which squares to one as required by the bosonic statistics of excitons. The product of T and σ_z commutes with H_x as well, and hence is a symmetry of H_x , too. We define the anti-unitary operator $T_{\text{F}} = \sigma_z T$. This is a fermionic TR-operator in the sense that $T_{\text{F}}^2 = i\sigma_y \mathcal{K}$ with $T_{\text{F}}^2 = -1$.

Enlarged polariton Hilbert space

The BHZ Hamiltonian [1] in the basis $\{|+1/2\rangle, |+3/2\rangle, |-1/2\rangle, |-3/2\rangle\}$ has the form

$$H_e(\vec{k}) = \begin{pmatrix} H_e^+(\vec{k}) & 0 \\ 0 & H_e^-(\vec{k}) \end{pmatrix}, \quad (\text{S.6})$$

where $H_e^+(\vec{k}) = \vec{d}(\vec{k}) \cdot \vec{\sigma}$ and $H_e^-(\vec{k}) = H_e^+(-\vec{k})^*$ with pseudospin $\alpha \in \{+, -\}$, two-dimensional wavevector \vec{k} and spin-orbit field \vec{d} . We found that optical transitions do not change the pseudospin α . Then, excitons can be characterized by a quantum number α , too. In order to study the topology of these excitons we embed the exciton Hilbert space for each pseudospin α into an enlarged Hilbert space; a four dimensional space spanned by the tensor-product states: $\{|\alpha 1/2\rangle_h \otimes |\alpha 1/2\rangle_e, |\alpha 1/2\rangle_h \otimes |\alpha 3/2\rangle_e, |\alpha 3/2\rangle_h \otimes |\alpha 1/2\rangle_e, |\alpha 3/2\rangle_h \otimes |\alpha 3/2\rangle_e\}$. Approximating $H_x^\alpha \approx H_h^\alpha \otimes \mathbb{1}_e + \mathbb{1}_h \otimes H_e^\alpha$ yields in this representation

$$H_x^+ = \begin{pmatrix} 0 & d_x - id_y & d_x + id_y & 0 \\ d_x + id_y & -2d_z & 0 & d_x + id_y \\ d_x - id_y & 0 & 2d_z & d_x - id_y \\ 0 & d_x - id_y & d_x + id_y & 0 \end{pmatrix}. \quad (\text{S.7})$$

Because of TR-symmetry $H_x^-(\vec{q}) = (H_x^+(-\vec{q}))^*$. The Hamiltonian Eq. (S.7) describes an exciton state with energy $\epsilon_x(\vec{q}) = 2|\vec{d}(\vec{q}/2)|$, and three unphysical pairs with holes in the conduction band and/or electrons in the valence band. The four bands of Eq. (S.7) have Chern numbers which result from adding the nontrivial Chern numbers of electronic conduction and/or valence band. This results in a doubling of the exciton (hole-electron) Chern number. We find $C_\pm = \mp 2$ for excitons and $C_\pm = \pm 2$ for artificial hole-electron pairs with negative energy $-\epsilon_x$. The two bands with electron and hole in the same band carry vanishing Chern numbers.

The Hamiltonian of polaritons in a QSH cavity embedded into the extended exciton space takes the form

$$H_P = \begin{pmatrix} H_x^+ & 0 & G_+ \\ 0 & H_x^- & G_- \\ G_+^\dagger & G_-^\dagger & H_{\text{ph}} \end{pmatrix}, \quad (\text{S.8})$$

where the exciton Hamiltonian is given in Eq. (S.7) and the photon Hamiltonian for right and left circularly polarized modes is of form $H_{\text{ph}} = \omega \mathbb{1}$ with dispersion ω . The coupling matrix is

$$G_+ = \frac{g_0}{8} \begin{pmatrix} (1 - \hat{d}_z) \hat{d}_\perp e^{-i\varphi} & -(1 + \hat{d}_z) \hat{d}_\perp e^{i\varphi} \\ (1 - \hat{d}_z)^2 & -\hat{d}_\perp^2 e^{2i\varphi} \\ \hat{d}_\perp^2 e^{-2i\varphi} & -(1 + \hat{d}_z)^2 \\ (1 - \hat{d}_z) \hat{d}_\perp e^{-i\varphi} & -(1 + \hat{d}_z) \hat{d}_\perp e^{i\varphi} \end{pmatrix}, \quad (\text{S.9})$$

with g_0 being a constant, $\hat{d}_z = d_z/|\vec{d}|$, and $\hat{d}_\perp e^{i\varphi} \equiv (d_x + id_y)/|\vec{d}|$. TR-symmetry demands that

$G_-(\vec{q}) = -G_+^*(-\vec{q})\sigma_x$. We emphasize that Eq. (S.9) is continuously defined over the entire Brillouin zone for a topologically nontrivial QSH insulator, and couples only the (physical) excitonic states to photons.

Polariton system on a cylindrical geometry

First, we analyze the QSH insulator on a cylindrical geometry with periodic boundary conditions in x -direction and hard wall boundary conditions in y -direction. We compute the spectrum and eigenstates by numerical diagonalization of the lattice Hamiltonian of Eq. (S.6). The eigenfunctions are plane waves in x -direction with quantum numbers k_x , and vanish at $y = 0, L$ with system size $L = L_y$. For given pseudospin α and wavevector k_x we find $l = 1, \dots, N$ conduction (valence) band eigenstates where $L = aN$ with N lattice sites and lattice constant a . These provide a basis set for electrons $|\psi_{\alpha k_x l}^e\rangle$ and holes $|\psi_{\alpha k_x l}^h\rangle$. For a topologically nontrivial QSH insulator the state with $l = 1$ is an edge state located near a boundary. From now on we will label any edge state by a tilde.

As long as momentum was a good quantum number an approximation for the exciton wave function was given by the direct product of hole and electron wave function: $|\psi_{\alpha \vec{q}}^x\rangle \approx |\psi_{\alpha \vec{q}/2}^h\rangle \otimes |\psi_{\alpha \vec{q}/2}^e\rangle$ with exciton momentum \vec{q} . This approximation fails on a cylindrical geometry, since k_y is no longer a good quantum number. Nonetheless, the exciton state can be expanded in product states of electron and hole: $|\psi_{\alpha q_x n}^x\rangle = \mathbb{1}_b |\psi_{\alpha q_x n}^x\rangle$ with

$$\mathbb{1}_b = \sum_{l'l'} |\psi_{\alpha k_x l}^h\rangle \langle \psi_{\alpha k_x l'}^e\rangle \langle \psi_{\alpha k_x l'}^e\rangle \langle \psi_{\alpha k_x l}^h|, \quad (\text{S.10})$$

where $|\psi_{\alpha k_x l}^{e,h}\rangle$ are the electron and hole eigenstates introduced above. For sufficiently large systems we can approximate the excitonic wave function on a cylindrical geometry by projecting the excitonic eigenstates with periodic boundary conditions onto the electron-hole basis states with boundaries, namely

$$|\psi_{\alpha q_x n}^x\rangle \approx \sum_{l'l'} c_{ll'}^{\alpha n}(q_x) |\psi_{\alpha q_x/2l}^h\rangle |\psi_{\alpha q_x/2l'}^e\rangle, \quad (\text{S.11})$$

$$c_{ll'}^{\alpha n}(q_x) = \langle \psi_{\alpha q_x/2l}^h\rangle \langle \psi_{\alpha q_x/2l'}^e\rangle \frac{1}{\sqrt{2}} (|\psi_{\alpha q_x q_n}^x\rangle \pm |\psi_{\alpha q_x - q_n}^x\rangle).$$

Above, the exciton state $|\psi_{\alpha q_x q_n}^x\rangle$ is the plane wave solution for periodic boundary conditions with wavevector $q_x = 2k_x$, and $q_n = 2(2\pi/L)n$, where n runs from $n = -N/2, \dots, N/2 - 1$. We use the even superposition (plus sign) for $n \leq 0$ (cosine eigenfunction) and the odd one (minus sign) for $n > 0$ (sine eigenfunctions).

We note that: i) The electron-hole Hilbert space is different for hard wall and periodic boundary conditions, so that $\mathbb{1}_b$ Eq. (S.10) is the identity in the former and a projector in the latter space. ii) In the presence of edge

states we replace the $n = 0$ state by the edge state wave function

$$|\tilde{\psi}_{\alpha q_x}^x\rangle \approx |\tilde{\psi}_{\alpha q_x/2}^h\rangle \otimes |\tilde{\psi}_{\alpha q_x/2}^e\rangle, \quad (\text{S.12})$$

i.e. $c_{ll'}^{\alpha 0} = \delta_{ll'}\delta_{1l'}$. iii) The wave function Eq. (S.11) has an energy

$$\epsilon_x(q_x, n) = \sum_{ll'} |c_{ll'}^{\alpha n}|^2 (\epsilon_h(q_x/2, l) + \epsilon_e(q_x/2, l')), \quad (\text{S.13})$$

where ϵ_e (ϵ_h) is the eigenvalue of the electron (hole) eigenfunction of the QSH insulator on a cylindrical geometry. iv) We note that the expansion Eq. (S.11) is somewhat analogous of projecting sine and cosine waves (free particles) onto a standing wave basis (particles in a box). v) In the limit of infinite system size, wave function Eq. (S.11) and its spectrum Eq. (S.13) converge to the solutions for periodic boundary conditions.

On a cylindrical geometry the photonic eigenmodes are

$$\vec{A}_{q_x m}^\sigma(x, y) = \sqrt{\frac{1}{L}} e^{iq_x x} \sqrt{\frac{2}{L}} \sin(q_m y) \vec{e}_\sigma \quad (\text{S.14})$$

with wavevector q_x , $q_m = \pi/L m$, $m = 1, 2, \dots$, polarization vector \vec{e}_σ , and energy

$$\omega(q_x, q_m) = \sqrt{\omega_0^2 + \hbar^2 c_{\text{ph}}^2 (q_x^2 + q_m^2)}, \quad (\text{S.15})$$

with c_{ph} as photon velocity and ω_0 determined by the thickness of the cavity. The coupling to excitons is

$$g_{nm}^{\alpha\sigma}(q_x) = \sum_{ll'} (c_{ll'}^{\alpha n}(q_x))^* \times \langle \psi_{\alpha q_x/2l'}^c | i[\hat{H}_e, \hat{x}] \cdot \frac{e\vec{A}_{q_x m}^\sigma}{\hbar} | \psi_{\alpha - q_x/2l}^v \rangle, \quad (\text{S.16})$$

where c, v label the conduction and valence band, respectively.

The polaritonic modes are obtained by evaluating the coupling Eq. (S.16) numerically and diagonalizing the corresponding polariton Hamiltonian with exciton energy Eq. (S.13) and photon energy Eq. (S.15) for given wavevector q_x and pseudospin α . We find pairs of polaritonic edge states lying energetically below the lower polariton branch.

Polaritonic edge state model

Replacing $k_y \rightarrow -i\partial_y$ in Eq. (S.6) allows us to calculate analytically the edge-state wave function for hard wall boundary conditions in y -direction, see Ref. 2–4. For wave functions located near $y = 0$ [5] we find

$$\tilde{\psi}_{\alpha k_x}^e(y) = \eta_{k_x}(y) \phi_{+1}^\alpha, \quad (\text{S.17})$$

with wavevector k_x , spinor $\phi_{\pm 1}^\alpha$ (eigenvector of the σ_x Pauli matrix with eigenvalue ± 1), and real-space function

$$\eta_{k_x}(y) = 2 \frac{\sqrt{\lambda(\lambda^2 - \nu^2)}}{\nu} e^{-\lambda y} \sinh(\nu y), \quad (\text{S.18})$$

satisfying the boundary condition $\eta_{k_x}(y = 0) = 0$. The two parameters λ, ν (measured in inverse lattice units) are defined as

$$\lambda \equiv \frac{A}{B}, \quad \nu(k_x) \equiv \sqrt{\lambda^2 - \frac{2|M|}{B} + k_x^2} \quad (\text{S.19})$$

respectively, where A, B, M are the BHZ-parameters. Above, all lengths (wavevectors) are measured in lattice units (inverse lattice units). The edge state exists if $|k_x| < \sqrt{2|M|/B}$, and has an energy

$$\tilde{\epsilon}_e^\alpha(k_x) = \alpha \hbar v_F k_x. \quad (\text{S.20})$$

Edge states located near $y = L$ have ϕ_{-1}^α spinors and energies $\tilde{\epsilon}_e^\alpha(k_x) = -\alpha \hbar v_F k_x$. In the following we will focus on the boundary $y = 0$.

Now, the coupling Eq. (S.16) is evaluated using the approximation Eq. (S.12) and the result Eq. (S.17). We find that only p-polarized light (linearly polarized light with electric field parallel to the plane of incident which is perpendicular to the y -direction) couples: $g_m^{\alpha\sigma=p} \equiv g_m^\alpha \neq 0$, whereas s-polarized light (electric field perpendicular to the boundary) does not: $g_m^{\alpha\sigma=s} = 0$. We find

$$g_m^\pm(k_x) = -\frac{i}{\sqrt{2}} \frac{g_0}{2} \sqrt{\frac{2}{L}} \int_y \eta_{k_x}(y)^2 \sin\left(\frac{\pi m}{L} y\right), \quad (\text{S.21})$$

for both pseudospins $\alpha = \pm$.

As long as the exciton bulk states are energetically much higher as the edge state, $\tilde{\epsilon}_x = \hbar v_F |q_x| \ll 2|M|$, we can neglect those and use an effective description,

$$H_E'(q_x) = \begin{pmatrix} \tilde{\epsilon}_x(q_x) & 0 & \underline{g}^+(q_x) \\ 0 & \tilde{\epsilon}_x(q_x) & \underline{g}^-(q_x) \\ (\underline{g}^+(q_x))^\dagger & (\underline{g}^-(q_x))^\dagger & \underline{\omega}(q_x) \end{pmatrix}, \quad (\text{S.22})$$

where \underline{g}^α is a row vector in the photon-space, see Eq. (S.21), and $\underline{\omega}(q_x) = \omega(q_x, q_m) \delta_{mm'}$ a diagonal matrix, see Eq. (S.15). In leading order degenerate perturbation theory we find

$$\begin{aligned} \tilde{\epsilon}(q_x) &\approx \tilde{\epsilon}_{(0)}(q_x) + \tilde{\epsilon}_{(2)}(q_x) \\ &= \tilde{\epsilon}_x(q_x) - \sum_m \frac{|g_m^\pm(q_x/2)|^2}{\Delta_m(q_x)}, \end{aligned} \quad (\text{S.23})$$

$$\begin{aligned} |\tilde{\Phi}_{\rho q_x}\rangle &\approx |\tilde{\Phi}_{\rho q_x}^{(0)}\rangle + |\tilde{\Phi}_{\rho q_x}^{(1)}\rangle \\ &= |\tilde{\psi}_{\rho q_x}^x\rangle - \sum_m \frac{(g_m^\pm(q_x/2))^*}{\Delta_m(q_x)} |\vec{A}_{q_x m}^{\sigma=p}\rangle. \end{aligned} \quad (\text{S.24})$$

Above, we have defined the detuning $\Delta_m(q_x) \equiv \omega(q_x, q_m) - \tilde{\epsilon}_x(q_x)$, and an index ρ which labels right (R)

and left (L) moving edge states. The excitonic component of the right (left) mover has pseudospin $\alpha = +(-)$, whereas the photonic component is p-polarized independently of the direction of motion. Since g_m^\pm is equal for both pseudospins, the edge-state energy is degenerate for $\rho = \{R, L\}$. Evaluating the photonic part of $\tilde{\Phi}_{\rho q_x}(y)$ Eq. (S.24) results in a wave function which is exponentially localized near the boundary, too. We define the photon fraction as $F \equiv \sqrt{|P_{\text{ph}} \tilde{\Phi}_{\rho q_x}|^2}$ where P_{ph} projects onto the photonic part, so that Eq. (S.24) yields

$$F(q_x) \approx \sqrt{\sum_m \frac{|g_m^\pm(q_x/2)|^2}{\Delta_m(q_x)^2}}. \quad (\text{S.25})$$

A simple effective model for right or left moving polaritonic edge states is

$$H_E(q_x) = \begin{pmatrix} \tilde{\epsilon}_x(q_x) & \tilde{g}(q_x) \\ (\tilde{g}(q_x))^* & \tilde{\omega}(q_x) \end{pmatrix}, \quad (\text{S.26})$$

where $\tilde{\epsilon}_x(q_x) = \hbar v_F |q_x|$ is the exciton energy, $\tilde{\omega}$ the energy of the localized photon wave function and \tilde{g} an effective coupling. Diagonalizing Eq. (S.26) and expanding in powers of $\tilde{g}/\tilde{\Delta}$ yields

$$\tilde{\epsilon}(q_x) \approx \tilde{\epsilon}_x(q_x) - \left(\frac{\tilde{g}(q_x)}{\tilde{\Delta}(q_x)} \right)^2 \tilde{\Delta}(q_x), \quad (\text{S.27})$$

$$|\tilde{\Phi}_{\rho q_x}\rangle \approx |\tilde{\psi}_{\rho q_x}^x\rangle - \frac{\tilde{g}(q_x)}{\tilde{\Delta}(q_x)} |\tilde{\psi}_{\rho q_x}^{\text{ph}}\rangle, \quad (\text{S.28})$$

with detuning $\tilde{\Delta} \equiv \tilde{\omega} - \tilde{\epsilon}_x$. This allows us to extract

$$\tilde{g}(q_x) = \frac{1}{F(q_x)} \sum_m \frac{|g_m^\pm(q_x/2)|^2}{\Delta_m(q_x)}, \quad (\text{S.29})$$

$$\tilde{\Delta}(q_x) = \frac{1}{F(q_x)^2} \sum_m \frac{|g_m^\pm(q_x/2)|^2}{\Delta_m(q_x)}, \quad (\text{S.30})$$

$$|\tilde{\psi}_{\rho q_x}^{\text{ph}}\rangle = \frac{1}{F(q_x)} \sum_m \frac{(g_m^\pm(q_x/2))^*}{\Delta_m(q_x)} |\tilde{A}_{q_x m}^{\sigma=p}\rangle, \quad (\text{S.31})$$

by comparing with Eq. (S.23) and Eq. (S.24).

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