Dispersive bands of bound states in the continuum: supplementary material

The supplementary material contains technical details concerning (i) The effective non-Hermitian description of indirect resonator coupling; (ii) Band dispersion curve of the BIC crystal; (iii) Friedrichs-Lee Hamiltonian of the exactly-solvable optical cavities-CROW system.

1. EFFECTIVE NON-HERMITIAN DESCRIPTION OF INDIRECT RESONATOR COUPLING

To derive an effective non-Hermitian description of indirect resonator coupling, we follow a rather standard procedure which is outlined, for example, in Refs. [1–3]. The starting point is provided by the exact coupled-mode equations (Eqs.(8) and (9) of the main manuscript)

$$i\frac{da_n}{dt} = \int dk \; G_n(k) c(k,t) \tag{S1}$$

$$i\frac{\partial c}{\partial t} = \{\omega(k) - \omega_0\} c(k,t) + \sum_n G_n^*(k) a_n(t) \tag{S2}$$

Equation (S2) can be formally integrated with the initial condition $c(k,0) = 0$, yielding

$$c(k,t) = -i \sum_n G_n^*(k) \int_0^t d\tau \; a_n(\tau) \exp\left\{-i[\omega(k) - \omega_0](t-\tau)\right\} \tag{S3}$$

Substitution of Eq.(S3) into Eq.(S1) yields the following set of integro-differential equations for the field amplitudes $a_n(t)$

$$i\frac{da_n}{dt} = \sum_l \int_0^t d\tau \; a_l(t-\tau) \mathcal{G}_{n,l}(\tau) \tag{S4}$$

where

$$\mathcal{G}_{n,l}(\tau) \equiv -i \int dk \; G_n(k) G_l^*(k) \exp\left\{-i[\omega(k) - \omega_0]\tau\right\} \tag{S5}$$

are the memory functions. Note that $\mathcal{G}_{n,l}(\tau)$ vanishes for long memory time τ, i.e. $\mathcal{G}_{n,l}(\tau) \rightarrow 0$ as $\tau \rightarrow \infty$, with some characteristic time $\tau_{n,l}$ which provides the typical memory time of the indirect coupling between resonators n and l. In the weak coupling (Markovian) limit, the change of the amplitudes $a_n(t)$ over the time scale of the memory times is small, so that Eq.(S4) can be approximated by the set of differential equations

$$i\frac{da_n}{dt} \simeq \sum_l H_{n,l} a_l(t) \tag{S6}$$

where we have set

$$H_{n,l} \equiv \int_0^\infty d\tau \mathcal{G}_{n,l}(\tau) = -i \int_0^\infty d\tau \int dk \; G_n(k) G_l^*(k) \exp\left\{-i[\omega(k) - \omega_0]\tau\right\} \tag{S7}$$

Note that $H_{n,l}$ can be written as

$$\begin{aligned} H_{n,l} &= -i \lim_{\epsilon \rightarrow 0^+} \int_0^\infty d\tau \int dk \; G_n(k) G_l^*(k) \exp\left\{-i[\omega(k) - \omega_0]\tau - \epsilon\tau\right\} \\ &= -i \int dk \; G_n(k) G_l^*(k) \lim_{\epsilon \rightarrow 0^+} \int_0^\infty \exp\left\{-i[\omega(k) - \omega_0]\tau - \epsilon\tau\right\} = \lim_{\epsilon \rightarrow 0^+} \int dk \frac{G_n(k) G_l^*(k)}{i\epsilon + \omega_0 - \omega(k)} \end{aligned} \tag{S8}$$

which is Eq.(11) given in the main text. In order to discuss some main properties of the coefficients $H_{n,l}$, let us consider a system with discrete translational invariance, so that $G_n(k) = G_0(k) \exp(ikdn)$ and $H_{n,l}$ is a function of $(n-l)$ solely, i.e. $H_{n,l} = H_{n-l}$ with

$$H_n = \lim_{\epsilon \rightarrow 0^+} \int dk \frac{|G_0(k)|^2 \exp(ikdn)}{i\epsilon + \omega_0 - \omega(k)}. \tag{S9}$$

In a typical situation where the coupling of the resonator mode with the forward and backward propagating waves in the waveguide is symmetric, one has $G_0(-k) = G_0(k)$, so that from Eq.(S9) it readily follows that

$$H_{-n} = H_n. \tag{S10}$$

Assuming that the resonance condition $\omega(k) = \omega_0$ is satisfied at the wave numbers $k = \pm k_0$, the main contribution to the integral on the right hand sides of Eq.(S9) is obtained when k varies in the neighborhood of $\pm k_0$. Therefore, after setting $\omega(k) \simeq v_g|k|$ for $k \sim \pm k_0$, where v_g is the group velocity of the propagating fields in the waveguide at the frequency ω_0, taking into account the identity

$$\lim_{\epsilon \to 0^+} \frac{1}{i\epsilon + x} = \mathcal{P}\left(\frac{1}{x}\right) - i\pi\delta(x), \tag{S11}$$

where $\mathcal{P}$ denotes the principal value, from Eq.(S9) one obtains

$$H_n = -\frac{2\pi i |G_0(k_0)|^2 \cos(k_0 n d)}{v_g} + \frac{1}{v_g}\mathcal{P}\int dk \left(\frac{1}{k+k_0} - \frac{1}{k-k_0}\right) |G_0(k)|^2 \exp(iknd). \tag{S12}$$

From Eq.(S12) it readily follows that H_n vanishes as $n \to \pm\infty$ if and only if

$$G_0(k_0) = 0. \tag{S13}$$

Equation (S13) also corresponds to a real value of H_0, i.e. to the vanishing of the decay rate for the coupling of a single resonator into the waveguide. The condition (S13), which ensures that the coupling H_n vanishes as $n \to \pm\infty$, is equivalent the existence of a BIC when *a single resonator* is side-coupled to the waveguide.

2. BAND DISPERSION CURVE OF THE BIC CRYSTAL

In a system with discrete translational invariance, $H_{n,l} = H_{n-l}$.Therefore, in the $N \to \infty$ limit the solutions to the coupled-mode equations (S6) of reduced non-Hermitian dynamics are of Bloch-Floquet form. By letting $a_n(t) = \exp[iqdn - i\Omega(q)t]$, where $-\pi/d \leq q < \pi/d$ is the Bloch wave number, the energy dispersion relation $\Omega(q)$ reads

$$\Omega(q) = \sum_l H_l \exp(-iqdl) \tag{S14}$$

where H_l is given by Eq.(S9). Substitution of Eq.(S9) into Eq.(S14) and using the identity

$$\sum_{l=-\infty}^{\infty} \exp(ilx) = 2\pi \sum_l \delta(x - 2\pi l) \tag{S15}$$

one obtains

$$\Omega(q) = \frac{2\pi}{d} \lim_{\epsilon \to 0^+} \sum_{l=-\infty}^{\infty} \frac{|G_0(q + 2\pi l/d)|^2}{i\epsilon + \omega_0 - \omega(q + 2\pi l/d)}. \tag{S16}$$

Clearly, since ω_0 is embedded in the continuous spectrum $\omega(k)$ of the waveguide modes, for q and l such that $q + 2\pi l/d = \pm k_0$, so as $\omega(\pm k_0) = \omega_0$, the corresponding term in the series on the right hand side of Eq.(S16) diverges in the $\epsilon \to 0^+$ limit, unless $G(\pm k_0) = 0$. As discussed above, this condition corresponds to the vanishing of H_n as $|n| \to \infty$ and to the existence of a BIC mode when a *single* resonator is coupled to the waveguide. In this case $\Omega(q)$ is non-singular for any value of Bloch wave number q and the dispersion curve reads

$$\Omega(q) = \frac{2\pi}{d} \sum_{l=-\infty}^{\infty} \frac{|G_0(q + 2\pi l/d)|^2}{\omega_0 - \omega(q + 2\pi l/d)} \tag{S17}$$

which is Eq.(16) given in the main manuscript. Conversely, if $G_0(\pm k_0) \neq 0$, i.e. when a single resonator coupled to the waveguide does not sustain a BIC mode and decay into the waveguide modes is allowed, $\Omega(q)$ converges to a real value for $q + 2\pi l/d \neq \pm k_0$, but displays a diverging behavior (with non-vanishing real and imaginary parts) for q near $q + 2\pi l/d \simeq \pm k_0$. Such a divergence stems from the fact that, when $G_0(\pm k_0) \neq 0$, the hopping amplitude H_n does not vanish as $n \to \pm\infty$, so as the $N \to \infty$ limit cannot be assumed within the asymptotic analysis based on the non-Hermitian effective Hamiltonian dynamics.

3. FRIEDRICHS-LEE HAMILTONIAN OF THE CAVITIES-CROW SYSTEM

Let us consider the optical structure of Fig.1B of the main manuscript, comprising a CROW and an array of side-coupled optical cavities with three contact points. Indicating by $\hat{a}_n^\dagger$ and $\hat{b}_n^\dagger$ the creation operators of photons in the optical modes of the n-th cavity and in the n-th resonator of the CROW, the full Hamiltonian of the photon field reads $\hat{H} = \hat{H}_s + \hat{H}_c + \hat{H}_i$, where

$$\hat{H}_s = \sum_n \omega_0 \hat{a}_n^\dagger \hat{a}_n \tag{S18}$$

is the Hamiltonian of uncoupled optical cavities,

$$\hat{H}_c = \sum_n J(\hat{b}_n^\dagger \hat{b}_{n+1} + \text{H.c.}) \tag{S19}$$

is the tight-binding Hamiltonian of the CROW, and

$$\hat{H}_i = \sum_n \left\{ \rho \hat{a}_n^\dagger b_n + \rho h \hat{a}_n^\dagger (\hat{b}_{n+1} + \hat{b}_{n-1}) + \text{H.c.} \right\} \tag{S20}$$

describes the coupling between the resonators in the CROW and the optical cavities. The full Hamiltonian $\hat{H}$ can be cast in the Friedrichs-Lee form [Eqs.(1-4) of the main text] after switching from the Wannier basis to the Bloch basis representations of the modes in the CROW. To this aim, let us introduce the destruction operators $\hat{c}(k)$ of Bloch photon modes in the CROW, with Bloch wave number k ($-\pi \leq k < \pi$), via the transformation

$$\hat{c}(k) = \frac{1}{\sqrt{2\pi}} \sum_n \hat{b}_n \exp(-ikn), \tag{S21}$$

i.e.

$$\hat{b}_n = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} dk \; \hat{c}(k) \exp(ikn). \tag{S22}$$

Note that, since $[\hat{b}_n, \hat{b}_m^\dagger] = \delta_{n,m}$ in the Wannier basis, one has $[\hat{c}(k), \hat{c}^\dagger(k')] = \delta(k - k')$ in Bloch basis. Substitution of Eq.(S22) into Eqs.(S19) and (S20) yields

$$\hat{H}_c = \int_{-\pi}^{\pi} dk \; \omega(k) \hat{c}^\dagger(k) \hat{c}(k) \tag{S23}$$

and

$$\hat{H}_i = \sum_n \int_{-\pi}^{\pi} dk \left\{ G_n(k) \hat{a}_n^\dagger \hat{c}(k) + \text{H.c.} \right\} \tag{S24}$$

where

$$\omega(k) = 2J \cos k \tag{S25}$$

is the dispersion relation of the tight-binding CROW band, and

$$G_n(k) = \frac{\rho}{\sqrt{2\pi}} (1 + 2h \cos k) \exp(ikn) \tag{S26}$$

is the spectral coupling function.

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