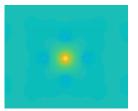
# Functional analytic methods for discrete approximation of subwavelength resonator systems

Habib Ammari

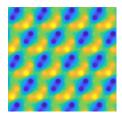
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#### Subwavelength resonances

- Focus, trap, guide, manipulate, and control waves at subwavelength scales.
- Construct a unified mathematical approach for modelling subwavelength confinement and guiding of waves as well as imaging and sensing using artificial materials.
- Microstructured resonant materials.
- Building block microstructure: subwavelength resonator.
- Evaluate the robustness of the proposed approaches for subwavelength confinement and guiding of waves with respect to uncertainties in the geometrical or physical parameters.







#### Subwavelength resonances

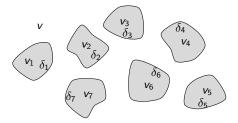
• PDE model for a single subwavelength resonator:

$$\begin{cases} & \Delta u + \omega^2 \frac{\rho}{\kappa} u = 0 \quad \text{in} \quad \mathbb{R}^3 \setminus \overline{D}, \\ & \Delta u + \omega^2 \frac{\rho r}{\kappa_r} u = 0 \quad \text{in} \quad D, \\ & u|_+ = u|_- \quad \text{on} \quad \partial D, \\ & \frac{\rho r}{\rho} \frac{\partial u}{\partial \nu} \bigg|_+ = \frac{\partial u}{\partial \nu} \bigg|_- \quad \text{on} \quad \partial D, \end{cases}$$

 $u^s:=u-u^{\mathrm{in}}$  satisfies the (outgoing) Sommerfeld radiation condition.

- $\kappa_r$ ,  $\rho_r$ ,  $\kappa$ ,  $\rho$ : material parameters inside and outside D.
- $k_r = \omega \sqrt{\rho_r/\kappa_r}$ ;  $v_r = \sqrt{\kappa_r/\rho_r}$ ;  $k = \omega \sqrt{\rho/\kappa}$ ;  $v = \sqrt{\kappa/\rho}$ .
- $v_r, v = O(1)$ ; High contrast:  $\delta := |\rho_r/\rho| \ll 1$ .
- Given  $\delta$ , a subwavelength resonant frequency  $\omega = \omega(\delta) \in \mathbb{C}$ :
  - (i) there exists a non-trivial solution to the PDE model with  $u^{in} = 0$ ;
  - (ii)  $\omega$  depends continuously on  $\delta$  and satisfies  $\omega \to 0$  as  $\delta \to 0$ .

- Finite system of subwavelength resonators<sup>1</sup>:
  - Let  $D = D_1 \cup \cdots \cup D_N$ ;  $D_1, D_2, \ldots, D_N \subset \mathbb{R}^d$ : N disjoint resonators;  $v_i$ : wave speed in resonator  $D_i$ ,  $k_i = \omega/v_i$ : wave number in  $D_i$ ;
  - $\delta_i = O(\delta)$ ,  $|\delta| \ll 1$ , for i = 1, ..., N.

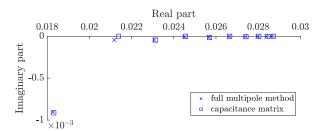


- There are N subwavelength resonances which can be computed by discretizing the boundary integral formulation  $\mathcal{A}(\omega,\delta)[\Psi]=0$  and using Muller's method.
- Use a discrete approximation of the PDE model to obtain accurate numerical approximations of the subwavelength resonances with significant reduction in computational power.



<sup>&</sup>lt;sup>1</sup>with B. Davies, E. Hiltunen, Submitted, 2020.

- Subwavelength resonant frequencies of a system of N=10 spherical resonators; Each resonator has unit radius and  $\delta=1/5000$ .
- Comparison between the values computed using the multipole expansion method to discretize the full boundary integral equation and the values computed using the discrete approximation.
- Computations using the full multipole method took 41 seconds while the the discrete approximation took just 0.02 seconds, on the same computer.



- Discrete approximation:
  - Generalized capacitance matrix:  $C = (C_{ij}) \in \mathbb{C}^{N \times N}$

$$\mathcal{C}_{ij} = rac{\delta_i v_i^2}{|D_i|} \mathcal{C}_{ij}, \quad i,j = 1,\ldots, \mathcal{N}.$$

• Capacitance matrix:  $C = (C_{ij}) \in \mathbb{R}^{N \times N}$ 

$$C_{ij} = -\int_{\partial D_i} \underbrace{\left(\mathcal{S}_D\right)^{-1} \left[\chi_{\partial D_j}
ight]}_{:=\psi_j} d\sigma, \quad i,j = 1,\ldots, N.$$

- $\chi_{\partial D_i}$ : characteristic function of  $\partial D_i$ ;
- $\mathcal{S}_D$ : Single-layer potential associated with the fundamental solution G to the Laplacian:  $\mathcal{S}_D[\phi] = \int_{\partial D} G(x-y)\phi(y) \, d\sigma(y)$ .
- Characterization of the subwavelength resonant frequencies:

•

$$\omega_n = \sqrt{\lambda_n} + O(\delta), \quad n = 1, \dots, N;$$

•  $\{\lambda_n: n=1,\ldots,N\}$ : eigenvalues of  $\mathcal{C}$ , which satisfy  $\lambda_n=O(\delta)$  as  $\delta\to 0$ .

- Characterization of the subwavelength resonant modes:
  - $\mathbf{v}_n$ : eigenvector of  $\mathcal{C}$  associated to  $\lambda_n$ .
  - Resonant mode  $u_n$  associated to  $\omega_n$ :

$$u_n(x) = \begin{cases} \mathbf{v}_n \cdot \mathbf{S}_D^k(x) + O(\delta^{1/2}), & x \in \mathbb{R}^3 \setminus \overline{D}, \\ \mathbf{v}_n \cdot \mathbf{S}_D^{kj}(x) + O(\delta^{1/2}), & x \in D_i. \end{cases}$$

•  $\mathbf{S}_D^k : \mathbb{R}^3 \to \mathbb{C}^N$ :

$$\mathbf{S}_{D}^{k}(x) = \begin{pmatrix} \mathcal{S}_{D}^{k}[\psi_{1}](x) \\ \vdots \\ \mathcal{S}_{D}^{k}[\psi_{N}](x) \end{pmatrix}, \quad x \in \mathbb{R}^{3} \setminus \partial D;$$

- $\psi_i := (\mathcal{S}_D)^{-1} [\chi_{\partial D_i}].$
- S<sub>D</sub><sup>k</sup>: single-layer potential associated with G<sub>k</sub>: outgoing fundamental solution of the Helmholtz operator Δ + k<sup>2</sup>.

- Modal decomposition:
  - V: matrix of eigenvectors of C.  $V = [\mathbf{v}_1, \dots, \mathbf{v}_N]$ .
  - If  $\omega = O(\sqrt{\delta})$  as  $\delta \to 0$ , then the solution u to the scattering problem can be written, uniformly for x in compact subsets of  $\mathbb{R}^3$ , as

$$u(x) - u^{\text{in}}(x) = \sum_{n=1}^{N} a_n u_n(x) - S_D^k \left[ \left( S_D^k \right)^{-1} [u^{\text{in}}] \right] (x) + O(\delta^{1/2});$$

•  $a_n = a_n(\omega)$  satisfy

$$V\begin{pmatrix} \omega^{2} - \omega_{1}^{2} & & \\ & \ddots & \\ & & \omega^{2} - \omega_{N}^{2} \end{pmatrix} \begin{pmatrix} a_{1} \\ \vdots \\ a_{N} \end{pmatrix} = \begin{pmatrix} \frac{v_{1}^{2} \delta_{1}}{|D_{1}|} \int_{\partial D_{1}} (\mathcal{S}_{D})^{-1} [u^{\mathrm{in}}] d\sigma \\ & \vdots \\ \frac{v_{N}^{2} \delta_{N}}{|D_{N}|} \int_{\partial D_{N}} (\mathcal{S}_{D})^{-1} [u^{\mathrm{in}}] d\sigma \end{pmatrix} + O(\delta^{3/2}).$$

#### Effective medium theory

- N = 1.
- Monopolar resonance frequency for a single subwavelength resonator:

$$\underbrace{\sqrt{\frac{\mathsf{Cap}_{D}}{|D|}} v_{r} \sqrt{\delta}}_{:=\omega_{M}} + i \underbrace{\left(-\frac{\mathsf{Cap}_{D}^{2} v_{r}^{2}}{8\pi v |D|} \delta\right)}_{:=\tau_{M}} + O(\delta^{\frac{3}{2}}).$$

- Capacity  $Cap_D := -\int_{\partial D} \mathcal{S}_D^{-1}[1] \, d\sigma.$
- Monopole approximation near the monopolar resonance frequency<sup>2</sup>:

$$u(x)-u^{\mathrm{in}}(x)=g(\omega,\delta,D)(1+o(1))u^{\mathrm{in}}(x_0)G_k(x,x_0).$$

Scattering coefficient g:

$$g(\omega, \delta, D) = \frac{\mathsf{Cap}_D}{1 - (\frac{\omega_M}{\omega})^2 + i\tau_M}.$$

Scattering enhancement near the monopolar resonance frequency.

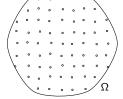


#### Effective medium theory

- Effective medium theory for dilute systems of subwavelength resonators<sup>3</sup>:
- Effective operator:  $\Delta + k^2 + V(x)$

$$V(x) = \frac{1}{\left(\frac{\omega_M}{\omega}\right)^2 - 1} \Lambda \widetilde{V}(x).$$

- $\omega_M := \sqrt{\lambda_1}$ ;
- Λ: depends only on the size and number of the subwavelength resonators;
- V: depends only on the distribution of the centers of the subwavelength resonators.



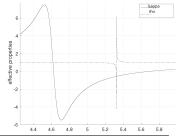
- ω slightly below ω<sub>M</sub>: high-contrast effective κ ⇒ superresolution imaging: imaginary part of the Green function sharper peak than the free-space one
- $\omega$  slightly above  $\omega_M$ : negative effective  $\kappa$ .
- Effective medium theory does not hold at  $\omega = \omega_M$ : adding or removal of one resonator from the system affects the total field by a magnitude  $O(u^{\text{in}})$ .

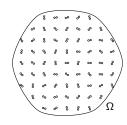


<sup>&</sup>lt;sup>3</sup>with H. Zhang, SIAM J. Math. Anal., 2017.

#### Effective medium theory

- Double-negative effective material properties<sup>4</sup>:
  - Dimer consisting of two identical resonators;
  - Resonator dimer: approximated as a point scatterer with resonant monopole mode at ω<sub>M,1</sub> and resonant dipole mode at ω<sub>M,2</sub>;
  - Resonances  $\omega_{M,1}$  and  $\omega_{M,2}$ : hybridized resonances of the resonator dimer.
- Obtain negative effective  $\kappa$  and  $\rho$  for frequencies near the hybridized resonant frequencies of a single dimer.

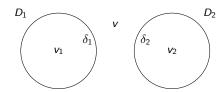




<sup>4</sup>with B. Fitzpatrick, H. Lee, S. Yu, H. Zhang, Quart. Appl. Math., 2019.

#### Exceptional points

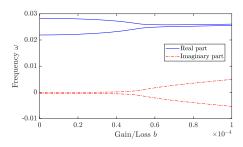
• Parity-time-symmetric system:  $D_1 = -D_2$  and  $v_1^2 \delta_1 = \overline{v_2^2 \delta_2}$ 



- $v_1^2 \delta_1 := a + ib$ ,  $v_2^2 \delta_2 := a ib$ , for  $a, b \in \mathbb{R}$ ; |b|: magnitude of the gain and the loss.
- Asymptotic exceptional points<sup>5</sup>: There is a magnitude of the gain/loss such that resonant frequencies and corresponding eigenmodes coincide to leading order in δ.
- PT-symmetry forces the spectrum of the capacitance matrix to be conjugate symmetric.
- The operator in the PDE model: not PT-symmetric due to the radiation condition ⇒ approximate nature of the exceptional points.

#### **Exceptional points**

- As  $\delta \to 0$ ,  $\omega_i = \sqrt{\lambda_i} + O(\delta)$ , i = 1, 2.
- $\lambda_i = \frac{1}{|D_1|} \left( aC_{11} + (-1)^i \sqrt{a^2 C_{12}^2 b^2 (C_{11}^2 C_{12}^2)} \right), \quad i = 1, 2.$
- $b_0 = \frac{aC_{12}}{\sqrt{c_{11}^2 c_{12}^2}}$  corresponds to the point where  $\mathcal C$  has a double eigenvalue corresponding to a one-dimensional eigenspace.



#### High-order exceptional points

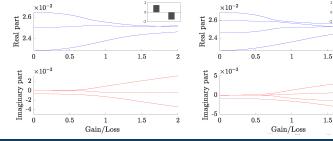
 Asymptotic Nth order exceptional point: eigenvalue of algebraic multiplicity = N and a corresponding eigenspace of dimension one

$$\det(\mathcal{C} - xI) = (\lambda - x)^N$$
,  $\dim \operatorname{Ker}(\mathcal{C} - \lambda I) = 1$ .

If a small particle is introduced into a structure with Nth order exceptional point, the splitting in one of the resonant frequencies is O(Nth root of the particle's volume) ⇒ enhanced sensing.



PT-symmetric systems with high-order exceptional points:



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1.5

# Time-modulated systems of subwavelength resonators

Wave equation in a time-modulated structure:

$$\left(\frac{\partial}{\partial t}\frac{1}{\kappa(x,t)}\frac{\partial}{\partial t}-\nabla\cdot\frac{1}{\rho(x,t)}\nabla\right)u(x,t)=0,\quad x\in\mathbb{R}^d,t\in\mathbb{R}.$$

Time-modulation of the resonators:

$$\kappa(x,t) = \begin{cases} \kappa, & x \in \mathbb{R}^d \setminus \overline{D}, \\ \kappa_r \kappa_i(t), & x \in D_i, \end{cases}, \qquad \rho(x,t) = \begin{cases} \rho, & x \in \mathbb{R}^d \setminus \overline{D}, \\ \rho_r \rho_i(t), & x \in D_i. \end{cases}$$

•  $\rho_i(t)$  and  $\kappa_i(t)$ : modulation inside the  $i^{\text{th}}$  resonator  $D_i$ ;  $\rho_i, \kappa_i$ : periodic with period T;  $\kappa_i \in C^1(\mathbb{R})$  and  $\kappa_i'(t) = O(\delta^{1/2})$  for each  $i = 1, \ldots, N$ .

#### Time-modulated systems of subwavelength resonators

• Floquet transform in t:

$$\left\{ \begin{array}{l} \left( \frac{\partial}{\partial t} \frac{1}{\kappa(x,t)} \frac{\partial}{\partial t} - \nabla \cdot \frac{1}{\rho(x,t)} \nabla \right) u(x,t) = 0, \\ u(x,t) e^{-i\omega t} \text{ is $T$-periodic in $t$.} \end{array} \right.$$

- Time-Brillouin zone:  $\omega \in Y_t^* := \mathbb{C}/(\Omega \mathbb{Z}); \Omega = (2\pi)/T = O(\delta^{1/2}).$
- A quasifrequency is a subwavelength quasifrequency if the corresponding solution is essentially supported in the subwavelength frequency regime:

$$u(x,t) = e^{i\omega t} \sum_{n=-\infty}^{\infty} v_n(x)e^{in\Omega t}, \quad \omega$$
: Floquet exponent,

where

$$\omega \to 0$$
 and  $M\Omega \to 0$  as  $\delta \to 0$ ,

for some integer-valued function  $M=M(\delta)$  such that, as  $\delta \to 0$ , we have

$$\sum_{n=-\infty}^{\infty}\|v_n\|_{L^2(K)}=\sum_{n=-M}^{M}\|v_n\|_{L^2(K)}+o(1),\qquad \text{$K$ compact set containing $D$}.$$

#### Time-modulated systems of subwavelength resonators

- Capacitance matrix formulation of the problem<sup>6</sup>:
  - As δ → 0, the quasifrequencies ω ∈ Y<sub>t</sub>\* are, to leading order, given by the quasifrequencies of the system of ordinary differential equations:

$$\sum_{j=1}^N \mathcal{C}_{ij} c_j(t) = -rac{1}{
ho_i(t)} rac{d}{dt} \left(rac{1}{\kappa_i(t)} rac{d(
ho_i c_i)}{dt}
ight),$$

for 
$$i = 1, ..., N$$
.  $(c_j(t) = e^{i\omega t} \sum_n c_{j,n} e^{in\Omega t})$ .

• Rewrite as a system of Hill equations:

$$\Psi''(t) + M(t)\Psi(t) = 0.$$

- Compute the Floquet exponents of the Hill system of equations.
- If  $\kappa_i(t) = 1, \rho_i(t) = \rho_1(t), t \in \mathbb{R}, i = 1, ..., N$ :

$$\Psi''(t) + \mathcal{C}\Psi(t) = 0.$$

•  $\Rightarrow$  Static case: Quasifrequencies  $\omega_i = \sqrt{\lambda_i}$  at leading order in  $\delta$ .

<sup>6</sup>with E.O. Hiltunen, J. Comp. Phys., 2021.



- d<sub>I</sub>: dimension of periodicity of the lattice. d: dimension of the ambient space.
   P<sub>⊥</sub>: ℝ<sup>d</sup> → ℝ<sup>d-d<sub>I</sub></sup>: projection onto the last d d<sub>I</sub> coordinates.
- Three different cases:
  - $d d_l = 0$ : crystal;
  - $d d_l = 1$ : screen;
  - $d d_l = 2$ : chain.
- $\Lambda$ : periodic lattice;  $l_1, \ldots, l_{d_l}$ : lattice vectors  $(P_{\perp}l_i = 0, i = 1, \ldots, d_l)$ .

$$\Lambda := \{m_1 I_1 + \ldots + m_{d_l} I_{d_l} | m_i \in \mathbb{Z}\}.$$

• Y: fundamental domain

Subwavelength resonator systems

$$Y := \{c_1 I_1 + \ldots + c_{d_l} I_{d_l} | 0 \le c_1, \ldots, c_{d_l} \le 1\}.$$

- $\Lambda^*$ : dual lattice of  $\Lambda$  generated by  $\alpha_1, \ldots, \alpha_{d_i}$  satisfying  $\alpha_i \cdot l_j = 2\pi \delta_{ij}$ ,  $P_{\perp} \alpha_i = 0, i = 1, \ldots, d_i$ ;
- Brillouin zone  $Y^* := (\mathbb{R}^{d_I} \times \{\mathbf{0}\})/\Lambda^*$ ; **0**: zero-vector in  $\mathbb{R}^{d-d_I}$ .



• Periodically repeated  $i^{\text{th}}$  resonator  $\mathcal{D}_i$  and the full periodic structure  $\mathcal{D}$ :

$$\mathcal{D}_i = \bigcup_{m \in \Lambda} D_i + m, \qquad \mathcal{D} = \bigcup_{i=1}^N \mathcal{D}_i.$$

Subwavelength spectrum of the original problem:

$$\sigma = \bigcup_{\alpha \in Y^*} \sigma(\alpha).$$

 For α ∈ Y\*, σ(α), the subwavelength spectrum of the quasiperiodic problem, consists of N discrete values ω<sub>i</sub>α:

$$\sigma(\alpha) = \{\omega_i^{\alpha}\}_{i=1}^{N}.$$

•  $\alpha \mapsto \omega_i^{\alpha}$ : band functions.

• Assume  $|\alpha|>c>0$  for some constant c independent of  $\omega$  and  $\delta$ . As  $\delta\to 0$ , the N subwavelength resonant frequencies satisfy the asymptotic formula

$$\omega_n^{\alpha} = \sqrt{\lambda_n^{\alpha}} + O(\delta^{3/2}), \quad n = 1, \dots, N.$$

- {λ<sub>n</sub><sup>α</sup> : n = 1,..., N}: eigenvalues of the generalized quasiperiodic capacitance matrix C<sup>α</sup>, which satisfy λ<sub>n</sub><sup>α</sup> = O(δ) as δ → 0.
- Resonant mode  $u_n^{\alpha}$  associated to  $\omega_n^{\alpha}$ :

$$u_n^{\alpha}(x) = \begin{cases} \mathbf{v}_n^{\alpha} \cdot \mathbf{S}_D^{\alpha,k}(x) + O(\delta^{1/2}), & x \in \mathbb{R}^d \setminus \overline{\mathcal{D}}, \\ \mathbf{v}_n^{\alpha} \cdot \mathbf{S}_D^{\alpha,k_i}(x) + O(\delta^{1/2}), & x \in \mathcal{D}_i. \end{cases}$$

•  $\mathbf{S}_{D}^{\alpha,k}: \mathbb{R}^{d} \to \mathbb{C}^{N}$ :

$$\mathbf{S}_{D}^{\alpha,k}(x) = \begin{pmatrix} S_{D}^{\alpha,k}[\psi_{1}^{\alpha}](x) \\ \vdots \\ S_{D}^{\alpha,k}[\psi_{N}^{\alpha}](x) \end{pmatrix}, \quad x \in \mathbb{R}^{d} \setminus \partial \mathcal{D},$$

with  $\psi_i^{\alpha} := (\mathcal{S}_D^{\alpha,0})^{-1} [\chi_{\partial D_i}].$ 



• Single layer potential associated with  $G^{\alpha,k}$ :

$$S_D^{\alpha,k}[\phi] = \int_{\partial D} G^{\alpha,k}(x,y)\phi(y) \, d\sigma(y).$$

• Quasi-periodic Green's function:

$$G^{\alpha,k}(x,y) = \sum_{m \in \Lambda} \frac{e^{ik|x-y-m|}}{4\pi|x-y-m|} e^{i\alpha \cdot m}.$$

- Uniform convergence for x and y in compact sets of  $\mathbb{R}^d$ ,  $x \neq y$ , and  $k \neq |\alpha + q|$  for all  $q \in \Lambda^*$ .
- $\mathcal{S}_{D}^{\alpha,k}: L^{2}(\partial D) \to H^{1}(\partial D)$  is invertible if k is small enough and  $k \neq |\alpha + q|$  for all  $q \in \Lambda^{*}$ .
- For  $\alpha \neq 0$ ,

$$\mathcal{S}^{lpha,k}_D = \mathcal{S}^{lpha,0}_D + O(k^2)$$
 as  $k o 0$ .



- System of N resonators  $D_1, \ldots, D_N$  in Y.
- Quasiperiodic capacitance matrix
  - For  $\alpha \neq 0$ ,  $C^{\alpha} = (C_{ii}^{\alpha}) \in \mathbb{C}^{N \times N}$ :

$$C_{ij}^{\alpha} = -\int_{\partial D_i} (\mathcal{S}_D^{\alpha,0})^{-1} [\chi_{\partial D_j}] d\sigma, \quad i,j = 1,\ldots,N.$$

- $C^{\alpha}$ : Hermitian.
- Generalized quasiperiodic capacitance matrix

• For 
$$\alpha \neq 0$$
,  $C^{\alpha} = (C_{ii}^{\alpha}) \in \mathbb{C}^{N \times N}$ :

$$\mathcal{C}^{lpha}_{ij} = rac{\delta_i v_i^2}{|D_i|} C^{lpha}_{ij}, \quad i,j = 1, \ldots, N.$$

#### Resonances in the first radiation continuum

- Resonances in the first radiation continuum  $|\alpha| < k = \omega/\nu < \inf_{q \in \Lambda^* \setminus \{0\}} |\alpha + q|$ .
- For any  $\alpha_0 \in Y^*$  with  $|\alpha_0| < 1/v$ ,  $(S_D^{\omega \alpha_0, \omega})^{-1}$ : holomorphic operator-valued function of  $\omega$  in a neighbourhood of  $\omega = 0$ :

$$\left(\mathcal{S}_{D}^{\omega\alpha_{0},\omega}\right)^{-1}=\mathcal{S}_{0}^{\alpha_{0}}+\omega\mathcal{S}_{-1}^{\alpha_{0}}+\mathcal{O}(\omega^{2}) \text{ as } \omega\to0.$$

• Periodic capacitance matrix: For  $\alpha_0$  with  $|\alpha_0| < 1/v$ :

$$C^0 = (C_{ij}^0) \in \mathbb{R}^{N \times N}, \quad C_{ij}^0 = -\int_{\partial D_j} S_0^{\alpha_0} [\chi_{\partial D_i}] d\sigma.$$

- $C^0$ : independent of  $\alpha_0$ .
- Generalized periodic capacitance matrix:

$$C_{ij}^0 = rac{\delta_i v_i^2}{|D_i|} C_{ij}^0, \quad i,j = 1,\ldots,N.$$

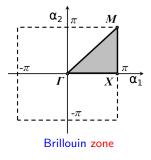
• Assume that  $\alpha = \omega \alpha_0$  for some  $\alpha_0$  independent of  $\omega$  and  $\delta$  such that  $|\alpha_0| < 1/\nu$ . As  $\delta \to 0$ , there are N subwavelength resonant frequencies

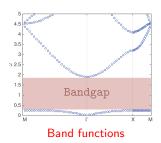
$$\omega_n^{lpha}=\sqrt{\lambda_n^0}+O(\delta),\quad n=1,\ldots,N,\quad \{\lambda_n^0\}: ext{ eigenvalues of } \mathcal{C}^0.$$



# Subwavelength bandgap opening

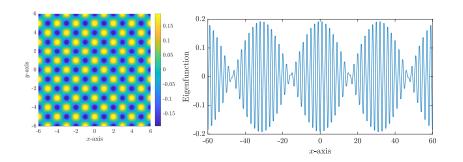
#### • Square crystal<sup>7</sup>:





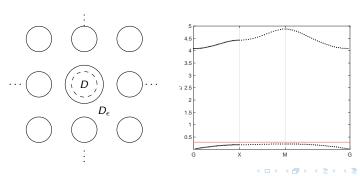
# Subwavelength bandgap opening

• Two-scale behaviour of the resonant mode of a square crystal for  $\alpha$  close to  $(\pi, \pi)$ : rapidly oscillating on the small scale, and a large scale envelope which satisfies a homogenized equation<sup>8</sup>.



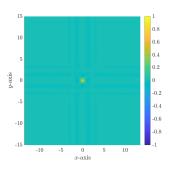
# Subwavelength defect modes

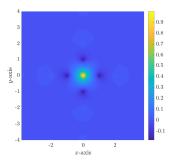
- Defect modes: Create a detuned resonator with an upward shifted resonance frequency (within the subwavelength band gap).
  - Weak interaction  $\Rightarrow$  decrease the radius of one resonator (from R to  $R + \epsilon$ ;  $\epsilon < 0$ );
  - Strong interaction ⇒ increase the radius of one resonator (from R to R + ε; ε > 0);
  - Shift at resonator radius = resonator separation.



# Subwavelength defect modes

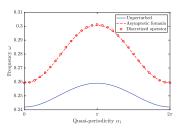
• Real part of the defect eigenmode:

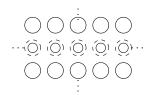


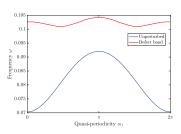


#### Subwavelength guided modes

- Line defect:<sup>9</sup>
- Defect band within the subwavelength band gap: large perturbation of the radius;
- Defect modes: localized to and guided along the line defect;
- Absence of bound modes.

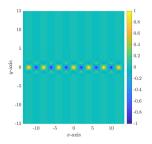


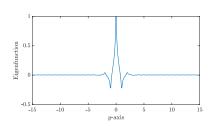




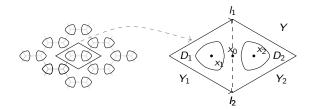
# Subwavelength guided modes

• Real part of the defect eigenmode for  $\alpha_1 = \pi/2$  in the dilute case. Each peak corresponds to one resonator, and the defect line is located at y=0:

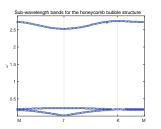


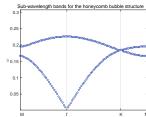


• Honeycomb lattice:



• Subwavelength band structure:





- At  $\alpha = \alpha^*$ , the first eigenfrequency  $\omega^* := \omega(\alpha^*)$  of multiplicity 2.
- Conical behavior of subwavelength bands  $^{10}$ : The first band and the second band form a Dirac cone at  $\alpha^*$ , i.e.,

$$\omega_1(\alpha) = \omega(\alpha^*) - \lambda |\alpha - \alpha^*| [1 + O(|\alpha - \alpha^*|)],$$
  

$$\omega_2(\alpha) = \omega(\alpha^*) + \lambda |\alpha - \alpha^*| [1 + O(|\alpha - \alpha^*|)];$$

 $\lambda = |c|\sqrt{\delta}\lambda_0 \neq 0$  for sufficiently small  $\delta$ .

• Dirac point at  $\alpha = \alpha^*$ .

Subwavelength resonator systems

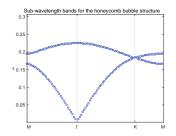
<sup>&</sup>lt;sup>10</sup>with B. Fitzpatrick, E.O. Hiltunen, H. Lee, S. Yu, SIAM J. Math. Anal., 2020.

• For  $\alpha$  close to  $\alpha^*$ , eigenmodes:

$$\tilde{u}_1(x)S_1(\frac{x}{5}) + \tilde{u}_2(x)S_2(\frac{x}{5}) + O(\delta + s);$$

• Effective equation:  $\tilde{u}_i$  satisfies

$$|c|^2 \lambda_0^2 \Delta \tilde{u}_j + \underbrace{\frac{(\omega - \omega^*)^2}{\delta}}_{\text{near zero}} \tilde{u}_j = 0.$$

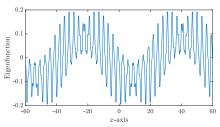


• Dirac equation:11

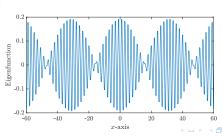
$$\lambda_0 \begin{bmatrix} 0 & (-ci)(\partial_1 - i\partial_2) \\ (-\overline{c}i)(\partial_1 + i\partial_2) & 0 \end{bmatrix} \begin{bmatrix} \tilde{u}_1 \\ \tilde{u}_2 \end{bmatrix} = \frac{\omega - \omega^*}{\sqrt{\delta}} \begin{bmatrix} \tilde{u}_1 \\ \tilde{u}_2 \end{bmatrix}.$$

- Single near-zero effective material property:  $1/\kappa$  near zero;
- Zero-phase shift propagation.

 One-dimensional plot along the x-axis of the real part of the Bloch eigenfunction of the honeycomb lattice shown over many unit cells:



• Square lattice:



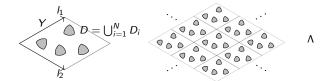
#### Periodic time-modulated systems

Wave equation in a periodic time-modulated structure:

$$\left(\frac{\partial}{\partial t}\frac{1}{\kappa(x,t)}\frac{\partial}{\partial t}-\nabla\cdot\frac{1}{\rho(x,t)}\nabla\right)u(x,t)=0,\quad x\in\mathbb{R}^d,t\in\mathbb{R}.$$

- Y: unit cell;  $\mathcal{D} = \bigcup_{m \in \Lambda} D + m$ ;  $\mathcal{D}_i = \bigcup_{m \in \Lambda} D_i + m$ ;  $D_i, i = 1, \dots, N$ .
- Time-modulation of the resonators:

$$\kappa(x,t) = \begin{cases} \kappa, & x \in \mathbb{R}^d \setminus \overline{\mathcal{D}}, \\ \kappa_r \kappa_i(t), & x \in \mathcal{D}_i, \end{cases}, \qquad \rho(x,t) = \begin{cases} \rho, & x \in \mathbb{R}^d \setminus \overline{\mathcal{D}}, \\ \rho_r \rho_i(t), & x \in \mathcal{D}_i. \end{cases}$$



#### Periodic time-modulated systems

Floquet transform in both x and t:

$$\begin{cases} \left(\frac{\partial}{\partial t} \frac{1}{\kappa(x,t)} \frac{\partial}{\partial t} - \nabla \cdot \frac{1}{\rho(x,t)} \nabla \right) u(x,t) = 0, \\ u(x,t) e^{-i\alpha \cdot x} \text{ is } \Lambda\text{-periodic in } x, \\ u(x,t) e^{-i\omega t} \text{ is } T\text{-periodic in } t. \end{cases}$$

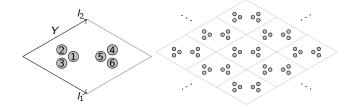
- Space-Brillouin zone:  $\alpha \in Y^* := \mathbb{R}^d / \Lambda^*$ ; Time-Brillouin zone:  $\omega \in Y^* := \mathbb{C}/(\Omega\mathbb{Z})$ ;  $\Omega = (2\pi)/T$ .
- As  $\delta \to 0$ , the quasifrequencies  $\omega = \omega(\alpha) \in Y_t^*$  are, to leading order, given by the quasifrequencies of the system of ordinary differential equations:

$$\sum_{j=1}^{N} \mathcal{C}_{ij}^{lpha} c_j(t) = -rac{1}{
ho_i(t)} rac{d}{dt} \left(rac{1}{\kappa_i(t)} rac{d(
ho_i c_i)}{dt}
ight),$$

for 
$$i = 1, ..., N$$
.  $(c_i(t) = e^{i\omega t} \sum_n c_{i,n} e^{in\Omega t})$ .

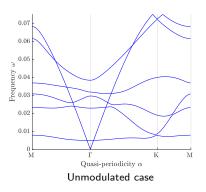
#### Trimer honeycomb lattice

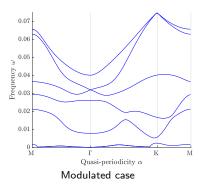
- Dirac cone degeneracy at Γ in trimer honeycomb lattice
- Fundamental domain Y now contains six resonators D<sub>i</sub>:



$$\begin{split} \bullet & \text{ Modulation given by } \kappa_i(t) = 1, \ i = 1, \ldots, 6 \text{ and } \\ & \rho_1(t) = \rho_4(t) = \frac{1}{1 + \varepsilon \cos(\Omega t)}, \quad \rho_2(t) = \rho_5(t) = \\ & \frac{1}{1 + \varepsilon \cos\left(\Omega t + \frac{2\pi}{3}\right)}, \quad \rho_3(t) = \rho_6(t) = \frac{1}{1 + \varepsilon \cos\left(\Omega t + \frac{4\pi}{3}\right)}, \text{ for } 0 \leq \varepsilon < 1. \end{split}$$

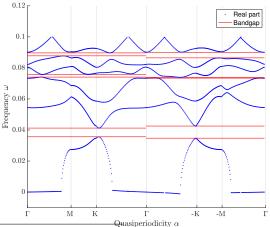
### Trimer honeycomb lattice





# Non-reciprocal wave propagation in time-modulated systems

• Band structure of honeycomb lattice with six subwavelength resonators with modulation frequency  $\Omega=0.2$  and  $\varepsilon=0.5^{12}$ :

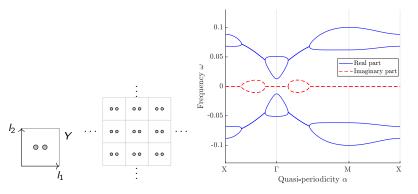


<sup>&</sup>lt;sup>12</sup>with J. Cao, E.O. Hiltunen, submitted, 2021.



#### Exceptional points in time-modulated systems

- Exceptional point degeneracy in square lattice of dimers<sup>13</sup>:
- $\bullet \ \ \rho_1(t) = \rho_2(t) = 1, \kappa_1(t) = \frac{1}{1 + \varepsilon \cos(\Omega t)}, \quad \kappa_2(t) = \frac{1}{1 + \varepsilon \cos(\Omega t + \pi)}, t \in \mathbb{R},$  for  $0 \le \varepsilon < 1$ .

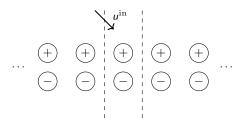


<sup>&</sup>lt;sup>13</sup>with E.O. Hiltunen, T. Kosche, submitted, 2021.



#### $\mathcal{PT}$ -symmetric screens

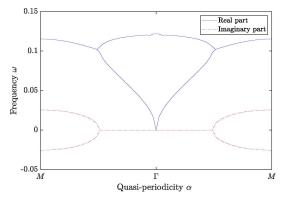
 Band structure and exceptional points of PT-symmetric screens (periodically repeated PT-symmetric dimers):



- $\omega_i^{\alpha} = \sqrt{\lambda_i^{\alpha}} + O(\delta), i = 1, 2;$  $\lambda_i^{\alpha} = \left(aC_{11}^{\alpha} \pm \sqrt{a^2|C_{12}^{\alpha}|^2 - b^2((C_{11}^{\alpha})^2 - |C_{12}^{\alpha}|^2)}\right)/|D_1|.$
- Exceptional point occurs when  $b=b_0(\alpha)=\frac{s|C_{12}^{\alpha}|}{\sqrt{(C_{11}^{\alpha})^2-|C_{12}^{\alpha}|^2}}.$
- Exceptional point depends both on the geometry and on the quasiperiodicity  $\alpha$ .

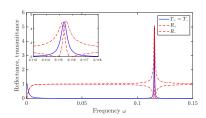
#### $\mathcal{PT}$ -symmetric screens

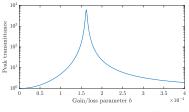
- Close to Γ, the system is always below the exceptional point.
- For larger  $\alpha$  and for large enough b, there is a point  $\alpha_0$  where  $b = b_0(\alpha_0)$ .
- For  $\alpha$  above  $\alpha_0$ , the band structure of the system has a non-zero imaginary part and the two bands are complex conjugate to each other.



#### $\mathcal{PT}$ -symmetric screens

- Unidirectional transmission: there is a frequency such that the screen's reflection
  coefficient is asymptotically close to zero when the incident wave is from one
  side and non-zero when the incident wave is from the other side of the screen.
- Critical frequency range: first radiation continuum  $|\alpha| < k = \omega/v < \inf_{q \in \Lambda^* \setminus \{0\}} |\alpha + q|$ .
- Extraordinarily high transmittance: for a critical gain/loss parameter b.
- Gain and loss allows the scattering matrix to be non-unitary and the reflectance and transmittance to exceed one.
- Compute explicit expressions for the subwavelength band structure close to the origin.



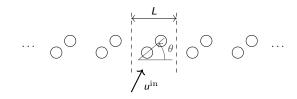


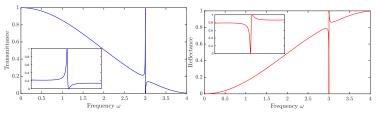
#### Bound states in the continuum and Fano resonances

- Subwavelength band structure close to the origin.
- Symmetric screen of dimers repeated periodically:
  - ω<sub>2</sub>: real and corresponds to an eigenvalue that is embedded within the continuous radiation spectrum, which is the spectrum of waves that can propagate into the far field.
  - Bound state in the continuum: eigenmode associated with this
    real-valued resonant frequency vanishes in the far field ⇒ it will not
    interact with incoming waves and the corresponding resonance peak
    will therefore not appear in the transmission spectrum.
- Symmetry broken: the real eigenvalue  $\omega_2$  will be shifted into the complex plane and the corresponding mode will be coupled to the far field.
- Design the system so that the two resonances interfere: ω<sub>1</sub> with large imaginary part.
- Derive an expression for the scattering matrix ⇒ demonstrate the occurrence of a Fano-type transmission anomaly<sup>14</sup>.
- Existence of asymmetric peaks in transmission spectra due to the interference between a "discrete state" and a "continuum".

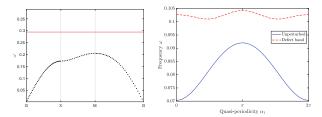
#### Bound states in the continuum and Fano resonances

• Resonators arranged in a symmetric dimer that is inclined at an angle of  $\theta$  to the plane of the screen.





- General principle for trapping and guiding waves at subwavelength scales: introduce a defect to a periodic arrangement of subwavelength resonators.
- Sensitivity to imperfections in the crystal's design:



- Goal: design subwavelength wave guides whose properties are robust with respect to imperfections.
- Idea: Topological invariant which captures the crystal's wave propagation properties.
- Topologically protected edge mode.

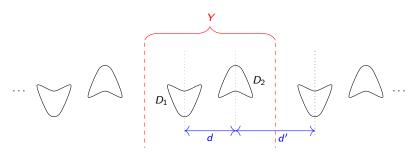
- Bulk-boundary correspondence:
  - Take two crystals with topologically different wave propagation properties (different values of the topological invariant);
  - Join half of crystal A to half of crystal B;
  - At the interface, a topologically protected edge mode will exist<sup>15</sup>.



Subwavelength resonator systems

<sup>15</sup>with B. Davies, E.O. Hiltunen, S. Yu, J. Math. Pures Appl., 2020. ★ ★ ★ ★ ★ ★ ★ ★ ◆ ◆ ◆ ◆ ◆

An infinite chain of resonator dimers: 16



Two assumptions of geometric symmetry:

- dimer is symmetric, in the sense that  $D(:=D_1 \cup D_2) = -D$ ,
- each resonator has reflective symmetry.

<sup>&</sup>lt;sup>16</sup> Analogue of the Su-Schrieffer-Heeger model in topological insulator theory in quantum mechanics.

• The Zak phase:

$$\varphi_n^z := \int_{Y^*} A_n(\alpha) \ d\alpha; \quad Y^* = \mathbb{R}/2\pi\mathbb{Z} \simeq (-\pi, \pi] \quad \text{(first Brillouin zone)};$$

• Berry-Simon connection:

$$A_n(\alpha) := i \int_D u_n^{\alpha} \frac{\partial}{\partial \alpha} \overline{u}_n^{\alpha} dx; \quad n = 1, 2.$$

• For any  $\alpha_1, \alpha_2 \in Y^*$ , parallel transport from  $\alpha_1$  to  $\alpha_2$  gives  $u_n^{\alpha_1} \mapsto e^{i\theta} u_n^{\alpha_2}$ , where  $\theta$  is given by

$$\theta = \int_{\alpha_1}^{\alpha_2} A_n d\alpha.$$

•  $\Rightarrow$  The Zak phase corresponds to parallel transport around the whole of  $Y^*$ .

- Quasi-periodic capacitance matrix:  $C = (C_{ij}^{\alpha})_{i,j=1,2}$ .
- The Zak phase is given by the change in the argument of  $C_{12}^{\alpha}$  as  $\alpha$  varies over the Brillouin zone:

$$\varphi_n^z = -\frac{1}{2} \left[ \operatorname{arg}(C_{12}^\alpha) \right]_{Y^*}.$$

• Further, it holds that

$$C_{12}^{\alpha'} = e^{-i\alpha} C_{12}^{\alpha}, \Rightarrow \text{if } d = d' \text{then } C_{12}^{\pi} = 0,$$

where the prime denotes that d and d' have been swapped.

• Thus,

$$|\varphi_n^{z\prime} - \varphi_n^z| = \pi,$$

i.e. the cases d > d' and d < d' have different Zak phases.

 Dilute computations: Assume that the dimer is a rescaling of fixed domains B<sub>1</sub> and B<sub>2</sub>:

$$D_1 = \epsilon B_1 - \left(\frac{d}{2},0,0\right), \quad D_2 = \epsilon B_2 + \left(\frac{d}{2},0,0\right),$$

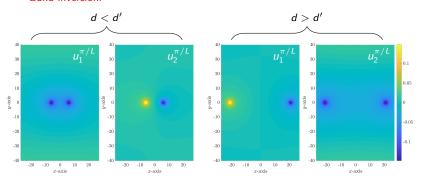
for  $0 < \epsilon$ .

• In the dilute regime, as  $\epsilon \to 0$ :

$$\varphi_n^z = \begin{cases} 0, & \text{if } d < d', \\ \pi, & \text{if } d > d', \end{cases}$$

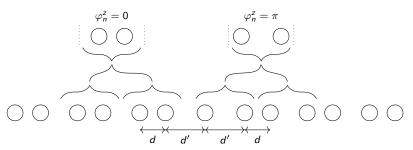
- There exists a band gap for all  $d \neq d'$ ,
- The dilute crystal has a degeneracy precisely when d = d'.
- The dispersion relation has a Dirac cone at  $\alpha = \pi$ .
- Band inversion occurs between d < d' and d > d'.

#### Band inversion:



The monopole/dipole natures of the  $1^{\rm st}$  and  $2^{\rm nd}$  eigenmodes have swapped between the d < d' and d > d' regimes.

A finite chain of resonators

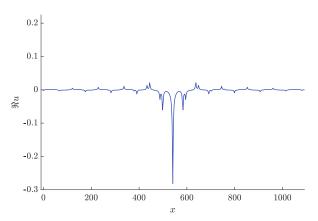


• Capacitance matrix of the finite chain  $D = \bigcup_{l=1}^{N} D_{l}$ :

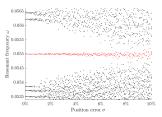
$$C = (C_{ij}), \quad C_{ij} := -\int_{\partial D_i} (\mathcal{S}_D)^{-1} [\chi_{\partial D_i}], \quad i,j = 1,\ldots, N.$$

 Odd number of resonators ⇒ odd number of eigenvalues; middle frequency: midgap frequency ⇒ robust to imperfections.

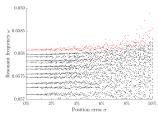
• Finite chain - localisation: There is a localized eigenmode



- Finite chain–stability to imperfections: Simulation of band gap frequency (red) and bulk frequencies (black) with Gaussian  $\mathcal{N}(0, \sigma^2)$  errors added to the resonator positions.  $\sigma$ : expressed as a percentage of the average resonator separation.
- Even for relatively small errors, the frequency associated with the point defect mode exhibits poor stability and is easily lost amongst the bulk frequencies.

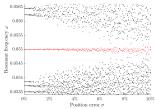


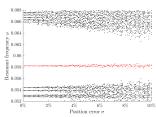
Finite chain with topological interface



Classical, point defect chain.

- Finite chain effect of diluteness.
- The variance of each frequency is consistent across both dilute and non-dilute regimes.
- In both the dilute and non-dilute regimes, the structure supports a localized mode whose resonant frequency is in the middle of the band gap.
- In the dilute regime, the nearest-neighborhood approximation,
   C<sub>ij</sub> = 0 if |i j| > 1 does not give an accurate approximation ⇒ significant difference between classical wave propagation problems and topological insulator theory in quantum mechanics.

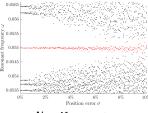




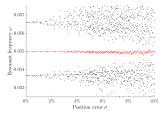
Dilute chain, d = 12, d' = 42, R = 1

Non-dilute chain, d = 3, d' = 6, R = 1

- Short finite chains: The stable mode exists also in very short chains of subwavelength resonators.
- With only 9 resonators, there is a midgap frequency which is much more stable than the bulk frequencies.



N = 41 resonators



N = 9 resonators

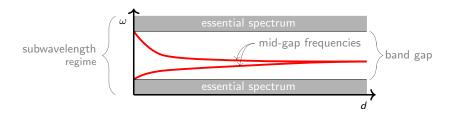
- A second approach for creating robust localized subwavelength modes <sup>17</sup>:
  - We start with an array of pairs of subwavelength resonators, known to have a subwavelength band gap. A dislocation (with size d>0) is introduced to create mid-gap frequencies.





<sup>&</sup>lt;sup>17</sup>with B. Davies, E.O. Hiltunen, submitted, 2020.

• As the dislocation size d increases from zero, a mid-gap frequency appears from each edge of the subwavelength band gap. These two frequencies converge to a single value within the subwavelength band gap as  $d \to \infty$ .



- Edge modes in the non-Hermitian case<sup>18</sup>:
  - Protected edge modes in crystals where the periodic geometry is intact, and a defect is placed in the parameters.
  - A topological winding number: the non-Hermitian Zak phase, which describes the winding of the complex eigenvalues.
  - Exceptional point degeneracies can open into non-trivial band gaps enabling topologically protected non-Hermitian edge modes.

$$m=-1$$
  $m=0$   $m=1$   $m=2$   $\cdots$   $\widehat{\kappa_1}$   $\widehat{\kappa_2}$   $\widehat{\kappa_1}$   $\widehat{\kappa_2}$   $\widehat{\kappa_1}$   $\cdots$   $\widehat{\kappa_2}$   $\widehat{\kappa_1}$   $\cdots$ 

<sup>&</sup>lt;sup>18</sup>with E.O. Hiltunen, submitted, 2020.

• Generalized quasiperiodic capacitance matrix:

$$\mathcal{C}^{lpha} = rac{1}{
ho |D_1|} egin{pmatrix} \kappa_1 \, \mathcal{C}_{11}^{lpha} & \kappa_1 \, \mathcal{C}_{12}^{lpha} \ \kappa_2 \, \mathcal{C}_{21}^{lpha} & \kappa_2 \, \mathcal{C}_{22}^{lpha} \end{pmatrix}.$$

• Eigenvalues  $\lambda_i^{\alpha}$  of  $\mathcal{C}^{\alpha}$ :

$$\lambda_j^{\alpha} = \frac{1}{\rho |D_1|} \left( C_{11}^{\alpha} \frac{\kappa_1 + \kappa_2}{2} + (-1)^j \sqrt{\left(\frac{\kappa_1 - \kappa_2}{2}\right)^2 (C_{11}^{\alpha})^2 + \kappa_1 \kappa_2 |C_{12}^{\alpha}|^2} \right).$$

- As  $\delta \to 0$ ,  $\omega_i^{\alpha} = \sqrt{\lambda_i^{\alpha}} + O(\delta)$ , i = 1, 2.
- Degeneracy to occur for small  $\delta$ :  $\lambda_1^{\alpha} = \lambda_2^{\alpha}$  at some  $\alpha \in Y^*$ .
- Non-Hermitian Zak phase:  $u_j^{\alpha}$ : right eigenmode;  $v_j^{\alpha}$ : left eigenmode corresponding to  $\overline{\omega_i^{\alpha}}$ ,

$$\varphi_j^{\mathrm{zak}} := \frac{i}{2} \int_{Y^*} \left( \left\langle v_j^{\alpha}, \frac{\partial u_j^{\alpha}}{\partial \alpha} \right\rangle + \left\langle u_j^{\alpha}, \frac{\partial v_j^{\alpha}}{\partial \alpha} \right\rangle \right) d\alpha.$$

Hermitian counterpart of the structure is topologically trivial:

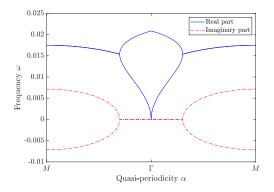
$$\varphi_j^{\mathrm{zak}}(\mathrm{Re}(\kappa_1),\mathrm{Re}(\kappa_2))=0.$$

• =

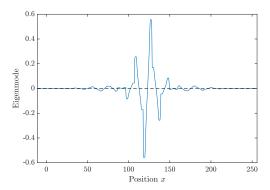
$$\varphi_j^{\mathrm{zak}}(\kappa_1,\kappa_2) = -\varphi_j^{\mathrm{zak}}(\kappa_2,\kappa_1) + \textit{O}(\delta), \quad \varphi_j^{\mathrm{zak}}(\overline{\kappa_1},\overline{\kappa_2}) = \varphi_j^{\mathrm{zak}}(\kappa_1,\kappa_2) + \textit{O}(\delta).$$

- $\Rightarrow$  If  $\kappa_1 = \overline{\kappa_2} := \kappa$ ,  $\varphi_j^{\mathbf{zak}}(\kappa, \overline{\kappa}) = O(\delta)$ .
- Degeneracy occurs when  $\kappa_1 = \overline{\kappa_2} = \kappa$  for sufficiently large  $\kappa$ :
  - $\beta_1 = C_{11}^{\pi} + C_{12}^{\pi}$ ,  $\beta_2 = 2C_{11}^0$ ;  $I = (\beta_1 + \beta_2)/(\beta_2 \beta_1)$ .
  - If  $\kappa_1 = \overline{\kappa_2} := \kappa$  with  $|\mathrm{Im}(\kappa)| \leq \frac{\mathrm{Re}(\kappa)}{\sqrt{\ell^2 1}}$  (unbroken  $\mathcal{PT}$ -symmetry), the structure does not support localized modes in the subwavelength regime.
  - If  $\kappa_1 = \overline{\kappa_2} := \kappa$  with  $|\mathrm{Im}(\kappa)| > \frac{\mathrm{Re}(\kappa)}{\sqrt{\ell^2 1}}$  (broken  $\mathcal{PT}$ -symmetry) or if  $\kappa_1 \neq \overline{\kappa_2}$  (no  $\mathcal{PT}$ -symmetry): characterization of the localized mode in the subwavelength regime.

- Non-Hermitian Zak phase: not quantized but can nevertheless predict the
  existence of localized edge modes. Edge modes can be achieved by swapping κ<sub>1</sub>
  and κ<sub>2</sub> while keeping the distance between the resonators fixed.
- Purely non-Hermitian effect: as  ${\rm Im}\kappa_1$  and  ${\rm Im}\kappa_2 \to 0$ , the effect disappears.



• Edge mode in a non-Hermitian system:



### Concluding remarks

- Mathematical and numerical framework for subwavelength wave physics: focus, guide, manipulate, and control waves at subwavelength scales.
- Quantitative explanation of the mechanisms behind the spectacular properties exhibited by subwavelength resonators in recent physical experiments.
- Non-Hermitian subwavelength resonators: existence and implications of exceptional points; non-quantized topological invariants to predict the existence of edge modes.
- Time-modulated subwavelength resonators: conceptually similar properties can arise, which nevertheless have fundamentally different physical implications.
- Avenue for understanding the topological properties of non-hermitian and time-modulated systems of subwavelength resonators.

# Concluding remarks

Classical wave problems	Quantum mechanics
PDE model	Hamiltonian
Capacitance matrix:	
discrete approximation of the differential problem	
resonant frequencies & resonant modes	
Dilute regime:	Tight-binding model:
approximation of the capacitance matrix	Hamiltonian: small correction to
	sum of Hamiltonians of single
	isolated atoms
Not accurate: slow decay of the off-diagonal	Nearest-neighborhood approximation:
terms of the capacitance matrix	Tridiagonal tight-binding matrix