Complex Band Structures in the Spectral Theory of Toeplitz Operators and Applications to Metamaterials

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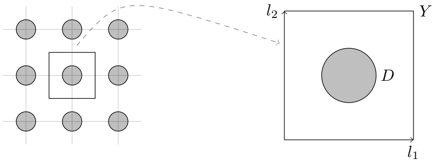
Floquet-Bloch Theory

- **Benefit:**
  - Reduce periodic structure to one unit cell.



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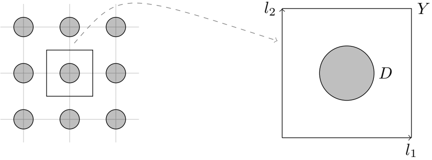
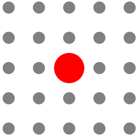
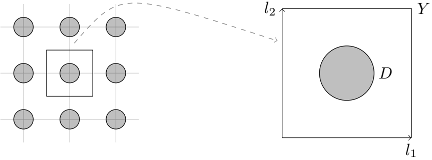
  - Finite systems.
  - Defected systems.

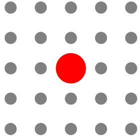




Floquet-Bloch Theory

- **Benefit:**
  - Reduce periodic structure to one unit cell.
- **Downside:**
  - Finite systems.
  - Defected systems.
- **Solution:**
  - Introduce Complex Floquet conditions.
  - Capture quantitative localisation behaviour.





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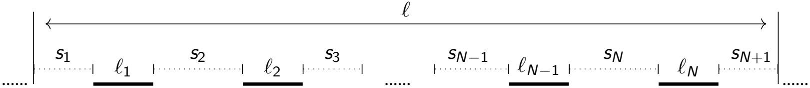
One Dimensional non-Hermitian Helmholtz scattering

- **Model setting:**



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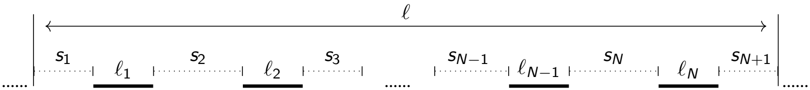


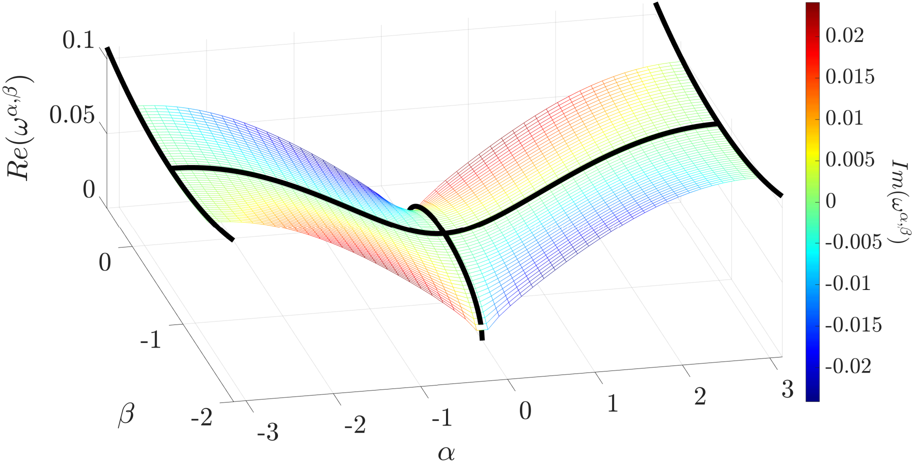
- **Wave equation:**

$$
\begin{cases}
u''(x) + \gamma u'(x) + \omega^2 u(x) = 0, & x \in D \\
u''(x) + \omega^2 u(x) = 0, & x \in \mathbb{R}\backslash D, \\
u|_+ - u|_- = 0, & \text{on } \partial D, \\
\left.\frac{\partial u}{\partial \nu}\right|_- - \delta \left.\frac{\partial u}{\partial \nu}\right|_+ = 0, & \text{on } \partial D \\
u(x+\ell) = e^{\mathrm{i}(\alpha + \mathrm{i}\beta)\ell} u(x), & \text{for all } \ell \in \Lambda,
\end{cases}
$$

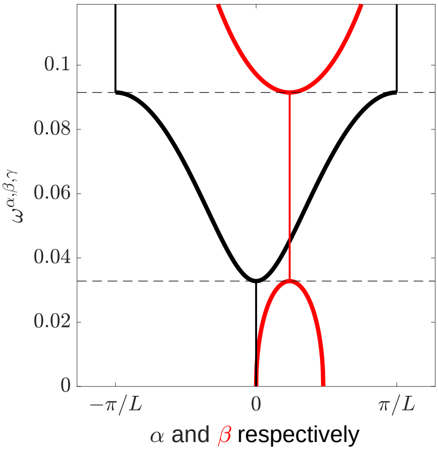
where

- Imaginary gauge potential $\gamma \in \mathbb{R} \setminus \{0\}$.
- Contrast parameter $0 < \delta \ll 1$.

Complex Band structure for Monomer chain



Projected visualisation



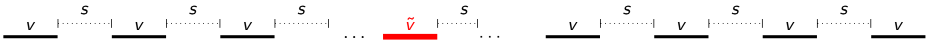
In the Spectrum:

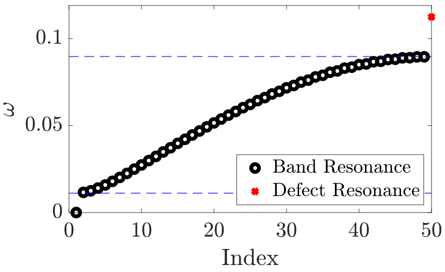
- β is fixed
- $\alpha \in Y^*$

In the Bandgap:

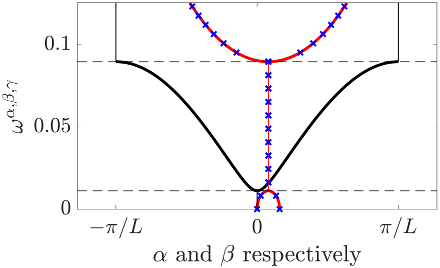
- $\beta \in \mathbb{R}$
- $\alpha \in \{0, \pm\pi/L\}$

- **Changed wave speed:**



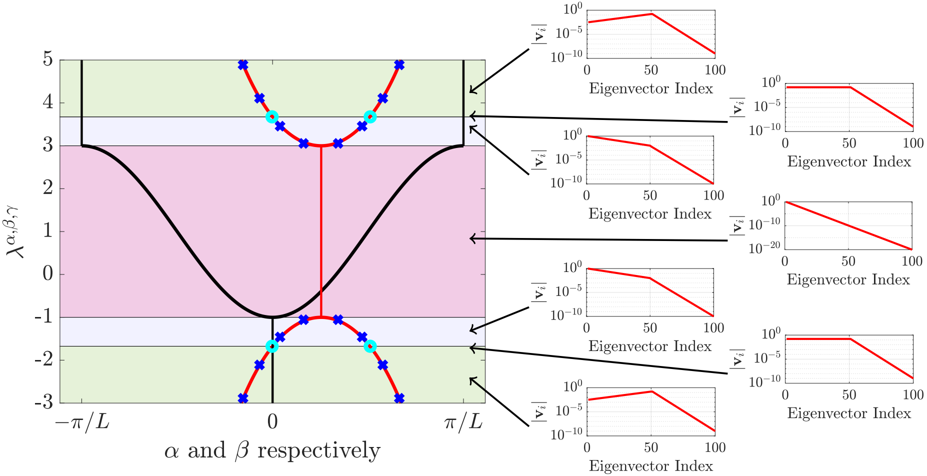


(a) Resonances

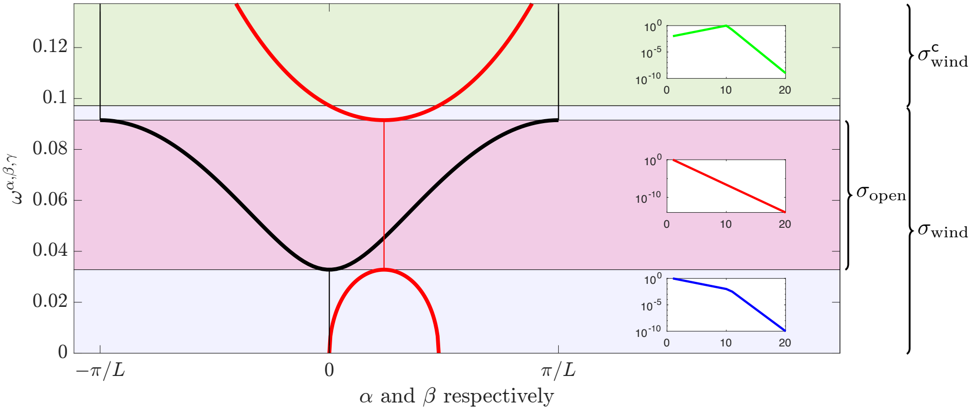


(b) Exponential decay vs Complex band structure

Defect-Induced Localization Transitions



Topological properties



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Tridiagonal k-Toeplitz operators.

Example: 2-Toeplitz operator

$$\mathbf{T}(\mathbf{f}) := \begin{pmatrix} a_1 & b_1 & 0 & 0 & & & \\ c_1 & a_2 & b_2 & 0 & & & \\ 0 & c_2 & a_1 & b_1 & 0 & 0 & \\ 0 & 0 & c_1 & a_2 & b_2 & 0 & \\ & & 0 & c_k & \ddots & & \ddots \\ & & 0 & 0 & & & \\ & & & & \ddots & & \end{pmatrix} = \begin{pmatrix} \mathbf{A}_0 & \mathbf{A}_{-1} & & \\ \mathbf{A}_1 & \mathbf{A}_0 & \mathbf{A}_{-1} & \\ & \mathbf{A}_1 & \ddots & \ddots \\ & & \ddots & \end{pmatrix}$$

- **Symbol function:**

$$f : \mathbb{C} \to \mathbb{C}^{2\times 2}$$

$$z \mapsto \mathbf{A}_{-1} z^{-1} + \mathbf{A}_0 + \mathbf{A}_1 z = \begin{pmatrix} a_1 & b_1 + c_2 z \\ c_1 + b_2 z^{-1} & a_2 \end{pmatrix}.$$

Spectrum of k-Toeplitz operators

- Let us define the sets:

$$\sigma_{\det}(f) := \left\{\lambda \in \mathbb{C} : \det\big(f(z) - \lambda\big) = 0,\ \exists z \in \mathbb{T}\right\},$$
$$\sigma_{\text{wind}}(f) := \left\{\lambda \in \mathbb{C} \setminus \sigma_{\det}(f) : \text{wind}\big(\det\big(f(\mathbb{T}) - \lambda\big), 0\big) \neq 0\right\}.$$

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Theorem (dB, Ammari, Liu, Thalhammer)

Let $f \in \mathbb{C}^{k\times k}(\mathbb{T})$ be the symbol of a tridiagonal k-Toeplitz operator $T(f)$ it holds that

$$\sigma_{\mathrm{det}}(f) \cup \sigma_{\mathrm{wind}}(f) \subseteq \sigma\big(T(f)\big) \subseteq \sigma_{\mathrm{det}}(f) \cup \sigma_{\mathrm{wind}}(f) \cup \sigma(B_0).$$

Similarity transform and eigenvector estimate

- Tridiagonal k-Toeplitz operators are *similar to symmetric* matrices $\implies$ real spectrum.

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- Let $\tilde{f}$ symbol of symmetrised operator.
  - $\sigma_{\text{det}}(\tilde{f}) = \{\lambda \in \mathbb{R} \mid 2Ae^r \cos(\alpha) \cosh(\beta - r) + g(\lambda) = 0\}$.
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Lemma (dB, Hiltunen)

Let $\lambda \in \mathbb{R}$ be an eigenfrequency, such that $\mathbf{T}(f)\mathbf{u} = \lambda\mathbf{u}$ then

$$\frac{|\mathbf{u}^{(i+k)}|}{|\mathbf{u}^{(i)}|} = \mathcal{O}\left(e^{-(r-\tilde{\beta})}\right),$$

where $r = \frac{1}{2}\log\left(\prod_{i=1}^{k}\frac{b_i}{c_i}\right)$ is fixed and $\tilde{\beta}(\lambda) = \operatorname{arccosh}\left(-\frac{g(\lambda)}{2Ae^r}\right)$, for $A = (-1)^{k+1}\prod_{i=1}^{k} c_i$, and $g(\lambda)$ a known polynomial.

Pseudospectra

- **Question:**
  - Why is the Complex Band Structure valid for finite media?

Definition

λ is ε-pseudoeigenvalue of $\mathbf{A}$ with ε-pseudoeigenvector if,

$$\|(\mathbf{A} - \lambda)\mathbf{u}\| < \varepsilon \text{ for some vector } u \text{ with } \|\mathbf{u}\| = 1.$$

- **Finite vs semi-infinite systems:**
  - Truncated eigenvectors of a semi-infinite system become ε_N-pseudoeigenvectors in the finite system

$$\varepsilon_N = e^{-\beta(\lambda)N}.$$

- **Conclusion:**
  - Exponentially localised mode insensitive to boundary conditions.

Possible Applications

- Disordered/random media systems.
- Topologically protected/edge interface modes (SSH chain).
- Defected materials.
- Wave guiding.
- Invisible Tunnelling.

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Two-Dimensional Crystal

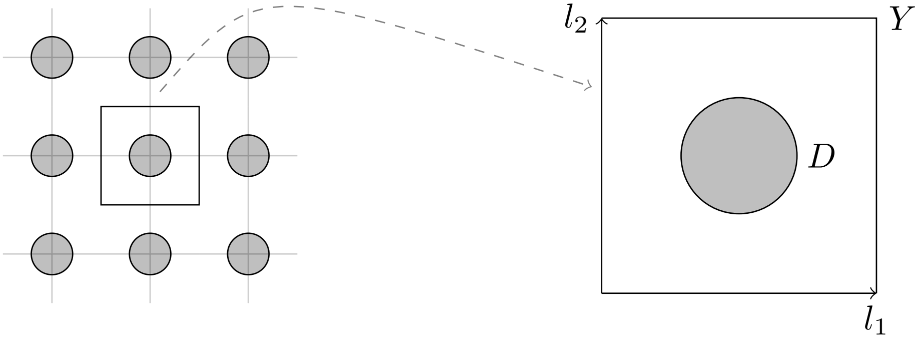

Figure: Square lattice with a single resonator inside the unit cell ($N = 1$).

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Bandgap Green's function

- Two-dimensional Helmholtz problem

$$\begin{cases} \Delta u + k^2 u = 0, & \text{in } Y \setminus \overline{D}, \\ \Delta u + k_i^2 u = 0, & \text{in } D_i, \\ u|_+ - u|_- = 0, & \text{on } \partial D, \\ \left.\dfrac{\partial u}{\partial \nu}\right|_- - \delta \left.\dfrac{\partial u}{\partial \nu}\right|_+ = 0, & \text{on } \partial D, \\ u(x+\ell) = e^{\mathrm{i}(\alpha + \mathrm{i}\beta)\cdot \ell} u(x), & \text{for all } \ell \in \Lambda. \end{cases}$$

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- For a real quasimomentum ($\beta = 0$), the α-quasiperiodic Green's function $G^{\alpha,k}$ satisfies

$$\Delta G^{\alpha,k}(x) + k^2 G^{\alpha,k}(x) = \sum_{m \in \Lambda} \delta(x - m) e^{\mathrm{i}\alpha \cdot m},$$

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and is given by

$$G^{\alpha,k}(x) = \frac{1}{|Y|} \sum_{q \in \Lambda^*} \frac{e^{\mathrm{i}(\alpha+q)\cdot x}}{k^2 - |\alpha + q|^2}.$$

Generalised Green's function

- Change of function,

$$v(x) := e^{\beta \cdot x} u(x), \quad \beta \in \mathbb{R}^2.$$

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- v satisfies the real Floquet-Condition.
- The band gap Green's function satisfies
$$\Delta\tilde{G}^{\alpha,\beta,k}(x) - 2\beta\cdot\nabla\tilde{G}^{\alpha,\beta,k}(x) + (k^2+|\beta|^2)\tilde{G}^{\alpha,\beta,k}(x) = \sum_{m\in\Lambda} e^{\mathrm{i}\alpha\cdot m}\delta(x-m).$$

Generalised Green's function

- Poisson summation formula,

$$\tilde{G}^{\alpha,\beta,k}(x) = \frac{1}{|Y|} \sum_{q \in \Lambda^*} \frac{e^{\mathrm{i}(\alpha+q)\cdot x}}{k^2 + |\beta|^2 - 2\mathrm{i}\beta \cdot (\alpha + q) - |\alpha + q|^2}.$$

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- **Computational Bottleneck:** $\tilde{G}^{\alpha,\beta,k}(x)$ is only conditionally convergent.
- **Solution:** Accelerated lattice sum methods have been introduced.

Layer Potential Techniques

- Let $D \subset Y$ be a domain in $\mathbb{R}^2$ with a boundary $\partial D \in C^{1,s}$, with some $0 < s < 1$.

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$$\tilde{\mathcal{S}}_{D_i}^{\alpha,\beta,k} : L^2(\partial D) \rightarrow H^1(\partial D)$$
$$\phi \mapsto \tilde{\mathcal{S}}_{D}^{\alpha,\beta,k}[\phi](x) = \int_{\partial D} \tilde{G}^{\alpha,\beta,k}(x-y)\phi(y)\mathrm{d}\sigma(y), \quad x \in \mathbb{R}^2.$$

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- Field solution

$$v(x) = \begin{cases} \tilde{\mathcal{S}}_{D}^{\alpha,\beta,k}[\phi](x), & \text{in } Y \setminus \overline{D}, \\ \tilde{\mathcal{S}}_{D_i}^{\alpha,\beta,k_i}[\psi](x), & \text{in } D_i, \end{cases} \qquad \text{and unknown } \phi, \psi \in L^2(\partial D).$$

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- Gap mode

$$u(x) = e^{-\beta\cdot x} v(x).$$

Quasiperiodic Capacitance

Subwavelength Regime:

- High contrast low frequency regime $\implies$ asymptotic expansion of resonances.
- Let $0 < \frac{\rho_1}{\rho_0} = \delta \ll 1$ such that $\omega(\delta) \xrightarrow{\delta \to 0} 0$.

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- High contrast low frequency regime $\Longrightarrow$ asymptotic expansion of resonances.
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Theorem (dB & Hiltunen)

Consider a system of N subwavelength resonators in the unit cell Y and assume $\tilde{G}^{\alpha,\beta,k}(x)$ is well-defined and $\tilde{\mathcal{S}}_D^{\alpha,\beta,0}$ is invertible. As $\delta \to 0$, the subwavelength resonant frequencies $\omega_n^{\alpha,\beta}$ satisfy the asymptotic formula

$$\omega^{\alpha,\beta} = \sqrt{\delta \lambda_n^{\alpha,\beta}} + \mathcal{O}(\delta), \quad n = 1, \dots, N,$$

where $\{\lambda_n^{\alpha,\beta}\}$ are the N eigenvalues of the generalised capacitance matrix $\mathcal{C}^{\alpha,\beta} \in \mathbb{C}^{N\times N}$, given by

$$\mathcal{C}_{ij}^{\alpha,\beta} = -\frac{v_i^2}{|D_i|} \int_{D_i} e^{-\mathrm{i}\beta\cdot x} \psi_j \mathrm{d}\sigma, \quad \psi_i = (\tilde{\mathcal{S}}_D^{\alpha,\beta,0})^{-1}[e^{\beta\cdot x}\chi_{\partial D_i}].$$

Spectral Plot and complex Band Functions

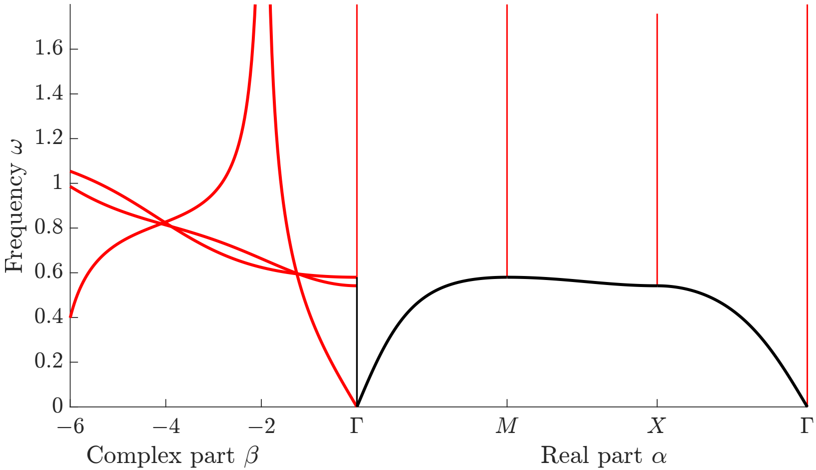

Figure: Generate the spectral plot in 0.5s and an expected error of $\mathcal{O}(10^{-3})$.

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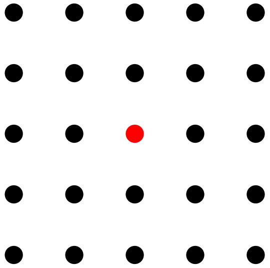
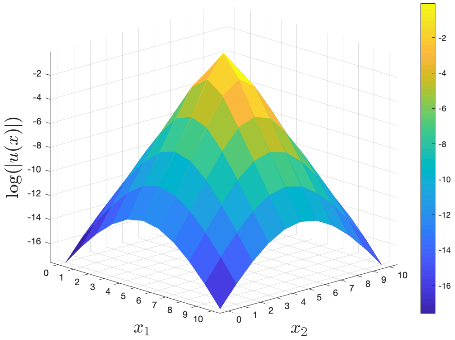
2D defect modes



(a) Truncated infinite defected resonator lattice.



(b) Defect eigenmode.

Defect Modes and Spectral Plot

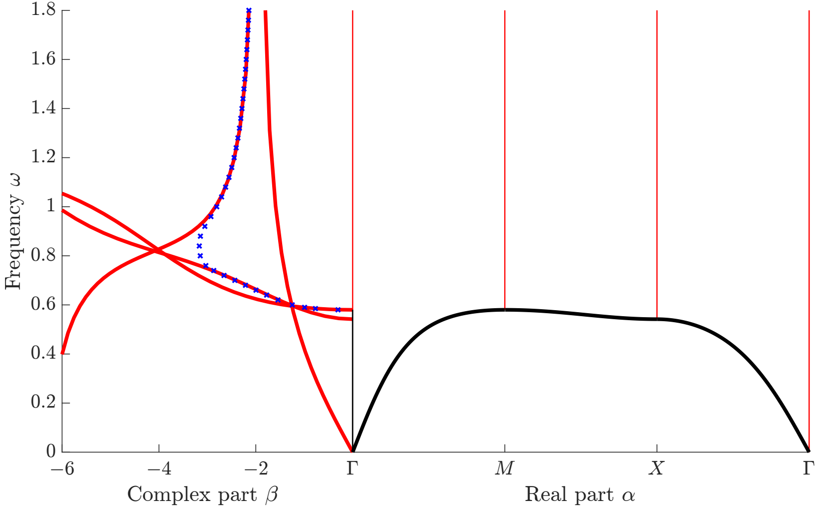


Figure: Decay for β horizontal ($\rightarrow$).

Complex Floquet transform

Theorem (dB & Hiltunen)

Let u be a complex Bloch mode for some $\beta \in \mathbb{R}^n \setminus \{0\}$, i.e.,

$$\left|u(x+\ell)\right| = e^{\beta\cdot\ell}\left|u(x)\right|, \quad \forall \ell \in \Lambda.$$

Then the complex Floquet transform is well-defined and given by,

$$u(x) \mapsto \mathcal{U}_\Lambda\left[u(x, \alpha + \mathrm{i}\beta)\right] := \sum_{\ell\in\Lambda} u(x-\ell)e^{\mathrm{i}(\alpha+\mathrm{i}\beta)\cdot\ell}.$$

Truncated complex Floquet transform

- Defect mode $\mathbf{u}_m$, with decay length $\tilde{\beta}$.

Truncated complex Floquet transform

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- Finite lattice Λ_t,

$$\|(\hat{u})_{\alpha,\tilde{\beta}}\|_2 := \left\| \sum_{m\in\Lambda_t} \mathbf{u}_m e^{\mathrm{i}(\alpha+\mathrm{i}\tilde{\beta})\cdot m} \right\|_2 .$$

Truncated complex Floquet transform

- Defect mode $\mathbf{u}_m$, with decay length $\tilde{\beta}$.
- Finite lattice Λ_t,

$$\|(\hat{u})_{\alpha,\tilde{\beta}}\|_2 := \left\| \sum_{m\in\Lambda_t} \mathbf{u}_m e^{\mathrm{i}(\alpha+\mathrm{i}\tilde{\beta})\cdot m} \right\|_2 .$$

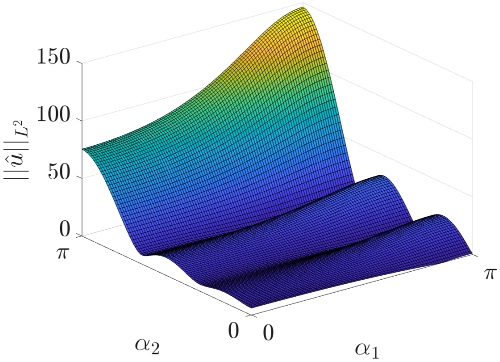


Figure: $\|(\hat{u})_{\alpha,\tilde{\beta}}\|_2$ at gap frequency $\omega = 0.6$.

Truncated complex Floquet transform

- Defect mode $\mathbf{u}_m$, with decay length $\tilde{\beta}$.
- Finite lattice Λ_t,

$$\|(\hat{u})_{\alpha,\tilde{\beta}}\|_2 := \left\| \sum_{m\in\Lambda_t} \mathbf{u}_m e^{\mathrm{i}(\alpha+\mathrm{i}\tilde{\beta})\cdot m} \right\|_2 .$$

- $\|(\hat{u})_{\alpha,\tilde{\beta}}\|_2$ has distinct peaks,

$$\alpha = \max_{\alpha\in Y^*} \|(\hat{u})_{\alpha,\tilde{\beta}}\|_2 .$$

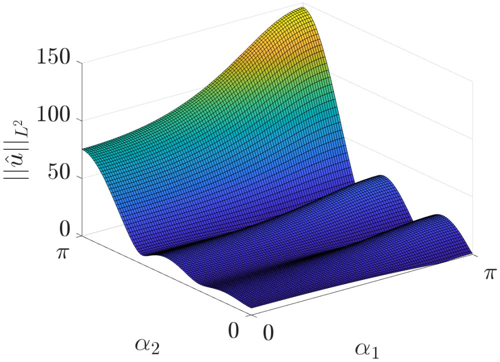
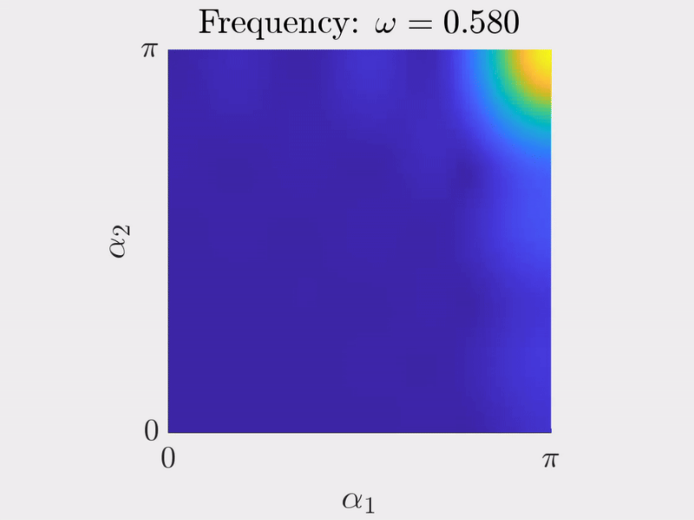
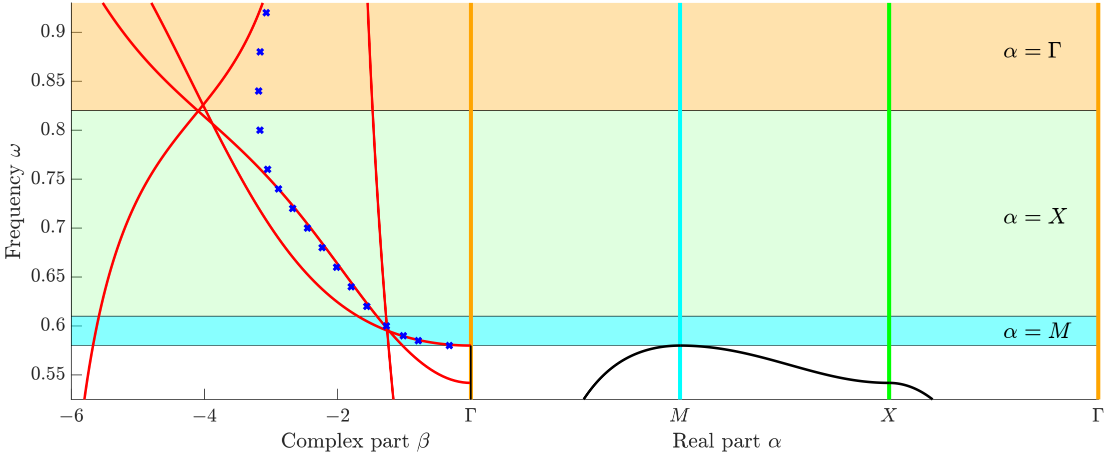


Figure: $\|(\hat{u})_{\alpha,\tilde{\beta}}\|_2$ at gap frequency $\omega = 0.6$.

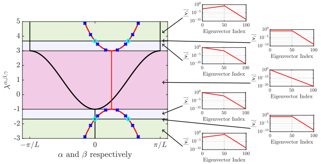
Phase-shift within the Band Gap



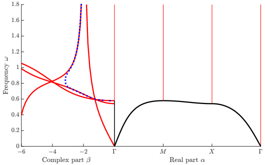
3 Phase-shift zones



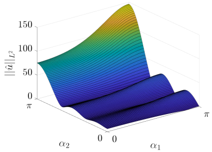
Questions?



(a) 1D Decay Transition.



(b) 2D Spectral Plot.



(c) Floquet Transform.

References and Code availability:

[1] dB, Ammari, Thalhammer, Liu, Barandun: *Spectra and pseudo-spectra of tridiagonal k-Toeplitz matrices and the topological origin of the non-Hermitian skin effect* 10.1088/1751-8121/add5ab
[2] dB, Hiltunen: *Complex Band Structure for Subwavelength Evanescent Waves* 10.1111/sapm.70022
[3] dB, Hiltunen: *Complex Brillouin Zone for Localised Modes in Hermitian and Non-Hermitian Problem* arXiv.2502.06620
[4] dB, Hiltunen: *Complex Band Structure and localisation transition for tridiagonal non-Hermitian k-Toeplitz operators with defects* arXiv.2505.23610
[5] dB, Hiltunen: *Github: PhotonicBandGaps* github.com/yannick2305/PhotonicBandGaps
[6] dB, Hiltunen: *Github: Non-Hermitian Localisation* github.com/yannick2305/Non-Hermitian-Localisation

Contact: yannicd@math.uio.no

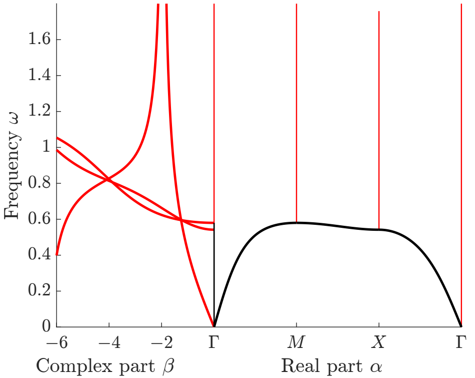
What does the spectral Plot mean?

- Band formulation, i.e. $\beta = 0$,

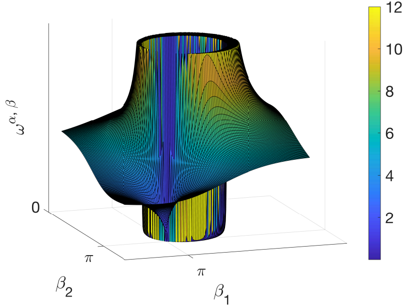
$$\begin{cases} \Delta u + k^2 u = 0, & \text{in } Y \setminus \overline{D}, \\ \Delta u + k_i^2 u = 0, & \text{in } D_i, \\ u|_+ - u|_- = 0, & \text{on } \partial D, \\ \left.\frac{\partial u}{\partial \nu}\right|_- - \delta \left.\frac{\partial u}{\partial \nu}\right|_+ = 0, & \text{on } \partial D, \\ u(x+\ell) = e^{\mathrm{i}(\alpha + \mathrm{i}\beta)\cdot \ell} u(x), & \text{for all } \ell \in \Lambda. \end{cases}$$

- Gap formulation i.e. $\beta \neq 0$, set $v(x) := e^{\beta \cdot x} u(x)$,

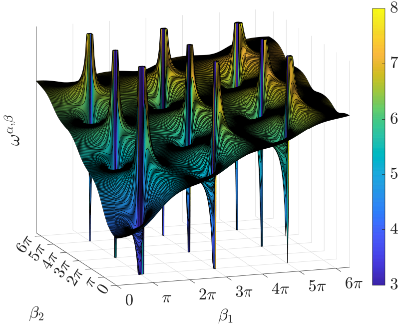
$$\begin{cases} \Delta v - 2\beta \cdot \nabla v + (k^2 + |\beta|^2) v = 0, & \text{in } Y \setminus \overline{D}, \\ \Delta v - 2\beta \cdot \nabla v + (k_i^2 + |\beta|^2) v = 0, & \text{in } D_i, \\ v|_+ - v|_- = 0, & \text{on } \partial D, \\ \left.\frac{\partial v}{\partial \nu}\right|_- - (\beta \cdot \nu) v - \delta \left(\left.\frac{\partial v}{\partial \nu}\right|_+ - (\beta \cdot \nu) v \right) = 0, & \text{on } \partial D, \\ v(x+\ell) = e^{\mathrm{i}\alpha \cdot \ell} v(x), & \text{for all } \ell \in \Lambda. \end{cases}$$



Motivation: Singularities in the Band functions



(d) Close View.



(e) Wide View.

Figure: Band function $\omega^{\alpha,\beta}$ for fixed $\alpha = [\pi, \pi]$ and Resonator radius $R = 0.005$.