



# Wave interaction of subwavelength resonators in one dimension

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## Outline

1. Motivation

- 2. Problem Formulation
- 3. Numerical Solution and Approximation
- 4. Conclusion & Outlook



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## Motivation

- Goal: Focus, trap, guide, manipulate and control waves at subwavelength scales.
- Why 1D?
  - Explicit calculations are possible;
  - Only neighboring resonators interact with each other;
  - Analogies with quantum mechanical phenomena (tight-binding approximation for quantum systems) ⇒ connects the field of high-contrast metamaterials to condensed-matter theory.
- Why time-modulated?
  - Formation of k-gaps;
  - Many wave operations such as signal amplification/compression, spacetime cloaking, ...
- Applications: Wireless communications, biomedical superresolution imaging, quantum computing.
- Tools: PDE model, capacitance matrix



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#### Problem Formulation Geometric Setup

- Subwavelength resonators: Objects exhibiting resonant phenomena in response to wavelengths much greater than their size. Subwavelength = size of resonators is much smaller than the operating wavelength.
- Unit cell: An interval Y := (0, L) containing N resonators D<sub>i</sub> := (x<sub>i</sub><sup>-</sup>, x<sub>i</sub><sup>+</sup>), ∀i = 1,..., N, each of length ℓ<sub>i</sub> and spacing ℓ<sub>i(i+1)</sub> between D<sub>i</sub> and D<sub>i+1</sub>.
- Infinite system: Infinitely many contiguous unit cells covering  $\mathbb{R}$ , the regime taken up by the resonators is denoted by  $D + L\mathbb{Z} := \{x + kL : x \in D, k \in \mathbb{Z}\}$ , where  $D := \bigcup_{i=1}^{N} D_i$ .





#### Problem Formulation Material Parameters

• Time-dependency: Periodic in x with period L and in t with period  $T := 2\pi/\Omega$ , given by

$$\kappa(x,t) = \begin{cases} \kappa_0, & x \notin D, \\ \kappa_r \kappa_i(t), & x \in D_i, \end{cases} \quad \frac{1}{\kappa_i(t)} = \sum_{n=-M}^M k_{i,n} e^{in\Omega t},$$
$$\rho(x,t) = \begin{cases} \rho_0, & x \notin D, \\ \rho_r \rho_i(t), & x \in D_i, \end{cases} \quad \frac{1}{\rho_i(t)} = \sum_{n=-M}^M r_{i,n} e^{in\Omega t}.$$

- High contrast assumption:  $\delta := \rho_r / \rho_0 \ll 1$ .
- Wave speed:  $v_0 := \sqrt{\kappa_0/\rho_0}$  outside D and  $v_r := \sqrt{\kappa_r/\rho_r}$  inside D.
- Difficulty: Folding of resonant frequencies into the first Brillouin zone in time. ⇒ Only consider resonant frequencies corresponding to eigenmodes essentially supported in the subwavelength regime. ⇒ subwavelength quasifrequencies

## Problem Formulation Goal

• Goal: For  $\Omega = O(\delta^{1/2})$  find  $\omega = O(\delta^{1/2})$  s.t.

$$\begin{cases} \left(\frac{\partial}{\partial t}\frac{1}{\kappa(x,t)}\frac{\partial}{\partial t} - \frac{\partial}{\partial x}\frac{1}{\rho(x,t)}\frac{\partial}{\partial x}\right)u(x,t) = 0, \quad x \in \mathbb{R}, \ t \in \mathbb{R}, \\ u(x,t)\mathrm{e}^{-\mathrm{i}\omega t} \text{ is } T-\mathrm{periodic}, \\ u(x,t)\mathrm{e}^{-\mathrm{i}\alpha x} \text{ is } L-\mathrm{periodic}, \end{cases}$$

has a non-trivial solution u(x, t).



#### Problem Formulation Governing Equations

• Fourier expansion + Floquet-Bloch in time domain + superposition of Bloch waves:

 $u(x,t) = e^{i\omega t} \sum_{n=-\infty}^{\infty} \int_{-\pi/L}^{\pi/L} \hat{v}_n(x,\alpha) e^{i\alpha x} d\alpha e^{in\Omega t}$ , where  $\alpha$  is the momentum.

• Coupled Helmholtz equations: Find  $v_n(x, \alpha) := \hat{v}_n(x, \alpha) e^{i\alpha x}$  s.t.

$$\begin{cases} \frac{\mathrm{d}^2}{\mathrm{d}x^2} v_n + \frac{\rho_0(\omega + n\Omega)^2}{\kappa_0} v_n = 0 & \text{ in } (0, L) \setminus D, \\ \frac{\mathrm{d}^2}{\mathrm{d}x^2} v_{i,n}^* + \frac{\rho_r(\omega + n\Omega)^2}{\kappa_r} v_{i,n}^{**} = 0 & \text{ in } D_i, \\ v_n|_- \left(x_i^{\pm}\right) = v_n|_+ \left(x_i^{\pm}\right) & \text{ for all } 1 \le i \le N, \\ \frac{\mathrm{d}v_{i,n}^*}{\mathrm{d}x}\Big|_{\pm} \left(x_i^{\mp}\right) = \delta \frac{\mathrm{d}v_n}{\mathrm{d}x}\Big|_{\mp} \left(x_i^{\mp}\right) & \text{ for all } 1 \le i \le N, \end{cases}$$

where

$$v_{i,n}^*(x,\alpha) = \sum_{m=-\infty}^{\infty} r_{i,m} v_{n-m}(x,\alpha), \quad v_{i,n}^{**}(x,\alpha) = \sum_{m=-\infty}^{\infty} k_{i,m} \frac{\omega + (n-m)\Omega}{\omega + n\Omega} v_{n-m}(x,\alpha).$$



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## Numerical Solution and Approximation Exterior Solution

#### Lemma (Exterior Solution) [FCA23, Lemma 2.1]

The following exponential Ansatz solves the Helmholtz equation in  $\mathbb{R}\setminus D$ :

$$v_n(x) = \alpha_i^n \mathrm{e}^{\mathrm{i}k^n x} + \beta_i^n \mathrm{e}^{-\mathrm{i}k^n x}, \quad \forall x \in \left(x_i^+, x_{i+1}^-\right),$$

for all i = 1, ..., N - 1. The coefficients  $(\alpha_i^n, \beta_i^n)_{i=1}^N \subset \mathbb{R}^2$  can be determined in terms of the boundary values v through

$$\begin{bmatrix} \alpha_i^n \\ \beta_i^n \end{bmatrix} = \frac{-1}{2\mathrm{i}\sin\left(k^n\ell_{i(i+1)}\right)} \begin{bmatrix} \mathrm{e}^{\mathrm{i}k^nx_{i+1}^-} & -\mathrm{e}^{-\mathrm{i}k^nx_i^+} \\ -\mathrm{e}^{\mathrm{i}k^nx_{i+1}^-} & \mathrm{e}^{\mathrm{i}k^nx_i^+} \end{bmatrix} \begin{bmatrix} v_n(x_i^+) \\ v_n(x_{i+1}^-) \end{bmatrix},$$

for all  $i = 1, \ldots, N$  and for all  $n \in \mathbb{Z}$ .

To do: determine  $(\alpha_i^n, \beta_i^n)_{i=1}^N \subset \mathbb{C}^2, \forall n \in \mathbb{Z}, i.e.$  determine the boundary values of  $v_n$ .

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## Numerical Solution and Approximation Interior Solution

#### Lemma (Interior Solution) [ACHR23, Lemma 3.3]

For each resonator  $D_i$ , for i = 1, ..., N, the interior problem can be written as an infinitely-dimensional system of ODEs  $\Delta \mathbf{v}_i + C_i \mathbf{v}_i = \mathbf{0}$  with the unknown  $\mathbf{v}_i(x, \alpha) := [v_n(x, \alpha)]_{n \in \mathbb{Z}} \in \mathbb{C}^{\infty}$  for all  $x \in D_i$ , for fixed  $\alpha$ . Let  $\{\tilde{\lambda}_n^i\}_{n \in \mathbb{Z}}$  be the set of all eigenvalues of  $C_i$  with corresponding eigenvectors  $\{\mathbf{f}^{n,i}\}_{n \in \mathbb{Z}}$ . Using the square-roots  $\pm \lambda_n^i$  of the eigenvalues  $\tilde{\lambda}_n^i$ , the solution to the interior problem over  $D_i$  takes the form

$$\mathbf{v}_i = \sum_{n=-\infty}^{\infty} \left( a_i^n \mathrm{e}^{\mathrm{i}\lambda_n^i x} + b_i^n \mathrm{e}^{-\mathrm{i}\lambda_n^i x} \right) \mathbf{f}^{n,i}, \quad \forall x \in \left( x_i^-, x_i^+ \right),$$

for coefficients  $\{(a_i^n, b_i^n)\}_{n \in \mathbb{Z}} \subset \mathbb{C}^2$ .

To do: determine  $\{(a_i^n, b_i^n)\}_{n \in \mathbb{Z}} \subset \mathbb{C}^2, \forall i = 1, ..., N.$ Truncation: choose  $K \in \mathbb{N}$  and truncate the solution,  $\mathbf{v}_i = \sum_{n=-K}^{K} \left(a_i^n e^{i\lambda_j^i x} + b_i^n e^{-i\lambda_j^i x}\right) \mathbf{f}^{n,i}, \forall x \in D_i.$ 

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#### Numerical Solution and Approximation Dirichlet-to-Neumann Map

#### Definition (Dirichlet-to-Neumann Map) [FCA23, Definition 2.1]

For any  $k^n \in \mathbb{C}$ , for fixed  $n \in \mathbb{Z}$ , which is not of the form  $m\pi/\ell_{i(i+1)}$  for some  $m \in \mathbb{Z} \setminus \{0\}$  and  $1 \le i \le N-1$ , the *Dirichlet-to-Neumann map* with wave number  $k^n := (\omega + n\Omega)/v_0$  is the linear operator  $\mathcal{T}^{k^n, \alpha}$ :  $\mathbb{C}^{2N, \alpha} \to \mathbb{C}^{2N, \alpha}$  defined by

$$\mathcal{T}^{k^n,\alpha}[(v_i^{\pm})_{1\leq i\leq N}] := \left(\pm \frac{\mathrm{d}v_n}{\mathrm{d}x}(x_i^{\pm})\right)_{1\leq i\leq N},$$

where  $v_n$  is the unique solution to the exterior Helmholtz equation and  $(v_i^{\pm})_{i=1}^N \subset \mathbb{C}^{2N,\alpha}$  is a sequence of quasi-periodic boundary data defined s.t.  $v_{i+N}^{\pm} = e^{i\alpha L}v_i^{\pm}$ .

The Dirichlet-to-Neumann map can be expressed explicitly through a matrix-vector multiplication, where we denote the matrix by  $\mathcal{T}^{k^n,\alpha} \in \mathbb{C}^{2N \times 2N}$ .

Transmission condition: 
$$\left. \frac{\mathrm{d}v_{i,n}^*}{\mathrm{d}x} \right|_{\pm} \left( x_i^{\mp} \right) = \left. \delta \frac{\mathrm{d}v_n}{\mathrm{d}x} \right|_{\mp} \left( x_i^{\mp} \right) \Rightarrow \pm \frac{\mathrm{d}}{\mathrm{d}x} v_{i,n}^*(x_i^{\pm}, \alpha) = \delta \mathcal{T}^{k^n, \alpha}[v_n]_i^{\pm}$$



#### Numerical Solution and Approximation Numerical Solution

#### Lemma (Transmission Condition) [ACHR23, Theorem 3.4]

The subwavelength quasifrequencies  $\omega$  are approximately satisfying, as  $\delta \to 0$ , the following truncated system of non-linear equations:

$$\sum_{j=-K}^{K} \left( \mathcal{G}^{n,j} - \delta \mathcal{T}^{k^{n},\alpha} \times \mathcal{V}^{n,j} \right) \mathbf{w}_{j} = \mathbf{0}, \, \forall -K \le n \le K, \quad \mathbf{w}_{j} := \begin{bmatrix} a_{i}^{j} \\ b_{i}^{j} \end{bmatrix}_{1 \le i \le N} \in \mathbb{C}^{2N}, \, \forall -K \le j \le K,$$

and the matrices  $\mathcal{G}^{n,j}=\mathcal{G}^{n,j}(\omega)$  and  $\mathcal{V}^{n,j}=\mathcal{V}^{n,j}(\omega)$  are given by

$$\begin{aligned} \mathcal{G}^{n,j} &:= \operatorname{diag} \left( \sum_{m=-M}^{M} r_{i,m} f_{K+1-n+m}^{j,i} \left[ \begin{matrix} -\mathrm{i}\lambda_j^i \mathrm{e}^{\mathrm{i}\lambda_j^j x_i^-} & \mathrm{i}\lambda_j^i \mathrm{e}^{-\mathrm{i}\lambda_j^j x_i^-} \\ \mathrm{i}\lambda_j^i \mathrm{e}^{\mathrm{i}\lambda_j^i x_i^+} & -\mathrm{i}\lambda_j^i \mathrm{e}^{-\mathrm{i}\lambda_j^i x_i^+} \end{matrix} \right] \right)_{1 \le i \le N} \in \mathbb{C}^{2N \times 2N}, \\ \mathcal{V}^{n,j} &:= \operatorname{diag} \left( f_{K+1-n}^{j,i} \left[ \begin{matrix} \mathrm{e}^{\mathrm{i}\lambda_j^j x_i^-} & \mathrm{e}^{-\mathrm{i}\lambda_j^j x_i^-} \\ \mathrm{e}^{\mathrm{i}\lambda_j^j x_i^+} & \mathrm{e}^{-\mathrm{i}\lambda_j^j x_i^+} \end{matrix} \right] \right)_{1 \le i \le N} \in \mathbb{C}^{2N \times 2N}. \end{aligned}$$



#### Numerical Solution and Approximation Numerical Solution

#### Theorem [ACHR23, Theorem 3.4]

The subwavelength quasifrequencies  $\omega$  are approximately satisfying  $\mathcal{A}(\omega, \delta)[\mathbf{w}_j]_{j=K}^{-K} = \mathbf{0}$ , where  $\mathcal{A}(\omega, \delta) \in \mathbb{C}^{2N(2K+1) \times 2N(2K+1)}$  and  $\mathbf{w}_j \in \mathbb{C}^{2N}$  are given by:

$$\mathcal{A}(\omega,\delta) := \begin{bmatrix} \mathcal{G}^{K,K} - \delta \mathcal{T}^{k^{K},\alpha} \times \mathcal{V}^{K,K} & \cdots & \mathcal{G}^{K,-K} - \delta \mathcal{T}^{k^{K},\alpha} \times \mathcal{V}^{K,-K} \\ \vdots & \vdots \\ \mathcal{G}^{0,K} - \delta \mathcal{T}^{k^{0},\alpha} \times \mathcal{V}^{0,K} & \cdots & \mathcal{G}^{0,-K} - \delta \mathcal{T}^{k^{0},\alpha} \times \mathcal{V}^{0,-K} \\ \vdots & \vdots \\ \mathcal{G}^{-K,K} - \delta \mathcal{T}^{k^{-K},\alpha} \times \mathcal{V}^{-K,K} & \cdots & \mathcal{G}^{-K,-K} - \delta \mathcal{T}^{k^{-K},\alpha} \times \mathcal{V}^{-K,-K} \end{bmatrix}, \mathbf{w}_{j} := \begin{bmatrix} a_{j}^{j} \\ b_{i}^{j} \end{bmatrix}_{1 \leq i \leq N}$$

Use Muller's method to find  $\omega$  for which  $\mathcal{A}(\omega, \delta)$  is not invertible.



## Numerical Solution and Approximation Problems

 $\triangle$  Run-time increases with increasing N and K, K must be sufficiently large for sufficient accuracy.



The run-time depends algebraically on K.

## We introduce the Capacitance matrix!



With increasing K, the absolute error decreases.



## Numerical Solution and Approximation

Capacitance Matrix Approximation

#### Lemma [AH21, Lemma 4.1]

As  $\delta \to 0$ , the functions  $v^*_{i,n}(x, \alpha)$  are approximately constant inside the resonator:

$$v_{i,n}^*(x,\alpha)\Big|_{(x_i^-,x_i^+)} = c_{i,n} + O(\delta^{(1-\gamma)/2}).$$

Define 
$$c_i(t) = e^{i\omega t} \sum_{n=-\infty}^{\infty} c_{i,n} e^{in\Omega t}$$
.

#### Definition [ACHR23]

For any smooth function 
$$f : \mathbb{R} \to \mathbb{R}$$
, we define  $I_{\partial D_j}[f]$  by  $I_{\partial D_j}[f] := \frac{df}{dx} \Big|_{-} (x_j^-) - \frac{df}{dx} \Big|_{+} (x_j^+)$ .



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## Numerical Solution and Approximation

Capacitance Matrix Approximation

Capacitance matrix:  $C^{\alpha} := \left(C_{ij}^{\alpha}\right)_{1 \le i,j \le N}$  (nearly tridiagonal) same as in the static case [FCA23].

#### Theorem [ACHR23, Theorem 5.3]

The quasifrequencies in the subwavelength regime are, at leading order, given by the quasifrequencies of the system of ordinary differential equations

 $M^{\alpha}(t)\Psi(t) + \Psi^{\prime\prime}(t) = 0,$ 

where  $M^{\alpha}(t) = \frac{\delta \kappa_r}{\rho_r} W_1(t) C^{\alpha} W_2(t) + W_3(t)$  with  $W_1, W_2$  and  $W_3$  being diagonal matrices defined as

$$(W_1)_{ii} = \frac{\sqrt{\kappa_i}}{\ell_i}, \quad (W_2)_{ii} = \sqrt{\kappa_i}, \quad (W_3)_{ii} = \frac{\sqrt{\kappa_i}}{2} \frac{\mathrm{d}}{\mathrm{d}t} \frac{\kappa'_i}{\kappa_i^{3/2}},$$

for  $i = 1, \ldots, N$ , with

$$\Psi(t) = \left(\frac{c_i(t)}{\sqrt{\kappa_i(t)}}\right)_{i=1,\dots,N}$$



#### Numerical Solution and Approximation Numerical Simulations



Observations:

- $\kappa_i(t) = \frac{1}{1 + \epsilon_{\kappa,i} \cos(\Omega t + \phi_{\kappa,i})}$
- k-gaps: undesirable α for which wave propagation is uncontrollable.
- *ρ* does not affect band structure at leading order.



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## **Conclusion & Outlook**

- Solve the coupled Helmholtz equations exactly up to numerical errors.
- Capacitance matrix approximation to the subwavelength quasifrequencies in one dimension for a quasi-periodic, time-modulated problem.
- Time-modulating  $\rho$  does not affect the subwavelength quasifrequencies at leading order.
- Time-modulating  $\kappa$  leads to the formation of k-gaps.
- Next step: Formulate the scattering problem in the dilute regime and let N → ∞ while the resonators have fixed size. Derive an approximation for N = 1. Obtain an effective medium theory.



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## **Additional Material**

Consider the solution  $V_i^{\alpha} : \mathbb{R} \to \mathbb{R}$  of the following problem:

$$\begin{cases} -\frac{\mathrm{d}^2}{\mathrm{d}x^2}V_i^\alpha = 0, & (0,L)\backslash D, \\ V_i^\alpha(x) = \delta_{ij}, & x \in D_j, \\ V_i^\alpha(x+mL) = \mathrm{e}^{\mathrm{i}\alpha mL}V_i^\alpha(x), & m \in \mathbb{Z}. \end{cases}$$

The corresponding capacitance matrix is defined by

$$\begin{split} C_{ij}^{\alpha} &= \left. \frac{\mathrm{d}V_{j}^{\alpha}}{\mathrm{d}x} \right|_{-} (x_{i}^{-}) - \left. \frac{\mathrm{d}V_{j}^{\alpha}}{\mathrm{d}x} \right|_{+} (x_{i}^{+}) \\ &= -\frac{1}{\ell_{(j-1)j}} \delta_{i(j-1)} + \left( \frac{1}{\ell_{(j-1)j}} + \frac{1}{\ell_{j(j+1)}} \right) \delta_{ij} - \frac{1}{\ell_{j(j+1)}} \delta_{i(j+1)} \\ &- \delta_{1j} \delta_{iN} \frac{\mathrm{e}^{-\mathrm{i}\alpha L}}{\ell_{N(N+1)}} - \delta_{1i} \delta_{jN} \frac{\mathrm{e}^{\mathrm{i}\alpha L}}{\ell_{N(N+1)}}, \end{split}$$



## **Additional Material**

or equivalently by

.



### Additional Material

For fixed  $n \in \mathbb{Z}$ , the Dirichlet-to-Neumann map  $\mathcal{T}^{k^n,\alpha}$  admits the following explicit matrix representation: for any  $k^n \in \mathbb{C} \setminus \{m\pi/\ell_{i(i+1)} : m \in \mathbb{Z} \setminus \{0\}, 1 \leq i \leq N-1\}, f \equiv (f_i^{\pm})_{1 \leq i \leq N}, \mathcal{T}^{k^n,\alpha}[f] \equiv (\mathcal{T}^{k^n,\alpha}[f]_i^{\pm})_{1 \leq i \leq N}$  is given by

$$\begin{bmatrix} \mathcal{T}^{k^{n},\alpha}[f]_{1}^{-} \\ \mathcal{T}^{k^{n},\alpha}[f]_{1}^{+} \\ \vdots \\ \mathcal{T}^{k^{n},\alpha}[f]_{N}^{-} \end{bmatrix} = \begin{bmatrix} -\frac{k^{n}\cos(k^{n}\ell_{N(N+1)})}{\sin(k^{n}\ell_{N(N+1)})} & \frac{k^{n}}{\sin(k^{n}\ell_{N(N+1)})} e^{-i\alpha L} \\ A^{k^{n}}(\ell_{12}) & \vdots \\ \ddots & & \\ \frac{k^{n}}{\sin(k^{n}\ell_{N(N+1)})} e^{i\alpha L} & \frac{k^{n}}{\sin(k^{n}\ell_{N(N+1)})} \end{bmatrix} \begin{bmatrix} f_{1}^{-} \\ f_{1}^{+} \\ \vdots \\ f_{n}^{-} \\ f_{N}^{+} \end{bmatrix}$$

•

where for any  $\ell \in \mathbb{R},$   $\boldsymbol{A}^{k^n}(\ell)$  denotes the  $2\times 2$  symmetric matrix

$$A^{k^n}(\ell) := \begin{bmatrix} -\frac{k^n \cos(k^n \ell)}{\sin(k^n \ell)} & \frac{k^n}{\sin(k^n \ell)} \\ \frac{k^n}{\sin(k^n \ell)} & -\frac{k^n \cos(k^n \ell)}{\sin(k^n \ell)} \end{bmatrix}.$$