2D plasmonic computation of layered heterostructures

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Collaborators

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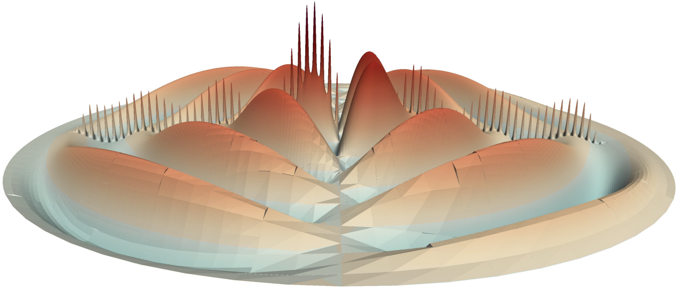

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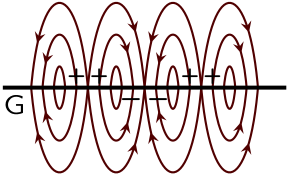
[3] School of Engineering and Applied Sciences, Harvard University

Motivation

Motivation

- Surface plasmon polaritons (SPPs) on graphene:



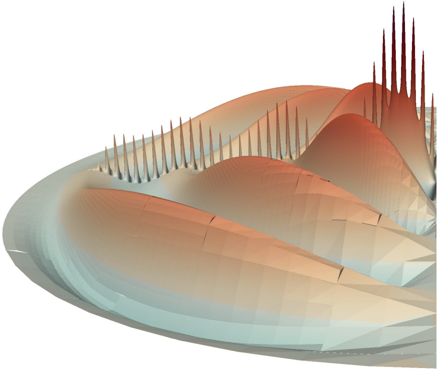
Optical properties of graphene

- On meso/macroscale:
  Effective surface conductivity σ,

$$\boldsymbol{J}_\Sigma = \sigma \boldsymbol{E}_\Sigma .$$

- $\operatorname{Im}\sigma \gg \operatorname{Re}\sigma$ in the Terahertz and mid-infrared regimes

- SPP wavelength is much smaller than the outer wave:



- *Subwavelength optics* beyond the diffraction limit

Motivation

(atomistic) microscale

optical phenomena on mesoscale (SPPs)

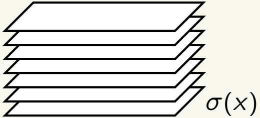
macroscale

Goals

- Analytical and numerical understanding of optical phenomena on meso/macroscale.
- Simulation of multiscale effects in time-harmonic Maxwell's equations

Metamaterials in optics

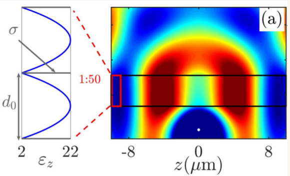
Layered heterostructures:



Manipulating the laws of optics:

- tuning of permittivity/permeability
- no/negative refraction index

$\varepsilon_z^{\text{eff}} \approx 0$:

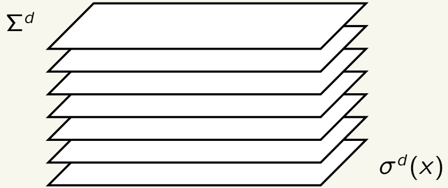


A Bloch-wave approach

A Bloch-wave approach

Scattering configuration

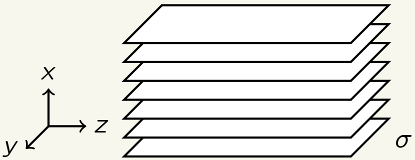
- Heterogeneous permittivity $\varepsilon^d(x)$,
- periodic layers Σ^d with heterogeneous surface conducitivity $\sigma^d(x)$
- Scaling parameter d



- Goal: understand effective properties assuming scale separation

A Bloch-wave approach

Microscale model



$$\varepsilon = \big(\varepsilon_x, \varepsilon_z(x), \varepsilon_z(x)\big), \qquad \sigma = \text{const.}$$

Find particular solutions,

$$\boldsymbol{E} = (E_x, 0, E_z), \qquad \boldsymbol{H} = (0, H_y, 0),$$

$$E_z(x,z) = \mathcal{E}(x)\, e^{ik_z z}.$$

Bloch-wave ansatz:

$$\mathcal{E}(x) = e^{ik_x d}\, \mathcal{E}(x-d)$$

Dispersion relation:

$$D[k_x, k_z] = \det\left(e^{ik_x d} \begin{bmatrix} 1 & 0 \\ -i\sigma/\omega\kappa(k_z) & 1 \end{bmatrix} - \Psi(d) \right) \;=\; 0,$$

and Ψ is the fundamental system of

$$-\partial_x^2 \mathcal{E}(x) + \kappa(k_z)\mathcal{E}(x) = 0, \qquad \kappa(k_z) = (k_z^2 - k_0^2\varepsilon_x)/\varepsilon_x.$$

A Bloch-wave approach

Expanding near $\boldsymbol{k}^*$:

$$D[\boldsymbol{k}^* + \delta\boldsymbol{k}] = -d\left(\frac{-\mathrm{i}\sigma}{\omega\varepsilon_x}\,2k_z\delta k_z - \delta\mathcal{E}'_{(1)}(d)[\delta k_z]\right) + \mathcal{O}((\delta\boldsymbol{k})^2),$$

$$\text{where}\quad \delta\mathcal{E}'_{(1)}(x) = 2k_z\delta k_z\left[\varepsilon_x\int_0^x \varepsilon_z(\xi)\,\mathrm{d}\xi\right]^{-1}.$$

For $\varepsilon_z^{\text{eff}}/\varepsilon_x \sim 1$ it can be shown that

$$D[\boldsymbol{k}^* + \delta\boldsymbol{k}] \approx -d^2\left[\delta k_x^2 + \frac{\varepsilon_z^{\text{eff}}}{\varepsilon_x}(k_z^* + \delta k_z)^2 - \frac{\varepsilon_z^{\text{eff}}}{\varepsilon_x}(k_z^*)^2\right].$$

- M. Maier, M. Mattheakis, E. Kaxiras, M. Luskin, and D. Margetis. Universal behavior of dispersive Dirac cone in gradient-index plasmonic metamaterials. *Physical Review B*, 97(3), 2018. doi: 10.1103/PhysRevB.97.035307. URL https://arxiv.org/abs/1711.02210

A Bloch-wave approach

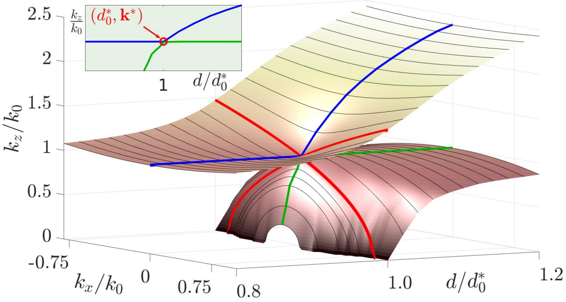
Theorem (Bifurcation)

Bifurcation occurs at

$$d_0^* = -\frac{i\sigma}{\omega}\left[\int_0^1 \varepsilon(x)\,dx\right]^{-1},$$

with

$$\varepsilon_z^{eff} = \int_0^1 \varepsilon(x)\,dx - \frac{\sigma}{i\omega d}.$$



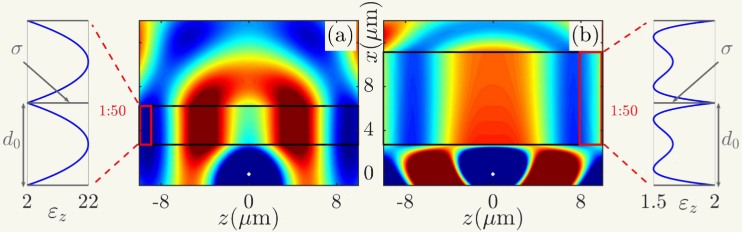
- M. Maier, M. Mattheakis, E. Kaxiras, M. Luskin, and D. Margetis. Universal behavior of dispersive Dirac cone in gradient-index plasmonic metamaterials. *Physical Review B*, 97(3), 2018. doi: 10.1103/PhysRevB.97.035307. URL https://arxiv.org/abs/1711.02210

A Bloch-wave approach

Effective permittivity:

$$\varepsilon = \begin{pmatrix} \varepsilon_x & & \\ & \varepsilon_z^{\text{eff}} & \\ & & \varepsilon_z^{\text{eff}} \end{pmatrix}, \qquad \varepsilon_z^{\text{eff}} = \int_0^1 \varepsilon(x)\,\mathrm{d}x - \frac{\sigma}{i\omega d}.$$

Epsilon near zero (ENZ) effect

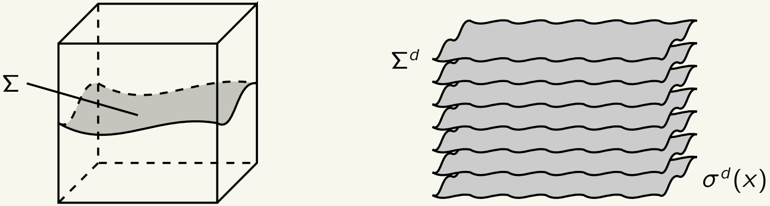


Layered heterostructures

Layered heterostructures

Scattering configuration, periodicity and scaling assumptions

- Unit cell $Y = [0, 1]^3$ with inscribed layer Σ:

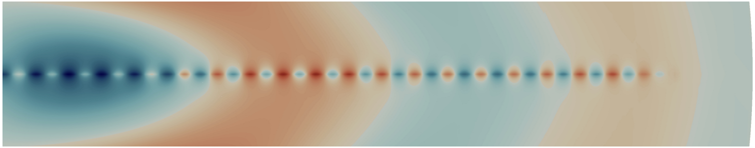


$$\Sigma^d = \Big\{ d\,\boldsymbol{z} + d\,\boldsymbol{\varsigma} \;:\; \boldsymbol{z} \in \mathbb{Z}^3,\ \boldsymbol{\varsigma} \in \Sigma \Big\},$$

- Material parameters: $\varepsilon^d(\boldsymbol{x}) = \varepsilon\big(\boldsymbol{x}, \boldsymbol{x}/d\big)$, $\sigma^d(\boldsymbol{x}) = d\,\sigma\big(\boldsymbol{x}, \boldsymbol{x}/d\big)$, where $\varepsilon, \sigma \;:\; \Omega \times Y \to \mathbb{R}^{3\times 3}$ are Y-periodic,

$$\varepsilon\big(\boldsymbol{x}, \boldsymbol{y} + \boldsymbol{e}_i\big) = \varepsilon\big(\boldsymbol{x}, \boldsymbol{y}\big), \text{ and } \sigma\big(\boldsymbol{x}, \boldsymbol{y} + \boldsymbol{e}_i\big) = \sigma\big(\boldsymbol{x}, \boldsymbol{y}\big), \quad \boldsymbol{x} \in \Omega,\ \boldsymbol{y} \in \mathbb{R}^3.$$

Layered heterostructures



On the choice of scaling of σ^d

$$\sigma^d(\boldsymbol{x}) = d\,\sigma\big(\boldsymbol{x}, \boldsymbol{x}/d\big)$$

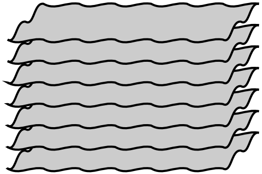
- Scale separation between

$$\lambda_0 \sim 1 \quad \text{ambient, incident wavelength, average of } \varepsilon^d$$

$$\lambda_{\text{SPP}} \sim d \quad \text{wavelength of SPP structures, average of } \sigma^d$$

- Coupling strength between layers remains constant

Layered heterostructures



Microscale model

Find $\boldsymbol{E}^d, \boldsymbol{H}^d : \Omega \to \mathbb{R}^3$ s. t.

$$\begin{cases} \nabla \times \boldsymbol{E}^d = i\omega\mu_0 \boldsymbol{H}^d, \\ \nabla \times \boldsymbol{H}^d = -i\omega\varepsilon^d \boldsymbol{E}^d + \boldsymbol{J}_a, \\ \nabla \cdot (\varepsilon^d \boldsymbol{E}^d) = \dfrac{1}{i\omega}\nabla \cdot \boldsymbol{J}_a, \\ \nabla \cdot \boldsymbol{H}^d = 0, \end{cases} \qquad \begin{cases} \left[\boldsymbol{\nu} \times \boldsymbol{E}^d\right]_{\Sigma^d} = 0, \\ \left[\boldsymbol{\nu} \times \boldsymbol{H}^d\right]_{\Sigma^d} = \sigma^d \boldsymbol{E}^d_T, \\ \left[\boldsymbol{\nu} \cdot (\varepsilon^d \boldsymbol{E}^d)\right]_{\Sigma^d} = \dfrac{1}{i\omega}\nabla_T \cdot (\sigma^d \boldsymbol{E}^d_T), \\ \left[\boldsymbol{\nu} \cdot \boldsymbol{H}^d\right]_{\Sigma^d} = 0. \end{cases}$$

Asymptotic analysis

Asymptotic analysis

Microscale model

$$\begin{cases} \nabla \times \boldsymbol{E}^d = i\omega\mu_0 \boldsymbol{H}^d, \\ \nabla \times \boldsymbol{H}^d = -i\omega\varepsilon^d \boldsymbol{E}^d + \boldsymbol{J}_a, \\ \nabla \cdot (\varepsilon^d \boldsymbol{E}^d) = \frac{1}{i\omega} \nabla \cdot \boldsymbol{J}_a, \\ \nabla \cdot \boldsymbol{H}^d = 0, \end{cases} \qquad \begin{cases} [\boldsymbol{\nu} \times \boldsymbol{E}^d]_{\Sigma^d} = 0, \\ [\boldsymbol{\nu} \times \boldsymbol{H}^d]_{\Sigma^d} = \sigma^d \boldsymbol{E}^d_T, \\ [\boldsymbol{\nu} \cdot (\varepsilon^d \boldsymbol{E}^d)]_{\Sigma^d} = \frac{1}{i\omega} \nabla_T \cdot (\sigma^d \boldsymbol{E}^d_T), \\ [\boldsymbol{\nu} \cdot \boldsymbol{H}^d]_{\Sigma^d} = 0. \end{cases}$$

- Formal multiscale expansion

$$\boldsymbol{E}^d \to \boldsymbol{E}^{(0)}(\boldsymbol{x}, \boldsymbol{y}) + d\boldsymbol{E}^{(1)}(\boldsymbol{x}, \boldsymbol{y}) + d^2 \boldsymbol{E}^{(2)}(\boldsymbol{x}, \boldsymbol{y}) + \ldots,$$
$$\boldsymbol{H}^d \to \boldsymbol{H}^{(0)}(\boldsymbol{x}, \boldsymbol{y}) + d\boldsymbol{H}^{(1)}(\boldsymbol{x}, \boldsymbol{y}) + d^2 \boldsymbol{H}^{(2)}(\boldsymbol{x}, \boldsymbol{y}) + \ldots.$$

$$\nabla \to \nabla_x + \frac{1}{d} \nabla_y$$

- Order d system:

$$\begin{cases} \nabla_x \times \boldsymbol{E}^{(0)} + \nabla_y \times \boldsymbol{E}^{(1)} = i\omega\mu_0 \boldsymbol{H}^{(0)}, \\ \nabla_x \times \boldsymbol{H}^{(0)} + \nabla_y \times \boldsymbol{H}^{(1)} = -i\omega\varepsilon \boldsymbol{E}^{(0)} + \boldsymbol{J}_a, \\ \nabla_x \cdot (\varepsilon \boldsymbol{E}^{(0)}) + \nabla_y \cdot (\varepsilon \boldsymbol{E}^{(1)}) = \frac{1}{i\omega} \nabla_x \cdot \boldsymbol{J}_a, \\ \nabla_x \cdot \boldsymbol{H}^{(0)} + \nabla_y \cdot \boldsymbol{H}^{(1)} = 0, \end{cases} \qquad \begin{cases} [\boldsymbol{\nu} \times \boldsymbol{E}^{(1)}]_\Sigma = 0, \\ [\boldsymbol{\nu} \times \boldsymbol{H}^{(1)}]_\Sigma = \sigma \boldsymbol{E}^{(0)}, \\ [\boldsymbol{\nu} \cdot (\varepsilon \boldsymbol{E}^{(1)})]_\Sigma = \frac{1}{i\omega} \left(\nabla_x \cdot (\sigma \boldsymbol{E}^{(0)}) + \nabla_y \cdot (\sigma \boldsymbol{E}^{(1)})\right), \\ [\boldsymbol{\nu} \cdot \boldsymbol{H}^{(1)}]_\Sigma = 0. \end{cases}$$

Asymptotic analysis

Homogenized system

Find $\mathcal{E}, \mathcal{H} : \Omega \to \mathbb{R}^3$, s. t.

$$\begin{cases} \nabla \times \mathcal{E} = i\omega\mu_0\mathcal{H}, \\ \nabla \times \mathcal{H} = -i\omega\varepsilon^{\text{eff}}\mathcal{E} + \boldsymbol{J}_a, \\ \nabla \cdot (\varepsilon^{\text{eff}}\mathcal{E}) = \frac{1}{i\omega}\nabla \cdot \boldsymbol{J}_a, \\ \nabla \cdot \mathcal{E} = 0, \end{cases}$$

where

$$\varepsilon^{\text{eff}}(\boldsymbol{x}) := \int_Y \varepsilon(\boldsymbol{x},\boldsymbol{y})(\mathcal{I} + \nabla_y \boldsymbol{\chi}(\boldsymbol{x},\boldsymbol{y}))\,\mathrm{d}y - \frac{1}{i\omega}\int_\Sigma \sigma(\boldsymbol{x},\boldsymbol{y})(\mathcal{I} + \nabla_y \boldsymbol{\chi}(\boldsymbol{x},\boldsymbol{y}))\,\mathrm{d}o_y.$$

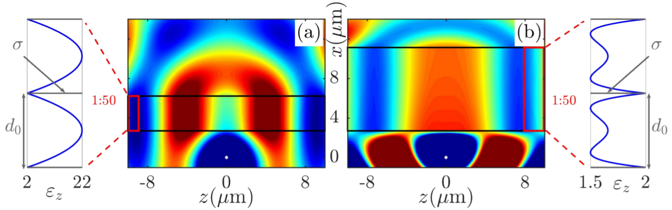
The corrector $\chi_j(\boldsymbol{x}, .) : Y \to \mathbb{R}$ solves a cell problem,

$$\begin{cases} \nabla_y \cdot \Big(\varepsilon(\boldsymbol{x},\boldsymbol{y})\big(\boldsymbol{e}_j + \nabla_y \chi_j(\boldsymbol{x},\boldsymbol{y})\big)\Big) = 0, \\ [\boldsymbol{\nu} \times (\boldsymbol{e}_j + \nabla_y \chi_j(\boldsymbol{x},\boldsymbol{y}))]_\Sigma = 0, \\ [\boldsymbol{\nu} \cdot (\boldsymbol{e}_j + \nabla_y \chi_j(\boldsymbol{x},\boldsymbol{y})]_\Sigma = \frac{1}{i\omega}\nabla_y \cdot \Big(\sigma(\boldsymbol{x},\boldsymbol{y})\big(\boldsymbol{e}_j + \nabla_y \chi_j(\boldsymbol{x},\boldsymbol{y})\big)\Big). \end{cases}$$

Asymptotic analysis

Effective permittivity

$$\varepsilon^{\text{eff}}(\boldsymbol{x}) := \int_Y \varepsilon(\boldsymbol{x},\boldsymbol{y})(\mathcal{I} + \nabla_y \boldsymbol{\chi}(\boldsymbol{x},\boldsymbol{y}))\,\mathrm{d}y - \frac{1}{i\omega}\int_\Sigma \sigma(\boldsymbol{x},\boldsymbol{y})(\mathcal{I} + \nabla_y \boldsymbol{\chi}(\boldsymbol{x},\boldsymbol{y}))\,\mathrm{d}o_y.$$

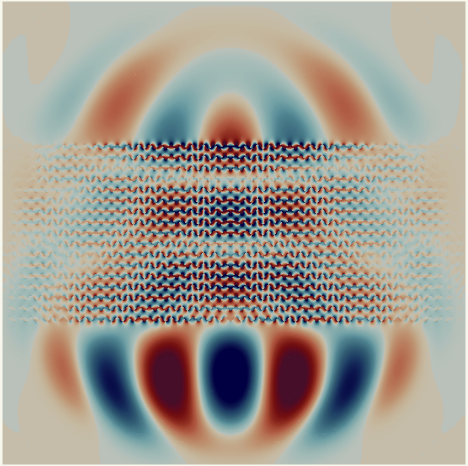


- M. Maier, M. Mattheakis, E. Kaxiras, M. Luskin, and D. Margetis. Homogenization of plasmonic crystals: Seeking the epsilon-near-zero effect. *Proceedings of the Royal Society A: Mathematical, Physical, and Engineering Sciences*, 475, 2019. doi: 10.1098/rspa.2019.0220. URL https://arxiv.org/abs/1809.08276

Example: Plasmonic crystal

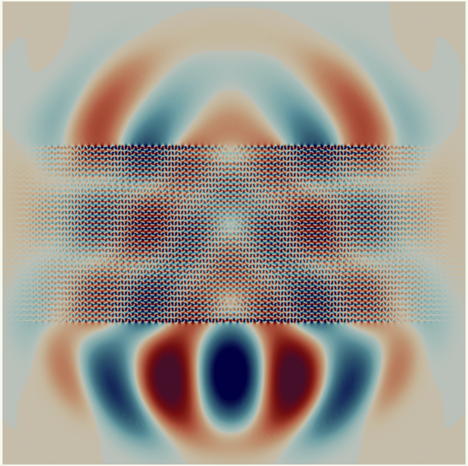
Example: Plasmonic crystal

$d = 2^{-4}$



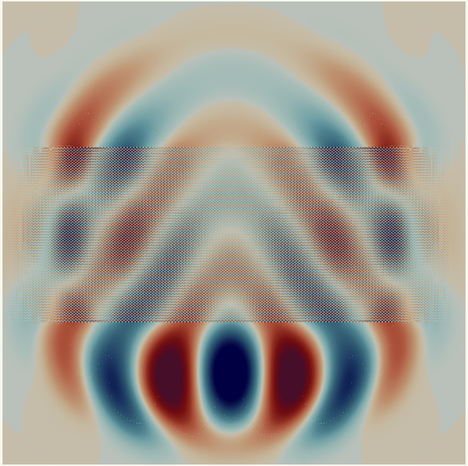
Example: Plasmonic crystal

$d = 2^{-5}$



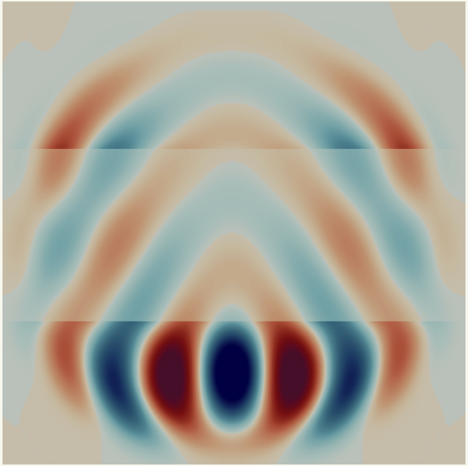
Example: Plasmonic crystal

$d = 2^{-6}$



Example: Plasmonic crystal

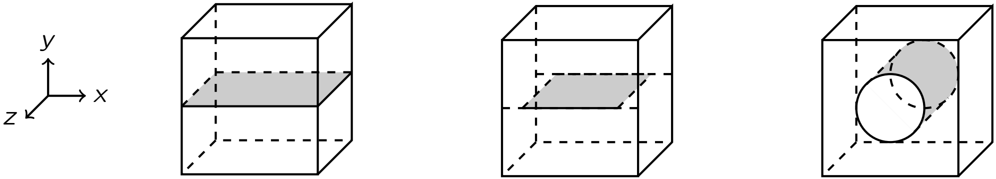
Homogenized system



Resonances and the role of the corrector

Resonances and the role of the corrector

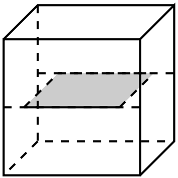
$$\varepsilon^{\text{eff}}(\boldsymbol{x}) := \int_Y \varepsilon(\boldsymbol{x},\boldsymbol{y})(\mathcal{I}+\nabla_y \boldsymbol{\chi}(\boldsymbol{x},\boldsymbol{y}))\,\mathrm{d}y - \frac{1}{i\omega}\int_\Sigma \sigma^{\text{Drude}}(\omega)P_T(\boldsymbol{y})(\mathcal{I}+\nabla_y \boldsymbol{\chi}(\boldsymbol{x},\boldsymbol{y}))\,\mathrm{d}o_y.$$



Stacked graphene layers | Stacked nano ribbons | Stacked nano tubes

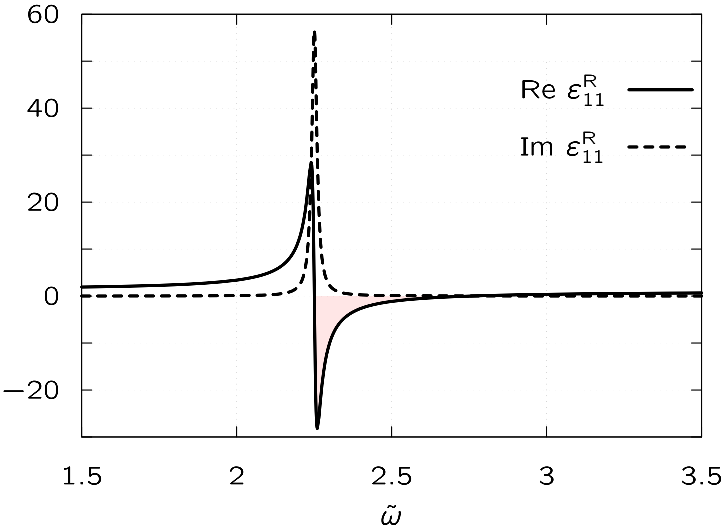
$$\varepsilon^{\text{eff}} = \begin{pmatrix} \varepsilon^S_{11} & 0 & 0 \\ 0 & \varepsilon & 0 \\ 0 & 0 & \varepsilon^S_{33} \end{pmatrix} \quad \begin{pmatrix} \varepsilon^R_{11} & 0 & 0 \\ 0 & \varepsilon & 0 \\ 0 & 0 & \varepsilon^R_{33} \end{pmatrix} \quad \begin{pmatrix} \varepsilon^T_{11} & 0 & 0 \\ 0 & \varepsilon^T_{22} & 0 \\ 0 & 0 & \varepsilon^T_{33} \end{pmatrix}$$

Numerical solution of cell problems

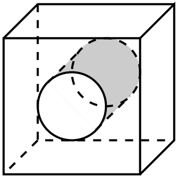


Stacked nano ribbons

$$\begin{pmatrix} \varepsilon_{11}^{R} & 0 & 0 \\ 0 & \varepsilon & 0 \\ 0 & 0 & \varepsilon_{33}^{R} \end{pmatrix}$$

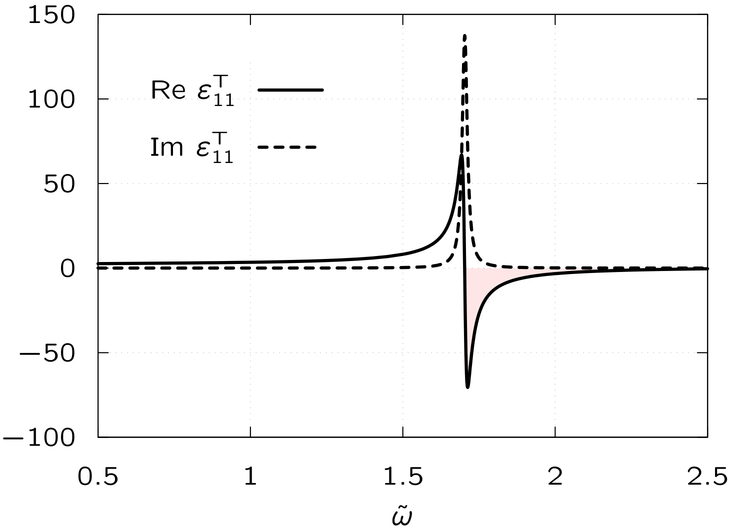


Numerical solution of cell problems



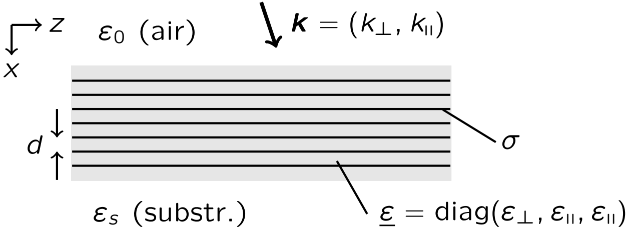
Stacked nano tubes

$$\begin{pmatrix} \varepsilon_{11}^{\mathrm{T}} & 0 & 0 \\ 0 & \varepsilon_{22}^{\mathrm{T}} & 0 \\ 0 & 0 & \varepsilon_{33}^{\mathrm{T}} \end{pmatrix}$$



Finite size structures

Finite size structures

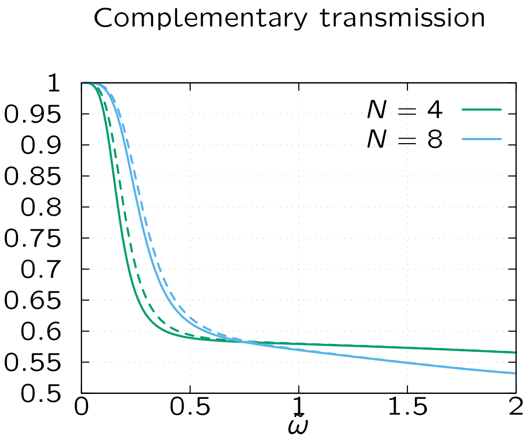


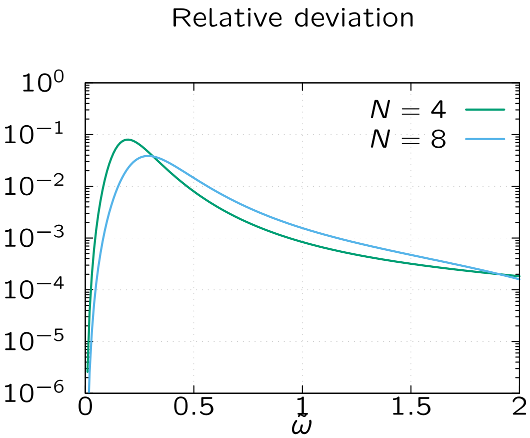
Compare homogenization result against complementary transmission of finite sized structures,

$$E(\tilde{\omega}) = 1 - \left|T(\tilde{\omega})\right|^2.$$

- M. Maier, D. Margetis, and M. Luskin. Finite-size effects in the fresnel coefficients for plasmonic crystals: A tale of two scales. *In Preparation*, 2020

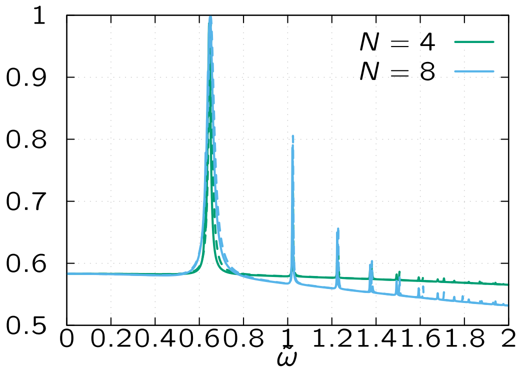
Sheets


Complementary transmission
$N = 4$
$N = 8$
1
0.95
0.9
0.85
0.8
0.75
0.7
0.65
0.6
0.55
0.5
0
0.5
1
1.5
2
$\tilde{\omega}$

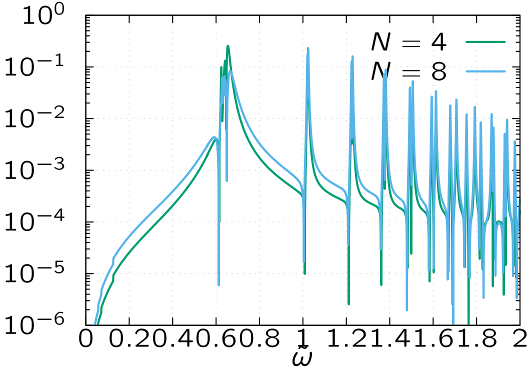

Relative deviation
$N = 4$
$N = 8$
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
0
0.5
1
1.5
2
$\tilde{\omega}$

Nano-ribbons

Complementary transmission



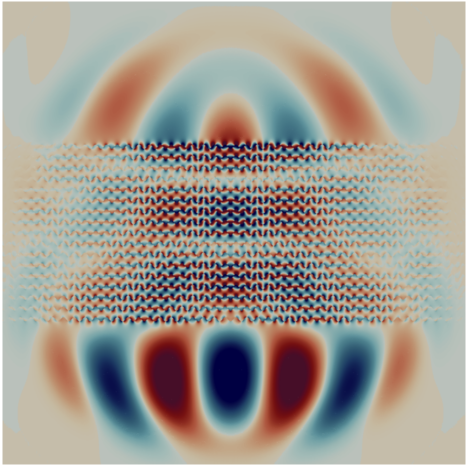
Relative deviation



Conclusion

Conclusion

- Bloch-wave approach for ideal plasmonic crystal
- Two-scale analysis of layered heterostructures
- Comparison to finite sized configurations



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