Nonlocal Multicomponent Metamaterials

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Collaborators

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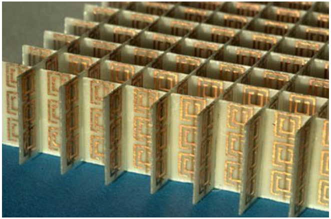
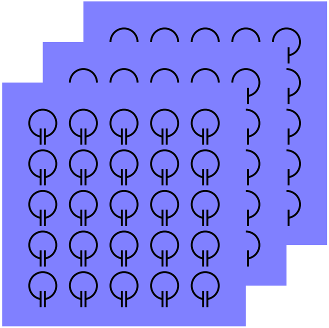
- José Samuel Pérez
- Bernardo Mendoza

(Thanks to DGAPA-UNAM IN111119)

Metamaterials



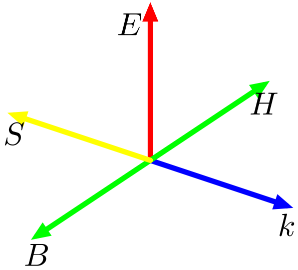


- Resonances in ϵ, μ.
- $\epsilon < 0$, $\mu < 0$.
- $n < 0$

Left-handed materials

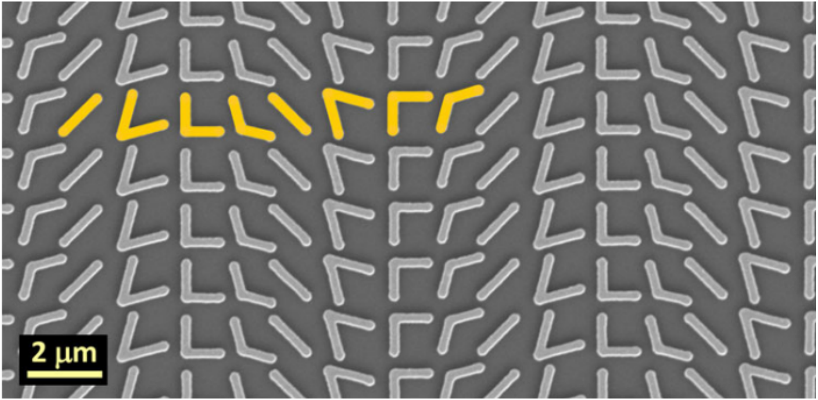
$$k^2 = \epsilon\mu\frac{\omega^2}{c^2}$$

- If $\epsilon < 0$ y $\mu < 0$, k is real $\Longrightarrow$ propagating field.



- but $\boldsymbol{S}$ would be opposite to $\boldsymbol{k}$.

Metasurfaces



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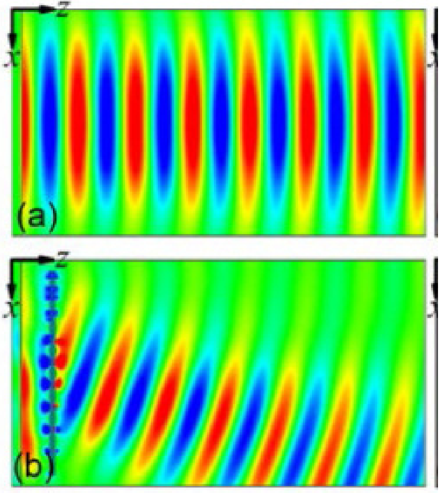
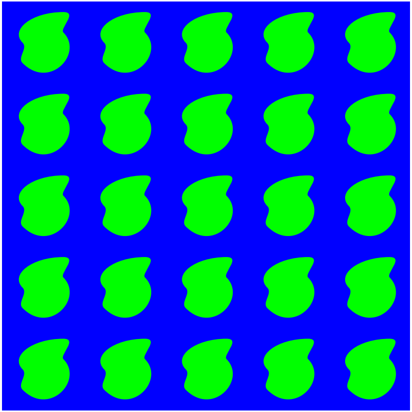


The problem

- The optical properties of these materials is determined not only by their composition,
- but also by their geometry (size, shape).
- ¿How to calculate them?
- Effective response.



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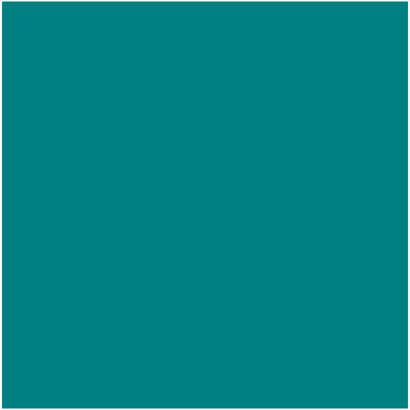

Macroscopic vs. average response

- $\boldsymbol{D} = \epsilon \boldsymbol{E}$
- $\boldsymbol{D}_M = \epsilon_M \boldsymbol{E}_M$
- $\epsilon_M \neq \langle \epsilon \rangle$ as $\langle \epsilon \boldsymbol{E} \rangle \neq \langle \epsilon \rangle \langle \boldsymbol{E} \rangle$
- Find some operator whose average does have a meaning.

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Macroscopic response

Small scale, no retardation

- $\boldsymbol{D}^L$ *obeys* the same equations with the same sources as the external longitudinal E field: $\nabla \times \boldsymbol{D}^L \equiv 0$, $\nabla \cdot \boldsymbol{D}^L = 4\pi\rho^{ex}$.
- $\boldsymbol{D}^L$ *is* the external longitudinal E field.
- $\boldsymbol{D}^L$ has no spatial fluctuations induced by the texture.
- $\boldsymbol{E}^L = (\epsilon^{LL})^{-1}\boldsymbol{D}^L$
- $\boldsymbol{E}^L_a = (\epsilon^{LL})^{-1}_{aa}\boldsymbol{D}^L_a$
- $(\epsilon^{LL}_M)^{-1} = (\epsilon^{LL})^{-1}_{aa}$
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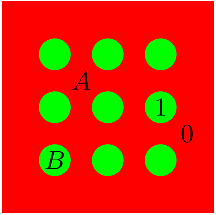
Binary system

- $\epsilon(\boldsymbol{r}) = \begin{cases} \epsilon_B & \text{if } \boldsymbol{r} \in \text{inclusion}, \\ \epsilon_A & \text{if } \boldsymbol{r} \in \text{matrix} \end{cases}$
- Characteristic function $B(\boldsymbol{r}) = \begin{cases} 1 & \text{if } \boldsymbol{r} \in \text{inclusion}, \\ 0 & \text{if } \boldsymbol{r} \in \text{host} \end{cases}$ (geometry)
- $\epsilon(\boldsymbol{r}) = (\epsilon_A - \epsilon_{AB} B(\boldsymbol{r})) = \epsilon_{AB}(u - B(\boldsymbol{r}))$
- $\epsilon_{AB} = \epsilon_A - \epsilon_B$
- Spectral variable $u \equiv (1 - \epsilon_B/\epsilon_A)^{-1} = \epsilon_A(\omega)/\epsilon_{AB}(\omega)$. (composition, frequency)



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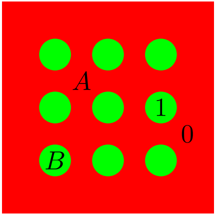

Analogy

- Periodic system, reciprocal lattice $\{\boldsymbol{G}\}$; average: $\boldsymbol{G} = 0$.
- $(\epsilon^{LL}_{GG'})^{-1} \equiv [\hat{\boldsymbol{G}} \cdot (\epsilon_{GG'} \hat{\boldsymbol{G}}')]^{-1} = \frac{1}{\epsilon_{ab}}[u\delta_{GG'} - B^{LL}_{GG'}]^{-1}$
- Interpreting $B^{LL}_{GG'} = \hat{\boldsymbol{G}} \cdot B_{\boldsymbol{G}-\boldsymbol{G}'} \hat{\boldsymbol{G}}'$ as a *Hermitian* Hamiltonian $\hat{H}$, u as an *energy* ε, then $(\epsilon^{LL}_{M})^{-1} = (u\hat{1} - B^{LL})^{-1}_{00} / \epsilon_{ab}$ is analogous to a Green's operator $\mathcal{G}(\varepsilon) = (\varepsilon\hat{1} - \hat{H})^{-1}$ projected onto the state $|0\rangle$.

Haydock's recursion

- Define $|0\rangle = |\boldsymbol{G}=0\rangle$, $|-1\rangle = 0$.
- Orthonormal basis $\{|n\rangle\}$
  $|\tilde{n}\rangle \equiv \hat{H}|n-1\rangle = b_n|n\rangle + a_{n-1}|n-1\rangle + b_{n-1}|n-2\rangle$
  in which $\hat{H}$ is tridiagonal. Apply $\hat{H}$ and orthogonalize.
- $a_{n-1} = \langle n-1|\tilde{n}\rangle = \langle n-1|\hat{H}|n-1\rangle$
  $b_n^2 = \langle\tilde{n}|\tilde{n}\rangle - a_{n-1}^2 - b_{n-1}^2$.
- $\hat{H} \to B^{LL}_{GG'} = \hat{\boldsymbol{G}} \cdot B_{\boldsymbol{G}-\boldsymbol{G}'} \hat{\boldsymbol{G}}'$
- $\hat{H}|n\rangle$ is obtained by multiplying $\langle\boldsymbol{G}|n\rangle$
  1. by $\hat{\boldsymbol{G}}$ in reciprocal space,
  2. $B(\boldsymbol{r})$ in real space,
  3. $\hat{\boldsymbol{G}}\cdot$ in reciprocal space,

  $\to a_n$ and b_n ¡without matrix multiplications!

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Continued fraction

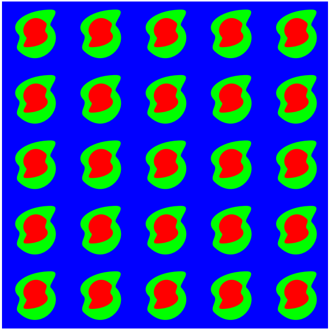
- We look for only one element (0,0) of the inverse of a tridiagonal symmetric matrix with elements $u - a_n$, $-b_n$,

$$\frac{1}{\epsilon_M^{LL}} = \frac{1}{\epsilon_{ab}} \frac{1}{u - a_0 - \frac{b_1^2}{u - a_1 - \frac{b_2^2}{u - a_2 - \frac{b_3^2}{\ddots}}}}, \qquad (1)$$

- a_n, b_n depend only on geometry.
- u has all the information about composition and frequency.
- Compute a_n, b_n once, obtain ϵ_M for many compositions and frequencies substituting $u = u(\omega) = 1/(1 - \epsilon_B(\omega)/\epsilon_A(\omega))$.
- Allows for dispersion and dissipation. Useful for dielectrics and/or metals

Limitations

- Doesn't work for three or more components (there is no characteristic function).
- Solution: Use $\hat{\epsilon}^{LL}$ directly, instead of $\hat{B}^{LL}$.
- Problem: Geometry and composition are no longer factored.
- Worse yet: Can't allow for dissipation. Non-Hermitian$\rightarrow$ no orthogonality, no Haydock basis.



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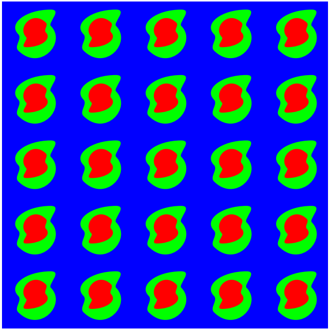

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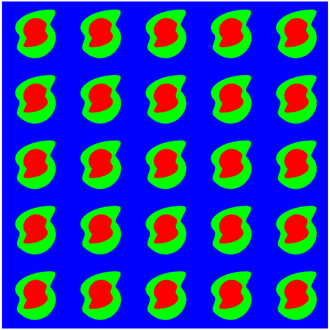

Euclidean vs. Hermitian Product

- Define $\langle\phi|\psi\rangle \equiv \int d^3r\, \phi(\boldsymbol{r})\psi(\boldsymbol{r})$, without conjugation!
- In reciprocal space
  $\langle\phi|\psi\rangle = \int \frac{d^3q}{(2\pi)^3}\, \phi(-\boldsymbol{q})\psi(\boldsymbol{q}) = \int \frac{d^3q}{(2\pi)^3}\, \phi(\boldsymbol{q})\psi(-\boldsymbol{q})$.
- With this product $\hat{\epsilon}^{LL}$ becomes symmetric!

$$\langle\phi|\hat{\epsilon}^{LL}|\psi\rangle = \int \frac{d^3q}{(2\pi)^3} \int \frac{d^3q'}{(2\pi)^3}\, \phi(-\boldsymbol{q})\hat{\boldsymbol{q}}\cdot\epsilon(\boldsymbol{q}-\boldsymbol{q}')\hat{\boldsymbol{q}}'\psi(\boldsymbol{q}')$$
$$= -\int \frac{d^3q}{(2\pi)^3} \int \frac{d^3q'}{(2\pi)^3}\, \phi(\boldsymbol{q})\hat{\boldsymbol{q}}\cdot\epsilon(-\boldsymbol{q}-\boldsymbol{q}')\hat{\boldsymbol{q}}'\psi(\boldsymbol{q}').$$

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Spinors

- Periodic system: Bloch's vector $\boldsymbol{k}$, reciprocal lattice $\{\boldsymbol{G}\}$.

$$\langle\phi|\hat{\epsilon}^{LL}|\psi\rangle = \int_{\mathrm{BZ}} \frac{d^3\boldsymbol{k}}{(2\pi)^3} \sum_{\boldsymbol{G}} \sum_{\boldsymbol{G}'} \phi(-\boldsymbol{k}-\boldsymbol{G}) \hat{\boldsymbol{G}} \cdot \epsilon_{\boldsymbol{G}-\boldsymbol{G}'} \hat{\boldsymbol{G}}' \psi(\boldsymbol{k}+\boldsymbol{G}'),$$

- mixes Bloch's vectors $\boldsymbol{k}$ with $-\boldsymbol{k}$!
- Bloch's vector is conserved by the response, $\pm\boldsymbol{k}$ are mixed by the metric!
- Spinor-like representation.

$$|\zeta\rangle \to \begin{pmatrix} \zeta(\boldsymbol{k}+\boldsymbol{G}) \\ \zeta(-\boldsymbol{k}+\boldsymbol{G}) \end{pmatrix}.$$

Matricial Formulation

- Dielectric response

$$\hat{\epsilon}^{LL} \rightarrow \begin{pmatrix} \hat{\boldsymbol{G}}_{\boldsymbol{k}} \cdot \epsilon_{\boldsymbol{G}-\boldsymbol{G}'} \hat{\boldsymbol{G}'}_{\boldsymbol{k}} & 0 \\ 0 & \hat{\boldsymbol{G}}_{-\boldsymbol{k}} \cdot \epsilon_{\boldsymbol{G}-\boldsymbol{G}'} \hat{\boldsymbol{G}'}_{-\boldsymbol{k}} \end{pmatrix}.$$

- Internal product

$$\langle \phi | \psi \rangle = \sum_{G} \left(\phi(-\boldsymbol{k} - \boldsymbol{G}) \psi(\boldsymbol{k} + \boldsymbol{G}) + \phi(\boldsymbol{k} - \boldsymbol{G}) \psi(-\boldsymbol{k} + \boldsymbol{G}) \right).$$

Haydock's recursion

- Initial state: macroscopic plane wave.

$$|0\rangle \rightarrow \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \delta_{\mathbf{G}0},$$

- Haydock recursion

$$b_{n+1} |n+1\rangle = \hat{\epsilon}^{LL} |n\rangle - a_n |n\rangle - b_n |n-1\rangle ,$$

$$\langle n|m\rangle = \delta_{nm}$$

$$a_n = \langle n|\hat{\epsilon}^{LL}|n\rangle$$

$$b_{n+1}^2 = (\langle n| \hat{\epsilon}^{LL} - a_n \langle n| - b_n \langle n-1|) (\hat{\epsilon}^{LL} |n\rangle - a_n |n\rangle - b_n |n-1\rangle).$$

Macroscopic response

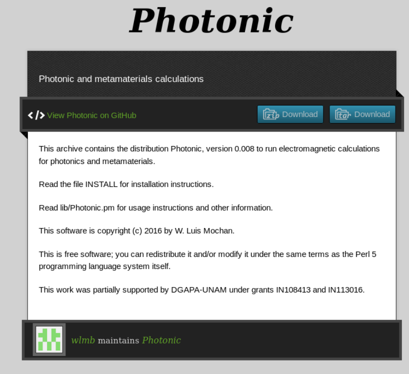
- In Haydock's basis, the response is a tridiagonal symmetric matrix

$$\hat{\epsilon}^{LL} \to T_{nn'} = \begin{pmatrix} a_0 & b_1 & 0 & 0 & \dots \\ b_1 & a_1 & b_2 & 0 & \dots \\ 0 & b_2 & a_2 & b_3 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

- Macroscopic response

$$\epsilon_M^{LL} = \left(a_0 - \cfrac{b_1^2}{a_1 - \cfrac{b_2^2}{a_2 - \cfrac{b_3^2}{\ddots}}} \right).$$

Photonic


Photonic

Photonic and metamaterials calculations

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This archive contains the distribution Photonic, version 0.008 to run electromagnetic calculations for photonics and metamaterials.

Read the file INSTALL for installation instructions.

Read lib/Photonic.pm for usage instructions and other information.

This software is copyright (c) 2016 by W. Luis Mochan.

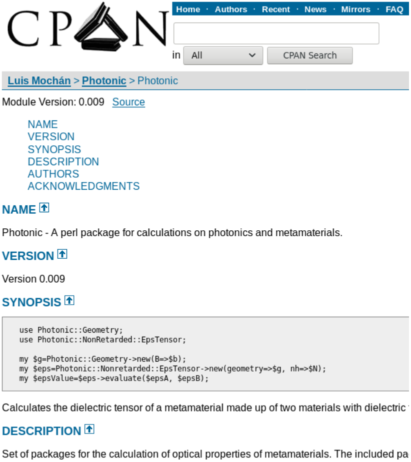
This is free software; you can redistribute it and/or modify it under the same terms as the Perl 5 programming language system itself.

This work was partially supported by DGAPA-UNAM under grants IN108413 and IN113016.

wlmb maintains *Photonic*

- PERL
- PDL
- Moose
- Public domain
  - Github
  - CPAN

Photonic



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Luis Mochán > Photonic > Photonic

Module Version: 0.009 Source

NAME
VERSION
SYNOPSIS
DESCRIPTION
AUTHORS
ACKNOWLEDGMENTS

NAME

Photonic - A perl package for calculations on photonics and metamaterials.

VERSION

Version 0.009

SYNOPSIS

```
use Photonic::Geometry;
use Photonic::NonRetarded::EpsTensor;

my $g=Photonic::Geometry->new(B=>$b);
my $eps=Photonic::Nonretarded::EpsTensor->new(geometry=>$g, nh=>$N);
my $epsValue=$eps->evaluate($epsA, $epsB);
```

Calculates the dielectric tensor of a metamaterial made up of two materials with dielectric

DESCRIPTION

Set of packages for the calculation of optical properties of metamaterials. The included pa

- PERL
- PDL
- Moose
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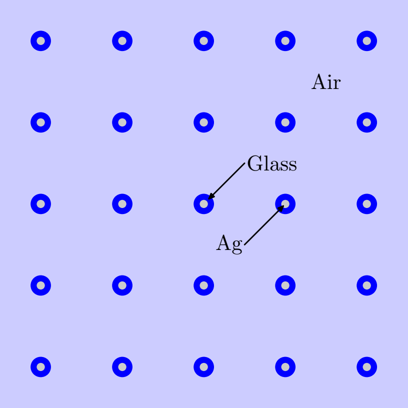
Coated cylinders



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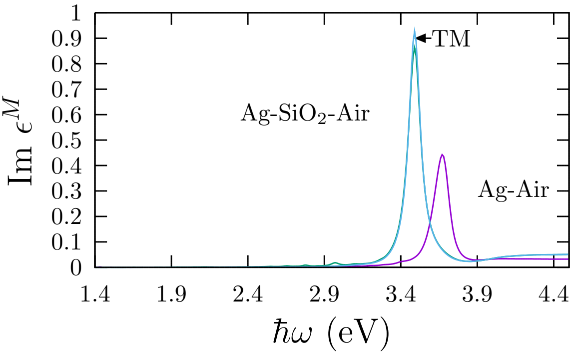
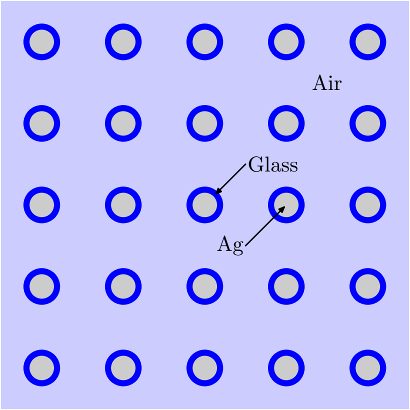


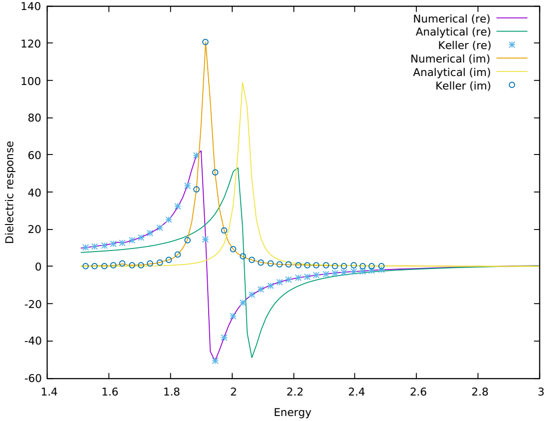
2D MG+cylindrical TM:

$$\epsilon_M = \frac{1 + 2\pi n\alpha}{1 - 2\pi n\alpha}$$

Coated cylinders

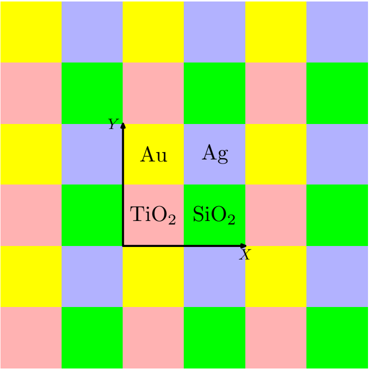


Coated cylinders



Generalized Keller: $\epsilon_M(\epsilon_1, \epsilon_2, \epsilon_3)\epsilon_M^R(1/\epsilon_1, 1/\epsilon_2, 1/\epsilon_3) = 1$

Mortola and Steffe



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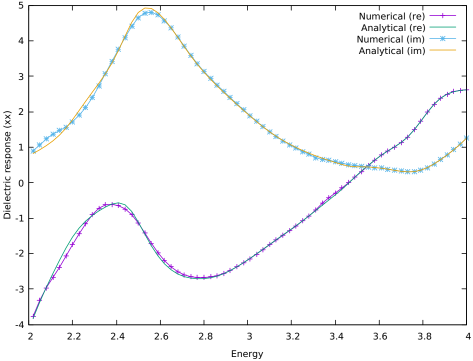


$$\begin{aligned}\epsilon_M^{xx} = & \{[(\epsilon_A+\epsilon_C)(\epsilon_B+\epsilon_D)(\epsilon_A\epsilon_B\epsilon_C+\epsilon_B\epsilon_C\epsilon_D \\ & +\epsilon_C\epsilon_D\epsilon_A+\epsilon_D\epsilon_A\epsilon_B)]/[(\epsilon_A+\epsilon_B)(\epsilon_C+\epsilon_D) \\ & \times(\epsilon_A+\epsilon_B+\epsilon_C+\epsilon_D)]\}^{1/2}.\end{aligned}$$

Retardation

- Wave equation:

$$\hat{\mathcal{W}}\boldsymbol{E} = \frac{4\pi}{i\omega}\boldsymbol{j}^{\text{ex}}$$

- Wave operator:

$$\hat{\mathcal{W}} = \hat{\epsilon} + \frac{c^2}{\omega^2}\nabla^2\hat{\mathcal{P}}_T$$

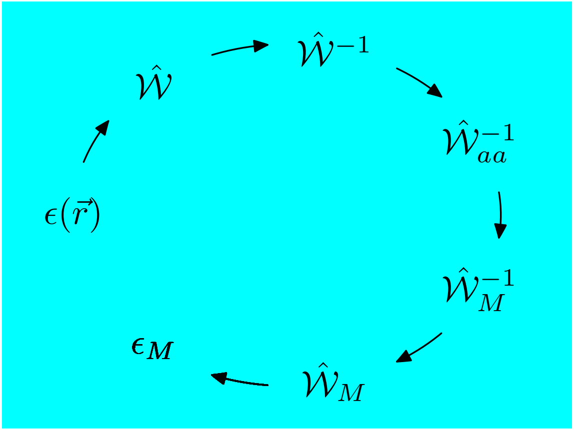
- Solution:

$$\boldsymbol{E} = \frac{4\pi}{i\omega}\hat{\mathcal{W}}^{-1}\boldsymbol{j}^{\text{ex}}$$

- Homogenization:

$$\hat{\mathcal{W}}_M^{-1} = \hat{\mathcal{W}}_{aa}^{-1}$$

Procedure



$$\Longrightarrow \epsilon_{ij}^{M}(\omega, \boldsymbol{k})$$

From spatial dispersion to magnetism

- $k^2 = \frac{\omega^2}{c^2}\epsilon(k,\omega)$
- $k^2 = \frac{\omega^2}{c^2}\left(\epsilon(k=0,\omega) + \frac{1}{2}k^2\frac{\partial^2}{\partial k^2}\epsilon(k=0,\omega)\right)$
- $k^2 = \frac{\omega^2}{c^2}\epsilon(\omega)\mu(\omega)$
- Local approximation:
  $\epsilon(\omega) = \epsilon(k=0,\omega)$,
  $\mu(\omega) = \frac{1}{1 - \frac{1}{2}\frac{\omega^2}{c^2}\frac{\partial^2}{\partial k^2}\epsilon(k=0,\omega)}$

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- $k^2 = \frac{\omega^2}{c^2}\left(\epsilon(k=0,\omega) + \frac{1}{2}k^2\frac{\partial^2}{\partial k^2}\epsilon(k=0,\omega)\right)$
- $k^2 = \frac{\omega^2}{c^2}\epsilon(\omega)\mu(\omega)$
- Local approximation:
  $\epsilon(\omega) = \epsilon(k=0,\omega)$,
  $\mu(\omega) = \frac{1}{1 - \frac{1}{2}\frac{\omega^2}{c^2}\frac{\partial^2}{\partial k^2}\epsilon(k=0,\omega)}$

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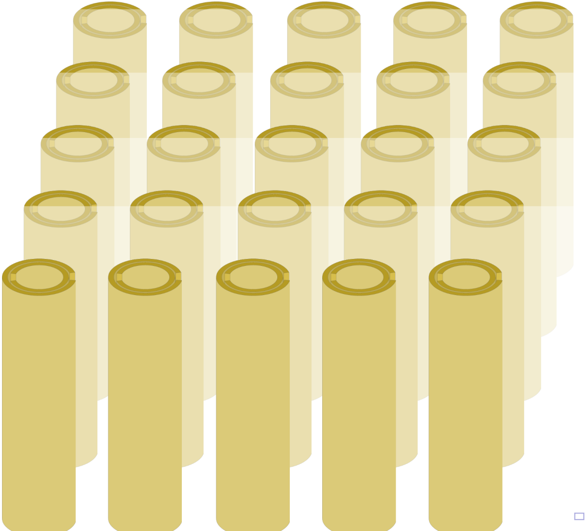
Split rings

$r_i = .26d, .32d, .34d, .4d$, hole$=.1d$, Drude: $\omega_p d/c = 20$



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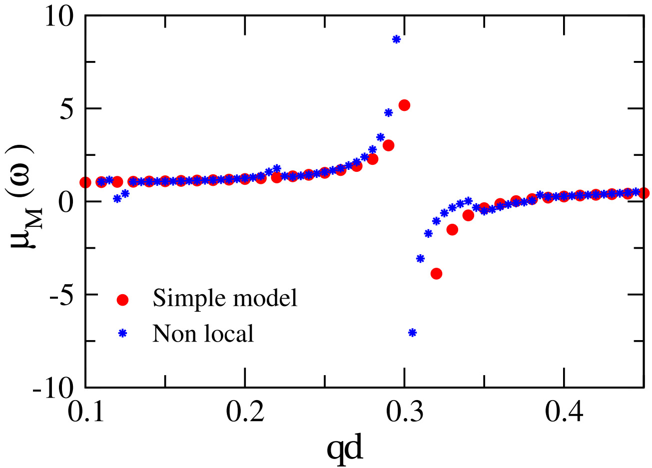

Conclusions

- Recursive procedure based on Haydock's representation.
- Macroscopic response (microscopic fields). Spectra.
- Metamaterials with arbitrary composition and geometry. Dielectric, metals, dispersive, dissipative...
- Efficient. For binary materials, geometry-response factorization.
- Generalization to arbitrary number of phases.
- Spinor representation $\rightarrow$ symmetric operators. Orthogonality theorems.
- Tested against analytical results.
- Generalization to retarded case $\rightarrow$ Spatial dispersion. Magnetism. (Chirality. Photonic bands.)
- Implemented in open/free computational package `Photonic`.