Photonic

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Collaborators

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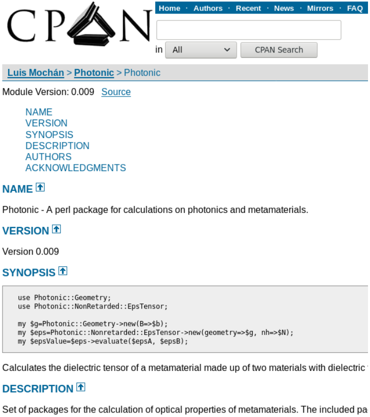
- Bernardo Mendoza
- Guillermo P. Ortiz

- Ed *mohawk2* (many improvements, contributions, suggestions, optimizations, modularization,. . .)

(Thanks to DGAPA-UNAM IN109822)

What is it?

A package to compute the optical properties of *metamaterials* and *photonic crystals*.



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Luis Mochán > Photonic > Photonic

Module Version: 0.009 Source

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SYNOPSIS
DESCRIPTION
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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

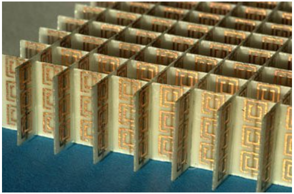
Set of packages for the calculation of optical properties of metamaterials. The included pa

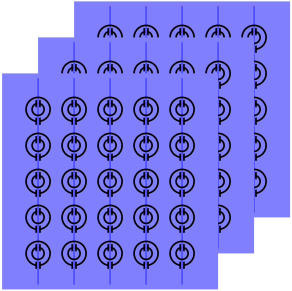
- Public domain
  - Github
  - CPAN
- Using
  - Perl
  - PDL
  - Moo

Metamaterials

Example: split rings

Material made from a mixture of *particles* of ordinary materials, properties usually differ from those of its components.





- *LC* like resonances in ϵ, μ.
- Can have $\epsilon < 0$ and $\mu < 0$, but $n^2 = \epsilon\mu > 0$, i.e., real index of refraction, propagation of e.m. waves.
- *Exotic* behavior from mix of ordinary materials, negative index of refraction $n < 0$.

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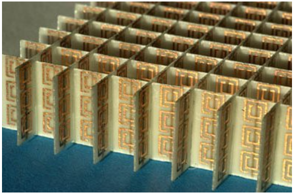

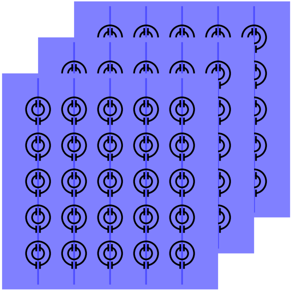

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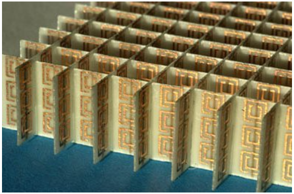

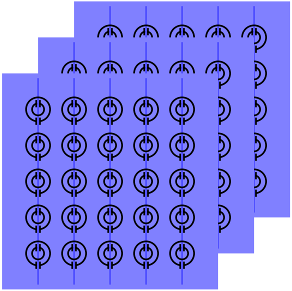

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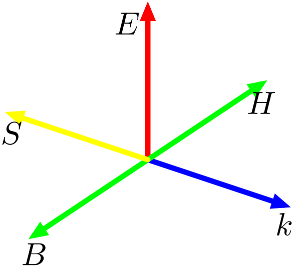
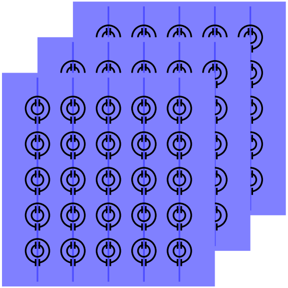
Left-handed materials

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

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

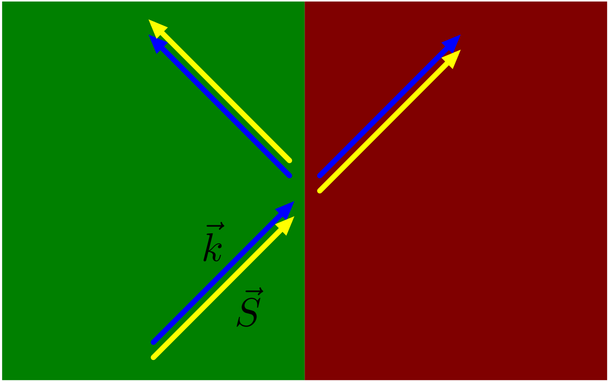




- but ***S*** (energy flux) would be opposite to ***k*** (phasae velocity). *Group velocity* opposes *phase velocity*.

Negative refraction

$n < 0$



Negative refraction

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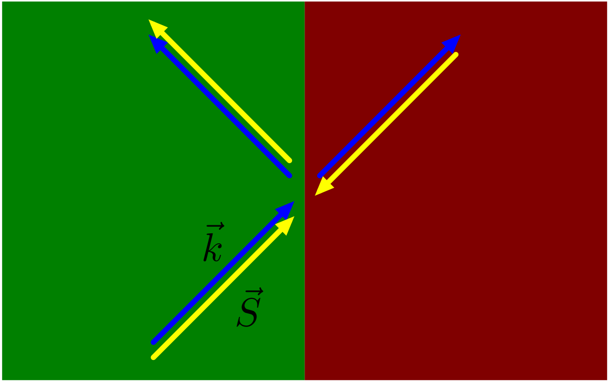

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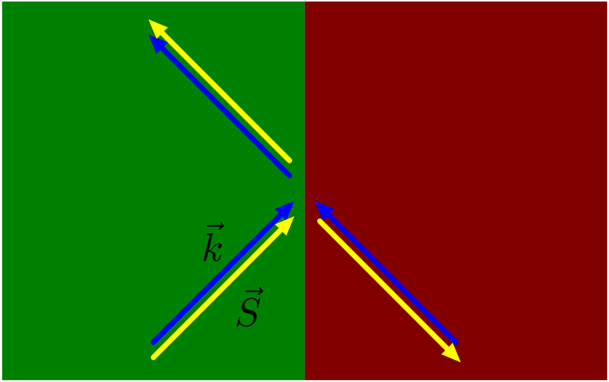
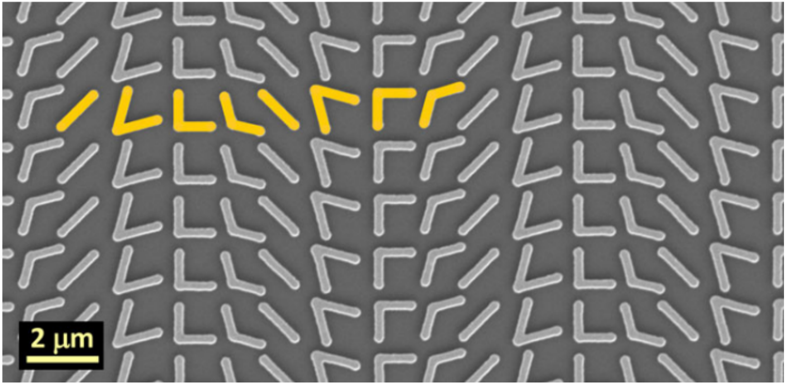


Metasurfaces



- Lateral phase controlled through geometry-dependent resonances. Controllable, polarization dependent refraction, *beyond* Snell's law.

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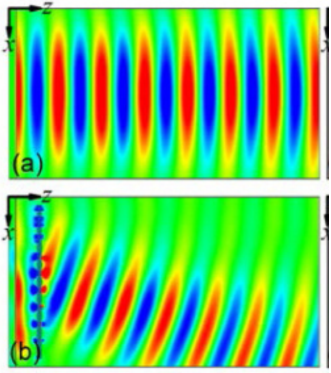

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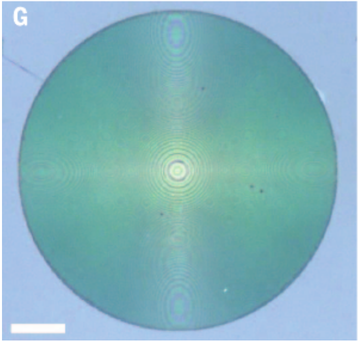

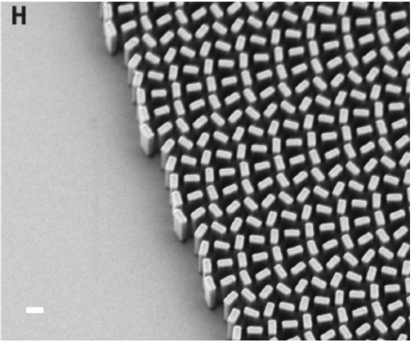

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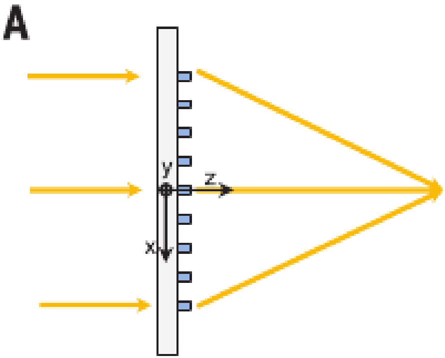
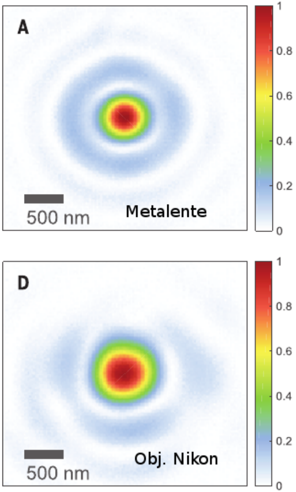
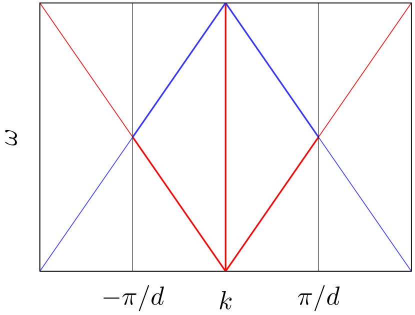




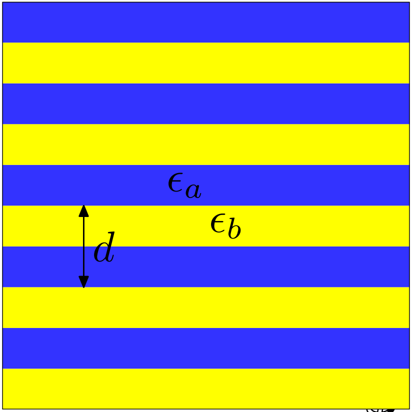
Photonic crystals

Superlattice

Photonic bands/gaps



$k \to k \pm 2\pi/d$



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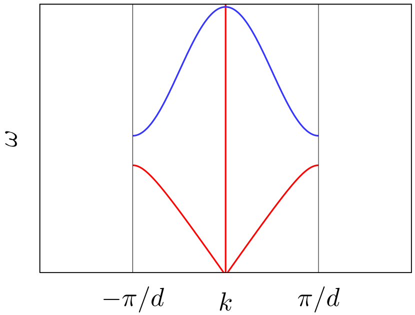

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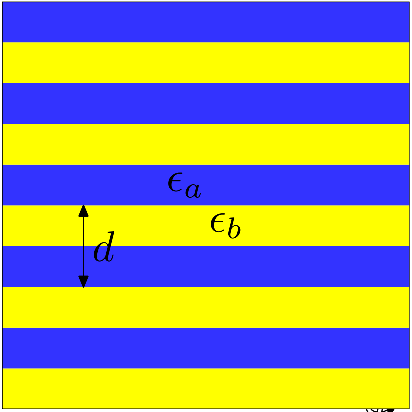
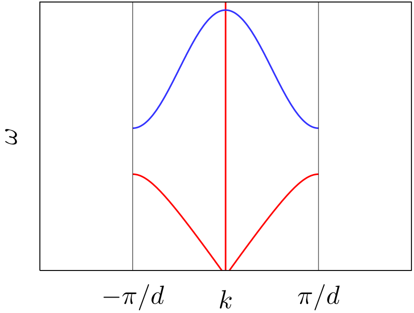
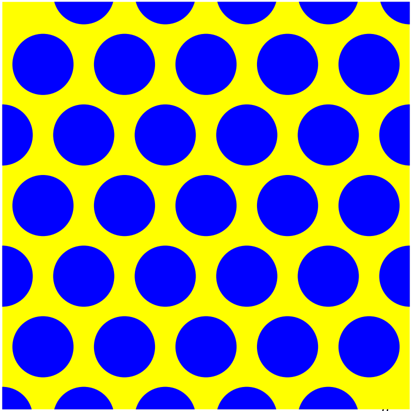


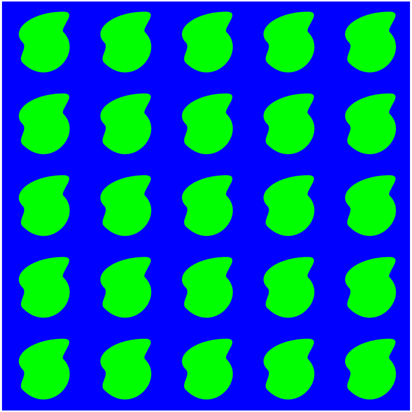
Photonic crystals
Absolute gap





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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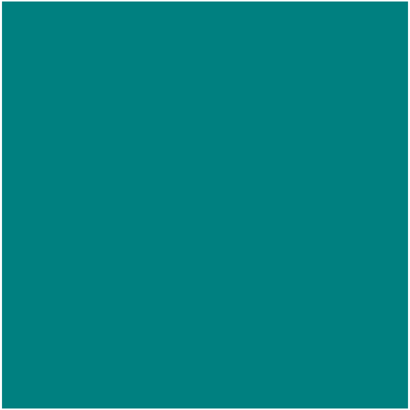

Theory

Macroscopic is not any *average*

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

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Macroscopic response

Example: Small scale, no retardation, longitudinal response

- $\boldsymbol{D}^L$ *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 $\boldsymbol{E}^{\mathrm{ex}}$ 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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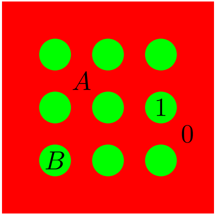
Periodic binary system

- $\epsilon(\boldsymbol{r}) = \begin{cases} \epsilon_B & \text{if } \boldsymbol{r} \in \text{inclusion}, \\ \epsilon_A & \text{if } \boldsymbol{r} \in \text{matrix} \end{cases}$
- Characteristic function of unit cell
  $B(\boldsymbol{r}) = \begin{cases} 1 & \text{if } \boldsymbol{r} \in \text{inclusion}, \\ 0 & \text{if } \boldsymbol{r} \in \text{host} \end{cases}$ (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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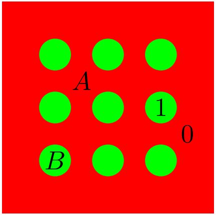

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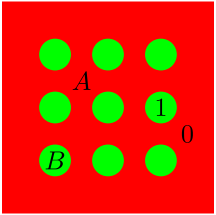

Quantum analogy

- Periodic system, reciprocal lattice (wavevectors) $\{\boldsymbol{G}\}$; average: $\boldsymbol{G} = 0$.
- $(\epsilon^{LL}_{GG'})^{-1} \equiv [\hat{\boldsymbol{G}} \cdot (\epsilon_{GG'} \hat{\boldsymbol{G}}')]^{-1} = \dfrac{1}{\epsilon_{ab}} [u - B^{LL}_{GG'}]^{-1}$
- $B^{LL}_{GG'} = \hat{\mathbf{G}} \cdot B_{\mathbf{G}-\mathbf{G}'} \hat{\mathbf{G}}' \longrightarrow \hat{H}$ *Hermitian operator* (like a Hamiltonian in QM),
  $u \longrightarrow \varepsilon$ *complex 'energy'*,

$$\frac{\epsilon_{ab}}{\epsilon^{LL}_{M}} = (u - B^{LL})^{-1}_{00} / \epsilon_{ab} \longrightarrow \hat{\mathcal{G}}_{00}(\varepsilon) = \langle 0 | (\varepsilon - \hat{H})^{-1} | 0 \rangle .$$

The macroscopic inverse longitudinal permittivity is analogous to a Q.M. *Green's* operator projected onto the *macroscopic state* $|0\rangle \equiv |\boldsymbol{G} = 0\rangle$.

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Haydock's recursion

- $|0\rangle \equiv |\boldsymbol{G} = 0\rangle$, $|-1\rangle \equiv 0$. Iteratively apply $\hat{H}$ and orthogonalize:
- $\hat{H}|n-1\rangle = b_n|n\rangle + a_{n-1}|n-1\rangle + b_{n-1}|n-2\rangle \longrightarrow$ Orthonormal basis $\{|n\rangle\}$ in which $\hat{H}$ is tridiagonal.
- $a_{n-1} = \langle n-1|\hat{H}|n-1\rangle$
  $b_n^2 = ||H\,|n-1\rangle\,||^2 - a_{n-1}^2 - b_{n-1}^2$.
- $\hat{H} \to B^{LL}_{GG'} = \hat{\boldsymbol{G}} \cdot B_{\boldsymbol{G}-\boldsymbol{G}'}\hat{\boldsymbol{G}}'$
- $\hat{H}|n\rangle$ is obtained by multiplying $\psi_n(\boldsymbol{G}) \equiv FT[\psi_n(\boldsymbol{r})] = \langle \boldsymbol{G}|n\rangle$
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$\rightarrow a_n$ and b_n without matrix multiplications!

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Theory summary

- There are *microscopic* operators $\hat{\mathcal{O}}$ whose *macroscopic* counterpart $\hat{\mathcal{O}}_M$ obeys

$$\hat{\mathcal{O}}_M^{-1} = \langle(\hat{\mathcal{O}}^{-1}\rangle = \langle 0|\hat{\mathcal{O}}^{-1}|0\rangle\,,$$

  i.e., they are *averagable*, invert some operator and project onto *macroscopic* state.
- For example $\dfrac{\hat{\epsilon}^{LL}}{\epsilon_{AB}} = u - \hat{B}^{LL}$ for binary metamaterials in the nonretarded regime.
- Haydock's *recursion*: Construct basis $\{|n\rangle\}$ and Haydock coefficients a_n, b_n: apply $\hat{\mathcal{O}}$, orthogonalize, normalize, repeat... Alternate between real and Fourier space, avoid big matrices.
- Initialize with macroscopic state $|0\rangle = |\boldsymbol{G} = 0\rangle$ in reciprocal (Fourier, wave-vector) space.
- $\hat{\mathcal{O}} \to$ tridiagonal matrix with a_n in the main diagonal, b_n in the sub- and supradiagonals, and 0 elsewhere.

Continued fraction

- Macroscopic response relates to element (0,0) of the inverse of a tridiagonal symmetric matrix with elements $u - a_n$, $-b_n$,

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

- 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.

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Extensions

- Retardation. Lengthscale of structure comparable to wavelength of light (or even larger).
- More than two components.
- Anisotropic components.
- All of the above.
- Obtain permittivity, temporal and spatial dispersion, electromagnetic fields, photonic bands, Green's functions, reflection amplitudes, optical activity (chirality), permeability, non-linear fields, non-linear response…

Example

- Full spectra as expensive as a single value.
- 2D binary case runs in a few seconds in one core of an old (12 years) laptop.
- Easily parallelizable using `PDL::ParallelCPU` (`set_autopthread_targ` and `set_autopthread_size`).
- Can be used to tune resonance frequencies, transmission, absorption and reflection spectra, polarization, etc. Allows design of photonic devices through optimization of their geometric parameters.

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Classes, Roles

- Join pieces to build programas (choose Geometry; Haydock; dielectric Tensor, Field, Green's function...).
- Obtain `Geometry` from characteristic function, 2D pixelated image, dielectric function, dielectric tensor: `Photonic::Geometry::FromB`, `::FromImage2D`, `::FromEpsilon`, `::FromEpsilonTensor` consume the `Photonic::Roles::Geometry` role.
- Calculate Haydock coefficients from the nonretarded, longitudinal permittivity ϵ of binary system, from the wave equation of retarded multicomponent system using spinor representation, etc. `Photonic::LE::NR2::Haydock`, `::WE::S::Haydock`...consume the `Photonic::Roles::Haydock` role.
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Application example

- Bouligand structure
- Bands, forbidden gap for circularly polarized light of one helicity $\longrightarrow$ strong metallic like reflections, circularly polarized.

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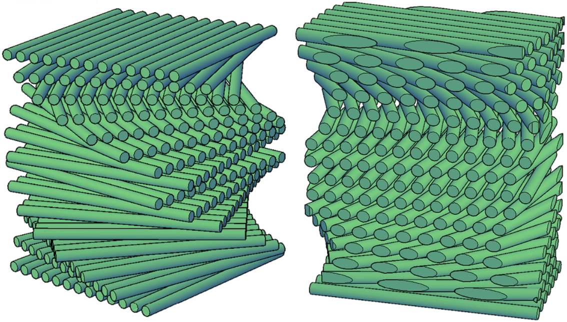

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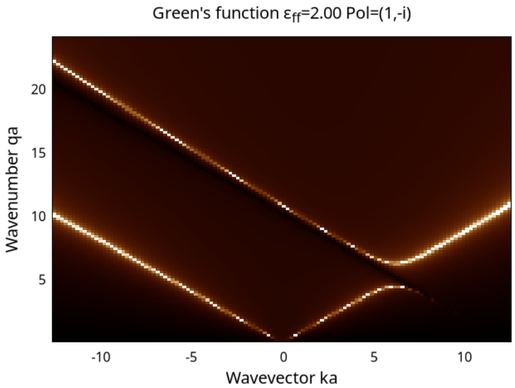

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Conclusions

- Recursive procedures based on Haydock's representation.
- Maxwell's equations translated to Hermitian or symmetric operators that act efficiently alternating between real and reciprocal (Fourier) space.
- Macroscopic response, temporal and spatial dispersion, spectra, photonic bands, microscopic fields.
- Metamaterials with arbitrary composition and geometry. Dielectric, metals, dispersive, dissipative. . .
- Implemented in open/free computational package **Photonic**
- using **Perl** with **Moo** objects (classes, roles) and the **Perl Data Language** PDL packages for efficient number crunching.

W. Luis Mochán, Guillermo P. Ortiz, doi:10.48550/arXiv.2309.11632