

Poor's Man Guide to 2D Metamaterial Optical Properties

Based on Haydock's Scheme

by

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## I. FOR THE IMPATIENTE

In Sec. XV you'll find an example that cuts through the chase, and perhaps this is where you should start, if you have read at least once this manual.

## II. INTRODUCTION

These are the steps to be followed in order to calculate the optical properties of a 2D binary metamaterial, characterized by  $\epsilon_a(\omega)$  and  $\epsilon_b(\omega)$ . Here  $a$  represents the host material and  $b$  the inclusion, that could have any shape.

Warning: So far it works for  $\epsilon_b$  a complex/real number and  $\epsilon_a$  a complex/real number or a file. For vacuum filled inclusions, chose  $\epsilon_b = 1.01$  and NOT  $\epsilon_b = 1$ .

Warning: Give the name of the dielectric functions as:

- If a file: `eps_name.dat`, where `name` is the name of the element or material. `name` is used by the scripts, so is very importnat to have this nomenclature.
- If a number: `R+i*I`, where `R` is the real part and `I` is the imaginary part. Either one could be positive or negative.

Glossary:

- WD: is the Working Directory. Try to use a nemotecnic name, for instance, making reference to the shape of the inclusion.

- **drawing**: the name of the original unit cell, try to use a mnemonic name, for instance, making reference to the shape of the inclusion.

**WARNING: Don't use underscore \_ in the name!**

- **path**: is the path to the directory with the programs.
- **>** : command line.
- **--od**: output directory.
- **gnuplot>**: gnuplot screen.

### III. SOFTWARE INSTALLATION

1 **untar** or **svn** the latest version of the software. In **programs/how-to-svn.txt** WLM has written partial instructions for **svn**.

2 The software tree is:

- **programs**
  - **programs/exec** the executables **perl** files and one **awk** auxiliary file.
  - **programs/exec/utilidades** auxiliary goodies files.
  - **programs/2torial/text** files and subdirectories for the **how-to-run.tex** file.
  - **programs/2torial/example** an example with all the files and subdirectories generated.

3 **WARNING** Edit **programs/exec/the-whole-enchilada.pl** and put the full path where you installed the **programs** directory.

In **programs/exec/the-whole-enchilada.pl** look for

```
##### PUT THE PATH #####
```

```
my $ruta="path/programs/exec";
```

and put your own path.

Do this every time you change the location of **programs**.

#### IV. CRIMES AND MISDEMEANORS

You must be warned that this software is under continuous development and you may correct/improve/play as you freaking wish. Here are some, but not all, minor caveats that may be handy, but please, by no means blame the, so far, only author of this, must humble, manual.

- `whole-enchilada.pl`

```
# scale factor for color maps  
my $sfcm=150;
```

change the 150 to control the color maps, I wish you good luck.

- `rm-angle.pl`

calculates the complex principal angles given  $\epsilon_M$  in the crystal axis.

#### V. INITIALIZATION

We suggest to use the following directories within your chosen Working Directory (WD)

- > `mkdir WD` (Try to use a mnemonic name, for instance, making reference to the shape of the inclusion.)
- > `cd WD`
  - **Warning:** Work in WD **always!**
- WD > `mkdir cases ucell hc res meps plots movies arrows rt`
- **cases:** unit cells
- **ucell:**  $3 \times 3$  array of a unit cells
- **hc:** Haydock Coefficients
- **res:** files with the E-fields and Polarization
- **epsm:** files with macroscopic dielectric function
- **plots:** file with the plots

- `movies`: file with movies
- `arrows`: files with arrows

## VI. INKSCAPE

Draw the unit cell with `Inkscape`

- 1 Open `Inkscape`
- 2 In `file`→`Document Properties`→`Page`→`Custom size`
  - Chose the `Width` and `Height` of the 2D unit cell in pixels.
    - They should be an odd number.
    - The higher (lower) the number of pixels the better (worse) the resolution.
    - Square unit cells have `W=H`.
    - **Example:**  $201 \times 201$ .
- 3 Click in `Background` and use 255 in option A, so the background is transparent.
- 4 In the lower right corner of the screen you can chose the viewing size of the unit cell, usually 200% is good enough.
- 5 Draw the inclusion and make sure that it is totally black.
  - Try not to fill the unit cell.
- 6 Position the inclusion as you wish within the unit cell. For fine tuning the position **click** on the figure and at the top menu will appear `X Y W H`, that are the  $(x, y)$  position and (width,height) of the inclusion.
- 7 Save: `file`→`save`, be sure tu put the `drawing.svg` in your chosen working directory (WD). For `drawing` try to use a mnemonic name, for instance, making reference to the shape of the inclusion.
- 8 Export: `file`→`Export Bitmap`→`Page`→`Export`.  
Be that sure that `Width` and `Height` are the same as those of 2. You must have `drawing.png` in your WD.

## VII. MAGICK

- WD> path/magick.pl
- follow instructions.
- We recommend to call --od=cases/
- The  $3 \times 3$ -tiled unit cells are in ucell/

## VIII. HAYDOCK COEFFICIENTS

- WD> path/corre-base.pl
- Follow instructions.
- The input file, which is the unit cell, is in WD/cases/
- You can select fixed-angle and variable-scale or viceversa, using  
  > ls path/files\*.png
- We recommend to call --od=hc/
- Output in pld format.

## IX. ELECTRIC FIELDS

- WD> path/corre-fields.pl
- Follow instructions.
- You can select fixed-angle and variable-scale or viceversa, using  
  > ls path/files\*.png
- We recommend to call --od=res/
- Output in ascii files (e,p)-\*.dat and (e,p)-\*.dat-v

---

## X. MACROSCOPIC DIELECTRIC FUNCTION

- WD> path/fracCont.pl
- Follow instructions.
- If you followed our humble recommendation the Haydock coefficients are in  
--haydock=hc/filename
- We recommend to call --od=epsm/
- Output in epsm/eps-\* with lots of information. See the header of the file. In particular the Normal Incidence Reflectivity,  $R_i$ , given by

$$R_i(\omega) = \left| \frac{\sqrt{\epsilon_i(\omega)} - 1}{\sqrt{\epsilon_i(\omega)} + 1} \right|^2, \quad (1) \quad \{\text{nir}\}$$

for Principal Axis  $i = 1, 2$  is in gnuplot variable `nir1` and `nir2`, so you can plot with

- gnuplot> p 'file' u "w":"nir(1,2)"

## XI. PLOTS

For Electric field and Polarization:

- For one plot:
  - WD> path/plots.pl
  - Follow instructions.
  - We recommend to call --od=plots/
- For several plots:
  - WD> path/corre-plots.pl
  - Follow instructions.
  - You can sort according to angles (`scale`) [`energy`] for fixed scale (`angle`) [`angle`] and energy (`energy`) [`scale`].
  - We recommend to call --od=plots/

- Output in png files.
- **Warning:** Calculate the plots for *both*  $(E, P)_x$  and  $(E, P)_y$  incident fields given as
  - `plots/(e,p)-*_dir_xx*` or `plots/(e,p)-*_dir_yy*`
- `--cell=[1,2]` chooses one unite cell [1] or a  $2 \times 2$  array [2] for most *biutiful* plots.

For Reflection

- WD> `path/plot-angles.pl`
  - Follow instructions.

## XII. MOVIES

We thank Liliana Wilson-Herrán for her help in developing these part of the Code, during a two week summer training.

To generate the movie for  $R_i(\omega)$  along with the intensity maps of the total electric field or polarization for both  $E_x$  and  $E_y$  incident fields follow:

- WD> `path/corre-arrows.pl`
  - Follow instructions.
  - We recommend to call `--od=arrows/`
  - If you followed our humble recommendation the  $R_i(\omega)$  data is in `--idf=epsm/`
  - We recommend to use `--tam=.1` for the arrows.
- WD> `path/corre-3g.pl` or `path/corre-4g.pl`
  - follow instructions.
  - We recommend to call `--od=movies/`
  - **Warning** use the name of the material in `--eps(a,b)` where the name comes from the \* in `eps_*.dat`. Here \* is the name of the material.

- To obtain the files that make up the movies, use the option “`--keep`”. We recommend to use `--od=keep`, so in the `WD/keep` you should get the `(e,p)-lrem_*` files, that you could use at your free will (although with a 300ms delay!, free will, of course!).

### XIII. DIPOLAR FIELDS

Run the following program to calculate the dipolar field of a square array of cylindrical inclusions.

- `dipolar.pl`

Follow instructions. In Sec. XVI B we show some results.

### XIV. THE-HOLE-ENCHILADA

We have prepared the file `the-whole-enchilada.pl` that as you may have guessed correctly, runs “the-whole-enchilada”. Edit `programs/exec/the-whole-enchilada.pl` to set up the following variables on your computer:

- `$ruta=path` to the place of the programs.
- The variable `$sfcm` is used to accentuate the color contrast in the color maps. `$sfcm=150` seems to work well.

`the-whole-enchilada.pl` follows these steps in the given order:

- 1 Calculates the Haydock Coefficients using the Crystal axes.
- 2 Calculates the Marcoscopic  $\epsilon^M(\omega)$  using the crystal axes  $X$  and  $Y$ .
- 3 Calculates the Marcoscopic (diagonal)  $\epsilon_{x,y}^M(\omega)$  along the principal axes  $x$  and  $y$ .
- 4 Calculates the Reflectivity  $R_{x,y}$  along principal axes.
- 5 Calculates the Haydock Coefficients using the principal axes.
- 6 Calculates the Electric Field and Polarization using the principal axes.
- 7 Does movies of the Electric Field and Polarization using the principal axes.

- 8 Draws the *ellipses representing the polarization*.
- 9 As it runs, shows on the screen the relevant signs explaining what is being done!
- 10 It does all the necessary steps and whatever else not mentioned here, so don't put the blame on me!

## XV. EXAMPLE

### A. Run

The steps for running are henceforth summarized:

- 1 Work in WD
- 2 WD > mkdir cases ucell hc res meps plots movies arrows rt
- 3 Copy a `eps_name.dat` dielectric function.
- 4 Draw the unit cell (see Sec. VI)
- 5 Run `magick.pl` (see Sec. VII)
- 6 Run `the-whole-enchilada.pl` (see Sec. XIV)

With option:

- `--cual=ronly` only calculates the Reflection.
- `--cual=all` calculates the Reflection and the fields.

- 7 **To run again:** well we need a daring young soul to code and avoid multiple recalculation of what was calculated and may not be needed again. But till brave soul comes along, follow these steps and let the computer do the job once more once

7.1 `rm -rf arrows/ meps/ plots/ res/ hc/ rt/ movies/`

- 8 **Isotropic Inclusions:** run using the `--fixedangle=0` option.
- 9 `programs/exec/tochito.sh` calculates the reflection and transmission of a thin film and makes a movie of the ellipses of polarization. You can copy the file to WD and modify it *ad libitum*.

10 In `programs/exec/2torial/example` there is an example, where `programs/exec/2torial/example/step-by-step.sh` has some of the required steps to run.

11 Indulge yourself and try `dipolar.pl`

The instructions of `the-whole-enchilada.pl` are simple to follow, and the “trick” is to give a set of units cells to be run in the variable `--case`, i.e.,

`--case=cases/elipse_A*S1.2*`

will select all the different angles chosen in `magick.pl` for the fixed scale factor `S=1.2`, where the shape of the inclusion is an `elipse`.

In `path/2torial/example` we have `elipse.png` and `eps_au.dat` for you to rejoice and run an example. The unit cell is  $51 \times 51$  pixels so it runs rather fast. So, if you follow above instructions and run (with 25 Haydock coefficients, so is fast)

```
PWD> path/the-whole-enchilada.pl --Nh=25 --epsa=eps_au.dat --epsb=4 --nem=ave  
--case=cases/elipse_A25.00_S1.200_f0.304.png
```

you should get the following movies, that can be played with `Acro Read` using the buttons!

Microscopic **E** field

Microscopic Polarization

## B. Redo the Plots

If for some reason you want to redo only the plots, like you changed a line style, or frequency range, etc. do the following easy steps, so you don not have to calculate unnecessary files.

1 Create a `new` directory within PWD

2 PWD/hc> `ls * > hoy`

3 PWD/new> `mv ../hc/hoy .`

4 PWD/new> `sort -tW -n -k 2 hoy > lista`

after `-t` put the identifier for the sorting, if any!

5 Edit `lista` or `hoy`, so you have the set you may want to redo the plots with. For instance select a few frequencies.

6 PWD/new> `awk '{print "ln -s","..../..../hc/"$1,$1}' lista >lista2`

7 PWD/new> `./lista2`

so now you have a symbolic link to the required files

8 Repeat from step 2 to step 7 for directory `res`

9 PWD/new> `rm arrows/* plots/* movies/*`

or any combination that you want to redo.

10 Run `the-whole-enchilada.pl` just as you did the last time, and voilà!

## XVI. INTERNAL CHECKUPS

### A. P · E approach

As an internal check up we compare the reflectivity of Eq. 1 calculated through the macroscopic dielectric function  $\epsilon$ , and the Polarization  $\mathbf{P}$ . We recall that

$$\mathbf{D}(\mathbf{r}) = \mathbf{E}(\mathbf{r}) + 4\pi\mathbf{P}(\mathbf{r}) = \epsilon(\mathbf{r}) \cdot \mathbf{E}(\mathbf{r}), \quad (2) \quad \{\text{pol1}\}$$

we multiply by  $\mathbf{E}(\mathbf{r})$  to obtain

$$\mathbf{E}(\mathbf{r}) \cdot \mathbf{E}(\mathbf{r}) + 4\pi \mathbf{P}(\mathbf{r}) \cdot \mathbf{E}(\mathbf{r}) = \epsilon(\mathbf{r}) \cdot \mathbf{E}(\mathbf{r}) \cdot \mathbf{E}(\mathbf{r}), \quad (3) \quad \{\text{pol12}\}$$

working on principal axis  $i$ ,

$$\begin{aligned} E_i^2(\mathbf{r}) + 4\pi P_i(\mathbf{r})E_i(\mathbf{r}) &= \epsilon_i(\mathbf{r})E_i^2(\mathbf{r}) \\ P_i(\mathbf{r})E_i(\mathbf{r}) &= \frac{1 - \epsilon_i(\mathbf{r})}{4\pi}E_i^2(\mathbf{r}). \end{aligned} \quad (4)$$

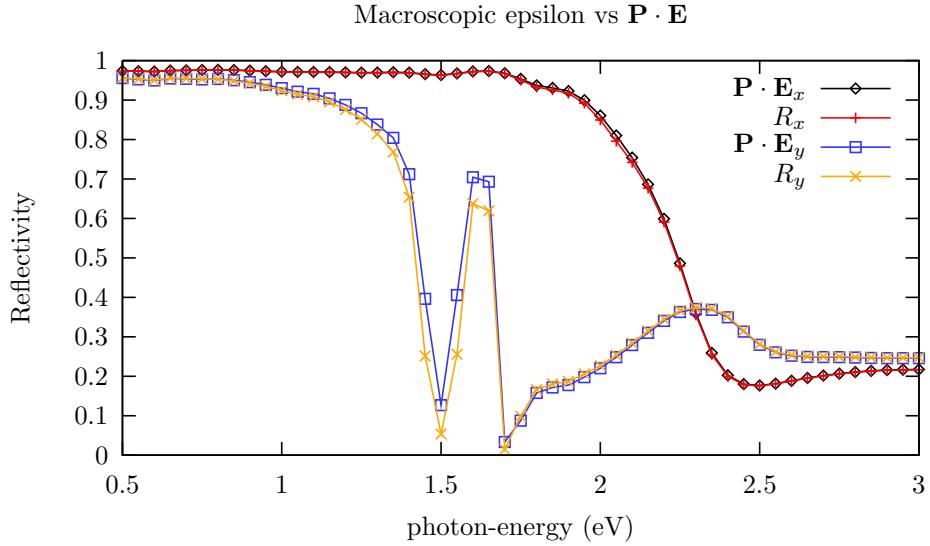
Above can be calculated inside ( $\epsilon_i(\mathbf{r}) = \epsilon_{bi}$ ) and outside ( $\epsilon_i(\mathbf{r}) = \epsilon_{ai}$ ) the inclusion, since we know the microscopic field  $\mathbf{E}(\mathbf{r})$  (in this case, along the principal axis). Once we have  $\mathbf{P} \cdot \mathbf{E}$  inside and outside the inclusion, we can calculate the macroscopic  $\epsilon_i^M$  as

$$\epsilon_i^M = 1 + 4\pi \left( [P_i(\mathbf{r})E_i(\mathbf{r})] \Big|_{\mathbf{r} \in \text{inclusion}} + [P_i(\mathbf{r})E_i(\mathbf{r})] \Big|_{\mathbf{r} \notin \text{inclusion}} \right), \quad (5) \quad \{\text{pol14}\}$$

from where we can calculate the reflectivity (Eq. 1).

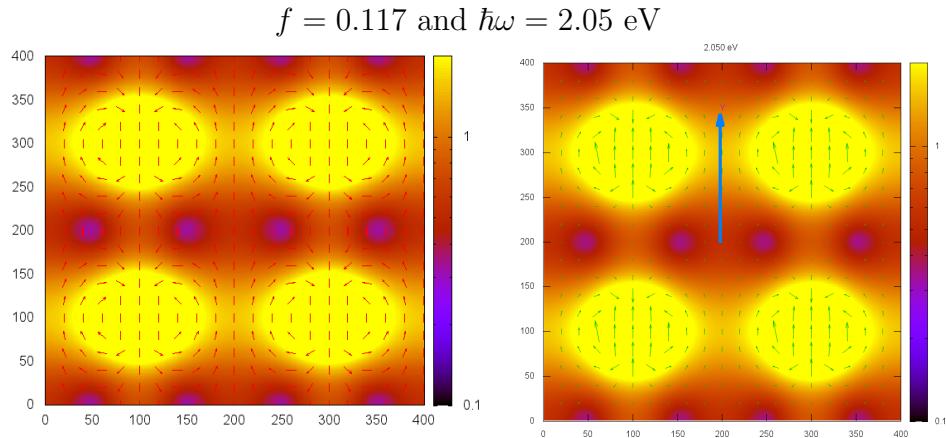
In the following figure we show the comparison of the two methods, from where we see a good agreement, confirming that the fields are correctly calculated. We do it for an ellipse, and the details are found in `programs/2torial/text/plots/A0`. In particular the file `pol1a.g` is used for the plot. We used a  $201 \times 201$  ellipse with  $\epsilon_a = \text{Au}$ ,  $ge_b = 4$  and  $N_H = 100$ .

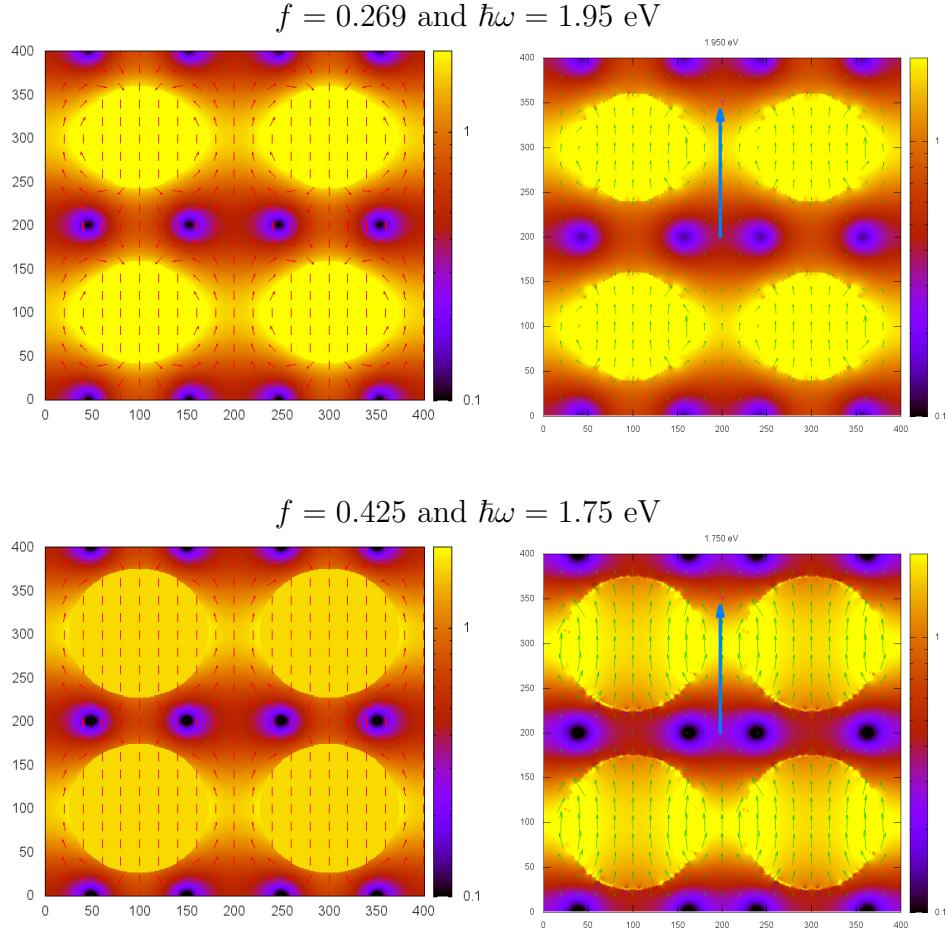
**Warning:** This check must be done by using the same axis for every energy value. So, it is recommended to do it for inclusions whose crystal axis are the same as the principal axis. That is why we choose the ellipse at  $0^\circ$ .



## B. Dipolar Approximation

Following the notes of WLM (yet to be L<sup>A</sup>T<sub>E</sub>X'ed), in the following plots we compare the full approach (Haydock's) with the analytical result of the Dipolar Field of an square array of cylindrical inclusions. We obtain that for small  $f$  both approaches are very similar, whereas for large  $f$ , the dipolar field differs from the full calculations, since the latter contains all different multipoles. However, for large  $f$  and low energy (high wavelength), the dipolar field could be rather similar to the full field. We dare the young soul to confirm such claim.





## XVII. NOTES

These are the notes for the calculation of the Fields as transcribed by SP

### A. General theory

We have shown how to get the macroscopic electromagnetic response of composite systems

We have propose an efficient homogenization procedure for the calculation of optical properties of nanostructured composites. we use Eq. (?) to obtain the optical properties of an artificial binary crystal made of two materials  $A$  and  $B$  with dielectric functions  $\epsilon_A$  and  $\epsilon_B$ . We assume that both media are local and isotropic so that  $\epsilon_A$  and  $\epsilon_B$  are simply complex functions of the frequency.

We introduce the characteristic function  $B(\mathbf{r})$  of the inclusions, such that  $B(\mathbf{r}) \equiv 1$  whenever  $\mathbf{r}$  is on the region  $B$  occupied by the inclusions, and  $B(\mathbf{r}) \equiv 0$  otherwise. Thus,

we may write the microscopic dielectric response as

$$\epsilon(\mathbf{r}) = \frac{\epsilon_A}{u} (u - B(\mathbf{r})) , \quad (6) \quad \{\text{epsmicr}\}$$

where we defined the spectral variable  $u \equiv 1/(1 - \epsilon_B/\epsilon_A)$ . The longitudinal projection of Eq. (6) may be written as

$$\hat{\epsilon}_{\mathbf{GG}'}^{LL} = \frac{\epsilon_A}{u} (u - B_{\mathbf{GG}'}^{LL}) , \quad (7) \quad \{\text{epsll1}\}$$

According to Eq. (??) we have to invert and take the **00** element

$$(\hat{\epsilon}_{\mathbf{GG}'}^{LL})_{\mathbf{00}}^{-1} = \frac{u}{\epsilon_A} (u - B_{\mathbf{GG}'}^{LL})_{\mathbf{00}}^{-1} , \quad (8) \quad \{\text{epsll1i}\}$$

Now we have used the recursion relation

$$\widetilde{|n+1\rangle} \equiv \hat{\mathcal{H}}|n\rangle = b_{n+1}|n+1\rangle + a_n|n\rangle + b_n|n-1\rangle , \quad (9) \quad \{\text{n+1}\}$$

where  $\hat{\mathcal{H}} = B_{\mathbf{GG}'}^{LL}$  and all the states  $|n\rangle$  are orthonormalized according to

$$\langle n|m \rangle = \delta_{nm} , \quad (10) \quad \{\text{ortonor}\}$$

with  $\delta_{nm}$  the Kronecker's delta function. The requirement of orthonormality yields the generalized Haydock coefficients  $a_n$ ,  $b_{n+1}$ , given the previous coefficients  $b_n$ , and  $a_{n-1}$ .

In the basis  $\{|n\rangle\}$ ,  $\hat{\mathcal{B}}$  is represented by a tridiagonal matrix with  $a_n$  along the main diagonal,  $b_n$  along the subdiagonal and  $b_n$  along the supradiagonal, so that

$$(u - \hat{\mathcal{B}}) \rightarrow \begin{pmatrix} u - a_0 & -b_1 & 0 & 0 & \dots \\ -b_1 & u - a_1 & -b_2 & 0 & \dots \\ 0 & -b_2 & u - a_2 & -b_3 & \dots \\ \vdots & \vdots & & \vdots & \ddots \end{pmatrix} . \quad (11) \quad \{\text{MWaveMa}\}$$

According to Eq. (?), we do not require the full inverse of the matrix (?), but only the element in the first row and first column. Following Ref. \cite{Mochan3}, we obtain that

element as a continued fraction, which substituted into Eq. (?) yields

$$(\hat{\epsilon}_{LL}^M)^{-1} = \frac{u}{\epsilon_A} \frac{1}{u - a_0 - \frac{b_1^2}{u - a_1 - \frac{b_2^2}{u - a_2 - \frac{b_3^2}{\ddots}}}}. \quad (12) \quad \{\text{chin}\}$$

The constitutive equation in the long wavelength limit is

$$\mathbf{D}_L = \hat{\epsilon}_{LL} \mathbf{E}_L, \quad (13) \quad \{\text{constit}\}$$

so electric field is

$$\mathbf{E}_L = (\hat{\epsilon}_{LL})^{-1} \mathbf{D}_L. \quad (14) \quad \{\text{EL}\}$$

Averaging  $\mathbf{E}_L$  we get

$$\mathbf{E}_L^a = (\hat{\epsilon}_{LL})_{aa}^{-1} \mathbf{D}_L^a + (\hat{\epsilon}_{LL})_{af}^{-1} \mathbf{D}_L^f, \quad (15) \quad \{\text{ELp}\}$$

but  $\mathbf{D}_L$  has not fluctuations,  $\mathbf{D}_L^f = \hat{\mathcal{P}}_f \mathbf{D}_L = \mathbf{0}$ . So

$$\mathbf{E}_L^a = (\hat{\epsilon}_{LL})_{aa}^{-1} \mathbf{D}_L^a. \quad (16) \quad \{\text{ELM}\}$$

or

$$\mathbf{E}_L^M = (\hat{\epsilon}_{LL})_{aa}^{-1} \mathbf{D}_L^M. \quad (17) \quad \{\text{ELMm}\}$$

In the basis  $\{|n\rangle\}$ ,  $\mathbf{D}^L$  is different of zero only in the first position,

$$\mathbf{D}_L \rightarrow \begin{pmatrix} \mathbf{D}_0 \\ \mathbf{0} \\ \vdots \\ \mathbf{0} \end{pmatrix}. \quad (18) \quad \{\text{d1}\}$$

but  $\mathbf{E}^L$  is a vector of the form

$$\mathbf{E}_L \rightarrow \begin{pmatrix} \mathbf{E}_0 \\ \mathbf{E}_1 \\ \vdots \\ \mathbf{E}_N \end{pmatrix}. \quad (19) \quad \{\text{e1}\}$$

So

$$\begin{pmatrix} \mathbf{D}_0 \\ \mathbf{0} \\ \vdots \\ \mathbf{0} \end{pmatrix} = \frac{\epsilon_A}{u} \begin{pmatrix} u - a_0 & -b_1 & 0 & 0 & \cdots & 0 \\ -b_1 & u - a_1 & -b_2 & 0 & \cdots & 0 \\ 0 & -b_2 & u - a_2 & -b_3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & -b_{N-1} & u - a_N \end{pmatrix} \cdot \begin{pmatrix} \mathbf{E}_0 \\ \mathbf{E}_1 \\ \vdots \\ \mathbf{E}_N \end{pmatrix}. \quad (20) \quad \{\text{consti}\}$$

therefore

$$-b_N \mathbf{E}_{N-1} + (u - a_N) \mathbf{E}_N = 0 \quad (21)$$

and gives for the last row

$$\mathbf{E}_{N-1} = \frac{u - a_N}{b_N} \mathbf{E}_N. \quad (22)$$

In general,

$$-b_n \mathbf{E}_{n-1} + (u - a_n) \mathbf{E}_n = b_{n+1} \mathbf{E}_n = 0 \quad (23)$$

so

$$\mathbf{E}_{n-1} = \frac{(u - a_n) \mathbf{E}_n - b_{n+1} \mathbf{E}_{n+1}}{b_n} \quad (24)$$

and finish as

$$(u - a_0) \mathbf{E}_0 - b_1 \mathbf{E}_1 = \frac{u}{\epsilon_A} \mathbf{D}_0 \quad (25)$$

cuidado, son vectores but

$$(u - a_0) - b_1 \mathbf{E}_1 / \mathbf{E}_0 = \frac{u}{\epsilon_A} \mathbf{D}_0 / \mathbf{E}_0 \equiv \frac{u}{\epsilon_A} \epsilon^M \quad (26)$$

and the microscopic field can be obtained as

$$\mathbf{E}_{\mathbf{G}} = \sum_n \mathbf{E}_n \hat{\mathbf{G}} \phi_n(\mathbf{G}) \quad (27)$$

where  $\phi_n(\mathbf{G}) = \langle \mathbf{G} | n \rangle$ , so

$$\mathbf{E}(\mathbf{r}) = \mathcal{F}^{-1}\{\mathbf{E}_{\mathbf{G}}\} \quad (28)$$

## XVIII. OPTICAL ACTIVITY

### A. Diagonalization

The eigenvalues and eigenvectors of a  $2 \times 2$  symmetric (complex) matrix  $M|\lambda_i\rangle = \lambda_i|\lambda_i\rangle$ , are obtained as follows. Let

$$M = \begin{pmatrix} M_{xx} & M_{xy} \\ M_{xy} & M_{yy} \end{pmatrix}. \quad (29) \quad \{\text{h.1}\}$$

Then,

$$\begin{aligned} \begin{vmatrix} M_{xx} - \lambda & M_{xy} \\ M_{xy} & M_{yy} - \lambda \end{vmatrix} &= (M_{xx} - \lambda)(M_{yy} - \lambda) - M_{xy}^2 \\ &= \lambda^2 - \lambda(M_{xx} + M_{yy}) + M_{xx}M_{yy} - M_{xy}^2 \\ &= \lambda^2 - \lambda\text{Tr}[M] + \text{Det}[M] = 0 \\ \rightarrow \lambda_{\pm} &= \frac{1}{2} \left( \text{Tr}[M] \pm \sqrt{(\text{Tr}[M])^2 - 4\text{Det}[M]} \right). \end{aligned} \quad (30)$$

The eigenvectors follow from

$$\begin{aligned} \begin{pmatrix} M_{xx} - \lambda & M_{xy} \\ M_{xy} & M_{yy} - \lambda \end{pmatrix} \begin{pmatrix} c \\ c \end{pmatrix} &= 0 \\ (M_{xx} - \lambda)c + M_{xy}d &= 0 \\ M_{xy}c + (M_{yy} - \lambda)d &= 0 \\ \rightarrow d &= \frac{\lambda - M_{xx}}{M_{xy}}c, \\ \rightarrow \mathbf{v} &= \frac{c}{M_{xy}} \begin{pmatrix} M_{xy} \\ \lambda - M_{xx} \end{pmatrix}, \end{aligned} \quad (31)$$

and use  $c$  to normalize the vector, then

$$\mathbf{v}_{\pm} = \frac{1}{\sqrt{|M_{xy}|^2 + |\lambda_{\pm} - M_{xx}|^2}} \begin{pmatrix} M_{xy} \\ \lambda_{\pm} - M_{xx} \end{pmatrix}, \quad (32) \quad \{\text{h.3}\}$$

with  $\mathbf{v}_{\pm} \cdot \mathbf{v}_{\pm}^T = 1$ , and  $\mathbf{v}_{\mp} \cdot \mathbf{v}_{\pm} = 0$  can be easily verified for the case of real  $M$ . If  $M$  is complex the complex eigenvectors are not necessarily perpendicular in the standard sense

(see A).

## B. Elliptical Polarization

To obtain the corresponding ellipse that represents the polarization of the Electric field, we proceed as follows.

We take any one of the  $\mathbf{v}_\pm$  (complex) eigenvectors, and write it as

$$\vec{v} = \vec{v}' + i\vec{v}'', \quad (33) \quad \{\text{w.1}\}$$

then, the electric field is

$$\mathbf{E}(t) \propto \vec{v}' \cos \omega t + \vec{v}'' \sin \omega t. \quad (34) \quad \{\text{w.2}\}$$

Taking the components

$$\begin{aligned} E_x &= v'_x \cos \omega t + v''_x \sin \omega t \\ E_y &= v'_y \cos \omega t + v''_y \sin \omega t, \end{aligned} \quad (35)$$

and eliminating  $\cos \omega t$  and  $\sin \omega t$ , respectively, we obtain

$$\begin{aligned} v'_y E_x - v'_x E_y &= (v'_y v''_x - v'_x v''_y) \sin \omega t \\ v''_y E_x - v''_x E_y &= (v''_y v'_x - v''_x v'_y) \cos \omega t, \end{aligned} \quad (36)$$

from where we obtain

$$\begin{aligned} \sin \omega t &= \frac{v'_y E_x - v'_x E_y}{v'_y v''_x - v'_x v''_y} \\ \cos \omega t &= -\frac{v''_y E_x - v''_x E_y}{v''_y v'_x - v''_x v'_y}. \end{aligned} \quad (37)$$

Using  $\cos^2 x + \sin^2 x = 1$ , we can eliminate the time by writing

$$\vec{E}^T M \vec{E} = 1, \quad (38) \quad \{\text{w.6}\}$$

where we write  $\vec{E}$  as a column vector and  $M$  is a matrix with components

$$\begin{aligned} M_{xx} &= |v_y|^2/D \\ M_{xy} &= -(v'_x v'_y + v''_x v''_y)/D \end{aligned} \quad (39)$$

$$M_{yy} = |v_x|^2/D, \quad (40)$$

with

$$D = (v'_y v''_x - v'_x v''_y)^2. \quad (41) \quad \{\text{w.9}\}$$

The secular equation follows from Eq. (30),

$$\lambda^2 - \lambda \text{tr}(M) + \det(M) = 0, \quad (42) \quad \{\text{w.39}\}$$

with solutions

$$\lambda_{\pm} = (\text{tr}(M) \pm \sqrt{\text{tr}(M)^2 - 4\det(M)})/2, \quad (43) \quad \{\text{h.56}\}$$

with the corresponding eigenvectors  $|+\rangle$  and  $|-\rangle$  (not to be confused with right-left circularly polarizations). Writing  $\vec{E} = E_+|+\rangle + E_-|-\rangle$  we obtain

$$\vec{E}^T M \vec{E} = \lambda_- E_-^2 + \lambda_+ E_+^2 = 1, \quad (44) \quad \{\text{w.51}\}$$

that is the equation of an ellipse with semi-major  $a$  and semi-minor  $b$  axis given by

$$a = \frac{1}{\sqrt{\lambda_-}} \quad (45)$$

$$b = \frac{1}{\sqrt{\lambda_+}}. \quad (46)$$

The directions *with respect to the crystal x axis* are given by

$$\tan \alpha_- = \frac{\lambda_- - M_{xx}}{M_{xy}} \quad (47)$$

$$\tan \alpha_+ = \frac{\lambda_+ - M_{xx}}{M_{xy}}, \quad (48)$$

with  $\alpha_+$  and  $\alpha_-$  real angles perpendicular to each other (we are using the same notation as M& M PRB **85**, 125418 (2012)). The helicity of the polarization ellipse is given by the sign

of

$$\begin{aligned} \text{Re}[\mathbf{v}_\pm] \times \text{Im}[\mathbf{v}_\pm] &= (v'_x \hat{x} + v'_y \hat{y}) \times (v''_x \hat{x} + v''_y \hat{y}) = (v'_x v''_y - v''_x v'_y) \hat{z} \\ \rightarrow \text{sgn}[v'_x v''_y - v''_x v'_y] &= \begin{cases} - \circlearrowleft \text{ left-polarized} \\ + \circlearrowright \text{ right-polarized} \end{cases} \end{aligned} \quad (49)$$

Above is implemented in `fracCont.pl`, `corre-principal-axes.pl`, `haydock2DNRBase.pl`. Also there is `gnuplot` program `semiejes.g` where above is implemented for any  $\mathbf{v}$  of the form given by Eq. (33).

## Appendix A: Complex Eigenvectors

After WLM, we show that  $\Theta_1 - \Theta_2 = \pi/2$ , where  $\Theta_\alpha = \theta_\alpha + i\text{Im}(\Theta_\alpha)$ . We have that

$$\begin{aligned} V_1^T \cdot \epsilon \cdot V_2 &= V_1^T \cdot (\epsilon \cdot V_2) = \lambda_2 V_1^T \cdot V_2 \rightarrow \text{scalar} = \text{scalar}^T \\ &= (V_1^T \cdot \epsilon \cdot V_2)^T = V_2^T \cdot \epsilon \cdot V_1 = \lambda_1 V_2^T \cdot V_1 = \lambda_1 (V_2^T \cdot V_1)^T = \lambda_1 V_1^T \cdot V_2 \\ (\lambda_1 - \lambda_2) V_1^T \cdot V_2 &= 0 \Rightarrow V_1^T \cdot V_2 = 0. \end{aligned} \quad (\text{A1})$$

Thus the eigenvectors are perpendicular, within the Euclidean metric, even if the eigenvalues,  $\lambda_{1,2}$ , are complex. Then, it follows that  $\Theta_1 - \Theta_2 = \pi/2$ , even if the angles,  $\Theta_{1,2}$ , are complex. But if  $\Theta_1 - \Theta_2 = \pi/2$ , the complex part of  $\Theta_1$  must be equal to the complex part of  $\Theta_2$ , and then  $\theta_1 - \theta_2 = \pi/2$ . Indeed, we have confirmed numerically that  $\text{Im}(\Theta_1) = \text{Im}(\Theta_2)$ , and that  $\theta_1 - \theta_2 = \text{sgn}(\theta_1 - \theta_2)\pi/2$ .

## Appendix B: Projection of the Electric Field

We can calculate the electric field  $\mathbf{E}(\mathbf{r})$  as follows. We begin by using two mutually perpendicular polarizations,  $\boldsymbol{\varepsilon}_{1,2}$  for the external (unitary) field  $\mathbf{E}_{\text{ext}}$ , say along the crystal axis  $x$  and  $y$ , then we can write,

$$\begin{aligned} \mathbf{E}(\mathbf{r}; \boldsymbol{\varepsilon}_1) &= E_x(\mathbf{r}; \boldsymbol{\varepsilon}_1) \hat{x} + E_y(\mathbf{r}; \boldsymbol{\varepsilon}_1) \hat{y} \quad \text{for } \mathbf{E}_{\text{ext}} = \boldsymbol{\varepsilon}_1 = \hat{x} \\ \mathbf{E}(\mathbf{r}; \boldsymbol{\varepsilon}_2) &= E_x(\mathbf{r}; \boldsymbol{\varepsilon}_2) \hat{x} + E_y(\mathbf{r}; \boldsymbol{\varepsilon}_2) \hat{y} \quad \text{for } \mathbf{E}_{\text{ext}} = \boldsymbol{\varepsilon}_2 = \hat{y}, \end{aligned} \quad (\text{B1})$$

where  $\mathbf{E}(\mathbf{r}; \boldsymbol{\varepsilon}_i)$  is the microscopic field for  $\mathbf{E}_{\text{ext}} = \boldsymbol{\varepsilon}_i$ . We want to express  $\mathbf{E}(\mathbf{r}; \boldsymbol{\varepsilon}_i)$  along any given direction  $\hat{\mathbf{v}}$ , then

$$\begin{aligned}
 \mathbf{E}(\mathbf{r}; \hat{\mathbf{v}}) &= (\mathbf{E}(\mathbf{r}; \boldsymbol{\varepsilon}_i) \cdot \hat{\mathbf{v}})\hat{\mathbf{v}} = (\mathbf{E}(\mathbf{r}; \boldsymbol{\varepsilon}_i) \cdot \hat{\mathbf{v}})(\hat{v}_x \hat{x} + \hat{v}_y \hat{y}) \\
 &= (\hat{v}_x E_x(\mathbf{r}; \boldsymbol{\varepsilon}_i) + \hat{v}_y E_y(\mathbf{r}; \boldsymbol{\varepsilon}_i))(\hat{v}_x \hat{x} + \hat{v}_y \hat{y}) \\
 &= E_x(\mathbf{r}; \hat{\mathbf{v}})\hat{x} + E_y(\mathbf{r}; \hat{\mathbf{v}})\hat{y} \\
 E_x(\mathbf{r}; \hat{\mathbf{v}}) &= (\hat{v}_x E_x(\mathbf{r}; \boldsymbol{\varepsilon}_i) + \hat{v}_y E_y(\mathbf{r}; \boldsymbol{\varepsilon}_i))\hat{v}_x \\
 E_y(\mathbf{r}; \hat{\mathbf{v}}) &= (\hat{v}_x E_x(\mathbf{r}; \boldsymbol{\varepsilon}_i) + \hat{v}_y E_y(\mathbf{r}; \boldsymbol{\varepsilon}_i))\hat{v}_y,
 \end{aligned} \tag{B2}$$

### Appendix C: Ellipses

```

corre-angles.pl --od=plots/ --idf=meps/eps-*--dat --tam=.1
corre-arrows.pl --od=arrows/ --idf=meps/eps-*--dat --tam=.1
corre-ellipses.pl --od=movies/ --scale=1.250 --angle=24 --Nh=100
--epsa=ag --epsb=1.001 --axes=principal -nem=vsw --ep=e

```

