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CODE PWE2D.F: DOCUMENTATION

Written by L.C. Andreani, Department of Physics "A. Volta", University of Pavia,
via Bassi 6, 27100 Pavia, Italy
andreani@fisicavolta.unipv.it
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INTRODUCTION

The code pwe2d.f is an implementation of the plane-wave expansion method to calculate the photonic band structure of 2D photonic crystals, assuming lossless, non-dispersive dielectric systems (the dielectric constants must be real and positive, metals cannot be treated). The spatially-dependent dielectric modulation is expanded in plane waves with reciprocal lattice vectors. The inverse dielectric matrix, which is needed to solve the second-order Maxwell equation for the magnetic field, is obtained by numerical inversion of the dielectric matrix which is calculated analytically for the different structures. The dielectric matrix is defined to be real (with double precision), thus only photonic structures with inversion symmetry can be calculated.

HOW TO INSTALL

The code is written in Fortran 77. There are three source files:
pwe2d.f : main program with several subroutines
ft2d.f   : subroutines with 2D Fourier transform of dielectric function
sub.f   : library subroutines for matrix diagonalization (from Eispack)
In order to compile with Linux o.s., copy the files in the same directory and run the compiler with one of the following commands which create the executable file pwe2d.e:

$ f77 -C -o pwe2d.e pwe2d.f ft2d.f sub.f (check mode: suggested for tests)
$ f77 -o pwe2d.e pwe2d.f ft2d.f sub.f (normal compilation mode)

A sample file pwe2d.gnu is provided for plotting the photonic bands: use command
$ gnuplot pwe2d.gnu
to create a postscript file pwe2d.ps, which can then be viewed with $ gv or similar.

INPUT FILE

All input data are read from data file pwe2d.dat
The following input variables are read:

Row number 1:
jlattice - defines the 2D Bravais lattice.
1= square, 2= triangular, 4=rectangular (use for W1 waveguide with supercell)

Row number 2:
jbasis - defines the basis in the unit cell, see comments in file pwe2d.dat
alength1, alength2, alength3, alength4 - used for defining the photonic lattice.
For example, in the triangular lattice of holes, alength1=r/a and all other "alength" are not used.
With the Fourier transforms provided in this version, alength4 is never used. It can be useful for generalization to other structures (e.g., point cavities).

Row number 3:
eps1, eps2 = dielectric constants: must be REAL and POSITIVE
For example, the triangular lattice of air holes is implemented by setting eps1=1, eps2=epsilon of dielectric material.

Row number 4:
jparxy,jparkz - parity w.r.t. mirror reflection in xy resp. kz plane (σ_{xy}, σ_{kz})
jparxy=1 for E or TM modes (electric field along z, odd under mirror symmetry σ_{xy})
jparxy=0 for H or TE modes (magnetic field along z, even under mirror symmetry σ_{xy})
jparxy=−1 for both modes together (necessary for out-of-plane dispersion)
jparkz=0 or 1 (even, odd under σ_{kz}) can be used only along special symmetry directions.
If jparkz=−1, parity separation is not used - SUGGESTED CHOICE

Row number 5:
akzmin, akzmax, nkw - values of kappa_z for calculating out-of-plane dispersion.
The code writes the kz dispersion for state with wavevector number "jkeigenv".

Row number 6:
nk - number of k-point subdivisions along each line in Brillouin zone

Row number 7:
npw - number of plane waves in expansion. It is advisable to use symmetry-adapted values, which include all reciprocal lattice vector with |G|<cutoff value. To find these values, run the code once and look into the file pwe2d_gvec.out . A few suggested values are indicated in the input file.
If you use values of npw which are not symmetry adapted...
... parity separation (if requested) may not work, execution stops because subroutine "DECOUPLE" does not find a symmetric wavevector
... unphysical splittings at symmetry points, including Γ, may arise

Row number 8:
jeigenv=0 only eigenvalues, =1 eigenvalues and eigenvectors (used for field plot)
jkeigenv= k-vector for which fields are calculated (variable jk in code)
jstate=number of band for which fields are calculated

Row number 9:
factor= multiplication factor for photonic bands
Use factor=1 for dimensionless units ($\omega a/2\pi c$=a/lambda)
Use factor=1240/a(nm) for eV

Row number 10:
xmin,xmax,ymin,ymax,ngrid= grid variables for plot of e.m. field

Row number 11:
jfreephotons=0 for usual calculation, =1 for free photon bands in average dielectric constant

Row number 12:
jloop,varmin,varmax,nvar=for loop over a variable (e.g., alength1 for gap map)
No loop: jloop=0, nvar=0
Loop: jloop=1, nvar=no. of subdivisions, change line "alength1=var" in code
WARNING: With jloop=1, output files are pwe2d001.out, pwe2d002.out, ...

OUTPUT FILES

pwe2d.out or pwe2d001.out, pwe2d002.out, ...
Main output file with wavevector (col.1) and energy (col.2). Wavevectors along main symmetry lines are in a single array from 0 to 1, as defined by subroutine "kline" in code. To change, find "kline" in code. To plot the results with gnuplot, use the vertical tic positions written at the end of the execution and copy them in file pwe2d.gnu (some are already there).

WARNING:
pwe2d.out is used when jloop=0 (no loop)
pwe2d001.out, pwe2d002.out, ... are used when jloop=1 (loop)

pwe2d_gvec.out - reciprocal lattice vectors in order of increasing modulus |G|, given in last column

pwe2d_vl.out - values of vertical lines to be used for plot of bands, e.g. with gnuplot

pwe2d_refrindex.out - effective refractive index (when out-of-plane dispersion is calculated)

pwe2d_gapwidth.out - gap widths, for gap map calculation

pwe2d_gapedge.out - gap edges, for gap map calculation
(DIFFICULT! you have to clean the file carefully before having reliable gap maps).

pwe2d_offplane.out - out of plane dispersion as a function of kz, at the wavevector given by input data "jkeigenv"

pwe2d_ll.out - light lines

fort.15, fort.16, fort.17, fort.18, fort.19 - field components when jeigenv=1

OTHER HINTS

I list a few common situations in which you may need to change the code:

1) If you need to change the symmetry lines along the BZ, look for "kline" in code and comment/uncomment relevant lines. Notice that vertical symmetry can be implemented only along a given line at once: i.e., to use jparkz=0 or 1 for triangular lattice you need to calculate only M-Γ or Γ-K directions separately.

2) If you need to perform a loop over a given variable, look for "=var" or "9995" in code and comment/uncomment.

3) If you need to change parameters, like
maxpw=maximum number of plane waves
maxg =maximum number of reciprocal lattice vectors in the linear array
look for "maxpw=" or "maxg=" in the code and change all relevant lines **in the main program and in the subroutines.**

4) If you need to calculated a new photonic structure with one of the Bravais lattices already implemented (jlattice=1,2,4) you must write a new subroutine for the Fourier transform and define a new "jbasis" accordingly. Look for "ft11" in code to see where to modify.

If you need to calculate a structure with a new Bravais lattice, you must define new "jlattice", "jbasis".

N.b. example of supercell for W1 waveguide, definition of alength2 and alength3

W1 waveguide with $l_2=1$, $l_3=4$

$w_0 = 3^{1/2}a$

$l_3 w_0 / 2$

$w = l_2 w_0$

$l_3 w_0 / 2$

$(l_2 + l_3) w_0$

a

y

x