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CODE GME.F: DOCUMENTATION

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

The code gme.f is an implementation of the guided-mode expansion (GME) method to calculate the photonic band structure of 2D photonic crystals (PhCs) embedded in planar waveguides, also called PhC slabs. Only dielectric systems with real and positive dielectric constants are considered (material losses or metallic systems cannot be treated). The second-order equation for the magnetic field is transformed into a linear eigenvalue problem, by expanding the field on the basis of guided modes of an effective homogeneous waveguide with an average dielectric constant in each layer. In practice, the basis consists of plane waves in the 2D plane (xy) and guided modes in the vertical (z) direction. The spatially-dependent dielectric modulation in each layer j=1,2,3 is expanded in plane waves with reciprocal lattice vectors, like in 2D PWE (see code "pwe2d.f"). The inverse dielectric matrix is obtained by numerical inversion of the direct dielectric matrix, which is calculated analytically for the different structures. The dielectric matrix in each layer is defined to be real (double precision), thus only photonic structures with inversion symmetry can be calculated. With this condition, and with the proper choice of phases, the "Hamiltonian" matrix of the linear eigenvalue problem is real symmetric. Diffraction losses of quasi-guided modes are calculated by perturbation theory, using the photonic analog of Fermi Golden rule for quantum mechanics.
Both dispersion and losses as obtained by the GME method are APPROXIMATE - beware of possible corrections and inaccuracies.

REFERENCE FOR THE METHOD AND DISCLAIMERS

The main reference for the GME method is:
[*] L.C. Andreani and D. Gerace, Phys. Rev. B 73, 235114 (2006).
You can freely use the code for scientific purposes. However, the code is provided "as is" and no responsibility is taken about correctness of the results for any specific application.
When publishing results obtained with the GME code, please refer to the method as follows: "Photonic mode dispersion and losses were obtained by a guided-mode expansion method, which consists of expanding the magnetic field on the basis of guided modes of an effective homogeneous waveguide and calculating out-of-plane diffraction losses by perturbation theory [*]".

HOW TO INSTALL

The code is written in Fortran 77. There are three source files:
gme.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 gme.e:
$ f77 -C -o gme.e gme.f ft2d.f sub.f (check mode: suggested for tests)
$ f77 -o gme.e gme.f ft2d.f sub.f (normal compilation mode)

N.b. subroutines in ft2d.f and sub.f are also used by code "pwe2d". When implementing new structures, I suggest to develop both codes together and to keep a single file "ft2d.f"

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

INPUT FILE
All input data are read from data file gme.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 gme.dat)
alength1, alength2, alength3, alength4 - lengths 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 the present version, alength4 is never used: it can be useful for generalization to other structures (e.g., point cavities).
N.b. the 2D lattice constant is called "aret" in the code and is a fixed parameter set equal to unity.

Rows number 3 to 5:
eps1_clad1, eps2_clad1 - dielectric constants for upper cladding layer 1, REAL and POSITIVE
eps1_core , eps2_core - dielectric constants for core layer 2, must be REAL and POSITIVE
eps1_clad3, eps2_clad3 - dielectric constants for lower cladding layer 3, REAL and POSITIVE

For example, the triangular lattice of air holes is implemented by setting eps1=1, eps2=epsilon of dielectric material in the core and, possibly, in the cladding(s).

Row number 6:
d = waveguide thickness, in unit of the 2D lattice constant

Row number 7:
npw - number of plane waves in expansion (2D plane)
nalpha - number of guided modes in expansion (vertical direction)
It is advisable to use symmetry-adapted values for npw, which include all reciprocal lattice vector with |G|<cutoff value. To find these values, run the code and look into the file gme_gvec.out, where the G-vectors are sorted with increasing modulus |G|, given in the last column. A few suggested values are indicated in the input file. If you use values of npw which are not symmetry adapted...
... vertical parity separation (if requested) may not work, execution stops because subroutine "DECOUWGA" does not find a symmetric wavevector
... unphysical splittings at symmetry points, including Gamma, may arise

Row number 8:
jparxy,jparkz - parity w.r.t. mirror reflection in xy resp. kz plane: σ_{xy}, σ_{kz}
jparxy=1 for odd states under σ_{xy} (often called quasi-TM modes)
jparxy=0 for even states under σ_{xy} (often called quasi-TE modes)
jparxy=−1 for both modes together (necessary for asymmetric slab, when layers 1,3 are different)
jparkz=0 or 1 (even, odd) can be used only along special symmetry directions.
If jparkz=−1, parity separation with respect to σ_{kz} is not used - SUGGESTED CHOICE

Row number 9:
nk - number of k-point subdivisions along each line in Brillouin zone

Row number 10:
jeigenv=0 find only eigenvalues, =1 eigenvalues and eigenvectors (used for losses and field plot)
jlossmin,jlossmax= mix, max band number for which losses are calculated

Row number 11:
nom, error, niter - parameters for search of zeros (guided-mode dispersion of effective waveguide).
nom = number of subdivisions in frequency interval
error = tolerance in finding a guided-mode frequency
niter = maximum number of bisection steps
I suggest not to change the values provided in the original file.

Row number 12:
factor - multiplication factor for photonic bands
Use factor=1 for dimensionless units (ωa/2πc=a/lambda)
Use factor=1240/a(nm) for eV
jshift - used to shift bands at k=0, sometimes necessary to get continuous curves in the case of a symmetric PhC slab.
If jshift=0 yields broken curves, try jshift=1 or higher...
WARNING: if the PhC slab is asymmetric, the photonic dispersion curves are ALWAYS broken due to the finite cutoffs of the fundamental modes. Plot with points (instead of lines).

Row number 13:
jfreephotons=0 for usual photonic bands calculation
jfreephotons=1 for free photon bands, i.e., for the dispersion of the effective waveguide folded in the Brillouin zone of the photonic lattice.

Row number 14:
jloop,varmin,varmax,nvar=use for loop over a variable (e.g., alength1 for gap map)
No loop: jloop=0, nvar=0
Loop: jloop=1, nvar= number of subdivisions, change line "alength1=var" in code
WARNING: With jloop=1, output files are gme001.out, gme002.out, ...

Row number 15:
jfields =0 no field, =1 calculates e.m. field (can be used only when jeigenv=1)
jkeigenv= number of k-vector (variable jk in code) for which fields are calculated
jstate=number of band for which fields are calculated

Row number 16:
xmin,xmax,nxgrid, ymin,ymax,nygrid, zmin,zmax,nzgrid = grid variables for plot of e.m. field

OUTPUT FILES
gme.out or gme001.out, gme002.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 execution and copy them in file gme.gnu (some are already there).

When losses are calculated, the file gme.out (or gme001.out, ...) contains also the imaginary part of frequency (col.3), the group velocity (col.4) and propagation losses in decibel/a (col.5). To plot these quantities, use file "gme.gnu" in the "multiplot" part. Losses in dB/mm are given by col(5)/lattice constant(mm).
The calculated Im(omega) is the main quantity characterizing losses in the GME method and is implemented as described in [*]. Obtaining the group velocity v_g and the losses $2Im(k)=2Im(omega)/v_g$ requires a numerical derivative: in some cases it may be better to use only columns 1,2,3 of the output file and elaborate the data separately in order to get better v_g and Im(k).

Warning:
gme.out is used when jloop=0 (no loop)
gme001.out, gme002.out, ... are used when jloop=1 (loop)

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

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

gme_ll.out - light lines

fort.13 to fort.18, - field components when jeigenv=1 and jfields=1

gmebis.out is a copy of gme.out (only columns 1 to 3)
gmeloss.out is a copy of gme.out, but only for the bands from jlossmin to jlossmax

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 MΓ or ΓK 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
maxalpha=maximum number of guided modes
maxham =maximum dimension of Hamiltonian matrix
maxg =maximum number of reciprocal lattice vectors in the linear array
look for "maxpw=" etc. in the file and change all relevant lines in the main program **and in the subroutines**.

4) If you need to calculate 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 and how to modify.
If you need to calculate a structure with a new Bravais lattice, you must define new "jlattice", "jbasis".
REMEMBER: there are three Fourier transforms ft1, ft2, ft3 for the three layers, thus each new structure has to be added three times.