Introduction to Nanophotonics: Numerical exercises

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INTRODUCTION

Class 0: Optical resonances (and training MATLAB!!)

1. Transfert matrix

   We use a transfer matrix T_c to describe the scattering process of a cavity coupled to a waveguide. The scattering matrix is [see S. Fan, "Sharp asymmetric line shapes in side-coupled waveguide-cavity systems." Applied Physics Letters 80, 908-910 (2002)]:

$$\begin{pmatrix} b_2 \\ a_2 \end{pmatrix} = T_c \begin{pmatrix} a_1 \\ b_1 \end{pmatrix} = \begin{bmatrix} 1 - \frac{i\gamma}{\omega-\omega_0} & \frac{-i\gamma}{\omega-\omega_0} \\ \frac{i\gamma}{\omega-\omega_0} & 1 + \frac{i\gamma}{\omega-\omega_0} \end{bmatrix} \begin{pmatrix} a_1 \\ b_1 \end{pmatrix} \tag{1}$$

   where a and b are the incoming and outgoing power from left (1) and right (2) sides. When no power is coming from the right, show that the reflected field is $b_1 = -a_1 T_{21}/T_{22}$. Using that $det(T_c) = 1$, show that the transmitted field is $b_2 = a_1/T_{c,22}$. Now compute numerically T_c using MATLAB, and plot the reflectivity and transmission for a cavity with a central energy of $1eV$, and a a relative width of 1%. Plot R and T as a function of energy in eV, wavelength in microns, and frequency ω in Hz.

   HINTS:

   - Use "class0.m" MATLAB code.
   - For units conversion use that λ(in microns) = 1.23984/Energy(in eV).

2. Fano resonance

   Now consider that there are two partially reflecting elements (mirrors) with reflectivity r^2, each one at a distance ℓ from the cavity. Compute numerically the reflectivity and transmission of the whole system when launching a wave from the left. Use the following transfert matrix for the reflecting element T_p and the free propagation in the waveguide T_ℓ:

$$T_p = \frac{1}{i\sqrt{1-r^2}} \begin{bmatrix} -1 & -r \\ r & 1 \end{bmatrix}; T_\ell = \begin{bmatrix} exp(i\phi) & 0 \\ 0 & exp(-i\phi) \end{bmatrix} \tag{2}$$

   where $\phi = \omega\ell/c$ is the accumulated phase upon propagation from the cavity to the mirror. Use $\gamma = 0.002(2\pi c/\ell)$ and choose for instance $r = 0.4$ (as in the paper) and

$\ell = 0.5$ microns. Plot the results as a function of $\omega/(2\pi c/\ell)$ for the following central frequencies: $0.175(2\pi c/\ell)$, $0.25(2\pi c/\ell)$, $0.325(2\pi c/\ell)$, and $0.375(2\pi c/\ell)$. Discuss the results: is the energy conserved? Is the background transmission something familiar to you? Why the asymmetry of the resonance is opposite at both sides of the maximum of the background transmission? Such an asymmetrical resonance shape is called "Fano resonance", and it is widespread in nanophotonics...

HINTS:

- Generate a loop similar to the one in "class0.m", including all matrices: T_c, T_p and T_l.
- Generate the total transfer matrix as a simple MATLAB product: $T_s = T_p * T_l * T_c * T_l * T_p$.

3. Multilayered 1D periodic medium

Simulate N periods of a multilayered structure, with a period consisting of: a propagation length ℓ, a partial reflecting element r, and a propagation ℓ, such that the period is $a = 2\ell$. Compute the reflectivity for different N. Can you predict the a/λ value for the band-gap in this simple structure?

HINTS:

- Generate a loop similar to the one in "class0.m", including the matrices T_p and T_l.
- Generate the total transfer matrix as a simple MATLAB product: $T_s = (T_l * T_p * T_l)^N$.
- For the band-gap frequency prediction, take into account that the transmission through a single reflecting element gives a phase $\pi/2$.

PART I. PHOTONIC CRYSTAL BAND DIAGRAMS

Class 1: 2D Photonic Crytals (Plane Wave Expansion, PWE)

1. 2D bands, square lattice.

   Calculate 2D photonic bands for the squared lattice of dielectric cylinders with $\epsilon = 9$ in air, $r/a = 0.38$, and find TE and TM photonic band gaps between $a/\lambda = 0$ and 0.7. Are there any total (both TE and TM) band gaps? Compare with Sakoda's calculation (p. 38). Suggested parameters: $N_{pw} = 97$.

   HINTS:

   - Use "gme_2Dcylinders.m" MATLAB code. Run "pwe" code over both horizontal symmetries. For this choose sy='xy' in "gme_2Dcylinders.m". This will run "pwe" twice for parameter jparxy=0 (even, TE) and jparxy=1 (odd, TM)
   - Use variable "path=1231" for ΓXMΓ path in the reciprocal lattice.

2. 2D bands, triangular lattice.

   Calculate 2D photonic bands for the triangular lattice of air holes with $\epsilon = 12$, $r/a = 0.45$ and verify that there is a complete photonic band gap for all directions and polarizations between $a/\lambda = 0.4$ and 0.44. Suggested parameters: $N_{pw} = 61$ (rough), $N_{pw} = 109$ (more accurate).

   HINTS:

   - Generate a new "myfile.m" file by changing the following parameters in "gme_2Dcylinders.m": jlattice; alength1; eps1 & eps2; npw to 61 or 109
   - Run "pwe" code over both horizontal symmetries. For this choose sy='xy' in "myfile.m" MATLAB code. This will run "pwe" twice for parameter jparxy=0 (even, TE) and jparxy=1 (odd, TM)
   - Use variable "path=2132" for MΓKM path in the reciprocal lattice. Change x-labels in plot accordingly.

PART I. PHOTONIC CRYSTAL BAND DIAGRAMS

Class 2: 2.5D Photonic Crytals (Guided Mode Expansion Method, GME)

1. 2D bands of PhC membrane in air.

   Calculate photonic bands in a membrane PhC slab, for the triangular lattice of air holes with $\epsilon = 12$, $d/a = 0.6$, $r/a = 0.45$. Suggested parameters: $N_{pw} = 61$, $N_\alpha = 2$ (rough), $N_{pw} = 109$, $N_\alpha = 4$ (more accurate). Compare with the results of S.G. Johnson et al., PRB 60, 5751 (1999). Try to answer the following questions: (a) why is there no complete PBG in the membrane PhC? (b) why is the value $d/a = 0.6$ considered to be the optimal one in PhC slabs with triangular lattice, as stated in the paper by Johnson et al? See also IEEE-JQE 38, 891 (2002).

   HINTS:

   - Use "gme_EX2.m" MATLAB code. Run "gme" code over both horizontal symmetries. For this choose sy='xy' in "gme_EX2.m". This will run "gme" twice for parameter jparxy=0 (even, TE) and jparxy=1 (odd, TM)
   - Use variable "path=1231" for ΓXMΓ path in the reciprocal lattice.

2. Losses in 1D PhC slab

   Calculate photonic bands and Im(ω) of vertically odd (TE) modes in a membrane PhC slab patterned with a 1D lattice: $\epsilon = 12$, $d/a = 0.2$, $r/a = 0.3$. Use jparxy=-1 (both horizontal parities) and jparkz=+1 (vertically odd modes, which are purely TE for the case of a 1D lattice). Plot the losses as a function of frequency, look at the behavior of losses as a function of wavevector and band index. Additionally: Calculate photonic bands and Im(ω) for a SOI PhC slab ($\epsilon_1 = 1, \epsilon_2 = 12, \epsilon_3 = 2.1$) with the same 1D lattice. Notice that the losses for each band are slightly higher for the asymmetric structure. What is the effect of slab asymmetry? See also PRE 69, 056603 (2004).

   HINTS:

   - Generate a new "myfileLoss.m" file by changing the following parameters in "gme_EX2.m": jlattice; jbasis; npw=21; nalpha=4; jparxy=-1; jeigenv=1 for loss calculation. Run "gme" code for odd vertical symmetry. For this choose

sy='kz' in "myfileLoss.m" file and jrun=[1]. This will run "gme" for jparkz=1 (odd, purely TE for a 1D lattice)

- Use variable "path=12" for ΓX path in the reciprocal lattice. Change x-labels in plot accordingly.

3. Losses in 2D PhC slab

   Calculate photonic bands and Im(ω) of horizontally even (TE-like) modes in a membrane PhC slab patterned with a triangular lattice of air holes: $\epsilon = 12, d/a = 0.5, r/a = 0.3$, jparxy=0. Consider only the ΓK symmetry direction and separate photonic modes according to vertical parity (σ_{kz}: jparkz=0 even, 1 odd). Plot the losses as a function of frequency, compare with the results of PRB 73, 235114 (2006) and also with T. Ochiai and K. Sakoda, PRB 63, 125107 (2001) (see lecture slides). N.b. It is possible to plot Im(ω) as a function of wavevector, as done in the above papers... but then it is more cumbersome to associate the losses with each corresponding band.

   HINTS:

   - Generate a new "myfile2D.m" file by changing the following parameters in "myfile2DLoss.m": jlattice; jbasis; npw=109; nalpha=4; jparxy=0; nk=100; jeigenv=1 for loss calculation. Run "gme" code over both vertical symmetries. For this choose sy='kz' in "myfile2DLoss.m" file. This will run "gme" twice for parameter jparkz=0 (even, TM-like) and jparkz=1 (odd, TE-like). Why are they called TE and TM-"like"?
   - Use variable "path=13" for ΓK path in the reciprocal lattice. Change x-labels in plot accordingly.

PART I. PHOTONIC CRYSTAL BAND DIAGRAMS

Class 3: Photonic Crystal defects (Guided Mode Expansion Method, GME)

1. W1 waveguide

   Calculate the dispersion of the line-defect modes in a W1 waveguide (missing row of holes in the ΓK direction of the triangular lattice) realized in a high-index membrane with $\epsilon = 12, d/a = 0.5, r/a = 0.3$. Calculate only horizontally even modes (jparxy=0) and separate the modes according to vertical parity (jparkz=0 or 1). A supercell in the ΓM direction has to be introduced: setting $w0 = \sqrt{3}a$, the channel width is alength2*w0 while the period in the ΓM direction is (alength2+alength3)*w0. Suggested parameters are alength3=4, $N_{pw} = 91$, $N_\alpha = 1$ (very rough), $N_{pw} = 161$, $N_\alpha = 2$ (rough). When changing the supercell period, the number of plane waves has also to be adjusted → keep a constant cutoff. Notice that the index-guided is odd under vertical parity, while the gap-guided mode is even. This is because the modes are quasi-TE, i.e., the dominant electric field component is perpendicular to the line defect: thus the jparkz=+1 or index-guided mode has a spatially even electric field, but is globally odd under vertical mirror symmetry. This is the most important defect mode for applications, because it has a dispersion region below the light line with high group velocity and low losses. See e.g. A. Chutinan and S. Noda, PRB 62, 4488 (2000); S.G. Johnson et al., PRB 62, 8212 (2000) and lecture slides. Additionally: try plotting the field components of the defect modes.

   HINTS:

   - Use "gme_EX7.m" MATLAB code. Run "gme" code over both vertical symmetries. For this choose sy='kz' in "gme_EX7.m". This will run "gme" twice for parameter jparkz=0 (even) and jparkz=1 (odd)
   - Use variable "path=12" for ΓK path in the reciprocal lattice. Change x-labels in plot accordingly.

2. Losses in W1 waveguide

   Calculate propagation losses of the line-defect mode in a W1 waweguide realized in a high-index membrane with $\epsilon = 12, d/a = 0.5, r/a = 0.3$. Consider only horizon-

tally even (jparxy=0) and vertically odd (jparkz=1) modes, according to the results of Exercise 2. A supercell in the ΓM direction has to be introduced: setting $w0 = \sqrt{3}a$, the channel width is alength2*w0 while the period in the ΓM direction is (alength2+alength3)*w0. Plot Im(ω), the group velocity $vg = d\omega/dk$ and the propagation loss 4.34*2*Im(k) as a function of frequency. The code yields the loss in decibel/lattice constant: in order to get the propagation loss in dB/mm, use a typical lattice constant a = 420 nm (yielding the defect-mode wavelength around 1.55 micron). Suggested parameters are alength3=4, $N_{pw} = 91$, $N_\alpha = 1$ (very rough), $N_{pw} = 161$, $N_\alpha = 2$ (rough). When changing the supercell period, the number of plane waves has also to be adjusted → keep a constant cutoff. The jumps in Im(ω) and in the propagation loss are unphysical, they arise because of the finite supercell width. In order to get the limit of an isolated defect with (relatively) smooth curves, an average over different supercell periods has to be performed, as in APL 82, 2011 (2003). Notice that a typical value of propagation loss for the line-defect mode above the light line is around 50 dB/mm: this is much too high for applications. The useful low-loss region is below the light line, where diffraction losses are purely extrinsic as they depend on the presence of fabrication disorder.

HINTS:

- Generate a new "myfileW1.m" file by changing the following parameters in "gme_EX7.m": jlattice; jbasis; npw=109; nalpha=4; jparxy=0; nk=100; jeigenv=1 for loss calculation. Run "gme" code over both vertical symmetries. For this choose sy='kz' in "myfileW1.m" file. This will run "gme" twice for parameter jparkz=0 (even, TE) and jparkz=1 (odd, TM)
- Use variable "path=13" for ΓK path in the reciprocal lattice. Change x-labels in plot accordingly.

PART II. PLASMONICS

Class 4: 1D Surface Plasmon Polaritons (RETICOLO 1D)

1. Dielectric constant of metals

   Plot real and imaginary parts of the dielectric permittivity of gold (Au) and silver (Ag) between 0 and 8 eV, using different models: "Drude model without dissipation ($\Gamma = 0$)", "Drude model with dissipation", and "Drude-Lorentz model (inter band transitions)". Compare them with experimental data from Johnson and Christie (1972). Also, trace real and imaginary index. At what energy range interband transitions become dominant?

   HINTS:

   - Use code "epsmetal.m" for the Drude models. Materials are chosen through the option 'Material' ('Au' or 'Ag'), and models are set with 'Method' ('Drude-real', 'Drude-complex' or Drude-Lorentz'). Example: eps=epsmetal(1.55e-6,'Material','Au','Method','Lorentz-complex') computes Drude model (with dissipation) for Au at $\lambda = 1.55\mu$m.
   - Use code "JC_data.m" to get the database from Johnson and Christie. Example: [wev_JC,eps1,eps2]=JC_data('Material','Ag') returns energy in eV, eps1=real(epsilon) and eps2=imag(epsilon) for Ag.

2. Reflectivity spectra of dielectric 1D PhC slabs

   Compute zero-order (i.e. specular), TE reflectivity of the 1D PhC slab in air from EXCERCISE 2, Class 2 ($\epsilon = 12$, thickness= 0.2a, air-slot width=0.3a), using RETICOLO-1D. Vary the normalized energy (a/λ) from 0 to 0.8, and the incident angle (θ) from 0 to 90°. Plot a/λ vs. $k(\pi/a)$. Is there any information below the light line? What can you say about the two second order bands (gap@$a/\lambda \sim 0.5$)? Does the lower band couple to a PW incident in the normal direction? Why? Looking at R(λ) plots at fixed angle, comment on the shape of the second order resonances ... What is the impact of radiative losses in the observed resonances?

   HINTS:

- Use code "ret_1Dgrating.m".

3. SPP in a metallic thin layer on SiO2

   Compute zero-order TM reflectivity and extinction of a 1D uniform 50nm-thick Ag layer (SiO2 on top, air underneath), with an incident PW from the top. Vary the normalized frequency (ω/ω_p) from 0 to 0.6, and the incident angle (θ) from 0 to 90°. Identify SPP band: is this SPP on the air or SiO2 sides? Confirm this by plotting Ey field on a xz cut. Notice that SPR modes lie between the air and SiO2 lines, hence angles are larger than total internal reflection angle (i.e. $41.81° < \theta < 90°$). A prism is needed to access these angles from free space!!

   HINTS:

   - Generate a new "myfile.m" file by changing the following parameters in "ret_1Dgrating.m": parm=res0(-1) (TM); profile=[0.5,0.05,0.5],[1,3,2];
   - In general compute the extinction by summing over all diffraction orders, e.g.: Ext(mw,ma)=1-(sum(one_D_TM.inc_top_reflected.efficiency)... ...+sum(one_D_TM.inc_top_transmitted.efficiency))
   - For plotting field (z vs x) define zpoints=[50,50,50] and use the function "plotfield1D.m". Example: plotfield1D(period,'temp_files/aa21-15',parm,profile,zpoints) plots fields for the following indexes of frequency and angle lists, mw=21 (frequency), and ma=15 (angle). To obtain these indexes, first identify frequency w (e.g. w=2.84e15) and incidence angle θ (e.g. 43.45 deg) of interest, then use: [mw,value]=min(abs(wlist-2.84e15/wp)); [ma,value]=min(abs(alist-43.45)).

4. Shallow grating coupler for SPPs

   "The most basic description of SPP launching by periodic set of ridges (period Λ) relies on the momentum conservation: $k_{SPP} = k_0 \sin\theta + nG$, where k_{SPP} and k_0 denote the wave-vector magnitudes of the excited SPP and incident light, respectively, θ is the angle of light incidence in the plane perpendicular to the ridges, n is an integer, and $G = 2\pi/\Lambda$ is the grating momentum. Efficient SPP excitation (in the first grating order) at normal incidence requires thereby that the grating period should be equal to the SPP wavelength: $\Lambda = \lambda_{SPP}$ " [I. Radko, et at, "Efficient unidirectional ridge excitation of surface plasmons," Opt. Express 17, 7228-7232 (2009)]

Compute zero-order TM transmission of a 1D uniform 50nm-thick Ag layer (SiO2 on top, air underneath), with a shallow (20 nm thickness) grating on the air side. Choose the period of the coupler in such a way to couple the SPP mode with $k_{SPP} = 0.3(c/\omega_p)$ with a normally incident PW from the top. Vary the normalized frequency (ω/ω_p) from 0 to 0.6, and the incident angle (θ) from 0 to 90°. Identify the folded SPP band. Plot the field corresponding to the SPP mode for $\theta = 0$.

HINTS:

- period=$2\pi/(0.4\omega_p/c) = 0.448$ (in microns); use e.g. width=period/2
- Generate a new "myfile1Dcoupler.m" file by changing the following parameters in "myfile.m":
  add textures{4}= {[-r/2,r/2],[n_transmitted_medium,n_metal(mw)] };
  profile=[0.5,0.05,0.02,0.5],[1,3,4,2];
- Increase the visibility of the bands by plotting log(Teff)
- For plotting field (z vs x) define zpoints=[50,50,50] and use the function "plotfield1D.m". Example: plotfield1D(period,'temp_files/aa46-1',parm,profile,zpoints), plots fields for the following indexes of frequency and angle lists, mw=46 (frequency), and ma=1 ($\theta = 0$). To obtain mw, first identify frequency w of interest (e.g. w=3.82e15) , then use: [mw,value]=min(abs(wlist-3.82e15/wp)).

PART II. PLASMONICS

Class 5: Localized Surface Plasmons (RETICOLO 2D)

1. 2D metal nanorods

   Using RETICOLO 2D, compute zero order transmission, reflection and extinction of a 2D square array of Au-rectangle parallelepipeds with the following parameters: period=250 nm, x-length=130nm, y-length=30nm and height=20nm. The rods are surrounded by air on the top and lie on a SiO2 substrate (n=1.5). Illuminate the system from the top with a PW polarized along the x-axis. Identify the main resonant LSP mode: is there any secondary resonance? Repeat the calculation with the incident E-field along y-axis. Conclude. Now increase the length of the long axis from 130 to 200 nm and repeat the calculation (E-field along x). Is the main resonance shifted with respect to the first result? Why?

   HINTS:

   - Use code "ret_2Drods.m".

2. LSPs in nano spheres

   Using RETICOLO 2D, compute the extinction of a 2D square array of Ag-spheres with the following parameters: period=200 nm and radius=50nm. The spheres are surrounded by air. Illuminate the system from the top with a PW polarized along the x-axis. Identify the main resonant LSP mode. Compare with the electrostatic model and the prediction of the resonant frequency from the Frohlich condition.

   HINTS:

   - Generate a new "myfile.m" from "ret_2Drods.m" by changing the following parameters: nn=[5,5]; remove textures{3}; change "Au" to "Ag";
     n_transmitted_medium=1.
   - Design the sphere as a stack of Ms+1 Ag layers with the following algorithm:
     ms=1;
     Ms=20;
     N=10;

for Z=linspace(0,2*R,Ms+1)

rho=R*sqrt(1-(Z-R)^2/R^2);

textures{2+ms}={n_incident_medium,[0,0,2*rho,2*rho,n_metal(ml),N] };

ms=ms+1;

end;

- profile={[0.1,ones(1,Ms+1)*(2*R/Ms),0.1],[1,3:(3+Ms),2]};