Introduction to Nanophotonics: Numerical exercises

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PART I. PLASMONICS

Class 1: Dielectric constant of metals (MATLAB only)

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. Metallic mirrors

   The reflectivity coefficient at an interface between air and a lossy material (as a metal) can be approximated by $r = (1-\tilde{n})/(1+\tilde{n})$, where $\tilde{n}$ is the complex refractive index. Plot the reflectivity $R = |r|^2$ for gold and silver as a function of energy, and also as a function of wavelength. For which range they behave as good mirrors? And as nearly perfect conductors? Discuss the conditions needed for these two regimes. Compare the Drude model ("Drude-complex") and Drude with interband transitions ("Drude-Lorentz").

   What is the best mirror choice if working in the visible?

Class 2: 1D Surface Plasmon Polaritons (RETICOLO 1D)

1. SPP in a metallic thin layer on SiO2

   Compute zero-order TM reflectivity and transmission 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. (a) Fix the incident angle (θ) to 0. Compare with exercise 2 (class 1). Are there any resonant features? (b) Now change θ to a value between the total internal reflection (TIR) angle and 90°, i.e. $41.81° < \theta < 90°$. Check for resonant features and interpret . (c) Is this SPP on the air or SiO2 side? Check this by plotting Hy field on a xz cut.

   HINTS:

   - Use "ret_1Dmetalslab0.m" for (a)
   - for (b): generate a new "myfile.m" file by changing the angle_theta0 parameter.
   - For plotting field (z vs x), first identify the index of the desired frequency w (e.g. the resonant frequency for theta=42 degrees is w=0.082 wp), then determine its index mw by doing [value,mw]=min(abs(wlist-0.082)). Finally define zpoints=[50,50,50] and use the function "plotfield1D.m".
     Example: plotfield1D(period,aalist{42},parm,profile,zpoints)

2. SPP band in a metallic thin layer on SiO2

   Compute zero-order TM reflectivity and total absorption 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 side? 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_1Dmetalslab0.m":
     - for ma=1:length(alist); angle_theta0=alist(ma); after texture definition

- Replace klist{mw} by klist{mw,ma} (same with aalist, Reff,Teff)
- Add "end" closing the "for ma=1:length(alist)" loop

- In general compute the absorption as:
  Abs(mw,ma)=1-(sum(one_D_TM.inc_top_reflected.efficiency)...
  ...+sum(one_D_TM.inc_top_transmitted.efficiency))

- For plotting the bands use e.g.:
  surface(klist,repmat(wlist',1,length(alist)),zeros(size(klist)),Abs,'EdgeColor',...
  ... 'none','LineStyle','none','FaceLighting','phong'); colormap(hot); shading interp

- For plotting field (z vs x), run the code again for a given (single) frequency and angle. To obtain indexes of wlist (frequency) and alist (angles), first identify frequency w (e.g. w=2.84e15) and incidence angle θ (e.g. 43.45 deg) of interest, then use: [value,mw]=min(abs(wlist-2.84e15/wp)); [value,ma]=min(abs(alist-43.45)). After running RETICOLO, define zpoints=[50,50,50] and use the function "plotfield1D.m".
  Example: plotfield1D(period,aa,parm,profile,zpoints)

3. 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=$2\pi/(0.3\omega_p/c) = 0.448$ (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), run the code again for a given (single) frequency and angle. To obtain the index of wlist (frequency), first identify w (e.g. w=3.82e15), then use: [value,mw]=min(abs(wlist-3.82e15/wp)); ma=1 ($\theta = 0$). After running RETICOLO, define zpoints=[50,50,50] and use the function "plotfield1D.m". Example: plotfield1D(period,aa,parm,profile,zpoints)

PART I. PLASMONICS

Class 3: 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=140nm, 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_Ex1.m".

2. LSPs in nano spheres

   a) 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. b) Compare with the the prediction of the resonant frequency from the Frohlich condition (electrostatic model). c) Compare with a Mie calculation.

   HINTS:

   - Generate a new "myfile.m" from "ret_2Drods_Ex1.m" by changing the following parameters: nn=[5,5]; remove textures{3}; change "Au" to "Ag" and use "Drude-Lorentz"; n_transmitted_medium=1; R=0.05; llist=linspace(0.3,0.5,41);
   - 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]};

PART II. PHOTONIC CRYSTAL BAND DIAGRAMS

Class 4: 1D Photonic Crytals (RETICOLO)

1. Reflectivity spectra of dielectric 1D PhC slabs (RETICOLO)

   a) Compute zero-order (i.e. specular), TE reflectivity of the 1D PhC slab in air with $\epsilon = 12$, thickness= 0.2a, air-slot width=0.3a, $a = 0.85\mu m$ 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? What is the impact of radiative losses in the observed resonances?. b) Repeat for SIO ($\epsilon_{substrate} = 2.1$) and compare, incidence from air.

   HINTS:

   - Use code "myfile1Dcoupler.m" from Ex3, Class 2. Generate a new file "myfile1Dphotoniccrystal.m"
   - Change wlist to a/lambda list, e.g., wlist=linspace(0,0.8,101); also change period and r.
   - Change parm to parm=res0(1) for TE excitation.
   - Change klist(mw,ma)=k_parallel*(2*pi/wavelength)*period/pi;
   - Remove textures3. Rename and change textures{4} as the new textures{3}= {[-r/2,r/2],[sqrt(12),n_incident_medium]};
   - Change wavelength=period/wlist(mw);
   - Change profile to profile={[1,0.17,1],[1,3,2]};
   - For plotting bands, use Reff in the "surface" command.

Class 5: 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. 29). 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 II. PHOTONIC CRYSTAL BAND DIAGRAMS

Class 6: 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) and jparxy=1 (odd)
   - 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. Compare with RETICOLO result (Ex. 1, Class 4). 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 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). 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. *Optional*: try to guess the domiant E-field distribution of the vertically even (jparkz=0) band between $a/\lambda = 0.36$ and $a/\lambda = 0.48$, and the dominant E-field distribution of the vertically even (jparkz=0) band along the light-line. Plot fields to check.

HINTS:

- Generate a new "myfile2D.m" file by changing the following parameters in "myfile2DLoss.m": jlattice; jbasis; npw=109; alpha=2; parxy=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) and jparkz=1 (odd).

- Identify the order of the guided modes for each band (i.e., those corresponding to the fundamental or excited guided modes of the slab) by running the code:

  i) With alpha=1 (fundamental guided mode of the effective slab) first: the resulting modes are TE-like ones (why are they called TE-"like"?).

  ii) With alpha=2 which gives the fundamental and first excited modes of the effective slab.

- Use variable "path=13" for ΓK path in the reciprocal lattice. Change x-labels in plot accordingly.

PART II. PHOTONIC CRYSTAL BAND DIAGRAMS

Class 7: 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.

OPTIONAL

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 $\pi/2$.