

18.325 Problem Set 6

Due Thursday, 17 November 2005.

Problem 1: Brillouin zones and band diagrams

In class, we derived the irreducible Brillouin zone for a lattice of cylindrical dielectric rods in air with lattice constant a : either a square lattice, where the lattice vectors differ by 90° , or a triangular lattice, where the lattice vectors differ by 60° (in class we used 120° , but you can get 60° just by flipping the sign of one of the lattice vectors).

- If you look in the MPB tutorial (<http://ab-initio.mit.edu/mpb/doc/user-tutorial.html>), it shows you how to compute the TM band diagrams in these two cases. Repeat these calculations, but use rods with radius $r = 0.2a$ and $\varepsilon = 8.9$ rather than the $\varepsilon = 12$ in the tutorial, and find the size of the first TM gap for both the square and triangular lattices. (See also the `sq-rods.ctf` and `tri-rods.ctf` files in the `/mit/mpb/examples` directory.)
- Now, consider an intermediate case: a lattice of the same circular rods in air where the primitive lattice vectors both have length a but the angle between them is 75° . Figure out what is the Brillouin zone in this case, and the irreducible Brillouin zone, and then run MPB to compute the size of the first TM gap.

Be careful about units (see the note on units in the MPB tutorial): in MPB, the \mathbf{k} points are specified in the basis of the reciprocal lattice vectors. If you work out the Brillouin zone in Cartesian coordinates, you can convert to the reciprocal basis by dividing by 2π and calling the (cartesian->reciprocal (vector3 x y z)) function in MPB as described in the reference section of the manual.

Problem 2: Line-defect modes

For this problem, you should make use of the file `/mit/mpb/examples/line-defect.ctf` in the MPB locker on Athena, which computes the bands of

a line defect formed by a missing row of rods in a triangular lattice of rods.

- Change ε to 8.9 to match problem 1. Compute and plot the TM projected band diagram of this mode. By increasing the supercell size (which folds more and more bands in the continuum regions but leaves the defect mode unchanged), identify the continuum regions on your plot (the projection of the bands of the perfect crystal).
- Sketch the Brillouin zone of the triangular lattice of rods, and show how it is projected for the line defect. *Careful*: for the line defect, we have to project this onto the $\Gamma - K$ direction (the nearest-neighbor direction), but the edge of the new 1d Brillouin zone is *not* K . Where is the edge of the projected 1d Brillouin zone?
- Consider the TM bands for the triangular lattice that you computed in problem 1. Project each one of these bands onto the irreducible Brillouin zone for the line-defect waveguide, and superimpose its projected plot onto your the projected band diagram you computed in (a). For each band of the original band diagram, you should have *more than one* projected band, corresponding to all rotations/reflections of the original band (e.g. there are six equivalent rotations of the $\Gamma - K$ direction, although some of these project onto the $-k$ axis and can be omitted.)

Problem 3: Galerkin methods

Consider the 1d Schrodinger equation for an eigenvalue (energy) E :

$$\left(-\frac{d^2}{dx^2} + V(x)\right)\psi(x) = E\psi(x),$$

with boundary conditions $\psi(0) = \psi(L) = 0$, for some smooth potential $V(x)$. Now suppose we want to express this problem on a computer via a discrete grid of $N - 1$ points with spacing $\Delta = L/N$, using a basis of “tent” functions $t(x)$ centered at each grid point:

$$\psi(x) \approx \psi_N(x) = \sum_{n=1}^{N-1} p_n t(x - n\Delta)$$

with some unknown coefficients p_n , where

$$t(x) = \begin{cases} 1 - |x|/\Delta & |x| < \Delta \\ 0 & \text{otherwise} \end{cases}.$$

Thus, $\psi_N(n\Delta) = p_n$ (i.e. the p_n are the values at the grid points) and ψ_N is linearly interpolated in between grid points. Note that the boundary conditions are automatically satisfied.

- (a) Using the Galerkin approach, express the Schrodinger equation above as an $(N - 1) \times (N - 1)$ matrix eigenvalue problem $A\mathbf{p} = EB\mathbf{p}$ in terms of Hermitian matrices A and B .
- (b) Show that the d^2/dx^2 operator just turned into a discrete-grid (finite-difference) version of the 2nd derivative. (Hint: in evaluating this integral in the Galerkin approach, it is probably easier if you integrate by parts to avoid taking the derivative of a discontinuous function.)
- (c) For $V(x) = 0$, recall that we solved this equation in class in the first week: the solutions are $\psi(x) = \sin(m\pi x/L)$, with eigenvalues $E_k = (m\pi/L)^2$ for $m = 1, 2, 3, \dots$. Compute your matrices A and B in this case for $L = 1$, $V(x) = 0$, and $N = 10$, and plug them into Matlab to get the corresponding 9 eigenvalues (with the eig(A,B) command), and give the fractional error in each eigenvalue compared to the analytical result. Which is most accurate, and why?

Problem 4: Meep!

For this problem, you will use the *Meep* finite-difference time-domain code, which is installed on the Athena Linux/Intel machines in the mpb locker (add mpb); see also the Meep manual at <http://ab-initio.mit.edu/meep>. As your starting point, you should use the rod-transmission.ctf example file, which is posted on the course web page, which computes the transmission spectrum of TM planewave source in the x direction through nx layers of the square-lattice rod crystal from problem 1.

- (a) Compute the transmission spectrum as a function of nx , for $nx=1, 2, 3, 4, 5, 6$, and

plot them (on a single plot). The transmission spectrum should be normalized by dividing by the transmission for $nx=0$ (no holes). Relate the features of this transmission spectrum to the band diagram of problem 1.

- (b) Compute the *TE* transmission spectrum for $nx=10$ layers, and relate it to the TE band diagram (which you can compute yourself with MPB, or you can look up from the band diagram in the handout). Careful: you need to change *three* places in the control file. (What happens to the symmetry?)
- (c) Try making the pulse frequency spectrum very broad, e.g. $df=2$ (computing the flux in a correspondingly wide frequency range), and plotting the TM transmission spectrum; in the original range from (a), does the new transmission spectrum match what you had before?
- (d) Predict analytically at what frequency ω_0 you should start to see additional diffracted orders in the reflected wave (i.e. reflected waves at angles in *addition* to the normal 0° reflection). Now, modify the simulation to use a TM *continuous-wave* (CW) source and output E_z at the end, as in the Meep tutorial, and show that there is a qualitative change in the reflected field pattern if you put in a frequency *just* below ω_0 versus a frequency *just* above ω_0 . If you look *just* below ω_0 , then you will have to increase the “pad” parameter in order to see an undisturbed 0° reflection pattern far from the crystal—why?