18.369 Problem Set 5 Solutions

Problem 1: (20 points)

Our derivation is similar to before, except that we have an additional term $-\varepsilon^{-2}\frac{\partial\varepsilon}{\partial\omega}\frac{d\omega}{dk}$ from the derivative $\frac{d}{dk}$ acting on the frequency argument of $\varepsilon^{-1}(\mathbf{x},\omega)$ inside $\hat{\Theta}_k$. This gives us:

$$\frac{d(\omega^2)}{dk} = 2\omega\frac{d\omega}{dk} = \frac{\langle H_k, \frac{\partial\hat{\Theta}_k}{\partial k}H_k\rangle - \frac{d\omega}{dk}\langle H_k, (\nabla+i\mathbf{k})\times\varepsilon^{-2}\frac{\partial\varepsilon}{\partial\omega}(\nabla+i\mathbf{k})\times H_k\rangle}{\langle H_k, H_k\rangle}.$$

If we solve for $\frac{d\omega}{dk}$, we obtain:

$$\frac{d\omega}{dk} = \frac{\langle H_k, \frac{\partial\hat{\Theta}_k}{\partial k}H_k\rangle}{2\omega\langle H_k, H_k\rangle + \langle H_k, (\nabla+i\mathbf{k})\times\varepsilon^{-2}\frac{\partial\varepsilon}{\partial\omega}(\nabla+i\mathbf{k})\times H_k\rangle},$$

where the only new term compared to class is

$$\begin{aligned}\langle H_k, (\nabla+i\mathbf{k})\times\varepsilon^{-2}\frac{\partial\varepsilon}{\partial\omega}(\nabla+i\mathbf{k})\times H_k\rangle &= \langle(\nabla+i\mathbf{k})\times H_k, \varepsilon^{-2}\frac{\partial\varepsilon}{\partial\omega}(\nabla+i\mathbf{k})\times H_k\rangle \\ &= \langle -i\omega\varepsilon E_k, \varepsilon^{-2}\frac{\partial\varepsilon}{\partial\omega}(-i\omega\varepsilon E_k)\rangle \\ &= \omega^2\int\frac{\partial\varepsilon}{\partial\omega}|E|^2,\end{aligned}$$

using Ampere's law and the fact that $E_k = Ee^{-ikx}$. From class, $2\langle H_k, H_k\rangle = 2\int|H|^2 = \int(|H|^2+\varepsilon|E|^2)$ for time-harmonic fields. So, putting it all together, and using $\frac{\partial(\omega\varepsilon)}{\partial\omega} = \varepsilon+\omega\frac{\partial\varepsilon}{\partial\omega}$, we have

$$\frac{d\omega}{dk} = \frac{\langle H_k, \frac{\partial\hat{\Theta}_k}{\partial k}H_k\rangle}{\omega\int\left[\frac{\partial(\omega\varepsilon)}{\partial\omega}|\mathbf{E}|^2+|\mathbf{H}|^2\right]} = \frac{\frac{1}{4\omega}\langle H_k, \frac{\partial\hat{\Theta}_k}{\partial k}H_k\rangle}{\frac{1}{4}\int\left[\frac{\partial(\omega\varepsilon)}{\partial\omega}|\mathbf{E}|^2+|\mathbf{H}|^2\right]},$$

and the numerator was shown in class (and in the book) to be the time-average Poynting flux. Thus the energy density is modified to the Brillouin formula $\frac{1}{4}\left[\frac{\partial(\omega\varepsilon)}{\partial\omega}|\mathbf{E}|^2+|\mathbf{H}|^2\right]$ as desired.

Problem 2: (10+5+5+5 points)

The accompanying Jupyter notebook gives an example calculation of the TM (E_z) band diagram and gap for a 2d hexagonal lattice of dielectric rods (radius $0.2a$, $\varepsilon = 12$) in air. Modify this calculation so that the angle between the primitive lattice vectors is **75**° instead of 60°.

(a) For this part, let us take the lattice vectors to be $\mathbf{R}_1 = a\hat{\mathbf{x}}$ and $\mathbf{R}_2 = a(\hat{\mathbf{x}}\cos\theta + \hat{\mathbf{y}}\sin\theta)$, where $\theta = 75°$, which are shown in fig. 1a—with cylindrical rods, this structure has C_2 symmetry plus the two mirror planes shown as dashed lines. The reciprocal lattice vectors, by the usual formula, are then $\mathbf{G}_1 = \frac{2\pi}{a}(\hat{\mathbf{x}} - \hat{\mathbf{y}}\cot\theta)$ and $\mathbf{G}_2 = \frac{2\pi}{a}\hat{\mathbf{y}}\csc\theta$, so that $\mathbf{R}_i\cdot\mathbf{G}_j = 2\pi\delta_{ij}$. Note that $|\mathbf{G}_i| = \frac{2\pi}{a}\csc\theta$, and that the angle ϕ between $\mathbf{G}_1$ and $\mathbf{G}_2$ is $\cos\phi = \mathbf{G}_1\cdot\mathbf{G}_2/|\mathbf{G}_1|^2 = -\cos\theta$, and thus $\phi = \pi-\theta = 105°$. Therefore, the reciprocal lattice (shown in fig. 1b) is the same lattice *rotated* by 90°, with with a different choice of lattice vectors (an obtuse instead of an acute angle between them). The first Brillouin zone, shaded yellow+blue in fig. 1b, is determined by the usual perpendicular bisectors (black lines), and is a sort of distorted hexagon. Note that the first Brillouin zone still has the C_2 and mirror symmetries of the lattice, as it must! Applying these symmetries, we find the irreducible Brillouin zone to be the blue shaded region in fig. 1b, whose special points we have labelled Γ, M, K, and J as shown. The K point is somewhat subtle, in that (as labeled) several corners are equivalent to K in non-obvious ways: if you take the K in the upper-right and translate it by $-\mathbf{G}_2$, you get the K in the upper-left,

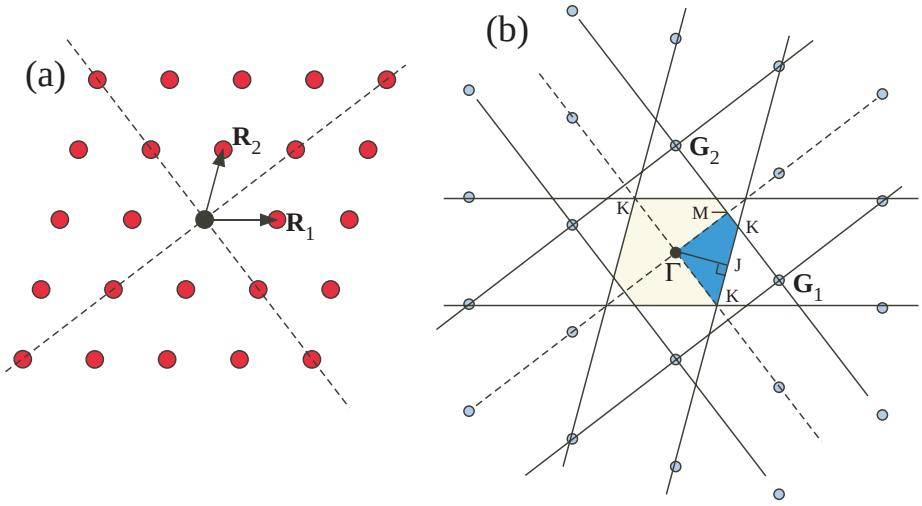

Figure 1: (a) Lattice of dielectric rods with $|\mathbf{R}_1| = |\mathbf{R}_2| = a$ and an an angle 75° between $\mathbf{R}_1$ and $\mathbf{R}_2$. (Lattice is to scale.) Dashed lines are mirror planes. (b) Reciprocal lattice (to scale), with the first Brillouin zone (shaded yellow+blue) surrounded by the perpendicular bisectors (black lines) between Γ and neighboring $\mathbf{G}$ vectors. Dashed lines are mirror planes. Irreducible B.Z. is shaded blue, with special points labelled; note that the three labelled K points are equivalent due to periodicity + symmetry.

which via C_2 rotation gives you the K at the lower-right. Because of this, we are treating J as a special point, even though it is not a corner (see below).

To compute the band diagram, we must find the actual coordinates of these points, in the $(\mathbf{G}_1, \mathbf{G}_2)$ reciprocal basis for MPB. The easiest ones (besides Γ) are the M and J points, which are clearly $M = (0.5, 0.5)$ and $J = (0.5, 0)$ in the reciprocal basis. To get the K point, we must find the intersections of the perpendicular bisectors. The perpendicular bisector between Γ and $\mathbf{G}_1$ is the line of points $(\mathbf{k} - \mathbf{G}_1/2) \cdot \mathbf{G}_1 = 0$, and the perpendicular bisector between Γ and $\mathbf{G}_+ = \mathbf{G}_1 + \mathbf{G}_2$ is the line of points $(\mathbf{k} - \mathbf{G}_+/2) \cdot \mathbf{G}_+ = 0$. The interesection of these two perpendicular bisectors is the K point (at the upper right), given by the solution to:

$$\mathbf{k}_K = \begin{pmatrix} \mathbf{G}_1 \\ \mathbf{G}_+ \end{pmatrix}^{-1} \begin{pmatrix} |\mathbf{G}_1|^2 \\ |\mathbf{G}_+|^2 \end{pmatrix} /2 = \begin{pmatrix} \frac{\csc\theta - \cot\theta}{2} + (1-\cos\theta)\cot\theta \\ -\frac{1}{2} + (1-\cos\theta) \end{pmatrix} \cdot \frac{2\pi}{a} \csc\theta.$$

Here, the first parenthesized quantity is the 2×2 matrix whose rows are $\mathbf{G}_1$ and $\mathbf{G}_+$, and we have used the fact that the inverse of a 2×2 matrix $\begin{pmatrix} a & b \\ c & d \end{pmatrix}$ is given by $\begin{pmatrix} d & -b \\ -c & a \end{pmatrix}/(ad-bc)$. However, for MPB we want to compute this vector in the basis of $\mathbf{G}_1$ and $\mathbf{G}_2$, which is related to the Cartesian $\mathbf{k}_K$ by the inverse of the matrix whose *columns* are $\mathbf{G}_1$ and $\mathbf{G}_2$:

$$K = \begin{pmatrix} \mathbf{G}_1 & \mathbf{G}_2 \end{pmatrix}^{-1} \mathbf{k}_K = \begin{pmatrix} \csc\theta & 0 \\ \cot\theta & 1 \end{pmatrix} \begin{pmatrix} \frac{\csc\theta - \cot\theta}{2} + (1-\cos\theta)\cot\theta \\ -\frac{1}{2} + (1-\cos\theta) \end{pmatrix} = \begin{pmatrix} 1-\alpha \\ \alpha \end{pmatrix},$$

where $\alpha = \sin^2(\theta/2)/\sin^2\theta$ (we have used several trig. identities to gratuitously simplify the result). *Let's check it:* for $\theta = 60°$, this gives us $K = (2/3, 1/3)$ which is equivalent to what MPB uses (via a 120° rotation); for $\theta = 90°$ it gives us the point $(0.5, 0.5)$, which is the same as the M point of the square lattice. For $\theta = 75°$, $K \approx (0.60280, 0.39720)$.

Let's check that the K point at the lower-right of fig. 1b is indeed related to the one at the upper-right. Denote the lower-right K point by K'; then K' is the intersection of the perpendicular bisectors

between Γ and $\mathbf{G}_1$ and between Γ and $-\mathbf{G}_2$, which is given by:

$$K' = \begin{pmatrix} \mathbf{G}_1 & \mathbf{G}_2 \end{pmatrix}^{-1} \begin{pmatrix} \mathbf{G}_1 \\ \mathbf{G}_2 \end{pmatrix}^{-1} \begin{pmatrix} |\mathbf{G}_1|^2 \\ -|\mathbf{G}_2|^2 \end{pmatrix} /2 = \begin{pmatrix} \alpha \\ -\alpha \end{pmatrix},$$

where α is the same as defined above. Now, we should have $K' = -(K - \mathbf{G}_1) = -K + (1,0)$, and indeed this is clearly the case (well, we helped by using lots of trig. identities in simplifying K above).

Now you can (hopefully) see why we are treating J as a special point, even though it isn't at a corner: the $\mathbf{k}$ range from upper-right K (K') is actually the same *along the boundary*, so we expect to get band extrema at J even though it is not a corner of the I.B.Z.! Note, however, that $\Gamma - J$ is *not* a mirror symmetry plane

(b) To compute the band structure we'll just look around the edge of the irreducible Brillouin zone plus $\Gamma - J$ for good measure: Γ to M to K to J and back to Γ and then from Γ to K'. which includes all of the high-symmetry directions (i.e. along the mirror planes) and no redundant points except for the repeated corners. This is implemented Jupyter notebook accompanying these solutions. Note that we don't have enough symmetry to have any exact degeneracies at the special points, though some bands come very close; we only get accidental degeneracies (crossings of even/odd modes) at intermediate points.) For $\theta = 75^\circ$, we find a 42.4% TM gap between band 1 at the M point to band 2 at the J point, which is in between the gap sizes of the square and triangular lattices as you might expect.

(c) The band diagram and the ε structure (over several periods) are plotted in the solutions

(d) As shown in the solutions, the gap size was 42.4%, compared to 47.4% for the hexagonal lattice. Breaking the symmetry often (though not always) decreases the gap, because in some directions the gap shrinks even if in other directions the gap increases.

Problem 3: (10+10 points)

Based on the sample code in the Jupyter notebook, compute the TM transmission spectrum for planewaves incident upon N_x layers of the hexagonal lattice of rods from problem 2.

(a) See the solution notebook for the calculatoins and plots.

In the band diagram, there was a TM gap from a frequency of 0.28 to $0.42\,c/a$. In the transmission spectrum, we clearly see a dip in the transmission—decreasing *exponentially* with N_x as expected (since fields are evanescent in the gap)—around these frequencies. However, if we look closely, we see that the transmission dip is **wider** than the overall band gap, from about 0.24 to 0.42. What's happening is that our structure is periodic in y, so k_y is conserved, and a normal-incident planewave **only couples to $k_y = 0$ bands**, which are those along the Γ–X portion of the band diagram. If we just look at Γ–X, then the gap is indeed wider, from 0.24 to 0.42 c/a!

Also as expected from class, the transmission dip is largest near the middle of the gap, since we showed that the evanescent decay rates increase away from the band edges.

Another feature that you might notice is that, as we increase N_x, we see that a transmission dip is appearing round 0.71–0.74 c/a. If you look closely at the Γ–X band diagram you will see that there is indeed **another gap** (just for Γ–X, not for the whole Brillouin zone) at those frequencies. Since that gap is much smaller, the evanescent decay rate is much slower, and so the transmission dip is weaker for the same N_x.

(b) From the analysis in class (and chapter 10), k_y is conserved up to integer multiples of $2\pi/a$. Since the incident wave is $k_y = 0$, the first diffracted order corresponds to $k_y = \pm 2\pi/a$. However, the corresponding $k_x = \sqrt{(\omega/c)^2 - k_y^2}$ is imaginary (evanescent) until $\omega \geq 2\pi c/a$, or a frequency $f \geq c/a$.

Since $c/a = 1$ in our Meep units, this means we expect to see an additional diffracted order actually propagating away in the reflected (and transmitted) wave for $\boxed{f \geq 1}$ in Meep units.

The resulting fields are shown for $f = 0.95c/a$ and $f = 1.05c/a$ in the solution notebook, and clearly exhibit the transition to additional diffracted orders for $f > 1\,c/a$.

The solution notebook also shows the results for $f = 0.995\,c/a$, much closer to the diffraction threshold. In this case, we needed to increase the "pad" parameter to increase the width of the air region. The reason for this is that, as $f \to 1^-$ (that is, approaching 1 from *below*), the first reflected diffracted order's evanescent decay rate gets slower and slower ($k_x \to i0^-$ from above), so we see its transverse oscillations in the field farther and farther from the crystal.