18.369 Midterm Exam Solutions (Spring 2014)

Problem 1: Irreps (50 pts)

(a) Trivially from the given identity,

$$\mathbf{J} = \frac{a}{2\pi} \int_0^{2\pi/a} \left[\sum_{n=-\infty}^{\infty} \delta(x - na) \delta(y) e^{ikna - i\omega t} \hat{z} \right] dk_y$$

where the term $[\cdots]$ is Bloch-periodic. Because irrep is conserved, from class and homework, the resulting steady-state/time-harmonic **E** field from each Bloch-periodic term is also Bloch-periodic (from periodicity) and TM-polarized (from $z \leftrightarrow -z$ mirror symmetry), i.e. the field of the current $[\cdots]$ is:

$$E_k(x,y)e^{ikx-i\omega t}\hat{z}_{j}$$

where $E_k(x+a, y) = E_k(x, y)$.

(b) To get an equation with *periodic* (*not* Bloch-periodic) boundary conditions, we have to write an equation for the Bloch envelope E_k rather than for the field $E_k e^{ikx}$. This is exactly the same as the process we went through in class to go from $\hat{\Theta}$ to $\hat{\Theta}_k$: just replace ∇ with $\nabla + i\mathbf{k}$ (where $\mathbf{k} = k\hat{x}$), the result of commuting e^{ikx} with ∇ . For convenience, define $\nabla_k = \nabla + i\mathbf{k}$. Then

$$(\nabla_k \times \nabla_k \times -\omega^2 \varepsilon) E_k \hat{z} = i\omega \delta(x) \delta(y),$$

defined on the unit cell $x \in [-a/2, a/2]$ with periodic boundary conditions in x. (The periodic boundary conditions mean that we don't need to sum an infinite series of sources: this is implied by the boundary conditions.)

(c) The total field, by superposition, is just

$$\mathbf{E} = \hat{z} \frac{a}{2\pi} \int_0^{2\pi/a} E_k(x, y) e^{ikx - i\omega t} dk.$$

(d) To get the total power, we also need

$$\mathbf{H} = \frac{1}{i\omega} \nabla \times \mathbf{E} = \frac{a}{2\pi} \int_0^{2\pi/a} \mathbf{H}_k(x, y) e^{ikx - i\omega t} dk,$$

where $\mathbf{H}_k = \nabla_k \times E_k \hat{z}$ is a periodic function. Hence, \mathbf{H} , like \mathbf{E} , is a superposition of Bloch-periodic functions. Because partners of different irreps are orthogonal, the $\int dx$ of $\hat{y} \cdot (E_k \hat{z} e^{ikx}) \times (\mathbf{H}_{k'} e^{ik'x})$ must necessarily be zero unless k = k', hence the total power P will be a superposition of terms P_k that are integrals of $\hat{y} \cdot (E_k \hat{z} e^{ikx}) \times (\mathbf{H}_k e^{ikx})$: the Poynting flux of one k at a time.

However, getting the exact form of this superposition, including the normalization, is a bit tricky because of the infinite bounds of the *x* integral. One straightforward approach is to adopt the same trick that we used to deriving the per-period LDOS (in fact, the notes on this were attached to the exam and are used in the next problem as well): instead of an infinite system in the *x* direction, we consider a supercell of *M* periods, with periodic boundaries $x \leftrightarrow x + Ma$, and take the $M \rightarrow \infty$ limit in the end. As in the notes, for such a supercell we

get a subset of the Bloch solutions, only $k_m = \frac{2\pi}{Ma}m$ for integers m = 0, ..., P-1, or equivalently one can easily show:

$$\mathbf{J} = \frac{1}{M} \sum_{m=0}^{M-1} \left[\sum_{n=0}^{M-1} \delta(x - na) \delta(y) e^{ik_m na - i\omega t} \hat{z} \right],$$
$$\mathbf{E} = \hat{z} \frac{1}{M} \sum_{m=0}^{M-1} E_{k_m}(x, y) e^{ik_m x - i\omega t}$$

for the same E_k solutions as above. The Poynting flux is then

$$P = \frac{1}{2} \int_{0}^{Ma} \hat{y} \cdot \operatorname{Re} \left[\mathbf{E}^{*}(x, y_{0}) \times \mathbf{H}(x, y_{0}) \right] dx$$

= $\frac{1}{2} \hat{y} \cdot \operatorname{Re} \int_{0}^{Ma} \left[\hat{z} \frac{1}{M} \sum_{m=0}^{M-1} E_{k_{m}}(x, y_{0}) e^{ik_{m}x - i\omega t} \right]^{*} \times \left[\frac{1}{M} \sum_{m'=0}^{M-1} \mathbf{H}_{k_{m'}}(x, y_{0}) e^{ik_{m'}x - i\omega t} \right] dx.$

As above, the $m \neq m'$ cross terms must integrate to zero (since they are partner functions of different irreps of the symmetry group: translations by *na* for n = 0, ..., M - 1). What remains is

$$P = \frac{1}{2}\hat{y} \cdot \operatorname{Re} \frac{1}{M^2} \sum_{m=0}^{M-1} \int_0^{Ma} [\hat{z}E_{k_m}(x, y_0)]^* \times [\mathbf{H}_{k_m}(x, y_0)] dx$$

= $\frac{1}{2}\hat{y} \cdot \operatorname{Re} \frac{1}{M} \sum_{m=0}^{M-1} \int_0^a [\hat{z}E_{k_m}(x, y_0)]^* \times [\mathbf{H}_{k_m}(x, y_0)] dx$
= $\frac{1}{M} \sum_{m=0}^{M-1} P_{k_m},$

where we have used the periodicity of E_k and \mathbf{H}_k and defined

$$P_k = \frac{1}{2}\hat{\mathbf{y}} \cdot \operatorname{Re} \int_0^a \left[\hat{z}E_k(x, y_0)\right]^* \times \left[\mathbf{H}_k(x, y_0)\right] dx$$

as the Poynting flux in a single unit cell from the Bloch solution for a single k. Finally, by multiplying and dividing by $\Delta k = \frac{2\pi}{Ma}$ as in class, we can take the $M \to \infty$ limit to recover the integral:

$$P = \frac{a}{2\pi} \int_0^{2\pi/a} P_k dk$$

Problem 2: LDOS (50 pts)

- (a) At $k = \pi/a$, the sign pattern should flip from one rod to the next, and should be even or odd mirror symmetric in both *x* and *y*. The first band should be concentrated in the high-dielectric rods, whereas the second band will have a sign oscillation in order to be orthogonal. This sign oscillation is probably in the *x* direction, for two reasons. First, if these two bands arise from "band-folding" of a guided mode, similar to the first and second bands in a 1d photonic crystal, then by the same arguments as in 1d they should come from $\cos(\pi x/a)$ and $\sin(\pi x/a)$ -like modes. Second, similarly to how we argued for 2d photonic crystals in class, a sign oscillation in the *x* direction is less oscillatory (and hence a smaller Rayleigh quotient) than a sign oscillation in the *y* direction, because this way there is no nodal plane halfway between the rods. The resulting field sketches are shown in Figure 1.
- (b) We will derive the LDOS in the same was as the per-period DOS in the notes: compute the LDOS for a point source in a periodic supercell of M periods, and then take the $M \to \infty$ limit. Suppose that the Bloch modes of the periodic system are $E_z^n(x,y) = E_k^n(x,y)e^{ikx}$, where E_k^n is the periodic Bloch envelope of the *n*-th band, with frequency $\omega_n(k)$, normalized to $\int \varepsilon |E_k|^2 = 1$ for an integral over the *unit cell* $x \in [0,a]$. In a periodic supercell, as in the notes and as above, the only allowed modes are those with $k_m = \frac{2\pi}{Ma}m$ for $m = 0, 1, \dots, M 1$. In this supercell, we can simply quote the LDOS formula:

$$\frac{1}{M}\sum_{m=0}^{M-1}\sum_{n}\varepsilon(\mathbf{x})|E_{k_m}^{(n)}(\mathbf{x})|^2\delta(\boldsymbol{\omega}-\boldsymbol{\omega}_n(k_m)),$$

where the 1/M factor is to convert the normalization of the modes to $\int \varepsilon |\mathbf{E}|^2 = 1$ over the *supercell*, as our LDOS derivation assumed. Then, we multiply and divide by $\Delta k = \frac{2\pi}{Ma}$, as in the notes and above, and take the limit $M \to \infty$ ($\Delta k \to 0$) to obtain an integral:

$$\frac{a}{2\pi}\int_0^{2\pi/a}\sum_n \varepsilon(\mathbf{x})|E_k^{(n)}(\mathbf{x})|^2\delta(\boldsymbol{\omega}-\boldsymbol{\omega}_n(k))dk$$

- (c) As in the notes, we expect a $\sim 1/\sqrt{\omega \omega_0}$ Van Hove singularity at the two band edges when we integrate the formula from part (b) (note that the same quadratic approximation applies to the LDOS as to the DOS, because $|E_k|^2$ should be a constant plus a quadratic term to lowest order in $k \pi/a$). However, the density of states is not zero in the "gap" because in *addition* to the guided bands we will also have an LDOS associated with the light cone, although the amplitude will be less than in vacuum because of the reduced radiation-field amplitude near the waveguide (in order to be orthogonal to the guided modes). (In two dimensions, it will turn out that this light-cone LDOS increases roughly linearly with *k* asymptotically, but I didn't expect you to show that.) As $|y_0|$ increases, moving away from the waveguide, the guided-mode contributions to the LDOS will decrease *exponentially* fast with y_0 , because of the exponential decay of the guided-mode fields. Neverthess, there will still be a singularity at the band edge, it will just get narrower because of the decreased amplitude, and the LDOS in the gap will approach that of vacuum. A sketch of the resulting LDOS is shown in the left panel of Figure 2.
- (d) From your sketch in part (a), the second band at k = π/a is zero at point 2 (which lis on the mirror plane). Naively, you might conclude that band 2 will not appear at all in the LDOS, but this is incorrect: the mode is mirror-symmetrical only at k = π/a, since k breaks the mirror symmetry at other points in the Brillouin zone



Figure 1: Sketches of E_z field (contour plot) for the first two bands, in problem 2(a).



Figure 2: Sketch of LDOS at point 1 in problem 2 (left) and at point 2 (right), where the latter differs because it lies on a mirror plane that is orthogonal to band 2 at $k = \pi/a$.

(except k = 0, but we don't have a guided mode there anyway). So, the second band will still contribute to the LDOS from $k \neq \pi/a$.

To work out this contribution, we will use the same Taylor-expansion trick as in the notes (approximating the band by a quadratic $\omega(k) \approx \omega_2 + \alpha (k - \pi/a)^2$ near the band edge). should first consider how $E_k^{(2)}(x_0, y_0)$ depends on k if we Taylor expand around $k = \pi/a$. The zero-th order term is $E_{\pi/a}^{(2)}(x_0, y_0) = 0$ as noted above, but generically we should expect a nonzero first-order term (since E_k does not need to be a particular sign). Hence, the $|E_k|^2$ term in the LDOS is proportional to $(k - \pi/a)^2$ to lowest order, and the band-2 contribution to the integral from part (b) becomes:

$$\sim \int (k - \pi/a)^2 \delta \left[\omega - \omega_2 - \alpha (k - \pi/a)^2 \right] dk$$
$$= \int \frac{k - \pi/a}{2\alpha} \delta \left[k - \pi/a \pm \sqrt{\frac{\omega - \omega_2}{\alpha}} \right] dk$$
$$\sim \sqrt{\omega - \omega_2},$$

i.e. a square-root singularity but *not* a divergence. This will look something like the sketch in the right panel of Figure 2.