18.369 Take-Home Midterm Exam SOLUTIONS: Spring 2024

Problem 1: (5+5+5 points)

Recall from class that if we have an x-periodic problem with period a, i.e. its symmetry group consists of translations $\hat{n}f(x) = f(x-na)$ for all integers n, then the eigenfunctions of $\hat{n}$ are Bloch-periodic functions $f_k(x)e^{ikx}$ where f_k is periodic, corresponding to eigenvalues $D^{(k)}(n) = e^{-ikna}$ for arbitrary real k (but $D^{(k)} = D^{(k+\frac{2\pi}{a})}$). Equivalently, these are the partner functions of the 1d irreps $D^{(k)}$ (which are, in fact, the only possible unitary irreps).

(a) Suppose that space is looped around in a torus/circle with period Na, so that translation $\hat{N}$ is equivalent to translation $\hat{0}$ (= identity). In this case, what are the irreps?

Solution: If $\hat{N} = \hat{0}$, then we must have the same property of the irreps: $D^{(k)}(N) = e^{-ikNa} = D^{(k)}(0) = 1$, which implies that $kNa = 2\pi m$ for some integer m. That is $k = \frac{2\pi m}{Na}$. However, not all integers m lead to distinct irreps, because we also know that k and $k + \frac{2\pi}{a} = \frac{2\pi}{Na}(m+N)$ are equivalent, so that m and $m+N$ are equivalent. Hence, the distinct irreps correspon to

$$\boxed{k_m = \frac{2\pi m}{Na} \text{ for } m = 0, \ldots, N-1}$$

(or equivalent, e.g. $m = 1 \ldots N$ or $m = -\lfloor N/2 \rfloor \ldots \lceil N/2 \rceil - 1$).

(b) For this finite N-period torus, what are the projection operators for your irreps, applied to some arbitrary function $f(x)$? The projection operator involves a sum, and (as you saw in pset 4) the sum of the projection operators over all irreps is the identity — show that in the limit $N \to \infty$ (infinite periodic systems), at least one of these two sums becomes an integral (you may need to rearrange a normalization factor).

Solution: The dimension d of these representations is 1, and the size of the group is N, so applying our general formula for projection operators, we have

$$\boxed{f_{k_m}(x) = \hat{P}^{(m)} f = \frac{1}{N}\sum_{n=0}^{N-1} D^{(k_m)}(n)^* \hat{n} f = \frac{1}{N}\sum_{n=0}^{N-1} e^{+i\frac{2\pi}{N}mn} f(x-na),}$$

which is in the form of a discrete Fourier transform (DFT) for each x, and $f(x) = \sum_{m=0}^{N-1} f_{k_m}(x)$. Note that $f_{k_m}(a)$ is *not* periodic, it is Bloch-periodic: by construction, $f_{k_m}(x-a) = e^{-i\frac{2\pi}{N}m} f_{k_m}(x)$ via the change of variables $n' = n+1$.

To take the $N \to \infty$ limit, we will want to shift the $1/N$ normalization factor to the $\sum_m$, so we will define $F_{k_m}(x) = Nf(x)$. It is also useful to rewrite the sums starting at zero to something like

$$\sum_{n=0}^{N-1} = \sum_{n=-\lfloor N/2 \rfloor}^{\lceil N/2 \rceil - 1}$$

so that we remove anything special about the origin $0 \leftrightarrow N$ from the sum (since it is weird to have $n = 0$ "wrap to infinity" in the $N \to \infty$ limit). Then, we have

$$F_{k_m}(x) = Nf_{k_m}(x) \longrightarrow \boxed{F_k(x) = \sum_{n=-\infty}^{\infty} e^{+ikna} f(x-na) \text{ for } k \in [0, \frac{2\pi}{a})}$$

and

$$f(x)=\frac{1}{N}\sum_{m=0}^{N-1}F_{k_m}(x)=\frac{a}{2\pi}\sum_m F_{k_m}(x)\underbrace{\frac{2\pi}{Na}}_{\Delta k}\longrightarrow\boxed{f(x)=\frac{a}{2\pi}\int_0^{2\pi/a}F_k(x)dk},$$

corresponding exactly to a **Fourier series** (or DTFT) and its inverse. The latter may not *look* like the inverse of a Fourier series, but remember that $F_k(x)$ is Bloch-periodic — if we change variables to a periodic coefficient $u_k(x)=e^{-ikx}F_k(x)=u(x+a)$, then we get something that looks more conventional:

$$u_k(x)=\sum_n e^{-ik(x-na)}f(x-na)\Longleftrightarrow f(x)=\frac{a}{2\pi}\int_0^{2\pi/a}e^{+ikx}u_k(x)dk\,.$$

(c) Suppose that we have Maxwell's equations in an x-periodic system $\varepsilon(x,y,z)=\varepsilon(x+a,y,z)$. You saw in pset 1 that the response to a time-harmonic current source is given by the solution to $(\nabla\times\nabla\times-\omega^2\varepsilon)\mathbf{E}=i\omega\mathbf{J}$ ($\varepsilon_0=\mu_0=c=1$ units); here, the operator on the left commutes with $\hat{n}$. Now, however, suppose that $\mathbf{J}$ is *not* periodic or Bloch-periodic, and just is some arbitrary current distribution (e.g. maybe it is localized in a finite region of space). Explain how we could still solve for $\mathbf{E}$ by solving a *set* of problems with Bloch-periodic boundaries and summing or integrating the results. (Hint: apply your projection operator.) (This is a very practical computational tool for modeling periodic systems with non-periodic sources!)

Solution: From above, $\mathbf{J}(x,y,z)=\frac{a}{2\pi}\int_0^{2\pi/a}\mathbf{J}_k(x,y,z)dk$ can be written as a superposition of Bloch-periodic sources by a projection operation:

$$\mathbf{J}_k(x,y,z)=\sum_{n=-\infty}^{\infty}e^{+ikna}\mathbf{J}(x-na,y,z)=e^{ika}\mathbf{J}_k(x-a,y,z)\,.$$

So, we can solve for $\mathbf{E}$ by:

(i) Approximate the integral $\mathbf{J}(x,y,z)=\frac{a}{2\pi}\int_0^{2\pi/a}\mathbf{J}_k(x,y,z)dk$ by a sum (a "quadrature rule") over a finite set $\{k_m\}$ of k values.

Comment: Since the integrand is periodic in k, a good choice is simply equally spaced points $k_m=\frac{2\pi m}{Na}$ for $m=0,\ldots,N$ for a sufficiently large N as we did in the previous part, i.e. $\mathbf{J}(x,y,z)\approx\frac{1}{N}\sum_{m=0}^{N-1}\mathbf{J}_{k_m}(x,y,z)$, exactly the reverse of the limit of the previous section (corresponding to approximating the infinite periodic system by a "supercell" of N unit cells).

(ii) For each "quadrature point" k_m, compute $\mathbf{J}_{k_m}$ by the projection operation above, for all x in the unit cell $x\in[0,a)$. If the current is localized in a finite region as suggested, then the sum can be truncated to n's for which $x-na$ lies within the support of $\mathbf{J}$. (More generally, assume that the sum is converging so that we can compute it easily to any desired accuracy.)

(iii) For each Bloch-periodic current $\mathbf{J}_{k_m}$, solve Maxwell's equations in the unit cell $x\in[0,a)$ with Bloch-periodic boundary conditions for the corresponding electric field $\mathbf{E}_{k_m}(x,y,z)$.

(iv) Compute $\mathbf{E}(x,y,z)=\frac{a}{2\pi}\int_0^{2\pi/a}\mathbf{E}_k(x,y,z)dk$ (for any desired x), where again the $\int dk$ is approximated by our sum over k_m (our quadrature rule). This is the desired solution!

Problem 2 (15 points)

Refer to the solutions for problem 3 of pset 2 (recently updated to fix a couple of typos), in which we put a time-harmonic current source $\mathbf{J}=f(x)\delta(y)e^{-i\omega t}\hat{x}$ into a PEC waveguide (waves traveling along the y direction) and found the (H_z-polarized) solutions as an infinite cosine series of propagating + evanescent modes.

Suppose that the cosine-series coefficients of $f(x)/2$ are $a_n=0$ for n even and $a_n=\frac{1}{n^2}$ for n odd (corresponding to $f(x)$ proportional to $x-L/2$, but you need not go through the integrals). Compute the rate of power $P(\omega)$ expended by the current source (e.g. with the help of Poynting's theorem), and sketch a plot of $P(\omega)$ a function of frequency $\omega \geq 0$ (capturing the main qualitative features).

Solution:

Recall from pset 2 that the solution for the magnetic field looked like:

$$H_z(x,y) = \sum_{n=0}^{\infty} a_n \cos\left(\frac{n\pi x}{L}\right) e^{ik_n|y|-i\omega t}\,\mathrm{sign}(y),$$

for propagating/evanescent modes $k_n = +\sqrt{\omega^2 - \left(\frac{n\pi}{L}\right)^2}$ (for $c=1$ units and $\omega > 0$) with Fourier cosine-series coefficients

$$a_n = \frac{1}{L}\int_0^L f(x)\cos\left(\frac{n\pi x}{L}\right)dx\,.$$

By Poynting's theorem, we can compute the (time-average) power $P(\omega)$ expended by the current source either by computing the Poynting flux or by computing the (time-average) work **expended** by the current source on the field (note the sign):

$$P(\omega) = -\frac{1}{2}\Re\left[\int \mathbf{J}^* \cdot \mathbf{E}\right].$$

Here, I will use the latter approach. Either way, we first need to compute E_x, which is given from Ampere's law $\nabla \times \mathbf{H} = -i\omega\varepsilon\mathbf{E} + \mathbf{J}$. For $y \neq 0$, where we have $\varepsilon = 1$, this gives

$$E_x = -\frac{1}{i\omega}\frac{\partial H_z}{\partial y} = -\sum_{n=0}^{\infty} a_n \frac{k_n}{\omega}\cos\left(\frac{n\pi x}{L}\right) e^{ik_n|y|-i\omega t},$$

(where the $\pm$ and i factors helpfully cancel out). Notice that the limits $y \to 0^{\pm}$ agree — E_x is continuous and well defined at $y=0$. (Recall from pset 2 that the derivative of H_z across its jump at $y=0$ gives the δ function in $\mathbf{J}$, so Ampere's law is now satisfied everywhere.) The power is now:

$$P(\omega) = -\frac{1}{2}\Re\left[\int \mathbf{J}^*\cdot\mathbf{E}\right] = \frac{1}{2}\Re\left[\sum_{n=0}^{\infty} a_n \frac{k_n}{\omega}\underbrace{\int_0^L f(x)^*\cos\left(\frac{n\pi x}{L}\right)dx}_{La_n^*}\right] = \boxed{\frac{L}{2\omega}\Re\left[\sum_{n=0}^{\infty}|a_n|^2 k_n\right]},$$

where the $\delta(y)$ eliminated the y integral, the $f(x)$ integral gave us an a_n^* term, and some other nice simplifications happened. In fact, a further simplication occurs because **most of the terms in the $\sum_n$ are zero** since k_n is imaginary (evanescent) for all but a finite number of terms $\boxed{n < \frac{L\omega}{\pi}}$. Hence, we can simplify this further to

$$P(\omega) = \frac{L}{2}\sum_{0\leq n<\frac{L\omega}{\pi}} |a_n|^2\sqrt{1-\left(\frac{n}{\omega L/\pi}\right)^2} \geq 0.$$

For $L\omega/\pi < 1$, so that this only has the $n=0$ term, we have a constant $P = |a_0|^2 L/2$. As $L\omega/\pi$ passes through each positive integer (corresponding to the cutoff of each successive propagating mode), we get a square-root singularity (infinite slope). Note that this power is always nonnegative as expected! An example of what this could look like is shown in Fig. 1.

Comment on solutions: van Hove Singularities

The singularities in the power $P(\omega)$ that occur when new propagating modes appear (i.e. at band edges) is called a *van Hove singularity*, and is well known in solid-state physics. However, if you are already familiar with van Hove singularities, you may have noticed something that seems mysterious at first glance:

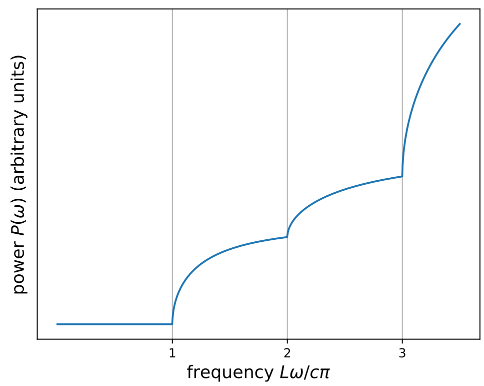

Figure 1: Problem 2 solution: typical power $P(\omega) \geq 0$ in arbitrary units as a function of nondimensionalized frequency $L\omega/c\pi$. It starts at some ≥ 0 constant value, then undergoes a square-root singularity (infinite slope) every time $L\omega/c\pi$ passes through a positive integer (corresponding to the cutoffs for additional propagating modes). The exact amplitudes of each term will depend on the Fourier cosine-series coefficients a_n of the current source, which here were chosen randomly.

the square root singularity that we see above is the "wrong singularity" for 1d. In a 1d band structure (only one direction of translational symmetry = one direction of k), the singularity in the power (or "local density of states") is genericaly an *inverse square root* singularity, corresponding to $\Re[k_n^{-1}]$. The "mere" square-root singularity $\Re[k_n]$ that we get here is much weaker, and is generically what one expects from van Hove singularities in *3d*. (These dependencies can be derived from density-of-states "counting" arguments where you integrate $\sum_n \int \delta(\omega - \omega_n(\mathbf{k}))\, dk$ around a band edge $\omega_n \sim \|\mathbf{k}\|^2 + \cdots$ in various dimensions, and are discussed in many solid-state physics textbooks.) What is going on here that is special?

In fact, you do see the "expected" $\Re[k_n^{-1}]$ singularity for a J_z current source exciting E_z-polarized modes, so the behavior here is unique to the H_z polarization. What's going on here originates from the fact that the H_z-polarized solution at cutoff ($k = 0$) is a standing wave of planewaves propagating in the $\pm x$ direction (orthogonal to the direction of translational symmetry), which for the H_z polarization have an electric field $\mathbf{E}$ that lies entirely in the y direction. But with this polarization, $\mathbf{E}$ at $k = 0$ is therefore **perpendicular** to our current source $\mathbf{J}$ (in the x direction), and hence contributes *nothing* to the power $P(\omega)$. This vanishing current–field overlap exactly at cutoff cancels some of the singularity, and is the reason $\Re[k_n^{-1}]$ is weakened to $\Re[k_n]$ for the H_z polarization. For the E_z polarization, in contrast, the electric field lies in the z direction for all k, and hence has a nonzero inner product with J_z for all k including cutoff, and one consequently observes the full $\Re[k_n^{-1}]$ singularity — precisely this case was analyzed in problem 2 of pset 3 from fall 2021, in fact.

Problem 3 (5+5+5 points)

In class, we have mostly considered the simplified case where the electric polarization density $\mathbf{P}$ responds *instantaneously* and linearly to the electric field at the same point in space: $\mathbf{P}(\mathbf{x}) = \chi_e \mathbf{E}(\mathbf{x})$ for some constant "susceptibility" $\chi_e = \varepsilon - 1$. More generally, however, changing $\mathbf{P}$ involves physically moving electric charges, and so it cannot happen instantaneously.

Imagine a simple model in which the charges are attached to immobile atoms with linear springs, so that they can bounce back and forth with some frequency ω_0 in the absence of external forces. (This actually turns out to be a reasonable semiclassical model of an atom with an "electric dipole transition" energy difference $\hbar\omega_0$ between a ground state and an excited state.) Of course, there also needs to be some "friction" so that the atom slowly settles down (to its ground state) when it is left alone. A simple model for this is to describe $\mathbf{P}$ by a damped harmonic oscillator at each point in space:

$$\ddot{\mathbf{P}} = -\omega_0^2 \mathbf{P} - \gamma_0 \dot{\mathbf{P}} + \sigma_0 \mathbf{E}$$

for a frequency ω_0, a damping rate $\gamma_0 > 0$, and a coupling coefficient $\sigma_0 > 0$ to the electric field at that point in space.

(a) Assuming time-harmonic fields $\mathbf{E}$ and $\mathbf{P}$ proportional to $e^{-i\omega t}$, show that you obtain the same Maxwell equations as in class but with a *frequency-dependent* permittivity $\varepsilon(\omega,\mathbf{x})$ (where the $\mathbf{x}$ dependence arises if your coefficients above vary with $\mathbf{x}$).

Solution: For time-harmonic solutions $\mathbf{E}(\mathbf{x})e^{-i\omega t}$ and $\mathbf{P}(\mathbf{x})e^{-i\omega t}$, the equation becomes $-\omega^2\mathbf{P} = -\omega_0^2\mathbf{P} + i\omega\gamma_0\mathbf{P} + \sigma_0\mathbf{E}$, and hence

$$\mathbf{P} = \underbrace{\frac{\sigma_0}{(\omega_0^2 - \omega^2) - i\omega\gamma_0}}_{\chi_e(\omega,\mathbf{x})}\mathbf{E},$$

where we have identified the proportionality factor as $\chi_e(\omega)$ (the electric susceptibility) from class. Hence (from class),

$$\boxed{\varepsilon(\omega,\mathbf{x}) = 1 + \chi_e(\omega,\mathbf{x}) = 1 + \frac{\sigma_0}{(\omega_0^2 - \omega^2) - i\omega\gamma_0}}.$$

where the $\mathbf{x}$ dependence (if any) comes from $\omega_0(\mathbf{x}), \gamma_0(\mathbf{x}), \sigma_0(\mathbf{x})$. For example, if we have a single kind of polarizable material in some regions of space and vacuum ($\varepsilon = 1$) in other regions, then ω_0 and γ_0 will be constants while σ_0 will be 0 in vacuum and some positive constant in the material.

(b) Sketch a plot of $\Re\varepsilon - 1 = \Re\chi_e$ and $\Im\varepsilon = \Im\chi_e$ versus ω/ω_0, in the regime where the friction term is fairly small (but not zero!) compared the ω_0 term (i.e. where the loss rate is small, say 5%, compared to ω_0). $\Im\varepsilon$ should have a peak—what parameters determine the width, amplitude, and location of this peak?

Solution: The real and imaginary parts of ε are

$$\Re\varepsilon = 1 + \frac{\sigma_0(\omega_0^2 - \omega^2)}{(\omega_0^2 - \omega^2)^2 + (\omega\gamma_0)^2},$$

$$\Im\varepsilon = \frac{\sigma_0(\omega\gamma_0)}{(\omega_0^2 - \omega^2)^2 + (\omega\gamma_0)^2}.$$

Let's plot this in the regime of *small damping*, where $\gamma_0 \ll \omega_0$, e.g. for $\gamma_0 = 0.05\omega_0$ (note that this is dimensionally correct—both have units of frequency). To make things nice and dimensionless, we'll plot $(\Re\varepsilon - 1)/\sigma_0\omega_0^2$ and $\Im\varepsilon/\sigma_0\omega_0^2$, both versus ω/ω_0.

By inspection of the formula, when γ_0 is small, it's pretty easy[1] to see that $\Im\varepsilon$ peaks in the vicinity of $\omega = \pm\omega_0$, with a peak amplitude proportional to $\sigma_0/(\omega_0\gamma_0)$ and a peak width proportional to γ_0. That is, it peaks near the resonance frequency, with a "linewidth" proportional to the loss.

We can solve for the peak more precisely by setting $\frac{d}{d\omega}\Im\varepsilon = 0$ and solving for ω. After some tedious algebra, keeping terms only to lowest order in γ_0/ω_0, I find that there are peaks at $\omega = \pm\omega_0\left[1 + \frac{\gamma_0^2}{8}\right]$ (plus terms proportional to γ_0^4 or larger).

Similarly, we can solve for the peak width (the "linewidth") more precisely by realizing that near

[1] For small $\gamma_0 \ll \omega_0$, the denominator of $\Im\varepsilon$ becomes very small when $(\omega_0^2 - \omega^2)^2 \lesssim (\omega\gamma_0)^2$, i.e. for $\omega \approx \omega_0$. Furthermore, in the vicinity of $\omega = \omega_0$ (similarly for $-\omega_0$), we can approximate $(\omega\gamma_0)^2 \approx (\omega_0\gamma_0)^2$ and $(\omega_0^2 - \omega^2)^2 = (\omega_0 - \omega)^2(\omega_0 + \omega)^2 \approx 4\omega_0^2(\omega_0 - \omega)^2$, so that the latter is smaller than the former for $|\omega - \omega_0| \lesssim \gamma_0/2$. This corresponds to a peak for $\omega \in [\omega_0 - \gamma_0/2, \omega_0 + \gamma_0/2]$, or a peak width $\sim \gamma_0$.

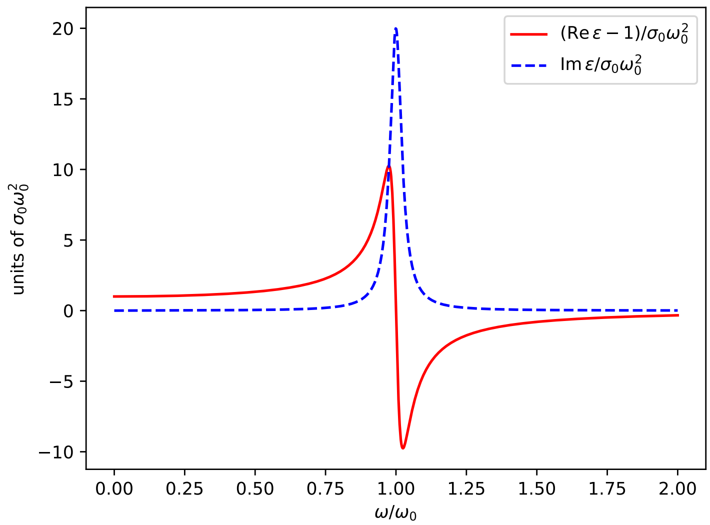

Figure 2: Plot of $\Re\varepsilon - 1$ and $\Im\varepsilon$, both in "nondimensionalized" units of $\sigma_0\omega_0^2$ for problem 3(c), with a relatively small loss $\gamma_0 = 0.05\omega_0$, as a function of ω/ω_0.

the peak for small γ_0 (narrow peaks), $|\omega|\gamma_0 \approx \omega_0\gamma_0$. With this approximation, we can compute the "width at half maximum" —i.e., over what width 2Γ is $\Im\varepsilon$ at least $1/2$ its peak? That is, what Γ solves $\Im\varepsilon(\omega_0 \pm \Gamma) \approx \frac{1}{2}\Im\varepsilon(\omega_0) \approx \sigma_0/2\omega_0\gamma_0$? After a little algebra, we find that this occurs at $\omega_0^2 - (\omega_0 \pm \Gamma)^2 = \pm\omega_0\gamma_0 \approx \mp 2\omega_0\Gamma$, and hence we find that the linewidth 2Γ is actually γ_0 at half-maximum! (Again, we could be even more precise by doing an expansion in powers of γ_0/ω_0.)

From the plot, notice also that $\Re\varepsilon - 1$ *oscillates in sign* around the resonance frequency ω_0. If this oscillation is large enough (if $\sigma_0/\omega_0\gamma_0$ is large enough), then $\Re\varepsilon$ can actually flip sign and become < 0 — it is totally possible to have a negative permittivity near a strong resonance (although this typically comes hand in hand with large absorption)!

(c) Show that your equations are consistent with the passivity condition $\omega\Im[\varepsilon] \geq 0$ from class.

Solution: From the formula in the previous part, it is obvious that

$$\omega\Im\varepsilon = \frac{\sigma_0(\omega^2\gamma_0)}{(\omega_0^2 - \omega^2)^2 + (\omega\gamma_0)^2} \geq 0$$

for all ω if and only if $\sigma_0\gamma_0 \geq 0$. Since $\gamma_0 \geq 0$ is required for our harmonic-oscillator equations for $\mathbf{P}$ to decay rather than grow (the friction force $-\gamma_0\dot{\mathbf{P}}$ must *oppose* the motion), it follows that we must have $\sigma_0 \geq 0$ (as assumed above).

From our notes on energy conservation in Maxwell's equations, it follows that $\sigma_0 \geq 0$ corresponds to the electric field $\mathbf{E}$ "doing net work" *on* the polarization $\mathbf{P}$ (rather than vice versa), called *passivity* of the medium, and we argued that this ultimately implies $\omega\Im\varepsilon \geq 0$ much more generally.