18.369 Problem Set 4 Solutions

Problem 1: Projection operators (5+5+5+5=20 points)

(a) Consider the action of $\hat{P}_i^{(\alpha)}$ on a partner function $\phi_j^{(\alpha')}$, as defined in the handout. We obtain $\hat{P}_i^{(\alpha)}\phi_j^{(\alpha')} = \frac{d_\alpha}{|G|}\sum_{g\in G} D_{ii}^{(\alpha)}(g)^*\hat{g}\phi_j^{(\alpha')} = \frac{d_\alpha}{|G|}\sum_{g\in G} D_{ii}^{(\alpha)}(g)^*[\sum_{i'}\phi_{i'}^{(\alpha')}D_{i'j}^{(\alpha')}(g)]$. If we perform the $\sum_g$ first, then from the Great Orthogonality Theorem we get $\sum_{i'}\delta_{ii'}\delta_{ij}\delta_{\alpha\alpha'}\phi_{i'}^{(\alpha')} = \delta_{ij}\delta_{\alpha\alpha'}\phi_i^{(\alpha)}$. Thus, for a $\psi = \sum_\alpha\sum_i c_i^{(\alpha)}\phi_i^{(\alpha)}$ decomposed into partner functions (as proved in the class notes), $\hat{P}_i^{(\alpha)}\psi = c_i^{(\alpha)}\phi_i^{(\alpha)}$. Q.E.D.

(b) $\sum_\alpha \hat{P}^{(\alpha)} = \sum_{g\in G}\left[\frac{1}{|G|}\sum_\alpha \chi^{(\alpha)*}(g)d_\alpha\right]\hat{g}$, interchanging the $\sum_\alpha$ and the $\sum_g$. But d_α, the dimension of the representation, is exactly the character $\chi^{(\alpha)}(E)$, the character of the identity element E, which is one column of the character table (E is in a conjugacy class by itself). So, the $[\cdots]$ inner sum is $\frac{1}{|G|}\sum_\alpha\chi^{(\alpha)*}(g)\chi^{(\alpha)}(E) = \delta_{gE}$ by the orthogonality of columns: it is zero unless $g = E$ and one otherwise. Hence, the outer sum $\sum_g$ disappears except for the E term, and $\sum_\alpha \hat{P}^{(\alpha)} = \hat{O}_E = 1$. Q.E.D.

Note that you can also prove $\sum_\alpha \hat{P}^{(\alpha)} = 1$ by combining the result from (a) with the fact that any function is a sum of irrep partners, which immediately gives $\sum_\alpha \hat{P}^{(\alpha)}\psi = \psi$ for any ψ. But I wanted you to see how the same fact arises from the character-table orthogonality.

(c) $\hat{P}_i^{(\alpha)\dagger} = \frac{d_\alpha}{|G|}\sum_{g\in G} D_{ii}^{(\alpha)}(g)\hat{g}^\dagger = \frac{d_\alpha}{|G|}\sum_{g\in G} D_{ii}^{(\alpha)}(g)\widehat{g^{-1}} = \frac{d_\alpha}{|G|}\sum_{g\in G} D_{ii}^{(\alpha)}(g^{-1})\hat{g}$, using unitarity $\hat{g}^\dagger = \hat{g}^{-1} = \widehat{g^{-1}}$ and changing variables $g \to g^{-1}$ in the summation. Note that the D_{ii}^* term in $\hat{P}_i$ is unconjugated in $\hat{P}_i^\dagger$. By definition of a representation, we must have $D^{(\alpha)}(g^{-1}) = D^{(\alpha)}(g)^{-1}$, and if D is unitary then we must have $D^{(\alpha)}(g)^{-1} = D^{(\alpha)}(g)^\dagger$ (the conjugate-transpose). Hence $D_{ii}^{(\alpha)}(g^{-1}) = D_{ii}^{(\alpha)}(g)^*$, and $\hat{P}_i^{(\alpha)\dagger} = \hat{P}_i^{(\alpha)}$. Q.E.D.

(d) Inserting $\sum_{k,\gamma}\hat{P}_k^{(\gamma)} = 1$, we obtain $\langle\phi_i^{(\alpha)},\psi_j^{(\beta)}\rangle = \langle\phi_i^{(\alpha)},\sum_{k,\gamma}\hat{P}_k^{(\gamma)}\psi_j^{(\beta)}\rangle = \langle\phi_i^{(\alpha)},\hat{P}_j^{(\beta)}\psi_j^{(\beta)}\rangle$ by definition of a projection operator (only the j,β projection operator can give a nonzero result for $\psi_j^{(\beta)}$). Alternatively, $\hat{P}_j^{(\beta)}\psi_j^{(\beta)} = \psi_j^{(\beta)}$ follows directly from the defining property of a projection operator, in (a). Because $\hat{P}_j^{(\beta)}$ is Hermitian (we always assume unitary irreps., which are guaranteed to be possible for finite groups), we then have $\langle\phi_i^{(\alpha)},\psi_j^{(\beta)}\rangle = \langle\phi_i^{(\alpha)},\hat{P}_j^{(\beta)}\psi_j^{(\beta)}\rangle = \langle\hat{P}_j^{(\beta)}\phi_i^{(\alpha)},\psi_j^{(\beta)}\rangle$, which is zero unless $i = j$ and $\alpha = \beta$. Q.E.D.

Figure 1: Electric fields (E_z) of eigenmodes inside a 2d metal box. Blue/white/red indicate positive/zero/negative fields.

Problem 2: A square metal box(5+15 points)

(a) For $\mathbf{E} = E_z(x,y)\hat{\mathbf{z}}$ in air ($\varepsilon = 1$), we get $\nabla\times\nabla\times\mathbf{E} = -\nabla^2 E_z\hat{\mathbf{z}} = \frac{\omega^2}{c^2}E_z$. The solutions of this are sines and cosines, and to satisfy the $E_z = 0$ boundary conditions at $x = 0, L$ and $y = 0, L$ we must have:

$$E_z = A\sin\left(\frac{n\pi}{L}x\right)\sin\left(\frac{m\pi}{L}y\right)$$

where n and m are positive integers and A is an amplitude. The corresponding frequency is $\omega = c\frac{\pi}{L}\sqrt{n^2+m^2}$. This solutions are plotted in Figure 1 for the first few values of n and m.

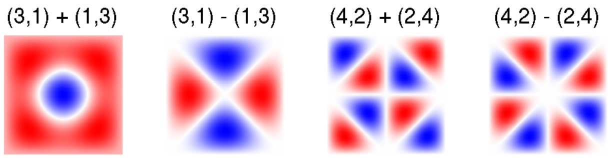

Figure 2: Electric fields (E_z) of eigenmodes inside a 2d metal box for accidentally degenerate (n, m) states $n \neq m$. By forming linear combinations as shown, we can create eigenmodes which transform as, from left to right: Γ_1, Γ_3, Γ_4, and Γ_2. Blue/white/red indicate positive/zero/negative fields.

(b) Since $\mathbf{E}$ is a vector, we can treat E_z as an ordinary scalar field here (no funny -1 factors under reflections). Therefore, from the field plots we can see that $n = m = 1$ (and, in fact, any $n = m =$ odd) transforms as Γ_1 (the trivial representation) and $n = m = 2$ (and any $n = m =$ even) transforms as Γ_4 (even with diagonal mirror planes and odd with horizontal/vertical mirrors). Any $n \neq m$ state is (at least) doubly degenerate [with the (m, n) state], such as the $(n, m) = (2, 1)$ and $(1, 2)$ states shown in Fig. 1. There are three cases [which can be understood in a variety of ways, e.g. by acting projection operators on the (n, m) solution]:

(i) If n is even and m is odd or vice versa, e.g. $(n, m) = (2, 1)$, then it transforms as Γ_5.

(ii) If both n and m are odd, e.g. $(n, m) = (3, 1)$, then it forms a 2×2 *reducible* representation with (m, n). To decompose it into irreducible representations, we just take the sum and difference of the two eigenmodes. The $(n, m) + (m, n)$ state transforms as Γ_1, and $(n, m) - (m, n)$ transforms as Γ_3. This is shown in the left two panels of Fig. 2.

(iii) If both n and m are even, e.g. $(n, m) = (4, 2)$, then it again forms a 2×2 reducible representation with (m, n). The $(n, m) + (m, n)$ state transforms as Γ_4, and $(n, m) - (m, n)$ transforms as Γ_2. This is shown in the right two panels of Fig. 2.

Problem 3: Group Velocity and Material Dispersion (20 points)

First, little bit of background info (you were *not* required to show this):

- We now technically have a "nonlinear eigenproblem" $\hat{\Theta}_k(\omega)\mathbf{H}_k = \omega^2 \mathbf{H}_k$, in which the eigen-operator $\hat{\Theta}_k$ depends on the eigenvalue ω^2. But if $\varepsilon(\omega)$ is still real, $\hat{\Theta}_k$ is still Hermitian. Our proof of real eigenvalues and positive-definiteness still work, so ω is still real. (But our proof of orthogonality of eigenfunctions no longer works, since eigenfunctions at distinct eigenvalues now have different operators $\hat{\Theta}_k$.)
- The derivation of first-order perturbation theory (from which we got $d\omega/dk$) carries through exactly as before, except that you now need to include an additional perturbation $\frac{\partial \hat{\Theta}}{\partial \omega}\Delta\omega$ in the operator due to the change in the eigenvalue. This is what gives us the "chain rule" term you were asked to include in $d\omega/dk$.

With that in mind, let's go ahead and solve the problem. As in class, we'll just set $c = \varepsilon_0 = \mu_0 = 1$ so that we don't have to deal with all of those annoying SI constant factors. (The book does it in SI units if you are curious.)

The derivation of group velocity is the same as in class, except that there is now an extra term in the numerator of the Hellman-Feynman theorem. In class, we dealt with the $\frac{\partial \hat{\Theta}_\mathbf{k}}{\partial \mathbf{k}}$ term and showed that it gave 2ω multipled by the flux (the integral of the time-averaged Poynting vector $\mathbf{S} = \frac{1}{2}\Re[\mathbf{E}^* \times \mathbf{H}]$). Now we have an additional term $\frac{\partial \hat{\Theta}}{\partial \varepsilon} \cdot \frac{d\varepsilon}{d\omega} \cdot \mathbf{v}_g$. The $\frac{\partial \hat{\Theta}}{\partial \varepsilon}$, however is precisely what we would get for a $\Delta\varepsilon = \frac{d\varepsilon}{d\omega} \cdot \mathbf{v}_g$ perturbation like when we first derived perturbation theory (we get $-\frac{\Delta\varepsilon}{\varepsilon^2}|\nabla \times \mathbf{H}|^2 = -\omega^2 \Delta\varepsilon |\mathbf{E}|^2$). Therefore, this term of the numerator becomes $-\frac{\omega^2}{c^2}\langle \mathbf{E}, (\frac{d\varepsilon}{d\omega} \cdot \mathbf{v}_g)\mathbf{E}\rangle$. In short, we have exactly the expression from class with the addition of this new term:

$$\mathbf{v}_g = \frac{1}{2\omega} \cdot \frac{4\omega \int \mathbf{S} - \omega^2 \mathbf{v}_g \int |\mathbf{E}|^2 \frac{d\varepsilon}{d\omega}}{\frac{1}{2}\int (|\mathbf{H}|^2 + \varepsilon |\mathbf{E}|^2)} = \frac{2\int \mathbf{S} - \frac{\omega}{2}\mathbf{v}_g \int |\mathbf{E}|^2 \frac{d\varepsilon}{d\omega}}{\frac{1}{2}\int (|\mathbf{H}|^2 + \varepsilon |\mathbf{E}|^2)}.$$

(Note that, in the denominator, we have used (as in class) the fact that $\int |\mathbf{H}|^2 = \int \varepsilon |\mathbf{E}|^2$, which is still true for dispersive media—our derivation from class only relied on $\nabla \times \mathbf{E} = i\frac{\omega}{c}\mathbf{H}$ and $\nabla \times \mathbf{H} = -i\frac{\omega}{c}\varepsilon\mathbf{E}$.) Now, however, we have $\mathbf{v}_g$ on both sides of the equation, so we must solve for it, and obtain:

$$\mathbf{v}_g = \frac{\int \mathbf{S}}{\frac{1}{4}\int (|\mathbf{H}|^2 + \varepsilon|\mathbf{E}|^2 + \omega\frac{d\varepsilon}{d\omega}|\mathbf{E}|^2)} = \frac{\int \mathbf{S}}{\frac{1}{4}\int \left[|\mathbf{H}|^2 + \frac{d(\omega\varepsilon)}{d\omega}|\mathbf{E}|^2\right]}$$

as desired: the Poynting flux divided by the Brillouin energy density of a lossless dispersive medium, both time-averaged and averaged over the unit cell.

A more complete derivation of this can be found in Appendix A of Welters *et al.*, “Speed-of-light limitations in passive linear media,” *Physical Review A*, vol. 90, p. 023847 (2014).