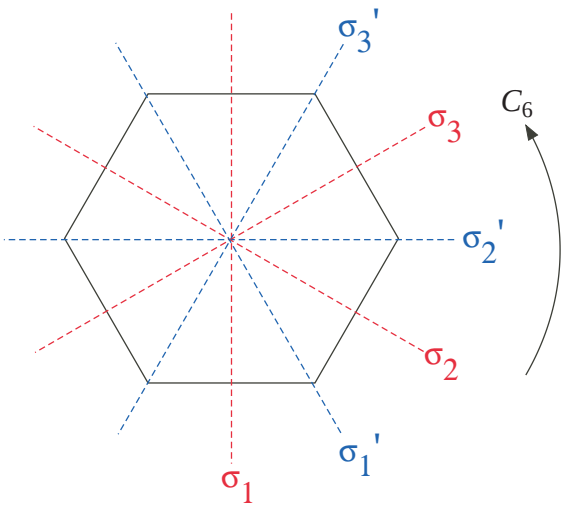

Figure 1: Symmetry operations, and in particular the mirror symmetries σ and σ' and the 60° rotation C_6, for the hexagon symmetry group ($C_{6\mathrm{v}}$).

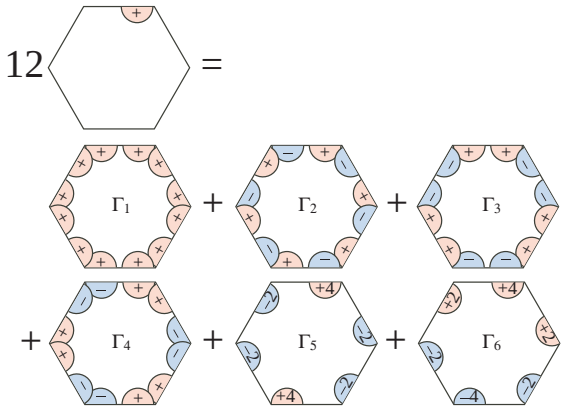

Figure 2: Projection operation for $C_{6\mathrm{v}}$ acting on a function $f(x, y) = 1$ in the small region shown at upper right, and zero elsewhere. The decompositions are labelled in terms of partner functions of the irreducible representations Γ_1 to Γ_5 from the table. Here, "+" and "−" by themselves refer to $+1$ and -1, respectively.

18.369 Mid-term Solutions

Problem 1: Hexagons (30 points)

(a) The symmetry operations, as summarized in Fig. 1, are: E (the identity), 3 mirror planes σ_k bisecting sides, 3 mirror planes σ'_k bisecting corners, C_6 and C_6^{-1}, $C_6^2 = C_3$ and C_3^{-1}, and $C_6^3 = C_2$—and these are also the 6 conjugacy classes. The character table is therefore:

C_{6v}	E	$2C_6$	$2C_3$	C_2	3σ	$3\sigma'$
Γ_1	1	1	1	1	1	1
Γ_2	1	1	1	1	−1	−1
Γ_3	1	−1	1	−1	1	−1
Γ_4	1	−1	1	−1	−1	1
Γ_5	2	−1	−1	2	0	0
Γ_6	2	1	−1	−2	0	0

Here, we have used several of the usual facts to fill in the table. The number of representations must equal the number of conjugacy classes (6). The sum of the squares of the first column (the dimensions) must equal the number of elements in the group (12), which sets the first column. The first row must be the trivial representation (all 1's). Subsequent rows must be orthogonal to this (and the columns must also be orthogonal).

However, there is still an ambiguity after all of these conditions—if you look at the table above, the $2C_6$ and $2C_3$ columns could be swapped without breaking the orthogonality, and the table would *not* be the equivalent (in contrast, if we swapped the 3σ and $3\sigma'$ columns, the table would be equivalent with Γ_3 and Γ_4 swapped). To resolve this ambiguity, it turns out that we need the final rule from the handout, about the product of character classes. In particular, $\{C_6, C_6^{-1}\} \cdot \{C_2, C_2^{-1}\} = \{C_6, C_6^{-1}\} + 2\{C_2\}$, just multiplying out the elements and counting how many times they appear. Then, if we look at the Γ_3 row of the table, this means that $(-1) \cdot (1) \cdot \{C_6, C_6^{-1}\} \cdot \{C_2, C_2^{-1}\} = (-1)\{C_6, C_6^{-1}\} + 2 \cdot (-1)\{C_2\}$, substituting the various characters according to the formula in the handout, and this works (both sides are multiplied by -1). However, if we had swapped the $2C_6$ and $2C_3$ columns, we would have gotten $(1) \cdot (-1) \cdot \{C_6, C_6^{-1}\} \cdot \{C_2, C_2^{-1}\} \neq (1)\{C_6, C_6^{-1}\} + 2 \cdot (-1)\{C_2\}$, ruling out this possibility. *As this ambiguity is rather subtle, and we didn't discuss the final rule on the handout in class, I didn't take off points if you failed to notice/resolve it.*

(b) This is shown in Fig. 2, using the proejction operator based on the character table above. Note

the normalization factors; we have pulled a factor of $\frac{1}{|G|} = \frac{1}{12}$ from the projection operator over to the left-hand side.

(c) The cases are:

(i) **Yes.** This has the full $C_{6\mathrm{v}}$ symmetry group, which we expect to have non-accidental degeneracies since it has two 2×2 irreducible representations from above.

(ii) **No.** Rotating the inner hexagon by $15°$ breaks the mirror symmetries, so our remaining group is $\{E, C_6, C_6^2, C_6^3, C_6^4, C_6^5\}$, which is commutative (it is the cyclic group of order 6). Because it is commutative, every element of the group is in its own conjugacy class. Thus we have six 1×1 irreducible representations, and there can be no non-accidental degeneracies.

(iii) **No**. The symmetry group is only $\{E, C_2, \sigma_1, \sigma_2'\}$, which again will have 4 conjugacy classes and four 1×1 irreducible representations.

(iv) **Yes**. This structure has the symmetry group $C_{3\mathrm{v}}$, which we saw in homework has a 2×2 irreducible representation, and therefore we expect non-accidental degeneracies.

Problem 2: Band Diagrams (30 points)

What Calvin has forgotten is that, with Bloch's theorem, the periodicity in $\mathbf{k}$ is determined by the choice of unit cell—if you employ a supercell, a periodicity larger than the minimum, then this leads to a labelling $\mathbf{k}$ that is "folded" onto the smaller Brillouin zone of the new unit cell.

In particular, the point $(k_x, 0, 0)$ in the *second* calculation (where the y direction has a non-zero periodicity a and thus a finite Brillouin zone $2\pi/a$ in the y direction) corresponds to the points $(k_x, \frac{2\pi n}{a}, 0)$, for all integers n, in the *first* calculation (where the y direction has zero periodicity and thus an infinite Brillouin zone where all k_y are distinct). The results are shown in Fig. 3.

For the 1d unit cell, shown in Fig. 3(top), we see the usual 1d quarter-wave band diagram of non-degenerate bands (considering the TM polarization only). Because the index contrast is so low, the bands

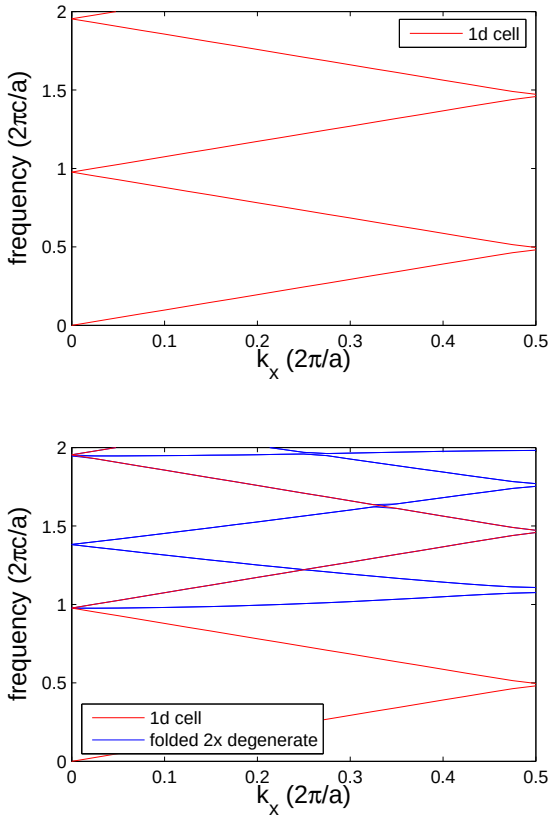

Figure 3: Band diagrams of quarter-wave stack ($\varepsilon = 1.1/1$). *Top*: 1d unit cell. *Bottom:* 2d unit cell (supercell), showing 1d bands (red) and double-degenerate folded bands from $k_y = \frac{2\pi n}{a}$ for $n \neq 0$ (blue).

are *nearly* the folded bands from $\varepsilon \approx 1.05$ (the mean ε). A small gap opens up at $k_x = \pi/a$, centered on $\omega a/2\pi c = 0.4884$. There is no gap at $k_x = 0$, due to the peculiar accidental degeneracy of the quarter-wave stack at this point.

For the $a \times a$ unit cell, we see two kinds of bands in Fig. 3(bottom). First, the (non-degenerate) bands of the 1d unit cell ($n = 0$) are still solutions, of course, shown in red. The first folded band is for $n = 1$, corresponding to the lowest band at $k_y = \pm\frac{2\pi}{a}$. Since this is *nearly* a homogeneous system, we expect this band to be *nearly* $\omega \approx c\sqrt{k_x^2 + (\pm 2\pi/a)^2}$, which is doubly-degenerate, curved, and is almost degenerate with the 1d bands at $k_x = 0$ (a little below $\omega a/2\pi c = 1$) and at $k_x = 0.5\frac{\pi}{a}$ should be a little below $\sqrt{0.5^2 + 1} = 1.12$. In fact, the first 3 folded bands correspond to the first 3 bands at $n = \pm 1$, with frequencies $\omega \approx c\sqrt{(k_x + \ell\frac{2\pi}{a})^2 + (\pm 2\pi/a)^2}$ for $\ell = 0, -1, 1$. Thus, the 2nd and 3rd folded bands at $k_x = 0$ should be at $\omega \approx \sqrt{2}$. It's hard to tell on this plot because the index contrast is so low, but there *is* a gap in the folded bands at $k_x = 0$, since we are no longer satisfying the quarter-wave condition when $k_y \neq 0$. For the 4th folded band, there is a crossing between two bands: first, the 4th band(s) at $n = \pm 1$, with $\omega \approx c\sqrt{(k_x - 2\frac{2\pi}{a})^2 + (\pm 2\pi/a)^2}$; and second, the 1st band at $n = \pm 2$, with $\omega \approx c\sqrt{k_x^2 + (\pm 4\pi/a)^2}$. The latter is lower ($\omega \approx 2$ vs. $\omega \approx \sqrt{5}$) at $k_x = 0$, and the former is lower ($\omega \approx \frac{\sqrt{13}}{2}$ vs. $\omega \approx \frac{\sqrt{17}}{2}$) at $k_x = \pi/a$. No bands are more than 2-fold degenerate (except at points where they cross, of course).

Problem 3: Operators (30 points)

(a) In general, at each ω we have a different Hermitian operator $\hat{\Theta}(\omega)$. All of the properties of Hermitian operators apply to *that* operator, too. The only things that *don't* apply are relationships between modes at *different* ω, since different ω have different operators. In particular:

(i) ω is real: **still true**. Real eigenvalues $\lambda = \omega^2/c^2$ only depended on the fact that $\langle H|\hat{\Theta}(\omega)|H\rangle = \lambda^* \langle H|H\rangle = \lambda \langle H|H\rangle$, from the fact that $\hat{\Theta}$ is Hermitian and so we can operate it either to the left or to the right. And from the fact that we have real eigenvalues, real ω follows from the fact that $\hat{\Theta}$ is positive semi-definite, which is still true since $\varepsilon > 0$ was given.

(ii) the solutions $\mathbf{H}$ can be chosen to transform as irreducible representations of the space group: **still true**. Our proof of this only depended on the degenerate modes at a *single* frequency ω, and therefore still holds.

(iii) $\omega \neq \omega'$ implies that $\int \mathbf{H}^* \cdot \mathbf{H}' = 0$: **no longer true**. Two modes at different frequencies now satisfy different eigenproblems, and therefore have no orthogonality relationship.

(b) We can derive this most simply by taking the ordinary perturbation-theory expression, derived in class, and substituting $\Delta\varepsilon = \frac{\partial\varepsilon}{\partial p}\Delta p + \frac{\partial\varepsilon}{\partial\omega}\frac{d\omega}{dp}\Delta p + O(\Delta p^2)$, obtaining:

$$\Delta\omega = -\frac{\omega}{2}\frac{\int (\frac{\partial\varepsilon}{\partial p} + \frac{\partial\varepsilon}{\partial\omega}\frac{d\omega}{dp})|\mathbf{E}|^2}{\int \varepsilon|\mathbf{E}|^2}\Delta p + O(\Delta p^2).$$

We then divide both sides by Δp and take the limit $\Delta p \to 0$ to get the derivative $d\omega/dp$, as in our previous derivation. However, we now have *two* terms in which $d\omega/dp$ appears: one on the left-hand side, and one in the numerator on the right-hand side. Solving for $d\omega/dp$, we obtain:

$$\begin{aligned}\frac{d\omega}{dp} &= -\frac{\omega}{2}\frac{\int \frac{\partial\varepsilon}{\partial p}|\mathbf{E}|^2}{\int \varepsilon|\mathbf{E}|^2 + \int \frac{\omega}{2}\frac{\partial\varepsilon}{\partial\omega}|\mathbf{E}|^2} \\ &= -\omega\frac{\int \frac{\partial\varepsilon}{\partial p}|\mathbf{E}|^2}{\int \frac{d(\omega\varepsilon)}{d\omega}|\mathbf{E}|^2 + \int |\mathbf{H}|^2}.\end{aligned}$$

In the last expression, we have used the fact that $\int |\mathbf{H}|^2 = \int \varepsilon|\mathbf{E}|^2$ to write the result in a suggestive form. If we interpret the denominator as the energy in the field, then we see that the energy density in the electric field for a dispersive medium (with negligible loss) must be $\frac{d(\omega\varepsilon)}{d\omega}|\mathbf{E}|^2$. Exactly this result is derived (in a more explicit way) in, e.g., Jackson, *Classical Electrodynamics*. Note that in the case of $\frac{\partial\varepsilon}{\partial\omega} = 0$ we obtain the usual result, of course.