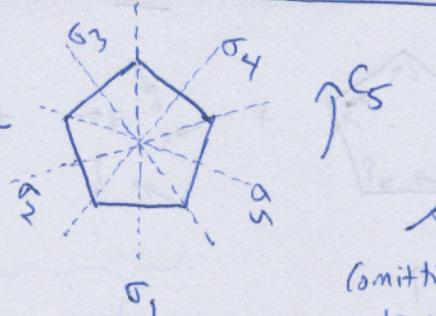


①

18.325 Mid-term / Pset #5 Solutions

Problem #1



a)

$$A = E, C_5, C_5^2, C_5^3 = C_5^{-2}, C_5^4 = C_5^{-1}, S_5$$

(omitting \vec{d} translations)

classes: $E, \{C_5, C_5^{-1}\}, \{C_5^2, C_5^{-2}\}, S_5$

\uparrow
equivalent
under any σ

\uparrow
equivalent
under any σ

\uparrow
equivalent
under C_5
rotations

\Rightarrow character table:

	E	$2C_5$	$2C_5^2$	S_5
Γ_1	1	1	1	1
Γ_2	1	1	1	-1
Γ_3	2	$-\frac{\sqrt{5}+1}{2}$	$\frac{\sqrt{5}-1}{2}$	0
Γ_4	2	$\frac{\sqrt{5}-1}{2}$	$-\frac{\sqrt{5}+1}{2}$	0

4 classes \Rightarrow 4 rep's

$$\sum d^2 = 1^2 + 1^2 + 2^2 + 2^2$$

$$= 12 = 10$$

$$\left. \begin{array}{l} \Gamma_1 \quad 1 \quad 1 \quad 1 \quad 1 \\ \Gamma_2 \quad 1 \quad 1 \quad 1 \quad -1 \\ \Gamma_3 \quad 2 \quad -\frac{\sqrt{5}+1}{2} \quad \frac{\sqrt{5}-1}{2} \quad 0 \\ \Gamma_4 \quad 2 \quad \frac{\sqrt{5}-1}{2} \quad -\frac{\sqrt{5}+1}{2} \quad 0 \end{array} \right\} \begin{array}{l} \text{by orthogonality,} \\ \text{of rows} \end{array}$$

see below

let $\Gamma_4 = 2 \times 2$ coord. transformations (given to be an irreducible rep.)

$$\Rightarrow D^{(4)}(C_5) = \begin{pmatrix} \cos \frac{2\pi}{5} & -\sin \frac{2\pi}{5} \\ \sin \frac{2\pi}{5} & \cos \frac{2\pi}{5} \end{pmatrix} \Rightarrow \chi^{(4)}(C_5) = 2 \cos \frac{2\pi}{5} = \frac{\sqrt{5}-1}{2}$$

$$\text{similarly, } \chi^{(4)}(C_5^2) = 2 \cos \frac{4\pi}{5} = -\frac{\sqrt{5}+1}{2}$$

$$D^{(4)}(\sigma_1) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \text{ by inspection} \Rightarrow \chi^{(4)}(\sigma_1) = \chi^{(4)}(\sigma) = 0$$

(we could also get this
by orthogonality of
rows in the char. table)

Note: Γ_4 row orthogonal to Γ_1, Γ_2 rows

$$\text{since } 2 + 2 \frac{\sqrt{5}-1}{2} - 2 \frac{\sqrt{5}+1}{2} = 0$$

Γ_3 row? by column orthogonality: $1 + 1 + 2\chi^{(3)}(C_5) + 2\left(\frac{\sqrt{5}-1}{2}\right) = 0$

$$\Rightarrow \chi^{(3)}(C_5) = \chi^{(3)}(C_5^{-1}) = -\left(\frac{\sqrt{5}+1}{2}\right); \text{ similarly for } \chi^{(3)}(C_5^2), \chi^{(3)}(\sigma)$$

(b)

$$\text{Pentagon} = \frac{1}{10} \left[\begin{array}{c} \Gamma_1 \\ \Gamma_2 \\ \Gamma_3 \\ \Gamma_4 \end{array} \right]$$

Γ_1 Γ_2 Γ_3 Γ_4

Γ_1 copy has arrows labeled: c_1, c_2, c_3, c_4, c_5 and E .
 Γ_2 copy has arrows labeled: a, b, c, d, e .
 Γ_3 copy has arrows labeled: b, a, b, a, b .
 Γ_4 copy has arrows labeled: c, b, c, b, c .

where $a = \sqrt{5} - 1$
 $b = \sqrt{5} + 1$

(we have labelled each $\tilde{\Gamma}$ copy by the symmetry operation that gives it)

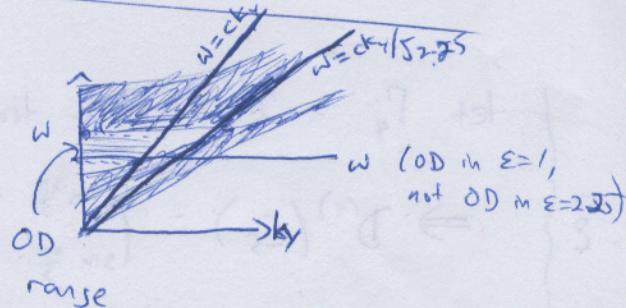
(c)

$\tilde{\Gamma}_1 = \delta(\vec{x}) \hat{z}$ excites Γ_1 only: $\tilde{\Gamma}_1$ is fully symmetric, so $\hat{P}^{(1)} \tilde{\Gamma}_1 = \tilde{\Gamma}_1$

$\tilde{\Gamma}_4 = \delta(\vec{x}) \hat{y}$ excites Γ_4 only: $\tilde{\Gamma}_4$ manifestly transforms as $(\vec{x}, \vec{y}) \Rightarrow \hat{P}^{(4)} \tilde{\Gamma}_4 = \tilde{\Gamma}_4$
 (or any combination of \hat{x}, \hat{y})

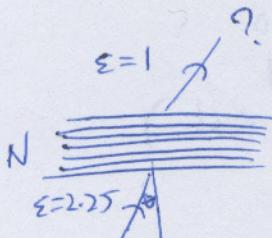
Problem 2 :

(a) mirror is OD from $\varepsilon = 1 \Rightarrow$ band diagram looks like



mirror is not OD from $\varepsilon = 2.25$
 at ω

\Rightarrow at ω , $\omega = ck_y / \sqrt{2.25}$ light line is inside (or below) mirror continuum, as shown above.



$\rightarrow k_y$
 is conserved

Two cases:

(1) incident light has k_y above $\omega > ck_y / \sqrt{2.25}$

\Rightarrow in this range, there are no modes in the mirror

\Rightarrow exponentially decaying transmission with N (due to tails that penetrate mirror)

(3)

(2) Incident light has k_y above $\epsilon=2.25$ light cone

but below $\epsilon=1$ light cone: $ck_y > \omega \geq ck_y/\sqrt{2.25}$

\Rightarrow cannot couple to propagating modes in $\epsilon=1 \Rightarrow 0$ transmission

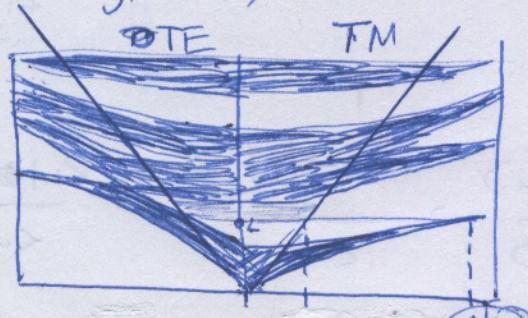
- We may couple to modes propagating in the mirrors, since this portion of the $\epsilon=2.25$ light cone overlaps the mirror modes, but these mirror modes are still reflected at the $\epsilon=1$ interface \Rightarrow reflection is still 1

Case (2) corresponds to $\theta > \theta_c = \sin^{-1}\left(\frac{1}{\sqrt{2.25}}\right)$,

In short: $\theta > \theta_c \Rightarrow 0$ transmission, 100% reflection

$\theta < \theta_c \Rightarrow$ transmission T exponentially decreasing with N ,
reflection = $1-T$

- this phenomenon does not depend on polarization, but polarization will affect transmission T in the $\theta < \theta_c$ regime by some constant factor

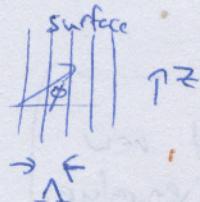


(i) Δ couples k_y to $k_y + \frac{2\pi}{\Delta}$
 \Rightarrow if Δ is small enough, we
 cannot couple light cone to mirror states

$$\Rightarrow \Delta < \frac{2\pi}{\max \Delta k_y} < \frac{2\pi}{\Delta k}$$

marked
on
graph
(limited by
TM modes)

(ii) No. If we look out of plane:



period at an angle ϕ

$$= \Delta \sec \phi$$

$\rightarrow \infty$ for $\phi \rightarrow \frac{\pi}{2}$

\Rightarrow there is always some out-of-plane angle ϕ
 so that $\Delta \sec \phi > 2\pi/\Delta k_y$

Problem 3

① O is Hermitian \Rightarrow use 1st-order perturbation theory

$$\Rightarrow \text{for non-degenerate case, } \Delta\text{eigenvalue} = \frac{\langle u | \Delta O | u \rangle}{\langle u | u \rangle} + O(\Delta O^2)$$

$$\Rightarrow \text{for } \begin{pmatrix} 1 \\ 0 \\ 0 \\ \pm 1 \end{pmatrix} : \Delta\text{eigenvalue} \approx \frac{\phi}{2} = \phi \text{ zero!}$$

for $\begin{pmatrix} 0 \\ 1 \\ \pm 1 \\ 0 \end{pmatrix}$ we must use degenerate perturbation theory

\Rightarrow find superposition that diagonalizes ΔO

$$\text{by inspection: } \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} = \frac{1}{2} \left(\begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ -1 \\ 0 \\ 0 \end{pmatrix} \right)$$

$$\begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} = \frac{1}{2} \left(\begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} - \begin{pmatrix} 0 \\ -1 \\ 0 \\ 0 \end{pmatrix} \right) \text{ works}$$

$$\Rightarrow \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \text{ has } \Delta\text{eigenvalue} = \frac{\delta}{1} = \delta \quad \left. \begin{array}{l} \text{degeneracy} \\ \text{is split} \\ \text{and these} \\ \text{are the new} \\ \text{eigenvectors} \end{array} \right\}$$

$$\begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \text{ has } \Delta\text{eigenvalue} = 0$$

⑤ 1st-order approx for new eigenvalue

$$= \text{old eigenvalue} + \frac{\langle u | \Delta O | u \rangle}{\langle u | u \rangle} = \frac{\langle u | O | u \rangle}{\langle u | u \rangle} + \frac{\langle u | \Delta O | u \rangle}{\langle u | u \rangle}$$

$$= \frac{\langle u | O + \Delta O | u \rangle}{\langle u | u \rangle} = \text{Rayleigh quotient, plusing old } |u\rangle \text{ into new } O + \Delta O$$

O Hermitian, ΔO Hermitian $\Rightarrow O + \Delta O$ Hermitian

\Rightarrow Variational thm. holds

$$\Rightarrow \left. \begin{array}{c} \text{smallest} \\ \text{new} \\ \text{eigenvalue} \end{array} \leq \text{1}^{\text{st}} \text{ order} \leq \text{largest new} \\ \text{approximation} \quad \text{eigenvalue} \end{array} \right\}$$

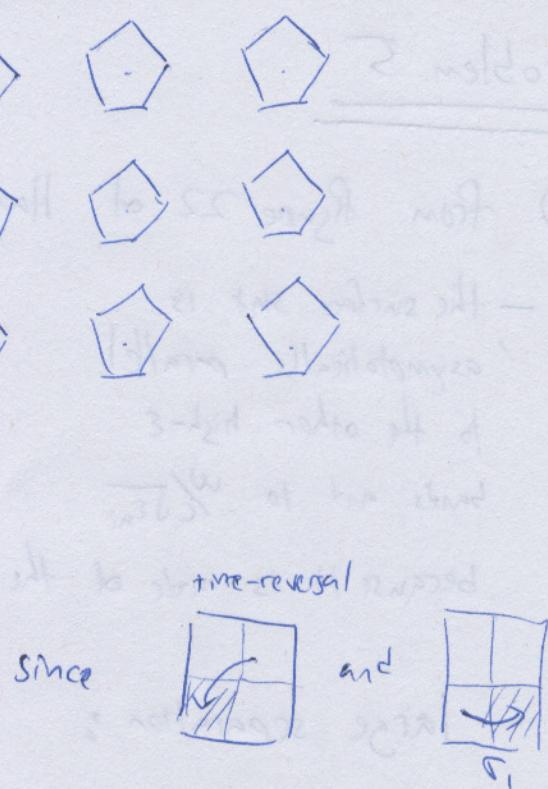
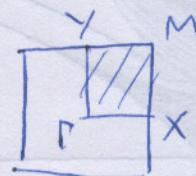
Problem 4

- (a) same lattice \Rightarrow same B.Z.
 point-group symmetries: E, σ_1 ,
 + time-reversal only!

$$B.Z. = \frac{2\pi}{a} \begin{array}{|c|} \hline \sigma_1 \\ \hline \end{array} \Rightarrow \text{by } \sigma_1 \text{ we only need } \begin{array}{|c|} \hline / \\ \hline \backslash \\ \hline \end{array}$$

by time-reversal, we only need
 $+ \sigma_1$

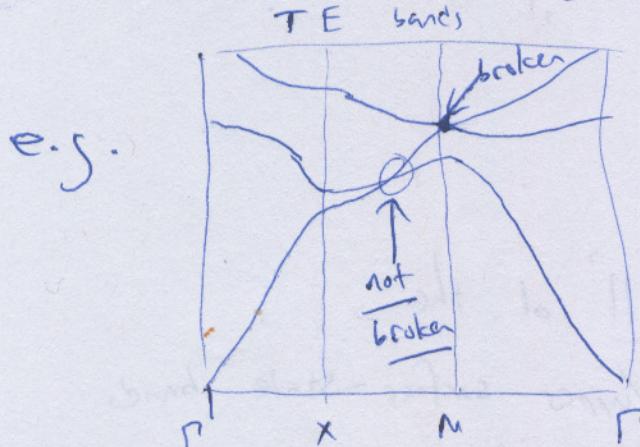
$\Rightarrow I.B.Z.$ is



- (b) $\{E, \sigma_1\}$ has no 2-dimensional irreducible representations

\Rightarrow degeneracies at Γ and M (which came from symmetry)
 are broken.

But, accidental degeneracies from band crossings remain



However, these crossing points will shift slightly to a new \vec{k}, ω

- (c) because of mirror σ_1 + time-reversal, ω 's just above and below $\Gamma-X$ line are equal $\Rightarrow \Gamma-X$ line is an extremum $\Rightarrow \frac{\partial \omega}{\partial k_x} = 0$ at $\Gamma-X$
 $\Rightarrow \vec{V} = \frac{du}{d\vec{k}}$ is in $\pm \hat{x}$ direction on $\Gamma-X$. On $\Gamma-M$, there is no such symmetry $\Rightarrow \vec{V}$ can point anywhere!

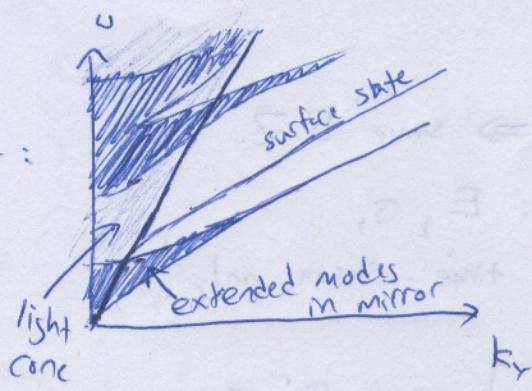
Problem 5

6

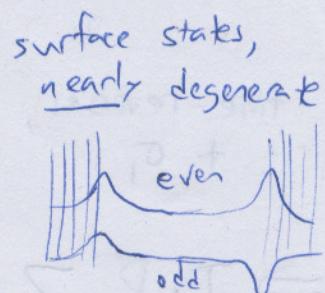
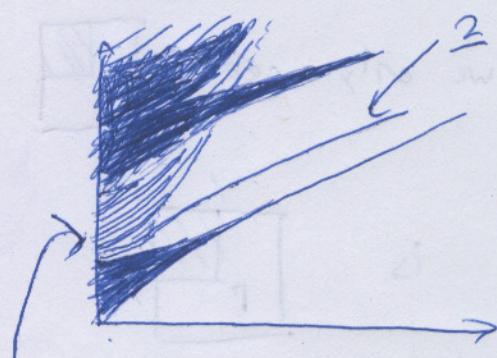
(a) from figure 22 of Handout:

- the surface state is asymptotically parallel to the other high- ϵ bands and to $\omega/c\sqrt{\epsilon_m}$

because it is made of the same material



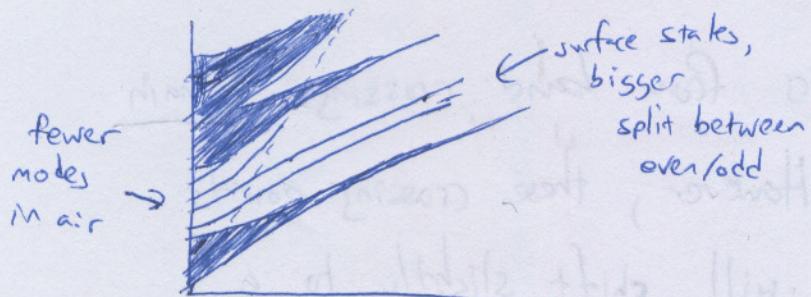
(b) large separation:



form even and odd superpositions
(by mirror symmetry)

- nearly degenerate since only coupled through exponential tails

smaller separation:



As separation goes to zero, all of the air modes disappear, and the lower/upper surface-state bands merge with the lower/upper continua. (Two half layers together = 1 whole layer = no defect.)