# UNIVERSITY OF MARYLAND

## DEPARTMENT OF PHYSICS

COLLEGE PARK, MARYLAND 20742

**PHYSICS 732** **HOMEWORK ASSIGNMENT #2**
**DR. H. D. DREW** Due Thursday, February 22, 2007

Read Marder, chapter 16.2, 19.3, Appendix C
Read Ashcroft and Mermin, chapter 10, 28, Appendix E

1. Consider the form of the absorption edge for a "forbidden" direct gap in which the valence band maximum and conduction band minimum are both at Γ but have the same parity so that the momentum matrix element $P_{vc}(k)$ vanishes at k=0. By expanding $P_{vc}(k)$ around k=0 and using phase space arguments find the power law governing $\varepsilon_2$.
For $\varepsilon_2(\omega) \propto (\hbar\omega - E_{gap})^n$, for $\hbar\omega > E_{gap}$ find n.

2. Marder, chapter 19, #1.

3. Ashcroft and Mermin, chapter 28, #3.

4. Consider the nearest-neighbor tight binding model for a simple cubic crystal where one includes both s and p orbitals. For simplicity, we ignore all overlap matrix elements except the ones involving ΔU. Furthermore, we assume that $|\gamma_{sp}| = |\gamma_{ps}|$.

i. Consider first a model involving only p-orbitals.
ii. Show that there is no splitting at the Γ point and that only two matrix elements $\gamma_0$ and $\gamma_1$ are required. Choose the definitions such that $|\gamma_0| > |\gamma_1|$. Assume for the sketching purposes that $|\gamma_0| > 2|\gamma_1|$. Is this reasonable?
iii. Is the result that only two γ's are required for p-orbitals a general one? In particular, is there any relation between the γ's defined in A&M problem 10.2? Note that the definitions and Equations (10.34) are different than for the simple cubic case. Hint: Are there any misprints in (10.34)?
iv. Sketch the p-bands along the ΓXMR path. Indicate degeneracies. What is the band width?
v. Now consider the effect of an s-orbital on the bands. For simplicity, look only along the ΓX direction. Produce a simple argument that the two bands are not affected. Derive analytic formula for the remaining two bands. Sketch these along ΓX for the case $|\gamma_s| > |\gamma_0|$, $4(|\gamma_s|+|\gamma_0|)>\Delta$, $E_s=E_p=0$, and where $\gamma_s$ is the "overlap" for the s-orbitals. What is the effect on the dispersion relation due to $\gamma_{sp}$?