

Physics 555 Fall 2003

Solid State Physics

Homework Assignment # 6, Due Wednesday Nov. 19

1. Band Structure of Silicon, (100) direction

The table below gives the Hamiltonian matrix $\mathcal{H}(\vec{k})$ for diamond structure C, Si, or Ge, in the “minimal basis” nearest-neighbor tight-binding model. There are 8 Bloch orbitals in the basis, labeled by $a = s, x, y, z$ and by 1 or 2 to indicate the two atoms in the unit cell.

	s1	s2	x1	x2	y1	y2	z1	z2
s1	E_s	$V_{ss}g_1$	0	$V_{sp}g_2$	0	$V_{sp}g_3$	0	$V_{sp}g_4$
s2	$V_{ss}g_1^*$	E_s	$-V_{sp}g_2^*$	0	$-V_{sp}g_3^*$	0	$-V_{sp}g_4^*$	0
x1	0	$-V_{sp}g_2$	E_p	$V_{xx}g_1$	0	$V_{xy}g_4$	0	$V_{xy}g_3$
x2	$V_{sp}g_2^*$	0	$V_{xx}g_1^*$	E_p	$V_{xy}g_4^*$	0	$V_{xy}g_3^*$	0
y1	0	$-V_{sp}g_3$	0	$V_{xy}g_4$	E_p	$V_{xx}g_1$	0	$V_{xy}g_2$
y2	$V_{sp}g_3^*$	0	$V_{xy}g_4^*$	0	$V_{xx}g_1^*$	E_p	$V_{xy}g_2^*$	0
z1	0	$-V_{sp}g_4$	0	$V_{xy}g_3$	0	$V_{xy}g_2$	E_p	$V_{xx}g_1$
z2	$V_{sp}g_4^*$	0	$V_{xy}g_3^*$	0	$V_{xy}g_2^*$	0	$V_{xx}g_1^*$	E_p

In this table, the parameters g_i contain the phase factors that accumulate from hopping along the four tetrahedral bonds when the Bloch state has wavevector $\vec{k} = (k_x, k_y, k_z)$, namely:

$$g_1 = \frac{1}{4} \left(e^{i\vec{k} \cdot \vec{d}_1} + e^{i\vec{k} \cdot \vec{d}_2} + e^{i\vec{k} \cdot \vec{d}_3} + e^{i\vec{k} \cdot \vec{d}_4} \right)$$

$$g_2 = \frac{1}{4} \left(e^{i\vec{k} \cdot \vec{d}_1} + e^{i\vec{k} \cdot \vec{d}_2} - e^{i\vec{k} \cdot \vec{d}_3} - e^{i\vec{k} \cdot \vec{d}_4} \right)$$

$$g_3 = \frac{1}{4} \left(e^{i\vec{k} \cdot \vec{d}_1} - e^{i\vec{k} \cdot \vec{d}_2} + e^{i\vec{k} \cdot \vec{d}_3} - e^{i\vec{k} \cdot \vec{d}_4} \right)$$

$$g_4 = \frac{1}{4} \left(e^{i\vec{k} \cdot \vec{d}_1} - e^{i\vec{k} \cdot \vec{d}_2} - e^{i\vec{k} \cdot \vec{d}_3} + e^{i\vec{k} \cdot \vec{d}_4} \right)$$

where the bonds \vec{d}_i are defined as

$$\vec{d}_1 = (a/4)(1, 1, 1) \quad \vec{d}_2 = (a/4)(1, \bar{1}, \bar{1}) \quad \vec{d}_3 = (a/4)(\bar{1}, 1, \bar{1}) \quad \vec{d}_4 = (a/4)(\bar{1}, \bar{1}, 1).$$

The parameters V_{ss} , etc., are Hamiltonian matrix elements of atomic orbitals which are defined as

$$V_{ss} = 4H_{ss\sigma}$$

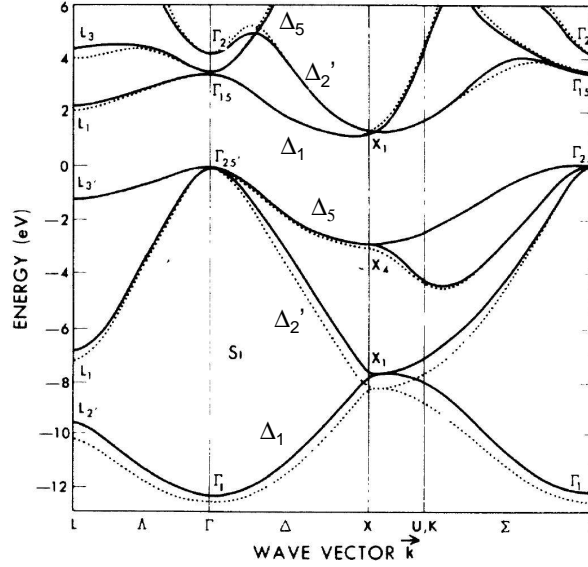


Figure 1: Empirical pseudopotential band structure of silicon, fitted to optical data by Chelikowsky and Cohen. The dashed bands used a local approximation, and the solid bands are an improved non-local fit.

$$V_{sp} = 4H_{sp\sigma}/\sqrt{3}$$

$$V_{xx} = (4H_{pp\sigma}/3) + (8V_{pp\pi}/3)$$

$$V_{xy} = (4H_{pp\sigma}/3) - (4V_{pp\pi}/3)$$

These combinations occur because of the geometric arrangement of bonds along (111)-type directions and orbitals defined along (100)-type directions. We should expect $V_{ss} < 0$, $V_{sp} > 0$, $V_{xx} > 0$, and $V_{xy} > 0$. The signs are negative for the ss integral because the product of wavefunctions is positive and the Hamiltonian is negative in the region of overlap. For the others, the product of wavefunctions is negative. For the integral $H_{sp\sigma}$, it is necessary to define it with the s function to the left and the p_x function to the right along the x axis. **Note:** This matrix and the corresponding notations are from Yu and Cardona, p84 ff. However, there are numerous typographical errors which hopefully are all corrected here. Also, a more convenient ordering of rows and columns is used here.

a. This matrix uses Bloch basis functions defined as

$$|\vec{k}a\vec{\tau}\rangle = \sqrt{\frac{1}{N}} \sum_{\vec{\ell}} e^{i\vec{k}\cdot(\vec{\ell}+\vec{\tau})} \phi_a(r - \vec{\ell} - \vec{\tau})$$

where a labels the atomic orbital (s , or x , or y , or z) and $\vec{\tau}$ has two values, $\tau_1 = 0$ and $\tau_2 = (1, 1, 1)/4$. There is an (unnecessary

but convenient) phase factor $\exp(i\vec{k} \cdot \vec{\tau})$ which is not needed to give the Bloch property. This factor sometimes simplifies the appearance of the Hamiltonian matrix, and is therefore included here, but is optional – omitting this phase factor would not change the answers. Explain the matrix elements $\langle s1|\mathcal{H}|s2 \rangle$ and $\langle s1|\mathcal{H}|x2 \rangle$.

- b. For the wavevector $\vec{k} = (2\pi/a)(\zeta, 0, 0)$ some of the g_i vanish and the matrix simplifies. Write the simplified form of the matrix. **Note:** It will break into two 4×4 matrices. A study of the accompanying figure (from Chelikowsky and Cohen, Phys. Rev. B **10**, 5095 (1974)) shows that bands in the (100) direction (this direction is called Δ) are labeled by quantum numbers $(\Delta_1, \Delta'_2, \Delta_5, \Delta_1, \Delta'_2, \Delta_5)$ (these are analogs of the atomic quantum number ℓ .) The state labeled Δ_5 is doubly degenerate, and the rest are singly degenerate. These symmetry labels indicate that it is possible to use symmetry to reduce the two 4×4 matrices to four 2×2 matrices. One will contain the two Δ_1 states, one will contain the two Δ'_2 states, one will contain the two Δ_5 states of type a , and one will contain the two Δ_5 states of type b , where a and b refer to some extra quantum number (analogous to m) used to designate the two partners of the doubly degenerate Δ_5 manifold.
- c. It would not be possible to solve an arbitrary 4×4 matrix by the method of “guess the eigenvectors.” But since we know from the argument above that symmetry can be used to reduce them to 2×2 matrices, we can be sure that the eigenvectors contain some symmetry. Even without knowing the details, we are allowed to guess and have the assurance that this can work. I suggest the following guesses:

$$|A\rangle = \begin{pmatrix} \alpha \\ \alpha \\ i\beta \\ i\beta \end{pmatrix} \quad |B\rangle = \begin{pmatrix} \alpha \\ -\alpha \\ i\beta \\ -i\beta \end{pmatrix} \quad |C\rangle = \begin{pmatrix} \alpha \\ \alpha \\ i\beta \\ -i\beta \end{pmatrix} \quad |D\rangle = \begin{pmatrix} \alpha \\ -\alpha \\ i\beta \\ i\beta \end{pmatrix}.$$

The first two of these are orthogonal and can be used for one of the 4 by 4 matrices, and the last two are orthogonal and can be used for the other. Show that these vectors can be used to reduce the problem to four 2×2 matrices.

- d. Find the eight eigenvalues and associate them with the six lowest curves on the accompanying figure between Γ and X .

2. Band Velocity

Crystalline solids differ from other large molecules or glasses in that the single particle eigenstates can propagate; they can have non-zero currents. There are two different ways to understand the fact that the Bloch state labeled (\vec{k}, n) (n is the “band index”) has velocity $\vec{v}(\vec{k}, n) = (1/\hbar)\partial\epsilon(\vec{k}, n)/\partial\vec{k}$. In both approaches we assume the one-electron Hamiltonian $\mathcal{H} = p^2/2m + V$.

- a. Consider a wave-packet built from a single band n , using states near some wavevector \vec{k} :

$$\psi(\vec{r}, t = 0) = \sum_{\vec{k}'} A(\vec{k}') \psi_{\vec{k}', n}(\vec{r}, t = 0)$$

where the envelope function $A(\vec{k}')$ can be taken to be a Gaussian $\exp[-b^2(\vec{k}' - \vec{k})^2]$ where the distance b is reasonable large compared with the lattice constant a . Show that as time evolves, the wave-packet propagates and find the velocity of propagation.

- b. The previous proof is the best. But it is also possible to prove by an algebraic manipulation that the Bloch state $|\vec{k}, n\rangle$ has the group velocity $\vec{v}(\vec{k}, n)$ given by the expectation value $\langle \vec{k}, n | \vec{p} / m | \vec{k}, n \rangle$, where \vec{p} is the momentum operator. The proof uses a slight modification of the single particle Schrödinger equation. If we write the Bloch eigenstate $\psi_{\vec{k}n}(\vec{r})$ as $\exp(i\vec{k} \cdot \vec{r})$ times a periodic function $u_{\vec{k}n}(\vec{r})$, then the periodic function obeys the equation

$$\mathcal{H}(\vec{k}) u_{\vec{k}n} = \epsilon(\vec{k}n) u_{\vec{k}n}$$

where the new Hamiltonian $\mathcal{H}(\vec{k})$ is

$$\mathcal{H}(\vec{k}) = \left(\frac{p^2}{2m} + \frac{\hbar \vec{k} \cdot \vec{p}}{m} + \frac{\hbar^2 k^2}{2m} \right) + V$$

and serves as the Hamiltonian for the states labeled by \vec{k} . We can also use the Feynman theorem

$$\frac{\partial \langle \psi(\alpha) | \mathcal{H}(\alpha) | \psi(\alpha) \rangle}{\partial \alpha} = \langle \psi(\alpha) | \partial \mathcal{H}(\alpha) / \partial \alpha | \psi(\alpha) \rangle$$

where α is a parameter, not an operator, and $|\psi(\alpha)\rangle$ is an eigenvector of $\mathcal{H}(\alpha)$. Construct the proof.