EECS 230

Problem Set 3 Solutions

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1) Semi-empirical Tight binding Method calculation of Si and GaAs band structure using only First nearest neighbors.

As discussed in class, the problems requires solving the energy eigenvalue equation:

$$H|\psi\rangle = E|\psi\rangle$$

where,

E = energy eigenvalues, which we want to solve

$|\psi\rangle$ = hybrid eigenfunction, a linear combination of atomic orbitals $|\mathcal{U}_{3s}^{A}\rangle$, $|\mathcal{U}_{3px}^{A}\rangle$, $|\mathcal{U}_{3py}^{A}\rangle$, $|\mathcal{U}_{3pz}^{A}\rangle$

$|\mathcal{U}_{3s}^{B}\rangle$, $|\mathcal{U}_{3px}^{B}\rangle$, $|\mathcal{U}_{3py}^{B}\rangle$, $|\mathcal{U}_{3pz}^{B}\rangle$

in GaAs: $A \equiv Ga$ $B = As$

Si: $A = B = Si$

$$H = \begin{bmatrix} [\varepsilon^A] & [AB] \\ [BA] & [\varepsilon^B] \end{bmatrix} \longrightarrow 8\times 8 \text{ matrix}$$

$$[\varepsilon] = \begin{bmatrix} \varepsilon_s & 0 & 0 & 0 \\ 0 & \varepsilon_p & 0 & 0 \\ 0 & 0 & \varepsilon_p & 0 \\ 0 & 0 & 0 & \varepsilon_p \end{bmatrix} \qquad AB = \begin{bmatrix} E_{ss}B_0 & E_{sp}^{AB}B_1 & E_{sp}^{AB}B_2 & E_{sp}^{AB}B_3 \\ -E_{sp}^{BA}B_1 & E_{xx}B_0 & E_{xy}B_3 & E_{xy}B_2 \\ -E_{sp}^{BA}B_2 & E_{xy}B_3 & E_{xx}B_0 & E_{xy}B_1 \\ -E_{sp}^{BA}B_3 & E_{xy}B_2 & E_{xy}B_1 & E_{xx}B_0 \end{bmatrix}$$

$$[BA] = [AB]^{+} = \left\{[AB]^{*}\right\}^{T}$$

E_{sp}^{AB}, E_{sp}^{BA}, E_{ss}, E_{xx}, E_{xy}, E_s^A, E_s^B, E_p^A and E_p^B are given (experiment values)

$$B_0(\vec{k}) = 4\left(\cos\frac{k_x a}{2}\cos\frac{k_y a}{2}\cos\frac{k_z a}{2} - i\sin\frac{k_x a}{2}\sin\frac{k_y a}{2}\sin\frac{k_z a}{2}\right)$$

$$B_1(\vec{k}) = 4\left(-\cos\frac{k_x a}{2}\sin\frac{k_y a}{2}\sin\frac{k_z a}{2} + i\sin\frac{k_x a}{2}\cos\frac{k_y a}{2}\cos\frac{k_z a}{2}\right)$$

$$B_2(\vec{k}) = 4\left(-\sin\frac{k_x a}{2}\cos\frac{k_y a}{2}\sin\frac{k_z a}{2} + i\cos\frac{k_x a}{2}\sin\frac{k_y a}{2}\cos\frac{k_z a}{2}\right)$$

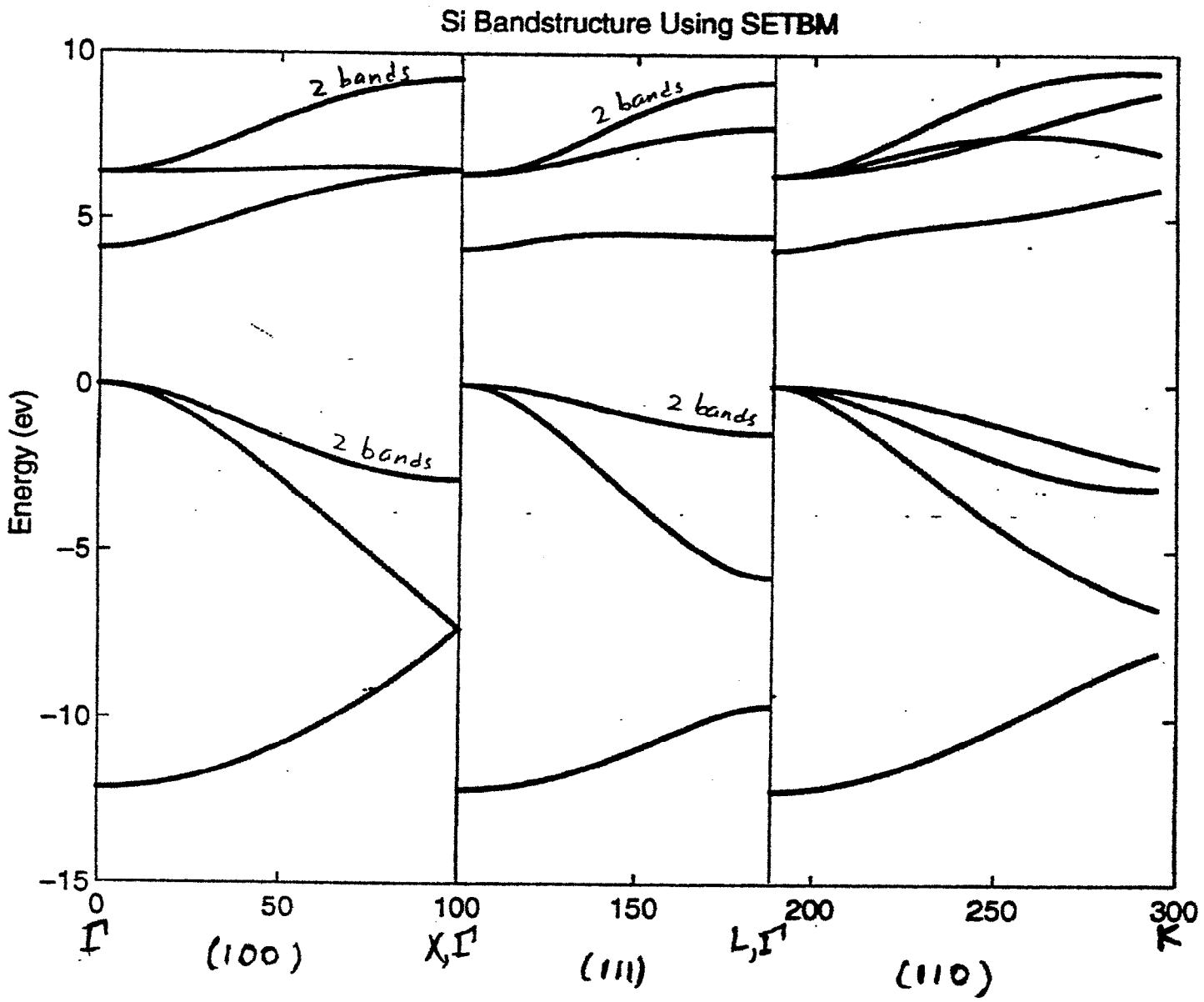
$$B_3(\vec{k}) = 4\left(-\sin\frac{k_x a}{2}\sin\frac{k_y a}{2}\cos\frac{k_z a}{2} + i\cos\frac{k_x a}{2}\cos\frac{k_y a}{2}\sin\frac{k_z a}{2}\right)$$

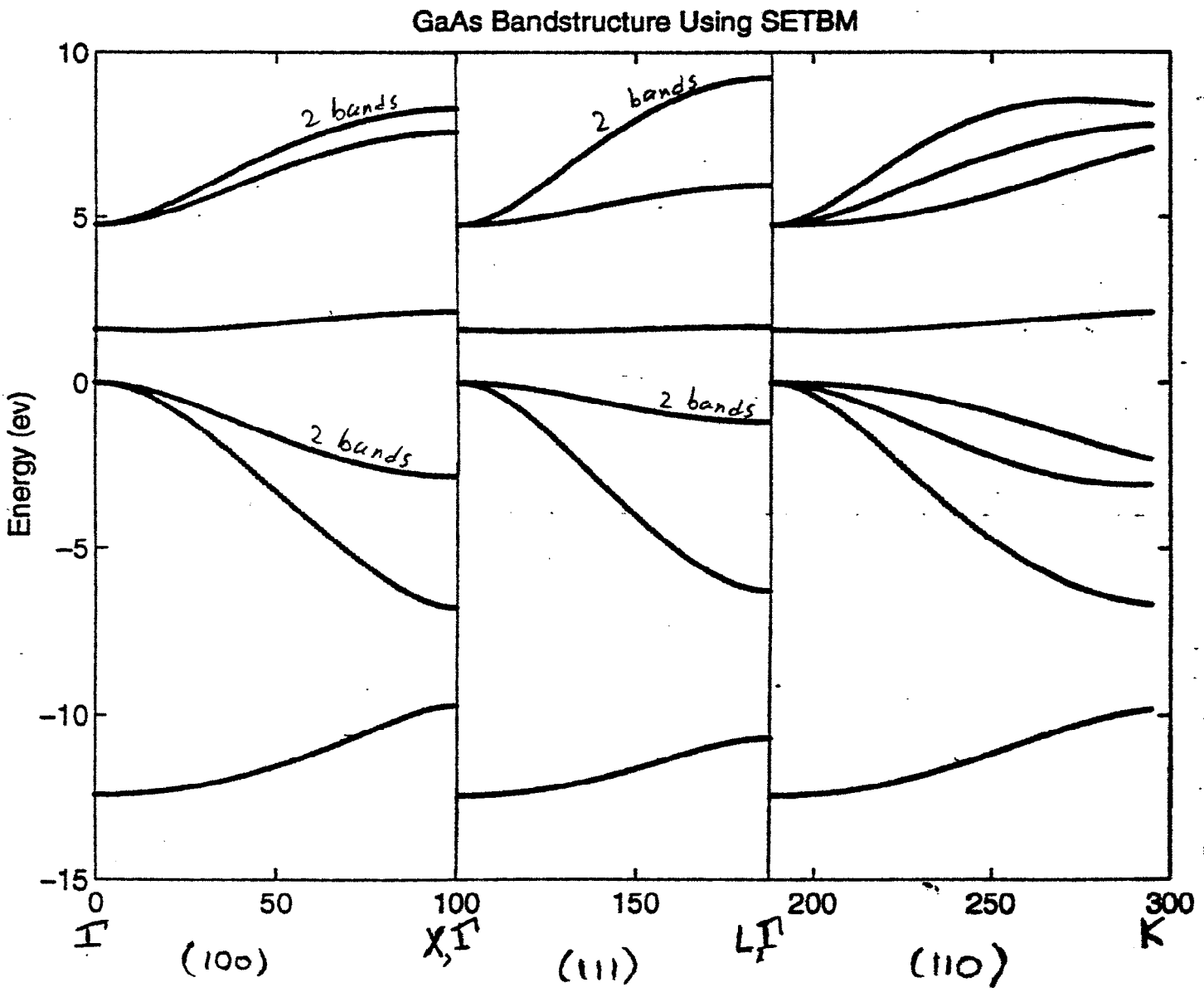
Solving the eigenvalue equation is accomplished by iteratively solving for

$$\det(H - EI) = 0$$

I = Identity Matrix

Since H is an 8×8 matrix, we will get 8 energy eigenvalues, corresponding to 8 energy bands for each $\vec{k}$


Si Bandstructure Using SETBM
Energy (ev)
10
5
0
−5
−10
−15
0
50
100
150
200
250
300
2 bands
2 bands
2 bands
2 bands
Γ
(100)
X,Γ
(111)
L,Γ
(110)
K


GaAs Bandstructure Using SETBM
Energy (ev)
10
5
0
−5
−10
−15
0
50
100
150
200
250
300
2 bands
2 bands
2 bands
2 bands
Γ
(100)
X,Γ
(111)
L,Γ
(110)
K