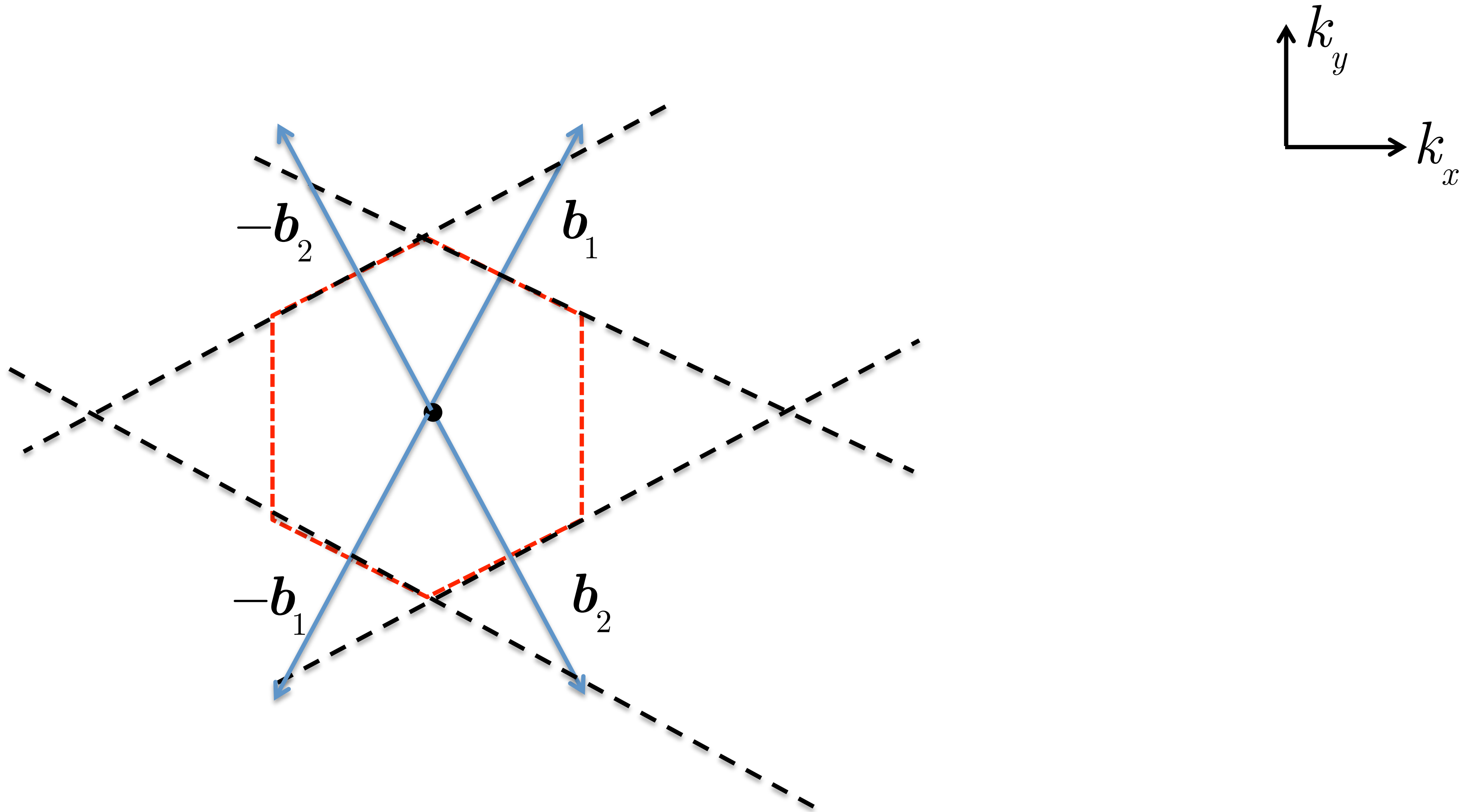
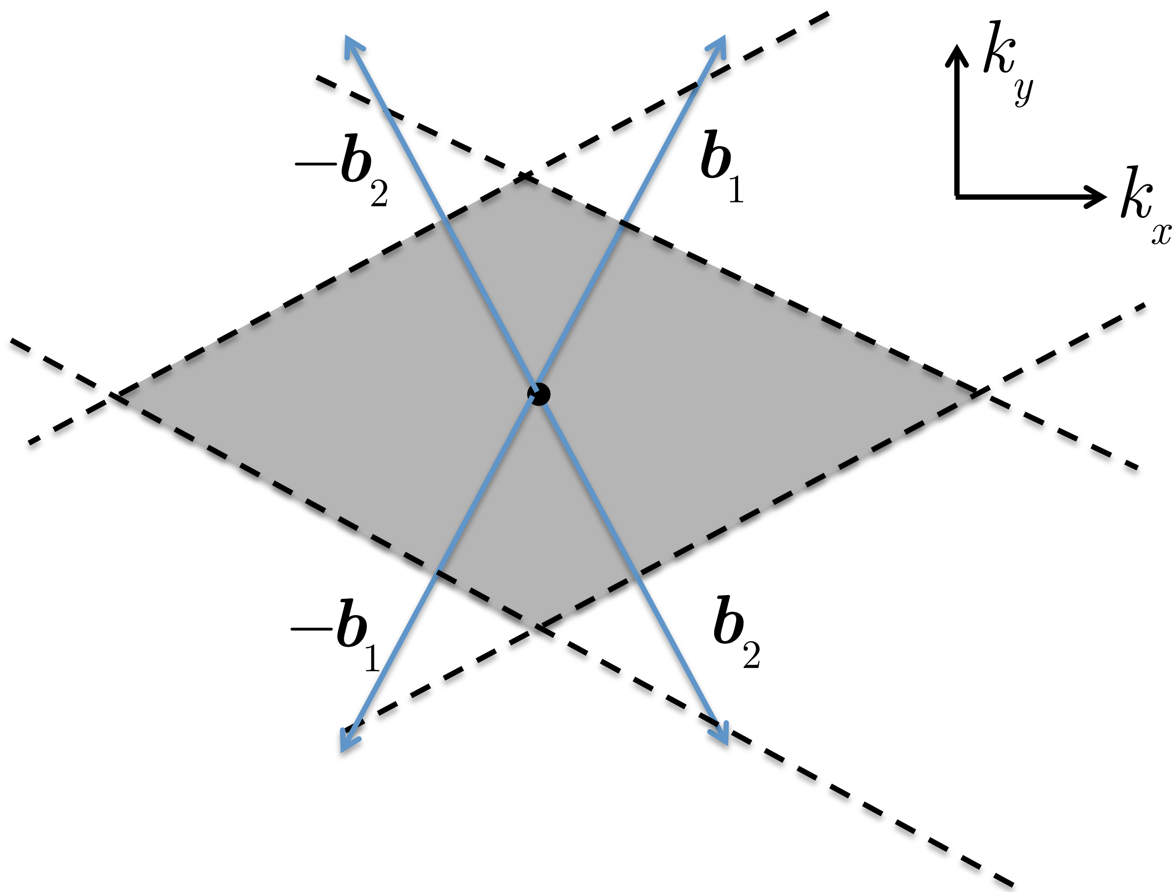
Física de Semiconductores

Lección 7

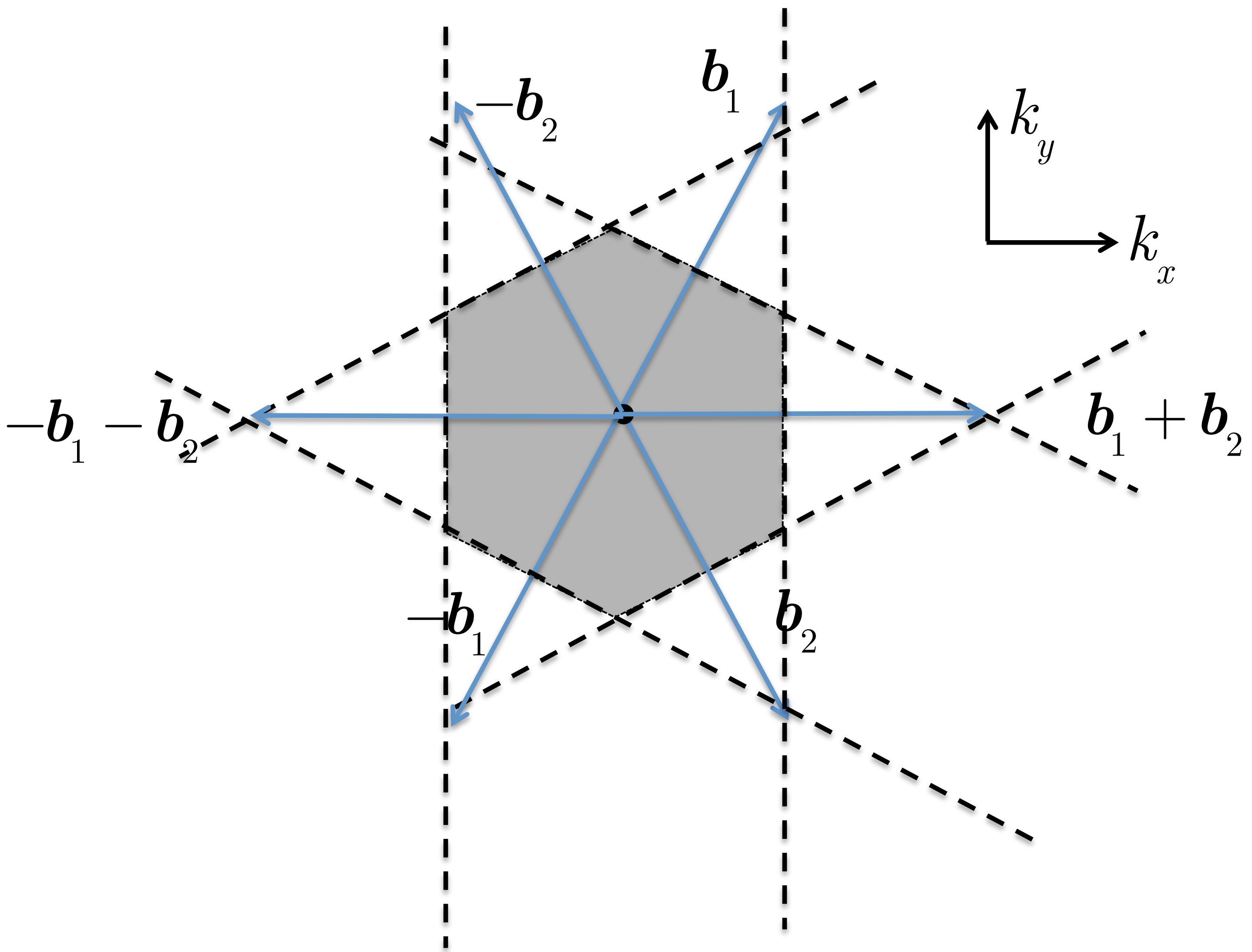
Brillouin zone del grafeno



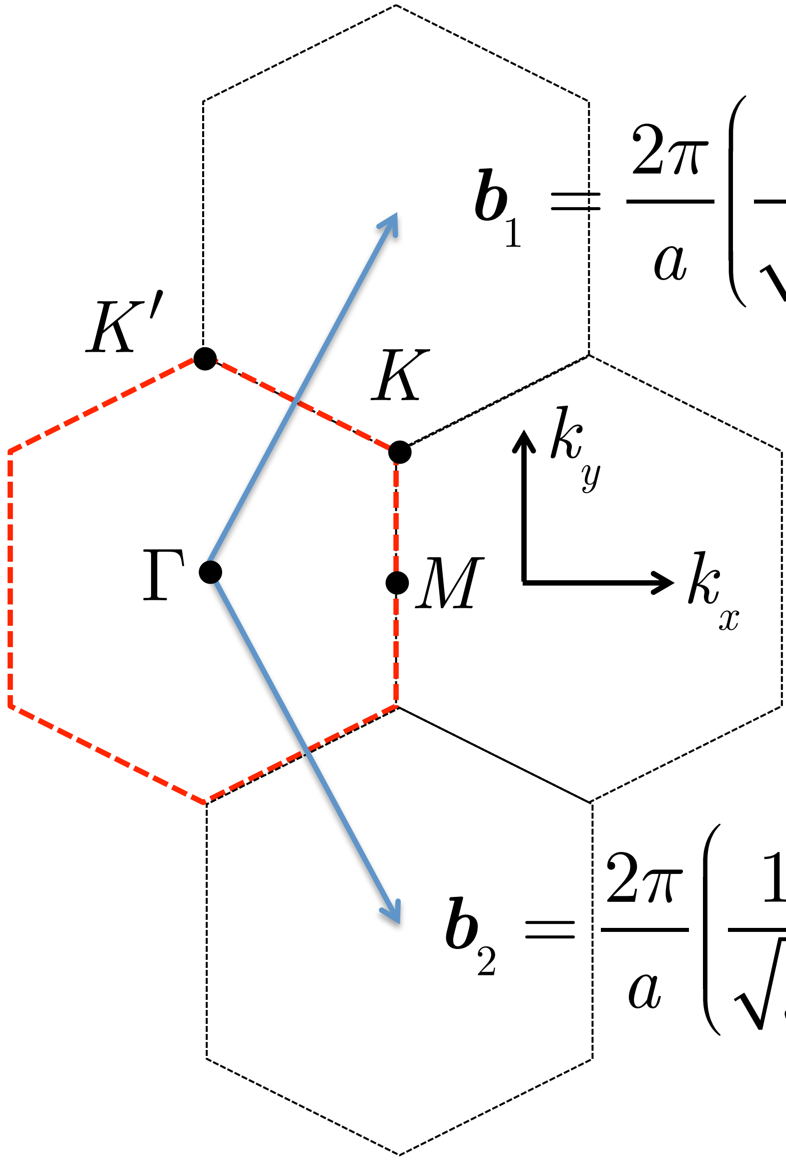
Brillouin zone del grafeno I



Brillouin zone del grafeno II



Brillouin zone del grafeno



$$\boldsymbol{b}_1 = \frac{2\pi}{a}\left(\frac{1}{\sqrt{3}}\hat{\mathbf{i}} + \hat{\mathbf{j}}\right)$$

$$\boldsymbol{b}_2 = \frac{2\pi}{a}\left(\frac{1}{\sqrt{3}}\hat{\mathbf{i}} - \hat{\mathbf{j}}\right)$$

$$\Gamma = 0$$

$$M = \frac{1}{2}\left(\boldsymbol{b}_1 + \boldsymbol{b}_2\right) = \frac{2\pi}{a\sqrt{3}}\mathbf{i}$$

$$K = \frac{2}{3}\boldsymbol{b}_1 + \frac{1}{3}\boldsymbol{b}_2 = \frac{2\pi}{a}\left(\frac{1}{\sqrt{3}}\mathbf{i} + \frac{1}{3}\mathbf{j}\right)$$

Plane wave expansion

$$\left(\frac{\hbar^2\left(\boldsymbol{k}\text{ - }\boldsymbol{K}\right)^2}{2m} - E\right)c_{\boldsymbol{k}\text{-}\boldsymbol{K}} + \sum_{\boldsymbol{K}'} c_{\boldsymbol{k}\text{-}\boldsymbol{K}'} U_{\boldsymbol{K}'\text{-}\boldsymbol{K}} = 0$$

$$H = \begin{pmatrix} \frac{\hbar^2\left(\boldsymbol{k}-\boldsymbol{K}_0\right)}{2m} & U_{\boldsymbol{K}_1-\boldsymbol{K}_0} & U_{\boldsymbol{K}_2-\boldsymbol{K}_0} & U_{\boldsymbol{K}_3-\boldsymbol{K}_0} & \cdots \\ U_{\boldsymbol{K}_0-\boldsymbol{K}_1} & \frac{\hbar^2\left(\boldsymbol{k}-\boldsymbol{K}_1\right)}{2m} & U_{\boldsymbol{K}_2-\boldsymbol{K}_1} & U_{\boldsymbol{K}_3-\boldsymbol{K}_1} & \cdots \\ U_{\boldsymbol{K}_0-\boldsymbol{K}_2} & U_{\boldsymbol{K}_1-\boldsymbol{K}_2} & \frac{\hbar^2\left(\boldsymbol{k}-\boldsymbol{K}_2\right)}{2m} & U_{\boldsymbol{K}_3-\boldsymbol{K}_2} & \cdots \\ U_{\boldsymbol{K}_0-\boldsymbol{K}_3} & U_{\boldsymbol{K}_1-\boldsymbol{K}_3} & U_{\boldsymbol{K}_2-\boldsymbol{K}_3} & \frac{\hbar^2\left(\boldsymbol{k}-\boldsymbol{K}_3\right)}{2m} & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix}$$

Empty cell band structure

$$H = \begin{pmatrix} \frac{\hbar^2\left(\boldsymbol{k}-\boldsymbol{K}_0\right)}{2m} & 0 & 0 & 0 & \cdots \\ 0 & \frac{\hbar^2\left(\boldsymbol{k}-\boldsymbol{K}_1\right)}{2m} & 0 & 0 & \cdots \\ 0 & 0 & \frac{\hbar^2\left(\boldsymbol{k}-\boldsymbol{K}_2\right)}{2m} & 0 & \cdots \\ 0 & 0 & 0 & \frac{\hbar^2\left(\boldsymbol{k}-\boldsymbol{K}_3\right)}{2m} & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix}$$

Γ-M line

$$\boldsymbol{k} = \frac{2\pi}{a}\left(\frac{\delta}{\sqrt{3}}, 0, 0\right) \qquad \delta = 0 \rightarrow 1$$

$$\boldsymbol{K}_0 = 0; \quad E(\delta) = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2 \frac{\delta^2}{3} = E_0 \frac{\delta^2}{3}; \quad E(0) = 0$$

$$\boldsymbol{K}_1 = \boldsymbol{b}_1; \quad E(\delta) = E_0\left[\frac{(\delta-1)^2}{3} + 1\right]; \quad E(0) = \frac{4}{3}E_0$$

$$\boldsymbol{K}_2 = \boldsymbol{b}_2; \quad E(\delta) = E_0\left[\frac{(\delta-1)^2}{3} + 1\right]; \quad E(0) = \frac{4}{3}E_0$$

$$\boldsymbol{K}_3 = -\boldsymbol{b}_1; \quad E(\delta) = E_0\left[\frac{(\delta+1)^2}{3} + 1\right]; \quad E(0) = \frac{4}{3}E_0$$

$$\boldsymbol{K}_4 = -\boldsymbol{b}_2; \quad E(\delta) = E_0\left[\frac{(\delta+1)^2}{3} + 1\right]; \quad E(0) = \frac{4}{3}E_0$$

Γ-M line (cont) $\boldsymbol{k} = \frac{2\pi}{a}\left(\frac{\delta}{\sqrt{3}}, 0, 0\right) \quad \delta = 0 \to 1$

$$\boldsymbol{K}_5 = \boldsymbol{b}_1 + \boldsymbol{b}_2; \quad E(\delta) = E_0\left[\frac{(\delta-2)^2}{3}\right]; \quad E(0) = \frac{4}{3}E_0$$

$$\boldsymbol{K}_6 = -\boldsymbol{b}_1 - \boldsymbol{b}_2; \quad E(\delta) = E_0\left[\frac{(\delta+2)^2}{3}\right]; \quad E(0) = \frac{4}{3}E_0$$

$$\boldsymbol{K}_7 = \boldsymbol{b}_1 - \boldsymbol{b}_2; \quad E(\delta) = E_0\left(\frac{\delta^2}{3} + 4\right); \quad E(0) = 4E_0$$

$$\boldsymbol{K}_8 = -\boldsymbol{b}_1 + \boldsymbol{b}_2; \quad E(\delta) = E_0\left(\frac{\delta^2}{3} + 4\right); \quad E(0) = 4E_0$$

Γ-M line (cont)

$$\boldsymbol{k} = \frac{2\pi}{a}\left(\frac{\delta}{\sqrt{3}}, 0, 0\right) \quad \delta = 0 \rightarrow 1$$

$$\boldsymbol{K}_9 = 2\boldsymbol{b}_1; \quad E(\delta) = E_0\left[\frac{(\delta - 2)^2}{3} + 4\right]; \quad E(0) = \frac{16}{3}E_0$$

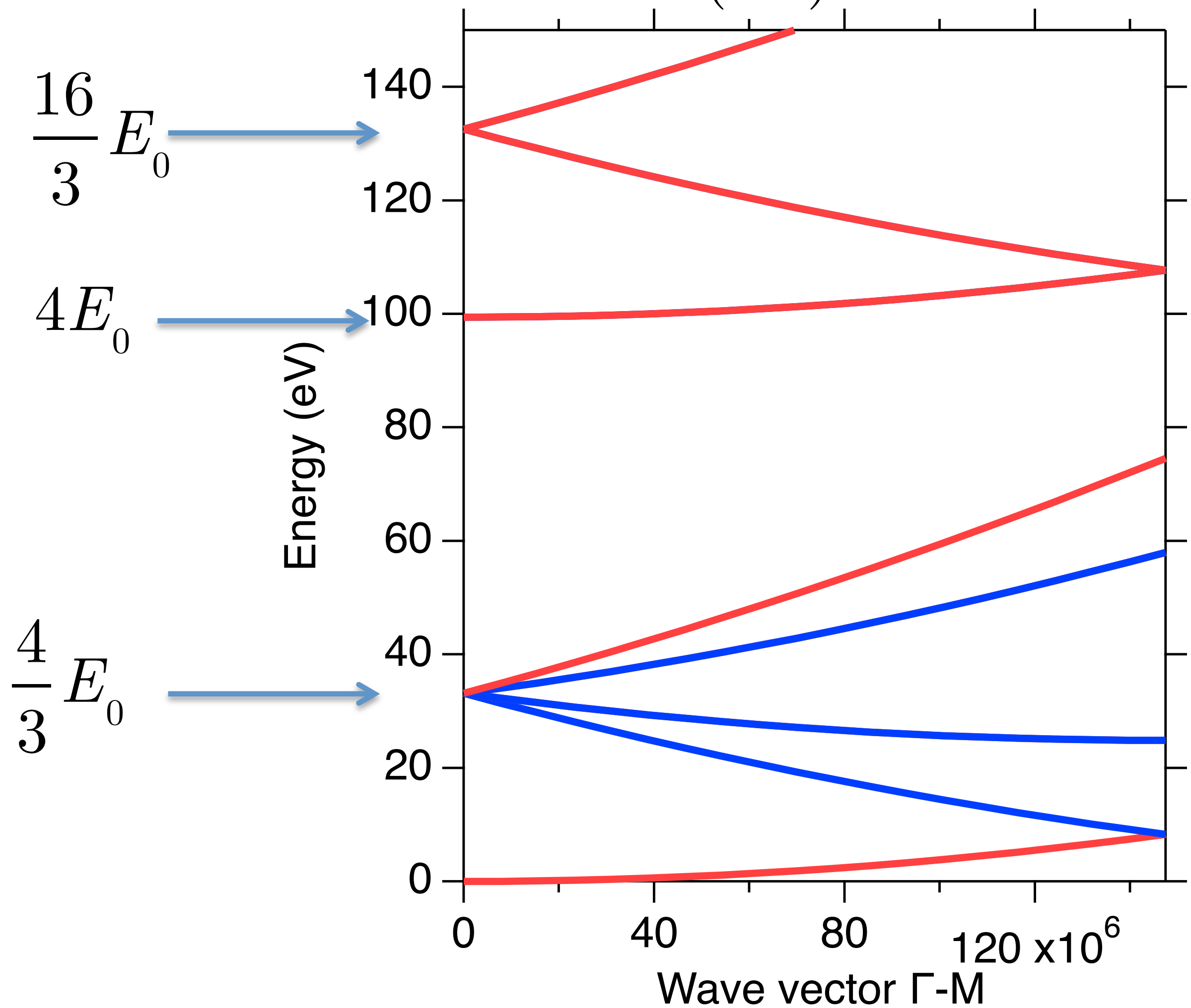
$$\boldsymbol{K}_{10} = 2\boldsymbol{b}_2; \quad E(\delta) = E_0\left[\frac{(\delta - 2)^2}{3} + 4\right]; \quad E(0) = \frac{16}{3}E_0$$

$$\boldsymbol{K}_{11} = -2\boldsymbol{b}_1; \quad E(\delta) = E_0\left[\frac{(\delta + 2)^2}{3} + 4\right]; \quad E(0) = \frac{16}{3}E_0$$

$$\boldsymbol{K}_{12} = -2\boldsymbol{b}_2; \quad E(\delta) = E_0\left[\frac{(\delta + 2)^2}{3} + 4\right]; \quad E(0) = \frac{16}{3}E_0$$

Graphene empty cell Γ-M line

$$E_0 = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2 = 24.86 \text{ eV}$$



Γ-K line

$$\boldsymbol{k} = \frac{2\pi}{a}\left(\frac{\lambda}{\sqrt{3}}, \frac{\lambda}{3}, 0\right) \quad \delta = 0 \rightarrow 1$$

$$\boldsymbol{K}_0 = 0; \quad E(\lambda) = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2 \left[\frac{\lambda^2}{3} + \frac{\lambda^2}{9}\right] = \frac{4}{9} E_0 \lambda^2; \quad E(0) = 0$$

$$\boldsymbol{K}_1 = \boldsymbol{b}_1; \quad E(\lambda) = E_0 \left[\frac{(\lambda - 1)^2}{3} + \left(\frac{\lambda}{3} - 1\right)^2\right]; \quad E(0) = \frac{4}{3} E_0$$

$$\boldsymbol{K}_2 = \boldsymbol{b}_2; \quad E(\lambda) = E_0 \left[\frac{(\lambda - 1)^2}{3} + \left(\frac{\lambda}{3} + 1\right)^2\right]; \quad E(0) = \frac{4}{3} E_0$$

$$\boldsymbol{K}_3 = -\boldsymbol{b}_1; \quad E(\lambda) = E_0 \left[\frac{(\lambda + 1)^2}{3} + \left(\frac{\lambda}{3} + 1\right)^2\right]; \quad E(0) = \frac{4}{3} E_0$$

$$\boldsymbol{K}_4 = -\boldsymbol{b}_2; \quad E(\lambda) = E_0 \left[\frac{(\lambda + 1)^2}{3} + \left(\frac{\lambda}{3} - 1\right)^2\right]; \quad E(0) = \frac{4}{3} E_0$$

Γ-K line (cont)

$$\boldsymbol{k} = \frac{2\pi}{a}\left(\frac{\lambda}{\sqrt{3}}, \frac{\lambda}{3}, 0\right) \quad \delta = 0 \rightarrow 1$$

$$\boldsymbol{K}_5 = \boldsymbol{b}_1 + \boldsymbol{b}_2; \quad E(\lambda) = E_0\left[\frac{(\lambda - 2)^2}{3}\right]; \quad E(0) = \frac{4}{3}E_0$$

$$\boldsymbol{K}_6 = -\boldsymbol{b}_1 - \boldsymbol{b}_2; \quad E(\lambda) = E_0\left[\frac{(\lambda + 2)^2}{3}\right]; \quad E(0) = \frac{4}{3}E_0$$

$$\boldsymbol{K}_7 = \boldsymbol{b}_1 - \boldsymbol{b}_2; \quad E(\lambda) = E_0\left(\frac{\lambda}{3} - 2\right)^2; \quad E(0) = 4E_0$$

$$\boldsymbol{K}_8 = -\boldsymbol{b}_1 + \boldsymbol{b}_2; \quad E(\lambda) = E_0\left(\frac{\lambda}{3} + 2\right)^2; \quad E(0) = 4E_0$$

Γ-K line (cont)

$$\boldsymbol{k} = \frac{2\pi}{a}\left(\frac{\lambda}{\sqrt{3}}, \frac{\lambda}{3}, 0\right) \quad \delta = 0 \rightarrow 1$$

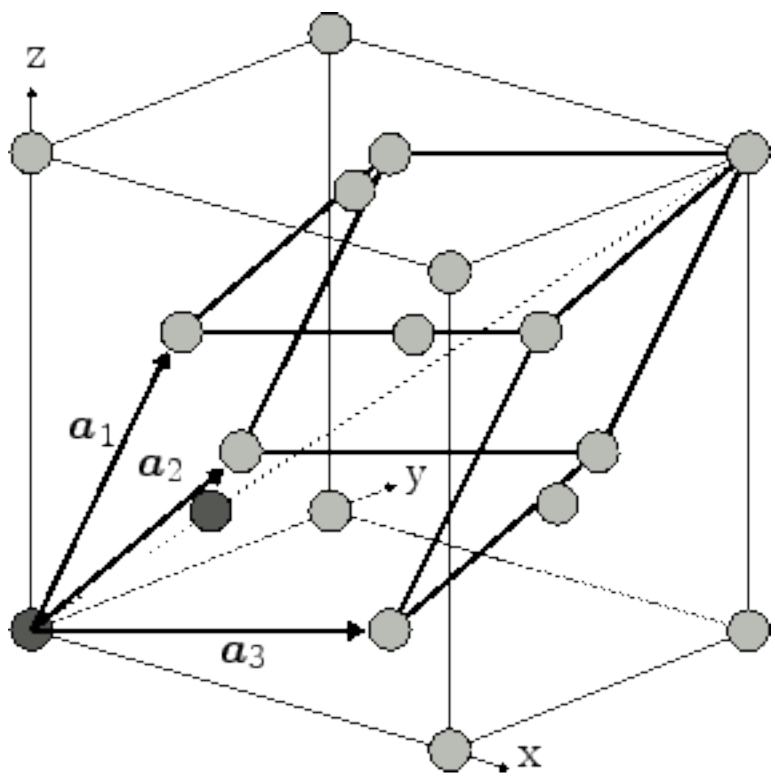
$$\boldsymbol{K}_9 = 2\boldsymbol{b}_1; \quad E\left(\lambda\right) = E_0\left[\frac{\left(\lambda - 2\right)^2}{3} + \left(\frac{\lambda}{3} - 2\right)^2\right]; \quad E\left(0\right) = \frac{16}{3}E_0$$

$$\boldsymbol{K}_{10} = 2\boldsymbol{b}_2; \quad E\left(\lambda\right) = E_0\left[\frac{\left(\lambda - 2\right)^2}{3} + \left(\frac{\lambda}{3} + 2\right)^2\right]; \quad E\left(0\right) = \frac{16}{3}E_0$$

$$\boldsymbol{K}_{11} = -2\boldsymbol{b}_1; \quad E\left(\lambda\right) = E_0\left[\frac{\left(\lambda + 2\right)^2}{3} + \left(\frac{\lambda}{3} + 2\right)^2\right]; \quad E\left(0\right) = \frac{16}{3}E_0$$

$$\boldsymbol{K}_{12} = -2\boldsymbol{b}_2; \quad E\left(\lambda\right) = E_0\left[\frac{\left(\lambda + 2\right)^2}{3} + \left(\frac{\lambda}{3} - 2\right)^2\right]; \quad E\left(0\right) = 4E_0$$

fcc unit cell

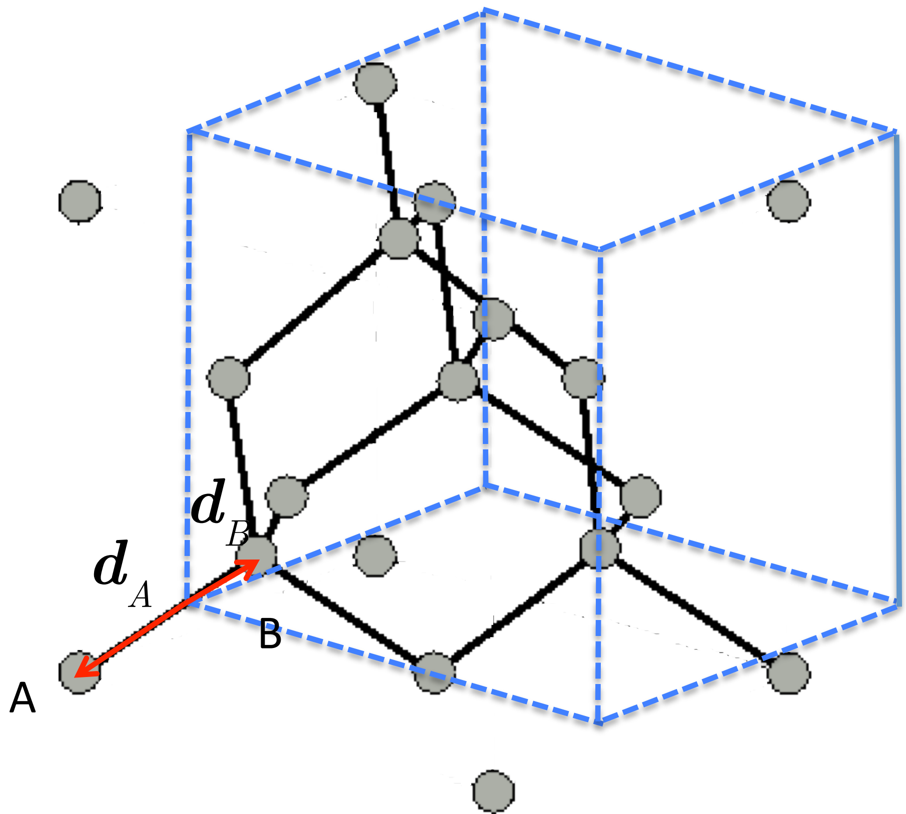


$$\boldsymbol{a}_1 = \frac{a}{2}\left(\hat{\mathbf{j}} + \hat{\mathbf{k}}\right)$$

$$\boldsymbol{a}_2 = \frac{a}{2}\left(\hat{\mathbf{i}} + \hat{\mathbf{k}}\right)$$

$$\boldsymbol{a}_3 = \frac{a}{2}\left(\hat{\mathbf{i}} + \hat{\mathbf{j}}\right)$$

Diamond structure (fcc +basis)



$$\boldsymbol{a}_1 = \tfrac{a}{2}\left(\hat{\mathbf{j}} + \hat{\mathbf{k}}\right)$$

$$\boldsymbol{a}_2 = \tfrac{a}{2}\left(\hat{\mathbf{i}} + \hat{\mathbf{k}}\right)$$

$$\boldsymbol{a}_3 = \tfrac{a}{2}\left(\hat{\mathbf{i}} + \hat{\mathbf{j}}\right)$$

$$\boldsymbol{n}_{AB}^{(1)} = \frac{a}{4}\left(\hat{\mathbf{i}} + \hat{\mathbf{j}} + \hat{\mathbf{k}}\right) = -\boldsymbol{n}_{BA}^{(1)}$$

$$\boldsymbol{n}_{AB}^{(2)} = \frac{a}{4}\left(\hat{\mathbf{i}} - \hat{\mathbf{j}} - \hat{\mathbf{k}}\right) = -\boldsymbol{n}_{BA}^{(2)}$$

$$\boldsymbol{n}_{AB}^{(3)} = \frac{a}{4}\left(-\hat{\mathbf{i}} + \hat{\mathbf{j}} - \hat{\mathbf{k}}\right) = -\boldsymbol{n}_{BA}^{(3)}$$

$$\boldsymbol{n}_{AB}^{(4)} = \frac{a}{4}\left(-\hat{\mathbf{i}} - \hat{\mathbf{j}} + \hat{\mathbf{k}}\right) = -\boldsymbol{n}_{BA}^{(4)}$$

$$\boldsymbol{d}_A = -\frac{a}{8}\left(\hat{\mathbf{i}} + \hat{\mathbf{j}} + \hat{\mathbf{k}}\right)$$

$$\boldsymbol{d}_B = \frac{a}{8}\left(\hat{\mathbf{i}} + \hat{\mathbf{j}} + \hat{\mathbf{k}}\right)$$

Complex tight binding factors

We define, to simplify the notation:

$$g_1 \equiv \frac{1}{4}\left[e^{i\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(1)}} + e^{i\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(2)}} + e^{i\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(3)}} + e^{i\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(4)}}\right]$$

$$g_2 \equiv \frac{1}{4}\left[e^{i\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(1)}} + e^{i\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(2)}} - e^{i\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(3)}} - e^{i\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(4)}}\right]$$

$$g_3 \equiv \frac{1}{4}\left[e^{i\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(1)}} - e^{i\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(2)}} + e^{i\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(3)}} - e^{i\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(4)}}\right]$$

$$g_4 \equiv \frac{1}{4}\left[e^{i\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(1)}} - e^{i\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(2)}} - e^{i\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(3)}} + e^{i\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(4)}}\right]$$

H(sA,sB) matrix elements

$$H_{sA,sB}\left(\boldsymbol{k}\right)=V_{ss\sigma}\sum_{m=1}^{N}e^{i\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(m)}}$$

$$H_{sB,sA}\left(\boldsymbol{k}\right)=V_{ss\sigma}\sum_{m=1}^{N}e^{i\boldsymbol{k}\cdot\boldsymbol{n}_{BA}^{(m)}}$$

$$H_{sA,sB}\left(\boldsymbol{k}\right)=V_{ss\sigma}\left(e^{i\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(1)}}+e^{i\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(2)}}+e^{i\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(3)}}+e^{i\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(4)}}\right)=4g_1V_{ss\sigma}$$

$$H_{sB,sA}\left(\boldsymbol{k}\right)=H^{*}_{sB,sA}\left(\boldsymbol{k}\right)=4g_1^{*}V_{ss\sigma}$$

H(sA,pB) matrix elements

$$H_{sA,p_xB}\left(\boldsymbol{k}\right)=V_{sp\sigma}\sum_{m=1}^{4}e^{i\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(m)}}\hat{n}_{AB,x}^{(m)}$$

$$=\frac{V_{sp\sigma}}{\sqrt{3}}\left[e^{i\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(1)}}+e^{i\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(2)}}+e^{i\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(3)}}\left(-1\right)+e^{i\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(4)}}\left(-1\right)\right]=\frac{4V_{sp\sigma}}{\sqrt{3}}g_2$$

$$H_{sA,p_yB}\left(\boldsymbol{k}\right)=V_{sp\sigma}\sum_{m=1}^{4}e^{i\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(m)}}n_{AB,y}^{(m)}=4V_{sp\sigma}g_3\Big/\sqrt{3}$$

$$H_{sA,p_zB}\left(\boldsymbol{k}\right)=V_{sp\sigma}\sum_{m=1}^{4}e^{i\boldsymbol{k}\cdot\boldsymbol{n}_{AB}^{(m)}}n_{AB,z}^{(m)}=4V_{sp\sigma}g_4\Big/\sqrt{3}$$

$$H_{sB,p_xA}\left(\boldsymbol{k}\right)=V_{sp\sigma}\sum_{m=1}^{4}e^{i\boldsymbol{k}\cdot\boldsymbol{n}_{BA}^{(m)}}n_{BA,x}^{(m)}=-4V_{sp\sigma}g_2\Big/\sqrt{3}$$

$$H_{sB,p_yA}\left(\boldsymbol{k}\right)=V_{sp\sigma}\sum_{m=1}^{4}e^{i\boldsymbol{k}\cdot\boldsymbol{n}_{BA}^{(m)}}n_{BA,y}^{(m)}=-4V_{sp\sigma}g_3\Big/\sqrt{3}$$

$$H_{sB,p_zA}\left(\boldsymbol{k}\right)=V_{sp\sigma}\sum_{m=1}^{N}e^{i\boldsymbol{k}\cdot\boldsymbol{n}_{BA}^{(m)}}n_{BA,z}^{(m)}=-V_{sp\sigma}g_4\Big/\sqrt{3}$$

Symmetrized elements in diamond

- Define

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

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

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

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

Tight binding hamiltonian diamond

$$H = \begin{bmatrix} \varepsilon_s & 0 & 0 & 0 & V_{ss}g_1 & V_{sp}g_2 & V_{sp}g_3 & V_{sp}g_4 \\ 0 & \varepsilon_p & 0 & 0 & -V_{sp}g_2 & V_{xx}g_1 & V_{xy}g_4 & V_{xy}g_3 \\ 0 & 0 & \varepsilon_p & 0 & -V_{sp}g_3 & V_{xy}g_4 & V_{xx}g_1 & V_{xy}g_2 \\ 0 & 0 & 0 & \varepsilon_p & -V_{sp}g_4 & V_{xy}g_3 & V_{xy}g_2 & V_{xx}g_1 \\ V_{ss}g_1^* & -V_{sp}g_2^* & -V_{sp}g_3^* & -V_{sp}g_4^* & \varepsilon_s & 0 & 0 & 0 \\ V_{sp}g_2^* & V_{xx}g_1^* & V_{xy}g_4^* & V_{xy}g_3^* & 0 & \varepsilon_p & 0 & 0 \\ V_{sp}g_3^* & V_{xy}g_4^* & V_{xx}g_1^* & V_{xy}g_2^* & 0 & 0 & \varepsilon_p & 0 \\ V_{sp}g_4^* & V_{xy}g_3^* & V_{xy}g_2^* & V_{xx}g_1^* & 0 & 0 & 0 & \varepsilon_p \end{bmatrix}$$

Diamond reciprocal lattice

$$\boldsymbol{b}_1 = \frac{2\pi}{a}\left(\hat{\mathbf{i}} - \hat{\mathbf{j}} - \hat{\mathbf{k}}\right); \quad \boldsymbol{b}_2 = \frac{2\pi}{a}\left(-\hat{\mathbf{i}} + \hat{\mathbf{j}} - \hat{\mathbf{k}}\right); \quad \boldsymbol{b}_3 = \frac{2\pi}{a}\left(-\hat{\mathbf{i}} - \hat{\mathbf{j}} + \hat{\mathbf{k}}\right)$$

$$-\boldsymbol{b}_1 = \frac{2\pi}{a}\left(-\hat{\mathbf{i}} + \hat{\mathbf{j}} + \hat{\mathbf{k}}\right); \quad -\boldsymbol{b}_2 = \frac{2\pi}{a}\left(\hat{\mathbf{i}} - \hat{\mathbf{j}} + \hat{\mathbf{k}}\right); \quad -\boldsymbol{b}_3 = \frac{2\pi}{a}\left(\hat{\mathbf{i}} + \hat{\mathbf{j}} - \hat{\mathbf{k}}\right)$$

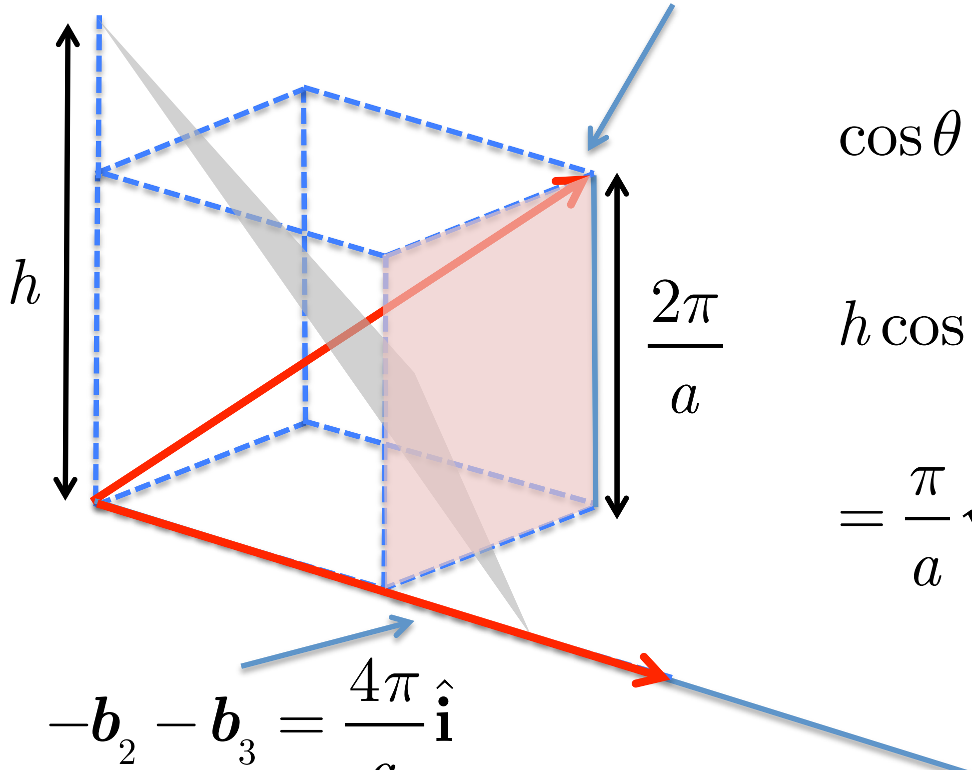
$$\boldsymbol{b}_1 + \boldsymbol{b}_2 + \boldsymbol{b}_3 = \frac{2\pi}{a}\left(-\hat{\mathbf{i}} - \hat{\mathbf{j}} - \hat{\mathbf{k}}\right); \quad -\boldsymbol{b}_1 - \boldsymbol{b}_2 - \boldsymbol{b}_3 = \frac{2\pi}{a}\left(\hat{\mathbf{i}} + \hat{\mathbf{j}} + \hat{\mathbf{k}}\right)$$

But these 8 vectors do not define the BZ:

$$-\boldsymbol{b}_2 - \boldsymbol{b}_3 = \frac{4\pi}{a}\hat{\mathbf{i}}$$

Diamond BZ: a truncated octahedron

$$-\boldsymbol{b}_1-\boldsymbol{b}_2-\boldsymbol{b}_3=\frac{2\pi}{a}\left(\hat{\mathbf{i}}+\hat{\mathbf{j}}+\hat{\mathbf{k}}\right)$$



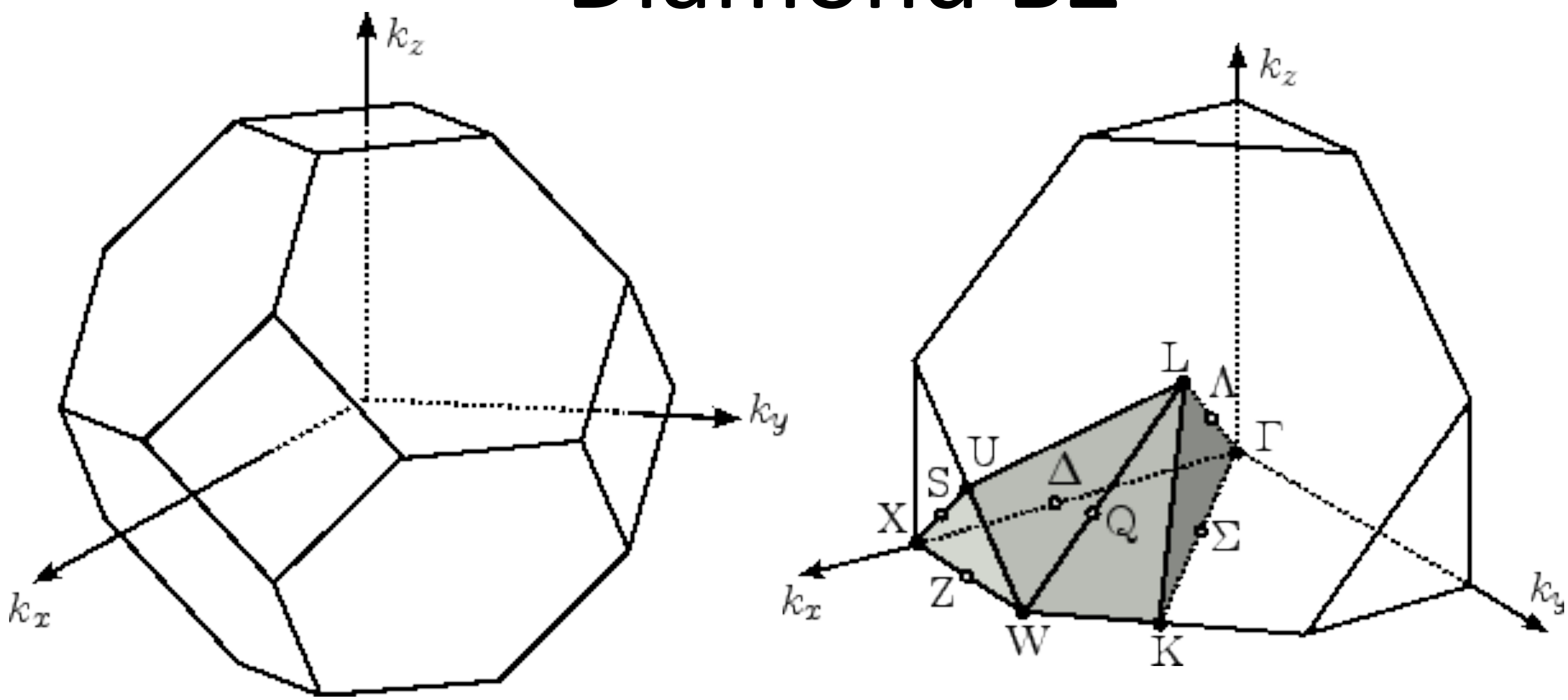
$$-\boldsymbol{b}_2-\boldsymbol{b}_3=\frac{4\pi}{a}\hat{\mathbf{i}}$$

$$\cos\theta=\frac{1}{\sqrt{3}}\left(1,1,1\right)\left(1,0,0\right)=\frac{1}{\sqrt{3}}$$

$$h\cos\theta=\frac{h}{\sqrt{3}}$$

$$=\frac{\pi}{a}\sqrt{1^2+1^2+1^2}\Rightarrow h=\frac{3\pi}{a}$$

Diamond BZ



$$\Gamma = \left(0,0,0\right)$$

$$X = \frac{2\pi}{a}\left(1,0,0\right); \quad \Delta = \frac{2\pi}{a}\left(\delta,0,0\right); \quad 0 < \delta < 1$$

$$L = \frac{\pi}{a}\left(1,1,1\right); \quad \Lambda = \frac{2\pi}{a}\left(\lambda,\lambda,\lambda\right); \quad 0 < \lambda < 1$$

Empty lattice band structure

- We consider the following reciprocal lattice vectors:

$$\boldsymbol{b}_1 = \frac{2\pi}{a}\left(\hat{\mathbf{i}} - \hat{\mathbf{j}} - \hat{\mathbf{k}}\right); \quad \boldsymbol{b}_2 = \frac{2\pi}{a}\left(-\hat{\mathbf{i}} + \hat{\mathbf{j}} - \hat{\mathbf{k}}\right); \quad \boldsymbol{b}_3 = \frac{2\pi}{a}\left(-\hat{\mathbf{i}} - \hat{\mathbf{j}} + \hat{\mathbf{k}}\right)$$

$$-\boldsymbol{b}_1 = \frac{2\pi}{a}\left(-\hat{\mathbf{i}} + \hat{\mathbf{j}} + \hat{\mathbf{k}}\right); \quad -\boldsymbol{b}_2 = \frac{2\pi}{a}\left(\hat{\mathbf{i}} - \hat{\mathbf{j}} + \hat{\mathbf{k}}\right); \quad -\boldsymbol{b}_3 = \frac{2\pi}{a}\left(\hat{\mathbf{i}} + \hat{\mathbf{j}} - \hat{\mathbf{k}}\right.$$

$$\boldsymbol{b}_1 + \boldsymbol{b}_2 + \boldsymbol{b}_3 = \frac{2\pi}{a}\left(-\hat{\mathbf{i}} - \hat{\mathbf{j}} - \hat{\mathbf{k}}\right); \quad -\boldsymbol{b}_1 - \boldsymbol{b}_2 - \boldsymbol{b}_3 = \frac{2\pi}{a}\left(\hat{\mathbf{i}} + \hat{\mathbf{j}} + \hat{\mathbf{k}}\right)$$

$$\boldsymbol{b}_1 + \boldsymbol{b}_2 = -\frac{4\pi}{a}\hat{\mathbf{k}}; \quad -\boldsymbol{b}_1 - \boldsymbol{b}_2 = \frac{4\pi}{a}\hat{\mathbf{k}}$$

$$\boldsymbol{b}_2 + \boldsymbol{b}_3 = -\frac{4\pi}{a}\hat{\mathbf{i}}; \quad -\boldsymbol{b}_2 - \boldsymbol{b}_3 = \frac{4\pi}{a}\hat{\mathbf{i}}$$

$$\boldsymbol{b}_1 + \boldsymbol{b}_3 = -\frac{4\pi}{a}\hat{\mathbf{j}}; \quad -\boldsymbol{b}_1 - \boldsymbol{b}_3 = \frac{4\pi}{a}\hat{\mathbf{j}}$$

Δ-line $\boldsymbol{k} = \frac{2\pi}{a}(\delta, 0, 0)$

$$\boldsymbol{K}_0 = 0; \quad E(\delta) = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2 \delta^2 = E_0\delta^2; \quad E(0) = 0; \quad E(1) = E_0$$

$$\boldsymbol{K}_1 = \boldsymbol{b}_1; \quad E(\delta) = E_0\left[(\delta - 1)^2 + 2\right]; \quad E(0) = 3E_0; \quad E(1) = 2E_0$$

$$\boldsymbol{K}_2 = \boldsymbol{b}_2; \quad E(\delta) = E_0\left[(\delta + 1)^2 + 2\right]; \quad E(0) = 3E_0; \quad E(1) = 6E_0$$

$$\boldsymbol{K}_3 = \boldsymbol{b}_3; \quad E(\delta) = E_0\left[(\delta + 1)^2 + 2\right]; \quad E(0) = 3E_0; \quad E(1) = 6E_0$$

$$\boldsymbol{K}_4 = -\boldsymbol{b}_1; \quad E(\delta) = E_0\left[(\delta + 1)^2 + 2\right]; \quad E(0) = 3E_0; \quad E(1) = 6E_0$$

$$\boldsymbol{K}_5 = -\boldsymbol{b}_2; \quad E(\delta) = E_0\left[(\delta - 1)^2 + 2\right]; \quad E(0) = 3E_0; \quad E(1) = 2E_0$$

$$\boldsymbol{K}_6 = -\boldsymbol{b}_3; \quad E(\delta) = E_0\left[(\delta - 1)^2 + 2\right]; \quad E(0) = 3E_0; \quad E(1) = 2E_0$$

Δ-line (cont) $\boldsymbol{k} = \frac{2\pi}{a}\left(\delta,0,0\right)$

$$\boldsymbol{K}_7 = \boldsymbol{b}_1 + \boldsymbol{b}_2 + \boldsymbol{b}_3; \quad E\left(\delta\right) = E_0\left[\left(\delta+1\right)^2 + 2\right]; E\left(0\right) = 3E_0; E\left(1\right) = 6E_0$$

$$\boldsymbol{K}_8 = -\boldsymbol{b}_1 - \boldsymbol{b}_2 - \boldsymbol{b}_3; \quad E\left(\delta\right) = E_0\left[\left(\delta-1\right)^2 + 2\right]; E\left(0\right) = 3E_0; E\left(1\right) = 2E_0$$

$$\boldsymbol{K}_9 = \boldsymbol{b}_1 + \boldsymbol{b}_2; \quad E\left(\delta\right) = E_0\left(\delta^2 + 4\right); \quad E\left(0\right) = 4E_0; \quad E\left(1\right) = 5E_0$$

$$\boldsymbol{K}_{10} = -\boldsymbol{b}_1 - \boldsymbol{b}_2; \quad E\left(\delta\right) = E_0\left(\delta^2 + 4\right); \quad E\left(0\right) = 4E_0; \quad E\left(1\right) = 5E_0$$

$$\boldsymbol{K}_{11} = \boldsymbol{b}_2 + \boldsymbol{b}_3; \quad E\left(\delta\right) = E_0\left(\delta + 2\right)^2; \quad E\left(0\right) = 4E_0; \quad E\left(1\right) = 9E_0$$

$$\boldsymbol{K}_{12} = -\boldsymbol{b}_2 - \boldsymbol{b}_3; \quad E\left(\delta\right) = E_0\left(\delta - 2\right)^2; \quad E\left(0\right) = 4E_0; \quad E\left(1\right) = E_0$$

$$\boldsymbol{K}_{13} = \boldsymbol{b}_1 + \boldsymbol{b}_3; \quad E\left(\delta\right) = E_0\left(\delta^2 + 4\right); \quad E\left(0\right) = 4E_0; \quad E\left(1\right) = 15E_0$$

$$\boldsymbol{K}_{14} = -\boldsymbol{b}_1 - \boldsymbol{b}_3; \quad E\left(\delta\right) = E_0\left(\delta^2 + 4\right); \quad E\left(0\right) = 4E_0; \quad E\left(1\right) = 15E_0$$

Λ-line

$$\boldsymbol{k} = \frac{\pi}{a}\left(\lambda, \lambda, \lambda\right) = \frac{2\pi}{a}\left(\frac{\lambda}{2}, \frac{\lambda}{2}, \frac{\lambda}{2}\right)$$

$$\boldsymbol{K}_0 = 0; \quad E\left(\lambda\right) = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2\left[\left(\frac{\lambda}{2}\right)^2 + \left(\frac{\lambda}{2}\right)^2 + \left(\frac{\lambda}{2}\right)^2\right] = \frac{3}{4}E_0\lambda^2; \quad E\left(0\right) = 0$$

$$\boldsymbol{K}_1 = \boldsymbol{b}_1; \quad E\left(\lambda\right) = E_0\left[\left(\lambda/2 - 1\right)^2 + 2\left(\lambda/2 + 1\right)^2\right]; \quad E\left(0\right) = 3E_0$$

$$\boldsymbol{K}_2 = \boldsymbol{b}_2; \quad E\left(\lambda\right) = E_0\left[2\left(\lambda/2 + 1\right)^2 + \left(\lambda/2 - 1\right)^2\right]; \quad E\left(0\right) = 3E_0$$

$$\boldsymbol{K}_3 = \boldsymbol{b}_3; \quad E\left(\lambda\right) = E_0\left[2\left(\lambda/2 + 1\right)^2 + \left(\lambda/2 - 1\right)^2\right]; \quad E\left(0\right) = 3E_0$$

$$\boldsymbol{K}_4 = -\boldsymbol{b}_1; \quad E\left(\lambda\right) = E_0\left[\left(\lambda/2 + 1\right)^2 + 2\left(\lambda/2 - 1\right)^2\right]; \quad E\left(0\right) = 3E_0$$

$$\boldsymbol{K}_5 = -\boldsymbol{b}_2; \quad E\left(\lambda\right) = E_0\left[\left(\lambda/2 + 1\right)^2 + 2\left(\lambda/2 - 1\right)^2\right]; \quad E\left(0\right) = 3E_0$$

$$\boldsymbol{K}_6 = -\boldsymbol{b}_3; \quad E\left(\lambda\right) = E_0\left[\left(\lambda/2 + 1\right)^2 + 2\left(\lambda/2 - 1\right)^2\right]; \quad E\left(0\right) = 3E_0$$

Λ-line (cont) $\boldsymbol{k} = \frac{\pi}{a}\left(\lambda,\lambda,\lambda\right) = \frac{2\pi}{a}\left(\frac{\lambda}{2},\frac{\lambda}{2},\frac{\lambda}{2}\right)$

$$\boldsymbol{K}_7 = \boldsymbol{b}_1 + \boldsymbol{b}_2 + \boldsymbol{b}_3; \quad E\left(\lambda\right) = E_0\left[3\left(\lambda/2+1\right)^2\right]; \quad E\left(0\right) = 3E_0$$

$$\boldsymbol{K}_8 = -\boldsymbol{b}_1 - \boldsymbol{b}_2 - \boldsymbol{b}_3; \quad E\left(\lambda\right) = E_0\left[\left(\lambda/2-1\right)^2\right]; \quad E\left(0\right) = 3E_0$$

$$\boldsymbol{K}_9 = \boldsymbol{b}_1 + \boldsymbol{b}_2; \quad E\left(\lambda\right) = E_0\left[2\left(\lambda/2\right)^2 + \left(\lambda/2+2\right)^2\right]; \quad E\left(0\right) = 4E_0$$

$$\boldsymbol{K}_{10} = -\boldsymbol{b}_1 - \boldsymbol{b}_2; \quad E\left(\lambda\right) = E_0\left[2\left(\lambda/2\right)^2 + \left(\lambda/2-2\right)^2\right]; \quad E\left(0\right) = 4E_0$$

$$\boldsymbol{K}_{11} = \boldsymbol{b}_2 + \boldsymbol{b}_3; \quad E\left(\lambda\right) = E_0\left[\left(\lambda/2+2\right)^2 + 2\left(\lambda/2\right)^2\right]; \quad E\left(0\right) = 4E_0$$

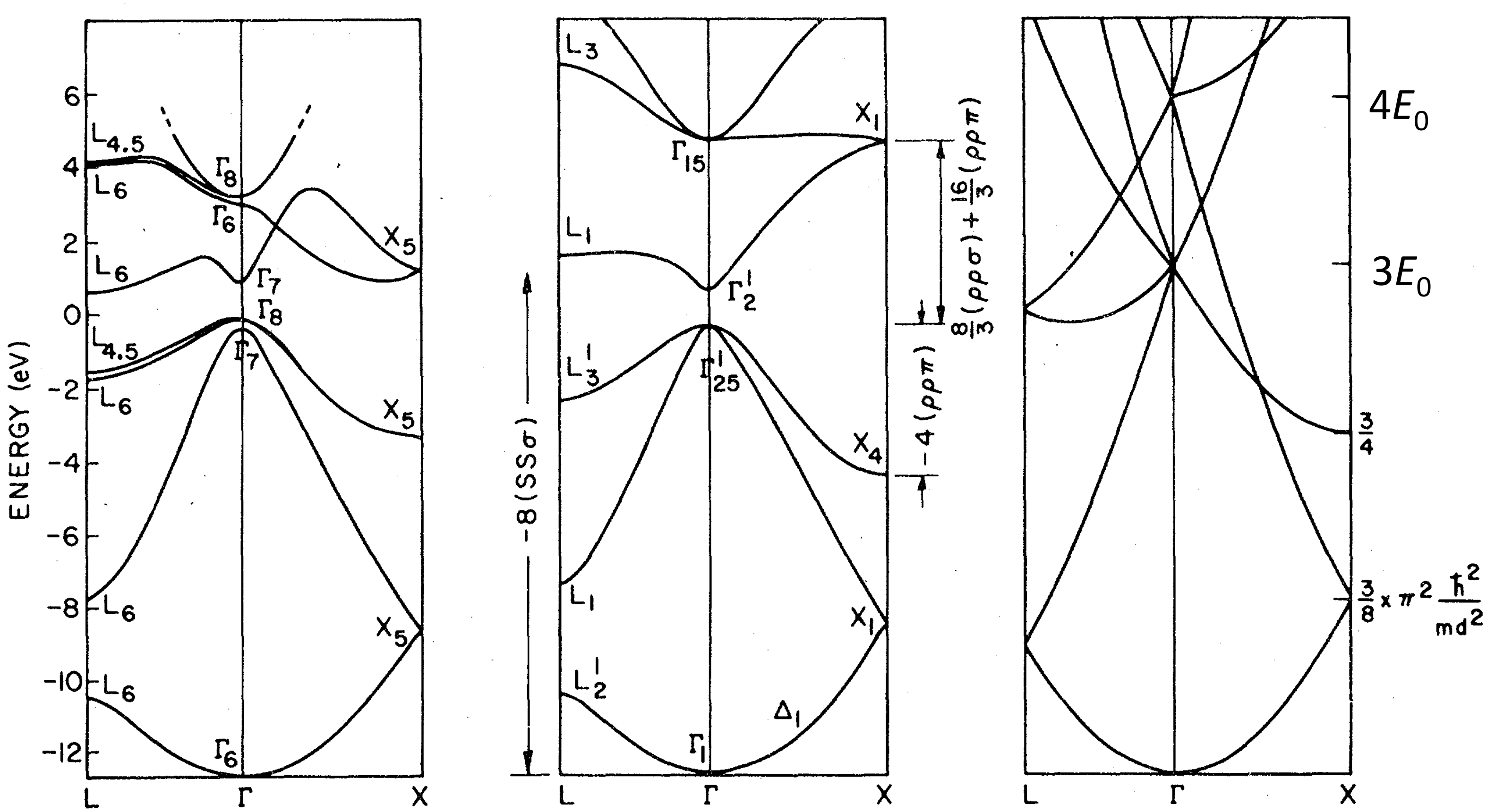
$$\boldsymbol{K}_{12} = -\boldsymbol{b}_2 - \boldsymbol{b}_3; \quad E\left(\lambda\right) = E_0\left[\left(\lambda/2-2\right)^2 + 2\left(\lambda/2\right)^2\right]; \quad E\left(0\right) = 4E_0$$

$$\boldsymbol{K}_{13} = \boldsymbol{b}_1 + \boldsymbol{b}_3; \quad E\left(\lambda\right) = E_0\left[\left(\lambda/2+2\right)^2 + 2\left(\lambda/2\right)^2\right]; \quad E\left(0\right) = 4E_0$$

$$\boldsymbol{K}_{14} = -\boldsymbol{b}_1 - \boldsymbol{b}_3; \quad E\left(\lambda\right) = E_0\left[\left(\lambda/2-2\right)^2 + 2\left(\lambda/2\right)^2\right]; \quad E\left(0\right) = 4E_0$$

Solution comparison

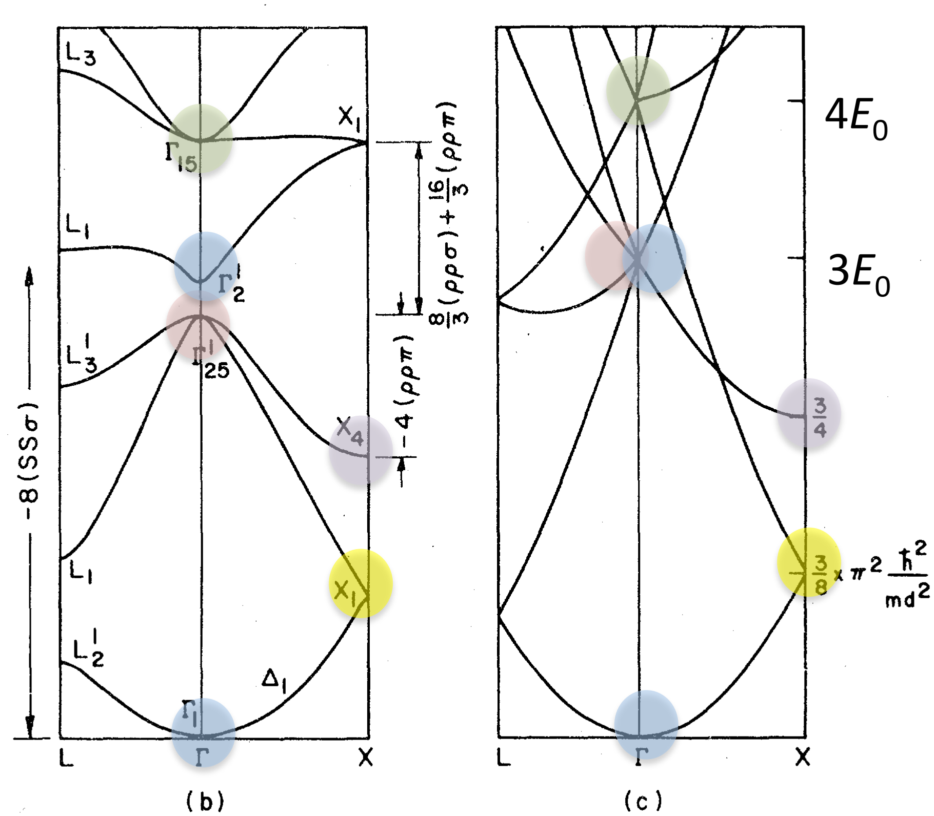
“Exact” **TB** **Empty cell**



(a) (b) (c)

Harrison's match (PRB 20, 2420 (1979))

- Harrison suggested matching the TB band structure to the empty cell eigenvalues and use these to determine universal tight binding parameters.



TB Hamiltonian k = 0

$$H = \begin{bmatrix} \varepsilon_s & 0 & 0 & 0 & V_{ss} & 0 & 0 & 0 \\ 0 & \varepsilon_p & 0 & 0 & 0 & V_{xx} & 0 & 0 \\ 0 & 0 & \varepsilon_p & 0 & 0 & 0 & V_{xx} & 0 \\ 0 & 0 & 0 & \varepsilon_p & 0 & 0 & 0 & V_{xx} \\ V_{ss} & 0 & 0 & 0 & \varepsilon_s & 0 & 0 & 0 \\ 0 & V_{xx} & 0 & 0 & 0 & \varepsilon_p & 0 & 0 \\ 0 & 0 & V_{xx} & 0 & 0 & 0 & \varepsilon_p & 0 \\ 0 & 0 & 0 & V_{xx} & 0 & 0 & 0 & \varepsilon_p \end{bmatrix}$$

s-states

$$H = \begin{pmatrix} \varepsilon_s & V_{ss} \\ V_{ss} & \varepsilon_s \end{pmatrix}$$

$$E = \varepsilon_s \pm \left| V_{ss} \right|$$

$$2\left| V_{ss} \right| = -8V_{ss\sigma} = 3E_0$$

$$V_{ss\sigma} = -\frac{3}{8}E_0 = -\frac{3}{8}\frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2 = -\frac{3}{4}\frac{\hbar^2}{m}\frac{\pi^2}{a^2} = -\left(\frac{9\pi^2}{64}\right)\frac{\hbar^2}{md^2}$$

p-states

$$H = \begin{pmatrix} \varepsilon_p & V_{xx} \\ V_{xx} & \varepsilon_p \end{pmatrix}$$

$$E = \varepsilon_p \pm \left| V_{xx} \right|$$

$$2\left|V_{xx}\right| = 2\left[\left(4V_{pp\sigma}/3\right) + \left(8V_{pp\pi}/3\right)\right] = 4E_0 - 3E_0 = E_0$$

Tight-binding Δ direction

$$g_1 \equiv \frac{1}{4}\left[e^{ik_x\frac{a}{4}} + e^{ik_x\frac{a}{4}} + e^{-ik_x\frac{a}{4}} + e^{-ik_x\frac{a}{4}}\right] = \cos\left(k_x\frac{a}{4}\right)$$

$$g_2 \equiv \frac{1}{4}\left[e^{ik_x\frac{a}{4}} + e^{ik_x\frac{a}{4}} - e^{-ik_x\frac{a}{4}} - e^{-ik_x\frac{a}{4}}\right] = i\sin\left(k_x\frac{a}{4}\right)$$

$$g_3 \equiv \frac{1}{4}\left[e^{ik_x\frac{a}{4}} - e^{ik_x\frac{a}{4}} + e^{-ik_x\frac{a}{4}} - e^{-ik_x\frac{a}{4}}\right] = 0$$

$$g_4 \equiv \frac{1}{4}\left[e^{ik_x\frac{a}{4}} - e^{ik_x\frac{a}{4}} - e^{-ik_x\frac{a}{4}} + e^{-ik_x\frac{a}{4}}\right] = 0$$

TB Hamiltonian Δ direction

$$H = \begin{bmatrix}
\varepsilon_s & 0 & 0 & 0 & V_{ss}\cos\left(k_x \frac{a}{4}\right) & iV_{sp}\sin\left(k_x \frac{a}{4}\right) & 0 & 0 \\
0 & \varepsilon_p & 0 & 0 & -iV_{sp}\sin\left(k_x \frac{a}{4}\right) & V_{xx}\cos\left(k_x \frac{a}{4}\right) & 0 & 0 \\
0 & 0 & \varepsilon_p & 0 & 0 & 0 & V_{xx}\cos\left(k_x \frac{a}{4}\right) & iV_{xy}\sin\left(k_x \frac{a}{4}\right) \\
0 & 0 & 0 & \varepsilon_p & 0 & 0 & iV_{xy}\sin\left(k_x \frac{a}{4}\right) & V_{xx}\cos\left(k_x \frac{a}{4}\right) \\
V_{ss}\cos\left(k_x \frac{a}{4}\right) & iV_{sp}\sin\left(k_x \frac{a}{4}\right) & 0 & 0 & \varepsilon_s & 0 & 0 & 0 \\
-iV_{sp}\sin\left(k_x \frac{a}{4}\right) & V_{xx}\cos\left(k_x \frac{a}{4}\right) & 0 & 0 & 0 & \varepsilon_p & 0 & 0 \\
0 & 0 & V_{xx}\cos\left(k_x \frac{a}{4}\right) & -iV_{xy}\sin\left(k_x \frac{a}{4}\right) & 0 & 0 & \varepsilon_p & 0 \\
0 & 0 & -iV_{xy}\sin\left(k_x \frac{a}{4}\right) & V_{xx}\cos\left(k_x \frac{a}{4}\right) & 0 & 0 & 0 & \varepsilon_p
\end{bmatrix}$$

TB Hamiltonian X-point

$$H = \begin{bmatrix} \varepsilon_s & 0 & 0 & 0 & 0 & iV_{sp} & 0 & 0 \\ 0 & \varepsilon_p & 0 & 0 & -iV_{sp} & 0 & 0 & 0 \\ 0 & 0 & \varepsilon_p & 0 & 0 & 0 & 0 & iV_{xy} \\ 0 & 0 & 0 & \varepsilon_p & 0 & 0 & iV_{xy} & 0 \\ 0 & iV_{sp} & 0 & 0 & \varepsilon_s & 0 & 0 & 0 \\ -iV_{sp} & 0 & 0 & 0 & 0 & \varepsilon_p & 0 & 0 \\ 0 & 0 & 0 & -iV_{xy} & 0 & 0 & \varepsilon_p & 0 \\ 0 & 0 & -iV_{xy} & 0 & 0 & 0 & 0 & \varepsilon_p \end{bmatrix}$$

s-p states at X

$$H = \begin{pmatrix} \varepsilon_s & iV_{sp} \\ -iV_{sp} & \varepsilon_p \end{pmatrix}$$

$$E = \frac{\left(\varepsilon_s + \varepsilon_p\right) \pm \sqrt{\left(\varepsilon_s + \varepsilon_p\right)^2 - 4\left(\varepsilon_s \varepsilon_p - V_{sp}^2\right)}}{2}$$

Pure p states at X

$$H = \begin{pmatrix} \varepsilon_p & iV_{xy} \\ -iV_{xy} & \varepsilon_p \end{pmatrix}$$

$$E = \varepsilon_p \pm \left|V_{xy}\right| = \varepsilon_p \pm \left|\left(4V_{pp\sigma}/3\right) - \left(4V_{pp\pi}/3\right)\right|$$

$$p\left(0\right) - p\left(X\right) = \left[-\left(4V_{pp\sigma}/3\right) - \left(8V_{pp\pi}/3\right)\right] + \left[\left(4V_{pp\sigma}/3\right) - \left(4V_{pp\pi}/3\right)\right]$$

$$= -\frac{12}{3}V_{pp\pi} = -4V_{pp\pi} = 3E_0 - 2E_0 = E_0 = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2 = \frac{\hbar^2}{md^2}\left(\frac{3}{8}\pi^2\right)$$

$$\Rightarrow V_{pp\pi} = -\left(\frac{3}{32}\pi^2\right)\frac{\hbar^2}{md^2}$$

TB universal parameters

$$V_{ll'm} = \eta_{ll'm} \frac{\hbar^2}{md^2}$$

TB parameters	$\eta_{ss\sigma}$	$\eta_{sp\sigma}$	$\eta_{pp\sigma}$	$\eta_{pp\pi}$
Ideal	$9\pi^2/64$	$3\sqrt{15}\pi^2/64$	$21\pi^2/64$	$-3\pi^2/32$
Ideal	1.39	1.79	3.24	-0.93
Fit Ge	-1.40	1.84	3.24	-0.81
Universal	-1.32	1.42	2.22	-0.63

Lattice parameters

	Si	Ge	Sn
$a(\text{Å})$	5.43	5.66	6.49
$d(\text{Å})$	2.35	2.45	2.81
ε_s	-14.79	-15.16	-13.04
ε_p	-7.59	-7.33	-6.76

Bonding in Si, Ge,Sn