PY4T01 Condensed Matter Theory: Lecture 12

Band Structure of Graphene: Corrections at E_F

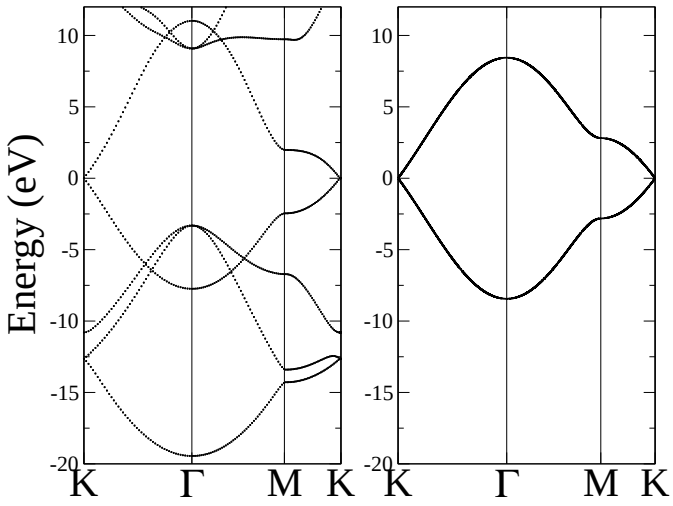
Remember the last result:

$$E(\vec{k}) = \epsilon_p \pm \gamma_{pp\pi}\sqrt{f(\vec{k})f(\vec{k})^*} = \epsilon_p \pm \gamma_{pp\pi}\sqrt{|f(\vec{k})|^2}$$

with

$$f(\vec{k}) = 1 + 2\,\mathrm{e}^{-ik_x\frac{\sqrt{3}}{2}a_0}\cos(\frac{k_y}{2}a_0)$$

This gives



This is somehow unsatisfactory since:

1. The π bands are symmetric with respect to $E = \epsilon_p$
2. One band is completely missed

Fixing the π band

The approximation we have to give up in this case is that of orthogonality of the basis set:

$$\langle \vec{R}'\, n' | \vec{R}\, n \rangle = \begin{cases} 1 & \text{if } (\vec{R}'\, n') = (\vec{R}\, n) \\ S & \text{if } (\vec{R}'\, n'), (\vec{R}\, n) \text{ nn} \\ 0 & \text{elsewhere} \end{cases}$$

we can still use the "molecular state"

$$|\psi_{\vec{k}}\rangle = \frac{1}{N^{1/2}} \sum_{\vec{R}} \sum_{n=1}^{2} \mathrm{e}^{i\vec{k}\cdot\vec{R}} A_n^{\vec{k}} |\vec{R}\, n\rangle$$

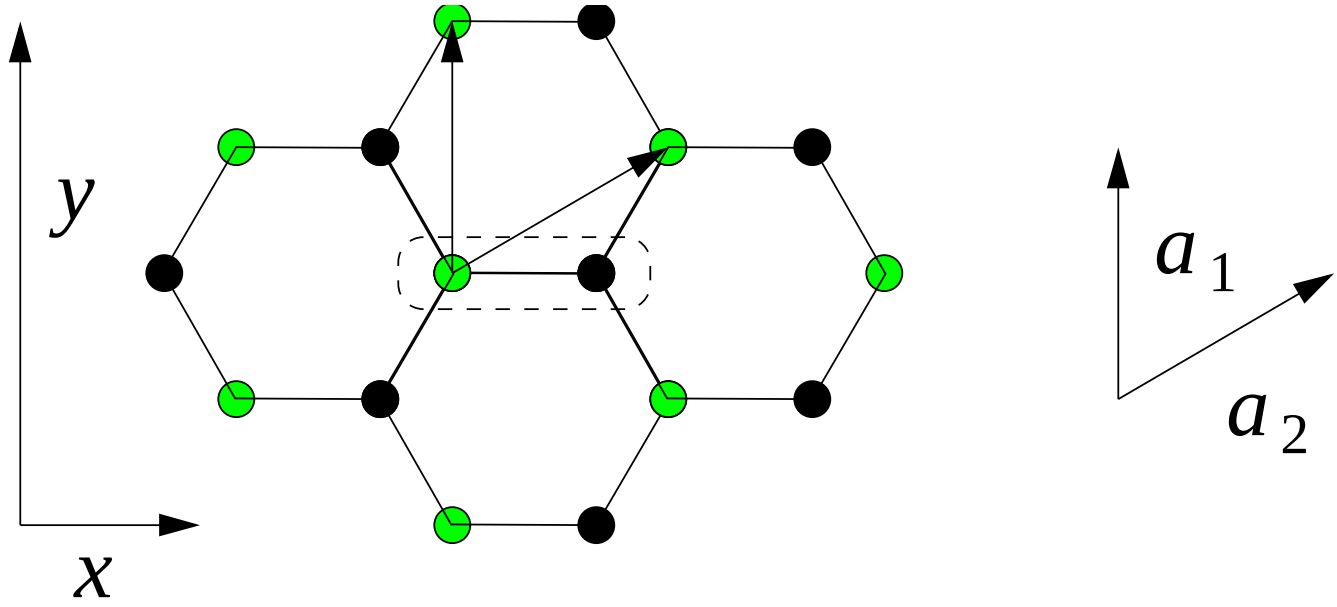
to solve the Schrödinger equation $H|\psi_{\vec{k}}\rangle = E|\psi_{\vec{k}}\rangle$

$$\sum_{\vec{R}} \sum_{n=1}^{2} A_n^{\vec{k}} \mathrm{e}^{i\vec{k}\cdot\vec{R}} H |\vec{R}\, n\rangle = E(\vec{k}) \sum_{\vec{R}} \sum_{n=1}^{2} A_n^{\vec{k}} \mathrm{e}^{i\vec{k}\cdot\vec{R}} |\vec{R}\, n\rangle$$

But now when we multiply by $\langle \vec{R}' n' |$, we obtain

$$\sum_{\vec{R}} \sum_{n=1}^{2} A_n^{\vec{k}} \mathrm{e}^{i\vec{k}\cdot\vec{R}} \langle \vec{R}' n' | H | \vec{R} n \rangle = E(\vec{k}) \sum_{\vec{R}} \sum_{n=1}^{2} A_n^{\vec{k}} \mathrm{e}^{i\vec{k}\cdot\vec{R}} \langle \vec{R}' n' | \vec{R} n \rangle$$

This is analogous to the case of the H_2 molecule. However the overlap matrix $\mathcal{S}$ now has some phases (as well as the Hamiltonian matrix elements).



On-site terms: overlap within the primitive cell

$$\langle \vec{R}'\, n' | \vec{R}'\, n \rangle = \begin{pmatrix} 1 & S \\ S & 1 \end{pmatrix}$$

The phase factor is $\mathrm{e}^{i\vec{k}\cdot\vec{R}'}$

Off-diagonal terms: overlap with other cells

Each cell has four nearest neighbor cells

1. Cell $\vec{a}_2$

$$\langle \vec{R}'\, n' | \vec{R}' + \vec{a}_2\, n \rangle = \begin{pmatrix} 0 & 0 \\ S & 0 \end{pmatrix}$$

The phase factor is $\mathrm{e}^{i\vec{k}\cdot(\vec{R}'+\vec{a}_2)}$

2. Cell $\vec{a}_2 - \vec{a}_1$

$$\langle \vec{R}'\, n' | H | \vec{R}' + \vec{a}_2 - \vec{a}_1\, n \rangle = \begin{pmatrix} 0 & 0 \\ S & 0 \end{pmatrix}$$

The phase factor is $\mathrm{e}^{i\vec{k}\cdot(\vec{R}'+\vec{a}_2-\vec{a}_1)}$

3. Cell $-\vec{a}_2$

$$\langle \vec{R}'\, n' | \vec{R}' - \vec{a}_2\, n \rangle = \begin{pmatrix} 0 & S \\ 0 & 0 \end{pmatrix}$$

The phase factor is $\mathrm{e}^{i\vec{k}\cdot(\vec{R}'-\vec{a}_2)}$

4. Cell $-\vec{a}_2 + \vec{a}_1$

$$\langle \vec{R}'\, n' | \vec{R}' - \vec{a}_2 + \vec{a}_1\, n \rangle = \begin{pmatrix} 0 & S \\ 0 & 0 \end{pmatrix}$$

The phase factor is $\mathrm{e}^{i\vec{k}\cdot(\vec{R}'-\vec{a}_2+\vec{a}_1)}$

Now let us put all together $(\mathcal{H} - E\mathcal{S})\Psi_{\vec{k}}$:

$$\begin{pmatrix} \epsilon_p & \gamma_{pp\pi}\, f(\vec{k}) \\ \gamma_{pp\pi}\, f(\vec{k})^* & \epsilon_p \end{pmatrix} \Psi_{\vec{k}} = E(\vec{k}) \begin{pmatrix} 1 & S\, f(\vec{k}) \\ S\, f(\vec{k})^* & 1 \end{pmatrix} \Psi_{\vec{k}}$$

It is easy to see that the solutions are:

$$E(\vec{k}) = \frac{\epsilon_p \pm \gamma_{pp\pi}\sqrt{|f(\vec{k})|^2}}{1 \pm S\sqrt{|f(\vec{k})|^2}}$$