

# Fundamentals of Nanoelectronics

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## Lecture 18: Bandstructure 3

Ref. Chapter 5.1 & 5.2



*Network for Computational Nanotechnology*

**nanoHUB** NCN  
online simulations and more

## Review

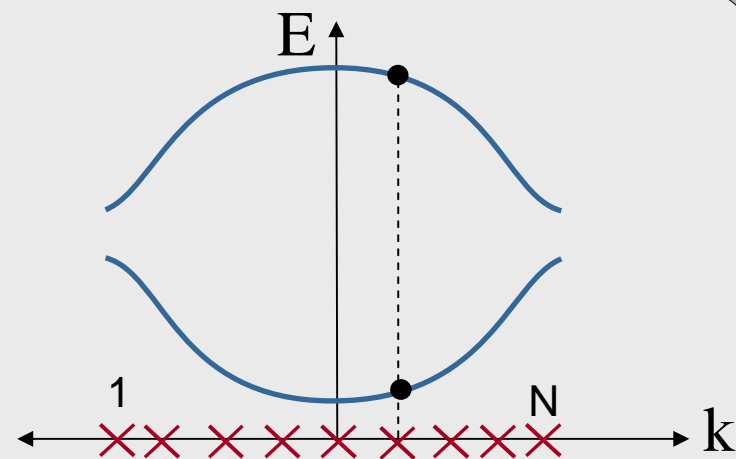


- Last time we talked about the principle of bandstructure which allows one to calculate the energy levels of a periodic structure. In particular we talked about a dimerized solid which has two atoms per unit cell.

$$\{\varphi_n\} = \{\varphi_0\} e^{ikna} \Rightarrow E\{\varphi_0\} = [h(k)]\{\varphi_0\}$$

$$E \begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_N \end{bmatrix} = \begin{bmatrix} \text{Every row looks} \\ \text{the same} \end{bmatrix} \begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_N \end{bmatrix}$$

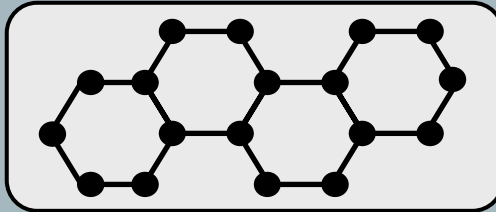
- The dispersion relation looks like:



- Today we want to expand this idea to a higher dimension: 2D.
- In particular we'll use the principle of bandstructure to describe the energy levels of graphene...

## • GRAPHENE

Hexagonal Lattice

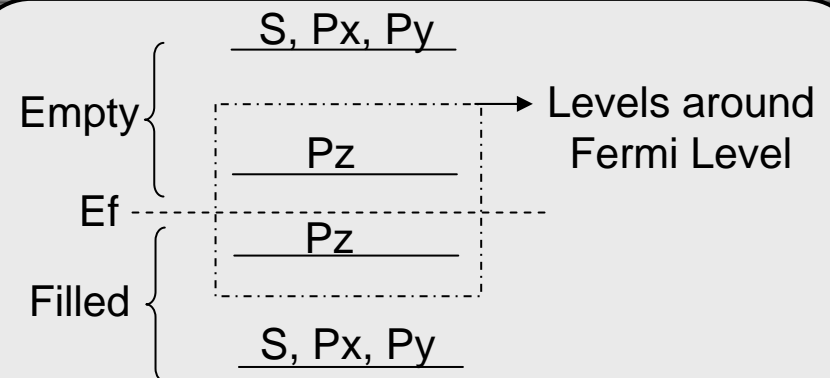


- The importance of this material comes in play when they role this up to become a carbon nanotube which is of great interest nowadays. Today we'll talk about the energy levels of a Graphene sheet.
- Remember that the starting point is the Schrödinger equation which can be turned into a matrix equation once a proper set of basis functions are has been chosen.
- How many basis functions do we need per atom? The basis functions are the atomic orbitals. There are 4 orbitals for the valence electrons of a carbon atom.

C6:	4	2p
	2	2s
	2	1s

- As it turns out we can talk only one of these four orbitals for our basis set. This makes the problem easier and tractable analytically.
- The reason that we can ignore the other 3 is that the “Pz” orbital does not mix with the other ones (the structure is planar). So the problem can be separated into two parts: the one for Pz orbital; and the one for S, Px, Py. At the end of the day it turns out that only the Pz orbitals play a major role in determining the electronic and optical properties.

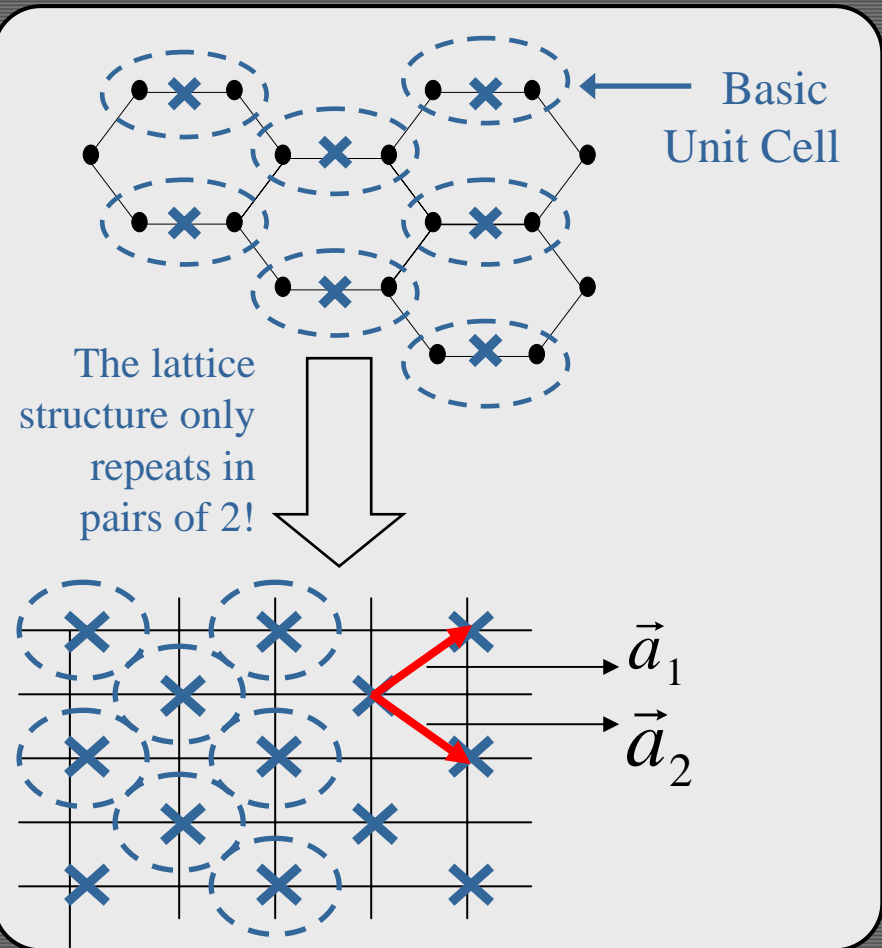
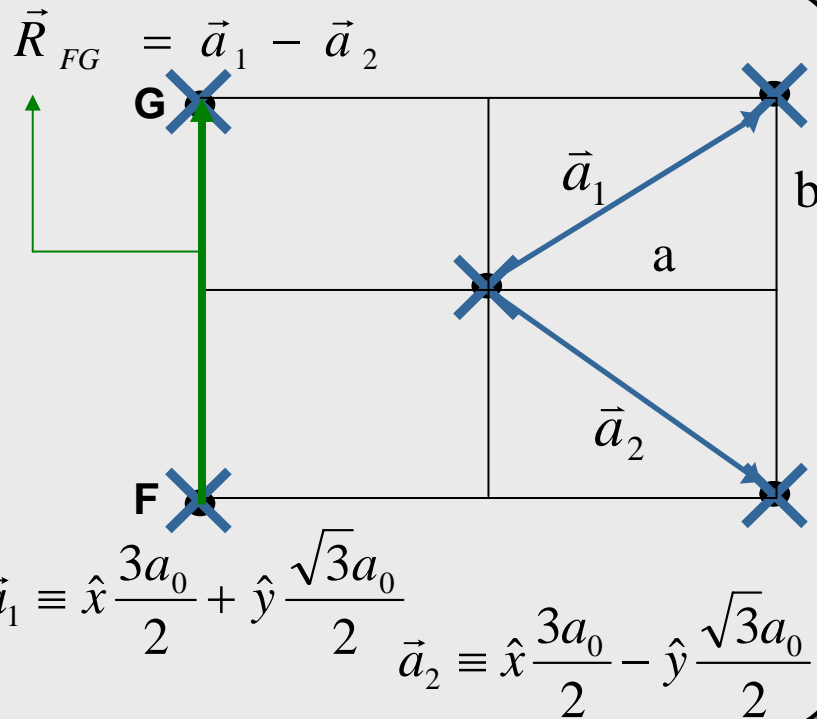
### Two Carbon Atoms in a Bond



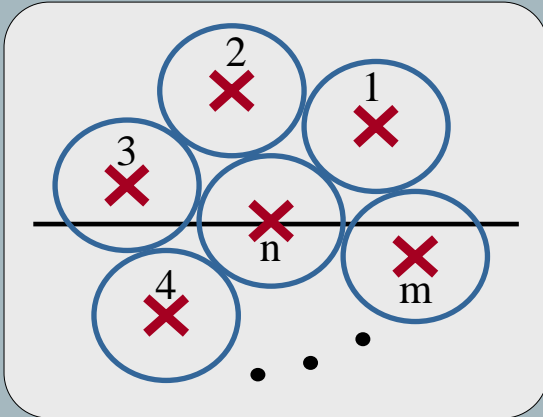
# Graphene: Unit Cell / Basis Vectors

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- To construct a basis set, the next question is: how many atoms are there per unit cell? In other words what is the minimal number of atoms that can be put together to construct a cell from which, the whole lattice can be constructed?
- The answer is: we need two atoms →

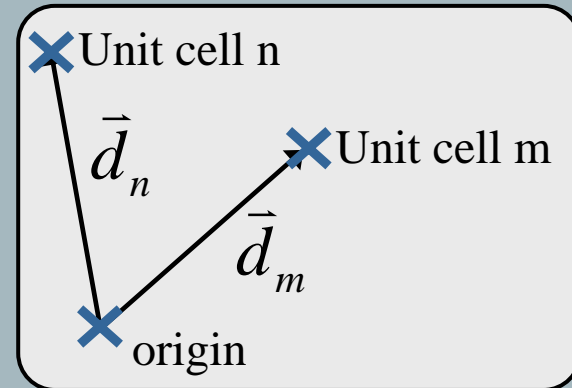


- Schrödinger equation reads:  $E\{\phi_n\} = \sum_m [H_{nm}]\{\phi_m\}$  (1)



- Equation 1 can be solved by:  $\{\phi_n\} = \{\phi_0\}e^{i\vec{k}\cdot\vec{d}_n}$  (2)

- Where vector  $\vec{d}_n$  is:



- Putting (2) in (1):

$$E\{\phi_0\}e^{i\vec{k}\cdot\vec{d}_n} = \sum_m [H_{nm}]\{\phi_0\}e^{i\vec{k}\cdot\vec{d}_m} \Rightarrow$$

$$E\{\phi_0\} = \sum_m [H_{nm}]e^{i\vec{k}\cdot(\vec{d}_m - \vec{d}_n)}\{\phi_0\}$$

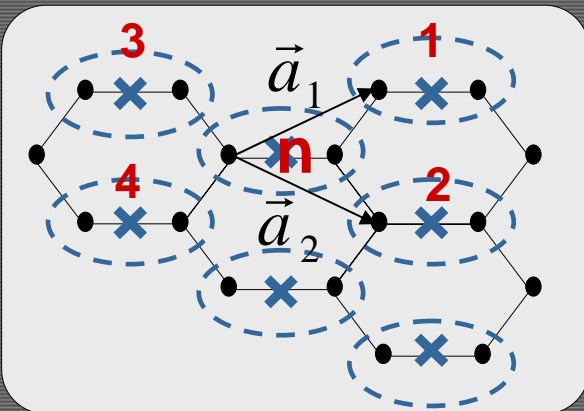
$$[h(\vec{k})]$$

# Graphene: $h(k)$

• Let's rewrite  $h(k)$ :

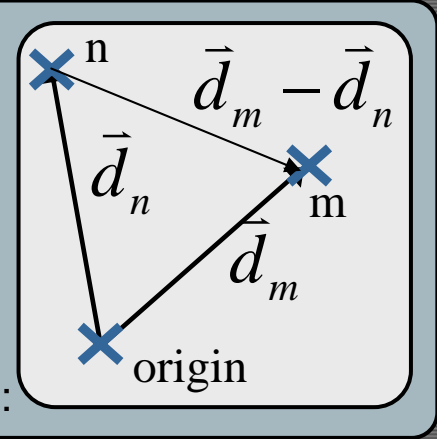
$$h(\vec{k}) = \sum_m [H_{nm}] e^{i\vec{k} \cdot (\vec{d}_m - \vec{d}_n)} \quad (1)$$

• To evaluate  $h(k)$ , we choose any unit cell  $n$  and then perform the summation over its nearest neighbors including  $n$  itself:



$m=1$	$m,1$	$m,2$
$n,1$	<b>0</b>	<b>0</b>
$n,2$	<b>t</b>	<b>0</b>

• To write the phase factor notice that  $d_m - d_n$  for  $m=2$  is actually  $a_1$ . Continuing like this, we can write all of the 4 terms that run through neighbors 1 to 4:



	$m=n$	$n,1$	$n,2$
<b>Phase factor is 1</b>	$n,1$	$\epsilon$	$t$
	$n,2$	$t$	$\epsilon$

$$\begin{aligned} & \begin{bmatrix} 0 & 0 \\ t & 0 \end{bmatrix} e^{i\vec{k} \cdot \vec{a}_1} + \begin{bmatrix} 0 & t \\ 0 & 0 \end{bmatrix} e^{i\vec{k} \cdot (-\vec{a}_2)} + \\ & \begin{bmatrix} 0 & t \\ 0 & 0 \end{bmatrix} e^{i\vec{k} \cdot (-\vec{a}_1)} + \begin{bmatrix} 0 & 0 \\ t & 0 \end{bmatrix} e^{i\vec{k} \cdot \vec{a}_2} \end{aligned}$$

# Graphene: h(k) / E-k relationship

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- All together we have the following 2by2 matrix for Graphene:

$$[h(\vec{k})] = \begin{bmatrix} \varepsilon & \Delta \\ \Delta^* & \varepsilon \end{bmatrix} \quad \Delta \equiv t \left( e^{-i\vec{k} \cdot \vec{a}_1} + e^{-i\vec{k} \cdot \vec{a}_2} + 1 \right)$$

eigenvalues :  $E = \varepsilon \pm \Delta$

## E-k Relationship

