## Fundamentals of Nanoelectronjics

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## Lecture 18: Bandstructure 3

 Ref. Chapter 5.1 \& 5.2
## 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.
$\left\{\varphi_{n}\right\}=\left\{\varphi_{0}\right\} e^{i k n a} \Rightarrow E\left\{\varphi_{0}\right\}=[h(k)]\left\{\varphi_{0}\right\}$
$E\left[\begin{array}{c}\phi_{1} \\ \phi_{2} \\ \vdots \\ \phi_{N}\end{array}\right]=\left[\begin{array}{c}\text { Every row looks } \\ \text { the same } \\ \vdots \\ \phi_{N}\end{array}\right]$


## - 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. $\qquad$ 2p

- 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: <br> Unit Cell / Basis Vectors

- 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 $\rightarrow$

$$
\vec{a}_{1} \equiv \hat{x} \frac{3 a_{0}}{2}+\hat{y} \frac{\sqrt{3} a_{0}}{2} \vec{a}_{2} \equiv \hat{x} \frac{3 a_{0}}{2}-\hat{y} \frac{\sqrt{3} a_{0}}{2}
$$



## Schrödinger Equation

- Schrödinger equation reads: $E\left\{\phi_{n}\right\}=\sum_{m}\left[H_{n m}\right]\left\{\phi_{m}\right\}$ (1)

- Equation 1 can be solved by: $\left\{\phi_{n}\right\}=\left\{\phi_{0}\right\} e^{i \vec{k} \bullet \bar{d}_{n}}$
- Where vector dn is:

- Putting (2) in (1):

$$
\begin{aligned}
& E\left\{\phi_{0}\right\} e^{i \vec{k} \cdot \bar{d}_{n}}=\sum_{m}\left[H_{n m}\right]\left\{\phi_{0}\right\} e^{i \bar{k} \cdot \bar{d}_{m}} \Rightarrow \\
& E\left\{\phi_{0}\right\}=\underbrace{\sum_{m}\left[H_{n m}\right] e^{i \bar{k} \cdot\left(\bar{d}_{m}-\bar{d}_{n}\right)}\left\{\phi_{0}\right\}} \\
& {[h(\bar{k})]}
\end{aligned}
$$

## Graphene: h(k)

- Let's rewrite $\mathrm{h}(\mathrm{k})$ :

$$
\begin{equation*}
[h(\vec{k})]=\sum_{m}\left[H_{n m}\right] e^{i \vec{k} \cdot\left(\vec{d}_{m}-\bar{d}_{n}\right)} \tag{1}
\end{equation*}
$$

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


| $m=1$ | $m, 1$ | $m, 2$ |
| :---: | :---: | :---: |
| $n, 1$ | 0 | 0 |
| $n, 2$ | $t$ | 0 |

- To write the phase factor notice that $d m-d n$ for $m=2$ is Actually a1.
Continuing like this, we can write all of the 4 terms that run through neighbors 1 to 4:


$$
\left[\begin{array}{ll}
0 & 0 \\
t & 0
\end{array}\right] e^{i \bar{k} \cdot \bar{a}_{1}}+\left[\begin{array}{ll}
0 & t \\
0 & 0
\end{array}\right] e^{i \bar{k} \bullet\left(-\bar{a}_{2}\right)}+
$$

$$
\left[\begin{array}{ll}
0 & t \\
0 & 0
\end{array}\right] e^{i \vec{\kappa} \cdot\left(-\bar{a}_{1}\right)}+\left[\begin{array}{ll}
0 & 0 \\
t & 0
\end{array}\right]^{i \vec{k} \cdot \bar{a}_{2}}
$$

- All together we have the following $2 b y 2$ matrix for Graphene:

$$
[h(\stackrel{\rightharpoonup}{k})]=\left[\begin{array}{cc}
\varepsilon & \Delta \\
\Delta^{*} & \varepsilon
\end{array}\right] \quad \Delta \equiv t\left(e^{-i \vec{k} \bullet \vec{a}_{1}}+e^{-i \vec{k} \bullet \vec{a}_{2}}+1\right)
$$

## E-k Relationship

eigenvalues : $\mathrm{E}=\varepsilon \pm \Delta$


