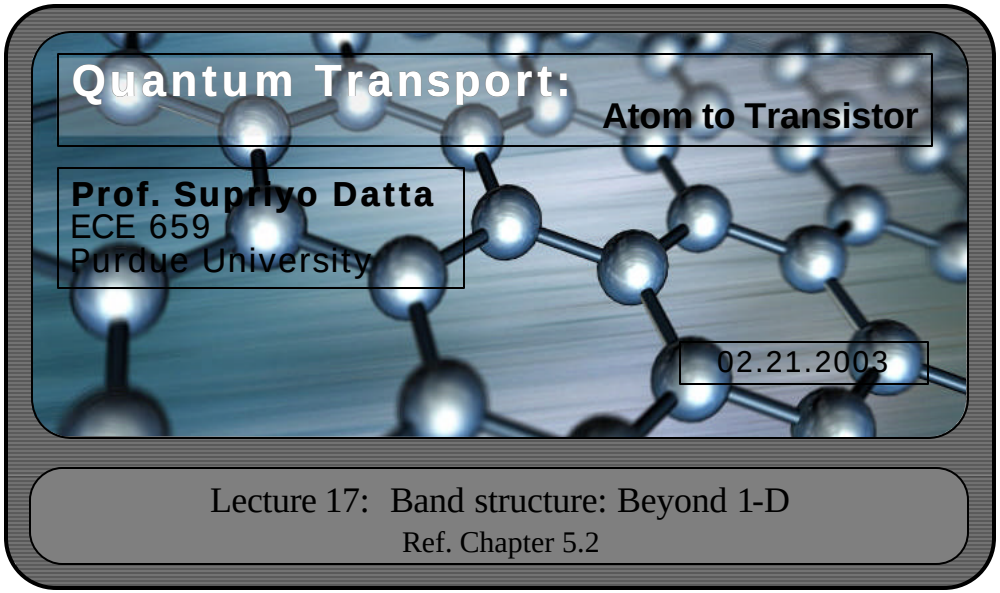


Lecture 17: Band structure: Beyond 1-D

Ref. Chapter 5.2

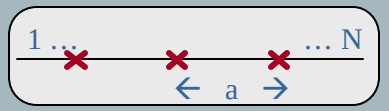
Network for Computational Nanotechnology

Bandstructure

00:00

• In determining bandstructure, we take advantage of the natural periodicity of a solid. This allows us to derive the eigenvalues and eigenfunctions analytically.

• Repeated unit cell



results in a periodic Hamiltonian

$$\begin{bmatrix} H_{11} & H_{12} & \\ H_{21} & H_{22} & \\ & & \ddots \end{bmatrix}$$

• Recall that all H_{nm} in $\begin{bmatrix} H_{11} & H_{12} & \\ H_{21} & H_{22} & \\ & & \ddots \end{bmatrix}$ are sub-matrices. The size of H_{nm} is directly dependent on the number of basis functions within a unit cell. Given b basis functions H_{nm} is of size bxb.

• As well, all basis functions

Ψ_{n_i} $n = (1, \cdots, N)$ $i = 1 \cdots b$ are grouped into $\{f_n\} = \begin{Bmatrix} \Psi_{n_1} \\ \Psi_{n_2} \\ \vdots \\ \Psi_{n_b} \end{Bmatrix}$

Multiple Basis Functions

03:30

• Finally, the Schrödinger Equation has the form

$$E\begin{Bmatrix} f_1 \\ f_2 \\ \vdots \\ f_N \end{Bmatrix} = \begin{bmatrix} H_{11} & H_{12} & & \\ H_{21} & H_{22} & & \\ & & \ddots & \end{bmatrix} \begin{Bmatrix} f_1 \\ f_2 \\ \vdots \\ f_N \end{Bmatrix}$$

and $$Ef_n = \sum_m H_{nm} f_m$$

As shown earlier, these equations may be solved via the ansatz

$$\{f_n\} = \{f_0\} e^{ikna}$$

• Such that,

$$E\{f_0\}e^{ikna} = \sum_m [H_{nm}] e^{ikma} \{f_0\}$$

or

$$E\{f_0\} = \sum_m [H_{nm}] e^{ik(ma-na)} \{f_0\}$$

• Let us define the matrix

$$[h(k)] = \sum_m [H_{nm}] e^{ik(m-n)a}$$

where the eigenvalue problem is now defined by

$$E\{f_0\} = [h(k)]\{f_0\}$$

(Remember: $\{f_0\}$ is a column vector and [h(k)] is a matrix of size bxb where b is the number of basis functions per unit cell)

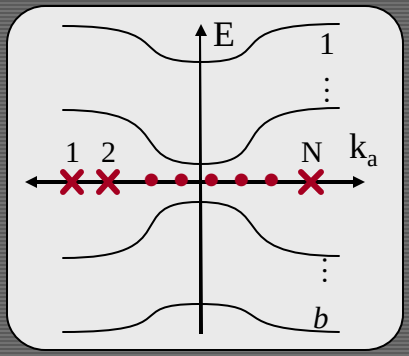
Beyond 1-Dimension

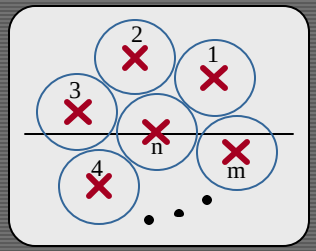
09:21

• Therefore N lattice points, N unit cells, and "b" basis functions will result in b•N eigenvalues

• It is relatively straight forward to go from 1-dimension to further dimensions. In the equation: $[h(k)] = \sum [H_{nm}] e^{ik(m-n)a}$ from the nth unit cell we sum over all "m" neighboring m cells

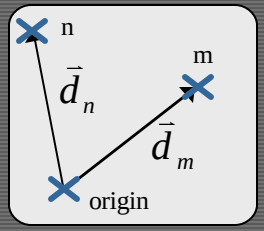
b•N eigenvalues





• Remember that ma and mb indicated position in1D case. What happens in general?

• To generalize, pick an origin and define the position of n and m by $\vec{d}_n$ and $\vec{d}_m$



Generalizing to Higher Dimensions

12:00

• Now, given $\vec{d}_n$ and $\vec{d}_m$ we claim that the ansatz

$$\{f_n\} = \{f_0\} e^{i\vec{k}\bullet\vec{d}_n}$$

Satisfies the Schrödinger equation. After substituting the above instead of eigenfunction, Sch. Eq. becomes:

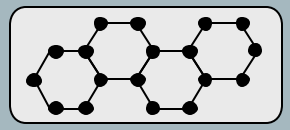
$$E\{f_0\} = [h(\vec{k})]\{f_0\}$$

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

which applicable to any number of dimensions!

(Don't forget: the **periodic** nature of a lattice makes this all possible. Visually, one can stand at any nth unit cell, sum over all m neighbors including itself, and the result will be the same)

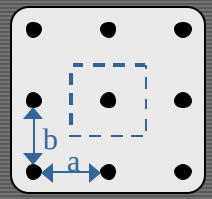
• We'll use this general procedure for Graphite:



Graphite is made up of carbon atoms bonded in a hexagonal 2D plane.

• But first, let's gain familiarity with two dimensions, and consider a simple rectangular lattice

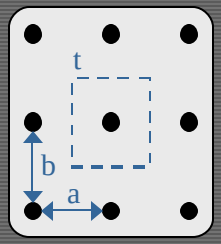
Rectangular Lattice

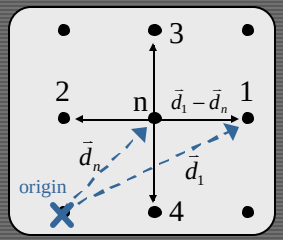


Rectangular Lattice

19:00

• Assume **one** basis orbital per unit cell. So $[h(\vec{k})]$ and $[H_{nm}]$ become **1** × **1**.





Want to evaluate: $h(\vec{k}) = \sum_m H_{nm} e^{i\vec{k}\bullet(\vec{d}_m - \vec{d}_n)}$

Evaluating Hnn results in E0 (self-energy) and evaluating Hnm results in a value that we call t. So we have 5 terms in our summation:

$$h(\vec{k}) = E_0 + \sum_{m=1}^{4} te^{i\vec{k}(\vec{d}_m - \vec{d}_n)}$$

• Take $\vec{k} = k_x\hat{x} + k_y\hat{y}$ and set the origin as shown…

• Exponents of "e" for the four terms become:

$$\vec{k}\bullet(d_1 - \vec{d}_n) = \vec{k}\bullet\hat{x}a = k_x a$$
$$\vec{k}\bullet(d_2 - \vec{d}_n) = \vec{k}\bullet(-\hat{x})a = -k_x a$$
$$\vec{k}\bullet(d_3 - \vec{d}_n) = \vec{k}\bullet\hat{y}b = k_y b$$
$$\vec{k}\bullet(d_4 - \vec{d}_n) = \vec{k}\bullet(-\hat{y})b = -k_y b$$

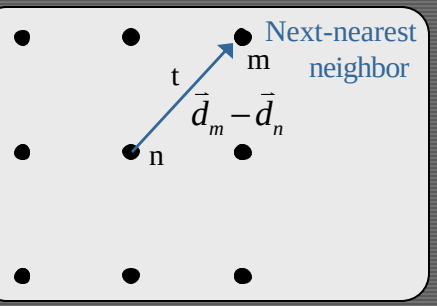
• Thus, after adding all of them we get:

$$h(\vec{k}) = E_0 + 2t(\cos k_x a + \cos k_y b)$$

Graphite

25:00

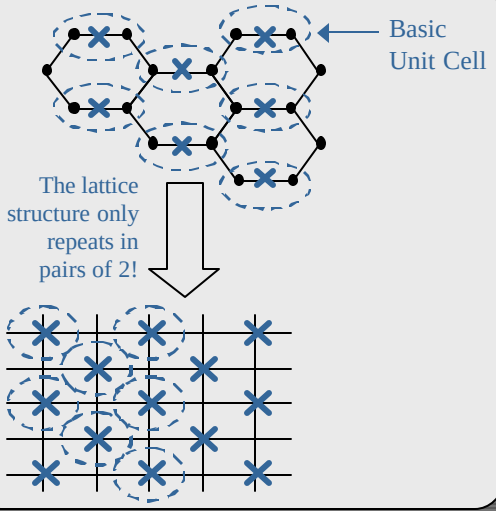
• In any lattice we can look beyond nearest neighbor interactions to next-nearest neighbor interactions. For example, in the rectangular lattice…



… here

$$\vec{k}\left(\vec{d}_m - \vec{d}_n\right) = \left(k_x\hat{x} + k_y\hat{y}\right) \bullet \left(a\hat{x} + b\hat{y}\right)$$

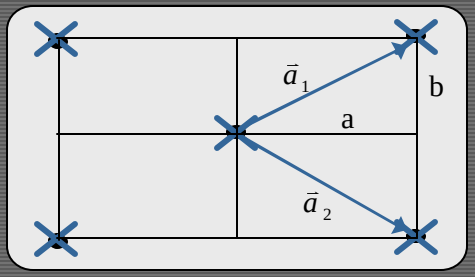
• Now let's move onto Graphite. First identify the basic unit cell



Graphite continued

28:11

• Next define two basis vectors, $\vec{a}_1$ and $\vec{a}_2$ such that the position of any cell in the lattice can be written as $\vec{R} = m\vec{a}_1 + n\vec{a}_2$ where m and n are integers

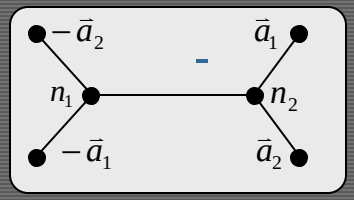


• In order to calculate $[h(\vec{k})]$ assume 1 basis function per carbon atom. This gives two basis functions per unit cell, $[h(\vec{k})]$ will be a 2x2 matrix

• Let t denote the overlap between 2 adjacent (nearest neighbor) carbon atoms. Denote n_1 and n_2 the atoms of the unit cell under consideration. Thus, H_{nn} is

$$\begin{array}{c} \\ n_1 \\ n_2 \end{array} \begin{array}{c} \begin{array}{cc} n_1 & n_2 \end{array} \\ \begin{bmatrix} E_0 & t \\ t & E_0 \end{bmatrix} \end{array}$$

• Overlap outside the unit cell will involve 4 nearest atoms. i.e …



Graphite continued

• Therefore, a total of 4 more matrices must be added (with phase factor!), they are:

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

• The final matrix looks like:

$$\left[h(\vec{k})\right] = \begin{bmatrix} E_0 & t\left(e^{-i\vec{k}\bullet\vec{a}_1} + e^{-i\vec{k}\bullet\vec{a}_2} + 1\right) \\ t\left(e^{i\vec{k}\bullet\vec{a}_1} + e^{i\vec{k}\bullet\vec{a}_2} + 1\right) & E_0 \end{bmatrix}$$

• If we let $\vec{a} = a\hat{x} + b\hat{y}$ and $\vec{a}_2 = a\hat{x} - b\hat{y}$ then $|h(\vec{k})|$ simplifies to:

$$\begin{bmatrix} E_0 & h_0^* \\ h_0 & E_0 \end{bmatrix}$$

where

$$h_0 = t\left(1 + e^{i(k_x a + k_y b)} + e^{i(k_x a - k_y b)}\right)$$

• To find the eigenvalues of $|h(\vec{k})|$ first recall the identity: given a matrix in the form

$$\begin{bmatrix} a & b^* \\ b & a \end{bmatrix}$$

then its eigenvalues are $a+|b|$ and $a-|b|$

Graphite Band Structure

46:00

• Thus the eigenvalues of $|h(\vec{k})|$ are $E_0 + |h_0|$ and $E_0 - |h_0|$

• What is $|h_0|$? Well, $h_0 = t\left(1 + 2e^{ik_x a}\cos k_y b\right)$

$$\therefore h_0 h_0^* = t^2\left(1 + 4\cos k_x a \cos k_y b + 4\cos^2 k_y b\right)$$

$$= |h_0|^2$$

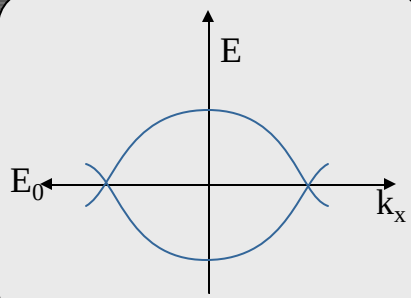
so,

$$|h_0| = t\sqrt{1 + 4\cos k_x a \cos k_y b + 4\cos^2 k_y b}$$

• More formally we say,

$$E(\vec{k}) = E_0 \pm |h_0|$$

• Note, a plot of graphite energy reveals the exact symmetry of the two eigenvalues



• Next lecture: Semiconductor Band Structure