

10/15/08

ECE 495N, Fall'08 ME118, MWF 1130A – 1220P

HW#5: Due Wednesday Oct.22 in class.

Problem 1: Use the principles of bandstructure to write down the eigenvalues and eigenvectors of the matrix (a, b are real numbers)

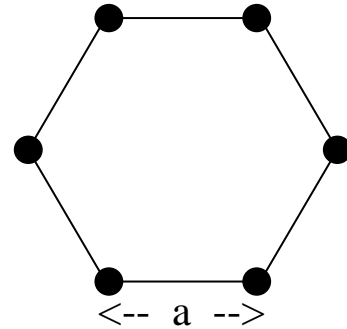
$$\begin{bmatrix} a & ib & -ib \\ -ib & a & ib \\ ib & -ib & a \end{bmatrix}$$

Problem 2: Benzene molecule consists of six carbon atoms arranged at the corners of a regular hexagon of side 'a'. Assume (1) one orbital per carbon atom as basis function ; (2) the overlap matrix [S] is a (6x6) identity matrix; and (3) the Hamiltonian matrix is given by

$$H_{n,n} = \varepsilon \quad (\text{site energy})$$

$$H_{n,m} = t \quad \text{if } n, m \text{ are neighboring atoms}$$

$$H_{n,m} = 0 \quad \text{if } n, m \text{ are NOT nearest neighbors}$$



What are the six energy eigenvalues in terms of 'ε' and 't' ?

What are the corresponding eigenvectors?

Problem 3: In class we have seen that an infinitely long linear 1-D lattice (lattice constant: a) with a Hamiltonian

$$H = \begin{bmatrix} \varepsilon & t & 0 & 0 & \dots \\ t & \varepsilon & t & 0 & \dots \\ 0 & t & \varepsilon & t & \dots \\ \dots & \dots & \dots & \dots & \dots \end{bmatrix}$$

has a dispersion relation $E(k) = \varepsilon + 2t \cos ka$ where $-\pi < ka < +\pi$ (1)

Do the same problem using a unit cell of **two** atoms (instead of one) and show that

$$E(k) = \varepsilon \pm 2t \cos ka \quad \text{where } -\pi/2 < ka < +\pi/2 \quad (2)$$

Are (1) and (2) equivalent? Explain.