10/9/09

ECE 495N, Fall'09 GRIS 280, MWF 1130A – 1220P

HW#4: Due Friday Oct.16 in class.

Problem 1: Consider the (2x2) matrix $A = \begin{bmatrix} \cos\theta & \sin\theta\, e^{-i\varphi} \\ \sin\theta\, e^{+i\varphi} & -\cos\theta \end{bmatrix}$

Show that the following

$$V_1 \equiv \begin{Bmatrix} \cos(\theta/2)\, e^{-i\varphi/2} \\ \sin(\theta/2)\, e^{+i\varphi/2} \end{Bmatrix} \text{ and } \quad V_2 \equiv \begin{Bmatrix} -\sin(\theta/2)\, e^{-i\varphi/2} \\ \cos(\theta/2)\, e^{+i\varphi/2} \end{Bmatrix}$$

are eigenvectors of [A]. What are the corresponding eigenvalues?
Are they orthogonal (that is, is $V_1^{+} V_2 = 0$) ?
Note: the superscript '+' denotes Hermitian conjugate.

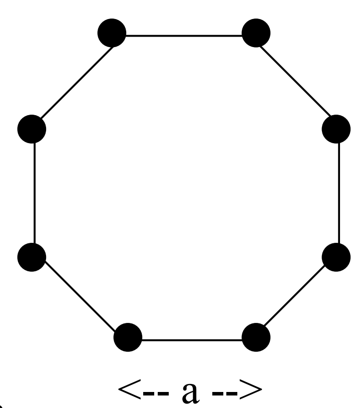
Problem 2: ***Use the principles of bandstructure*** to write down the eigenvalues and eigenvectors of the matrix $\begin{bmatrix} 0 & b & 0 & b \\ b & 0 & b & 0 \\ 0 & b & 0 & b \\ b & 0 & b & 0 \end{bmatrix}$. Please do not diagonalize directly.

Problem 3: A molecule (NOT a solid) consists of eight carbon atoms arranged at the corners of a regular octagon of side 'a'. Assume (1) one orbital per carbon atom as basis function and (2) the Hamiltonian matrix is given by

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

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

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



What are the eight energy eigenvalues in terms of 'ε' and 't' ?
Write down the corresponding eigenvectors.
Assume the basis functions to be orthogonal so that the overlap matrix [S] is a (8x8) identity matrix;

HW# 4 Solution

1)

$$A.V_1 = \begin{bmatrix} \cos\theta & \sin\theta\, e^{-i\varphi} \\ \sin\theta\, e^{i\varphi} & -\cos\theta \end{bmatrix} \begin{Bmatrix} \cos\frac{\theta}{2}\, e^{-i\varphi/2} \\ \sin\frac{\theta}{2}\, e^{i\varphi/2} \end{Bmatrix}$$

$$= \begin{Bmatrix} \left(\cos\theta\cos\frac{\theta}{2} + \sin\theta . \sin\frac{\theta}{2}\right) e^{-i\varphi/2} \\ \left(\sin\theta\cos\frac{\theta}{2} - \cos\theta\sin\frac{\theta}{2}\right) e^{i\varphi/2} \end{Bmatrix}$$

Notice: $\cos\theta\cos\frac{\theta}{2} + \sin\theta\sin\frac{\theta}{2} = \cos\left(\theta - \frac{\theta}{2}\right) = \cos\frac{\theta}{2}$.

$\sin\theta\cos\frac{\theta}{2} - \cos\theta\sin\frac{\theta}{2} = \sin\left(\theta - \frac{\theta}{2}\right) = \sin\frac{\theta}{2}$.

So $A.V_1 = \begin{Bmatrix} \cos\frac{\theta}{2}\, e^{-i\varphi/2} \\ \sin\frac{\theta}{2}\, e^{i\varphi/2} \end{Bmatrix} = V_1 \Rightarrow$ $\boxed{\text{eigenvalue is } 1}$

* $$AV_2 = \begin{bmatrix} \cos\theta & \sin\theta\, e^{-i\varphi} \\ \sin\theta & -\cos\theta \end{bmatrix} \begin{Bmatrix} -\sin\theta/2\; e^{-i\varphi/2} \\ \cos\frac{\theta}{2}\, e^{i\varphi/2} \end{Bmatrix}$$

$$= \begin{Bmatrix} \left(-\cos\theta\sin\frac{\theta}{2} + \sin\theta\cos\frac{\theta}{2}\right) e^{-i\varphi/2} \\ \left(-\sin\theta . \sin\frac{\theta}{2} - \cos\theta\cos\frac{\theta}{2}\right) e^{i\varphi/2} \end{Bmatrix} = \begin{Bmatrix} -\sin\frac{\theta}{2}\, e^{-i\varphi/2} \\ -\cos\frac{\theta}{2}\, e^{i\varphi/2} \end{Bmatrix}$$

$$= -V_2$$

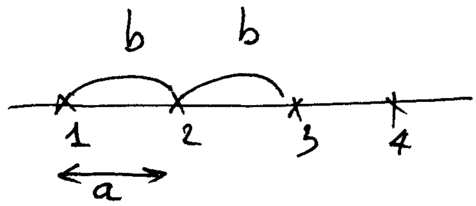
$\boxed{\Rightarrow \text{eigenvalue is } -1}$

Take $\quad V_1^{+} V_2 = \left[\cos\frac{\theta}{2}\, e^{+i\varphi/2} \quad \sin\frac{\theta}{2}\, e^{-i\varphi/2}\right] \begin{bmatrix} -\sin\frac{\theta}{2}\, e^{-i\varphi/2} \\ \cos\theta/_2\, e^{i\varphi/2} \end{bmatrix}$

$$= -\cos\frac{\theta}{2}\sin\frac{\theta}{2} + \sin\frac{\theta}{2}\cos\frac{\theta}{2} = 0$$

So V_1 and U_2 are orthogonal.

Problem 2.



$\psi_n = \psi_0 e^{iKx_n}$ $\qquad\qquad n = 1 \ldots 4$

And $\quad E\psi_n = \epsilon\psi_n + b\psi_{n+1} + b\psi_{n-1}$ $\quad$ here $\underline{\epsilon = 0}$

$\Rightarrow E\psi_0 e^{ikna} = b\psi_0 e^{ikna} \cdot e^{ika} + b e^{ikna} e^{-ika}$

$\Rightarrow \cancel{\psi_0}\; E = b e^{ika} + b e^{-ika} = b\left(e^{ika} + e^{-ika}\right)$

$$= 2b\cos ka.$$

So the eigenvalue of the matrix is

$$E = 2b\cos ka.$$

And since we have 4 sites: $\Rightarrow e^{iK4a} = 1$

$\Rightarrow K = \frac{2\pi}{4a}\cdot\nu \qquad \nu = 1, 2, 3, 4.$

$= \frac{\pi}{2a}\cdot\nu$

$$\Rightarrow \quad ka = \frac{\pi}{2}\cdot\nu$$

So $\quad ka = \frac{\pi}{2}, \ \pi, \ \frac{3\pi}{2}, \ 2\pi.$

Then

$$\boxed{\begin{aligned} E &= 2b\cos\frac{\pi}{2}, \ 2b\cos\pi, \ 2b\cos\frac{3\pi}{2}, \ 2b\cos 2\pi \\ &= 0, \ -2b, \ 0, \ 2b. \quad \text{4 eigenvalues} \end{aligned}}$$

* The eigenvectors:

$$\Psi = \begin{Bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{Bmatrix} = \psi_0 \begin{Bmatrix} e^{ika} \\ e^{2ika} \\ e^{3ika} \\ e^{4ika} \end{Bmatrix}$$

, we can choose $\psi_0 = 1$

Then $\quad \Psi_1 = \begin{Bmatrix} e^{i\pi/2} \\ e^{i\pi} \\ e^{i3\pi/2} \\ e^{2i\pi} \end{Bmatrix} = \begin{Bmatrix} i \\ -1 \\ -i \\ 1 \end{Bmatrix}$ when $ka = \frac{\pi}{2}$.

In general:

$$\Psi_\nu = \begin{Bmatrix} e^{i\nu\pi/2} \\ e^{i\nu\pi} \\ e^{i\nu\frac{3\pi}{2}} \\ e^{i\nu 2\pi} \end{Bmatrix}$$

$\nu = 1, 2, 3, 4$.

4 eigenvectors

Problem 3: (conti.)

So we have the matrix

$$E\Psi = \begin{bmatrix} \epsilon & t_0 & & & & & & t_0 \\ t_0 & \epsilon & t_0 & & & & & \\ & t_0 & \epsilon & t_0 & & & & \\ & & t_0 & \epsilon & t_0 & & & \\ & & & t_0 & \epsilon & t_0 & & \\ & & & & t_0 & \epsilon & t_0 & \\ & & & & & t_0 & \epsilon & t_0 \\ t_0 & & & & & & t_0 & \epsilon \end{bmatrix} \underbrace{\begin{Bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \\ \vdots \\ \psi_8 \end{Bmatrix}}_{\Psi}$$

8×8

$\boxed{\text{Here } t_0 \equiv t}$

$\Rightarrow$ the energy or eigenvalues are: (Similarly to problem 2)

$$E = \epsilon + 2t\cos ka.$$

And 8 sites $\rightarrow e^{ik8a} = 1 \Rightarrow ka = \frac{2\pi}{8} \cdot \nu$

$\nu = 1, 2 \ldots 8.$

$$\boxed{\text{So} \quad E_\nu = \epsilon + 2t\cos k_\nu a}$$

$k_\nu a = \frac{2\pi}{8} \cdot \nu = \frac{\pi}{4}\nu$

$\nu = 1, 2, \ldots 8$

The eigenvectors

$$\Psi_\nu = \begin{Bmatrix} \psi_1 \\ \vdots \\ \psi_8 \end{Bmatrix} = \begin{Bmatrix} e^{i\frac{\pi}{4}\nu} \\ e^{2i\frac{\pi}{4}\nu} \\ e^{3i\frac{\pi}{4}\nu} \\ \vdots \\ e^{8i\frac{\pi}{4}\nu} \end{Bmatrix}$$

$\nu = 1 \ldots 8$

(8 eigenvectors)