ECE 659, EXAM II

Friday, Feb.21, 2014, FNY B124, 330-420PM

NAME : SOLUTION

CLOSED BOOK

Useful relation $$\left[h(\vec{k})\right] = \sum_m [H_{nm}]\, e^{+i\vec{k}.(\vec{r}_m-\vec{r}_n)}$$

All five questions carry equal weight

Please show all work.
No credit for just writing down the answer, even if correct.

2.1. The spherical harmonics $Y_\ell^m(\theta,\phi)$ satisfy the differential equation:

$$\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\,\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)Y_\ell^m \quad = \quad -\,\ell(\ell+1)\,Y_l^m \tag{A}$$

(a) Is the following function one of the spherical harmonics

$$\frac{1}{4}\sqrt{\frac{5}{\pi}}\left(3\cos^2\theta-1\right)$$

(b) If so, what is the value of ℓ it corresponds to?

SOLUTION:

$$\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\,\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)(3\cos^2\theta-1)$$

$$= \quad -\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(6\sin^2\theta\,\cos\theta\right)$$

$$= \quad -\frac{6}{\sin\theta}\left(2\sin\theta\cos^2\theta-\sin^3\theta\right)$$

$$= \quad -6\left(2\cos^2\theta-\sin^2\theta\right)$$

$$= \quad -6\left(3\cos^2\theta-1\right)$$

Hence the given function satisfies the differential equation for the spherical harmonics with

$$\ell(\ell+1) = \quad 6 \quad \rightarrow \quad \ell = 2: \quad d-orbital$$

2.2. Use the principles of bandtructure to write down the eigenvalues of this 4x4 matrix

$$\begin{bmatrix} \varepsilon & t & 0 & t \\ t & \varepsilon & t & 0 \\ 0 & t & \varepsilon & t \\ t & 0 & t & \varepsilon \end{bmatrix}$$

and the corresponding eigenvectors.

SOLUTION:

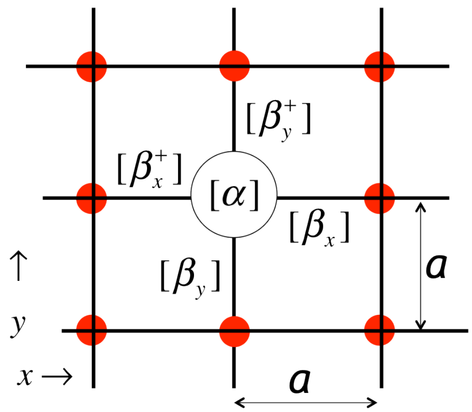
$$\varepsilon + 2t\cos[-2 \quad -1 \quad 0 \quad +1].*2\pi/4$$
$$= \varepsilon + 2t[-1 \quad 0 \quad 1 \quad 0]$$

$$\begin{Bmatrix} 1 \\ \exp(-i\pi) \\ 1 \\ \exp(-i\pi) \end{Bmatrix}, \quad \begin{Bmatrix} 1 \\ \exp(-i\pi/2) \\ \exp(-i\pi) \\ \exp(-i3\pi/2) \end{Bmatrix}, \quad \begin{Bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{Bmatrix}, \quad \begin{Bmatrix} 1 \\ \exp(i\pi/2) \\ \exp(i\pi) \\ \exp(i3\pi/2) \end{Bmatrix}$$

2.3. A 2-D square lattice has ***two*** basis functions per atom with (η is a real constant)

$$\alpha = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$$

$$\beta_x = \frac{\eta}{2a}\begin{bmatrix} 0 & +1 \\ -1 & 0 \end{bmatrix}, \quad \beta_y = \frac{\eta}{2a}\begin{bmatrix} 0 & -i \\ -i & 0 \end{bmatrix}$$



(a) Find the 2x2 matrix

$$\left[h(\vec{k})\right] = \sum_m [H_{nm}]\, e^{+i\vec{k}.(\vec{r}_m-\vec{r}_n)}$$

whose eigenvalues give the dispersion relation.

(b) What is the dispersion relation for $k_x a, k_y a \to 0$?

SOLUTION:

$$\left[h(\vec{k})\right] = [\alpha]+[\beta_x]\,e^{ik_xa}+[\beta_x]^+\,e^{-ik_xa}+\left[\beta_y\right]e^{-ik_ya}+\left[\beta_y\right]^+\,e^{ik_ya}$$

$$= \frac{\eta}{2a}\begin{bmatrix} 0 & +1 \\ -1 & 0 \end{bmatrix} e^{ik_xa} + \frac{\eta}{2a}\begin{bmatrix} 0 & -1 \\ +1 & 0 \end{bmatrix} e^{-ik_xa}$$

$$+\frac{\eta}{2a}\begin{bmatrix} 0 & -i \\ -i & 0 \end{bmatrix} e^{-ik_ya} + \frac{\eta}{2a}\begin{bmatrix} 0 & +i \\ +i & 0 \end{bmatrix} e^{ik_ya}$$

$$= \frac{i\eta}{a}\sin k_xa\begin{bmatrix} 0 & +1 \\ -1 & 0 \end{bmatrix} + \frac{\eta}{a}\sin k_ya\begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}$$

$$= \frac{\eta}{a}\begin{bmatrix} 0 & -\sin k_ya + i\sin k_xa \\ -\sin k_ya - i\sin k_xa & 0 \end{bmatrix}$$

(b)

$$E = \frac{\eta}{a}\sqrt{\sin^2 k_ya+\sin^2 k_xa} \;\to\; \eta\sqrt{k_x^2+k_y^2}\;, as\;\; k_{x,y}\,a \to 0$$

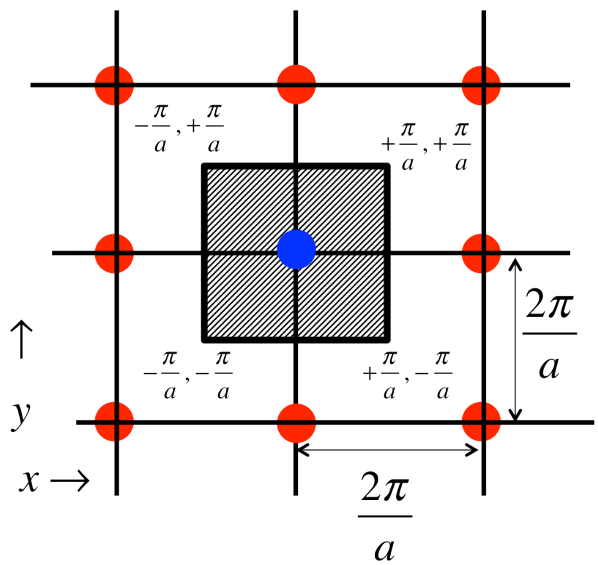
2.4. For the same 2-D square lattice with two basis functions per atom as in ***Prob.2.3***,
(a) What are the basis vectors for the reciprocal lattice?
(b) Sketch the reciprocal lattice and show the first Brillouin zone, ***clearly labeling its corners.***
(c) If the overall solid has dimensions (N atoms x N atoms) , how many allowed k-values are there in the first Brillouin zone and what is the total number of energy eigenvalues ?

SOLUTION:

(a) For the real space lattice $\vec{a}_1 = \hat{x}\, a \,, \vec{a}_2 = \hat{y}\, a$

For the reciprocal lattice $\vec{A}_1 = \hat{x}\,\dfrac{2\pi}{a} \,, \vec{A}_2 = \hat{y}\,\dfrac{2\pi}{a}$

(b)



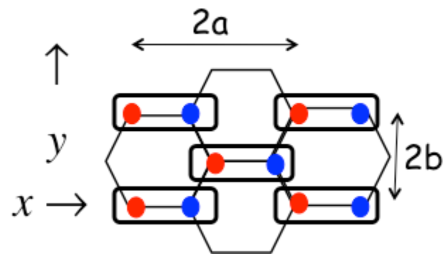
(c) N^2 allowed k-values, each with two energy eigenvalues, total of $2N^2$ energy eigenvalues.

2.5. A nearest neighbor tight-binding model for graphene with

$H_{n,n} = \varepsilon$

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

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



yields

$$h(k_x, k_y) = \begin{bmatrix} \varepsilon & h_0^* \\ h_0 & \varepsilon \end{bmatrix}, \qquad \text{where}$$

$$h_0 \equiv \quad t(1 + 2e^{ik_x a}\cos k_y b)$$

Suppose a graphene sheet is rolled up to form a nanotube with a circumferential vector along the x-direction: $\vec{c} = \hat{x}\, 2a\, m$, m being an integer. Consider the subband $\nu = 0$ with $\vec{k}.\vec{c} = 0$.

(a) What is its dispersion relation $E(k_y)$ over the range $-\frac{\pi}{b} < k_y < +\frac{\pi}{b}$?

(Please do not use Taylor expansion,
we would like the ***exact*** relation over the entire range)

(b) At what values of k_y are the eigenvalues equal to ε ?

(c) What is the group velocity $\frac{1}{\hbar}\frac{\partial E}{\partial k_y}$ at these points (where the eigenvalues equal ε)?

(d) Why are these points (“valleys”) so important in modeling current flow?

SOLUTION:

(a) $h_0(k_x = 0, k_y) = \quad t(1 + 2\cos k_y b)$

$E(k_y) = \quad \varepsilon \pm |h_0| = \quad \varepsilon \pm t(1 + 2\cos k_y b)$

(b) $1 + 2\cos k_y b = 0 \quad \rightarrow \quad \cos k_y b = -\frac{1}{2} \quad \rightarrow \quad k_y b = \pm 2\pi/3$

(c) $$\frac{\partial E}{\partial k_y} = \quad \mp\left[2bt\sin k_y b\right]_{k_y b = 2\pi/3} \quad = \quad \mp\sqrt{3}\,bt$$

$$\frac{\partial E}{\partial k_y} = \quad \mp\left[2bt\sin k_y b\right]_{k_y b = -2\pi/3} \quad = \quad \pm\sqrt{3}\,bt$$

(d) Because in intrinsic neutral graphene the Fermi level is located at ε and current flow is controlled by energy levels around the equilibrium Fermi level.