Useful relation

\[ h(\vec{k}) = \sum_{m} H_{nm} e^{i\vec{k} \cdot (\vec{r}_m - \vec{r}_n)} \]

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:

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

(A)

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

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

(b) If so, what is the value of $\ell$ it corresponds to?

**SOLUTION:**

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

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

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

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

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

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

$$
\ell (\ell + 1) = 6 \quad \rightarrow \quad \ell = 2 : \quad d \text{ – orbital}
$$
2.2. Use the principles of bandstructure 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:

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

\[
\begin{bmatrix}
1 \\
\exp(-i\pi) \\
1 \\
\exp(-i\pi) \\
\end{bmatrix}, \begin{bmatrix}
1 \\
\exp(-i\pi / 2) \\
1 \\
\exp(-i\pi) \\
\end{bmatrix}, \begin{bmatrix}
1 \\
\exp(i\pi / 2) \\
1 \\
\exp(i\pi) \\
\end{bmatrix}, \begin{bmatrix}
1 \\
\exp(i3\pi / 2) \\
1 \\
\exp(i3\pi / 2) \\
\end{bmatrix}
\]
2.3. A 2-D square lattice has two basis functions per atom with ($\eta$ 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

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

whose eigenvalues give the dispersion relation.

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

**SOLUTION:**

\[ \left[ h(\vec{k}) \right] = [\alpha] + [\beta_x] e^{i k_x a} + [\beta_x^+] e^{-i k_x a} + [\beta_y] e^{-i k_y a} + [\beta_y^+] e^{i k_y a} \]

\[ = \frac{\eta}{2a} \begin{bmatrix} 0 & +1 \\ -1 & 0 \end{bmatrix} e^{i k_x a} + \frac{\eta}{2a} \begin{bmatrix} 0 & -1 \\ +1 & 0 \end{bmatrix} e^{-i k_x a} \]

\[ + \frac{\eta}{2a} \begin{bmatrix} 0 & -i \\ -i & 0 \end{bmatrix} e^{-i k_y a} + \frac{\eta}{2a} \begin{bmatrix} 0 & +i \\ +i & 0 \end{bmatrix} e^{i k_y a} \]

\[ = \frac{i \eta}{a} \sin k_x a \begin{bmatrix} 0 & +1 \\ -1 & 0 \end{bmatrix} + \frac{\eta}{a} \sin k_y a \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix} \]

\[ = \frac{\eta}{a} \begin{bmatrix} 0 & -\sin k_y a + i \sin k_x a \\ -\sin k_y a - i \sin k_x a & 0 \end{bmatrix} \]

(b)

\[ E = \frac{\eta}{a} \sqrt{\sin^2 k_y a + \sin^2 k_x a} \to \eta \sqrt{k_x^2 + k_y^2}, \text{ as } k_{x,y} a \to 0 \]
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 \( \vec{A}_1 = \hat{x} \frac{2\pi}{a}, \vec{A}_2 = \hat{y} \frac{2\pi}{a} \)

(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
\[ H_{n,m} = \epsilon \]
if \( n, m \) are neighboring atoms
\[ H_{n,m} = t \]
if \( n, m \) are NOT nearest neighbors
yields
\[ h(k_x,k_y) = \begin{bmatrix} \epsilon & h_0^* \\ h_0 & \epsilon \end{bmatrix}, \quad \text{where} \]
\[ h_0 \equiv t(1 + 2e^{ik_ya} \cos k_yb) \]
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 \( \vec{k} \cdot \vec{c} = 0 \).

(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 \( \epsilon \) ?

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

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

**SOLUTION:**

(a) \[ h_0(k_x = 0,k_y) = t(1 + 2\cos k_yb) \]
\[ E(k_y) = \epsilon \pm h_0 = \epsilon \pm t(1 + 2\cos k_yb) \]

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

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

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