Assignment - 7:

Derivation of Graphene Hamiltonian (Bilayer)

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Q) From the Hamiltonian of the Bernally stacked Bilayer Graphene ie. two Graphene sheets oriented at 60° relative to each other. A & B sublattice atoms get coupled across the planes & $A_2 - B_1$ coupling exists.

$$H = \begin{array}{cccc} A_1 & B_1 & A_2 & B_2 \\ \hline \end{array}$$
$$\begin{bmatrix} 0 & \hbar v_F(k_x - ik_y) & 0 & 0 \\ \hbar v_F(k_x + ik_y) & 0 & \gamma_1 & 0 \\ 0 & \gamma_I & 0 & \hbar v_F(k_x - ik_y) \\ 0 & 0 & \hbar v_F(k_x + ik_y) & 0 \end{bmatrix}$$

Show that the hamiltonian can be written as:

$$H = \frac{\hbar^2}{2m^*} \begin{bmatrix} 0 & \pi_-^2 \\ \pi_+^2 & 0 \end{bmatrix}$$

See ArXiv: 1208.6953 V2

where

$$\pi_+ = k_x + i k_y - q(A_x + i A_y)$$

$$\pi_- = k_x - i k_y - q(A_x - i A_y)$$

Solution:

From the schrodinger equation:

$$H \psi = E \psi ,$$

$$
\begin{bmatrix}
0 & \hbar v_F(k_x - ik_y) & 0 & 0 \\
\hbar v_F(k_x + ik_y) & 0 & \gamma_1 & 0 \\
0 & \gamma_1 & 0 & \hbar v_F(k_x - ik_y) \\
0 & 0 & \hbar v_F(k_x + ik_y) & 0
\end{bmatrix}
\begin{bmatrix}
\psi_{A_1} \\ \psi_{B_1} \\ \psi_{A_2} \\ \psi_{B_2}
\end{bmatrix}
= E
\begin{bmatrix}
\psi_{A_1} \\ \psi_{B_1} \\ \psi_{A_2} \\ \psi_{B_2}
\end{bmatrix}
$$

Thus, the equations are in magnetic field

$k_x \to k_x - qA_x$, $k_y \to k_y - qA_y$:

① $(\hbar v_F \Pi_-)\psi_{B_1} = E\psi_{A_1}$

② $(\hbar v_F \Pi_+)\psi_{A_1} + \gamma_1 \psi_{A_2} = E\psi_{B_1}$

③ $\gamma_1 \psi_{B_1} + (\hbar v_F \pi_-)\psi_{B_2} = E\psi_{A_2}$

④ $(\hbar v_F \pi_+)\psi_{A_2} = E\psi_{B_2}$

Since we find energy near a dirac point, $E \ll \gamma_1$. Thus, in Eqn ② & ③, $E\psi_{B_1}$ and $E\psi_{A_2}$ terms can be neglected. Thus, we have

$$\boxed{(\hbar v_F \pi_+)\psi_{A_1} = -\gamma_1 \psi_{A_2}}, \quad \boxed{(\hbar v_F \pi_-)\psi_{B_2} = -\gamma_1 \psi_{B_1}} \rightarrow (5,6)$$

Substituting equations ⑤ & ⑥ in ④ & ① respectively,

$$\left.\begin{aligned} \hbar v_F \, \Pi_+ \left(\frac{\hbar v_F \Pi_+}{-\gamma_1} \right) \psi_{A_1} &= E \, \psi_{B_2} \\ \hbar v_F \, \Pi_- \left(\frac{\hbar v_F \Pi_-}{-\gamma_1} \right) \psi_{B_2} &= E \, \psi_{A_1} \end{aligned}\right\} (7, 8)$$

Simplifying Eqns 7 & 8 we get:

$$\left(\frac{\hbar v_F}{-\gamma_1} \right)^2 \left(\Pi_- \right)^2 \psi_{B_2} = E \, \psi_{A_1} \qquad \text{— I}$$

$$\left(\frac{\hbar v_F}{-\gamma_1} \right)^2 \left(\Pi_+ \right)^2 \psi_{A_1} = E \, \psi_{B_2} \qquad \text{— II}$$

Thus,

$$\left(\frac{\hbar v_F}{-\gamma_1} \right)^2 \begin{bmatrix} 0 & (\Pi_-)^2 \\ (\Pi_+)^2 & 0 \end{bmatrix} \begin{bmatrix} \psi_{A_1} \\ \psi_{B_2} \end{bmatrix} = E \begin{bmatrix} \psi_{A_1} \\ \psi_{B_2} \end{bmatrix}$$

where $\frac{(\hbar v_F)^2}{-\gamma_1}$ can be identified with $\frac{\hbar^2}{2m^*}$

or $m^* = \frac{-2\gamma_1}{v_F^2} = \left|\frac{2\gamma_1}{v_F^2}\right|$ (γ_1 is negative for bilayer coupling).

Therefore the hamiltonian can be written as:

$$\boxed{H = \frac{\hbar^2}{2m^*}\begin{bmatrix} 0 & (\pi_-)^2 \\ (\pi_+)^2 & 0 \end{bmatrix}}$$

$$
H_{bi} = \begin{array}{c} \begin{array}{cccc} A_1 & B_1 & A_2 & B_2 \end{array} \\ \begin{bmatrix} 0 & \hbar v_F(k_x - ik_y) & 0 & 0 \\ \hbar v_F(k_x + ik_y) & 0 & \gamma_1 & 0 \\ 0 & \gamma_1 & 0 & \hbar v_F(k_x - ik_y) \\ 0 & 0 & \hbar v_F(k_x + ik_y) & 0 \end{bmatrix} \end{array}
$$

interlayer coupling $\gamma_1 = 0.4\,eV$

First we transform our basis from $[A_1, B_1, A_2\, B_2]$ to $[A_1\, B_2\;\; A_2\, B_1]$

$$
H_{bi} = \begin{array}{c} \begin{array}{cccc} A_1 & B_2 & A_2 & B_1 \end{array} \\ \begin{bmatrix} 0 & 0 & 0 & \hbar v_F(k_x - ik_y) \\ 0 & 0 & \hbar v_F(k_x + ik_y) & 0 \\ 0 & \hbar v_F(k_x - ik_y) & 0 & \gamma_1 \\ \hbar v_F(k_x + ik_y) & 0 & \gamma_1 & 0 \end{bmatrix} \end{array} \Rightarrow
$$

Spinor $S_{bi} = \begin{pmatrix} |\psi_{A_1}\rangle \\ |\psi_{B_2}\rangle \\ |\psi_{A_2}\rangle \\ |\psi_{B_1}\rangle \end{pmatrix} = \begin{pmatrix} u_{A_1B_2} \\ u_{A_2B_1} \end{pmatrix}$

Generally, for 2×2 block diagonal Hamiltonians:

$$
\begin{bmatrix} h_\theta & u \\ u^\dagger & h_\chi \end{bmatrix} \begin{pmatrix} \theta \\ \chi \end{pmatrix} = E \begin{pmatrix} \theta \\ \chi \end{pmatrix}
$$

$$
\left.\begin{aligned} h_\theta \theta + u\chi &= E\theta \\ u^\dagger \theta + h_\chi \chi &= E\chi \end{aligned}\right\} \quad u\chi = (E - h_\theta)\theta, \quad u^\dagger\theta = (E - h_\chi)\chi
$$

$$
\chi = (E - h_\chi)^{-1} u^\dagger \theta.
$$

$$
H_{bi} S_{bi} = E S_{bi} \Rightarrow \begin{bmatrix} 0 & h_{mono} \\ h_{mono} & \gamma_1\sigma_x \end{bmatrix} \begin{pmatrix} u_{A_1B_2} \\ u_{A_2B_1} \end{pmatrix} = E \begin{pmatrix} u_{A_1B_2} \\ u_{A_2B_1} \end{pmatrix}
$$

$$
u_{A_2B_1} = (E - \gamma_1\sigma_x)^{-1} h_{mono} u_{A_1B_2}
$$

$$
h_{mono} u_{A_2B_1} = E u_{A_1B_2}
$$

$$
\boxed{(1-x)^{-1} = 1 + x + x^2 + \dots}
$$

$$
\Rightarrow u_{A_2B_1} = (E - \gamma_1\sigma_x)^{-1} h_{mono} u_{AB_2}
$$

$$
\Rightarrow h_{mono} (E - \gamma_1\sigma_x)^{-1} h_{mono} u_{AB_2} = E u_{A_1B_2}
$$

$$
\Rightarrow h_{mono} \frac{1}{-\gamma_1\sigma_x\left(1 - \frac{E}{\gamma_1\sigma_x}\right)} h_{mono} u_{A_1B_2} = E u_{A_1B_2}
$$

$$
\Rightarrow -h_{mono}(\gamma_1\sigma_x)^{-1}\left(1 + \frac{E}{\gamma_1\sigma_x} + \frac{E^2}{(\gamma_1\sigma_x)^2} + \dots\right) h_{mono} u_{A_1B_2} = E u_{A_1B_2}
$$

$$
\Rightarrow h_{effective,bi} = -\frac{h_{mono}\,\sigma_x\,h_{mono}}{\gamma_1} = \frac{-\hbar^2 v_F^2}{\gamma_1} \begin{pmatrix} 0 & (k_x - ik_y)^2 \\ (k_x + ik_y)^2 & 0 \end{pmatrix}
$$