# Thesis

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Từ Hamiltonian $H^{jj'}_{\mu\mu'}(\mathbf{k}) = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} E^{jj'}_{\mu\mu'}(\mathbf{R})$ trong đó

$$E^{jj'}_{\mu\mu'}(\mathbf{R}) = \langle \phi^{j}_{\mu}(\mathbf{r})| \hat{H} |\phi^{j'}_{\mu'}(\mathbf{r}-\mathbf{R})\rangle$$

$$|\phi^1_1\rangle = d_{z^2}, \quad |\phi^2_1\rangle = d_{xy}, \quad |\phi^2_2\rangle = d_{x^2-y^2}$$

$$\begin{aligned} H^{jj'}_{\mu\mu'}(\mathbf{k}) = &\sum_{\mu\mu'jj'} e^{i\mathbf{k}\cdot\mathbf{R_1}} E^{jj'}_{\mu\mu'}(\mathbf{R_1}) + \sum_{\mu\mu'jj'} e^{i\mathbf{k}\cdot\mathbf{R_2}} E^{jj'}_{\mu\mu'}(\mathbf{R_2}) + \sum_{\mu\mu'jj'} e^{i\mathbf{k}\cdot\mathbf{R_3}} E^{jj'}_{\mu\mu'}(\mathbf{R_3}) \\ &+ \sum_{\mu\mu'jj'} e^{i\mathbf{k}\cdot\mathbf{R_4}} E^{jj'}_{\mu\mu'}(\mathbf{R_4}) + \sum_{\mu\mu'jj'} e^{i\mathbf{k}\cdot\mathbf{R_5}} E^{jj'}_{\mu\mu'}(\mathbf{R_5}) + \sum_{\mu\mu'jj'} e^{i\mathbf{k}\cdot\mathbf{R_6}} E^{jj'}_{\mu\mu'}(\mathbf{R_6}) \end{aligned}$$

$$H^{NN} = \begin{pmatrix} h_0 & h_1 & h_2 \\ h_1^* & h_{11} & h_{12} \\ h_2^* & h_{12}^* & h_{22} \end{pmatrix}$$

$$\begin{aligned} h_0 &= \sum_R e^{i\mathbf{k}\cdot\mathbf{R}} \langle \phi^1_1(\mathbf{r})| H |\phi^1_1(\mathbf{r}-\mathbf{R})\rangle; \quad & h_1 &= \sum_R e^{i\mathbf{k}\cdot\mathbf{R}} \langle \phi^1_1(\mathbf{r})| H |\phi^2_1(\mathbf{r}-\mathbf{R})\rangle \\ h_2 &= \sum_R e^{i\mathbf{k}\cdot\mathbf{R}} \langle \phi^1_1(\mathbf{r})| H |\phi^2_2(\mathbf{r}-\mathbf{R})\rangle; \quad & h_{11} &= \sum_R e^{i\mathbf{k}\cdot\mathbf{R}} \langle \phi^2_1(\mathbf{r})| H |\phi^2_1(\mathbf{r}-\mathbf{R})\rangle \\ h_{12} &= \sum_R e^{i\mathbf{k}\cdot\mathbf{R}} \langle \phi^2_1(\mathbf{r})| H |\phi^2_2(\mathbf{r}-\mathbf{R})\rangle; \quad & h_{22} &= \sum_R e^{i\mathbf{k}\cdot\mathbf{R}} \langle \phi^2_2(\mathbf{r})| H |\phi^2_2(\mathbf{r}-\mathbf{R})\rangle \end{aligned}$$

Lại có $E^{jj'}(\hat{g_n}\mathbf{R}) = D^j(\hat{g_n})E^{jj'}(\mathbf{R})\left[D^j(\hat{g_n})\right]^\dagger$

trong đó $\hat{g_n} = \{E, C_3, C_3^2, \sigma_\nu, \sigma'_\nu, \sigma''_\nu\}$

trong đó $D^1(\hat{g_n}) = 1$

$$D^2(E) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$D^2(\hat{C}_3) = \begin{pmatrix} cos\phi & -sin\phi \\ sin\phi & cos\phi \end{pmatrix} = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$$

$$D^2(\hat{C_3}^2) = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$$

Để tìm được $D^2(\sigma_\nu)$ ta cố định $\triangle$ ABC : A$(\dfrac{1}{2},\dfrac{\sqrt{3}}{2})$,B(1,0), C(0,0).

Khi đổi chỗ A $\leftrightarrow$ B, ta được ma trận:

$$\begin{pmatrix}1\\0\end{pmatrix} = D^2(\sigma_\nu)\begin{pmatrix}\frac{1}{2}\\ \frac{\sqrt{3}}{2}\end{pmatrix} \Rightarrow D^2(\sigma_\nu) = \begin{pmatrix}\frac{1}{2} & \frac{\sqrt{3}}{2}\\ \frac{\sqrt{3}}{2} & -\frac{1}{2}\end{pmatrix}$$

Ta có $\overrightarrow{R_5} = \sigma'_\nu \overrightarrow{R_4}$ mà $C_3^2 \overrightarrow{R_5} = \overrightarrow{R_1} \Rightarrow C_3^2 \sigma'_\nu \overrightarrow{R_4} = \overrightarrow{R_1}$

$$\Rightarrow \begin{pmatrix}-\frac{1}{2} & \frac{\sqrt{3}}{2}\\ -\frac{\sqrt{3}}{2} & -\frac{1}{2}\end{pmatrix}\begin{pmatrix}a & b\\ c & d\end{pmatrix}\begin{pmatrix}-1\\0\end{pmatrix} = \begin{pmatrix}1\\0\end{pmatrix}$$

$$\Rightarrow D^2\left(\sigma'_\nu\right) = \begin{pmatrix}\frac{1}{2} & -\frac{\sqrt{3}}{2}\\ -\frac{\sqrt{3}}{2} & -\frac{1}{2}\end{pmatrix}$$

Tương tự ta tính cho

$$D^2\left(\sigma''_\nu\right) = \begin{pmatrix}-1 & 0\\ 0 & 1\end{pmatrix}$$

Toán tử $C_3$ đánh lên $\mathbf{R}_1$ ta được $\rightarrow \mathbf{R}_5$ (dưới dạng ma trận)

Toán tử $C_3^2$ đánh lên $\mathbf{R}_1$ ta được $\rightarrow \mathbf{R}_3$ (dưới dạng ma trận)

Toán tử $\sigma_\nu$ đánh lên $\mathbf{R}_1$ ta được $\rightarrow \mathbf{R}_6$ (dưới dạng ma trận)

Toán tử $\sigma'_\nu$ đánh lên $\mathbf{R}_1$ ta được $\rightarrow \mathbf{R}_2$ (dưới dạng ma trận)

Toán tử $\sigma''_\nu$ đánh lên $\mathbf{R}_1$ ta được $\rightarrow \mathbf{R}_4$ (dưới dạng ma trận)

Kiểm tra điều trên:

$$D^2\left(C_3^2\right) R_1 = \begin{pmatrix}-\frac{1}{2} & \frac{\sqrt{3}}{2}\\ -\frac{\sqrt{3}}{2} & -\frac{1}{2}\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}-\frac{1}{2}\\ -\frac{\sqrt{3}}{2}\end{pmatrix} = \mathbf{R}_3$$

$$D^2\left(\sigma'_\nu\right) R_1 = \begin{pmatrix}\frac{1}{2} & -\frac{\sqrt{3}}{2}\\ -\frac{\sqrt{3}}{2} & -\frac{1}{2}\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}\frac{1}{2}\\ -\frac{\sqrt{3}}{2}\end{pmatrix} = \mathbf{R}_2$$

$*$ **h0**

$$\begin{aligned}
h_0 &= \sum_{\mathbf{R}\neq 0} e^{i\mathbf{k}\cdot\mathbf{R}} \left\langle \phi_1^1(\mathbf{r})\right| H \left|\phi_1^1(\mathbf{r}-\mathbf{R})\right\rangle + \left\langle \phi_1^1(\mathbf{r})\right| H \left|\phi_1^1(\mathbf{r})\right\rangle\\
&= e^{i\mathbf{k}\cdot\mathbf{R_1}} \left\langle \phi_1^1(\mathbf{r})\right| H \left|\phi_1^1(\mathbf{r}-\mathbf{R_1})\right\rangle + e^{i\mathbf{k}\cdot\mathbf{R_4}} \left\langle \phi_1^1(\mathbf{r})\right| H \left|\phi_1^1(\mathbf{r}-\mathbf{R_4})\right\rangle\\
&+ e^{i\mathbf{k}\cdot\mathbf{R_2}} \left\langle \phi_1^1(\mathbf{r})\right| H \left|\phi_1^1(\mathbf{r}-\mathbf{R_2})\right\rangle + e^{i\mathbf{k}\cdot\mathbf{R_5}} \left\langle \phi_1^1(\mathbf{r})\right| H \left|\phi_1^1(\mathbf{r}-\mathbf{R_5})\right\rangle\\
&+ e^{i\mathbf{k}\cdot\mathbf{R_3}} \left\langle \phi_1^1(\mathbf{r})\right| H \left|\phi_1^1(\mathbf{r}-\mathbf{R_3})\right\rangle + e^{i\mathbf{k}\cdot\mathbf{R_6}} \left\langle \phi_1^1(\mathbf{r})\right| H \left|\phi_1^1(\mathbf{r}-\mathbf{R_6})\right\rangle + \epsilon_1\\
&= e^{ik_x a} E_{11}^{11}(\mathbf{R_1}) + e^{-ik_x a} E_{11}^{11}(\mathbf{R_4}) + e^{i\left(k_x \frac{a}{2} - k_y \frac{a\sqrt{3}}{2}\right)} E_{11}^{11}(\mathbf{R_2}) + e^{-i\left(k_x \frac{a}{2} - k_y \frac{a\sqrt{3}}{2}\right)} E_{11}^{11}(\mathbf{R_5})\\
&+ e^{-i\left(k_x \frac{a}{2} + k_y \frac{a\sqrt{3}}{2}\right)} E_{11}^{11}(\mathbf{R_3}) + e^{i\left(k_x \frac{a}{2} + k_y \frac{a\sqrt{3}}{2}\right)} E_{11}^{11}(\mathbf{R_6}) + \epsilon_1\\
&= 2E_{11}^{11}(\mathbf{R_1})\left(cos2\alpha + 2cos\alpha\, cos\beta\right) + \epsilon_1
\end{aligned}$$

$*$ **h1**

$$
\begin{aligned}
h_1 &= \sum_{\mathbf{R}\neq 0} e^{i\mathbf{k}\cdot\mathbf{R}} \left\langle \phi_1^1\left(\mathbf{r}\right)\right| H \left|\phi_1^2\left(\mathbf{r}-\mathbf{R}\right)\right\rangle \\
&= e^{ik_x a} E_{11}^{12}\left(\mathbf{R_1}\right) + e^{-ik_x a} E_{11}^{12}\left(\mathbf{R_4}\right) + e^{i\left(k_x \frac{a}{2} - k_y \frac{a\sqrt{3}}{2}\right)} E_{11}^{12}\left(\mathbf{R_2}\right) + e^{-i\left(k_x \frac{a}{2} - k_y \frac{a\sqrt{3}}{2}\right)} E_{11}^{12}\left(\mathbf{R_5}\right) \\
&+ e^{-i\left(k_x \frac{a}{2} + k_y \frac{a\sqrt{3}}{2}\right)} E_{11}^{12}\left(\mathbf{R_3}\right) + e^{i\left(k_x \frac{a}{2} + k_y \frac{a\sqrt{3}}{2}\right)} E_{11}^{12}\left(\mathbf{R_6}\right)
\end{aligned}
$$

trong đó

$$
\begin{aligned}
E^{12}(\mathbf{R_2}) &= E^{12}(\sigma_\nu' \mathbf{R_1}) = D^1(\sigma_\nu') E^{12}(\mathbf{R_1}) \left[D^2(\sigma_\nu')\right]^\dagger \\
&= \begin{pmatrix} 1 \end{pmatrix} \begin{pmatrix} E_{11}^{12}(\mathbf{R_1}) & E_{12}^{12}(\mathbf{R_1}) \end{pmatrix} \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \\
&= \begin{pmatrix} \dfrac{E_{11}^{12}(\mathbf{R_1}) - \sqrt{3} E_{12}^{12}(\mathbf{R_1})}{2} & \dfrac{-E_{11}^{12}(\mathbf{R_1})\sqrt{3} - E_{12}^{12}(\mathbf{R_1})}{2} \end{pmatrix}
\end{aligned}
$$

$$
\Rightarrow E_{11}^{12}(\mathbf{R_2}) = \frac{E_{11}^{12}(\mathbf{R_1}) - \sqrt{3} E_{12}^{12}(\mathbf{R_1})}{2}
$$

Tương tự ta có cho:

$$
\begin{aligned}
E_{11}^{12}(\mathbf{R_3}) &= \frac{-E_{11}^{12}(\mathbf{R_1}) + \sqrt{3} E_{12}^{12}(\mathbf{R_1})}{2} \quad ; E_{11}^{12}(\mathbf{R_4}) = -E_{11}^{12}(\mathbf{R_1}) \\
E_{11}^{12}(\mathbf{R_5}) &= \frac{-E_{11}^{12}(\mathbf{R_1}) - \sqrt{3} E_{12}^{12}(\mathbf{R_1})}{2} \quad ; E_{11}^{12}(\mathbf{R_6}) = \frac{E_{11}^{12}(\mathbf{R_1}) + \sqrt{3} E_{12}^{12}(\mathbf{R_1})}{2}
\end{aligned}
$$

$$
\begin{aligned}
h_1 &= e^{i2\alpha} E_{11}^{12}(\mathbf{R_1}) - e^{i2\alpha} E_{11}^{12}(\mathbf{R_1}) \\
&+ e^{i(\alpha-\beta)} \frac{E_{11}^{12}(\mathbf{R_1}) - \sqrt{3} E_{12}^{12}(\mathbf{R_1})}{2} + e^{-i(\alpha+\beta)} \frac{-E_{11}^{12}(\mathbf{R_1}) + \sqrt{3} E_{12}^{12}(\mathbf{R_1})}{2} \\
&+ e^{i(-\alpha+\beta)} \frac{-E_{11}^{12}(\mathbf{R_1}) - \sqrt{3} E_{12}^{12}(\mathbf{R_1})}{2} + e^{i(\alpha+\beta)} \frac{E_{11}^{12}(\mathbf{R_1}) + \sqrt{3} E_{12}^{12}(\mathbf{R_1})}{2} \\
&= 2isin2\alpha E_{11}^{12}(\mathbf{R_1}) + 2i \frac{E_{11}^{12}(\mathbf{R_1})}{2} sin(\alpha-\beta) - 2\frac{E_{12}^{12}(\mathbf{R_1}\sqrt{3})}{2} cos(\alpha-\beta) \\
&+ 2i \frac{E_{11}^{12}(\mathbf{R_1})}{2} sin(\alpha+\beta) + 2\frac{E_{12}^{12}(\mathbf{R_1}\sqrt{3})}{2} cos(\alpha+\beta) \\
&= -2\sqrt{3} t_2 sin\alpha\ sin\beta + 2it_1(sin2\alpha + sin\alpha\ \cos\beta)
\end{aligned}
$$

Đặt

$$
t_0 = E_{11}^{11}(\mathbf{R_1}); \quad t_1 = E_{11}^{12}(\mathbf{R_1}); \quad t_2 = E_{12}^{12}(\mathbf{R_1});
$$

$$
t_{11} = E_{11}^{22}(\mathbf{R_1}); \quad t_{12} = E_{12}^{22}(\mathbf{R_1}); \quad t_{21} = E_{21}^{22}(\mathbf{R_1}); \quad t_{22} = E_{22}^{22}(\mathbf{R_1});
$$

$*$ **h22**

$$
\begin{aligned}
h_{22} &= \sum_{R} e^{i\mathbf{k}\cdot\mathbf{R}} E^{22}_{22}(\mathbf{R}) \\
&= e^{i\mathbf{k}\cdot\mathbf{R_1}} E^{22}_{22}(\mathbf{R_1}) + e^{i\mathbf{k}\cdot\mathbf{R_2}} E^{22}_{22}(\mathbf{R_2}) + e^{i\mathbf{k}\cdot\mathbf{R_3}} E^{22}_{22}(\mathbf{R_3}) \\
&+ e^{i\mathbf{k}\cdot\mathbf{R_4}} E^{22}_{22}(\mathbf{R_4}) + e^{i\mathbf{k}\cdot\mathbf{R_5}} E^{22}_{22}(\mathbf{R_5}) + e^{i\mathbf{k}\cdot\mathbf{R_6}} E^{22}_{22}(\mathbf{R_6}) + E^{22}_{22}(\mathbf{0})
\end{aligned}
$$

$$
\begin{aligned}
E^{22}(\mathbf{R_2}) &= E^{22}(\sigma'_\nu \mathbf{R_1}) \\
&= D^2(\sigma'_\nu) E^{22}(\mathbf{R_1}) \left[D^2(\sigma'_\nu)\right]^\dagger
\end{aligned}
$$

$$
= \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} E^{22}_{11}(\mathbf{R_1}) & E^{22}_{12}(\mathbf{R_1}) \\ E^{22}_{21}(\mathbf{R_1}) & E^{22}_{22}(\mathbf{R_1}) \end{pmatrix} \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}
$$

$$
= \begin{pmatrix} \frac{t_{11} - t_{12}\sqrt{3} - t_{21}\sqrt{3} + 3t_{22}}{4} & \frac{-t_{11}\sqrt{3} - t_{12} + 3t_{21} + \sqrt{3}t_{22}}{4} \\ \frac{-t_{11}\sqrt{3} + 3t_{12} - t_{21} + \sqrt{3}t_{22}}{4} & \frac{3t_{11} + t_{12}\sqrt{3} + c\sqrt{3} + t_{22}}{4} \end{pmatrix}
$$

$$\Rightarrow E^{22}_{22}(\mathbf{R_2}) = \frac{3t_{11} + t_{12}\sqrt{3} + c\sqrt{3} + t_{22}}{4}$$

Tương tự ta có cho:

$$
\begin{aligned}
E^{22}_{22}(\mathbf{R_3}) &= \frac{3t_{11} - t_{12}\sqrt{3} - c\sqrt{3} + t_{22}}{4} \\
E^{22}_{22}(\mathbf{R_4}) &= t_{22} \\
E^{22}_{22}(\mathbf{R_5}) &= \frac{3t_{11} + t_{12}\sqrt{3} + c\sqrt{3} + t_{22}}{4} \\
E^{22}_{22}(\mathbf{R_6}) &= \frac{3t_{11} - t_{12}\sqrt{3} - c\sqrt{3} + t_{22}}{4}
\end{aligned}
$$

Ta được:

$$
\begin{aligned}
h_{22} &= e^{i2\alpha}t_{22} + e^{-i2\alpha}t_{22}\\
&+ e^{i(\alpha-\beta)}\left(\frac{3t_{11}+t_{12}\sqrt{3}+c\sqrt{3}+t_{22}}{4}\right) + e^{-i(\alpha+\beta)}\left(\frac{3t_{11}-t_{12}\sqrt{3}-c\sqrt{3}+t_{22}}{4}\right)\\
&+ e^{i(-\alpha+\beta)}\left(\frac{3t_{11}+t_{12}\sqrt{3}+c\sqrt{3}+t_{22}}{4}\right) + e^{i(\alpha+\beta)}\left(\frac{3t_{11}-t_{12}\sqrt{3}-c\sqrt{3}+t_{22}}{4}\right)\\
&= 2cos(2\alpha)t_{22} + \frac{1}{4}3t_{11}\left(e^{i\alpha}+e^{-i\alpha}\right)\left(e^{-i\beta}+e^{i\beta}\right) + \frac{1}{4}t_{22}\left(e^{i\alpha}+e^{-i\alpha}\right)\left(e^{-i\beta}+e^{i\beta}\right)\\
&+ c\sqrt{3}(e^{i(\alpha-\beta)} - e^{i(-\alpha+\beta)} + e^{i(-\alpha+\beta)} - e^{i(\alpha+\beta)})\\
&+ t_{12}\sqrt{3}(e^{i(\alpha-\beta)} - e^{i(-\alpha+\beta)} + e^{i(-\alpha+\beta)} - e^{i(\alpha+\beta)})\\
&= 2cos(2\alpha)t_{22} + (3t_{11}+t_{22})cos\alpha\, cos\beta
\end{aligned}
$$

Sử dụng tính Hermite của Hamiltonian $h_{22}$ là số thực, nên $t_{12} = -t_{21}$

***h11**

$$
\begin{aligned}
H_{11}^{22} &= \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}}E_{11}^{22}(\mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R_1}}E_{11}^{22}(\mathbf{R_1}) + e^{i\mathbf{k}\cdot\mathbf{R_2}}E_{11}^{22}(\mathbf{R_2}) + e^{i\mathbf{k}\cdot\mathbf{R_3}}E_{11}^{22}(\mathbf{R_3})\\
&+ e^{i\mathbf{k}\cdot\mathbf{R_4}}E_{11}^{22}(\mathbf{R_4}) + e^{i\mathbf{k}\cdot\mathbf{R_5}}E_{11}^{22}(\mathbf{R_5}) + e^{i\mathbf{k}\cdot\mathbf{R_6}}E_{11}^{22}(\mathbf{R_6}) + E_{11}^{22}(\mathbf{0})\\
&= e^{ik_xa}E_{11}^{22}(\mathbf{R_1}) + e^{i\left(k_x\frac{a}{2}-k_y\frac{a\sqrt{3}}{2}\right)}E_{11}^{22}(\mathbf{R_2}) + e^{i\left(-k_x\frac{a}{2}-k_y\frac{a\sqrt{3}}{2}\right)}E_{11}^{22}(\mathbf{R_3})\\
&+ e^{-ik_xa}E_{11}^{22}(\mathbf{R_4}) + e^{i\left(-k_x\frac{a}{2}+k_y\frac{a\sqrt{3}}{2}\right)}E_{11}^{22}(\mathbf{R_5}) + e^{i\left(k_x\frac{a}{2}+k_y\frac{a\sqrt{3}}{2}\right)}E_{11}^{22}(\mathbf{R_6}) + \epsilon_2\\
&= e^{2i\alpha}t_{11} + e^{i(\alpha-\beta)}\frac{t_{11}-\sqrt{3}t_{12}-\sqrt{3}t_{21}+3t_{22}}{4}\\
&+ e^{i(-\alpha-\beta)}\frac{t_{11}-\sqrt{3}t_{12}-\sqrt{3}t_{21}+3t_{22}}{4} + e^{-2i\alpha}t_{11}\\
&+ e^{i(-\alpha+\beta)}\frac{t_{11}+\sqrt{3}t_{12}+\sqrt{3}t_{21}+3t_{22}}{4} + e^{i(\alpha+\beta)}\frac{t_{11}+\sqrt{3}t_{12}+\sqrt{3}t_{21}+3t_{22}}{4} + \epsilon_2\\
&= 2t_{11}cos(2\alpha) + (t_{11}+3t_{22})\,cos(\alpha)cos(\beta) + \epsilon_2
\end{aligned}
$$

**Lưu ý ở đây đã sử dụng tính chất Hermite của $h_{11}$ phải là số thực**

$\Rightarrow t_{12} = -t_{21}$

$$E^{22}(\mathbf{R_2}) = E^{22}(\sigma_\nu^{'}\mathbf{R_1}) = D^2(\sigma_\nu^{'})E^{22}(\mathbf{R_1})[D^2(\sigma_\nu^{'})]^\dagger$$

$$= \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \text{Trong đó} \begin{pmatrix} a = t_{11} \\ b = t_{12} \\ c = t_{21} \\ d = t_{22} \end{pmatrix}$$

$$\Rightarrow E_{11}^{22}(\mathbf{R_2}) = \frac{a - \sqrt{3}b - \sqrt{3}c + 3d}{4}$$

Tương tự ta tìm được:

$$E_{11}^{22}(\mathbf{R_3}) = \frac{a - \sqrt{3}b - \sqrt{3}c + 3d}{4}$$

$$E_{11}^{22}(\mathbf{R_4}) = a$$

$$E_{11}^{22}(\mathbf{R_5}) = \frac{a + \sqrt{3}b + \sqrt{3}c + 3d}{4}$$

$$E_{11}^{22}(\mathbf{R_6}) = \frac{a + \sqrt{3}b + \sqrt{3}c + 3d}{4}$$

***h12**

$$
\begin{aligned}
H_{12}^{22} &= \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} E_{12}^{22}(\mathbf{R}) \\
&= e^{i\mathbf{k}\cdot\mathbf{R_1}} E_{12}^{22}(\mathbf{R_1}) + e^{i\mathbf{k}\cdot\mathbf{R_2}} E_{12}^{22}(\mathbf{R_2}) + e^{i\mathbf{k}\cdot\mathbf{R_3}} E_{12}^{22}(\mathbf{R_3}) \\
&\quad + e^{i\mathbf{k}\cdot\mathbf{R_4}} E_{12}^{22}(\mathbf{R_4}) + e^{i\mathbf{k}\cdot\mathbf{R_5}} E_{12}^{22}(\mathbf{R_5}) + e^{i\mathbf{k}\cdot\mathbf{R_6}} E_{12}^{22}(\mathbf{R_6}) + E_{12}^{22}(\mathbf{0}) \\
&= e^{ik_x a} E_{12}^{22}(\mathbf{R_1}) + e^{i\left(k_x \frac{a}{2} - k_y \frac{a\sqrt{3}}{2}\right)} E_{12}^{22}(\mathbf{R_2}) \\
&\quad + e^{i\left(-k_x \frac{a}{2} - k_y \frac{a\sqrt{3}}{2}\right)} E_{12}^{22}(\mathbf{R_3}) \\
&\quad + e^{-ik_x a} E_{12}^{22}(\mathbf{R_4}) + e^{i\left(-k_x \frac{a}{2} + k_y \frac{a\sqrt{3}}{2}\right)} E_{12}^{22}(\mathbf{R_5}) \\
&\quad + e^{i\left(k_x \frac{a}{2} + k_y \frac{a\sqrt{3}}{2}\right)} E_{12}^{22}(\mathbf{R_6}) \\
&= e^{2i\alpha} t_{12} + e^{i(\alpha-\beta)} \frac{-\sqrt{3}t_{11} - t_{12} + 3t_{21} + \sqrt{3}t_{22}}{4} \\
&\quad + e^{i(-\alpha-\beta)} \frac{\sqrt{3}t_{11} + t_{12} - 3t_{21} - \sqrt{3}t_{22}}{4} \\
&\quad - e^{-2i\alpha} t_{12} + e^{i(-\alpha+\beta)} \frac{-\sqrt{3}t_{11} + t_{12} - 3t_{21} + \sqrt{3}t_{22}}{4} \\
&\quad + e^{i(\alpha+\beta)} \frac{\sqrt{3}t_{11} - t_{12} + 3t_{21} - \sqrt{3}t_{22}}{4} \\
&= \sqrt{3}(t_{22} - t_{11}) \sin\alpha \sin\beta + 4it_{12} \sin\alpha \cos\alpha - it_{12} \sin\alpha \cos\beta + 3it_{21} \sin\alpha \cos\beta
\end{aligned}
$$

$$
\begin{aligned}
E^{22}(\mathbf{R_2}) &= E^{22}(\sigma_\nu^{'} \mathbf{R_1}) = D^2(\sigma_\nu^{'}) E^{22}(\mathbf{R_1}) [D^2(\sigma_\nu^{'})]^\dagger \\
&= \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \text{Trong đó} \begin{pmatrix} a = t_{11} \\ b = t_{12} \\ c = t_{21} \\ d = t_{22} \end{pmatrix} \\
&\Rightarrow E_{12}^{22}(\mathbf{R_2}) = \frac{-\sqrt{3}a - b + 3c + \sqrt{3}d}{4}
\end{aligned}
$$

Tương tự ta tìm được:

$$E_{12}^{22}(\mathbf{R_3}) = \frac{\sqrt{3}a + b - 3c - \sqrt{3}d}{4}$$

$$E_{12}^{22}(\mathbf{R_4}) = -b$$

$$E_{12}^{22}(\mathbf{R_5}) = \frac{\sqrt{3}a + b - 3c + \sqrt{3}d}{4}$$

$$E_{12}^{22}(\mathbf{R_6}) = \frac{\sqrt{3}a - b + 3c - \sqrt{3}d}{4}$$

Chọn hướng từ trường là $B = \begin{pmatrix} 0 \\ 0 \\ B \end{pmatrix}$.

Lại có $B = \overrightarrow{\nabla} \times \overrightarrow{A} = \begin{vmatrix} \overrightarrow{i} & \overrightarrow{j} & \overrightarrow{k} \\ \dfrac{\partial}{\partial x} & \dfrac{\partial}{\partial y} & \dfrac{\partial}{\partial z} \\ A_x & A_y & A_z \end{vmatrix}$

$= (\dfrac{\partial}{\partial y}A_z - \dfrac{\partial}{\partial z}A_y)\overrightarrow{i} + (\dfrac{\partial}{\partial z}A_x - \dfrac{\partial}{\partial x}A_z)\overrightarrow{j} + (\dfrac{\partial}{\partial x}A_y - \dfrac{\partial}{\partial y}A_x)\overrightarrow{k}$

Có thể chọn $A = \begin{pmatrix} 0 \\ B \cdot x \\ 0 \end{pmatrix}$

$$H^{jj'}_{\mu\mu'}(\mathbf{k}) = \sum_{\mu\mu' jj'} \sum_{\mathbf{R}} e^{\frac{ie}{\hbar}\int_0^{\mathbf{R}} \mathbf{A}(\mathbf{r}')d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R}} E^{jj'}_{\mu\mu'}(\mathbf{R})$$

$*$ **h0**

$$\begin{aligned} h_0 = H^{11}_{11}(\mathbf{k}) &= \sum_{\mathbf{R}} e^{\frac{ie}{\hbar}\int_0^{\mathbf{R}} A(\mathbf{r}')d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R}} E^{11}_{11}(\mathbf{R}) \\ &= e^{\frac{ie}{\hbar}\int_0^{\mathbf{R_1}} A(\mathbf{r}')d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R_1}} E^{11}_{11}(\mathbf{R_1}) + e^{\frac{ie}{\hbar}\int_0^{\mathbf{R_2}} A(\mathbf{r}')d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R_2}} E^{11}_{11}(\mathbf{R_2}) \\ &+ e^{\frac{ie}{\hbar}\int_0^{\mathbf{R_3}} A(\mathbf{r}')d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R_3}} E^{11}_{11}(\mathbf{R_3}) + e^{\frac{ie}{\hbar}\int_0^{\mathbf{R_4}} A(\mathbf{r}')d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R_4}} E^{11}_{11}(\mathbf{R_4}) \\ &+ e^{\frac{ie}{\hbar}\int_0^{\mathbf{R_5}} A(\mathbf{r}')d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R_5}} E^{11}_{11}(\mathbf{R_5}) + e^{\frac{ie}{\hbar}\int_0^{\mathbf{R_6}} A(\mathbf{r}')d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R_6}} E^{11}_{11}(\mathbf{R_6}) \end{aligned}$$

Xét $e^{\frac{ie}{\hbar}\int_0^{\mathbf{R}} A(\mathbf{r}')d\mathbf{r}'}$

Đặt $A = \big(P(x,y), Q(x,y), R(x,y)\big) = (0, Bx, 0)$. Do hướng của từ trường là theo trục $y$ nên khi electron hopping theo hướng $x(m,n) \rightarrow x(m+1,n)$ là không có pha vì $A$ không có thành phần theo trục $x$. Khi electron hopping theo hướng $y(m,n) \rightarrow y(m,n+1)$ thì có pha

Phương trình tham số cho $x, y$:

$$x = ma$$

$$y = y(t) = y_0 + \beta t$$

$*\underset{(0,0)}{\mathbf{R_0}} \longrightarrow \underset{(a,0)}{\mathbf{R_1}}$

Ta có:

$$\begin{aligned}
&y = 0\\
&\Rightarrow \int_C \mathbf{A}(\mathbf{r}')\cdot d\mathbf{r}' = \int_{t_B}^{t_A}\left[P(x,y)\frac{dx}{dt} + Q(x,y)\frac{dy}{dt} + R(x,y)\frac{dz}{dt}\right]dt\\
&= \int_0^1 \left[0\frac{dx}{dt} + Bx0 + 0\frac{dz}{dt}\right]dt = 0
\end{aligned}$$

$*\underset{(0,0)}{\mathbf{R_0}} \longrightarrow \underset{(\frac{a}{2},-\frac{a\sqrt{3}}{2})}{\mathbf{R_2}}$

Ta có:

$$\begin{aligned}
&y = -\frac{a\sqrt{3}}{2}t\\
&\Rightarrow \int_C \mathbf{A}(\mathbf{r}')\cdot d\mathbf{r}' = \int_{t_B}^{t_A}\left[P(x,y)\frac{dx}{dt} + Q(x,y)\frac{dy}{dt} + R(x,y)\frac{dz}{dt}\right]dt\\
&= \int_0^1 \left[0\frac{dx}{dt} + Bma^2\left(-\frac{a\sqrt{3}}{2}\right) + 0\frac{dz}{dt}\right]dt = -\frac{Bma^2\sqrt{3}}{2}
\end{aligned}$$

$*\underset{(0,0)}{\mathbf{R_0}} \longrightarrow \underset{(-\frac{a}{2},-\frac{a\sqrt{3}}{2})}{\mathbf{R_3}}$

Ta có:

$$\begin{aligned}
&y = -\frac{a\sqrt{3}}{2}t\\
&\Rightarrow \int_C \mathbf{A}(\mathbf{r}')\cdot d\mathbf{r}' = \int_{t_B}^{t_A}\left[P(x,y)\frac{dx}{dt} + Q(x,y)\frac{dy}{dt} + R(x,y)\frac{dz}{dt}\right]dt\\
&= \int_0^1 \left[0\frac{dx}{dt} + Bx\left(-\frac{a\sqrt{3}}{2}\right) + 0\frac{dz}{dt}\right]dt = Bma^2\left(-\frac{a\sqrt{3}}{2}\right)\int_0^1 dt\\
&= -\frac{Bma^2\sqrt{3}}{2}
\end{aligned}$$

$*\underset{(0,0)}{\mathbf{R_0}} \longrightarrow \underset{(0,-a)}{\mathbf{R_4}}$

Ta có:

$$\begin{aligned}
&y = 0 \\
&\Rightarrow \int_C \mathbf{A}(\mathbf{r}')\cdot d\mathbf{r}' = \int_{t_B}^{t_A}\left[P(x,y)\frac{dx}{dt} + Q(x,y)\frac{dy}{dt} + R(x,y)\frac{dz}{dt}\right]dt \\
&= \int_0^1 \left[0\frac{dx}{dt} + Bx0 + 0\frac{dz}{dt}\right]dt = 0
\end{aligned}$$

$*\underset{(0,0)}{\mathbf{R_0}} \longrightarrow \underset{(-\frac{a}{2},\frac{a\sqrt{3}}{2})}{\mathbf{R_5}}$

Ta có:

$$\begin{aligned}
&y = \frac{a\sqrt{3}}{2}t \\
&\Rightarrow \int_C \mathbf{A}(\mathbf{r}')\cdot d\mathbf{r}' = \int_{t_B}^{t_A}\left[P(x,y)\frac{dx}{dt} + Q(x,y)\frac{dy}{dt} + R(x,y)\frac{dz}{dt}\right]dt \\
&= \int_0^1 \left[0\frac{dx}{dt} + Bx\frac{a\sqrt{3}}{2} + 0\frac{dz}{dt}\right]dt = \frac{Bma^2\sqrt{3}}{2}
\end{aligned}$$

$*\underset{(0,0)}{\mathbf{R_0}} \longrightarrow \underset{(\frac{a}{2},\frac{a\sqrt{3}}{2})}{\mathbf{R_6}}$

Ta có:

$$\begin{aligned}
&y = \frac{a\sqrt{3}}{2}t \\
&\Rightarrow \int_C \mathbf{A}(\mathbf{r}')\cdot d\mathbf{r}' = \int_{t_B}^{t_A}\left[P(x,y)\frac{dx}{dt} + Q(x,y)\frac{dy}{dt} + R(x,y)\frac{dz}{dt}\right]dt \\
&= \int_0^1 \left[0\frac{dx}{dt} + Bx\frac{a\sqrt{3}}{2} + 0\frac{dz}{dt}\right]dt = \frac{Bma^2\sqrt{3}}{2}
\end{aligned}$$

Vậy $h_0$ có dạng:

$$\begin{aligned}
h_0 = H_{11}^{11}(\mathbf{k}) &= e^0 e^{i\mathbf{k}\cdot\mathbf{R_1}} E_{11}^{11}(\mathbf{R_1}) + e^{-\frac{ie}{\hbar}\frac{Bma^2\sqrt{3}}{2}} e^{i\mathbf{k}\cdot\mathbf{R_2}} E_{11}^{11}(\mathbf{R_2}) \\
&+ e^{-\frac{ie}{\hbar}\frac{Bma^2\sqrt{3}}{2}} e^{i\mathbf{k}\cdot\mathbf{R_3}} E_{11}^{11}(\mathbf{R_3}) + e^0 e^{i\mathbf{k}\cdot\mathbf{R_4}} E_{11}^{11}(\mathbf{R_4}) \\
&+ e^{\frac{ie}{\hbar}\frac{Bma^2\sqrt{3}}{2}} e^{i\mathbf{k}\cdot\mathbf{R_5}} E_{11}^{11}(\mathbf{R_5}) + e^{\frac{ie}{\hbar}\frac{Bma^2\sqrt{3}}{2}} e^{i\mathbf{k}\cdot\mathbf{R_6}} E_{11}^{11}(\mathbf{R_6}) + \epsilon_1 \\
&= e^{ik_x a} E_{11}^{11}(\mathbf{R_1}) + e^{-ik_x a} E_{11}^{11}(\mathbf{R_4}) + e^{-\frac{ie}{\hbar}\frac{Bma^2\sqrt{3}}{2}} e^{i\left(k_x\frac{a}{2} - k_y\frac{a\sqrt{3}}{2}\right)} E_{11}^{11}(\mathbf{R_2}) \\
&+ e^{-\frac{ie}{\hbar}\frac{Bma^2\sqrt{3}}{2}} e^{i\left(-k_x\frac{a}{2} - k_y\frac{a\sqrt{3}}{2}\right)} E_{11}^{11}(\mathbf{R_3}) + e^{\frac{ie}{\hbar}\frac{Ba^2\sqrt{3}}{2}} e^{i\left(-k_x\frac{a}{2} + k_y\frac{a\sqrt{3}}{2}\right)} E_{11}^{11}(\mathbf{R_5}) \\
&+ e^{\frac{ie}{\hbar}\frac{Bma^2\sqrt{3}}{2}} e^{i\left(k_x\frac{a}{2} + k_y\frac{a\sqrt{3}}{2}\right)} E_{11}^{11}(\mathbf{R_6}) + \epsilon_1
\end{aligned}$$

Đặt $k_x \dfrac{a}{2q} =, \quad k_y \dfrac{a\sqrt{3}}{2} = \beta, \quad \dfrac{e}{\hbar}\dfrac{Bma^2\sqrt{3}}{2} = 2\pi \dfrac{\Phi}{\Phi_0} m = \eta, \quad \alpha - \beta = \delta, \quad \alpha + \beta = \gamma$, với $\Phi_0 = 2\pi \dfrac{\hbar}{e}$ và $\Phi = Ba^2$ là thông lượng đi qua ô đơn vị. Áp dụng các toán tử quay để biểu diễn $\mathbf{R}_n$ theo $\mathbf{R}_1$.

$$
\begin{aligned}
E^{11}(\mathbf{R_4}) &= E^{11}(\sigma''\mathbf{R_4}) = D^1(\sigma'')E^{11}(\mathbf{R_1})\left[D^1(\sigma'')\right]^\dagger = E^{11}(\mathbf{R_1})\\
E^{11}(\mathbf{R_2}) &= E^{11}(\sigma'\mathbf{R_1}) = D^1(\sigma')E^{11}(\mathbf{R_1})\left[D^1(\sigma')\right]^\dagger = E^{11}(\mathbf{R_1})\\
E^{11}(\mathbf{R_3}) &= E^{11}(C_3^2\mathbf{R_1}) = D^1(C_3^2)E^{11}(\mathbf{R_1})\left[D^1(C_3^2)\right]^\dagger = E^{11}(\mathbf{R_1})\\
E^{11}(\mathbf{R_5}) &= E^{11}(C_3\mathbf{R_1}) = D^1(C_3)E^{11}(\mathbf{R_1})\left[D^1(C_3)\right]^\dagger = E^{11}(\mathbf{R_1})\\
E^{11}(\mathbf{R_6}) &= E^{11}(\sigma\mathbf{R_1}) = D^1(\sigma)E^{11}(\mathbf{R_1})\left[D^1(\sigma)\right]^\dagger = E^{11}(\mathbf{R_1})
\end{aligned}
$$

$$
\begin{aligned}
\Rightarrow h_0 &= E_{11}^{11}(\mathbf{R_1})(e^{ik_xa} + e^{-ik_xa}) + (e^{-i\eta}e^{i\delta} + e^{i\eta}e^{-i\gamma} + e^{i\eta}e^{-i\delta} + e^{-i\eta}e^{i\gamma})E_{11}^{11}(\mathbf{R_1}) + \epsilon_1\\
&= 2E_{11}^{11}(\mathbf{R_1})\cos(2\alpha) + E_{11}^{11}(\mathbf{R_1})\left[(\cos\eta - i\sin\eta)e^{i\delta} + (\cos\eta + i\sin\eta)e^{-i\delta}\right]\\
&+ E_{11}^{11}\mathbf{R_1}\left[(\cos\eta + i\sin\eta)e^{-i\gamma} + (\cos\eta - i\sin\eta)e^{i\gamma}\right] + \epsilon_1\\
&= 2E_{11}^{11}(\mathbf{R_1})\cos(2\alpha) + E_{11}^{11}(\mathbf{R_1})\left[2\cos\eta\cos\delta - i\sin\eta(2i\sin\delta)\right]\\
&+ E_{11}^{11}(\mathbf{R_1})\left[2\cos\eta\cos\gamma - i\sin\eta(2i\sin\gamma)\right] + \epsilon_1\\
&= 2E_{11}^{11}(\mathbf{R_1})\cos(2\alpha) + 2E_{11}^{11}(\mathbf{R_1})\left[\cos\eta(\cos\gamma + \cos\delta) + \sin\eta(\sin\gamma + \sin\delta)\right] + \epsilon_1\\
&= 2t_0\left[\cos(2\alpha) + 2\cos\eta\cos\alpha\cos\beta + 2\sin\eta\sin\alpha\cos\beta\right] + \epsilon_1
\end{aligned}
$$

$*$ **h1**

$$
\begin{aligned}
h_1 = H_{11}^{12}(\mathbf{k}) = \sum_{\mathbf{R}} e^{\frac{ie}{\hbar}\int_0^{\mathbf{R}} A(\mathbf{r}')d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R}} E_{11}^{12}(\mathbf{R}\\
&= e^{\frac{ie}{\hbar}\int_0^{\mathbf{R_1}} A(\mathbf{r}')d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R_1}} E_{11}^{12}(\mathbf{R_1}) + e^{\frac{ie}{\hbar}\int_0^{\mathbf{R_2}} A(\mathbf{r}')d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R_2}} E_{11}^{12}(\mathbf{R_2})\\
&+ e^{\frac{ie}{\hbar}\int_0^{\mathbf{R_3}} A(\mathbf{r}')d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R_3}} E_{11}^{12}(\mathbf{R_3}) + e^{\frac{ie}{\hbar}\int_0^{\mathbf{R_4}} A(\mathbf{r}')d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R_4}} E_{11}^{12}(\mathbf{R_4})\\
&+ e^{\frac{ie}{\hbar}\int_0^{\mathbf{R_5}} A(\mathbf{r}')d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R_5}} E_{11}^{12}(\mathbf{R_5}) + e^{\frac{ie}{\hbar}\int_0^{\mathbf{R_6}} A(\mathbf{r}')d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R_6}} E_{11}^{12}(\mathbf{R_6})
\end{aligned}
$$

Trong đó:

$$
\begin{aligned}
*E^{12}(\mathbf{R_4}) &= E^{12}(\sigma''\mathbf{R_4}) = D^1(\sigma'')E^{12}(\mathbf{R_1})\left[D^2(\sigma'')\right]^\dagger \\
&= 1\begin{pmatrix} E^{12}_{11}(\mathbf{R_1}) & E^{12}_{12}(\mathbf{R_1}) \end{pmatrix}\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \\
&= \begin{pmatrix} -E^{12}_{11}(\mathbf{R_1}) & E^{12}_{12}(\mathbf{R_1}) \end{pmatrix} \\
\Rightarrow E^{12}_{11}(\mathbf{R_4}) &= -E^{12}_{11}(\mathbf{R_1}), \quad E^{12}_{12}(\mathbf{R_4}) = E^{12}_{11}(\mathbf{R_1})
\end{aligned}
$$

$$
\begin{aligned}
*E^{12}(\mathbf{R_2}) &= E^{12}(\sigma'\mathbf{R_2}) = D^1(\sigma')E^{12}(\mathbf{R_1})\left[D^2(\sigma')\right]^\dagger \\
&= 1\begin{pmatrix} E^{12}_{11}(\mathbf{R_1}) & E^{12}_{12}(\mathbf{R_1}) \end{pmatrix}\begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \\
&= \begin{pmatrix} \dfrac{E^{12}_{11}(\mathbf{R_1}) - \sqrt{3}E^{12}_{12}(\mathbf{R_1})}{2} & \dfrac{-\sqrt{3}E^{12}_{11}(\mathbf{R_1}) - E^{12}_{12}(\mathbf{R_1})}{2} \end{pmatrix} \\
\Rightarrow E^{12}_{11}(\mathbf{R_2}) &= \frac{E^{12}_{11}(\mathbf{R_1}) - \sqrt{3}E^{12}_{12}(\mathbf{R_1})}{2} \\
E^{12}_{12}(\mathbf{R_2}) &= \frac{-\sqrt{3}E^{12}_{11}(\mathbf{R_1}) - E^{12}_{12}(\mathbf{R_1})}{2}
\end{aligned}
$$

Một cách tương tự ta có cho:

$$
\begin{aligned}
E^{12}_{11}(\mathbf{R_3}) &= \frac{-E^{12}_{11}(\mathbf{R_1}) + \sqrt{3}E^{12}_{12}(\mathbf{R_1})}{2} \quad ; E^{12}_{11}(\mathbf{R_4}) = -E^{12}_{11}(\mathbf{R_1}) \\
E^{12}_{11}(\mathbf{R_5}) &= \frac{-E^{12}_{11}(\mathbf{R_1}) - \sqrt{3}E^{12}_{12}(\mathbf{R_1})}{2} \quad ; E^{12}_{11}(\mathbf{R_6}) = \frac{E^{12}_{11}(\mathbf{R_1}) + \sqrt{3}E^{12}_{12}(\mathbf{R_1})}{2}
\end{aligned}
$$

$$
\begin{aligned}
h_1 =& E_{11}^{12}(\mathbf{R_1})\left(e^{ik_xa} - e^{-ik_xa}\right) + e^{-i\eta}e^{i\delta}\frac{E_{11}^{12}(\mathbf{R_1}) - \sqrt{3}E_{12}^{12}(\mathbf{R_1})}{2} \\
&+ e^{i\eta}e^{-i\gamma}\frac{-E_{11}^{12}(\mathbf{R_1}) + \sqrt{3}E_{12}^{12}(\mathbf{R_1})}{2} + e^{i\eta}e^{-i\delta}\frac{-E_{11}^{12}(\mathbf{R_1}) - \sqrt{3}E_{12}^{12}(\mathbf{R_1})}{2} \\
&+ e^{-i\eta}e^{i\gamma}\frac{E_{11}^{12}(\mathbf{R_1}) + \sqrt{3}E_{12}^{12}(\mathbf{R_1})}{2} \\
=& E_{11}^{12}(\mathbf{R_1})\left(e^{ik_xa} - e^{-ik_xa}\right) + \frac{E_{11}^{12}(\mathbf{R_1})}{2}\left(e^{-i\eta}e^{i\delta} - e^{i\eta}e^{-i\gamma} - e^{i\eta}e^{-i\delta} + e^{-i\eta}e^{i\gamma}\right) \\
&+ \frac{\sqrt{3}E_{12}^{12}(\mathbf{R_1})}{2}\left(-e^{-i\eta}e^{i\delta} + e^{i\eta}e^{-i\gamma} - e^{i\eta}e^{-i\delta} + e^{-i\eta}e^{i\gamma}\right) \\
=& E_{11}^{12}(\mathbf{R_1})\left(2i\sin 2\alpha\right) + \frac{E_{11}^{12}(\mathbf{R_1})}{2}4i(\cos\eta\sin\alpha\cos\beta - \sin\eta\cos\alpha\cos\beta) \\
&+ \frac{\sqrt{3}E_{12}^{12}(\mathbf{R_1})}{2}4(-\cos\eta\sin\alpha\sin\beta + \sin\eta\sin\alpha\cos\beta) \\
\Rightarrow h_1 =& 2it_1(\sin 2\alpha + \cos\eta\sin\alpha\cos\beta - \sin\eta\cos\alpha\cos\beta) \\
&- 2\sqrt{3}t_2\left[\cos\eta\sin\alpha\sin\beta - \sin\eta\cos\alpha\sin\beta\right]
\end{aligned}
$$

∗ **h2**

$$
\begin{aligned}
h_2 = H_{12}^{12}(\mathbf{k}) = \sum_{\mathbf{R}} & e^{\frac{ie}{\hbar}\int_0^{\mathbf{R}} A(\mathbf{r}')d\mathbf{r}'}e^{i\mathbf{k}\cdot\mathbf{R}}E_{12}^{12}(\mathbf{R}) \\
=& e^{\frac{ie}{\hbar}\int_0^{\mathbf{R_1}} A(\mathbf{r}')d\mathbf{r}'}e^{i\mathbf{k}\cdot\mathbf{R_1}}E_{12}^{12}(\mathbf{R_1}) + e^{\frac{ie}{\hbar}\int_0^{\mathbf{R_2}} A(\mathbf{r}')d\mathbf{r}'}e^{i\mathbf{k}\cdot\mathbf{R_2}}E_{12}^{12}(\mathbf{R_2}) \\
&+ e^{\frac{ie}{\hbar}\int_0^{\mathbf{R_3}} A(\mathbf{r}')d\mathbf{r}'}e^{i\mathbf{k}\cdot\mathbf{R_3}}E_{12}^{12}(\mathbf{R_3}) + e^{\frac{ie}{\hbar}\int_0^{\mathbf{R_4}} A(\mathbf{r}')d\mathbf{r}'}e^{i\mathbf{k}\cdot\mathbf{R_4}}E_{12}^{12}(\mathbf{R_4}) \\
&+ e^{\frac{ie}{\hbar}\int_0^{\mathbf{R_5}} A(\mathbf{r}')d\mathbf{r}'}e^{i\mathbf{k}\cdot\mathbf{R_5}}E_{12}^{12}(\mathbf{R_5}) + e^{\frac{ie}{\hbar}\int_0^{\mathbf{R_6}} A(\mathbf{r}')d\mathbf{r}'}e^{i\mathbf{k}\cdot\mathbf{R_6}}E_{12}^{12}(\mathbf{R_6})
\end{aligned}
$$

Trong đó:

$$
\begin{aligned}
E_{12}^{12}(\mathbf{R_2}) &= \frac{-\sqrt{3}E_{11}^{12}(\mathbf{R_1}) - E_{12}^{12}(\mathbf{R_1})}{2} \\
E_{12}^{12}(\mathbf{R_3}) &= \frac{-\sqrt{3}E_{11}^{12}(\mathbf{R_1}) - E_{12}^{12}(\mathbf{R_1})}{2} \quad ; E_{12}^{12}(\mathbf{R_4}) = E_{11}^{12}(\mathbf{R_1}) \\
E_{12}^{12}(\mathbf{R_5}) &= \frac{\sqrt{3}E_{11}^{12}(\mathbf{R_1}) - E_{12}^{12}(\mathbf{R_1})}{2} \quad ; E_{12}^{12}(\mathbf{R_6}) = \frac{\sqrt{3}E_{11}^{12}(\mathbf{R_1}) - E_{12}^{12}(\mathbf{R_1})}{2}
\end{aligned}
$$

Thế vô:

$$
\begin{aligned}
h_2 =& E_{12}^{12}(\mathbf{R_1})\left(e^{ik_xa}+e^{-ik_xa}\right)+e^{-i\eta}e^{i\delta}\frac{-\sqrt{3}E_{11}^{12}(\mathbf{R_1})-E_{12}^{12}(\mathbf{R_1})}{2}\\
&+e^{i\eta}e^{-i\gamma}\frac{-\sqrt{3}E_{11}^{12}(\mathbf{R_1})-E_{12}^{12}(\mathbf{R_1})}{2}+e^{i\eta}e^{-i\delta}\frac{\sqrt{3}E_{11}^{12}(\mathbf{R_1})-E_{12}^{12}(\mathbf{R_1})}{2}\\
&+e^{-i\eta}e^{i\gamma}\frac{\sqrt{3}E_{11}^{12}(\mathbf{R_1})-E_{12}^{12}(\mathbf{R_1})}{2}\\
=&2E_{12}^{12}(\mathbf{R_1})\cos 2\alpha+\frac{\sqrt{3}E_{11}^{12}(\mathbf{R_1})}{2}\left(-e^{-i\eta}e^{i\delta}-e^{i\eta}e^{-i\gamma}+e^{i\eta}e^{-i\delta}+e^{-i\eta}e^{i\gamma}\right)\\
&+\frac{E_{12}^{12}(\mathbf{R_1})}{2}\left(-e^{-i\eta}e^{i\delta}-e^{i\eta}e^{-i\gamma}-e^{i\eta}e^{-i\delta}-e^{-i\eta}e^{i\gamma}\right)\\
=&2t_2\cos 2\alpha+2i\sqrt{3}t_1(\cos\eta\cos\alpha\sin\beta+\sin\eta\sin\alpha\cos\beta)\\
&-2t_2(\cos\eta\cos\alpha\cos\beta+\sin\eta\sin\alpha\sin\beta)\\
h_2 =&2t_2(\cos 2\alpha-\cos\eta\cos\alpha\cos\beta-\sin\eta\sin\alpha\cos\beta)\\
&+2i\sqrt{3}t_1(\cos\eta\cos\alpha\sin\beta+\sin\eta\sin\alpha\sin\beta)
\end{aligned}
$$

Các ma trận $E^{22}(\mathbf{R})$

$$
\begin{aligned}
*E^{22}(\mathbf{R_2}) &= E^{22}(\sigma'_\nu\mathbf{R_1})\\
&= D^2(\sigma'_\nu)E^{22}(\mathbf{R_1})\left[D^2(\sigma'_\nu)\right]^\dagger\\
&=\begin{pmatrix}\frac{1}{2} & -\frac{\sqrt{3}}{2}\\ -\frac{\sqrt{3}}{2} & -\frac{1}{2}\end{pmatrix}\begin{pmatrix}E_{11}^{22}(\mathbf{R_1}) & E_{12}^{22}(\mathbf{R_1})\\ E_{21}^{22}(\mathbf{R_1}) & E_{22}^{22}(\mathbf{R_1})\end{pmatrix}\begin{pmatrix}\frac{1}{2} & -\frac{\sqrt{3}}{2}\\ -\frac{\sqrt{3}}{2} & -\frac{1}{2}\end{pmatrix}\\
&=\begin{pmatrix}\frac{t_{11}-\sqrt{3}t_{12}-\sqrt{3}t_{21}+3t_{22}}{4} & \frac{-\sqrt{3}t_{11}-t_{12}+3t_{21}+\sqrt{3}t_{22}}{4}\\ \frac{-\sqrt{3}t_{11}+3t_{12}-t_{21}+\sqrt{3}t_{22}}{4} & \frac{3t_{11}+\sqrt{3}t_{12}+\sqrt{3}t_{21}+t_{22}}{4}\end{pmatrix}
\end{aligned}
$$

$$
\begin{aligned}
\Rightarrow E_{11}^{22}(\mathbf{R_2}) &= \frac{t_{11}-\sqrt{3}t_{12}-\sqrt{3}t_{21}+3t_{22}}{4}\\
E_{12}^{22}(\mathbf{R_2}) &= \frac{-\sqrt{3}t_{11}-t_{12}+3t_{21}+\sqrt{3}t_{22}}{4}\\
E_{21}^{22}(\mathbf{R_2}) &= \frac{-\sqrt{3}t_{11}+3t_{12}-t_{21}+\sqrt{3}t_{22}}{4}\\
E_{22}^{22}(\mathbf{R_2}) &= \frac{3t_{11}+\sqrt{3}t_{12}+\sqrt{3}t_{21}+t_{22}}{4}
\end{aligned}
$$

$$
\begin{aligned}
*E^{22}(\mathbf{R_3}) &= E^{22}(C_3^2\mathbf{R_1}) \\
&= D^2(C_3^2)E^{22}(\mathbf{R_1})\left[D^2(C_3^2)\right]^\dagger \\
&= \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} E_{11}^{22}(\mathbf{R_1}) & E_{12}^{22}(\mathbf{R_1}) \\ E_{21}^{22}(\mathbf{R_1}) & E_{22}^{22}(\mathbf{R_1}) \end{pmatrix} \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \\
&= \begin{pmatrix} \frac{t_{11}-\sqrt{3}t_{12}-\sqrt{3}t_{21}+3t_{22}}{4} & \frac{\sqrt{3}t_{11}+t_{12}-3t_{21}-\sqrt{3}t_{22}}{4} \\ \frac{\sqrt{3}t_{11}-3t_{12}+t_{21}-\sqrt{3}t_{22}}{4} & \frac{3t_{11}+\sqrt{3}t_{12}+\sqrt{3}t_{21}+t_{22}}{4} \end{pmatrix}
\end{aligned}
$$

$$
\begin{aligned}
\Rightarrow E_{11}^{22}(\mathbf{R_3}) &= \frac{t_{11}-\sqrt{3}t_{12}-\sqrt{3}t_{21}+3t_{22}}{4} \\
E_{12}^{22}(\mathbf{R_3}) &= \frac{\sqrt{3}t_{11}+t_{12}-3t_{21}-\sqrt{3}t_{22}}{4} \\
E_{21}^{22}(\mathbf{R_3}) &= \frac{\sqrt{3}t_{11}-3t_{12}+t_{21}-\sqrt{3}t_{22}}{4} \\
E_{22}^{22}(\mathbf{R_3}) &= \frac{3t_{11}+\sqrt{3}t_{12}+\sqrt{3}t_{21}+t_{22}}{4}
\end{aligned}
$$

$$
\begin{aligned}
*E^{22}(\mathbf{R_5}) &= E^{22}(C_3\mathbf{R_1}) \\
&= D^2(C_3)E^{22}(\mathbf{R_1})\left[D^2(C_3)\right]^\dagger \\
&= \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} E_{11}^{22}(\mathbf{R_1}) & E_{12}^{22}(\mathbf{R_1}) \\ E_{21}^{22}(\mathbf{R_1}) & E_{22}^{22}(\mathbf{R_1}) \end{pmatrix} \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \\
&= \begin{pmatrix} \frac{t_{11}+\sqrt{3}t_{12}+\sqrt{3}t_{21}+3t_{22}}{4} & \frac{-\sqrt{3}t_{11}+t_{12}-3t_{21}+\sqrt{3}t_{22}}{4} \\ \frac{-\sqrt{3}t_{11}-3t_{12}+t_{21}+\sqrt{3}t_{22}}{4} & \frac{3t_{11}-\sqrt{3}t_{12}-\sqrt{3}t_{21}+t_{22}}{4} \end{pmatrix}
\end{aligned}
$$

$$
\begin{aligned}
\Rightarrow E_{11}^{22}(\mathbf{R_5}) &= \frac{t_{11}+\sqrt{3}t_{12}+\sqrt{3}t_{21}+3t_{22}}{4} \\
E_{12}^{22}(\mathbf{R_5}) &= \frac{-\sqrt{3}t_{11}+t_{12}-3t_{21}+\sqrt{3}t_{22}}{4} \\
E_{21}^{22}(\mathbf{R_5}) &= \frac{-\sqrt{3}t_{11}-3t_{12}+t_{21}+\sqrt{3}t_{22}}{4} \\
E_{22}^{22}(\mathbf{R_5}) &= \frac{3t_{11}-\sqrt{3}t_{12}-\sqrt{3}t_{21}+t_{22}}{4}
\end{aligned}
$$

$$
\begin{aligned}
*E^{22}(\mathbf{R_4}) &= E^{22}(\sigma''_\nu \mathbf{R_1}) \\
&= D^2(\sigma''_\nu) E^{22}(\mathbf{R_1}) \left[ D^2(\sigma''_n u) \right]^\dagger \\
&= \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} E^{22}_{11}(\mathbf{R_1}) & E^{22}_{12}(\mathbf{R_1}) \\ E^{22}_{21}(\mathbf{R_1}) & E^{22}_{22}(\mathbf{R_1}) \end{pmatrix} \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \\
&= \begin{pmatrix} t_{11} & -t_{12} \\ -t_{21} & t_{22} \end{pmatrix}
\end{aligned}
$$

$$
\begin{aligned}
\Rightarrow E^{22}_{11}(\mathbf{R_4}) &= t_{11} \\
E^{22}_{12}(\mathbf{R_4}) &= -t_{12} \\
E^{22}_{21}(\mathbf{R_4}) &= -t_{21} \\
E^{22}_{22}(\mathbf{R_4}) &= t_{22}
\end{aligned}
$$

$$
\begin{aligned}
*E^{22}(\mathbf{R_6}) &= E^{22}(\sigma_\nu \mathbf{R_1}) \\
&= D^2(\sigma_\nu) E^{22}(\mathbf{R_1}) \left[ D^2(\sigma_\nu) \right]^\dagger \\
&= \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} E^{22}_{11}(\mathbf{R_1}) & E^{22}_{12}(\mathbf{R_1}) \\ E^{22}_{21}(\mathbf{R_1}) & E^{22}_{22}(\mathbf{R_1}) \end{pmatrix} \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \\
&= \begin{pmatrix} \frac{t_{11}+\sqrt{3}t_{12}+\sqrt{3}t_{21}+3t_{22}}{4} & \frac{-\sqrt{3}t_{11}-t_{12}+3t_{21}-\sqrt{3}t_{22}}{4} \\ \frac{\sqrt{3}t_{11}+3t_{12}-t_{21}-\sqrt{3}t_{22}}{4} & \frac{3t_{11}-\sqrt{3}t_{12}-\sqrt{3}t_{21}+t_{22}}{4} \end{pmatrix}
\end{aligned}
$$

$$
\begin{aligned}
\Rightarrow E^{22}_{11}(\mathbf{R_6}) &= \frac{t_{11} + \sqrt{3}t_{12} + \sqrt{3}t_{21} + 3t_{22}}{4} \\
E^{22}_{12}(\mathbf{R_6}) &= \frac{\sqrt{3}t_{11} - t_{12} + 3t_{21} - \sqrt{3}t_{22}}{4} \\
E^{22}_{21}(\mathbf{R_6}) &= \frac{\sqrt{3}t_{11} + 3t_{12} - t_{21} - \sqrt{3}t_{22}}{4} \\
E^{22}_{22}(\mathbf{R_6}) &= \frac{3t_{11} - \sqrt{3}t_{12} - \sqrt{3}t_{21} + t_{22}}{4}
\end{aligned}
$$

* **h11**

$$
\begin{aligned}
h_{11} = H_{11}^{22}(\mathbf{k}) = \sum_{\mathbf{R}} & e^{\frac{ie}{\hbar}\int_0^{\mathbf{R}} A(\mathbf{r}')d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R}} E_{11}^{22}(\mathbf{R}) \\
=& e^{\frac{ie}{\hbar}\int_0^{\mathbf{R_1}} A(\mathbf{r}')d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R_1}} E_{11}^{22}(\mathbf{R_1}) + e^{\frac{ie}{\hbar}\int_0^{\mathbf{R_2}} A(\mathbf{r}')d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R_2}} E_{11}^{22}(\mathbf{R_2}) \\
&+ e^{\frac{ie}{\hbar}\int_0^{\mathbf{R_3}} A(\mathbf{r}')d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R_3}} E_{11}^{22}(\mathbf{R_3}) + e^{\frac{ie}{\hbar}\int_0^{\mathbf{R_4}} A(\mathbf{r}')d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R_4}} E_{11}^{22}(\mathbf{R_4}) \\
&+ e^{\frac{ie}{\hbar}\int_0^{\mathbf{R_5}} A(\mathbf{r}')d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R_5}} E_{11}^{22}(\mathbf{R_5}) + e^{\frac{ie}{\hbar}\int_0^{\mathbf{R_6}} A(\mathbf{r}')d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R_6}} E_{11}^{22}(\mathbf{R_6})
\end{aligned}
$$

Trong đó:

$$
\begin{aligned}
E_{11}^{22}(\mathbf{R_2}) &= \frac{t_{11} - \sqrt{3}t_{12} - \sqrt{3}t_{21} + 3t_{22}}{4} \\
E_{11}^{22}(\mathbf{R_3}) &= \frac{t_{11} - \sqrt{3}t_{12} - \sqrt{3}t_{21} + 3t_{22}}{4} \\
E_{11}^{22}(\mathbf{R_4}) &= t_{11} \\
E_{11}^{22}(\mathbf{R_5}) &= \frac{t_{11} + \sqrt{3}t_{12} + \sqrt{3}t_{21} + 3t_{22}}{4} \\
E_{11}^{22}(\mathbf{R_6}) &= \frac{t_{11} + \sqrt{3}t_{12} + \sqrt{3}t_{21} + 3t_{22}}{4}
\end{aligned}
$$

Thế vô:

$$
\begin{aligned}
h_{11} =& t_{11}\left(e^{ik_xa} + e^{-ik_xa}\right) + e^{-i\eta}e^{i\delta}\frac{t_{11} - \sqrt{3}t_{12} - \sqrt{3}t_{21} + 3t_{22}}{4} \\
&+ e^{i\eta}e^{-i\gamma}\frac{t_{11} - \sqrt{3}t_{12} - \sqrt{3}t_{21} + 3t_{22}}{4} + e^{i\eta}e^{-i\delta}\frac{t_{11} + \sqrt{3}t_{12} + \sqrt{3}t_{21} + 3t_{22}}{4} \\
&+ e^{-i\eta}e^{i\gamma}\frac{t_{11} + \sqrt{3}t_{12} + \sqrt{3}t_{21} + 3t_{22}}{4}
\end{aligned}
$$

Do tính Hermite của Hamiltonian, ta có thể đưa $t_{12} = -t_{21}$, nên $h_{11}$ đơn giản thành:

$$
\begin{aligned}
h_{11} =& e^{-i\eta}e^{i\delta}\frac{t_{11} + 3t_{22}}{4} + e^{i\eta}e^{-i\gamma}\frac{t_{11} + 3t_{22}}{4} + e^{i\eta}e^{-i\delta}\frac{t_{11} + 3t_{22}}{4} + e^{-i\eta}e^{i\gamma}\frac{t_{11} + 3t_{22}}{4} \\
&+ t_{11}\left(e^{ik_xa} + e^{-ik_xa}\right) + \epsilon_2 \\
=& (e^{-i\eta}e^{i\delta} + e^{i\eta}e^{-i\gamma} + e^{i\eta}e^{-i\delta} + e^{-i\eta}e^{i\gamma})\frac{t_{11} + 3t_{22}}{4} + t_{11}\left(e^{ik_xa} + e^{-ik_xa}\right) + \epsilon_2 \\
=& \frac{t_{11} + 3t_{22}}{2}\left[2\cos\eta\cos\alpha\cos\beta + 2\sin\eta\sin\alpha\cos\beta\right] + 2t_{11}\cos 2\alpha + \epsilon_2 \\
\Rightarrow h_{11} =& (t_{11} + 3t_{22})\left[\cos\eta\cos\alpha\cos\beta + \sin\eta\sin\alpha\cos\beta\right] + 2t_{11}\cos 2\alpha + \epsilon_2
\end{aligned}
$$

* **h22**

$$
\begin{aligned}
h_{22} = H_{22}^{22}(\mathbf{k}) = \sum_{\mathbf{R}} e^{\frac{ie}{\hbar}\int_0^{\mathbf{R}} A(\mathbf{r}')d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R}} E_{22}^{22}(\mathbf{R}) + \epsilon_2 \\
=& e^{\frac{ie}{\hbar}\int_0^{\mathbf{R_1}} A(\mathbf{r}')d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R_1}} E_{22}^{22}(\mathbf{R_1}) + e^{\frac{ie}{\hbar}\int_0^{\mathbf{R_2}} A(\mathbf{r}')d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R_2}} E_{22}^{22}(\mathbf{R_2}) \\
&+ e^{\frac{ie}{\hbar}\int_0^{\mathbf{R_3}} A(\mathbf{r}')d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R_3}} E_{22}^{22}(\mathbf{R_3}) + e^{\frac{ie}{\hbar}\int_0^{\mathbf{R_4}} A(\mathbf{r}')d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R_4}} E_{22}^{22}(\mathbf{R_4}) \\
&+ e^{\frac{ie}{\hbar}\int_0^{\mathbf{R_5}} A(\mathbf{r}')d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R_5}} E_{22}^{22}(\mathbf{R_5}) + e^{\frac{ie}{\hbar}\int_0^{\mathbf{R_6}} A(\mathbf{r}')d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R_6}} E_{22}^{22}(\mathbf{R_6}) + \epsilon_2
\end{aligned}
$$

Trong đó:

$$
\begin{aligned}
E_{22}^{22}(\mathbf{R_2}) &= \frac{3t_{11} + \sqrt{3}t_{12} + \sqrt{3}t_{21} + t_{22}}{4} \\
E_{22}^{22}(\mathbf{R_3}) &= \frac{3t_{11} + \sqrt{3}t_{12} + \sqrt{3}t_{21} + t_{22}}{4} \\
E_{22}^{22}(\mathbf{R_4}) &= t_{22} \\
E_{22}^{22}(\mathbf{R_5}) &= \frac{3t_{11} - \sqrt{3}t_{12} - \sqrt{3}t_{21} + t_{22}}{4} \\
E_{22}^{22}(\mathbf{R_6}) &= \frac{3t_{11} - \sqrt{3}t_{12} - \sqrt{3}t_{21} + t_{22}}{4}
\end{aligned}
$$

$$
\begin{aligned}
h_{22} =& e^{-i\eta} e^{i\delta} \frac{3t_{11} + \sqrt{3}t_{12} + \sqrt{3}t_{21} + t_{22}}{4} + e^{i\eta} e^{-i\gamma} \frac{3t_{11} + \sqrt{3}t_{12} + \sqrt{3}t_{21} + t_{22}}{4} \\
&+ e^{i\eta} e^{-i\delta} \frac{3t_{11} - \sqrt{3}t_{12} - \sqrt{3}t_{21} + t_{22}}{4} + e^{-i\eta} e^{i\gamma} \frac{3t_{11} - \sqrt{3}t_{12} - \sqrt{3}t_{21} + t_{22}}{4} \\
&+ t_{22}\left(e^{ik_x a} + e^{-ik_x a}\right) + \epsilon_2 \\
=& e^{-i\eta} e^{i\delta} \frac{3t_{11} + t_{22}}{4} + e^{i\eta} e^{-i\gamma} \frac{3t_{11} + t_{22}}{4} + e^{i\eta} e^{-i\delta} \frac{3t_{11} + t_{22}}{4} + e^{-i\eta} e^{i\gamma} \frac{3t_{11} + t_{22}}{4} \\
&+ t_{22}\left(e^{ik_x a} + e^{-ik_x a}\right) + \epsilon_2 \\
=& (e^{-i\eta} e^{i\delta} + e^{i\eta} e^{-i\gamma} + e^{i\eta} e^{-i\delta} + e^{-i\eta} e^{i\gamma}) \frac{3t_{11} + t_{22}}{4} + t_{11}\left(e^{ik_x a} + e^{-ik_x a}\right) + \epsilon_2 \\
=& \frac{3t_{11} + t_{22}}{2}\left[2\cos\eta\cos\alpha\cos\beta + 2\sin\eta\sin\alpha\cos\beta\right] + 2t_{22}\cos 2\alpha + \epsilon_2 \\
\Rightarrow h_{22} =& (3t_{11} + t_{22})\left[\cos\eta\cos\alpha\cos\beta + \sin\eta\sin\alpha\cos\beta\right] + 2t_{22}\cos 2\alpha + \epsilon_2
\end{aligned}
$$

$*$ **h12**

$$
\begin{aligned}
h_{12} = H_{12}^{22}(\mathbf{k}) = \sum_{\mathbf{R}} & e^{\frac{ie}{\hbar}\int_0^{\mathbf{R}} A(\mathbf{r}')d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R}} E_{12}^{22}(\mathbf{R}) + \epsilon_2 \\
=& e^{\frac{ie}{\hbar}\int_0^{\mathbf{R_1}} A(\mathbf{r}')d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R_1}} E_{12}^{22}(\mathbf{R_1}) + e^{\frac{ie}{\hbar}\int_0^{\mathbf{R_2}} A(\mathbf{r}')d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R_2}} E_{12}^{22}(\mathbf{R_2}) \\
&+ e^{\frac{ie}{\hbar}\int_0^{\mathbf{R_3}} A(\mathbf{r}')d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R_3}} E_{12}^{22}(\mathbf{R_3}) + e^{\frac{ie}{\hbar}\int_0^{\mathbf{R_4}} A(\mathbf{r}')d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R_4}} E_{12}^{22}(\mathbf{R_4}) \\
&+ e^{\frac{ie}{\hbar}\int_0^{\mathbf{R_5}} A(\mathbf{r}')d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R_5}} E_{12}^{22}(\mathbf{R_5}) + e^{\frac{ie}{\hbar}\int_0^{\mathbf{R_6}} A(\mathbf{r}')d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R_6}} E_{12}^{22}(\mathbf{R_6}) + \epsilon_2
\end{aligned}
$$

Trong đó:

$$
\begin{aligned}
E_{12}^{22}(\mathbf{R_2}) &= \frac{-\sqrt{3}t_{11} - t_{12} + 3t_{21} + \sqrt{3}t_{22}}{4} \\
E_{12}^{22}(\mathbf{R_3}) &= \frac{\sqrt{3}t_{11} + t_{12} - 3t_{21} - \sqrt{3}t_{22}}{4} \\
E_{12}^{22}(\mathbf{R_4}) &= -t_{12} \\
E_{12}^{22}(\mathbf{R_5}) &= \frac{-\sqrt{3}t_{11} + t_{12} - 3t_{21} + \sqrt{3}t_{22}}{4} \\
E_{12}^{22}(\mathbf{R_6}) &= \frac{\sqrt{3}t_{11} - t_{12} + 3t_{21} - \sqrt{3}t_{22}}{4}
\end{aligned}
$$

Thế vô:

$$
\begin{aligned}
h_{12} =& e^{-i\eta}e^{i\delta}\frac{-\sqrt{3}t_{11}-t_{12}+3t_{21}+\sqrt{3}t_{22}}{4}+e^{i\eta}e^{-i\gamma}\frac{\sqrt{3}t_{11}+t_{12}-3t_{21}-\sqrt{3}t_{22}}{4} \\
&+e^{i\eta}e^{-i\delta}\frac{-\sqrt{3}t_{11}+t_{12}-3t_{21}+\sqrt{3}t_{22}}{4}+e^{-i\eta}e^{i\gamma}\frac{\sqrt{3}t_{11}-t_{12}+3t_{21}-\sqrt{3}t_{22}}{4} \\
&+t_{12}\left(e^{ik_xa}-e^{-ik_xa}\right) \\
=& e^{-i\eta}e^{i\delta}\frac{-\sqrt{3}t_{11}-4t_{12}+\sqrt{3}t_{22}}{4}+e^{i\eta}e^{-i\gamma}\frac{\sqrt{3}t_{11}+4t_{12}-\sqrt{3}t_{22}}{4} \\
&+e^{i\eta}e^{-i\delta}\frac{-\sqrt{3}t_{11}+4t_{12}+\sqrt{3}t_{22}}{4}+e^{-i\eta}e^{i\gamma}\frac{\sqrt{3}t_{11}-4t_{12}-\sqrt{3}t_{22}}{4}+t_{12}\left(e^{ik_xa}-e^{-ik_xa}\right) \\
=& \frac{\sqrt{3}t_{11}}{4}\left(-e^{-i\eta}e^{i\delta}+e^{i\eta}e^{-i\gamma}-e^{i\eta}e^{-i\delta}+e^{-i\eta}e^{i\gamma}\right)+t_{12}\left(-e^{-i\eta}e^{i\delta}+e^{i\eta}e^{-i\gamma}+e^{i\eta}e^{-i\delta}-e^{-i\eta}e^{i\gamma}\right) \\
&+\frac{\sqrt{3}t_{22}}{4}\left(e^{-i\eta}e^{i\delta}-e^{i\eta}e^{-i\gamma}+e^{i\eta}e^{-i\delta}-e^{-i\eta}e^{i\gamma}\right)+t_{12}\left(e^{ik_xa}-e^{-ik_xa}\right) \\
=& 2it_{12}\sin 2\alpha+\frac{\sqrt{3}t_{11}}{4}4\left[-\cos\eta\sin\alpha\sin\beta+\sin\eta\cos\alpha\sin\beta\right] \\
&-4it_{12}(\cos\eta\sin\alpha\cos\beta-\sin\eta\cos\alpha\cos\beta)+\sqrt{3}t_{22}\left[\cos\eta\sin\alpha\sin\beta-\sin\eta\cos\alpha\sin\beta\right]
\end{aligned}
$$

$$
\begin{aligned}
\Rightarrow h_{12} =& 4it_{12}(\sin\alpha\cos\alpha-\cos\eta\sin\alpha\cos\beta+\sin\eta\cos\alpha\cos\beta) \\
&+\frac{\sqrt{3}(t_{22}-t_{11})}{4}4\left[\cos\eta\sin\alpha\sin\beta-\sin\eta\cos\alpha\sin\beta\right]
\end{aligned}
$$

Vậy Hamiltonian:

$$H_{TB}^{NN}(\mathbf{k}) = \begin{pmatrix} h_0 & h_1 & h_2 \\ h_1^* & h_{11} & h_{12} \\ h_2^* & h_{12}^* & h_{22} \end{pmatrix} \tag{1}$$

Với:

$$\begin{aligned}
h_0 =& 2t_0 \left[\cos(2\alpha) + 2\cos\eta\cos\alpha\cos\beta + 2\sin\eta\sin\alpha\cos\beta\right] + \epsilon_1, && (2)\\
h_1 =& 2it_1(\sin 2\alpha + \cos\eta\sin\alpha\cos\beta - \sin\eta\cos\alpha\cos\beta) \\
& - 2\sqrt{3}t_2\left(\cos\eta\sin\alpha\sin\beta - \sin\eta\cos\alpha\sin\beta\right), && (3)\\
h_2 =& 2t_2(\cos 2\alpha - \cos\eta\cos\alpha\cos\beta - \sin\eta\sin\alpha\cos\beta) && (4)\\
& + 2i\sqrt{3}t_1(\cos\eta\cos\alpha\sin\beta + \sin\eta\sin\alpha\sin\beta), && (5)\\
h_{11} =& (t_{11} + 3t_{22})\left[\cos\eta\cos\alpha\cos\beta + \sin\eta\sin\alpha\cos\beta\right] + 2t_{11}\cos 2\alpha + \epsilon_2, && (6)\\
h_{22} =& (3t_{11} + t_{22})\left[\cos\eta\cos\alpha\cos\beta + \sin\eta\sin\alpha\cos\beta\right] + 2t_{22}\cos 2\alpha + \epsilon_2, && (7)\\
h_{12} =& 4it_{12}(\sin\alpha\cos\alpha - \cos\eta\sin\alpha\cos\beta + \sin\eta\cos\alpha\cos\beta) \\
& + \sqrt{3}(t_{22} - t_{11})\left[\cos\eta\sin\alpha\sin\beta - \sin\eta\cos\alpha\sin\beta\right], && (8)
\end{aligned}$$

$$\begin{aligned}
(\alpha, \beta) &= \left(\frac{1}{2q}k_x a, \frac{\sqrt{3}}{2}k_y a\right), \\
\eta &= 2\pi\frac{\Phi}{\Phi_0}m = 2\pi\frac{p}{q}m,
\end{aligned} \tag{9}$$

$$\begin{aligned}
t_0 = E_{11}^{11}(\mathbf{R_1}); \quad t_1 = E_{11}^{12}(\mathbf{R_1}); \quad t_2 = E_{12}^{12}(\mathbf{R_1}); \\
t_{11} = E_{11}^{22}(\mathbf{R_1}); \quad t_{12} = E_{12}^{22}(\mathbf{R_1}); \quad t_{22} = E_{22}^{22}(\mathbf{R_1});
\end{aligned} \tag{10}$$

$*$ **Phương trình Harper cho Hamiltonian 3 bands:**

Phương trình Schrödinger độc lập thời gian cho Hamiltonian 3 bands

*content...*

$*$ **Hamiltonian Zeeman:**

Chọn các cơ sở:

$$\left|\phi_1^1,\uparrow\right\rangle = \left|\phi_1^1\right\rangle\chi_+ \quad , \quad \left|\phi_1^2,\uparrow\right\rangle = \left|\phi_1^2\right\rangle\chi_+ \quad , \quad \left|\phi_2^2,\uparrow\right\rangle = \left|\phi_2^2\right\rangle\chi_+$$

$$\left|\phi_1^1,\downarrow\right\rangle = \left|\phi_1^1\right\rangle\chi_- \quad , \quad \left|\phi_1^2,\downarrow\right\rangle = \left|\phi_1^2\right\rangle\chi_- \quad , \quad \left|\phi_2^2,\downarrow\right\rangle = \left|\phi_2^2\right\rangle\chi_-$$

$$\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad , \quad \chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Trong đó $\left|\phi_\mu^j\right\rangle$ là các hàm sóng không gian,$\chi$ là các hàm spinor.

Do các hàm Spinor $\chi$ chỉ tác động lên spin $\sigma_z$ và không tác động lên Hamiltonian nằm trong không gian Hilbert. Đồng thời Hamiltonian (1) không có sự tách spin nên ta có thể viết thành:

$$H = H_{space} + H_{1/2} = \mathbb{1}_{2\times 2} \otimes H_{TB}^{NN} + H_{Zeeman} \tag{11}$$

Nhờ vào tính trực giao của các hàm cơ sở $\left|\phi_\mu^j\right\rangle$ và spinor $\chi$, ta tính được:

$*H_{11}^{11(z)}\uparrow$

$$\begin{aligned}
H_{11}^{11(z)}\uparrow &= -\sum_{\mathbf{R}} e^{\frac{ie}{\hbar}\int_0^{\mathbf{R}}\mathbf{A}(\mathbf{r}')\cdot d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R}} \left\langle \phi_1^1(\mathbf{r}),\uparrow \middle| \boldsymbol{\mu}\cdot\mathbf{B} \middle| \phi_1^1(\mathbf{r}-\mathbf{R}),\uparrow \right\rangle \\
&= -\sum_{\mathbf{R}} e^{\frac{ie}{\hbar}\int_0^{\mathbf{R}}\mathbf{A}(\mathbf{r}')\cdot d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R}} \left\langle \phi_1^1(\mathbf{r}),\uparrow \middle| \gamma\mathbf{B}\cdot\mathbf{S} \middle| \phi_1^1(\mathbf{r}-\mathbf{R}),\uparrow \right\rangle \\
&= -\gamma B\sum_{\mathbf{R}} e^{\frac{ie}{\hbar}\int_0^{\mathbf{R}}\mathbf{A}(\mathbf{r}')\cdot d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R}} \left\langle \phi_1^1(\mathbf{r}),\uparrow \middle| S_z \middle| \phi_1^1(\mathbf{r}-\mathbf{R}),\uparrow \right\rangle \\
&= -\gamma B\sum_{\mathbf{R}} e^{\frac{ie}{\hbar}\int_0^{\mathbf{R}}\mathbf{A}(\mathbf{r}')\cdot d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R}} \left\langle \phi_1^1(\mathbf{r}) \middle| \phi_1^1(\mathbf{r}-\mathbf{R}) \right\rangle \left\langle\uparrow\right| S_z \left|\uparrow\right\rangle \\
&= \frac{-\gamma B\hbar}{2}\sum_{\mathbf{R}} e^{\frac{ie}{\hbar}\int_0^{\mathbf{R}}\mathbf{A}(\mathbf{r}')\cdot d\mathbf{r}'}\delta_{11}1 \\
&= \frac{-\gamma B\hbar}{2}(e^0 + e^{-\frac{ie}{\hbar}\frac{Ba^2\sqrt{3}}{8}} + e^{\frac{ie}{\hbar}\frac{Ba^2\sqrt{3}}{8}} + e^0 + e^{\frac{ie}{\hbar}\frac{Ba^2\sqrt{3}}{8}} + e^{-\frac{ie}{\hbar}\frac{Ba^2\sqrt{3}}{8}}) \\
&= \frac{-\gamma B\hbar}{2}(2 + 4\cos\eta) = -\gamma B\hbar(1 + 2\cos\eta)
\end{aligned}$$

$*H_{11}^{22(z)}\uparrow$

$$\begin{aligned}
H_{11}^{22(z)}\uparrow &= -\sum_{\mathbf{R}} e^{\frac{ie}{\hbar}\int_0^{\mathbf{R}}\mathbf{A}(\mathbf{r}')\cdot d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R}} \left\langle \phi_1^2(\mathbf{r}),\uparrow \middle| \boldsymbol{\mu}\cdot\mathbf{B} \middle| \phi_1^2(\mathbf{r}-\mathbf{R}),\uparrow \right\rangle \\
&= \frac{-\gamma B\hbar}{2}(e^0 + e^{-\frac{ie}{\hbar}\frac{Ba^2\sqrt{3}}{8}} + e^{\frac{ie}{\hbar}\frac{Ba^2\sqrt{3}}{8}} + e^0 + e^{\frac{ie}{\hbar}\frac{Ba^2\sqrt{3}}{8}} + e^{-\frac{ie}{\hbar}\frac{Ba^2\sqrt{3}}{8}}) \\
&= \frac{-\gamma B\hbar}{2}(2 + 4\cos\eta) = -\gamma B\hbar(1 + 2\cos\eta)
\end{aligned}$$

$*H_{22}^{22(z)}\uparrow$

$$
\begin{aligned}
H_{22}^{22(z)}\uparrow &= -\sum_{\mathbf{R}} e^{\frac{ie}{\hbar}\int_0^{\mathbf{R}}\mathbf{A}(\mathbf{r}')\cdot d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R}} \left\langle \phi_2^2\left(\mathbf{r}\right), \uparrow \right| \boldsymbol{\mu}\cdot\mathbf{B} \left| \phi_2^2\left(\mathbf{r}-\mathbf{R}\right), \uparrow \right\rangle \\
&= \frac{-\gamma B\hbar}{2}\left(e^0 + e^{-\frac{ie}{\hbar}\frac{Ba^2\sqrt{3}}{8}} + e^{\frac{ie}{\hbar}\frac{Ba^2\sqrt{3}}{8}} + e^0 + e^{\frac{ie}{\hbar}\frac{Ba^2\sqrt{3}}{8}} + e^{-\frac{ie}{\hbar}\frac{Ba^2\sqrt{3}}{8}}\right) \\
&= \frac{-\gamma B\hbar}{2}(2+4\cos\eta) = -\gamma B\hbar(1+2\cos\eta).
\end{aligned}
$$

$*H_{11}^{11(z)}\downarrow$

$$
\begin{aligned}
H_{11}^{11(z)}\downarrow &= -\sum_{\mathbf{R}} e^{\frac{ie}{\hbar}\int_0^{\mathbf{R}}\mathbf{A}(\mathbf{r}')\cdot d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R}} \left\langle \phi_1^1\left(\mathbf{r}\right), \downarrow \right| \boldsymbol{\mu}\cdot\mathbf{B} \left| \phi_1^1\left(\mathbf{r}-\mathbf{R}\right), \downarrow \right\rangle \\
&= -\sum_{\mathbf{R}} e^{\frac{ie}{\hbar}\int_0^{\mathbf{R}}\mathbf{A}(\mathbf{r}')\cdot d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R}} \left\langle \phi_1^1\left(\mathbf{r}\right), \downarrow \right| \gamma\mathbf{B}\cdot\mathbf{S} \left| \phi_1^1\left(\mathbf{r}-\mathbf{R}\right), \downarrow \right\rangle \\
s &= -\gamma B\sum_{\mathbf{R}} e^{\frac{ie}{\hbar}\int_0^{\mathbf{R}}\mathbf{A}(\mathbf{r}')\cdot d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R}} \left\langle \phi_1^1\left(\mathbf{r}\right), \downarrow \right| S_z \left| \phi_1^1\left(\mathbf{r}-\mathbf{R}\right), \downarrow \right\rangle \\
&= -\gamma B\sum_{\mathbf{R}} e^{\frac{ie}{\hbar}\int_0^{\mathbf{R}}\mathbf{A}(\mathbf{r}')\cdot d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R}} \left\langle \phi_1^1(\mathbf{r}) \middle| \phi_1^1(\mathbf{r}-\mathbf{R}) \right\rangle \left\langle\downarrow\right| S_z \left|\downarrow\right\rangle \\
&= \frac{-\gamma B\hbar}{2}\sum_{\mathbf{R}} e^{\frac{ie}{\hbar}\int_0^{\mathbf{R}}\mathbf{A}(\mathbf{r}')\cdot d\mathbf{r}'}\delta_{11}1 \\
&= \frac{-\gamma B\hbar}{2}\left(e^0 + e^{-\frac{ie}{\hbar}\frac{Ba^2\sqrt{3}}{8}} + e^{\frac{ie}{\hbar}\frac{Ba^2\sqrt{3}}{8}} + e^0 + e^{\frac{ie}{\hbar}\frac{Ba^2\sqrt{3}}{8}} + e^{-\frac{ie}{\hbar}\frac{Ba^2\sqrt{3}}{8}}\right) \\
&= \frac{-\gamma B\hbar}{2}(2+4\cos\eta) = \gamma B\hbar(1+2\cos\eta)
\end{aligned}
$$

$*H_{11}^{22(z)}\downarrow$

$$
\begin{aligned}
H_{11}^{22(z)}\downarrow &= -\sum_{\mathbf{R}} e^{\frac{ie}{\hbar}\int_0^{\mathbf{R}}\mathbf{A}(\mathbf{r}')\cdot d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R}} \left\langle \phi_1^2\left(\mathbf{r}\right), \downarrow \right| \boldsymbol{\mu}\cdot\mathbf{B} \left| \phi_1^2\left(\mathbf{r}-\mathbf{R}\right), \downarrow \right\rangle \\
&= \frac{-\gamma B\hbar}{2}\left(e^0 + e^{-\frac{ie}{\hbar}\frac{Ba^2\sqrt{3}}{8}} + e^{\frac{ie}{\hbar}\frac{Ba^2\sqrt{3}}{8}} + e^0 + e^{\frac{ie}{\hbar}\frac{Ba^2\sqrt{3}}{8}} + e^{-\frac{ie}{\hbar}\frac{Ba^2\sqrt{3}}{8}}\right) \\
&= \frac{-\gamma B\hbar}{2}(2+4\cos\eta) = \gamma B\hbar(1+2\cos\eta)
\end{aligned}
$$

$*H_{22}^{22(z)}\downarrow$

$$
\begin{aligned}
H_{22}^{22(z)}\downarrow &= -\sum_{\mathbf{R}} e^{\frac{ie}{\hbar}\int_0^{\mathbf{R}}\mathbf{A}(\mathbf{r}')\cdot d\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{R}} \left\langle \phi_2^2\left(\mathbf{r}\right), \downarrow \right| \boldsymbol{\mu}\cdot\mathbf{B} \left| \phi_2^2\left(\mathbf{r}-\mathbf{R}\right), \downarrow \right\rangle \\
&= \frac{-\gamma B\hbar}{2}\left(e^0 + e^{-\frac{ie}{\hbar}\frac{Ba^2\sqrt{3}}{8}} + e^{\frac{ie}{\hbar}\frac{Ba^2\sqrt{3}}{8}} + e^0 + e^{\frac{ie}{\hbar}\frac{Ba^2\sqrt{3}}{8}} + e^{-\frac{ie}{\hbar}\frac{Ba^2\sqrt{3}}{8}}\right) \\
&= \frac{-\gamma B\hbar}{2}(2+4\cos\eta) = \gamma B\hbar(1+2\cos\eta)
\end{aligned}
$$

với $\gamma = -\dfrac{e}{m}$

Hamiltonian cho thành phần Zeeman:

$$H_{Zeeman} = \frac{e\hbar B}{m}(1+\cos\eta)\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix}$$

Ta có thể xây dựng Hamiltonian thành:

$$\begin{aligned} H &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \bigotimes \begin{pmatrix} h_0 & h_1 & h_2 \\ h_1^* & h_{11} & h_{12} \\ h_2^* & h_{12}^* & h_{22} \end{pmatrix} + H_{Zeeman} \\ &= \begin{pmatrix} h_0 & h_1 & h_2 & 0 & 0 & 0 \\ h_1^* & h_{11} & h_{12} & 0 & 0 & 0 \\ h_2^* & h_{12}^* & h_{22} & 0 & 0 & 0 \\ 0 & 0 & 0 & h_0 & h_1 & h_2 \\ 0 & 0 & 0 & h_1^* & h_{11} & h_{12} \\ 0 & 0 & 0 & h_2^* & h_{12}^* & h_{22} \end{pmatrix} + \frac{e\hbar B}{m}(1+\cos\eta)\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix} \end{aligned}$$

**Two bands $\mathbf{k}\cdot\mathbf{p}$ model**

| $g_n$ | $x'$ | $y'$ | $z'$ | $z'^2$ | $x'y'$ | $\frac{1}{2}(x'^2-y'^2)$ |
|---|---|---|---|---|---|---|
| $E$ | $x$ | $y$ | $z$ | $z^2$ | $xy$ | $\frac{1}{2}(x^2-y^2)$ |
| $C_3(\frac{-2\pi}{3})$ | $-\frac{1}{2}x+\frac{\sqrt{3}}{2}y$ | $-\frac{\sqrt{3}}{2}x-\frac{1}{2}y$ | $z$ | $z^2$ | $-\frac{1}{2}xy+\frac{\sqrt{3}}{4}(x^2+y^2)$ | $-\frac{\sqrt{3}}{2}xy-\frac{1}{4}(x^2-y^2)$ |
| $C_3(\frac{-4\pi}{3})$ | $-\frac{1}{2}x-\frac{\sqrt{3}}{2}y$ | $\frac{\sqrt{3}}{2}x+\frac{1}{2}y$ | $z$ | $z^2$ | $-\frac{1}{2}xy-\frac{\sqrt{3}}{4}(x^2+y^2)$ | $\frac{\sqrt{3}}{2}xy-\frac{1}{4}(x^2-y^2)$ |
| $\sigma_\nu$ | $-x$ | $y$ | $z$ | $z^2$ | $-xy$ | $\frac{1}{2}(x^2-y^2)$ |
| $\sigma'_\nu$ | $\frac{1}{2}x-\frac{\sqrt{3}}{2}$ | $-\frac{\sqrt{3}}{2}x-\frac{1}{2}y$ | $z$ | $z^2$ | $\frac{1}{2}xy-\frac{\sqrt{3}}{4}(x^2+y^2)$ | $-\frac{\sqrt{3}}{2}xy-\frac{1}{4}(x^2-y^2)$ |
| $\sigma''_\nu$ | $\frac{1}{2}x+\frac{\sqrt{3}}{2}$ | $\frac{\sqrt{3}}{2}x-\frac{1}{2}y$ | $z$ | $z^2$ | $\frac{1}{2}xy+\frac{\sqrt{3}}{4}(x^2+y^2)$ | $\frac{\sqrt{3}}{2}xy-\frac{1}{4}(x^2-y^2)$ |

Nếu bỏ qua tương tác Coulomb giữa các điện tử, Hamiltonian của hệ nhiều điện tử đơn giản là tổng các Hamiltonian một điện tử:

$$H = \sum_i H_{1e}(\mathbf{r}_i) = \sum_i \left( -\frac{\hbar^2 \nabla_i^2}{2m_0} + V_0(\mathbf{r}_i) \right). \tag{12}$$

Hàm sóng trong mạng tinh thể thỏa định lý Bloch:

$$\left|\psi_{m\mathbf{k}}(\mathbf{r})\right\rangle = e^{i\mathbf{k}\cdot\mathbf{r}} \left|u_{m\mathbf{k}}(\mathbf{r})\right\rangle. \tag{13}$$

Thay (13) vào (12), ta được phương trình Schrödinger cho mạng tinh thể tuần hoàn theo $u_{m\mathbf{k}}$:

$$\left[ \frac{p^2}{2m_0} + V_0(\mathbf{r}) + \frac{\hbar^2 k^2}{2m_0} + \frac{\hbar}{m_0}\mathbf{k}\cdot\mathbf{p} \right] \left|u_{m\mathbf{k}}(\mathbf{r})\right\rangle = E_{m\mathbf{k}} \left|u_{m\mathbf{k}}(\mathbf{r})\right\rangle. \tag{14}$$

Giả định rằng chúng ta đã biết trị riêng năng lượng và trạng thái riêng tại một điểm $k_0$ trong vùng Brillouin. Để giải phương trình (14), ta có thể khai triển hàm riêng $\left|u_{m\mathbf{k}}(\mathbf{r})\right\rangle$ qua một tập hợp các hàm cơ sở trực chuẩn, đầy đủ $\{|u_n\rangle\}$:

$$\left|u_{m\mathbf{k}}(\mathbf{r})\right\rangle = \sum_n a^n_{m\mathbf{k}} \left|u_n(\mathbf{r})\right\rangle. \tag{15}$$

Thay (15) vào (14) và nhân trái với $\left\langle u_n(\mathbf{r})\right|$, ta được:

$$\sum_{n'} H_{nn'}(\mathbf{k}) a^{n'}_{m\mathbf{k}} = E_{m\mathbf{k}} a^n_{m\mathbf{k}}, \tag{16}$$

trong đó

$$H_{nn'}(\mathbf{k}) = \left( E^0_n + \frac{\hbar^2 k^2}{2m_0} \right) \delta_{nn'} + \frac{\hbar}{m_0}\mathbf{k}\cdot \langle u_n|\, \mathbf{p}\, |u_{n'}\rangle. \tag{17}$$

$H_{\mathbf{k}\cdot\mathbf{p}} = \dfrac{\hbar}{m_0}\mathbf{k}\cdot \langle u_n|\, \mathbf{p}\, |u_{n'}\rangle$

Ta đi khai triển nhiễu loạn cho $H_{\mathbf{k}\cdot\mathbf{p}}$ tới bậc 3 lân cận $\mathbf{k}$:

$$H_{\mathbf{k}\cdot\mathbf{p}} = \frac{\hbar}{m_0}\mathbf{k}\cdot\langle u_n|\,\mathbf{p}\,|u_{n'}\rangle\,, \tag{18}$$

$\langle u_n|\,\mathbf{p}\,|u_n\rangle = 0$.

Hamiltonian cho tập hợp con $A = \{|u_m\rangle\}$:

$$\breve{H}_A = H^{(0)} + H^{(1)} + H^{(2)} + H^{(3)} \tag{19}$$

trong đó

$$\begin{aligned}
H^{(1)}_{ii'} &= H^{'}_{ii'},\\
H^{(2)}_{ii'} &= \frac{1}{2}\sum_{l} H^{'}_{in}H^{'}_{ni'}\left[\frac{1}{E_i - E_n} + \frac{1}{E_{i'} - E_n}\right],\\
H^{(3)}_{ii'} &= -\frac{1}{2}\sum_{n,i''}\left[\frac{H^{'}_{in}H^{'}_{ni''}H^{'}_{i''i'}}{(E_{i'} - E_n)(E_{i''} - E_n)} + \frac{H^{'}_{ii''}H^{'}_{i''n}H^{'}_{ni'}}{(E_i - E_n)(E_{i''} - E_n)}\right],\\
&\quad + \frac{1}{2}\sum_{n,n'} H^{'}_{in}H^{'}_{nn'}H^{'}_{n'i'}\left[\frac{1}{(E_i - E_n)(E_i - E_{n'})} + \frac{1}{(E_{i'} - E_n)(E_{i'} - E_{n'})}\right],
\end{aligned}$$

với $i, i', i'' \in A$ và $n, n' \in B$ $(i = \pm 2, 0)$ và $(n = \pm 1)$. Ứng với đó là $d_{\pm 2} = \frac{1}{\sqrt{2}}(d_{x^2-y^2} \pm i d_{xy}), d_0 = d_{z^2}, d_{\pm 1} = \frac{1}{\sqrt{2}}(d_{xz} \pm i d_{yz})$.

Khi SOC chưa được xét đến, các orbitals trong tập chẵn không thể tương tác với các orbitals trong tập lẻ. Do đó ta chọn các cơ sở dựa trên trị riêng của toán tử xung lượng góc $L^2$ và $L_z$ với các chỉ số lượng tử $l = 2, m = 0, \pm 2$:

$$\left|\tilde{\phi}_1\right\rangle = |d_{m=2}\rangle\,, \tag{20}$$

$$\left|\tilde{\phi}_2\right\rangle = |d_{m=0}\rangle\,, \tag{21}$$

$$\left|\tilde{\phi}_3\right\rangle = |d_{m=-2}\rangle\,. \tag{22}$$

Các cơ sở mới cho thể có dẫn ra được từ cơ sở cũ bằng phép biến đổi tuyến tính sau

$$\left|\tilde{\phi}_j\right\rangle = \sum_j W_{jj'}\,|\phi_j\rangle\,,$$

trong đó

$$W = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \\ 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \end{pmatrix}$$

Hamiltonian TB ở cơ sở mới có dạng

$$\begin{aligned}
\tilde{H}^{\mathrm{NN}}(\mathbf{k}) &= W H^{\mathrm{NN}}(\mathbf{k}) W^{\dagger} \\
&= \begin{pmatrix}
\frac{1}{2}(h_{11} + h_{22} + 2\,\mathrm{Im}\{h_{12}\}) & \frac{1}{\sqrt{2}}\left(h_1^* + i h_2^*\right) & \frac{1}{2}\left(h_{11} - h_{22} + 2i\,\mathrm{Re}\{h_{12}\}\right) \\
\dfrac{1}{\sqrt{2}}\left(h_1 - i h_2\right) & h_0 & \dfrac{1}{\sqrt{2}}\left(h_1 + i h_2\right) \\
\frac{1}{2}(h_{11} - h_{22} - 2\,\mathrm{Im}\{h_{12}\}) & \frac{1}{\sqrt{2}}\left(h_1^* - i h_2^*\right) & \frac{1}{2}\left(h_{11} + h_{22} - 2i\,\mathrm{Re}\{h_{12}\}\right)
\end{pmatrix}
\end{aligned}$$

và đặt

$$\left\langle \tilde{\phi}_c^{\tau}, \pm\mathbf{K} \right| p_x \left| \tilde{\phi}_v^{\tau}, \pm\mathbf{K} \right\rangle = \pm i \left\langle \tilde{\phi}_c^{\tau}, \pm\mathbf{K} \right| p_y \left| \tilde{\phi}_v^{\tau}, \pm\mathbf{K} \right\rangle [3] \tag{23}$$

Thành phần ma trận của Hamiltonian không nhiễu loạn $H^0$:

$$\begin{aligned}
H_{\mu\mu'}(\mathbf{k}, \tau) &= \sum_R e^{i\mathbf{k}\cdot\mathbf{R}} E_{\mu\mu'}(\mathbf{R}) \\
&= \sum_R e^{i\mathbf{k}\cdot\mathbf{R}} \left\langle \psi_\mu^\tau(\mathbf{r}) \right| \hat{H} \left| \psi_{\mu'}^\tau(\mathbf{r} - \mathbf{R}) \right\rangle
\end{aligned}$$

$*H_{cc}(\mathbf{k}, \tau)$

$$\begin{aligned}
H_{cc}(\mathbf{k}, \tau) &= \sum_R e^{i\mathbf{k}\cdot\mathbf{R}} \left\langle \psi_c^\tau(\mathbf{r}) \right| \hat{H} \left| \psi_c^\tau(\mathbf{r} - \mathbf{R}) \right\rangle \\
&= h_0 \\
&= 2t_0 \left(\cos 2\alpha + 2\cos\alpha\cos\beta\right) + \epsilon_1
\end{aligned}$$

$*H_{cv}(\mathbf{k}, \tau)$

$$\begin{aligned}
H_{cv}(\mathbf{k}, \tau) &= \sum_R e^{i\mathbf{k}\cdot\mathbf{R}} \left\langle \psi_c^\tau(\mathbf{r}) \right| \hat{H} \left| \psi_v^\tau(\mathbf{r} - \mathbf{R}) \right\rangle \\
&= \frac{1}{\sqrt{2}} \sum_R e^{i\mathbf{k}\cdot\mathbf{R}} \left[ \left\langle \phi_1^1(\mathbf{r}) \right| \hat{H} \left| \phi_2^2(\mathbf{r} - \mathbf{R}) \right\rangle + i\tau \left\langle \phi_1^1(\mathbf{r}) \right| \hat{H} \left| \phi_1^2(\mathbf{r} - \mathbf{R}) \right\rangle \right] \\
&= \frac{1}{\sqrt{2}} (h_2 + i\tau h_1) \\
&= \frac{1}{\sqrt{2}} \Bigg[ 2t_2(\cos 2\alpha - \cos\alpha\cos\beta) + 2i\sqrt{3}t_1 \cos\alpha \sin\beta \\
&+ i\tau \left( -2\sqrt{3}t_2 \sin\alpha\sin\beta + 2it_1(\sin 2\alpha + \sin\alpha\cos\beta) \right) \Bigg]
\end{aligned}$$

$*H_{vc}(\mathbf{k},\tau)$

$$
\begin{aligned}
H_{vc}(\mathbf{k},\tau) &= \sum_R e^{i\mathbf{k}\cdot\mathbf{R}} \left\langle \psi_v^\tau(\mathbf{r}) \right| \hat{H} \left| \psi_c^\tau(\mathbf{r}-\mathbf{R}) \right\rangle \\
&= \frac{1}{\sqrt{2}} \sum_R e^{i\mathbf{k}\cdot\mathbf{R}} \left[ \left\langle \phi_2^2(\mathbf{r}) \right| \hat{H} \left| \phi_1^1(\mathbf{r}-\mathbf{R}) \right\rangle - i\tau \left\langle \phi_1^2(\mathbf{r}) \right| \hat{H} \left| \phi_1^1(\mathbf{r}-\mathbf{R}) \right\rangle \right] \\
&= \frac{1}{\sqrt{2}} (h_2^* - i\tau h_1^*) \\
&= \frac{1}{\sqrt{2}} \Big[ 2t_2(\cos 2\alpha - \cos\alpha\cos\beta) - 2i\sqrt{3}t_1 \cos\alpha \sin\beta \\
&- i\tau \left( -2\sqrt{3}t_2 \sin\alpha\sin\beta - 2it_1(\sin 2\alpha + \sin\alpha\cos\beta) \right) \Big]
\end{aligned}
$$

$*H_{vv}(\mathbf{k},\tau)$

$$
\begin{aligned}
H_{vv}(\mathbf{k},\tau) &= \sum_R e^{i\mathbf{k}\cdot\mathbf{R}} \left\langle \psi_v^\tau(\mathbf{r}) \right| \hat{H} \left| \psi_v^\tau(\mathbf{r}-\mathbf{R}) \right\rangle \\
&= \frac{1}{2} \sum_R e^{i\mathbf{k}\cdot\mathbf{R}} \Big[ \left\langle \phi_2^2(\mathbf{r}) \right| \hat{H} \left| \phi_2^2(\mathbf{r}-\mathbf{R}) \right\rangle + i\tau \left\langle \phi_2^2(\mathbf{r}) \right| \hat{H} \left| \phi_1^2(\mathbf{r}-\mathbf{R}) \right\rangle \\
&- i\tau \left\langle \phi_1^2(\mathbf{r}) \right| \hat{H} \left| \phi_2^2(\mathbf{r}-\mathbf{R}) \right\rangle + \tau^2 \left\langle \phi_1^2(\mathbf{r}) \right| \hat{H} \left| \phi_1^2(\mathbf{r}-\mathbf{R}) \right\rangle \Big] \\
&= \frac{1}{2} \Big( h_{22} + i\tau h_{12}^* - i\tau h_{12} + \tau h_{11} \Big) \\
&= \frac{1}{2} \Big[ 2t_{22}\cos 2\alpha + (3t_{11} + t_{22})\cos\alpha\cos\beta + \tau^2 \left( 2t_{11}\cos 2\alpha + (t_{11} + 3t_{22})\cos\alpha\cos\beta + 2\epsilon_2 \right) \\
&- i\tau(8it_{12}\sin\alpha(\cos\alpha - \cos\beta)) \Big]
\end{aligned}
$$

Tại $\pm K$ valley

$$\mathbf{k} = (k_x, k_y) = \left(\tau\frac{4\pi}{3a}, 0\right)$$
$$(\alpha, \beta) = \left(\frac{1}{2}k_x a, \frac{\sqrt{3}}{2}k_y a\right)$$

với $\tau = \pm 1$

$$H_{cc}(\mathbf{k}, \tau) = -3t_0 + \epsilon_1$$

$$H_{cv}(\mathbf{k}, \tau) = 0$$

$$H_{vc}(\mathbf{k}, \tau) = 0$$

$$H_{vv}(\mathbf{k}, \tau) = \epsilon_2 - \frac{3}{2}(t_{11} + t_{22}) - \tau 3\sqrt{3}t_{12}$$

$*H^{(1)}_{mm'}$

$$H^{(1)}_{cc} = H^{'}_{0,0} = 0$$

$$H^{(1)}_{vv} = H^{'}_{2,2} = 0$$

$$\begin{aligned} H^{(1)}_{vc} &= H^{'}_{vc} \\ &= H^{'*}_{0,2} \end{aligned}$$

$$\begin{aligned} H^{(1)}_{cv} &= H^{'}_{0,2} \\ &= \frac{\hbar}{m_0}\mathbf{k} \cdot \langle u_c| \, \mathbf{p} \, |u_v\rangle \\ &= \frac{\hbar}{m_0}\left(k_x \langle u_c| \, p_x \, |u_v\rangle + k_y \langle u_c| \, p_y \, |u_v\rangle\right) \\ &= \frac{\hbar}{m_0}\left(k_x \langle u_c| \, p_x \, |u_v\rangle - ik_y \langle u_c| \, p_x \, |u_v\rangle\right) \\ &= \frac{\hbar}{m_0}\left(k_x \langle u_c| \, p_x \, |u_v\rangle - ik_y \langle u_c| \, p_x \, |u_v\rangle\right) \\ &= \frac{a\hbar}{am_0}\left(k_x - ik_y\right) \langle u_c| \, p_x \, |u_v\rangle \\ &= at\left(k_x - ik_y\right) \end{aligned}$$

đặt $t = \dfrac{\hbar}{am_0} \langle u_c | p_x | u_v \rangle$ (ta nhân thêm $a$ và chia cho $a$ ở mẫu để không bị vi phạm thứ nguyên).

Ta sử dụng định nghĩa mới là $k_\pm = k_x \pm ik_y$ và $p_\pm = p_x \pm ip_y$

$$k_x = \frac{k_+ + k_-}{2};\ k_y = \frac{k_+ - k_-}{2i}, \tag{24}$$

$$p_x = \frac{k_+ + k_-}{2};\ p_y = \frac{k_+ - k_-}{2i}. \tag{25}$$

, viết lại phương trình (18) dưới dạng:

$$H_{\mathbf{k}\cdot\mathbf{p}} = \frac{1}{2}\frac{\hbar}{m_0}(k_+\hat{p}_- + k_-\hat{p}_+) = H^-_{\mathbf{k}\cdot\mathbf{p}} + H^+_{\mathbf{k}\cdot\mathbf{p}}, \tag{26}$$

với $k_\pm = k_x \pm iq_y$, $\hat{p}_\pm = \hat{p}_x \pm i\hat{p}_y$

| irrep | Basics funtioncs | Band |
|---|---|---|
| $A_1^{'}$ | $\left\|\Psi_{2,0}\right\rangle$ | VB |
| $E^{'}$ | $\{\left\|\Psi_{2,2}\right\rangle, \left\|\Psi_{2,-2}\right\rangle\}$ | VB-3 |
| $E^{''}$ | $\{\left\|\Psi_{2,1}\right\rangle, \left\|\Psi_{2,-1}\right\rangle\}$ | VB-1 |

Bảng 1: Cơ sở cho biểu diễn bất khả quy của nhóm $D_{3h}$ tại điểm $K$.

Sử dụng toán tử quay $C_3$ tác dụng lên $p_\pm$:

$$\begin{aligned} C_3\hat{p}_+ &= \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} p_x \\ p_y \end{pmatrix} = \begin{pmatrix} p'_x \\ p'_y \end{pmatrix} \\ &= \left(-\frac{1}{2}p_x - \frac{\sqrt{3}}{2}p_y\right) + i\left(\frac{\sqrt{3}}{2}p_x - \frac{1}{2}p_y\right) \\ &= e^{-\frac{2\pi i}{3}}p_+ \end{aligned}$$

Tương tự cho $p_-$, ta có:

$$C_3\hat{p}_\pm = e^{\mp\frac{2\pi i}{3}}p_\pm \tag{27}$$

$$\left\langle \psi_f \right| \hat{p}_\pm \left|\psi_i\right\rangle = e^{\frac{2\pi i(m_f - m_i \mp 1)}{3}} \left\langle \psi_f \right| \hat{p}_\pm \left|\psi_i\right\rangle$$

Sử dụng kết quả (22), ta tính được nhiễu loạn bậc 1 như sau:

$*H^{(1)}_{mm'}$

$$H^{(1)}_{cc} = H^{'}_{0,0} = 0$$

$$H^{(1)}_{vv} = H^{'}_{2,2} = 0$$

$$\begin{aligned} H^{(1)}_{vc} &= H^{'}_{vc} \\ &= H^{'*}_{0,2} \end{aligned}$$

$$\begin{aligned} H^{(1)}_{cv} &= H^{'}_{0,2} \\ &= \frac{1}{2}\frac{\hbar}{m_0}\left(k_+ \langle 0| \hat{p}_- |2\rangle + k_- \langle 0| \hat{p}_+ |2\rangle\right) \\ &= \frac{1}{2}\frac{\hbar}{m_0}\left(k_+ \langle 0| C_3^\dagger C_3 \hat{p}_- C_3^\dagger C_3 |2\rangle + k_- \langle 0| C_3^\dagger C_3 \hat{p}_+ C_3^\dagger C_3 |2\rangle\right) \\ &= \frac{1}{2}\frac{\hbar}{m_0}\left(e^{\frac{2i\pi}{3}} e^{\frac{2i\pi}{3}} k_+ \cancelto{0}{\langle 0| p_- |2\rangle} + e^{-\frac{2i\pi}{3}} e^{\frac{4i\pi}{3}} k_- \langle 0| \hat{p}_+ |2\rangle\right) \end{aligned}$$

$*H_{mm'}^{(2)}$

$$
\begin{aligned}
H_{0,0}^{(2)} &= \frac{1}{2}\sum_{l} H_{0,l}^{'}H_{l,0}^{'}\left[\frac{1}{E_0-E_l}+\frac{1}{E_0-E_l}\right]\\
&= \frac{1}{2}H_{0,-1}^{'}H_{-1,0}^{'}\left[\frac{1}{E_0-E_{-1}}+\frac{1}{E_0-E_{-1}}\right]+\frac{1}{2}H_{0,1}^{'}H_{1,0}^{'}\left[\frac{1}{E_0-E_1}+\frac{1}{E_0-E_1}\right]\\
&= \frac{1}{4}\frac{\hbar}{m_0}\big(k_+\langle 0|\,\hat{p}_-\,|{-1}\rangle + k_-\langle 0|\,\hat{p}_+\,|{-1}\rangle\big)\big(k_+\langle -1|\,\hat{p}_-\,|0\rangle + k_-\langle -1|\,\hat{p}_+\,|0\rangle\big)\left[\frac{1}{E_0-E_{-1}}+\frac{1}{E_0-E_{-1}}\right]\\
&+\frac{1}{4}\frac{\hbar}{m_0}\big(k_+\langle 0|\,\hat{p}_-\,|1\rangle + k_-\langle 0|\,\hat{p}_+\,|1\rangle\big)\big(k_+\langle 1|\,\hat{p}_-\,|0\rangle + k_-\langle 1|\,\hat{p}_+\,|0\rangle\big)\left[\frac{1}{E_0-E_1}+\frac{1}{E_0-E_1}\right]\\
&= \frac{1}{4}\frac{\hbar}{m_0}\Big(k_+\langle 0|\,C_3^\dagger C_3\hat{p}_- C_3^\dagger C_3\,|{-1}\rangle + k_-\langle 0|\,C_3^\dagger C_3\hat{p}_+ C_3^\dagger C_3\,|{-1}\rangle\Big)\\
&\times\Big(k_+\langle -1|\,C_3^\dagger C_3\hat{p}_- C_3^\dagger C_3\,|0\rangle + k_-\langle -1|\,C_3^\dagger C_3\hat{p}_+ C_3^\dagger C_3\,|0\rangle\Big)\left[\frac{1}{E_0-E_{-1}}+\frac{1}{E_0-E_{-1}}\right]\\
&+\frac{1}{4}\frac{\hbar}{m_0}\Big(k_+\langle 0|\,C_3^\dagger C_3\hat{p}_- C_3^\dagger C_3\,|1\rangle + k_-\langle 0|\,C_3^\dagger C_3\hat{p}_+ C_3^\dagger C_3\,|1\rangle\Big)\\
&\times\Big(k_+\langle 1|\,C_3^\dagger C_3\hat{p}_- C_3^\dagger C_3\,|0\rangle + k_-\langle 1|\,C_3^\dagger C_3\hat{p}_+ C_3^\dagger C_3\,|0\rangle\Big)\left[\frac{1}{E_0-E_1}+\frac{1}{E_0-E_1}\right]\\
&= \frac{1}{4}\frac{\hbar}{m_0}\left(k_+e^{\frac{2i\pi}{3}}e^{-\frac{2i\pi}{3}}\langle 0|\,\hat{p}_-\,|{-1}\rangle + k_-e^{-\frac{2i\pi}{3}}e^{-\frac{2i\pi}{3}}\cancelto{0}{\langle 0|\,\hat{p}_+\,|{-1}\rangle}\right)\\
&\times\left(k_+e^{\frac{2i\pi}{3}}e^{\frac{2i\pi}{3}}\cancelto{0}{\langle -1|\,\hat{p}_-\,|0\rangle} + k_-e^{-\frac{2i\pi}{3}}e^{\frac{2i\pi}{3}}\langle -1|\,\hat{p}_+\,|0\rangle\right)\left[\frac{1}{E_0-E_{-1}}+\frac{1}{E_0-E_{-1}}\right]\\
&+\frac{1}{4}\frac{\hbar}{m_0}\left(k_+e^{\frac{2i\pi}{3}}e^{\frac{2i\pi}{3}}\cancelto{0}{\langle 0|\,\hat{p}_-\,|1\rangle} + k_-e^{-\frac{2i\pi}{3}}e^{\frac{2i\pi}{3}}\langle 0|\,\hat{p}_+\,|1\rangle\right)\\
&\times\left(k_+e^{\frac{2i\pi}{3}}e^{-\frac{2i\pi}{3}}\langle 1|\,\hat{p}_-\,|0\rangle + k_-e^{-\frac{2i\pi}{3}}e^{\frac{-2i\pi}{3}}\cancelto{0}{\langle 1|\,\hat{p}_+\,|0\rangle}\right)\left[\frac{1}{E_0-E_1}+\frac{1}{E_0-E_1}\right]\text{ (để dấu “=” xảy ra)}
\end{aligned}
$$

Vậy, rút gọn những thành phần ma trận không cần thiết ta được:

$$
\begin{aligned}
H_{0,0}^{(2)} &= \frac{1}{4}\frac{\hbar}{m_0}\big(k_+\langle 0|\,\hat{p}_-\,|{-1}\rangle\big)\big(k_-\langle -1|\,\hat{p}_+\,|0\rangle\big)\left[\frac{2}{E_0-E_{-1}}\right]\\
&+\frac{1}{4}\frac{\hbar}{m_0}\big(k_-\langle 0|\,\hat{p}_+\,|1\rangle\big)\big(k_+\langle 1|\,\hat{p}_-\,|0\rangle\big)\left[\frac{2}{E_0-E_1}\right]\\
&= \frac{1}{2}\frac{\hbar}{m_0}q^2\left[\langle 0|\,\hat{p}_-\,|{-1}\rangle\langle -1|\,\hat{p}_+\,|0\rangle\frac{1}{E_0-E_{-1}}+\langle 0|\,\hat{p}_+\,|1\rangle\langle 1|\,\hat{p}_-\,|0\rangle\frac{1}{E_0-E_1}\right]\\
&= q^2a^2\underbrace{\frac{1}{2}\frac{\hbar}{a^2m_0}\left[\langle 0|\,\hat{p}_-\,|{-1}\rangle\langle -1|\,\hat{p}_+\,|0\rangle\frac{1}{E_0-E_{-1}}+\langle 0|\,\hat{p}_+\,|1\rangle\langle 1|\,\hat{p}_-\,|0\rangle\frac{1}{E_0-E_1}\right]}_{\gamma_1}\\
&= a^2k^2\gamma_1
\end{aligned}
$$

với $q^2 = k_x^2 + k_y^2$.

$$
\begin{aligned}
H^{(2)}_{2,2} &= \frac{1}{2}\sum_{l} H^{'}_{2,l}H^{'}_{l,-2}\left[\frac{1}{E_2-E_l}+\frac{1}{E_2-E_l}\right]\\
&= \frac{1}{2}H^{'}_{2,-1}H^{'}_{-1,2}\left[\frac{1}{E_2-E_{-1}}+\frac{1}{E_2-E_{-1}}\right]+\frac{1}{2}H^{'}_{2,1}H^{'}_{1,2}\left[\frac{1}{E_2-E_1}+\frac{1}{E_{-2}-E_1}\right]\\
&= \frac{1}{4}\frac{\hbar}{m_0}\left(k_+\left\langle 2\right| p_-\left|-1\right\rangle + k_-\left\langle 2\right| p_+\left|-1\right\rangle\right)\left(k_+\left\langle -1\right| p_-\left|2\right\rangle + k_-\left\langle -1\right| p_+\left|2\right\rangle\right)\\
&\times\left[\frac{1}{E_2-E_{-1}}+\frac{1}{E_{-2}-E_{-1}}\right]+\frac{1}{4}\frac{\hbar}{m_0}\left(k_+\left\langle 2\right| p_-\left|1\right\rangle + k_-\left\langle 2\right| p_+\left|1\right\rangle\right)\\
&\times\left(k_+\left\langle 1\right| p_-\left|2\right\rangle + k_-\left\langle 1\right| p_+\left|2\right\rangle\right)\left[\frac{1}{E_2-E_1}+\frac{1}{E_{-2}-E_1}\right]\\
&= \frac{1}{4}\frac{\hbar}{m_0}\left(k_+\left\langle 2\right| C_3^\dagger C_3 p_- C_3^\dagger C_3\left|-1\right\rangle + k_-\left\langle 2\right| C_3^\dagger C_3 p_+ C_3^\dagger C_3\left|-1\right\rangle\right)\\
&\times\left(k_+\left\langle -1\right| C_3^\dagger C_3 p_- C_3^\dagger C_3\left|2\right\rangle + k_-\left\langle -1\right| C_3^\dagger C_3 p_+ C_3^\dagger C_3\left|2\right\rangle\right)\times\left[\frac{1}{E_2-E_{-1}}+\frac{1}{E_{-2}-E_{-1}}\right]\\
&+\frac{1}{4}\frac{\hbar}{m_0}\left(k_+\left\langle 2\right| C_3^\dagger C_3 p_- C_3^\dagger C_3\left|1\right\rangle + k_-\left\langle 2\right| C_3^\dagger C_3 p_+ C_3^\dagger C_3\left|1\right\rangle\right)\\
&\times\left(k_+\left\langle 1\right| C_3^\dagger C_3 p_- C_3^\dagger C_3\left|2\right\rangle + k_-\left\langle 1\right| C_3^\dagger C_3 p_+ C_3^\dagger C_3\left|2\right\rangle\right)\left[\frac{1}{E_2-E_1}+\frac{1}{E_{-2}-E_1}\right]\\
&= \frac{1}{4}\frac{\hbar}{m_0}\left(k_+e^{\frac{4\pi i}{3}}e^{\frac{2\pi i}{3}}e^{\frac{2\pi i}{3}}\cancelto{0}{\left\langle 2\right| p_-\left|-1\right\rangle} + k_-e^{\frac{4\pi i}{3}}e^{-\frac{2\pi i}{3}}e^{\frac{2\pi i}{3}}\cancelto{0}{\left\langle 2\right| p_+\left|-1\right\rangle}\right)^{0}\\
&\times\left(k_+e^{-\frac{2\pi i}{3}}e^{\frac{2\pi i}{3}}e^{-\frac{4\pi i}{3}}\cancelto{0}{\left\langle -1\right| p_-\left|2\right\rangle} + k_-e^{-\frac{2\pi i}{3}}e^{-\frac{2\pi i}{3}}e^{-\frac{4\pi i}{3}}\cancelto{}{\left\langle -1\right| p_+\left|2\right\rangle}\right)^{0}\times\left[\frac{1}{E_2-E_{-1}}+\frac{1}{E_{-2}-E_{-1}}\right]\\
&+\frac{1}{4}\frac{\hbar}{m_0}\left(k_+e^{\frac{4\pi i}{3}}e^{\frac{2\pi i}{3}}e^{-\frac{2\pi i}{3}}\cancelto{0}{\left\langle 2\right| p_-\left|1\right\rangle} + k_-e^{\frac{4\pi i}{3}}e^{-\frac{2\pi i}{3}}e^{-\frac{2\pi i}{3}}\left\langle 2\right| p_+\left|1\right\rangle\right)\\
&\times\left(k_+e^{\frac{2\pi i}{3}}e^{\frac{2\pi i}{3}}e^{-\frac{4\pi i}{3}}\left\langle 1\right| p_-\left|2\right\rangle + k_-e^{\frac{2\pi i}{3}}e^{-\frac{2\pi i}{3}}e^{\frac{-4\pi i}{3}}\cancelto{}{\left\langle 1\right| p_+\left|2\right\rangle}\right)^{0}\left[\frac{1}{E_2-E_1}+\frac{1}{E_{-2}-E_1}\right]
\end{aligned}
$$

(để dấu "=" xảy ra)

$$
\begin{aligned}
&= \frac{1}{4}\frac{\hbar}{m_0}\left(k_-\left\langle 2\right| p_+\left|1\right\rangle\right)\left(k_+\left\langle 1\right| p_-\left|2\right\rangle\right)\left[\frac{1}{E_2-E_1}+\frac{1}{E_{-2}-E_1}\right]\\
&= a^2k_-k_+\underbrace{\frac{1}{4}\frac{\hbar}{a^2m_0}\left(\left\langle 2\right| p_+\left|1\right\rangle\right)\left(\left\langle 1\right| p_-\left|2\right\rangle\right)\left[\frac{1}{E_2-E_1}+\frac{1}{E_{-2}-E_1}\right]}_{\gamma_2}\\
&= a^2k^2\gamma_2
\end{aligned}
$$

$$
\begin{aligned}
H_{0,2}^{(2)} &= \frac{1}{2}\sum_l H_{0,l}^{'} H_{l,2}^{'} \left[\frac{1}{E_0 - E_l} + \frac{1}{E_2 - E_l}\right] \\
&= \frac{1}{2} H_{0,-1}^{'} H_{-1,2}^{'} \left[\frac{1}{E_0 - E_{-1}} + \frac{1}{E_2 - E_{-1}}\right] + \frac{1}{2} H_{0,1}^{'} H_{1,2}^{'} \left[\frac{1}{E_0 - E_1} + \frac{1}{E_2 - E_1}\right] \\
&= \frac{1}{4}\frac{\hbar}{m_0}\Big(k_+ \langle 0| p_- |-1\rangle + k_- \langle 0| p_+ |-1\rangle\Big)\Big(k_+ \langle -1| p_- |2\rangle + k_- \langle -1| p_+ |2\rangle\Big)\left[\frac{1}{E_0 - E_{-1}} + \frac{1}{E_2 - E_{-1}}\right] \\
+&\frac{1}{4}\frac{\hbar}{m_0}\Big(k_+ \langle 0| p_- |1\rangle + k_- \langle 0| p_+ |1\rangle\Big)\Big(k_+ \langle 1| p_- |2\rangle + k_- \langle 1| p_+ |2\rangle\Big)\left[\frac{1}{E_0 - E_1} + \frac{1}{E_2 - E_1}\right] \\
&= \frac{1}{4}\frac{\hbar}{m_0}\Big(k_+ \langle 0| C_3^\dagger C_3 p_- C_3^\dagger C_3 |-1\rangle + k_- \langle 0| C_3^\dagger C_3 p_+ C_3^\dagger C_3 |-1\rangle\Big) \\
\times&\Big(k_+ \langle -1| C_3^\dagger C_3 p_- C_3^\dagger C_3 |2\rangle + k_- \langle -1| C_3^\dagger C_3 p_+ C_3^\dagger C_3 |2\rangle\Big)\left[\frac{1}{E_0 - E_{-1}} + \frac{1}{E_2 - E_{-1}}\right] \\
+&\frac{1}{4}\frac{\hbar}{m_0}\Big(k_+ \langle 0| C_3^\dagger C_3 p_- C_3^\dagger C_3 |1\rangle + k_- \langle 0| C_3^\dagger C_3 p_+ C_3^\dagger C_3 |1\rangle\Big) \\
\times&\Big(k_+ \langle 1| C_3^\dagger C_3 p_- C_3^\dagger C_3 |2\rangle + k_- \langle 1| C_3^\dagger C_3 p_+ C_3^\dagger C_3 |2\rangle\Big)\left[\frac{1}{E_0 - E_1} + \frac{1}{E_2 - E_1}\right] \\
&= \frac{1}{4}\frac{\hbar}{m_0}\left(k_+ e^{\frac{2i\pi(0-(-1)+1)}{3}} \cancelto{0}{\langle 0| p_- |-1\rangle} + k_- e^{\frac{2i\pi(0-(-1)-1)}{3}} \langle 0| p_+ |-1\rangle\right) \\
\times&\left(k_+ e^{\frac{2i\pi(-1-2+1)}{3}} \cancelto{0}{\langle -1| p_- |2\rangle} + k_- e^{\frac{2i\pi(-1-2-1)}{3}} \cancel{\langle -1| p_+ |2\rangle}\right)^{0}\left[\frac{1}{E_0 - E_{-1}} + \frac{1}{E_2 - E_{-1}}\right] \\
+&\frac{1}{4}\frac{\hbar}{m_0}\left(k_+ e^{\frac{2i\pi(0-1+1)}{3}} \langle 0| p_- |1\rangle + k_- e^{\frac{2i\pi(0-1-1)}{3}} \cancel{\langle 0| p_+ |1\rangle}\right)^{0} \\
\times&\left(k_+ e^{\frac{2i\pi(1-2+1)}{3}} \langle 1| p_- |2\rangle + k_- e^{\frac{2i\pi(1-2-1)}{3}} \cancel{\langle 1| p_+ |2\rangle}\right)^{0}\left[\frac{1}{E_0 - E_1} + \frac{1}{E_2 - E_1}\right] \\
&= \frac{1}{4}\frac{\hbar}{m_0}\Big(k_+ \langle 0| p_- |1\rangle\Big)\Big(k_+ \langle 1| p_- |2\rangle\Big)\left[\frac{1}{E_0 - E_1} + \frac{1}{E_2 - E_1}\right] \\
&= a^2 k_+^2 \underbrace{\frac{1}{4}\frac{\hbar}{a^2 m_0}\Big(\langle 0| p_+ |1\rangle\Big)\Big(\langle 1| p_+ |2\rangle\Big)\left[\frac{1}{E_0 - E_1} + \frac{1}{E_2 - E_1}\right]}_{\gamma_3} \\
&= a^2 k_+^2 \gamma_3
\end{aligned}
$$

To describe the presence of the magnetic field, we replace the wave vector $\mathbf{k}$, by canonial wave vector $\hat{\mathbf{k}} = -i\boldsymbol{\nabla} + \dfrac{e}{\hbar}\mathbf{A}$, where $\mathbf{A}$ is vector potential and $\mathbf{B} = \boldsymbol{\nabla} \times \mathbf{A}$.

$$D(C_3(-\tfrac{2\pi}{3})) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1/2 & \sqrt{3}/2 \\ 0 & -\sqrt{3}/2 & -1/2 \end{pmatrix}, \quad D(C_3(-\tfrac{4\pi}{3})) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1/2 & -\sqrt{3}/2 \\ 0 & \sqrt{3}/2 & -1/2 \end{pmatrix},$$

$$D(\sigma_\nu) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad D(\sigma'_\nu) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1/2 & -\sqrt{3}/2 \\ 0 & -\sqrt{3}/2 & -1/2 \end{pmatrix}, \tag{28}$$

$$D(\sigma''_\nu) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1/2 & \sqrt{3}/2 \\ 0 & \sqrt{3}/2 & -1/2 \end{pmatrix}.$$

$$\begin{aligned} \mathcal{E}(\mathbf{R}_2) &= D(\sigma'_\nu)\mathcal{E}(\mathbf{R}_1)D^\dagger(\sigma'_\nu) \\ &= \begin{pmatrix} t_0 & \frac{1}{2}t_1 - \frac{\sqrt{3}}{2}t_2 & -\frac{\sqrt{3}}{2}t_1 - \frac{1}{2}t_2 \\ -\frac{1}{2}t_1 - \frac{\sqrt{3}}{2}t_2 & \frac{1}{4}t_{11} + \frac{3}{4}t_{22} & -\frac{\sqrt{3}}{4}t_{11} - t_{12} + \frac{\sqrt{3}}{4}t_{22} \\ \frac{\sqrt{3}}{2}t_1 - \frac{1}{2}t_2 & -\frac{\sqrt{3}}{4}t_{11} + t_{12} + \frac{\sqrt{3}}{4}t_{22} & \frac{3}{4}t_{11} + \frac{1}{4}t_{22} \end{pmatrix}, \end{aligned} \tag{29}$$

$$\begin{aligned} \mathcal{E}(\mathbf{R}_3) &= D(C(-\tfrac{2\pi}{3}))\mathcal{E}(\mathbf{R}_1)D^\dagger(C(-\tfrac{2\pi}{3})) \\ &= \begin{pmatrix} t_0 & -\frac{1}{2}t_1 + \frac{\sqrt{3}}{2}t_2 & -\frac{\sqrt{3}}{2}t_1 - \frac{1}{2}t_2 \\ \frac{1}{2}t_1 + \frac{\sqrt{3}}{2}t_2 & \frac{1}{4}t_{11} + \frac{3}{4}t_{22} & \frac{\sqrt{3}}{4}t_{11} + t_{12} - \frac{\sqrt{3}}{4}t_{22} \\ \frac{\sqrt{3}}{2}t_1 - \frac{1}{2}t_2 & \frac{\sqrt{3}}{4}t_{11} - t_{12} - \frac{\sqrt{3}}{4}t_{22} & \frac{3}{4}t_{11} + \frac{1}{4}t_{22} \end{pmatrix}, \end{aligned} \tag{30}$$

$$\mathcal{E}(\mathbf{R}_4) = D(\sigma_\nu)\mathcal{E}(\mathbf{R}_1)D^\dagger(\sigma_\nu) = \begin{pmatrix} t_0 & -t_1 & t_2 \\ t_1 & t_{11} & -t_{12} \\ t_2 & t_{12} & t_{22} \end{pmatrix}, \tag{31}$$

$$\begin{aligned} \mathcal{E}(\mathbf{R}_5) &= D(C(-\tfrac{4\pi}{3}))\mathcal{E}(\mathbf{R}_1)D^\dagger(C(-\tfrac{4\pi}{3})) \\ &= \begin{pmatrix} t_0 & -\frac{1}{2}t_1 - \frac{\sqrt{3}}{2}t_2 & \frac{\sqrt{3}}{2}t_1 - \frac{1}{2}t_2 \\ \frac{1}{2}t_1 - \frac{\sqrt{3}}{2}t_2 & \frac{1}{4}t_{11} + \frac{3}{4}t_{22} & -\frac{\sqrt{3}}{4}t_{11} + t_{12} + \frac{\sqrt{3}}{4}t_{22} \\ -\frac{\sqrt{3}}{2}t_1 - \frac{1}{2}t_2 & -\frac{\sqrt{3}}{4}t_{11} - t_{12} + \frac{\sqrt{3}}{4}t_{22} & \frac{3}{4}t_{11} + \frac{1}{4}t_{22} \end{pmatrix}, \end{aligned} \tag{32}$$

$$\begin{aligned} \mathcal{E}(\mathbf{R}_6) &= D(\sigma''_\nu)\mathcal{E}(\mathbf{R}_1)D^\dagger(\sigma''_\nu) \\ &= \begin{pmatrix} t_0 & \frac{1}{2}t_1 + \frac{\sqrt{3}}{2}t_2 & \frac{\sqrt{3}}{2}t_1 - \frac{1}{2}t_2 \\ -\frac{1}{2}t_1 + \frac{\sqrt{3}}{2}t_2 & \frac{1}{4}t_{11} + \frac{3}{4}t_{22} & \frac{\sqrt{3}}{4}t_{11} - t_{12} - \frac{\sqrt{3}}{4}t_{22} \\ -\frac{\sqrt{3}}{2}t_1 - \frac{1}{2}t_2 & \frac{\sqrt{3}}{4}t_{11} - t_{12} - \frac{\sqrt{3}}{4}t_{22} & \frac{3}{4}t_{11} + \frac{1}{4}t_{22} \end{pmatrix}, \end{aligned} \tag{33}$$

$$\begin{aligned}\mathcal{E}(\mathbf{R}_9) &= D(\sigma'_\nu)\mathcal{E}(\mathbf{R}_7)D^\dagger(\sigma'_\nu) \\ &= \end{aligned} \tag{34}$$

$$\mathcal{E}(\mathbf{R}_{10}) = \tag{35}$$

$$\mathcal{E}(\mathbf{R}_{11}) = D(C(-\frac{2\pi}{3}))\mathcal{E}(\mathbf{R}_7)D^\dagger(C(-\frac{2\pi}{3})) \tag{36}$$

$$\mathcal{E}(\mathbf{R}_{12}) = D(\sigma_\nu)\mathcal{E}(\mathbf{R}_8)D^\dagger(\sigma_\nu) \tag{37}$$

$$\mathcal{E}(\mathbf{R}_9) = D(\sigma'_\nu)\mathcal{E}(\mathbf{R}_7)D^\dagger(\sigma'_\nu) \tag{38}$$

$$\mathcal{E}(\mathbf{R}_9) = D(\sigma'_\nu)\mathcal{E}(\mathbf{R}_7)D^\dagger(\sigma'_\nu) \tag{39}$$

$$\mathcal{E}(\mathbf{R}_9) = D(\sigma'_\nu)\mathcal{E}(\mathbf{R}_7)D^\dagger(\sigma'_\nu) \tag{40}$$

$$\mathcal{E}(\mathbf{R}_9) = D(\sigma'_\nu)\mathcal{E}(\mathbf{R}_7)D^\dagger(\sigma'_\nu) \tag{41}$$

$$\mathcal{E}(\mathbf{R}_9) = D(\sigma'_\nu)\mathcal{E}(\mathbf{R}_7)D^\dagger(\sigma'_\nu) \tag{42}$$

$$\mathcal{E}(\mathbf{R}_9) = D(\sigma'_\nu)\mathcal{E}(\mathbf{R}_7)D^\dagger(\sigma'_\nu) \tag{43}$$

The nearest-neighbor tight-binding Hamiltonian now can be written as

$$H^{\mathrm{NN}}(\mathbf{k}) = \begin{pmatrix} h_0 & h_1 & h_2 \\ h_1^* & h_{11} & h_{12} \\ h_2^* & h_{12}^* & h_{22} \end{pmatrix}, \tag{44}$$

$$\mathbf{R}_1 = \begin{pmatrix} r_0 & r_1 & \frac{r_1}{\sqrt{3}} \\ h.c & r_{11} & r_{12} \\ h.c & h.c & r_{11} + \frac{2r_{12}}{\sqrt{3}} \end{pmatrix}, \tag{45}$$

$$\mathbf{R}_2 = \begin{pmatrix} r_0 & 0 & \frac{2r_2}{\sqrt{3}} \\ h.c & r_{11} + \sqrt{3}r_{12} & 0 \\ h.c & h.c & -r_{11} - \frac{r_{12}}{\sqrt{3}} \end{pmatrix}, \tag{46}$$

$$\mathbf{R}_3 = \begin{pmatrix} r_0 & -r_1 & -\frac{r_1}{\sqrt{3}} \\ h.c & r_{11} & -r_{12} \\ h.c & h.c & r_{11} + \frac{2r_{12}}{\sqrt{3}} \end{pmatrix}, \tag{47}$$

$$\mathbf{R}_4 = \begin{pmatrix} r_0 & r_2 & -\frac{r_2}{\sqrt{3}} \\ h.c & r_{11} & r_{12} \\ h.c & h.c & r_{11} + \frac{2r_{12}}{\sqrt{3}} \end{pmatrix}, \tag{48}$$

$$\mathbf{R}_5 = \begin{pmatrix} r_0 & 0 & \frac{2r_1}{\sqrt{3}} \\ h.c & r_{11} + \sqrt{3}r12 & 0 \\ h.c & h.c & -r_{11} - \frac{r_{12}}{\sqrt{3}} \end{pmatrix}, \tag{49}$$

$$\mathbf{R}_6 = \begin{pmatrix} r_0 & -r_2 & -\frac{r_2}{\sqrt{3}} \\ h.c & r_{11} & -r_{12} \\ h.c & h.c & r_{11} + \frac{2r_{12}}{\sqrt{3}} \end{pmatrix}, \tag{50}$$

# Tài liệu tham khảo

[1] Andor Kormányos, Viktor Zólyomi, Neil D. Drummond, Péter Rakyta, Guido Burkard, and Vladimir I. Fal'ko. Monolayer $mos_2$: Trigonal warping, the $\Gamma$ valley, and spin-orbit coupling effects. *Phys. Rev. B*, 88:045416, Jul 2013.

[2] Jun John Sakurai and Jim Napolitano. *Modern quantum mechanics.* Cambridge University Press, 2020.

[3] Fengyuan Xuan and Su Ying Quek. Valley zeeman effect and landau levels in two-dimensional transition metal dichalcogenides. *Phys. Rev. Res.*, 2:033256, Aug 2020.