

Thesis

TRẦN KHÔI NGUYỄN
VẬT LÝ LÝ THUYẾT

Ngày 12 tháng 10 năm 2024

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

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

$$|\phi_1^1\rangle = d_{z^2}, \quad |\phi_1^2\rangle = d_{xy}, \quad |\phi_2^2\rangle = d_{x^2-y^2}$$

$$\begin{aligned} H_{\mu\mu'}^{jj'}(\mathbf{k}) = & \sum_{\mu\mu'jj'} e^{i\mathbf{k}\cdot\mathbf{R}_1} E_{\mu\mu'}^{jj'}(\mathbf{R}_1) + \sum_{\mu\mu'jj'} e^{i\mathbf{k}\cdot\mathbf{R}_2} E_{\mu\mu'}^{jj'}(\mathbf{R}_2) + \sum_{\mu\mu'jj'} e^{i\mathbf{k}\cdot\mathbf{R}_3} E_{\mu\mu'}^{jj'}(\mathbf{R}_3) \\ & + \sum_{\mu\mu'jj'} e^{i\mathbf{k}\cdot\mathbf{R}_4} E_{\mu\mu'}^{jj'}(\mathbf{R}_4) + \sum_{\mu\mu'jj'} e^{i\mathbf{k}\cdot\mathbf{R}_5} E_{\mu\mu'}^{jj'}(\mathbf{R}_5) + \sum_{\mu\mu'jj'} e^{i\mathbf{k}\cdot\mathbf{R}_6} E_{\mu\mu'}^{jj'}(\mathbf{R}_6) \end{aligned}$$

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

$$\begin{aligned} h_0 &= \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \langle \phi_1^1(\mathbf{r}) | H | \phi_1^1(\mathbf{r} - \mathbf{R}) \rangle; \quad h_1 = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \langle \phi_1^1(\mathbf{r}) | H | \phi_1^2(\mathbf{r} - \mathbf{R}) \rangle \\ h_2 &= \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \langle \phi_1^1(\mathbf{r}) | H | \phi_2^2(\mathbf{r} - \mathbf{R}) \rangle; \quad h_{11} = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \langle \phi_1^2(\mathbf{r}) | H | \phi_1^2(\mathbf{r} - \mathbf{R}) \rangle \\ h_{12} &= \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \langle \phi_1^2(\mathbf{r}) | H | \phi_2^2(\mathbf{r} - \mathbf{R}) \rangle; \quad h_{22} = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \langle \phi_2^2(\mathbf{r}) | H | \phi_2^2(\mathbf{r} - \mathbf{R}) \rangle \end{aligned}$$

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

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

trong đó $D^1(\hat{g}_n) = 1$

$$\begin{aligned} D^2(E) &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\ D^2(\hat{C}_3) &= \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix} = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \\ D^2(\hat{C}_3^2) &= \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \end{aligned}$$

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

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 $\vec{R}_5 = \sigma'_\nu \vec{R}_4$ mà $C_3^2 \vec{R}_5 = \vec{R}_1 \Rightarrow C_3^2 \sigma'_\nu \vec{R}_4 = \vec{R}_1$

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

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

Tương tự ta tính cho

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

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 σ_ν đánh lên \mathbf{R}_1 ta được $\rightarrow \mathbf{R}_6$ (dưới dạng ma trận)

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

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

Kiểm tra điều trên:

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

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

* **h0**

$$\begin{aligned} h_0 &= \sum_{\mathbf{R} \neq 0} e^{i\mathbf{k} \cdot \mathbf{R}} \langle \phi_1^1(\mathbf{r}) | H | \phi_1^1(\mathbf{r} - \mathbf{R}) \rangle + \langle \phi_1^1(\mathbf{r}) | H | \phi_1^1(\mathbf{r}) \rangle \\ &= e^{i\mathbf{k} \cdot \mathbf{R}_1} \langle \phi_1^1(\mathbf{r}) | H | \phi_1^1(\mathbf{r} - \mathbf{R}_1) \rangle + e^{i\mathbf{k} \cdot \mathbf{R}_4} \langle \phi_1^1(\mathbf{r}) | H | \phi_1^1(\mathbf{r} - \mathbf{R}_4) \rangle \\ &+ e^{i\mathbf{k} \cdot \mathbf{R}_2} \langle \phi_1^1(\mathbf{r}) | H | \phi_1^1(\mathbf{r} - \mathbf{R}_2) \rangle + e^{i\mathbf{k} \cdot \mathbf{R}_5} \langle \phi_1^1(\mathbf{r}) | H | \phi_1^1(\mathbf{r} - \mathbf{R}_5) \rangle \\ &+ e^{i\mathbf{k} \cdot \mathbf{R}_3} \langle \phi_1^1(\mathbf{r}) | H | \phi_1^1(\mathbf{r} - \mathbf{R}_3) \rangle + e^{i\mathbf{k} \cdot \mathbf{R}_6} \langle \phi_1^1(\mathbf{r}) | H | \phi_1^1(\mathbf{r} - \mathbf{R}_6) \rangle + \epsilon_1 \\ &= e^{ik_x a} E_{11}^{11}(\mathbf{R}_1) + e^{-ik_x a} E_{11}^{11}(\mathbf{R}_4) + e^{i\left(k_x \frac{a}{2} - k_y \frac{a\sqrt{3}}{2}\right)} E_{11}^{11}(\mathbf{R}_2) + e^{-i\left(k_x \frac{a}{2} - k_y \frac{a\sqrt{3}}{2}\right)} E_{11}^{11}(\mathbf{R}_5) \\ &+ e^{-i\left(k_x \frac{a}{2} + k_y \frac{a\sqrt{3}}{2}\right)} E_{11}^{11}(\mathbf{R}_3) + e^{i\left(k_x \frac{a}{2} + k_y \frac{a\sqrt{3}}{2}\right)} E_{11}^{11}(\mathbf{R}_6) + \epsilon_1 \\ &= 2E_{11}^{11}(\mathbf{R}_1) (\cos 2\alpha + 2\cos \alpha \cos \beta) + \epsilon_1 \end{aligned}$$

* h1

$$\begin{aligned}
h_1 &= \sum_{\mathbf{R} \neq 0} e^{i\mathbf{k} \cdot \mathbf{R}} \langle \phi_1^1(\mathbf{r}) | H | \phi_1^2(\mathbf{r} - \mathbf{R}) \rangle \\
&= e^{ik_x a} E_{11}^{12}(\mathbf{R}_1) + e^{-ik_x a} E_{11}^{12}(\mathbf{R}_4) + e^{i\left(k_x \frac{a}{2} - k_y \frac{a\sqrt{3}}{2}\right)} E_{11}^{12}(\mathbf{R}_2) + e^{-i\left(k_x \frac{a}{2} - k_y \frac{a\sqrt{3}}{2}\right)} E_{11}^{12}(\mathbf{R}_5) \\
&\quad + e^{-i\left(k_x \frac{a}{2} + k_y \frac{a\sqrt{3}}{2}\right)} E_{11}^{12}(\mathbf{R}_3) + e^{i\left(k_x \frac{a}{2} + k_y \frac{a\sqrt{3}}{2}\right)} E_{11}^{12}(\mathbf{R}_6)
\end{aligned}$$

trong đó

$$\begin{aligned}
E^{12}(\mathbf{R}_2) &= E^{12}(\sigma'_\nu \mathbf{R}_1) = D^1(\sigma'_\nu) E^{12}(\mathbf{R}_1) \left[D^2(\sigma'_\nu) \right]^\dagger \\
&= \begin{pmatrix} 1 \\ 1 \end{pmatrix} \begin{pmatrix} E_{11}^{12}(\mathbf{R}_1) & E_{12}^{12}(\mathbf{R}_1) \end{pmatrix} \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \\
&= \begin{pmatrix} \frac{E_{11}^{12}(\mathbf{R}_1) - \sqrt{3}E_{12}^{12}(\mathbf{R}_1)}{2} & \frac{-E_{11}^{12}(\mathbf{R}_1)\sqrt{3} - E_{12}^{12}(\mathbf{R}_1)}{2} \end{pmatrix} \\
\Rightarrow E_{11}^{12}(\mathbf{R}_2) &= \frac{E_{11}^{12}(\mathbf{R}_1) - \sqrt{3}E_{12}^{12}(\mathbf{R}_1)}{2}
\end{aligned}$$

Tương tự ta có cho:

$$\begin{aligned}
E_{11}^{12}(\mathbf{R}_3) &= \frac{-E_{11}^{12}(\mathbf{R}_1) + \sqrt{3}E_{12}^{12}(\mathbf{R}_1)}{2} ; E_{11}^{12}(\mathbf{R}_4) = -E_{11}^{12}(\mathbf{R}_1) \\
E_{11}^{12}(\mathbf{R}_5) &= \frac{-E_{11}^{12}(\mathbf{R}_1) - \sqrt{3}E_{12}^{12}(\mathbf{R}_1)}{2} ; E_{11}^{12}(\mathbf{R}_6) = \frac{E_{11}^{12}(\mathbf{R}_1) + \sqrt{3}E_{12}^{12}(\mathbf{R}_1)}{2}
\end{aligned}$$

$$\begin{aligned}
h_1 &= e^{i2\alpha} E_{11}^{12}(\mathbf{R}_1) - e^{i2\alpha} E_{11}^{12}(\mathbf{R}_1) \\
&\quad + e^{i(\alpha-\beta)} \frac{E_{11}^{12}(\mathbf{R}_1) - \sqrt{3}E_{12}^{12}(\mathbf{R}_1)}{2} + e^{-i(\alpha+\beta)} \frac{-E_{11}^{12}(\mathbf{R}_1) + \sqrt{3}E_{12}^{12}(\mathbf{R}_1)}{2} \\
&\quad + e^{i(-\alpha+\beta)} \frac{-E_{11}^{12}(\mathbf{R}_1) - \sqrt{3}E_{12}^{12}(\mathbf{R}_1)}{2} + e^{i(\alpha+\beta)} \frac{E_{11}^{12}(\mathbf{R}_1) + \sqrt{3}E_{12}^{12}(\mathbf{R}_1)}{2} \\
&= 2i \sin 2\alpha E_{11}^{12}(\mathbf{R}_1) + 2i \frac{E_{11}^{12}(\mathbf{R}_1)}{2} \sin(\alpha - \beta) - 2 \frac{E_{12}^{12}(\mathbf{R}_1) \sqrt{3}}{2} \cos(\alpha - \beta) \\
&\quad + 2i \frac{E_{11}^{12}(\mathbf{R}_1)}{2} \sin(\alpha + \beta) + 2 \frac{E_{12}^{12}(\mathbf{R}_1) \sqrt{3}}{2} \cos(\alpha + \beta) \\
&= -2\sqrt{3}t_2 \sin \alpha \sin \beta + 2it_1 (\sin 2\alpha + \sin \alpha \cos \beta)
\end{aligned}$$

Đặt

$$\begin{aligned}
t_0 &= E_{11}^{11}(\mathbf{R}_1); \quad t_1 = E_{11}^{12}(\mathbf{R}_1); \quad t_2 = E_{12}^{12}(\mathbf{R}_1); \\
t_{11} &= E_{11}^{22}(\mathbf{R}_1); \quad t_{12} = E_{12}^{22}(\mathbf{R}_1); \quad t_{21} = E_{21}^{22}(\mathbf{R}_1); \quad t_{22} = E_{22}^{22}(\mathbf{R}_1);
\end{aligned}$$

* **h22**

$$\begin{aligned}
h_{22} &= \sum_R e^{i\mathbf{k}\cdot\mathbf{R}} E_{22}^{22}(\mathbf{R}) \\
&= e^{i\mathbf{k}\cdot\mathbf{R}_1} E_{22}^{22}(\mathbf{R}_1) + e^{i\mathbf{k}\cdot\mathbf{R}_2} E_{22}^{22}(\mathbf{R}_2) + e^{i\mathbf{k}\cdot\mathbf{R}_3} E_{22}^{22}(\mathbf{R}_3) \\
&\quad + e^{i\mathbf{k}\cdot\mathbf{R}_4} E_{22}^{22}(\mathbf{R}_4) + e^{i\mathbf{k}\cdot\mathbf{R}_5} E_{22}^{22}(\mathbf{R}_5) + e^{i\mathbf{k}\cdot\mathbf{R}_6} E_{22}^{22}(\mathbf{R}_6) + E_{22}^{22}(\mathbf{0})
\end{aligned}$$

$$\begin{aligned}
E_{22}^{22}(\mathbf{R}_2) &= E^{22}(\sigma'_\nu \mathbf{R}_1) \\
&= D^2(\sigma'_\nu) E^{22}(\mathbf{R}_1) \left[D^2(\sigma'_\nu) \right]^\dagger \\
&= \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} E_{11}^{22}(\mathbf{R}_1) & E_{12}^{22}(\mathbf{R}_1) \\ E_{21}^{22}(\mathbf{R}_1) & E_{22}^{22}(\mathbf{R}_1) \end{pmatrix} \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \\
&= \begin{pmatrix} \frac{t_{11}-t_{12}\sqrt{3}-t_{21}\sqrt{3}+3t_{22}}{4} & \frac{-t_{11}\sqrt{3}-t_{12}+3t_{21}+\sqrt{3}t_{22}}{4} \\ \frac{-t_{11}\sqrt{3}+3t_{12}-t_{21}+\sqrt{3}t_{22}}{4} & \frac{3t_{11}+t_{12}\sqrt{3}+c\sqrt{3}+t_{22}}{4} \end{pmatrix}
\end{aligned}$$

$$\Rightarrow E_{22}^{22}(\mathbf{R}_2) = \frac{3t_{11} + t_{12}\sqrt{3} + c\sqrt{3} + t_{22}}{4}$$

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:

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

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

***h11**

$$\begin{aligned}
H_{11}^{22} &= \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} E_{11}^{22}(\mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}_1} E_{11}^{22}(\mathbf{R}_1) + e^{i\mathbf{k}\cdot\mathbf{R}_2} E_{11}^{22}(\mathbf{R}_2) + e^{i\mathbf{k}\cdot\mathbf{R}_3} E_{11}^{22}(\mathbf{R}_3) \\
&+ e^{i\mathbf{k}\cdot\mathbf{R}_4} E_{11}^{22}(\mathbf{R}_4) + e^{i\mathbf{k}\cdot\mathbf{R}_5} E_{11}^{22}(\mathbf{R}_5) + e^{i\mathbf{k}\cdot\mathbf{R}_6} E_{11}^{22}(\mathbf{R}_6) + E_{11}^{22}(\mathbf{0}) \\
&= e^{ik_x a} E_{11}^{22}(\mathbf{R}_1) + e^{i\left(k_x \frac{a}{2} - k_y \frac{a\sqrt{3}}{2}\right)} E_{11}^{22}(\mathbf{R}_2) + e^{i\left(-k_x \frac{a}{2} - k_y \frac{a\sqrt{3}}{2}\right)} E_{11}^{22}(\mathbf{R}_3) \\
&+ e^{-ik_x a} E_{11}^{22}(\mathbf{R}_4) + e^{i\left(-k_x \frac{a}{2} + k_y \frac{a\sqrt{3}}{2}\right)} E_{11}^{22}(\mathbf{R}_5) + e^{i\left(k_x \frac{a}{2} + k_y \frac{a\sqrt{3}}{2}\right)} E_{11}^{22}(\mathbf{R}_6) + \epsilon_2 \\
&= e^{2i\alpha}t_{11} + e^{i(\alpha-\beta)} \frac{t_{11} - \sqrt{3}t_{12} - \sqrt{3}t_{21} + 3t_{22}}{4} \\
&+ e^{i(-\alpha-\beta)} \frac{t_{11} - \sqrt{3}t_{12} - \sqrt{3}t_{21} + 3t_{22}}{4} + e^{-2i\alpha}t_{11} \\
&+ e^{i(-\alpha+\beta)} \frac{t_{11} + \sqrt{3}t_{12} + \sqrt{3}t_{21} + 3t_{22}}{4} + e^{i(\alpha+\beta)} \frac{t_{11} + \sqrt{3}t_{12} + \sqrt{3}t_{21} + 3t_{22}}{4} + \epsilon_2 \\
&= 2t_{11}\cos(2\alpha) + (t_{11} + 3t_{22})\cos(\alpha)\cos(\beta) + \epsilon_2
\end{aligned}$$

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

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

$$\begin{aligned}
E^{22}(\mathbf{R}_2) &= E^{22}(\sigma'_\nu \mathbf{R}_1) = D^2(\sigma'_\nu) E^{22}(\mathbf{R}_1) [D^2(\sigma'_\nu)]^\dagger \\
&= \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \text{ Trong đó } \begin{pmatrix} a = t_{11} \\ b = t_{12} \\ c = t_{21} \\ d = t_{22} \end{pmatrix} \\
\Rightarrow E^{22}_{11}(\mathbf{R}_2) &= \frac{a - \sqrt{3}b - \sqrt{3}c + 3d}{4}
\end{aligned}$$

Tương tự ta tìm được:

$$\begin{aligned}
E^{22}_{11}(\mathbf{R}_3) &= \frac{a - \sqrt{3}b - \sqrt{3}c + 3d}{4} \\
E^{22}_{11}(\mathbf{R}_4) &= a \\
E^{22}_{11}(\mathbf{R}_5) &= \frac{a + \sqrt{3}b + \sqrt{3}c + 3d}{4} \\
E^{22}_{11}(\mathbf{R}_6) &= \frac{a + \sqrt{3}b + \sqrt{3}c + 3d}{4}
\end{aligned}$$

*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 $B = \begin{pmatrix} 0 \\ 0 \\ B \end{pmatrix}$.

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

$$= \left(\frac{\partial}{\partial y} A_z - \frac{\partial}{\partial z} A_y \right) \vec{i} + \left(\frac{\partial}{\partial z} A_x - \frac{\partial}{\partial x} A_z \right) \vec{j} + \left(\frac{\partial}{\partial x} A_y - \frac{\partial}{\partial y} A_x \right) \vec{k}$$

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

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

* $\mathbf{h0}$

$$h_0 = H_{11}^{11}(\mathbf{k}) = \sum_{\mathbf{R}} e^{\frac{ie}{\hbar} \int_0^{\mathbf{R}} A(\mathbf{r}') d\mathbf{r}'} e^{i\mathbf{k} \cdot \mathbf{R}} E_{11}^{11}(\mathbf{R})$$

$$= e^{\frac{ie}{\hbar} \int_0^{\mathbf{R}_1} A(\mathbf{r}') d\mathbf{r}'} e^{i\mathbf{k} \cdot \mathbf{R}_1} E_{11}^{11}(\mathbf{R}_1) + e^{\frac{ie}{\hbar} \int_0^{\mathbf{R}_2} A(\mathbf{r}') d\mathbf{r}'} e^{i\mathbf{k} \cdot \mathbf{R}_2} E_{11}^{11}(\mathbf{R}_2)$$

$$+ e^{\frac{ie}{\hbar} \int_0^{\mathbf{R}_3} A(\mathbf{r}') d\mathbf{r}'} e^{i\mathbf{k} \cdot \mathbf{R}_3} E_{11}^{11}(\mathbf{R}_3) + e^{\frac{ie}{\hbar} \int_0^{\mathbf{R}_4} A(\mathbf{r}') d\mathbf{r}'} e^{i\mathbf{k} \cdot \mathbf{R}_4} E_{11}^{11}(\mathbf{R}_4)$$

$$+ e^{\frac{ie}{\hbar} \int_0^{\mathbf{R}_5} A(\mathbf{r}') d\mathbf{r}'} e^{i\mathbf{k} \cdot \mathbf{R}_5} E_{11}^{11}(\mathbf{R}_5) + e^{\frac{ie}{\hbar} \int_0^{\mathbf{R}_6} A(\mathbf{r}') d\mathbf{r}'} e^{i\mathbf{k} \cdot \mathbf{R}_6} E_{11}^{11}(\mathbf{R}_6)$$

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

Đặt $A = (P(x, y), Q(x, y), R(x, y)) = (0, Bx, 0)$

Phương trình tham số cho x, y :

$$x = x(t) = x_0 + \alpha t$$

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

C là đường cong đi từ $\mathbf{R}_0 \rightarrow \mathbf{R}$

$$*\mathbf{R}_0 \longrightarrow \mathbf{R}_1$$

$$(0,0) \quad (a,0)$$

Ta có:

$$x = at$$

$$y = 0$$

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

$$= \int_0^1 \left[0 \frac{dx}{dt} + Bx0 + 0 \frac{dz}{dt} \right] dt = 0$$

$$*\mathbf{R}_0 \longrightarrow \mathbf{R}_2$$

$$(0,0) \quad \left(\frac{a}{2}, -\frac{a\sqrt{3}}{2}\right)$$

Ta có:

$$x = \frac{a}{2}t$$

$$y = -\frac{a\sqrt{3}}{2}t$$

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

$$= \int_0^1 \left[0 \frac{dx}{dt} + Bx \left(-\frac{a\sqrt{3}}{2} \right) + 0 \frac{dz}{dt} \right] dt = -\frac{Ba^2\sqrt{3}}{8}$$

$$*\mathbf{R}_0 \longrightarrow \mathbf{R}_3$$

$$(0,0) \quad \left(-\frac{a}{2}, -\frac{a\sqrt{3}}{2}\right)$$

Ta có:

$$x = -\frac{a}{2}t$$

$$y = -\frac{a\sqrt{3}}{2}t$$

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

$$= \int_0^1 \left[0 \frac{dx}{dt} + Bx \left(-\frac{a\sqrt{3}}{2} \right) + 0 \frac{dz}{dt} \right] dt = B \left(-\frac{a}{2} \right) \left(-\frac{a\sqrt{3}}{2} \right) \int_0^1 t dt$$

$$= \frac{Ba^2\sqrt{3}}{8}$$

Xét $\mathbf{R}_4, \mathbf{R}_5, \mathbf{R}_6$: ta nhận thấy có thể đưa đường cong \mathbf{C} từ \mathbf{R}_0 cho tới \mathbf{R} về các dạng của $\mathbf{R}_1, \mathbf{R}_2, \mathbf{R}_3$. Lúc này đường cong sẽ là $-\mathbf{C}$

Dựa vào tính chất của tích phân đường:

$$\begin{aligned}\int_C \vec{f} d\vec{r} &= - \int_{-C} \vec{f} d\vec{r} \\ \Rightarrow - \int_C \vec{f} d\vec{r} &= \int_{-C} \vec{f} d\vec{r}\end{aligned}$$

$$*\mathbf{R}_0 \longrightarrow \mathbf{R}_4$$

$$(0,0) \quad (0,-a)$$

Ta có:

$$x = -at$$

$$y = 0$$

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

$$*\mathbf{R}_0 \longrightarrow \mathbf{R}_5$$

$$(0,0) \quad \left(-\frac{a}{2}, \frac{a\sqrt{3}}{2}\right)$$

Ta có:

$$x = -\frac{a}{2}t$$

$$y = \frac{a\sqrt{3}}{2}t$$

$$\begin{aligned}\Rightarrow \int_{-C} \mathbf{A}(\mathbf{r}') \cdot d\mathbf{r}' &= - \int_C \mathbf{A}(\mathbf{r}') \cdot d\mathbf{r}' = \int_{t_B}^{t_A} \left[P(x, y) \frac{dx}{dt} + Q(x, y) \frac{dy}{dt} + R(x, y) \frac{dz}{dt} \right] dt \\ &= - \int_0^1 \left[0 \frac{dx}{dt} + Bx \frac{a\sqrt{3}}{2} + 0 \frac{dz}{dt} \right] dt = \frac{Ba^2\sqrt{3}}{8}\end{aligned}$$

$$*\mathbf{R}_0 \xrightarrow{(0,0)} \mathbf{R}_6 \xrightarrow{(\frac{a}{2}, \frac{a\sqrt{3}}{2})}$$

Ta có:

$$\begin{aligned} x &= \frac{a}{2}t \\ y &= \frac{a\sqrt{3}}{2}t \\ \Rightarrow \int_{-C} \mathbf{A}(\mathbf{r}') \cdot d\mathbf{r}' &= - \int_C \mathbf{A}(\mathbf{r}') \cdot d\mathbf{r}' = \int_{t_B}^{t_A} \left[P(x, y) \frac{dx}{dt} + Q(x, y) \frac{dy}{dt} + R(x, y) \frac{dz}{dt} \right] dt \\ &= - \int_0^1 \left[0 \frac{dx}{dt} + Bx \frac{a\sqrt{3}}{2} + 0 \frac{dz}{dt} \right] dt = - \frac{Ba^2\sqrt{3}}{8} \end{aligned}$$

Vậy h_0 có dạng:

$$\begin{aligned} h_0 = H_{11}^{11}(\mathbf{k}) &= e^0 e^{i\mathbf{k} \cdot \mathbf{R}_1} E_{11}^{11}(\mathbf{R}_1) + e^{-\frac{ie}{\hbar} \frac{Ba^2\sqrt{3}}{8}} e^{i\mathbf{k} \cdot \mathbf{R}_2} E_{11}^{11}(\mathbf{R}_2) \\ &+ e^{\frac{ie}{\hbar} \frac{Ba^2\sqrt{3}}{8}} e^{i\mathbf{k} \cdot \mathbf{R}_3} E_{11}^{11}(\mathbf{R}_3) + e^0 e^{i\mathbf{k} \cdot \mathbf{R}_4} E_{11}^{11}(\mathbf{R}_4) \\ &+ e^{\frac{ie}{\hbar} \frac{Ba^2\sqrt{3}}{8}} e^{i\mathbf{k} \cdot \mathbf{R}_5} E_{11}^{11}(\mathbf{R}_5) + e^{-\frac{ie}{\hbar} \frac{Ba^2\sqrt{3}}{8}} e^{i\mathbf{k} \cdot \mathbf{R}_6} E_{11}^{11}(\mathbf{R}_6) + \epsilon_1 \\ &= e^{ik_x a} E_{11}^{11}(\mathbf{R}_1) + e^{-ik_x a} E_{11}^{11}(\mathbf{R}_4) + e^{-\frac{ie}{\hbar} \frac{Ba^2\sqrt{3}}{8}} e^{i\left(k_x \frac{a}{2} - k_y \frac{a\sqrt{3}}{2}\right)} E_{11}^{11}(\mathbf{R}_2) \\ &+ e^{\frac{ie}{\hbar} \frac{Ba^2\sqrt{3}}{8}} e^{i\left(-k_x \frac{a}{2} - k_y \frac{a\sqrt{3}}{2}\right)} E_{11}^{11}(\mathbf{R}_3) + e^{\frac{ie}{\hbar} \frac{Ba^2\sqrt{3}}{8}} e^{i\left(-k_x \frac{a}{2} + k_y \frac{a\sqrt{3}}{2}\right)} E_{11}^{11}(\mathbf{R}_5) \\ &+ e^{-\frac{ie}{\hbar} \frac{Ba^2\sqrt{3}}{8}} e^{i\left(k_x \frac{a}{2} + k_y \frac{a\sqrt{3}}{2}\right)} E_{11}^{11}(\mathbf{R}_6) + \epsilon_1 \end{aligned}$$

Đặt $k_x \frac{a}{2} = \alpha$, $k_y \frac{a\sqrt{3}}{2} = \beta$, $\frac{e}{\hbar} \frac{Ba^2\sqrt{3}}{8} = \eta$, $\alpha - \beta = \delta$, $\alpha + \beta = \gamma$ và áp dụng các toán tử quay để biểu diễn \mathbf{R}_1 theo \mathbf{R}_1 .

$$\begin{aligned} E^{11}(\mathbf{R}_4) &= E^{11}(\sigma'' \mathbf{R}_4) = D^1(\sigma'') E^{11}(\mathbf{R}_1) \left[D^1(\sigma'') \right]^\dagger = E^{11}(\mathbf{R}_1) \\ E^{11}(\mathbf{R}_2) &= E^{11}(\sigma' \mathbf{R}_1) = D^1(\sigma') E^{11}(\mathbf{R}_1) \left[D^1(\sigma') \right]^\dagger = E^{11}(\mathbf{R}_1) \\ E^{11}(\mathbf{R}_3) &= E^{11}(C_3^2 \mathbf{R}_1) = D^1(C_3^2) E^{11}(\mathbf{R}_1) \left[D^1(C_3^2) \right]^\dagger = E^{11}(\mathbf{R}_1) \\ E^{11}(\mathbf{R}_5) &= E^{11}(C_3 \mathbf{R}_1) = D^1(C_3) E^{11}(\mathbf{R}_1) \left[D^1(C_3) \right]^\dagger = E^{11}(\mathbf{R}_1) \\ E^{11}(\mathbf{R}_6) &= E^{11}(\sigma \mathbf{R}_1) = D^1(\sigma) E^{11}(\mathbf{R}_1) \left[D^1(\sigma) \right]^\dagger = E^{11}(\mathbf{R}_1) \end{aligned}$$

$$\begin{aligned}
\Rightarrow h_0 &= 2E_{11}^{11}(\mathbf{R}_1) \cos(2\alpha) + (e^{-i\eta}e^{i\delta} + e^{i\eta}e^{-i\gamma} + e^{i\eta}e^{-i\delta} + e^{-i\eta}e^{i\gamma})E_{11}^{11}(\mathbf{R}_1) + \epsilon_1 \\
&= 2E_{11}^{11}(\mathbf{R}_1) \cos(2\alpha) + E_{11}^{11}(\mathbf{R}_1) \left[(\cos \eta - i \sin \eta)e^{i\delta} + (\cos \eta + i \sin \eta)e^{-i\delta} \right] \\
&+ E_{11}^{11}(\mathbf{R}_1) \left[(\cos \eta + i \sin \eta)e^{-i\gamma} + (\cos \eta - i \sin \eta)e^{i\gamma} \right] + \epsilon_1 \\
&= 2E_{11}^{11}(\mathbf{R}_1) \cos(2\alpha) + E_{11}^{11}(\mathbf{R}_1) \left[2 \cos \eta \cos \delta - i \sin \eta (2i \sin \delta) \right] \\
&+ E_{11}^{11}(\mathbf{R}_1) \left[2 \cos \eta \cos \gamma - i \sin \eta (2i \sin \gamma) \right] + \epsilon_1 \\
&= 2E_{11}^{11}(\mathbf{R}_1) \cos(2\alpha) + 2E_{11}^{11}(\mathbf{R}_1) \left[\cos \eta (\cos \gamma + \cos \delta) + \sin \eta (\sin \gamma + \sin \delta) \right] + \epsilon_1 \\
&= 2t_0 \left[\cos(2\alpha) + 2 \cos \eta \cos \alpha \cos \beta + 2 \sin \eta \sin \alpha \cos \beta \right] + \epsilon_1
\end{aligned}$$

* h1

$$\begin{aligned}
h_1 &= H_{11}^{12}(\mathbf{k}) = \sum_{\mathbf{R}} e^{\frac{i\epsilon}{\hbar} \int_0^{\mathbf{R}} A(\mathbf{r}') d\mathbf{r}'} e^{i\mathbf{k} \cdot \mathbf{R}} E_{11}^{12}(\mathbf{R}) \\
&= e^{\frac{i\epsilon}{\hbar} \int_0^{\mathbf{R}_1} A(\mathbf{r}') d\mathbf{r}'} e^{i\mathbf{k} \cdot \mathbf{R}_1} E_{11}^{12}(\mathbf{R}_1) + e^{\frac{i\epsilon}{\hbar} \int_0^{\mathbf{R}_2} A(\mathbf{r}') d\mathbf{r}'} e^{i\mathbf{k} \cdot \mathbf{R}_2} E_{11}^{12}(\mathbf{R}_2) \\
&+ e^{\frac{i\epsilon}{\hbar} \int_0^{\mathbf{R}_3} A(\mathbf{r}') d\mathbf{r}'} e^{i\mathbf{k} \cdot \mathbf{R}_3} E_{11}^{12}(\mathbf{R}_3) + e^{\frac{i\epsilon}{\hbar} \int_0^{\mathbf{R}_4} A(\mathbf{r}') d\mathbf{r}'} e^{i\mathbf{k} \cdot \mathbf{R}_4} E_{11}^{12}(\mathbf{R}_4) \\
&+ e^{\frac{i\epsilon}{\hbar} \int_0^{\mathbf{R}_5} A(\mathbf{r}') d\mathbf{r}'} e^{i\mathbf{k} \cdot \mathbf{R}_5} E_{11}^{12}(\mathbf{R}_5) + e^{\frac{i\epsilon}{\hbar} \int_0^{\mathbf{R}_6} A(\mathbf{r}') d\mathbf{r}'} e^{i\mathbf{k} \cdot \mathbf{R}_6} E_{11}^{12}(\mathbf{R}_6)
\end{aligned}$$

Trong đó:

$$\begin{aligned}
*E^{12}(\mathbf{R}_4) &= E^{12}(\sigma''\mathbf{R}_4) = D^1(\sigma'')E^{12}(\mathbf{R}_1) \left[D^2(\sigma'') \right]^\dagger \\
&= 1 \begin{pmatrix} E_{11}^{12}(\mathbf{R}_1) & E_{12}^{12}(\mathbf{R}_1) \end{pmatrix} \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \\
&= \begin{pmatrix} -E_{11}^{12}(\mathbf{R}_1) & E_{12}^{12}(\mathbf{R}_1) \end{pmatrix} \\
\Rightarrow E_{11}^{12}(\mathbf{R}_4) &= -E_{11}^{12}(\mathbf{R}_1), \quad E_{12}^{12}(\mathbf{R}_4) = E_{11}^{12}(\mathbf{R}_1)
\end{aligned}$$

$$\begin{aligned}
*E^{12}(\mathbf{R}_2) &= E^{12}(\sigma' \mathbf{R}_2) = D^1(\sigma') E^{12}(\mathbf{R}_1) \left[D^2(\sigma') \right]^\dagger \\
&= 1 \begin{pmatrix} E_{11}^{12}(\mathbf{R}_1) & E_{12}^{12}(\mathbf{R}_1) \end{pmatrix} \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \\
&= \begin{pmatrix} \frac{E_{11}^{12}(\mathbf{R}_1) - \sqrt{3}E_{12}^{12}(\mathbf{R}_1)}{2} & \frac{-\sqrt{3}E_{11}^{12}(\mathbf{R}_1) - E_{12}^{12}(\mathbf{R}_1)}{2} \end{pmatrix} \\
\Rightarrow E_{11}^{12}(\mathbf{R}_2) &= \frac{E_{11}^{12}(\mathbf{R}_1) - \sqrt{3}E_{12}^{12}(\mathbf{R}_1)}{2} \\
E_{12}^{12}(\mathbf{R}_2) &= \frac{-\sqrt{3}E_{11}^{12}(\mathbf{R}_1) - E_{12}^{12}(\mathbf{R}_1)}{2}
\end{aligned}$$

Một cách tương tự ta có cho:

$$\begin{aligned}
E_{11}^{12}(\mathbf{R}_3) &= \frac{-E_{11}^{12}(\mathbf{R}_1) + \sqrt{3}E_{12}^{12}(\mathbf{R}_1)}{2} ; E_{11}^{12}(\mathbf{R}_4) = -E_{11}^{12}(\mathbf{R}_1) \\
E_{11}^{12}(\mathbf{R}_5) &= \frac{-E_{11}^{12}(\mathbf{R}_1) - \sqrt{3}E_{12}^{12}(\mathbf{R}_1)}{2} ; E_{11}^{12}(\mathbf{R}_6) = \frac{E_{11}^{12}(\mathbf{R}_1) + \sqrt{3}E_{12}^{12}(\mathbf{R}_1)}{2}
\end{aligned}$$

$$\begin{aligned}
h_1 &= E_{11}^{12}(\mathbf{R}_1) \left(e^{ik_x a} - e^{-ik_x a} \right) + e^{-i\eta} e^{i\delta} \frac{E_{11}^{12}(\mathbf{R}_1) - \sqrt{3}E_{12}^{12}(\mathbf{R}_1)}{2} \\
&\quad + e^{i\eta} e^{-i\gamma} \frac{-E_{11}^{12}(\mathbf{R}_1) + \sqrt{3}E_{12}^{12}(\mathbf{R}_1)}{2} + e^{i\eta} e^{-i\delta} \frac{-E_{11}^{12}(\mathbf{R}_1) - \sqrt{3}E_{12}^{12}(\mathbf{R}_1)}{2} \\
&\quad + e^{-i\eta} e^{i\gamma} \frac{E_{11}^{12}(\mathbf{R}_1) + \sqrt{3}E_{12}^{12}(\mathbf{R}_1)}{2} \\
&= E_{11}^{12}(\mathbf{R}_1) \left(e^{ik_x a} - e^{-ik_x a} \right) + \frac{E_{11}^{12}(\mathbf{R}_1)}{2} \left(e^{-i\eta} e^{i\delta} - e^{i\eta} e^{-i\gamma} - e^{i\eta} e^{-i\delta} + e^{-i\eta} e^{i\gamma} \right) \\
&\quad + \frac{\sqrt{3}E_{12}^{12}(\mathbf{R}_1)}{2} \left(-e^{-i\eta} e^{i\delta} + e^{i\eta} e^{-i\gamma} - e^{i\eta} e^{-i\delta} + e^{-i\eta} e^{i\gamma} \right) \\
&= E_{11}^{12}(\mathbf{R}_1) (2i \sin 2\alpha) + \frac{E_{11}^{12}(\mathbf{R}_1)}{2} 4i (\cos \eta \sin \alpha \cos \beta - \sin \eta \cos \alpha \cos \beta) \\
&\quad + \frac{\sqrt{3}E_{12}^{12}(\mathbf{R}_1)}{2} 4(-\cos \eta \sin \alpha \sin \beta + \sin \eta \sin \alpha \cos \beta) \\
\Rightarrow h_1 &= 2it_1 (\sin 2\alpha + \cos \eta \sin \alpha \cos \beta - \sin \eta \cos \alpha \cos \beta) \\
&\quad - 2\sqrt{3}t_2 [\cos \eta \sin \alpha \sin \beta - \sin \eta \cos \alpha \sin \beta]
\end{aligned}$$

* 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 vào:

$$\begin{aligned}
h_2 &= E_{12}^{12}(\mathbf{R}_1) \left(e^{ik_x a} + e^{-ik_x a} \right) + e^{-i\eta} e^{i\delta} \frac{-\sqrt{3}E_{11}^{12}(\mathbf{R}_1) - E_{12}^{12}(\mathbf{R}_1)}{2} \\
&+ e^{i\eta} e^{-i\gamma} \frac{-\sqrt{3}E_{11}^{12}(\mathbf{R}_1) - E_{12}^{12}(\mathbf{R}_1)}{2} + e^{i\eta} e^{-i\delta} \frac{\sqrt{3}E_{11}^{12}(\mathbf{R}_1) - E_{12}^{12}(\mathbf{R}_1)}{2} \\
&+ e^{-i\eta} e^{i\gamma} \frac{\sqrt{3}E_{11}^{12}(\mathbf{R}_1) - E_{12}^{12}(\mathbf{R}_1)}{2} \\
&= 2E_{12}^{12}(\mathbf{R}_1) \cos 2\alpha + \frac{\sqrt{3}E_{11}^{12}(\mathbf{R}_1)}{2} \left(-e^{-i\eta} e^{i\delta} - e^{i\eta} e^{-i\gamma} + e^{i\eta} e^{-i\delta} + e^{-i\eta} e^{i\gamma} \right) \\
&+ \frac{E_{12}^{12}(\mathbf{R}_1)}{2} \left(-e^{-i\eta} e^{i\delta} - e^{i\eta} e^{-i\gamma} - e^{i\eta} e^{-i\delta} - e^{-i\eta} e^{i\gamma} \right) \\
&= 2t_2 \cos 2\alpha + 2i\sqrt{3}t_1 (\cos \eta \cos \alpha \sin \beta + \sin \eta \sin \alpha \cos \beta) \\
&\quad - 2t_2 (\cos \eta \cos \alpha \cos \beta + \sin \eta \sin \alpha \sin \beta) \\
h_2 &= 2t_2 (\cos 2\alpha - \cos \eta \cos \alpha \cos \beta - \sin \eta \sin \alpha \cos \beta) \\
&\quad + 2i\sqrt{3}t_1 (\cos \eta \cos \alpha \sin \beta + \sin \eta \sin \alpha \sin \beta)
\end{aligned}$$

Các ma trận $E^{22}(\mathbf{R})$

$$\begin{aligned}
*E^{22}(\mathbf{R}_2) &= E^{22}(\sigma'_\nu \mathbf{R}_1) \\
&= D^2(\sigma'_\nu) E^{22}(\mathbf{R}_1) \left[D^2(\sigma'_\nu) \right]^\dagger \\
&= \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} E_{11}^{22}(\mathbf{R}_1) & E_{12}^{22}(\mathbf{R}_1) \\ E_{21}^{22}(\mathbf{R}_1) & E_{22}^{22}(\mathbf{R}_1) \end{pmatrix} \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \\
&= \begin{pmatrix} \frac{t_{11}-\sqrt{3}t_{12}-\sqrt{3}t_{21}+3t_{22}}{4} & \frac{-\sqrt{3}t_{11}-t_{12}+3t_{21}+\sqrt{3}t_{22}}{4} \\ \frac{-\sqrt{3}t_{11}+3t_{12}-t_{21}+\sqrt{3}t_{22}}{4} & \frac{3t_{11}+\sqrt{3}t_{12}+\sqrt{3}t_{21}+t_{22}}{4} \end{pmatrix} \\
\Rightarrow E_{11}^{22}(\mathbf{R}_2) &= \frac{t_{11} - \sqrt{3}t_{12} - \sqrt{3}t_{21} + 3t_{22}}{4} \\
E_{12}^{22}(\mathbf{R}_2) &= \frac{-\sqrt{3}t_{11} - t_{12} + 3t_{21} + \sqrt{3}t_{22}}{4} \\
E_{21}^{22}(\mathbf{R}_2) &= \frac{-\sqrt{3}t_{11} + 3t_{12} - t_{21} + \sqrt{3}t_{22}}{4} \\
E_{22}^{22}(\mathbf{R}_2) &= \frac{3t_{11} + \sqrt{3}t_{12} + \sqrt{3}t_{21} + t_{22}}{4}
\end{aligned}$$

$$\begin{aligned}
*E^{22}(\mathbf{R}_3) &= E^{22}(C_3^2 \mathbf{R}_1) \\
&= D^2(C_3^2) E^{22}(\mathbf{R}_1) \left[D^2(C_3^2) \right]^\dagger \\
&= \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} E_{11}^{22}(\mathbf{R}_1) & E_{12}^{22}(\mathbf{R}_1) \\ E_{21}^{22}(\mathbf{R}_1) & E_{22}^{22}(\mathbf{R}_1) \end{pmatrix} \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \\
&= \begin{pmatrix} \frac{t_{11}-\sqrt{3}t_{12}-\sqrt{3}t_{21}+3t_{22}}{4} & \frac{\sqrt{3}t_{11}+t_{12}-3t_{21}-\sqrt{3}t_{22}}{4} \\ \frac{\sqrt{3}t_{11}-3t_{12}+t_{21}-\sqrt{3}t_{22}}{4} & \frac{3t_{11}+\sqrt{3}t_{12}+\sqrt{3}t_{21}+t_{22}}{4} \end{pmatrix} \\
\Rightarrow E_{11}^{22}(\mathbf{R}_3) &= \frac{t_{11} - \sqrt{3}t_{12} - \sqrt{3}t_{21} + 3t_{22}}{4} \\
E_{12}^{22}(\mathbf{R}_3) &= \frac{\sqrt{3}t_{11} + t_{12} - 3t_{21} - \sqrt{3}t_{22}}{4} \\
E_{21}^{22}(\mathbf{R}_3) &= \frac{\sqrt{3}t_{11} - 3t_{12} + t_{21} - \sqrt{3}t_{22}}{4} \\
E_{22}^{22}(\mathbf{R}_3) &= \frac{3t_{11} + \sqrt{3}t_{12} + \sqrt{3}t_{21} + t_{22}}{4}
\end{aligned}$$

$$\begin{aligned}
*E^{22}(\mathbf{R}_5) &= E^{22}(C_3\mathbf{R}_1) \\
&= D^2(C_3)E^{22}(\mathbf{R}_1) \left[D^2(C_3) \right]^\dagger \\
&= \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} E_{11}^{22}(\mathbf{R}_1) & E_{12}^{22}(\mathbf{R}_1) \\ E_{21}^{22}(\mathbf{R}_1) & E_{22}^{22}(\mathbf{R}_1) \end{pmatrix} \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \\
&= \begin{pmatrix} \frac{t_{11}+\sqrt{3}t_{12}+\sqrt{3}t_{21}+3t_{22}}{4} & \frac{-\sqrt{3}t_{11}+t_{12}-3t_{21}+\sqrt{3}t_{22}}{4} \\ \frac{-\sqrt{3}t_{11}-3t_{12}+t_{21}+\sqrt{3}t_{22}}{4} & \frac{3t_{11}-\sqrt{3}t_{12}-\sqrt{3}t_{21}+t_{22}}{4} \end{pmatrix} \\
\Rightarrow E_{11}^{22}(\mathbf{R}_5) &= \frac{t_{11} + \sqrt{3}t_{12} + \sqrt{3}t_{21} + 3t_{22}}{4} \\
E_{12}^{22}(\mathbf{R}_5) &= \frac{-\sqrt{3}t_{11} + t_{12} - 3t_{21} + \sqrt{3}t_{22}}{4} \\
E_{21}^{22}(\mathbf{R}_5) &= \frac{-\sqrt{3}t_{11} - 3t_{12} + t_{21} + \sqrt{3}t_{22}}{4} \\
E_{22}^{22}(\mathbf{R}_5) &= \frac{3t_{11} - \sqrt{3}t_{12} - \sqrt{3}t_{21} + t_{22}}{4}
\end{aligned}$$

$$\begin{aligned}
*E^{22}(\mathbf{R}_4) &= E^{22}(\sigma''_\nu\mathbf{R}_1) \\
&= D^2(\sigma''_\nu)E^{22}(\mathbf{R}_1) \left[D^2(\sigma''_\nu) \right]^\dagger \\
&= \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} E_{11}^{22}(\mathbf{R}_1) & E_{12}^{22}(\mathbf{R}_1) \\ E_{21}^{22}(\mathbf{R}_1) & E_{22}^{22}(\mathbf{R}_1) \end{pmatrix} \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \\
&= \begin{pmatrix} t_{11} & -t_{12} \\ -t_{21} & t_{22} \end{pmatrix}
\end{aligned}$$

$$\Rightarrow E_{11}^{22}(\mathbf{R}_4) = t_{11}$$

$$E_{12}^{22}(\mathbf{R}_4) = -t_{12}$$

$$E_{21}^{22}(\mathbf{R}_4) = -t_{21}$$

$$E_{22}^{22}(\mathbf{R}_4) = t_{22}$$

$$\begin{aligned}
*E^{22}(\mathbf{R}_6) &= E^{22}(\sigma_\nu \mathbf{R}_1) \\
&= D^2(\sigma_\nu) E^{22}(\mathbf{R}_1) \left[D^2(\sigma_\nu) \right]^\dagger \\
&= \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} E_{11}^{22}(\mathbf{R}_1) & E_{12}^{22}(\mathbf{R}_1) \\ E_{21}^{22}(\mathbf{R}_1) & E_{22}^{22}(\mathbf{R}_1) \end{pmatrix} \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \\
&= \begin{pmatrix} \frac{t_{11} + \sqrt{3}t_{12} + \sqrt{3}t_{21} + 3t_{22}}{4} & \frac{-\sqrt{3}t_{11} - t_{12} + 3t_{21} - \sqrt{3}t_{22}}{4} \\ \frac{\sqrt{3}t_{11} + 3t_{12} - t_{21} - \sqrt{3}t_{22}}{4} & \frac{3t_{11} - \sqrt{3}t_{12} - \sqrt{3}t_{21} + t_{22}}{4} \end{pmatrix} \\
\Rightarrow E_{11}^{22}(\mathbf{R}_6) &= \frac{t_{11} + \sqrt{3}t_{12} + \sqrt{3}t_{21} + 3t_{22}}{4} \\
E_{12}^{22}(\mathbf{R}_6) &= \frac{\sqrt{3}t_{11} - t_{12} + 3t_{21} - \sqrt{3}t_{22}}{4} \\
E_{21}^{22}(\mathbf{R}_6) &= \frac{\sqrt{3}t_{11} + 3t_{12} - t_{21} - \sqrt{3}t_{22}}{4} \\
E_{22}^{22}(\mathbf{R}_6) &= \frac{3t_{11} - \sqrt{3}t_{12} - \sqrt{3}t_{21} + t_{22}}{4}
\end{aligned}$$

* h11

$$\begin{aligned}
h_{11} = H_{11}^{22}(\mathbf{k}) &= \sum_{\mathbf{R}} e^{\frac{ie}{\hbar} \int_0^{\mathbf{R}} A(\mathbf{r}') d\mathbf{r}'} e^{i\mathbf{k} \cdot \mathbf{R}} E_{11}^{22}(\mathbf{R}) \\
&= e^{\frac{ie}{\hbar} \int_0^{\mathbf{R}_1} A(\mathbf{r}') d\mathbf{r}'} e^{i\mathbf{k} \cdot \mathbf{R}_1} E_{11}^{22}(\mathbf{R}_1) + e^{\frac{ie}{\hbar} \int_0^{\mathbf{R}_2} A(\mathbf{r}') d\mathbf{r}'} e^{i\mathbf{k} \cdot \mathbf{R}_2} E_{11}^{22}(\mathbf{R}_2) \\
&\quad + e^{\frac{ie}{\hbar} \int_0^{\mathbf{R}_3} A(\mathbf{r}') d\mathbf{r}'} e^{i\mathbf{k} \cdot \mathbf{R}_3} E_{11}^{22}(\mathbf{R}_3) + e^{\frac{ie}{\hbar} \int_0^{\mathbf{R}_4} A(\mathbf{r}') d\mathbf{r}'} e^{i\mathbf{k} \cdot \mathbf{R}_4} E_{11}^{22}(\mathbf{R}_4) \\
&\quad + e^{\frac{ie}{\hbar} \int_0^{\mathbf{R}_5} A(\mathbf{r}') d\mathbf{r}'} e^{i\mathbf{k} \cdot \mathbf{R}_5} E_{11}^{22}(\mathbf{R}_5) + e^{\frac{ie}{\hbar} \int_0^{\mathbf{R}_6} A(\mathbf{r}') d\mathbf{r}'} e^{i\mathbf{k} \cdot \mathbf{R}_6} E_{11}^{22}(\mathbf{R}_6)
\end{aligned}$$

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:

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

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

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

* **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:

$$\begin{aligned}
E_{22}^{22}(\mathbf{R}_2) = & \frac{3t_{11} + \sqrt{3}t_{12} + \sqrt{3}t_{21} + t_{22}}{4} \\
E_{22}^{22}(\mathbf{R}_3) = & \frac{3t_{11} + \sqrt{3}t_{12} + \sqrt{3}t_{21} + t_{22}}{4} \\
E_{22}^{22}(\mathbf{R}_4) = & t_{22} \\
E_{22}^{22}(\mathbf{R}_5) = & \frac{3t_{11} - \sqrt{3}t_{12} - \sqrt{3}t_{21} + t_{22}}{4} \\
E_{22}^{22}(\mathbf{R}_6) = & \frac{3t_{11} - \sqrt{3}t_{12} - \sqrt{3}t_{21} + t_{22}}{4}
\end{aligned}$$

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

* **h12**

$$\begin{aligned}
h_{12} &= H_{12}^{22}(\mathbf{k}) = \sum_{\mathbf{R}} e^{\frac{ie}{\hbar} \int_0^{\mathbf{R}} A(\mathbf{r}') d\mathbf{r}'} e^{i\mathbf{k} \cdot \mathbf{R}} E_{12}^{22}(\mathbf{R}) + \epsilon_2 \\
&= e^{\frac{ie}{\hbar} \int_0^{\mathbf{R}_1} A(\mathbf{r}') d\mathbf{r}'} e^{i\mathbf{k} \cdot \mathbf{R}_1} E_{12}^{22}(\mathbf{R}_1) + e^{\frac{ie}{\hbar} \int_0^{\mathbf{R}_2} A(\mathbf{r}') d\mathbf{r}'} e^{i\mathbf{k} \cdot \mathbf{R}_2} E_{12}^{22}(\mathbf{R}_2) \\
&\quad + e^{\frac{ie}{\hbar} \int_0^{\mathbf{R}_3} A(\mathbf{r}') d\mathbf{r}'} e^{i\mathbf{k} \cdot \mathbf{R}_3} E_{12}^{22}(\mathbf{R}_3) + e^{\frac{ie}{\hbar} \int_0^{\mathbf{R}_4} A(\mathbf{r}') d\mathbf{r}'} e^{i\mathbf{k} \cdot \mathbf{R}_4} E_{12}^{22}(\mathbf{R}_4) \\
&\quad + e^{\frac{ie}{\hbar} \int_0^{\mathbf{R}_5} A(\mathbf{r}') d\mathbf{r}'} e^{i\mathbf{k} \cdot \mathbf{R}_5} E_{12}^{22}(\mathbf{R}_5) + e^{\frac{ie}{\hbar} \int_0^{\mathbf{R}_6} A(\mathbf{r}') d\mathbf{r}'} e^{i\mathbf{k} \cdot \mathbf{R}_6} E_{12}^{22}(\mathbf{R}_6) + \epsilon_2
\end{aligned}$$

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:

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

Vậy Hamiltonian:

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

Với:

$$h_0 = 2t_0 [\cos(2\alpha) + 2\cos\eta\cos\alpha\cos\beta + 2\sin\eta\sin\alpha\cos\beta] + \epsilon_1, \quad (2)$$

$$h_1 = 2it_1(\sin 2\alpha + \cos\eta\sin\alpha\cos\beta - \sin\eta\cos\alpha\cos\beta) \\ - 2\sqrt{3}t_2(\cos\eta\sin\alpha\sin\beta - \sin\eta\cos\alpha\sin\beta), \quad (3)$$

$$h_2 = 2t_2(\cos 2\alpha - \cos\eta\cos\alpha\cos\beta - \sin\eta\sin\alpha\cos\beta) \quad (4)$$

$$+ 2i\sqrt{3}t_1(\cos\eta\cos\alpha\sin\beta + \sin\eta\sin\alpha\sin\beta), \quad (5)$$

$$h_{11} = (t_{11} + 3t_{22}) [\cos\eta\cos\alpha\cos\beta + \sin\eta\sin\alpha\cos\beta] + 2t_{11}\cos 2\alpha + \epsilon_2, \quad (6)$$

$$h_{22} = (3t_{11} + t_{22}) [\cos\eta\cos\alpha\cos\beta + \sin\eta\sin\alpha\cos\beta] + 2t_{22}\cos 2\alpha + \epsilon_2, \quad (7)$$

$$h_{12} = 4it_{12}(\sin\alpha\cos\alpha - \cos\eta\sin\alpha\cos\beta + \sin\eta\cos\alpha\cos\beta) \\ + \sqrt{3}(t_{22} - t_{11}) [\cos\eta\sin\alpha\sin\beta - \sin\eta\cos\alpha\sin\beta], \quad (8)$$

$$(\alpha, \beta) = \left(\frac{1}{2}k_x a, \frac{\sqrt{3}}{2}k_y a \right), \quad (9)$$

$$\eta = \frac{eBa^2\sqrt{3}}{\hbar 8},$$

$$t_0 = E_{11}^{11}(\mathbf{R}_1); \quad t_1 = E_{11}^{12}(\mathbf{R}_1); \quad t_2 = E_{12}^{12}(\mathbf{R}_1); \\ t_{11} = E_{11}^{22}(\mathbf{R}_1); \quad t_{12} = E_{12}^{22}(\mathbf{R}_1); \quad t_{22} = E_{22}^{22}(\mathbf{R}_1); \quad (10)$$

* **Hamiltonian Zeeman:**

Chọn các cơ sở:

$$\begin{aligned} |\phi_1^1, \uparrow\rangle &= |\phi_1^1\rangle \chi_+ \quad , \quad |\phi_1^2, \uparrow\rangle = |\phi_1^2\rangle \chi_+ \quad , \quad |\phi_2^2, \uparrow\rangle = |\phi_2^2\rangle \chi_+ \\ |\phi_1^1, \downarrow\rangle &= |\phi_1^1\rangle \chi_- \quad , \quad |\phi_1^2, \downarrow\rangle = |\phi_1^2\rangle \chi_- \quad , \quad |\phi_2^2, \downarrow\rangle = |\phi_2^2\rangle \chi_- \\ \chi_+ &= \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad , \quad \chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \end{aligned}$$

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

Do các hàm Spinor χ chỉ tác động lên spin σ_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:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\text{với } \gamma = -\frac{e}{m}$$

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:

$$H = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} h_0 & h_1 & h_2 \\ h_1^* & h_{11} & h_{12} \\ h_2^* & h_{12}^* & h_{22} \end{pmatrix} + H_{Zeeman}$$

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

Chéo hóa Hamiltonian, ta có phương trình hàm riêng trị riêng:

$$H_{TB}^{NN}(\mathbf{k})f = \lambda f$$

$$\begin{pmatrix} h_0 & h_1 & h_2 \\ h_1^* & h_{11} & h_{12} \\ h_2^* & h_{12}^* & h_{22} \end{pmatrix} f = \lambda \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} f$$

$$\Rightarrow \begin{pmatrix} h_0 - \lambda & h_1 & h_2 \\ h_1^* & h_{11} - \lambda & h_{12} \\ h_2^* & h_{12}^* & h_{22} - \lambda \end{pmatrix} f = 0$$

Để phương trình có nghiệm không tầm thường: $\Leftrightarrow \begin{vmatrix} h_0 - \lambda & h_1 & h_2 \\ h_1^* & h_{11} - \lambda & h_{12} \\ h_2^* & h_{12}^* & h_{22} - \lambda \end{vmatrix} = 0$

$$h_1 [h_{12}h_2^* - h_1^*(h_{22} - \lambda)] + h_2 [h_{12}^*h_1^* - h_2^*(h_{11} - \lambda)] + (h_0 - \lambda) [(h_{11} - \lambda)(h_{22} - \lambda) - h_{12}h_{12}^*] = 0$$

$$\Leftrightarrow h_1 h_{12} h_2^* - h_1 h_1^* h_{22} + h_1 h_1^* \lambda + h_2 h_{12}^* h_1^* - h_2 h_2^* h_{11} + h_2 h_2^* \lambda$$

$$+ (h_0 - \lambda)(h_{11} - \lambda)(h_{22} - \lambda) - h_0 h_{12} h_{12}^* + h_{12} h_{12}^* \lambda = 0$$

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

Sử dụng Hamiltonian:

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

chọn các cơ sở:

$$\begin{aligned} |\psi_c^\tau\rangle &= |d_{z^2}\rangle \equiv |\phi_1^1\rangle \\ |\psi_v^\tau\rangle &= \frac{1}{\sqrt{2}} \left(|d_{x^2-y^2}\rangle + i\tau |d_{xy}\rangle \right) \equiv \frac{1}{\sqrt{2}} \left(|\phi_2^2\rangle + i\tau |\phi_1^2\rangle \right) \end{aligned}$$

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

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

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

$$\begin{aligned} H_{cc}(\mathbf{k}, \tau) &= \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \langle \psi_c^\tau(\mathbf{r}) | \hat{H} | \psi_c^\tau(\mathbf{r} - \mathbf{R}) \rangle \\ &= h_0 \\ &= 2t_0 (\cos 2\alpha + 2 \cos \alpha \cos \beta) + \epsilon_1 \\ &= 2t_0 (1 + 2) + \epsilon_1 \end{aligned}$$

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

$$\begin{aligned}
H_{cv}(\mathbf{k}, \tau) &= \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \langle \psi_c^\tau(\mathbf{r}) | \hat{H} | \psi_v^\tau(\mathbf{r} - \mathbf{R}) \rangle \\
&= \frac{1}{\sqrt{2}} \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \left[\langle \phi_1^1(\mathbf{r}) | \hat{H} | \phi_2^2(\mathbf{r} - \mathbf{R}) \rangle + i\tau \langle \phi_1^1(\mathbf{r}) | \hat{H} | \phi_1^2(\mathbf{r} - \mathbf{R}) \rangle \right] \\
&= \frac{1}{\sqrt{2}} (h_2 + i\tau h_1) \\
&= \frac{1}{\sqrt{2}} \left[2t_2(\cos 2\alpha - \cos \alpha \cos \beta) + 2i\sqrt{3}t_1 \cos \alpha \sin \beta \right. \\
&\quad \left. + i\tau \left(-2\sqrt{3}t_2 \sin \alpha \sin \beta + 2it_1(\sin 2\alpha + \sin \alpha \cos \beta) \right) \right] \\
&= \frac{1}{\sqrt{2}} \left[2t_2(0) + 2i\sqrt{3}t_1\beta + i\tau \left(-2\sqrt{3}t_2\alpha\beta + 2it_1(2\alpha + \alpha) \right) \right] \\
&= \frac{2}{\sqrt{2}} \left[i\sqrt{3}t_1\beta - \sqrt{3}i\tau t_2\alpha\beta - t_1\tau 3\alpha \right] \\
&= \frac{2}{\sqrt{2}} \left[i\sqrt{3}t_1 \frac{\sqrt{3}}{2} k_y a - \sqrt{3}i\tau t_2 \frac{1}{2} k_x a \frac{\sqrt{3}}{2} k_y a - t_1\tau 3 \frac{1}{2} k_x a \right] \\
&= \frac{1}{\sqrt{2}} \left[3it_1 k_y a + \frac{3}{2} i\tau t_2 k_x k_y a^2 - 3t_1\tau k_x a \right] \\
&= \frac{3}{\sqrt{2}} \left[it_1 k_y a + i\tau t_2 k_x k_y a^2 - t_1\tau k_x a \right] \\
&= \frac{3}{\sqrt{2}} \left[at_1(ik_y - \tau k_x) + \frac{i}{2} \tau t_2 k_x k_y a^2 \right]
\end{aligned}$$

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

$$\begin{aligned}
H_{vc}(\mathbf{k}, \tau) &= \sum_R e^{i\mathbf{k}\cdot\mathbf{R}} \langle \psi_v^\tau(\mathbf{r}) | \hat{H} | \psi_c^\tau(\mathbf{r} - \mathbf{R}) \rangle \\
&= \frac{1}{\sqrt{2}} \sum_R e^{i\mathbf{k}\cdot\mathbf{R}} \left[\langle \phi_2^2(\mathbf{r}) | \hat{H} | \phi_1^1(\mathbf{r} - \mathbf{R}) \rangle - i\tau \langle \phi_1^2(\mathbf{r}) | \hat{H} | \phi_1^1(\mathbf{r} - \mathbf{R}) \rangle \right] \\
&= \frac{1}{\sqrt{2}} (h_2^* - i\tau h_1^*) \\
&= \frac{1}{\sqrt{2}} \left[2t_2(\cos 2\alpha - \cos \alpha \cos \beta) - 2i\sqrt{3}t_1 \cos \alpha \sin \beta \right. \\
&\quad \left. - i\tau \left(-2\sqrt{3}t_2 \sin \alpha \sin \beta - 2it_1(\sin 2\alpha + \sin \alpha \cos \beta) \right) \right] \\
&= \frac{1}{\sqrt{2}} \left[2t_2(0) - 2i\sqrt{3}t_1\beta - 2\sqrt{3}i\tau t_2\alpha\beta - 2t_1\tau 3\alpha \right] \\
&= \frac{1}{\sqrt{2}} \left[-2i\sqrt{3}t_1 \frac{\sqrt{3}}{2} k_y a - 2\sqrt{3}i\tau t_2 \frac{1}{2} k_x a \frac{\sqrt{3}}{2} k_y a - 2t_1\tau 3 \frac{1}{2} k_x a \right] \\
&= \frac{1}{\sqrt{2}} \left[-it_1 3k_y a - \frac{3i}{2} \tau t_2 k_x a k_y a - t_1\tau 3k_x a \right] \\
&= \frac{3}{\sqrt{2}} \left[-at_1(\tau k_x + ik_y) - \frac{i}{2} \tau t_2 k_x k_y a^2 \right]
\end{aligned}$$

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

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