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($\frac{1}{2}, \frac{\sqrt{3}}{2}$),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 $C_3^2\vec{R_5} = \vec{R_1} \Rightarrow C_3^2\sigma'_\nu\vec{R_4} = \vec{R_1}$

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

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

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 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:

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

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

$*$ **h0**

$$h_0 = \sum_{\mathbf{R}\neq 0} e^{i\mathbf{k}\cdot\mathbf{R}}\left\langle\phi_1^1(\mathbf{r})\right| H \left|\phi_1^1(\mathbf{r}-\mathbf{R})\right\rangle + \left\langle\phi_1^1(\mathbf{r})\right| H \left|\phi_1^1(\mathbf{r})\right\rangle$$

$$= e^{i\mathbf{k}\cdot\mathbf{R_1}}\left\langle\phi_1^1(\mathbf{r})\right| H \left|\phi_1^1(\mathbf{r}-\mathbf{R_1})\right\rangle + e^{i\mathbf{k}\cdot\mathbf{R_4}}\left\langle\phi_1^1(\mathbf{r})\right| H \left|\phi_1^1(\mathbf{r}-\mathbf{R_4})\right\rangle$$

$$+ e^{i\mathbf{k}\cdot\mathbf{R_2}}\left\langle\phi_1^1(\mathbf{r})\right| H \left|\phi_1^1(\mathbf{r}-\mathbf{R_2})\right\rangle + e^{i\mathbf{k}\cdot\mathbf{R_5}}\left\langle\phi_1^1(\mathbf{r})\right| H \left|\phi_1^1(\mathbf{r}-\mathbf{R_5})\right\rangle$$

$$+ e^{i\mathbf{k}\cdot\mathbf{R_3}}\left\langle\phi_1^1(\mathbf{r})\right| H \left|\phi_1^1(\mathbf{r}-\mathbf{R_3})\right\rangle + e^{i\mathbf{k}\cdot\mathbf{R_6}}\left\langle\phi_1^1(\mathbf{r})\right| H \left|\phi_1^1(\mathbf{r}-\mathbf{R_6})\right\rangle + \epsilon_1$$

$$= e^{ik_x a}E_{11}^{11}(\mathbf{R_1}) + e^{-ik_x a}E_{11}^{11}(\mathbf{R_4}) + e^{i\left(k_x\frac{a}{2}-k_y\frac{a\sqrt{3}}{2}\right)}E_{11}^{11}(\mathbf{R_2}) + e^{-i\left(k_x\frac{a}{2}-k_y\frac{a\sqrt{3}}{2}\right)}E_{11}^{11}(\mathbf{R_5})$$

$$+ e^{-i\left(k_x\frac{a}{2}+k_y\frac{a\sqrt{3}}{2}\right)}E_{11}^{11}(\mathbf{R_3}) + e^{i\left(k_x\frac{a}{2}+k_y\frac{a\sqrt{3}}{2}\right)}E_{11}^{11}(\mathbf{R_6}) + \epsilon_1$$

$$= 2E_{11}^{11}(\mathbf{R_1})\left(cos2\alpha + 2cos\alpha\ cos\beta\right) + \epsilon_1$$

$*$ **h1**

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

trong đó

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

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

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**

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

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

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

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

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

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

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**

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

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

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

$$
\Rightarrow E_{12}^{22}(\mathbf{R_2}) = \frac{-\sqrt{3}a - b + 3c + \sqrt{3}d}{4}
$$

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

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

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

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 $\mathbf{R_0} \to \mathbf{R}$

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

Ta có:

$$x = at$$

$$y = 0$$

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

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

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

Ta có:

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

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

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

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

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

Ta có:

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

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

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

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

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

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:

$$\int_C \vec{f} d\vec{\mathbf{r}} = -\int_{-C} \vec{f} d\vec{\mathbf{r}}$$
$$\Rightarrow -\int_C \vec{f} d\vec{\mathbf{r}} = \int_{-C} \vec{f} d\vec{\mathbf{r}}$$

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

Ta có:

$x = -at$

$y = 0$

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

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

Ta có:

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

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

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 $k_x\dfrac{a}{2} = \alpha$, $\quad k_y\dfrac{a\sqrt{3}}{2} = \beta$, $\quad \dfrac{e}{\hbar}\dfrac{Ba^2\sqrt{3}}{8} = \eta$, $\quad \alpha - \beta = \delta$, $\quad \alpha + \beta = \gamma$ 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**

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

Trong đó:

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

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

Một cách tương tự ta có cho:

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

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

∗ **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:

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

$$
\begin{aligned}
h_2 =& 2t_2(\cos 2\alpha - \cos\eta\cos\alpha\cos\beta - \sin\eta\sin\alpha\cos\beta) \\
&+ 2i\sqrt{3}t_1(\cos\eta\cos\alpha\sin\beta + \sin\eta\sin\alpha\sin\beta)
\end{aligned}
$$

Các ma trận $E^{22}(\mathbf{R})$

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

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

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

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

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

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

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

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

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

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

$*$ **h11**

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

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:

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

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

$*$ **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:

$$h_0 = 2t_0 \left[\cos(2\alpha) + 2\cos\eta\cos\alpha\cos\beta + 2\sin\eta\sin\alpha\cos\beta\right] + \epsilon_1, \tag{2}$$

$$\begin{aligned} h_1 =& 2it_1(\sin 2\alpha + \cos\eta\sin\alpha\cos\beta - \sin\eta\cos\alpha\cos\beta) \\ & - 2\sqrt{3}t_2\left(\cos\eta\sin\alpha\sin\beta - \sin\eta\cos\alpha\sin\beta\right), \end{aligned} \tag{3}$$

$$h_2 = 2t_2(\cos 2\alpha - \cos\eta\cos\alpha\cos\beta - \sin\eta\sin\alpha\cos\beta) \tag{4}$$

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

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

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

$$\begin{aligned} h_{12} =& 4it_{12}(\sin\alpha\cos\alpha - \cos\eta\sin\alpha\cos\beta + \sin\eta\cos\alpha\cos\beta) \\ & + \sqrt{3}(t_{22} - t_{11})\left[\cos\eta\sin\alpha\sin\beta - \sin\eta\cos\alpha\sin\beta\right], \end{aligned} \tag{8}$$

$$\begin{gathered} (\alpha, \beta) = \left(\frac{1}{2}k_x a, \frac{\sqrt{3}}{2}k_y a\right), \\ \eta = \frac{e}{\hbar}\frac{Ba^2\sqrt{3}}{8}, \end{gathered} \tag{9}$$

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

$*$ **Hamiltonian Zeeman:**

Chọn các cơ sở:

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

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:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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:

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

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: $\Leftrightarrow \begin{vmatrix} h_0-\lambda & h_1 & h_2 \\ h_1^* & h_{11}-\lambda & h_{12} \\ h_2^* & h_{12}^* & h_{22}-\lambda \end{vmatrix} = 0$

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

$$\begin{aligned}\Leftrightarrow & h_1h_{12}h_2^* - h_1h_1^*h_{22} + h_1h_1^*\lambda + h_2h_{12}^*h_1^* - h_2h_2^*h_{11} + h_2h_2^*\lambda \\ & + (h_0-\lambda)(h_{11}-\lambda)(h_{22}-\lambda) - h_0h_{12}h_{12}^* + h_{12}h_{12}^*\lambda = 0\end{aligned}$$

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

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

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

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

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

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

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

Do đó ta chọn các cơ sở:

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

$$\left\langle u_c, \pm\mathbf{K}\right| p_x \left|u_v, \pm\mathbf{K}\right\rangle = \pm i \left\langle u_c, \pm\mathbf{K}\right| p_y \left|u_v, \pm\mathbf{K}\right\rangle \tag{20}$$

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

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

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

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

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

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

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

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

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

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

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 $\tau = \pm 1$

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

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

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

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

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

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

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

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

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

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 $\mathbf{k} = \mathbf{q} + \mathbf{K}$, và viết lại phương trình (18) dưới dạng:

$$H_{\mathbf{k}\cdot\mathbf{p}} = \frac{1}{2}\frac{\hbar}{m_0}(q_+\hat{p}_- + q_-\hat{p}_+) = H^-_{\mathbf{k}\cdot\mathbf{p}} + H^+_{\mathbf{k}\cdot\mathbf{p}}, \tag{21}$$

với $q_\pm = q_x \pm iq_y$, $\hat{p}_\pm = \hat{p}_x \pm i\hat{p}_y$

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 cho biểu diễn bất khả quy của nhóm D_{3h} tại điểm Γ

.

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:

$$C_3\hat{p}_\pm = e^{\mp\frac{2\pi i}{3}}p_\pm \tag{22}$$

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

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

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

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

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

$$
\begin{aligned}
H_{cv}^{(1)} &= H_{0,2}^{'} \\
&= \frac{1}{2}\frac{\hbar}{m_0}\Big(q_+ \langle 0|\,\hat{p}_-\,|2\rangle + q_- \langle 0|\,\hat{p}_+\,|2\rangle\Big) \\
&= \frac{1}{2}\frac{\hbar}{m_0}\left(q_+ \langle 0|\,C_3^\dagger C_3 \hat{p}_- C_3^\dagger C_3\,|2\rangle + q_- \langle 0|\,C_3^\dagger C_3 \hat{p}_+ C_3^\dagger C_3\,|2\rangle\right) \\
&= \frac{1}{2}\frac{\hbar}{m_0}\left(e^{\frac{2i\pi}{3}}e^{\frac{2i\pi}{3}}q_+ \cancelto{0}{\langle 0|\,p_-\,|2\rangle} + e^{-\frac{2i\pi}{3}}e^{\frac{2i\pi}{3}}q_- \langle 0|\,\hat{p}_+\,|2\rangle\right) \text{(để dấu “=” xảy ra)} \\
&= \frac{a\hbar}{am_0}q_- \langle u_c|\,\hat{p}_+\,|u_v\rangle \\
&= atq_-
\end{aligned}
$$

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

$$
\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(q_+ \langle 0|\,\hat{p}_-\,|-1\rangle + q_- \langle 0|\,\hat{p}_+\,|-1\rangle\Big)\Big(q_+ \langle -1|\,\hat{p}_-\,|0\rangle + q_- \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(q_+ \langle 0|\,\hat{p}_-\,|1\rangle + q_- \langle 0|\,\hat{p}_+\,|1\rangle\Big)\Big(q_+ \langle 1|\,\hat{p}_-\,|0\rangle + q_- \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}\left(q_+ \langle 0|\,C_3^\dagger C_3 \hat{p}_- C_3^\dagger C_3\,|-1\rangle + q_- \langle 0|\,C_3^\dagger C_3 \hat{p}_+ C_3^\dagger C_3\,|-1\rangle\right) \\
&\times\left(q_+ \langle -1|\,C_3^\dagger C_3 \hat{p}_- C_3^\dagger C_3\,|0\rangle + q_- \langle -1|\,C_3^\dagger C_3 \hat{p}_+ C_3^\dagger C_3\,|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(q_+ \langle 0|\,C_3^\dagger C_3 \hat{p}_- C_3^\dagger C_3\,|1\rangle + q_- \langle 0|\,C_3^\dagger C_3 \hat{p}_+ C_3^\dagger C_3\,|1\rangle\right) \\
&\times\left(q_+ \langle 1|\,C_3^\dagger C_3 \hat{p}_- C_3^\dagger C_3\,|0\rangle + q_- \langle 1|\,C_3^\dagger C_3 \hat{p}_+ C_3^\dagger C_3\,|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(q_+e^{\frac{2i\pi}{3}}e^{-\frac{2i\pi}{3}}\langle 0|\,\hat{p}_-\,|-1\rangle + q_-e^{-\frac{2i\pi}{3}}e^{-\frac{2i\pi}{3}}\cancelto{0}{\langle 0|\,\hat{p}_+\,|-1\rangle}\right) \\
&\times\left(q_+e^{\frac{2i\pi}{3}}e^{\frac{2i\pi}{3}}\cancelto{0}{\langle -1|\,\hat{p}_-\,|0\rangle} + q_-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(q_+e^{\frac{2i\pi}{3}}e^{\frac{2i\pi}{3}}\cancelto{0}{\langle 0|\,\hat{p}_-\,|1\rangle} + q_-e^{-\frac{2i\pi}{3}}e^{\frac{2i\pi}{3}}\langle 0|\,\hat{p}_+\,|1\rangle\right) \\
&\times\left(q_+e^{\frac{2i\pi}{3}}e^{-\frac{2i\pi}{3}}\langle 1|\,\hat{p}_-\,|0\rangle + q_-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:

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

với $q^2 = q_x^2 + q_y^2$.

$$
\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}\big(q_+\left\langle 2\right| p_-\left|-1\right\rangle + q_-\left\langle 2\right| p_+\left|-1\right\rangle\big)\big(q_+\left\langle -1\right| p_-\left|2\right\rangle + q_-\left\langle -1\right| p_+\left|2\right\rangle\big)\\
&\times\left[\frac{1}{E_2-E_{-1}}+\frac{1}{E_{-2}-E_{-1}}\right]+\frac{1}{4}\frac{\hbar}{m_0}\big(q_+\left\langle 2\right| p_-\left|1\right\rangle + q_-\left\langle 2\right| p_+\left|1\right\rangle\big)\\
&\times\big(q_+\left\langle 1\right| p_-\left|2\right\rangle + q_-\left\langle 1\right| p_+\left|2\right\rangle\big)\left[\frac{1}{E_2-E_1}+\frac{1}{E_{-2}-E_1}\right]\\
&= \frac{1}{4}\frac{\hbar}{m_0}\Big(q_+\left\langle 2\right| C_3^\dagger C_3 p_- C_3^\dagger C_3\left|-1\right\rangle + q_-\left\langle 2\right| C_3^\dagger C_3 p_+ C_3^\dagger C_3\left|-1\right\rangle\Big)\\
&\times\Big(q_+\left\langle -1\right| C_3^\dagger C_3 p_- C_3^\dagger C_3\left|2\right\rangle + q_-\left\langle -1\right| C_3^\dagger C_3 p_+ C_3^\dagger C_3\left|2\right\rangle\Big)\times\left[\frac{1}{E_2-E_{-1}}+\frac{1}{E_{-2}-E_{-1}}\right]\\
&+\frac{1}{4}\frac{\hbar}{m_0}\Big(q_+\left\langle 2\right| C_3^\dagger C_3 p_- C_3^\dagger C_3\left|1\right\rangle + q_-\left\langle 2\right| C_3^\dagger C_3 p_+ C_3^\dagger C_3\left|1\right\rangle\Big)\\
&\times\Big(q_+\left\langle 1\right| C_3^\dagger C_3 p_- C_3^\dagger C_3\left|2\right\rangle + q_-\left\langle 1\right| C_3^\dagger C_3 p_+ C_3^\dagger C_3\left|2\right\rangle\Big)\left[\frac{1}{E_2-E_1}+\frac{1}{E_{-2}-E_1}\right]\\
&= \frac{1}{4}\frac{\hbar}{m_0}\left(q_+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} + q_-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(q_+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} + q_-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}\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(q_+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 + q_-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)\\
&\times\left(q_+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} + q_-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\right)\left[\frac{1}{E_2-E_1}+\frac{1}{E_{-2}-E_1}\right]
\end{aligned}
$$

(để dấu "=" xảy ra)

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

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