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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

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

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

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

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

$$h_0 = \sum_R e^{i\mathbf{k}\cdot\mathbf{R}} \langle \phi^1_1(\mathbf{r})| H |\phi^1_1(\mathbf{r}-\mathbf{R})\rangle; \quad h_1 = \sum_R e^{i\mathbf{k}\cdot\mathbf{R}} \langle \phi^1_1(\mathbf{r})| H |\phi^2_1(\mathbf{r}-\mathbf{R})\rangle$$

$$h_2 = \sum_R e^{i\mathbf{k}\cdot\mathbf{R}} \langle \phi^1_1(\mathbf{r})| H |\phi^2_2(\mathbf{r}-\mathbf{R})\rangle; \quad h_{11} = \sum_R e^{i\mathbf{k}\cdot\mathbf{R}} \langle \phi^2_1(\mathbf{r})| H |\phi^2_1(\mathbf{r}-\mathbf{R})\rangle$$

$$h_{12} = \sum_R e^{i\mathbf{k}\cdot\mathbf{R}} \langle \phi^2_1(\mathbf{r})| H |\phi^2_2(\mathbf{r}-\mathbf{R})\rangle; \quad h_{22} = \sum_R e^{i\mathbf{k}\cdot\mathbf{R}} \langle \phi^2_2(\mathbf{r})| H |\phi^2_2(\mathbf{r}-\mathbf{R})\rangle$$

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 $D^1(\hat{g_n}) = 1$

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

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

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

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:

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

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

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

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

Tương tự ta tính cho

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

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:

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

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

$*$ **h0**

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

$*$ **h1**

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

trong đó

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

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

Tương tự ta có cho:

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

$$h_1 = e^{i2\alpha} E_{11}^{12}(\mathbf{R_1}) - e^{i2\alpha} E_{11}^{12}(\mathbf{R_1})$$
$$+ e^{i(\alpha-\beta)} \frac{E_{11}^{12}(\mathbf{R_1}) - \sqrt{3}E_{12}^{12}(\mathbf{R_1})}{2} + e^{-i(\alpha+\beta)} \frac{-E_{11}^{12}(\mathbf{R_1}) + \sqrt{3}E_{12}^{12}(\mathbf{R_1})}{2}$$
$$+ e^{i(-\alpha+\beta)} \frac{-E_{11}^{12}(\mathbf{R_1}) - \sqrt{3}E_{12}^{12}(\mathbf{R_1})}{2} + e^{i(\alpha+\beta)} \frac{E_{11}^{12}(\mathbf{R_1}) + \sqrt{3}E_{12}^{12}(\mathbf{R_1})}{2}$$
$$= 2isin2\alpha E_{11}^{12}(\mathbf{R}_1) + 2i\frac{E_{11}^{12}(\mathbf{R_1})}{2} sin(\alpha-\beta) - 2\frac{E_{12}^{12}(\mathbf{R_1}\sqrt{3})}{2} cos(\alpha-\beta)$$
$$+ 2i\frac{E_{11}^{12}(\mathbf{R_1})}{2} sin(\alpha+\beta) + 2\frac{E_{12}^{12}(\mathbf{R_1}\sqrt{3})}{2} cos(\alpha+\beta)$$
$$= -2\sqrt{3}t_2 sin\alpha\ sin\beta + 2it_1(sin2\alpha + sin\alpha\ \cos\beta)$$

Đặt

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

$$t_{11} = E_{11}^{22}(\mathbf{R}_1); \quad t_{12} = E_{12}^{22}(\mathbf{R}_1); \quad c_{21} = E_{21}^{22}(\mathbf{R}_1); \quad t_{22} = E_{22}^{22}(\mathbf{R}_1);$$

$*$ **h22**

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

$$\begin{aligned} E^{22}(\mathbf{R}_2) &= E^{22}(\sigma_\nu' \mathbf{R}_1) \\ &= D^2(\sigma_\nu') E^{22}(\mathbf{R}_1) \left[D^2(\sigma_\nu') \right]^\dagger \end{aligned}$$

$$= \begin{bmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{3}{2} & -\frac{1}{2} \end{bmatrix} \begin{bmatrix} E_{11}^{22}(\mathbf{R}_1) & E_{12}^{22}(\mathbf{R}_1) \\ E_{21}^{22}(\mathbf{R}_1) & E_{22}^{22}(\mathbf{R}_1) \end{bmatrix} \begin{bmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{3}{2} & -\frac{1}{2} \end{bmatrix}$$

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

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

Tương tự ta có cho:

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

Ta được:

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

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

***h11**

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

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

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

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

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

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

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**

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

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

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

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

Tương tự ta tìm được:

$$
\begin{aligned}
E_{12}^{22}(\mathbf{R_3}) &= \frac{\sqrt{3}a + b - 3c - \sqrt{3}d}{4} \\
E_{12}^{22}(\mathbf{R_4}) &= -b \\
E_{12}^{22}(\mathbf{R_5}) &= \frac{\sqrt{3}a + b - 3c + \sqrt{3}d}{4} \\
E_{12}^{22}(\mathbf{R_6}) &= \frac{\sqrt{3}a - b + 3c - \sqrt{3}d}{4}
\end{aligned}
$$

Ta đưa điện trường vào. 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 $e^{\frac{ie}{\hbar}\int_0^{\mathbf{R}} A(\mathbf{r}')d\mathbf{r}'}$

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

Phương trình tham số cho x, y:

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

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

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

Ta có:

$$
\begin{aligned}
&x = at \\
&y = 0 \\
&\Rightarrow \int_0^{\mathbf{R_1}} \mathbf{A}(\mathbf{r}') \cdot d\mathbf{r}' = \int_{t_B}^{t_A} \left[P(x,y)\frac{dx}{dt} + Q(x,y)\frac{dy}{dt} + R(x,y)\frac{dz}{dt} \right] dt \\
&= \int_0^1 \left[0\frac{dx}{dt} + Bx0 + 0\frac{dz}{dt} \right] dt = 0
\end{aligned}
$$

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

Ta có:

$$
\begin{aligned}
&x = \frac{a}{2}t \\
&y = -\frac{a\sqrt{3}}{2}t \\
&\Rightarrow \int_0^{\mathbf{R_1}} \mathbf{A}(\mathbf{r}') \cdot d\mathbf{r}' = \int_{t_B}^{t_A} \left[P(x,y)\frac{dx}{dt} + Q(x,y)\frac{dy}{dt} + R(x,y)\frac{dz}{dt} \right] dt \\
&= \int_0^1 \left[0\frac{dx}{dt} + Bx\left(-\frac{a\sqrt{3}}{2}\right) + 0\frac{dz}{dt} \right] dt = -\frac{Ba^2\sqrt{3}}{8}
\end{aligned}
$$

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

Ta có:

$$
\begin{aligned}
&x = -\frac{a}{2}t \\
&y = -\frac{a\sqrt{3}}{2}t \\
&\Rightarrow \int_0^{\mathbf{R_1}} \mathbf{A}(\mathbf{r}') \cdot d\mathbf{r}' = \int_{t_B}^{t_A} \left[P(x,y)\frac{dx}{dt} + Q(x,y)\frac{dy}{dt} + R(x,y)\frac{dz}{dt} \right] dt \\
&= \int_0^1 \left[0\frac{dx}{dt} + Bx\left(-\frac{a\sqrt{3}}{2}\right) + 0\frac{dz}{dt} \right] dt = B\left(-\frac{a}{2}\right)\left(-\frac{a\sqrt{3}}{2}\right)\int_0^1 tdt \\
&= \frac{Ba^2\sqrt{3}}{8}
\end{aligned}
$$

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

Ta có:

$$x = -at$$

$$y = 0$$

$$\Rightarrow \int_0^{\mathbf{R_4}} \mathbf{A}(\mathbf{r}') \cdot d\mathbf{r}' = \int_{t_B}^{t_A} \left[P(x,y)\frac{dx}{dt} + Q(x,y)\frac{dy}{dt} + R(x,y)\frac{dz}{dt} \right] dt$$

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

$*\underset{(0,0)}{\mathbf{R_0}} \longrightarrow \underset{(0,a)}{\mathbf{R_5}}$

Ta có:

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

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

$$\Rightarrow \int_0^{\mathbf{R_5}} \mathbf{A}(\mathbf{r}') \cdot d\mathbf{r}' = \int_{t_B}^{t_A} \left[P(x,y)\frac{dx}{dt} + Q(x,y)\frac{dy}{dt} + R(x,y)\frac{dz}{dt} \right] dt$$

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

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

Ta có:

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

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

$$\Rightarrow \int_0^{\mathbf{R_6}} \mathbf{A}(\mathbf{r}') \cdot d\mathbf{r}' = \int_{t_B}^{t_A} \left[P(x,y)\frac{dx}{dt} + Q(x,y)\frac{dy}{dt} + R(x,y)\frac{dz}{dt} \right] dt$$

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

Vậy h_0 có dạng:

$$
\begin{aligned}
h_0 = H_{11}^{11}(\mathbf{k}) &= e^0 e^{i\mathbf{k}\cdot\mathbf{R_1}} E_{11}^{11}(\mathbf{R_1}) + e^{-\frac{ie}{\hbar}\frac{Ba^2\sqrt{3}}{8}} e^{i\mathbf{k}\cdot\mathbf{R_2}} E_{11}^{11}(\mathbf{R_2}) \\
&+ e^{\frac{ie}{\hbar}\frac{Ba^2\sqrt{3}}{8}} e^{i\mathbf{k}\cdot\mathbf{R_3}} E_{11}^{11}(\mathbf{R_3}) + e^0 e^{i\mathbf{k}\cdot\mathbf{R_4}} E_{11}^{11}(\mathbf{R_4}) \\
&+ e^{-\frac{ie}{\hbar}\frac{Ba^2\sqrt{3}}{8}} e^{i\mathbf{k}\cdot\mathbf{R_5}} E_{11}^{11}(\mathbf{R_5}) + e^{\frac{ie}{\hbar}\frac{Ba^2\sqrt{3}}{8}} e^{i\mathbf{k}\cdot\mathbf{R_6}} E_{11}^{11}(\mathbf{R_6}) \\
&= e^{ik_x a} E_{11}^{11}(\mathbf{R_1}) + e^{-ik_x a} E_{11}^{11}(\mathbf{R_4}) + e^{-\frac{ie}{\hbar}\frac{Ba^2\sqrt{3}}{8}} e^{i\left(k_x\frac{a}{2} - k_y\frac{a\sqrt{3}}{2}\right)} E_{11}^{11}(\mathbf{R_2}) \\
&+ e^{\frac{ie}{\hbar}\frac{Ba^2\sqrt{3}}{8}} e^{i\left(-k_x\frac{a}{2} - k_y\frac{a\sqrt{3}}{2}\right)} E_{11}^{11}(\mathbf{R_3}) + e^{-\frac{ie}{\hbar}\frac{Ba^2\sqrt{3}}{8}} e^{i\left(-k_x\frac{a}{2} + k_y\frac{a\sqrt{3}}{2}\right)} E_{11}^{11}(\mathbf{R_5}) \\
&+ e^{\frac{ie}{\hbar}\frac{Ba^2\sqrt{3}}{8}} e^{i\left(k_x\frac{a}{2} + k_y\frac{a\sqrt{3}}{2}\right)} E_{11}^{11}(\mathbf{R_6}) + \epsilon_1
\end{aligned}
$$

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 $\mathbf{R}_1$.

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

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

$*$ **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:

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

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

Một cách tương tự ta có cho:

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

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

$$
\begin{aligned}
h_2 =& E_{11}^{12}(\mathbf{R_1}) \left(e^{ik_x a} + e^{-ik_x a} \right) + e^{-i\eta} e^{i\delta} \frac{-\sqrt{3}E_{11}^{12}(\mathbf{R_1}) - E_{12}^{12}(\mathbf{R_1})}{2} \\
& + e^{i\eta} e^{-i\gamma} \frac{-\sqrt{3}E_{11}^{12}(\mathbf{R_1}) - E_{12}^{12}(\mathbf{R_1})}{2} + e^{-i\eta} e^{-i\delta} \frac{\sqrt{3}E_{11}^{12}(\mathbf{R_1}) - E_{12}^{12}(\mathbf{R_1})}{2} \\
& + e^{i\eta} e^{i\gamma} \frac{\sqrt{3}E_{11}^{12}(\mathbf{R_1}) - E_{12}^{12}(\mathbf{R_1})}{2} \\
=& 2E_{11}^{12}(\mathbf{R_1}) \cos 2\alpha + \frac{\sqrt{3}E_{11}^{12}(\mathbf{R_1})}{1} \left(-e^{i\eta} e^{i\delta} - e^{i\eta} e^{-i\gamma} + e^{-i\eta} e^{-i\delta} + e^{i\eta} e^{i\gamma} \right)
\end{aligned}
$$