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

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

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

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

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

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

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

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

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

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

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**

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

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

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

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

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

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

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

$*$ **h1**

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

trong đó

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

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

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

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

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

$*$ **h22**

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

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

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

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

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

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**

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

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

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

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

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

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

Tương tự ta tìm được:

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

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

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

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

**h12

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

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

Tương tự ta tìm được:

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

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:

$$x = at$$

$$y = 0$$

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

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

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

Ta có:

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

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

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

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

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

Ta có:

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

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

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

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

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

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

Ta có:

$$
\begin{aligned}
&x = -at \\
&y = 0 \\
&\Rightarrow \int_0^{\mathbf{R_4}} \mathbf{A}(\mathbf{r}') \cdot d\mathbf{r}' = \int_{t_B}^{t_A} \left[P(x,y)\frac{dx}{dt} + Q(x,y)\frac{dy}{dt} + R(x,y)\frac{dz}{dt} \right] dt \\
&= \int_0^1 \left[0\frac{dx}{dt} + Bx0 + 0\frac{dz}{dt} \right] dt = 0
\end{aligned}
$$

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

Ta có:

$$
\begin{aligned}
&x = -\frac{a}{2}t \\
&y = \frac{a\sqrt{3}}{2}t \\
&\Rightarrow \int_0^{\mathbf{R_5}} \mathbf{A}(\mathbf{r}') \cdot d\mathbf{r}' = \int_{t_B}^{t_A} \left[P(x,y)\frac{dx}{dt} + Q(x,y)\frac{dy}{dt} + R(x,y)\frac{dz}{dt} \right] dt \\
&= \int_0^1 \left[0\frac{dx}{dt} + Bx\frac{a\sqrt{3}}{2} + 0\frac{dz}{dt} \right] dt = -\frac{Ba^2\sqrt{3}}{8}
\end{aligned}
$$

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

Ta có:

$$
\begin{aligned}
&x = \frac{a}{2}t \\
&y = \frac{a\sqrt{3}}{2}t \\
&\Rightarrow \int_0^{\mathbf{R_6}} \mathbf{A}(\mathbf{r}') \cdot d\mathbf{r}' = \int_{t_B}^{t_A} \left[P(x,y)\frac{dx}{dt} + Q(x,y)\frac{dy}{dt} + R(x,y)\frac{dz}{dt} \right] dt \\
&= \int_0^1 \left[0\frac{dx}{dt} + Bx\frac{a\sqrt{3}}{2} + 0\frac{dz}{dt} \right] dt = \frac{Ba^2\sqrt{3}}{8}
\end{aligned}
$$

Vậy h_0 có dạng:

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