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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$(\dfrac{1}{2}, \dfrac{\sqrt{3}}{2})$,B(1,0), C(0,0).

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

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

trong đó $D^2\left(\sigma'_\nu\right) = D^2\left(C_3\right) D^2\left(\sigma_\nu\right) \quad ; D^2\left(\sigma''_\nu\right) = D^2\left(C_3^2\right) D^2\left(\sigma_\nu\right)$

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

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

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 $\rightarrow \mathbf{R}_4$ (dưới dạng ma trận)

Toán tử σ''_ν đánh lên $\mathbf{R}_1$ ta được $\rightarrow \mathbf{R}_2$ (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**

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

∗ **h1**

$$h_1 = \sum_{\mathbf{R}\neq 0} e^{i\mathbf{k}\cdot\mathbf{R}} \left\langle \phi_1^1(\mathbf{r})\right| H \left|\phi_1^2(\mathbf{r}-\mathbf{R})\right\rangle$$

$$= e^{ik_x a}E_{11}^{12}(\mathbf{R_1}) + e^{-ik_x a}E_{11}^{12}(\mathbf{R_4}) + e^{i\left(k_x\frac{a}{2}-k_y\frac{a\sqrt{3}}{2}\right)}E_{11}^{12}(\mathbf{R_2}) + e^{-i\left(k_x\frac{a}{2}-k_y\frac{a\sqrt{3}}{2}\right)}E_{11}^{12}(\mathbf{R_5})$$
$$+ e^{-i\left(k_x\frac{a}{2}+k_y\frac{a\sqrt{3}}{2}\right)}E_{11}^{12}(\mathbf{R_3}) + e^{i\left(k_x\frac{a}{2}+k_y\frac{a\sqrt{3}}{2}\right)}E_{11}^{12}(\mathbf{R_6})$$

trong đó

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

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

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

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

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

∗ **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 $t_{12} = -t_{21}$