

## 121<sup>st</sup> Eigenvector

$$N_e = 4 \quad s = 0 \quad m_s = 0$$

Irred. Representation :  $\Gamma_{3,2}$

$$E_{121} = -J + U + 10W + \left( \frac{\cos(\theta_1)}{\sqrt{3}} - \sin(\theta_1) \right) \sqrt{A_1}$$

$$\begin{aligned} |\Psi_{121}\rangle &= |4, 0, 0, \Gamma_{3,2}\rangle \\ &= C_{121,1} (|0022\rangle - |0220\rangle - |2002\rangle + |2200\rangle) \\ &+ C_{121,2} (|02du\rangle - |02ud\rangle - |0du2\rangle + |0ud2\rangle + |20du\rangle - |20ud\rangle - |2du0\rangle + |2ud0\rangle \\ &\quad - |d02u\rangle - |d20u\rangle + |du02\rangle + |du20\rangle + |u02d\rangle + |u20d\rangle - |ud02\rangle - |ud20\rangle) \\ &+ C_{121,3} (|dduu\rangle + |duud\rangle + |uddu\rangle + |uudd\rangle) \\ &+ C_{121,4} (|dudu\rangle + |udud\rangle) \end{aligned}$$

$$\begin{aligned} C_{121-1} &= t(J + U) \\ &+ \left( t(U - 2W) + \left( \frac{t \cos(\theta_1)}{\sqrt{3}} - t \sin(\theta_1) \right) \sqrt{A_1} \right) \end{aligned}$$

$$\begin{aligned} C_{121-2} &= \frac{1}{4} (-J^2 - 2UJ + 4WJ - U^2) \\ &+ \left( (J + U - W)W - \frac{1}{12} (\cos(2\theta_1) + \sqrt{3} \sin(2\theta_1) - 2) A_1 \right) \end{aligned}$$

$$\begin{aligned} C_{121-3} &= -t(J + U) \\ &+ \left( \left( \frac{t \cos(\theta_1)}{\sqrt{3}} - t \sin(\theta_1) \right) \sqrt{A_1} - t(U - 2W) \right) \end{aligned}$$

$$\begin{aligned} C_{121-4} &= 2t(J + U) \\ &+ \left( \frac{2}{3} t (3(U - 2W) + (3 \sin(\theta_1) - \sqrt{3} \cos(\theta_1)) \sqrt{A_1}) \right) \end{aligned}$$

$$N_{121} = \sqrt{4C_{121,1}^2 + 16C_{121,2}^2 + 4C_{121,3}^2 + 2C_{121,4}^2}$$