

# Hamiltonian matrix in GVB-BCCC formula derivation

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To derive the GVB-BCCC formula, all possible types of excited states need to be constructed firstly.

In total, there are 1 ground state and 3836 excited types.

When  $\hat{H}$  operator project onto a wavefunction state, it will be converted to a linear combination of other states. that is

$$\hat{H}|\Phi_u\rangle = \sum_{u,v} c_{u,v} \Phi_v$$

where  $c_{u,v}$  is Hamiltonian matrix, and listed separately in other files.

Specifically, state  $u, v =$

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$$(A_{15}, B_7, C_2, D_9)$$

$$(A_{15}, B_7, C_2, D_{10})$$

$$(A_{15}, B_7, C_3, D_9)$$

$$(A_{15}, B_7, C_3, D_{10})$$

$$(A_{15}, B_7, C_5, D_7)$$

$$(A_{15}, B_7, C_5, D_8)$$

$$(A_{15}, B_7, C_6, D_{13})$$

$$(A_{15}, B_7, C_6, D_{14})$$

$$(A_{15}, B_7, C_7, D_5)$$

$$(A_{15}, B_7, C_8, D_5)$$

$$(A_{15}, B_7, C_9, D_1)$$

$$(A_{15}, B_7, C_9, D_2)$$

$$(A_{15}, B_7, C_9, D_3)$$

$$(A_{15}, B_7, C_{10}, D_1)$$

$$(A_{15}, B_7, C_{10}, D_2)$$

$$(A_{15}, B_7, C_{10}, D_3)$$

$$(A_{15}, B_7, C_{13}, D_6)$$

$$(A_{15}, B_7, C_{14}, D_6)$$

$(A_{15}, B_8, C_1, D_9)$   
 $(A_{15}, B_8, C_1, D_{10})$   
 $(A_{15}, B_8, C_2, D_9)$   
 $(A_{15}, B_8, C_2, D_{10})$   
 $(A_{15}, B_8, C_3, D_9)$   
 $(A_{15}, B_8, C_3, D_{10})$   
 $(A_{15}, B_8, C_5, D_7)$   
 $(A_{15}, B_8, C_5, D_8)$   
 $(A_{15}, B_8, C_6, D_{13})$   
 $(A_{15}, B_8, C_6, D_{14})$   
 $(A_{15}, B_8, C_7, D_5)$   
 $(A_{15}, B_8, C_8, D_5)$   
 $(A_{15}, B_8, C_9, D_1)$   
 $(A_{15}, B_8, C_9, D_2)$   
 $(A_{15}, B_8, C_9, D_3)$   
 $(A_{15}, B_8, C_{10}, D_1)$   
 $(A_{15}, B_8, C_{10}, D_2)$   
 $(A_{15}, B_8, C_{10}, D_3)$   
 $(A_{15}, B_8, C_{13}, D_6)$   
 $(A_{15}, B_8, C_{14}, D_6)$   
 $(A_{15}, B_9, C_1, D_7)$   
 $(A_{15}, B_9, C_1, D_8)$   
 $(A_{15}, B_9, C_2, D_7)$   
 $(A_{15}, B_9, C_2, D_8)$   
 $(A_{15}, B_9, C_3, D_7)$   
 $(A_{15}, B_9, C_3, D_8)$   
 $(A_{15}, B_9, C_4, D_9)$   
 $(A_{15}, B_9, C_4, D_{10})$   
 $(A_{15}, B_9, C_6, D_{11})$

$$(A_{15}, B_9, C_6, D_{12})$$

$$(A_{15}, B_9, C_7, D_1)$$

$$(A_{15}, B_9, C_7, D_2)$$

$$(A_{15}, B_9, C_7, D_3)$$

$$(A_{15}, B_9, C_8, D_1)$$

$$(A_{15}, B_9, C_8, D_2)$$

$$(A_{15}, B_9, C_8, D_3)$$

$$(A_{15}, B_9, C_9, D_4)$$

$$(A_{15}, B_9, C_{10}, D_4)$$

$$(A_{15}, B_9, C_{11}, D_6)$$

$$(A_{15}, B_9, C_{12}, D_6)$$

$$(A_{15}, B_{10}, C_1, D_7)$$

$$(A_{15}, B_{10}, C_1, D_8)$$

$$(A_{15}, B_{10}, C_2, D_7)$$

$$(A_{15}, B_{10}, C_2, D_8)$$

$$(A_{15}, B_{10}, C_3, D_7)$$

$$(A_{15}, B_{10}, C_3, D_8)$$

$$(A_{15}, B_{10}, C_4, D_9)$$

$$(A_{15}, B_{10}, C_4, D_{10})$$

$$(A_{15}, B_{10}, C_6, D_{11})$$

$$(A_{15}, B_{10}, C_6, D_{12})$$

$$(A_{15}, B_{10}, C_7, D_1)$$

$$(A_{15}, B_{10}, C_7, D_2)$$

$$(A_{15}, B_{10}, C_7, D_3)$$

$$(A_{15}, B_{10}, C_8, D_1)$$

$$(A_{15}, B_{10}, C_8, D_2)$$

$$(A_{15}, B_{10}, C_8, D_3)$$

$$(A_{15}, B_{10}, C_9, D_4)$$

$$(A_{15}, B_{10}, C_{10}, D_4)$$

$$(A_{15}, B_{10}, C_{11}, D_6)$$

$$(A_{15}, B_{10}, C_{12}, D_6)$$

$$(A_{15}, B_{11}, C_6, D_9)$$

$$(A_{15}, B_{11}, C_6, D_{10})$$

$$(A_{15}, B_{11}, C_9, D_6)$$

$$(A_{15}, B_{11}, C_{10}, D_6)$$

$$(A_{15}, B_{12}, C_6, D_9)$$

$$(A_{15}, B_{12}, C_6, D_{10})$$

$$(A_{15}, B_{12}, C_9, D_6)$$

$$(A_{15}, B_{12}, C_{10}, D_6)$$

$$(A_{15}, B_{13}, C_6, D_7)$$

$$(A_{15}, B_{13}, C_6, D_8)$$

$$(A_{15}, B_{13}, C_7, D_6)$$

$$(A_{15}, B_{13}, C_8, D_6)$$

$$(A_{15}, B_{14}, C_6, D_7)$$

$$(A_{15}, B_{14}, C_6, D_8)$$

$$(A_{15}, B_{14}, C_7, D_6)$$

$$(A_{15}, B_{14}, C_8, D_6)$$

$$(A_{15}, B_{15}, C_6, D_6)$$