Calculation of Three-Body Density within GCM Method

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Outline

1. **Definition and Motivation**

2. **Calculation of Three-Body $\rho^{(3)}$ and $\lambda^{(3)}$**

3. **Numerical Check**

Definition (J-scheme and M-scheme) of $\rho^{(3)}$

$$\rho^{(3)^J} \equiv \left\langle 0_f^+ \middle| \left[\left[\left[\hat{c}_{j_1}^{(\tau_1)\dagger} \ \hat{c}_{j_2}^{(\tau_2)\dagger} \right]^{J_{12}} \ \hat{c}_{j_3}^{(\tau_3)\dagger} \right]^{J} \cdot \left[\left[\hat{c}_{\tilde{j}_4}^{(\tau_4)} \ \hat{c}_{\tilde{j}_5}^{(\tau_5)} \right]^{J_{45}} \ \hat{c}_{\tilde{j}_6}^{(\tau_6)} \right]^{J} \right]^{0} \middle| 0_i^+ \right\rangle \quad (1)$$

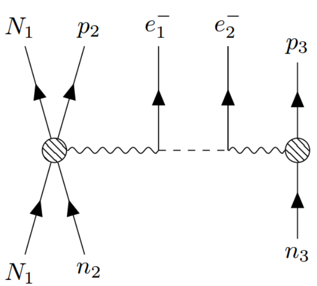
$$\rho^{(3)^M} \equiv \left\langle 0_f^+ \middle| \hat{c}^\dagger_{\tau_1 j_1 m_1} \hat{c}^\dagger_{\tau_2 j_2 m_2} \hat{c}^\dagger_{\tau_3 j_3 m_3} \hat{c}_{\tau_4 j_4 m_4} \hat{c}_{\tau_5 j_5 m_5} \hat{c}_{\tau_6 j_6 m_6} \middle| 0_i^+ \right\rangle \quad (2)$$

From M-scheme to J-scheme

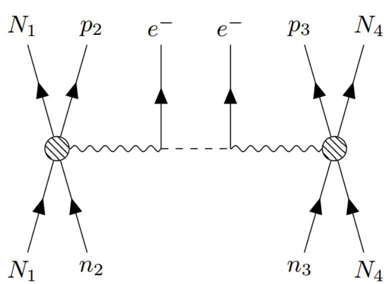
$$\rho^{(3)^J} = \sum_{(m_1 m_2 m_3 m_4 m_5 m_6)}{}' \text{Coeff}(123456, J_{12}, J_{45}, J, \text{Sig}) \cdot \rho^{(3)^M} \quad (3)$$

Important for NME of $0\nu\beta\beta$

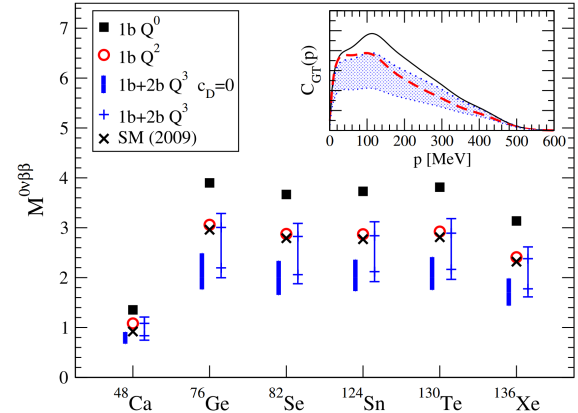
Menendez: PRL (2011); Engel: PRC (2014)



(b) 1B plus 2B



(d) Double 2B



From Wendt's notes

From PRL 107, 062501

Definition (M-scheme) of $\lambda^{(3)}$

$$A^{a\cdots k}_{l\cdots q} = c^\dagger_a \cdots c^\dagger_k c_q \cdots c_l \tag{4}$$

$$\rho^k_r = \langle\Psi|A^k_r|\Psi\rangle = \rho_{rk}, \tag{5}$$
$$\rho^{kl}_{rs} = \langle\Psi|A^{kl}_{rs}|\Psi\rangle = \rho^{(2)}_{rs,kl}, \tag{6}$$
$$\rho^{klm}_{rst} = \langle\Psi|A^{klm}_{rst}|\Psi\rangle = \rho^{(3)}_{rst,klm}. \tag{7}$$

$$\rho^k_r \equiv \lambda^k_r, \tag{8}$$
$$\rho^{kl}_{rs} \equiv \lambda^{kl}_{rs} + \mathcal{A}(\lambda^k_r\lambda^l_s), \tag{9}$$
$$\rho^{klm}_{rst} \equiv \lambda^{klm}_{rst} + \mathcal{A}(\lambda^k_r\lambda^l_s\lambda^m_t + \lambda^k_r\lambda^{lm}_{st}). \tag{10}$$

The antisymmetrizer $\mathcal{A}$ generates all unique permutations of the indices of the product of tensors it is applied to.

H. Hergert: In-Medium SRG Notes (2015)

$\rho^{(3)}$: from M- to J-scheme

$$
\begin{aligned}
&\left[\left[\left[\hat{c}^{(\tau_1)\dagger}_{j_1}\ \hat{c}^{(\tau_2)\dagger}_{j_2}\right]^{J_{12}}\ \hat{c}^{(\tau_3)\dagger}_{j_3}\right]^{J} \cdot \left[\left[\hat{c}^{(\tau_4)}_{\tilde{j}_4}\ \hat{c}^{(\tau_5)}_{\tilde{j}_5}\right]^{J_{45}}\ \hat{c}^{(\tau_6)}_{\tilde{j}_6}\right]^{J}\right]^{0} \\
&= \sum_{MM'} C^{00}_{JMJM'} \left[\left[\hat{c}^{(\tau_1)\dagger}_{j_1}\ \hat{c}^{(\tau_2)\dagger}_{j_2}\right]^{J_{12}}\ \hat{c}^{(\tau_3)\dagger}_{j_3}\right]^{JM} \cdot \left[\left[\hat{c}^{(\tau_4)}_{\tilde{j}_4}\ \hat{c}^{(\tau_5)}_{\tilde{j}_5}\right]^{J_{45}}\ \hat{c}^{(\tau_6)}_{\tilde{j}_6}\right]^{JM'} \\
&= \sum_{MM'} \sum_{M_{12}m_3} \sum_{M_{45}m_6} C^{00}_{JMJM'} C^{JM}_{J_{12}M_{12}j_3m_3} C^{JM'}_{J_{45}M_{45}j_6m_6} \left[\hat{c}^{(\tau_1)\dagger}_{j_1}\ \hat{c}^{(\tau_2)\dagger}_{j_2}\right]^{J_{12}M_{12}}\ \hat{c}^{(\tau_3)\dagger}_{j_3m_3} \cdot \left[\hat{c}^{(\tau_4)}_{\tilde{j}_4}\ \hat{c}^{(\tau_5)}_{\tilde{j}_5}\right]^{J_{45}M_{45}}\ \hat{c}^{(\tau_6)}_{\tilde{j}_6m_6} \\
&= \sum_{MM'} \sum_{M_{12}m_3} \sum_{M_{45}m_6} \sum_{m_1m_2} \sum_{m_4m_5} C^{00}_{JMJM'} C^{JM}_{J_{12}M_{12}j_3m_3} C^{JM'}_{J_{45}M_{45}j_6m_6} C^{J_{12}M_{12}}_{j_1m_1j_2m_2} C^{J_{45}M_{45}}_{j_4m_4j_5m_5} \\
&\qquad \times \hat{c}^{(\tau_1)\dagger}_{j_1m_1}\ \hat{c}^{(\tau_2)\dagger}_{j_2m_2}\ \hat{c}^{(\tau_3)\dagger}_{j_3m_3} \cdot \hat{c}^{(\tau_4)}_{\tilde{j}_4m_4}\ \hat{c}^{(\tau_5)}_{\tilde{j}_5m_5}\ \hat{c}^{(\tau_6)}_{\tilde{j}_6m_6} \\
&= \sum_{M} \sum_{M_{12}m_3} \sum_{M_{45}m_6} \sum_{m_1m_2} \sum_{m_4m_5} (-)^{J-M} \frac{1}{\sqrt{2J+1}} C^{JM}_{J_{12}M_{12}j_3m_3} C^{J-M}_{J_{45}M_{45}j_6m_6} C^{J_{12}M_{12}}_{j_1m_1j_2m_2} C^{J_{45}M_{45}}_{j_4m_4j_5m_5} \\
&\qquad \times \hat{c}^{(\tau_1)\dagger}_{j_1m_1}\ \hat{c}^{(\tau_2)\dagger}_{j_2m_2}\ \hat{c}^{(\tau_3)\dagger}_{j_3m_3} \cdot \hat{c}^{(\tau_4)}_{\tilde{j}_4m_4}\ \hat{c}^{(\tau_5)}_{\tilde{j}_5m_5}\ \hat{c}^{(\tau_6)}_{\tilde{j}_6m_6}
\end{aligned} \tag{11}
$$

$\rho^{(3)}$: from M- to J-scheme

- In the signature basis

$$\hat{d}_k \equiv \frac{1}{\sqrt{2}}(\hat{c}_{\tilde{k}} + \hat{c}_k), \qquad \hat{d}^\dagger_{\bar{k}} \equiv \frac{1}{\sqrt{2}}(\hat{c}^\dagger_{\tilde{k}} - \hat{c}^\dagger_k), \tag{12}$$

$$\hat{d}_{\bar{k}} \equiv \frac{1}{\sqrt{2}}(\hat{c}_{\tilde{k}} - \hat{c}_k), \qquad \hat{d}^\dagger_k \equiv \frac{1}{\sqrt{2}}(\hat{c}^\dagger_{\tilde{k}} + \hat{c}^\dagger_k). \tag{13}$$

$$e^{-i\pi \hat{J}_x} \begin{pmatrix} \hat{d}^\dagger_k \\ \hat{d}^\dagger_{\bar{k}} \end{pmatrix} e^{i\pi \hat{J}_x} = \pm i \begin{pmatrix} \hat{d}^\dagger_k \\ \hat{d}^\dagger_{\bar{k}} \end{pmatrix} \tag{14}$$

- Where $+(-)$ for $m = \frac{1}{2}, -\frac{3}{2}, \frac{5}{2} \cdots (-\frac{1}{2}, \frac{3}{2}, -\frac{5}{2} \cdots)$, i.e., $m =$ even$+\frac{1}{2}$ for positive signature.

- Rotated matrix elements in signature basis

$$\left\langle \phi_f \middle| \hat{d}^\dagger_{\tau_1 j_1 m_1} \hat{d}^\dagger_{\tau_2 j_2 m_2} \hat{d}^\dagger_{\tau_3 j_3 m_3} \hat{d}_{\tau_4 j_4 m_4} \hat{d}_{\tau_5 j_5 m_5} \hat{d}_{\tau_6 j_6 m_6} \middle| \tilde{\phi}_i \right\rangle \tag{15}$$

N. Hinohara: Notes (2015)

$\rho^{(3)}$: from M- to J-scheme

$$
= \sum_{(m_1m_2m_3m_4m_5m_6)}^{\prime} \sum_{(M_{12}M_{45}M)} (-)^{J-M} \frac{1}{\sqrt{2J+1}} \times
$$

$$
\left\{
\begin{array}{ll}
C^{JM}_{J_{12}M_{12}j_3m_3} C^{J-M}_{J_{45}M_{45}j_6m_6} C^{J_{12}M_{12}}_{j_1m_1j_2m_2} C^{J_{45}M_{45}}_{j_4m_4j_5m_5} & \hat{c}^{(\tau_1)\dagger}_{j_1m_1} \hat{c}^{(\tau_2)\dagger}_{j_2m_2} \hat{c}^{(\tau_3)\dagger}_{j_3m_3} \cdot \hat{c}^{(\tau_4)}_{\tilde{j}_4m_4} \hat{c}^{(\tau_5)}_{\tilde{j}_5m_5} \hat{c}^{(\tau_6)}_{\tilde{j}_6m_6} \\
+C^{JM}_{J_{12}M_{12}j_3m_3} C^{J-M}_{J_{45}M_{45}j_6-m_6} C^{J_{12}M_{12}}_{j_1m_1j_2m_2} C^{J_{45}M_{45}}_{j_4m_4j_5m_5} & \hat{c}^{(\tau_1)\dagger}_{j_1m_1} \hat{c}^{(\tau_2)\dagger}_{j_2m_2} \hat{c}^{(\tau_3)\dagger}_{j_3m_3} \cdot \hat{c}^{(\tau_4)}_{\tilde{j}_4m_4} \hat{c}^{(\tau_5)}_{\tilde{j}_5m_5} \hat{c}^{(\tau_6)}_{\tilde{j}_6-m_6} \\
+C^{JM}_{J_{12}M_{12}j_3m_3} C^{J-M}_{J_{45}M_{45}j_6m_6} C^{J_{12}M_{12}}_{j_1m_1j_2m_2} C^{J_{45}M_{45}}_{j_4m_4j_5-m_5} & \hat{c}^{(\tau_1)\dagger}_{j_1m_1} \hat{c}^{(\tau_2)\dagger}_{j_2m_2} \hat{c}^{(\tau_3)\dagger}_{j_3m_3} \cdot \hat{c}^{(\tau_4)}_{\tilde{j}_4m_4} \hat{c}^{(\tau_5)}_{\tilde{j}_5-m_5} \hat{c}^{(\tau_6)}_{\tilde{j}_6m_6} \\
+C^{JM}_{J_{12}M_{12}j_3m_3} C^{J-M}_{J_{45}M_{45}j_6-m_6} C^{J_{12}M_{12}}_{j_1m_1j_2m_2} C^{J_{45}M_{45}}_{j_4m_4j_5-m_5} & \hat{c}^{(\tau_1)\dagger}_{j_1m_1} \hat{c}^{(\tau_2)\dagger}_{j_2m_2} \hat{c}^{(\tau_3)\dagger}_{j_3m_3} \cdot \hat{c}^{(\tau_4)}_{\tilde{j}_4m_4} \hat{c}^{(\tau_5)}_{\tilde{j}_5-m_5} \hat{c}^{(\tau_6)}_{\tilde{j}_6-m_6} \\
+C^{JM}_{J_{12}M_{12}j_3m_3} C^{J-M}_{J_{45}M_{45}j_6m_6} C^{J_{12}M_{12}}_{j_1m_1j_2m_2} C^{J_{45}M_{45}}_{j_4-m_4j_5m_5} & \hat{c}^{(\tau_1)\dagger}_{j_1m_1} \hat{c}^{(\tau_2)\dagger}_{j_2m_2} \hat{c}^{(\tau_3)\dagger}_{j_3m_3} \cdot \hat{c}^{(\tau_4)}_{\tilde{j}_4-m_4} \hat{c}^{(\tau_5)}_{\tilde{j}_5m_5} \hat{c}^{(\tau_6)}_{\tilde{j}_6m_6} \\
+C^{JM}_{J_{12}M_{12}j_3m_3} C^{J-M}_{J_{45}M_{45}j_6-m_6} C^{J_{12}M_{12}}_{j_1m_1j_2m_2} C^{J_{45}M_{45}}_{j_4-m_4j_5m_5} & \hat{c}^{(\tau_1)\dagger}_{j_1m_1} \hat{c}^{(\tau_2)\dagger}_{j_2m_2} \hat{c}^{(\tau_3)\dagger}_{j_3m_3} \cdot \hat{c}^{(\tau_4)}_{\tilde{j}_4-m_4} \hat{c}^{(\tau_5)}_{\tilde{j}_5m_5} \hat{c}^{(\tau_6)}_{\tilde{j}_6-m_6} \\
+C^{JM}_{J_{12}M_{12}j_3m_3} C^{J-M}_{J_{45}M_{45}j_6m_6} C^{J_{12}M_{12}}_{j_1m_1j_2m_2} C^{J_{45}M_{45}}_{j_4-m_4j_5-m_5} & \hat{c}^{(\tau_1)\dagger}_{j_1m_1} \hat{c}^{(\tau_2)\dagger}_{j_2m_2} \hat{c}^{(\tau_3)\dagger}_{j_3m_3} \cdot \hat{c}^{(\tau_4)}_{\tilde{j}_4-m_4} \hat{c}^{(\tau_5)}_{\tilde{j}_5-m_5} \hat{c}^{(\tau_6)}_{\tilde{j}_6m_6} \\
+C^{JM}_{J_{12}M_{12}j_3m_3} C^{J-M}_{J_{45}M_{45}j_6-m_6} C^{J_{12}M_{12}}_{j_1m_1j_2m_2} C^{J_{45}M_{45}}_{j_4-m_4j_5-m_5} & \hat{c}^{(\tau_1)\dagger}_{j_1m_1} \hat{c}^{(\tau_2)\dagger}_{j_2m_2} \hat{c}^{(\tau_3)\dagger}_{j_3m_3} \cdot \hat{c}^{(\tau_4)}_{\tilde{j}_4-m_4} \hat{c}^{(\tau_5)}_{\tilde{j}_5-m_5} \hat{c}^{(\tau_6)}_{\tilde{j}_6-m_6} \\
+C^{JM}_{J_{12}M_{12}j_3-m_3} C^{J-M}_{J_{45}M_{45}j_6m_6} C^{J_{12}M_{12}}_{j_1m_1j_2m_2} C^{J_{45}M_{45}}_{j_4m_4j_5m_5} & \hat{c}^{(\tau_1)\dagger}_{j_1m_1} \hat{c}^{(\tau_2)\dagger}_{j_2m_2} \hat{c}^{(\tau_3)\dagger}_{j_3-m_3} \cdot \hat{c}^{(\tau_4)}_{\tilde{j}_4m_4} \hat{c}^{(\tau_5)}_{\tilde{j}_5m_5} \hat{c}^{(\tau_6)}_{\tilde{j}_6m_6} \\
+C^{JM}_{J_{12}M_{12}j_3-m_3} C^{J-M}_{J_{45}M_{45}j_6-m_6} C^{J_{12}M_{12}}_{j_1m_1j_2m_2} C^{J_{45}M_{45}}_{j_4m_4j_5m_5} & \hat{c}^{(\tau_1)\dagger}_{j_1m_1} \hat{c}^{(\tau_2)\dagger}_{j_2m_2} \hat{c}^{(\tau_3)\dagger}_{j_3-m_3} \cdot \hat{c}^{(\tau_4)}_{\tilde{j}_4m_4} \hat{c}^{(\tau_5)}_{\tilde{j}_5m_5} \hat{c}^{(\tau_6)}_{\tilde{j}_6-m_6} \\
+C^{JM}_{J_{12}M_{12}j_3-m_3} C^{J-M}_{J_{45}M_{45}j_6m_6} C^{J_{12}M_{12}}_{j_1m_1j_2m_2} C^{J_{45}M_{45}}_{j_4m_4j_5-m_5} & \hat{c}^{(\tau_1)\dagger}_{j_1m_1} \hat{c}^{(\tau_2)\dagger}_{j_2m_2} \hat{c}^{(\tau_3)\dagger}_{j_3-m_3} \cdot \hat{c}^{(\tau_4)}_{\tilde{j}_4m_4} \hat{c}^{(\tau_5)}_{\tilde{j}_5-m_5} \hat{c}^{(\tau_6)}_{\tilde{j}_6m_6} \\
+C^{JM}_{J_{12}M_{12}j_3-m_3} C^{J-M}_{J_{45}M_{45}j_6-m_6} C^{J_{12}M_{12}}_{j_1m_1j_2m_2} C^{J_{45}M_{45}}_{j_4m_4j_5-m_5} & \hat{c}^{(\tau_1)\dagger}_{j_1m_1} \hat{c}^{(\tau_2)\dagger}_{j_2m_2} \hat{c}^{(\tau_3)\dagger}_{j_3-m_3} \cdot \hat{c}^{(\tau_4)}_{\tilde{j}_4m_4} \hat{c}^{(\tau_5)}_{\tilde{j}_5-m_5} \hat{c}^{(\tau_6)}_{\tilde{j}_6-m_6} \\
+\cdots \ \cdots & \\
+\cdots \ \cdots &
\end{array}
\right\} \quad (16)
$$

$\rho^{(3)}$: from M- to J-scheme

$$\left[\left[\left[\hat{c}_{j_1}^{(\tau_1)\dagger}\ \hat{c}_{j_2}^{(\tau_2)\dagger}\right]^{J_{12}}\ \hat{c}_{j_3}^{(\tau_3)\dagger}\right]^{J}\cdot\left[\left[\hat{c}_{\tilde{j}_4}^{(\tau_4)}\ \hat{c}_{\tilde{j}_5}^{(\tau_5)}\right]^{J_{45}}\ \hat{c}_{\tilde{j}_6}^{(\tau_6)}\right]^{J}\right]^{0}$$
$$=\sum_{(m_1m_2m_3m_4m_5m_6)}^{\prime} C(123456, J_{12}, J_{45}, J)\ \hat{d}_{j_1,m_1}^{(\tau_1)\dagger}\hat{d}_{j_2,m_2}^{(\tau_2)\dagger}\hat{d}_{j_3,m_3}^{(\tau_3)\dagger}\hat{d}_{j_4,m_4}^{(\tau_4)}\hat{d}_{j_5,m_5}^{(\tau_5)}\hat{d}_{j_6,m_6}^{(\tau_6)} \tag{17}$$

where

$$\begin{aligned}
C(123456, J_{12}, J_{45}, J) &= +P1+P2+P3+P4+P5+P6+P7+P8+P9+P10+P11+P12+P13+P14+P15+P16\\
C(\bar{1}\bar{2}3456, J_{12}, J_{45}, J) &= +P1+P2+P3+P4+P5+P6+P7+P8-P9-P10-P11-P12-P13-P14-P15-P16\\
C(\bar{1}2\bar{3}456, J_{12}, J_{45}, J) &= +P1+P2+P3+P4-P5-P6-P7-P8+P9+P10+P11+P12-P13-P14-P15-P16\\
C(\bar{1}23\bar{4}56, J_{12}, J_{45}, J) &= -P1-P2+P3+P4-P5-P6+P7+P8-P9-P10+P11+P12-P13-P14+P15+P16\\
C(\bar{1}234\bar{5}6, J_{12}, J_{45}, J) &= -P1+P2-P3+P4-P5+P6-P7+P8-P9+P10-P11+P12-P13+P14-P15+P16\\
C(\bar{1}2345\bar{6}, J_{12}, J_{45}, J) &= +P1-P2-P3+P4-P5+P6+P7-P8-P9+P10+P11-P12+P13-P14-P15+P16\\
C(1\bar{2}\bar{3}456, J_{12}, J_{45}, J) &= +P1+P2+P3+P4-P5-P6-P7-P8-P9-P10-P11-P12+P13+P14+P15+P16\\
&\cdots\ \cdots\ \cdots
\end{aligned} \tag{18}$$

where

$$\begin{aligned}
P1 &= \sum_{(M_{12}M_{45}M)}\frac{1}{\sqrt{2J+1}}\frac{1}{4}C^{JM}_{J_{12}M_{12}j_3m_3}C^{J-M}_{J_{45}M_{45}j_6-m_6}C^{J_{12}M_{12}}_{j_1m_1j_2m_2}C^{J_{45}M_{45}}_{j_4m_4j_5m_5}(-)^{j_6-m_6+J-M}\\
P2 &= \sum_{(M_{12}M_{45}M)}\frac{1}{\sqrt{2J+1}}\frac{1}{4}C^{JM}_{J_{12}M_{12}j_3m_3}C^{J-M}_{J_{45}M_{45}j_6m_6}C^{J_{12}M_{12}}_{j_1m_1j_2m_2}C^{J_{45}M_{45}}_{j_4m_4j_5-m_5}(-)^{j_5-m_5+J-M}\\
P3 &= \sum_{(M_{12}M_{45}M)}\frac{1}{\sqrt{2J+1}}\frac{1}{4}C^{JM}_{J_{12}M_{12}j_3m_3}C^{J-M}_{J_{45}M_{45}j_6m_6}C^{J_{12}M_{12}}_{j_1m_1j_2m_2}C^{J_{45}M_{45}}_{j_4-m_4j_5m_5}(-)^{j_4-m_4+J-M}\\
&\cdots\ \cdots\ \cdots
\end{aligned} \tag{19}$$

Matrix elements in signature basis

$$\langle \phi_f | \hat{d}_i^{(\tau_1)\dagger} \hat{d}_j^{(\tau_2)\dagger} \hat{d}_k^{(\tau_3)\dagger} \hat{d}_l^{(\tau_4)} \hat{d}_m^{(\tau_5)} \hat{d}_n^{(\tau_6)} | \tilde{\phi}_i \rangle = \langle \phi_f | \tilde{\phi}_i \rangle \langle \tilde{\phi}_i | \bar{\alpha}_i^{(\tau_1)} \bar{\alpha}_j^{(\tau_2)} \bar{\alpha}_k^{(\tau_3)} \alpha_l^{(\tau_4)} \alpha_m^{(\tau_5)} \alpha_n^{(\tau_6)} | \tilde{\phi}_i \rangle \tag{20}$$

$$\bar{\alpha}_k^{(\tau)} = e^{\hat{Z}^\dagger} \hat{d}_k^{(\tau)\dagger} e^{-\hat{Z}^\dagger}, \qquad \alpha_m^{(\tau)} = e^{\hat{Z}^\dagger} \hat{d}_m^{(\tau)} e^{-\hat{Z}^\dagger}. \tag{21}$$

where

$$\hat{Z} = \sum_{\mu<\nu} Z_{\mu\nu} \hat{a}_\mu^\dagger \hat{a}_\nu^\dagger, \qquad Z = (VU^{-1})^* \tag{22}$$

$$\bar{\alpha}_k^{(\tau)} = \sum_\mu \left\{ A_{k\mu}^{(\tau)} \hat{a}_\mu^\dagger + B_{k\mu}^{(\tau)} \hat{a}_\mu \right\}, \tag{23}$$

$$\alpha_k = \sum_\mu \left\{ C_{k\mu}^{(\tau)} \hat{a}_\mu + D_{k\mu}^{(\tau)} \hat{a}_\mu^\dagger \right\}. \tag{24}$$

where

$$A_{k\mu}^{(\tau)} \equiv \left(U_i^{(\tau)*}\right)_{k\mu}, \qquad B_{k\mu}^{(\tau)} \equiv \left(V_i^{(\tau)} + U_i^{(\tau)*} Z^*\right)_{k\mu},$$
$$C_{k\mu}^{(\tau)} \equiv \left(U_i^{(\tau)} + V_i^{(\tau)*} Z^*\right)_{k\mu}, \quad D_{k\mu}^{(\tau)} \equiv \left(V_i^{(\tau)*}\right)_{k\mu}.$$

Ring and Schuck: Nuclear many-body problem (1980)

Matrix elements in signature basis: explicit

$$
\begin{aligned}
&\langle\tilde{\phi}_I|\bar{\alpha}_i^{(\tau_1)}\bar{\alpha}_j^{(\tau_2)}\bar{\alpha}_k^{(\tau_3)}\alpha_l^{(\tau_4)}\alpha_m^{(\tau_5)}\alpha_n^{(\tau_6)}|\tilde{\phi}_I\rangle \\
=&+\left[\left(B^{(\tau_1)}A^{(\tau_2)T}\right)_{ij}\left(C^{(\tau_4)}D^{(\tau_5)T}\right)_{lm}\left(B^{(\tau_3)}D^{(\tau_6)T}\right)_{kn}\right]-\left[\left(B^{(\tau_1)}A^{(\tau_2)T}\right)_{ij}\left(B^{(\tau_3)}D^{(\tau_5)T}\right)_{km}\left(C^{(\tau_4)}D^{(\tau_6)T}\right)_{ln}\right] \\
&+\left[\left(B^{(\tau_1)}A^{(\tau_2)T}\right)_{ij}\left(B^{(\tau_3)}D^{(\tau_4)T}\right)_{kl}\left(C^{(\tau_5)}D^{(\tau_6)T}\right)_{mn}\right]-\left[\left(B^{(\tau_1)}A^{(\tau_3)T}\right)_{ik}\left(C^{(\tau_4)}D^{(\tau_5)T}\right)_{lm}\left(B^{(\tau_2)}D^{(\tau_6)T}\right)_{jn}\right] \\
&+\left[\left(B^{(\tau_1)}A^{(\tau_3)T}\right)_{ik}\left(B^{(\tau_2)}D^{(\tau_5)T}\right)_{jm}\left(C^{(\tau_4)}D^{(\tau_6)T}\right)_{ln}\right]+\left[\left(B^{(\tau_2)}A^{(\tau_3)T}\right)_{jk}\left(C^{(\tau_4)}D^{(\tau_5)T}\right)_{lm}\left(B^{(\tau_1)}D^{(\tau_6)T}\right)_{in}\right] \\
&-\left[\left(B^{(\tau_2)}A^{(\tau_3)T}\right)_{jk}\left(B^{(\tau_1)}D^{(\tau_5)T}\right)_{im}\left(C^{(\tau_4)}D^{(\tau_6)T}\right)_{ln}\right]+\left[\left(B^{(\tau_2)}A^{(\tau_3)T}\right)_{jk}\left(B^{(\tau_1)}D^{(\tau_4)T}\right)_{il}\left(C^{(\tau_5)}D^{(\tau_6)T}\right)_{mn}\right] \\
&-\left[\left(B^{(\tau_1)}A^{(\tau_3)T}\right)_{ik}\left(B^{(\tau_2)}D^{(\tau_4)T}\right)_{jl}\left(C^{(\tau_5)}D^{(\tau_6)T}\right)_{mn}\right]+\left[\left(B^{(\tau_1)}D^{(\tau_4)T}\right)_{il}\left(B^{(\tau_3)}D^{(\tau_5)T}\right)_{km}\left(B^{(\tau_2)}D^{(\tau_6)T}\right)_{jn}\right] \\
&-\left[\left(B^{(\tau_1)}D^{(\tau_4)T}\right)_{il}\left(B^{(\tau_2)}D^{(\tau_5)T}\right)_{jm}\left(B^{(\tau_3)}D^{(\tau_6)T}\right)_{kn}\right]-\left[\left(B^{(\tau_2)}D^{(\tau_4)T}\right)_{jl}\left(B^{(\tau_3)}D^{(\tau_5)T}\right)_{km}\left(B^{(\tau_1)}D^{(\tau_6)T}\right)_{in}\right] \\
&+\left[\left(B^{(\tau_2)}D^{(\tau_4)T}\right)_{jl}\left(B^{(\tau_1)}D^{(\tau_5)T}\right)_{im}\left(B^{(\tau_3)}D^{(\tau_6)T}\right)_{kn}\right]+\left[\left(B^{(\tau_3)}D^{(\tau_4)T}\right)_{kl}\left(B^{(\tau_2)}D^{(\tau_5)T}\right)_{jm}\left(B^{(\tau_1)}D^{(\tau_6)T}\right)_{in}\right] \\
&-\left[\left(B^{(\tau_3)}D^{(\tau_4)T}\right)_{kl}\left(B^{(\tau_1)}D^{(\tau_5)T}\right)_{im}\left(B^{(\tau_2)}D^{(\tau_6)T}\right)_{jn}\right]
\end{aligned}
\tag{25}
$$

Matrix elements in signature basis: Pfaffian

- Define basic contractions

$$\langle\tilde{\phi}_I|\bar{\alpha}_i^{(\tau_i)}\bar{\alpha}_j^{(\tau_j)}|\tilde{\phi}_I\rangle = \left(B^{(\tau_i)}A^{(\tau_j)T}\right)_{ij} \tag{26a}$$

$$\langle\tilde{\phi}_I|\bar{\alpha}_i^{(\tau_i)}\alpha_j^{(\tau_j)}|\tilde{\phi}_I\rangle = \left(B^{(\tau_i)}D^{(\tau_j)T}\right)_{ij} \tag{26b}$$

$$\langle\tilde{\phi}_I|\alpha_i^{(\tau_i)}\alpha_j^{(\tau_j)}|\tilde{\phi}_I\rangle = \left(C^{(\tau_i)}D^{(\tau_j)T}\right)_{ij} \tag{26c}$$

- By the definition of Pfaffian, we get

$$\langle\tilde{\phi}_I|\bar{\alpha}_i^{(\tau_1)}\bar{\alpha}_j^{(\tau_2)}\bar{\alpha}_k^{(\tau_3)}\alpha_l^{(\tau_4)}\alpha_m^{(\tau_5)}\alpha_n^{(\tau_6)}|\tilde{\phi}_I\rangle = Pf(X) \tag{27}$$

- where

$$X = \begin{pmatrix} \left(B^{(\tau)}A^{(\tau')T}\right) & \left(B^{(\tau)}D^{(\tau')T}\right) \\ -\left(B^{(\tau)}D^{(\tau')T}\right)^T & \left(C^{(\tau)}D^{(\tau')T}\right) \end{pmatrix} \tag{28}$$

From $\rho^{(3)}$ to $\lambda^{(3)}$ (J-schcme)

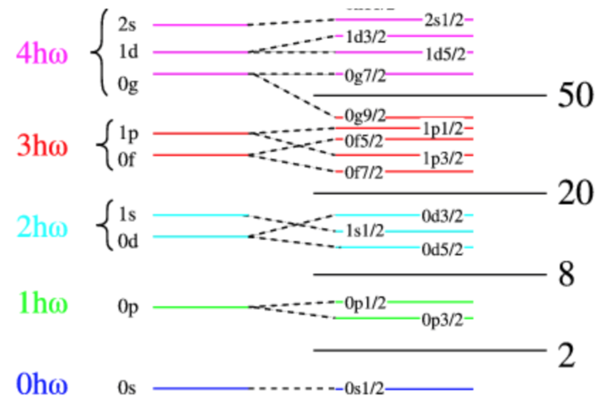
$$
\begin{aligned}
\lambda^{KLM}_{RST} = &+ \rho^{KLM}_{RST}/\sqrt{2J+1} \\
&- (-)^{J_{ts}+j_l+j_m+1}\delta_{JJ'}\delta_{MM'}\hat{J}_{kl}\left\{\begin{array}{ccc} j_k & j_l & J_{kl} \\ j_m & J & J_{ts}\end{array}\right\}\frac{\delta_{j_kj_r}}{\hat{j}_k}[c^\dagger_K\tilde{c}_R]^0_0\Big[[c^\dagger_Lc^\dagger_M]^{J_{ts}}[\tilde{c}_T\tilde{c}_S]^{J_{ts}}\Big]^0 \\
&- \sum_{J_{lm}}\delta_{JJ'}\delta_{MM'}(-)^{j_l+j_m+j_t+j_k+J_{ts}+J_{lm}}\left\{\begin{array}{ccc} j_t & j_k & J_{ts} \\ J & j_r & J_{lm}\end{array}\right\}\left\{\begin{array}{ccc} j_l & j_m & J_{lm} \\ J & j_k & J_{kl}\end{array}\right\} \\
&\qquad\times\frac{\delta_{j_kj_s}\hat{J}_{kl}\hat{J}_{ts}\hat{J}_{lm}}{\hat{j}_k}[c^\dagger_K\tilde{c}_S]^0_0\Big[[c^\dagger_Lc^\dagger_M]^{J_{lm}}[\tilde{c}_R\tilde{c}_T]^{J_{lm}}\Big]^0 \\
&- \delta_{JJ'}\delta_{MM'}\sum_{J_{lm}}(-)^{j_l+j_m+j_s+j_r}\left\{\begin{array}{ccc} j_s & j_k & J_{ts} \\ J & j_r & J_{lm}\end{array}\right\}\left\{\begin{array}{ccc} j_l & j_m & J_{lm} \\ J & j_k & J_{kl}\end{array}\right\} \\
&\qquad\times\frac{\delta_{j_kj_t}\hat{J}_{kl}\hat{J}_{ts}\hat{J}_{lm}}{\hat{j}_k}[c^\dagger_K\tilde{c}_T]^0_0\Big[[c^\dagger_Lc^\dagger_M]^{J_{lm}}[\tilde{c}_S\tilde{c}_R]^{J_{lm}}\Big]^0 \\
&- \delta_{JJ'}\delta_{MM'}(-)^{j_l-J_{kl}+j_k+1}\left\{\begin{array}{ccc} j_l & j_k & J_{kl} \\ j_m & J & J_{ts}\end{array}\right\}\frac{\delta_{j_lj_r}\hat{J}_{kl}}{\hat{j}_l}[c^\dagger_L\tilde{c}_R]^0_0\Big[[c^\dagger_Mc^\dagger_K]^{J_{ts}}[\tilde{c}_T\tilde{c}_S]^{J_{ts}}\Big]^0 \\
&- \delta_{JJ'}\delta_{MM'}(-)^{j_t+j_k+J_{kl}+J_{ts}+1}\sum_{J_{mk}}\left\{\begin{array}{ccc} j_t & j_l & J_{ts} \\ J & j_r & J_{mk}\end{array}\right\}\left\{\begin{array}{ccc} j_k & j_m & J_{mk} \\ J & j_l & J_{kl}\end{array}\right\} \\
&\qquad\times\frac{\delta_{j_lj_s}\hat{J}_{kl}\hat{J}_{ts}\hat{J}_{mk}}{\hat{j}_l}[c^\dagger_L\tilde{c}_S]^0_0\Big[[c^\dagger_Mc^\dagger_K]^{J_{mk}}[\tilde{c}_R\tilde{c}_T]^{J_{mk}}\Big]^0 \\
&- \delta_{JJ'}\delta_{MM'}\sum_{J_{mk}}(-)^{j_k+J_{kl}+j_l+j_r+j_s+J_{mk}}\left\{\begin{array}{ccc} j_s & j_l & J_{ts} \\ J & j_r & J_{mk}\end{array}\right\}\left\{\begin{array}{ccc} j_k & j_m & J_{mk} \\ J & j_l & J_{kl}\end{array}\right\}
\end{aligned}
$$

From $\rho^{(3)}$ to $\lambda^{(3)}$ (J-schcme)

$$
\begin{aligned}
&\times \frac{\delta_{j_l j_t}\hat{J}_{kl}\hat{J}_{ts}\hat{J}_{mk}}{\hat{j}_l}\left[c^\dagger_L\tilde{c}_T\right]^0_0\left[\left[c^\dagger_M c^\dagger_K\right]^{J_{mk}}\left[\tilde{c}_S\tilde{c}_R\right]^{J_{mk}}\right]^0 \\
&- \delta_{JJ'}\delta_{MM'}\frac{\delta_{j_m j_r}\delta_{J_{kl}J_{ts}}}{\hat{j}_m\hat{J}_{kl}}\left[c^\dagger_M\tilde{c}_R\right]^0_0\left[\left[c^\dagger_K c^\dagger_L\right]^{J_{kl}}\left[\tilde{c}_T\tilde{c}_S\right]^{J_{kl}}\right]^0 \\
&- \delta_{JJ'}\delta_{MM'}(-)^{j_t+j_m+J_{ts}+1}\begin{Bmatrix} j_t & j_m & J_{ts} \\ J & j_r & J_{kl}\end{Bmatrix}\frac{\delta_{j_m j_s}\hat{J}_{ts}}{\hat{j}_m}\left[c^\dagger_M\tilde{c}_S\right]^0_0\left[\left[c^\dagger_K c^\dagger_L\right]^{J_{kl}}\left[\tilde{c}_R\tilde{c}_T\right]^{J_{kl}}\right]^0 \\
&- \delta_{JJ'}\delta_{MM'}(-)^{J_{kl}+j_s+j_r+1}\begin{Bmatrix} j_s & j_m & J_{ts} \\ J & j_r & J_{kl}\end{Bmatrix}\frac{\delta_{j_m j_t}\hat{J}_{ts}}{\hat{j}_m}\left[c^\dagger_M\tilde{c}_T\right]^0_0\left[\left[c^\dagger_K c^\dagger_L\right]^{J_{kl}}\left[\tilde{c}_S\tilde{c}_R\right]^{J_{kl}}\right]^0 \\
&- 2\hat{J}_{kl}\hat{J}_{ts}\begin{Bmatrix} j_k & j_l & J_{kl} \\ j_m & J & J_{ts}\end{Bmatrix}\frac{\delta_{j_k j_r}\delta_{j_l j_s}\delta_{j_m j_t}}{\hat{j}_k\hat{j}_l\hat{j}_m}\rho^K_R\rho^L_S\rho^M_T \\
&- 2(-)^{J_{ts}+j_l+j_m+1}\hat{J}_{kl}\hat{J}_{ts}\begin{Bmatrix} j_k & j_l & J_{kl} \\ j_m & J & J_{ts}\end{Bmatrix}\frac{\delta_{j_k j_r}\delta_{j_l j_t}\delta_{j_m j_s}}{\hat{j}_k\hat{j}_l\hat{j}_m}\rho^K_R\rho^L_T\rho^M_S \\
&- 2(-)^{j_k+j_l-J_{kl}+1}\hat{J}_{kl}\hat{J}_{ts}\begin{Bmatrix} j_l & j_k & J_{kl} \\ j_m & J & J_{ts}\end{Bmatrix}\frac{\delta_{j_k j_s}\delta_{j_l j_r}\delta_{j_m j_t}}{\hat{j}_k\hat{j}_l\hat{j}_m}\rho^K_S\rho^L_R\rho^M_T \\
&+ 2\delta_{JJ'}\delta_{MM'}(-)^{j_k+j_l-J_{kl}}\frac{\delta_{j_k j_s}\delta_{j_l j_t}\delta_{j_m j_r}\delta_{J_{kl}J_{ts}}}{\hat{j}_k\hat{j}_l\hat{j}_m}\rho^K_S\rho^L_T\rho^M_R \\
&+ 2(-)^{-J_{kl}+j_l+J_{ts}+j_m}\hat{J}_{kl}\hat{J}_{ts}\begin{Bmatrix} j_l & j_k & J_{kl} \\ j_m & J & J_{ts}\end{Bmatrix}\frac{\delta_{j_k j_t}\delta_{j_l j_r}\delta_{j_m j_s}}{\hat{j}_k\hat{j}_l\hat{j}_m}\rho^K_T\rho^L_R\rho^M_S \\
&- 2\delta_{JJ'}\delta_{MM'}\frac{\delta_{j_k j_t}\delta_{j_l j_s}\delta_{j_m j_r}\delta_{J_{kl}J_{ts}}}{\hat{j}_k\hat{j}_l\hat{j}_m}\rho^K_T\rho^L_S\rho^M_R
\end{aligned}
\tag{29}
$$

Numerical details

- **Model space: for ^{76}Ge, ^{76}Se:** $2p_{3/2}, 1f_{5/2}, 2p_{1/2}, 1g_{9/2}$
- **Computation time:** $\sim$ **24 CPU hours for HFB with PNP**



Numerical check

- **Trace of $\rho^{(3)}$: Tr**$(\rho^{(3)}_{ij}) = -N(N-1)(N-2)$
- **Anti-symmetry of $\rho^{(3)}$ in M-scheme:**

$$\rho^{(3)^M} \equiv \left\langle 0_f^+ \middle| \hat{c}^\dagger_{\tau_1 j_1 m_1} \hat{c}^\dagger_{\tau_2 j_2 m_2} \hat{c}^\dagger_{\tau_3 j_3 m_3} \hat{c}_{\tau_4 j_4 m_4} \hat{c}_{\tau_5 j_5 m_5} \hat{c}_{\tau_6 j_6 m_6} \middle| 0_i^+ \right\rangle \qquad (30)$$

- **Symmetry in J-scheme:** $\rho^{(3)^J}_{ij} = \rho^{(3)^J}_{ji}, \qquad \lambda^{(3)^J}_{ij} = \lambda^{(3)^J}_{ji}$
- **Reproduce $\lambda^{(3)^J}_{ij}$ in Spherical case.**

Thank you for your attention!