An algebraic approach for the six nucleon systems

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The ab-initio algebraic model for nucleus

- Nucleus – many body quantum system, invariant for the translations in space.
- Strong correlations between two and three particles (NN and NNN forces).
- No Core Shell Model - All the nucleons are active in the model space

Problem: A set of wavefunctions depending on one particle variables $\mathbf{r}_i$ contain center of mass motion.
Solution: Transition to intrinsic coordinates $\boldsymbol{\rho}_i \rightarrow$ explicit removal of the center of mass coordinate.

Jacobi coordinates!

- Traditional No Core Shell Model approach with **intrinsic** coordinates N$\leq$4
- New interest in N$\geq$4 using intrinsic coordinates[1] [2] [3]

We have a different approach!

[1] A.Gnech, Theoretical calculation of nuclear reactions of interest for Big Bang Nucleosynthesis, Thesis, 2020.
[2] H.L. Thi, Jacobi No-Core Shell Model for P-shell Hypernuclei, Thesis, 2020
[3] S. Liebig, Antisymmetrisation in a Jacobi coordinate based no-core shell model approach, Thesis, 2013

The goal and the tasks

- Develop an **algebraic model** for the six nucleon systems.
  - Formulate **a systematic treatment of the transpositions of the Jacobi coordinates** and their representations in the HO basis (Applicable for large systems).
  - Create a **computationally efficient** approach for the accurate state vector construction (High performance computing).
  - **Develop** generic computational **tools** for the construction of the antisymmetric state vectors (Reusability).

Construct antisymmetric model space

Normalized Jacobi coordinates

Basically a graph to show intrinsic partition of the nucleus:

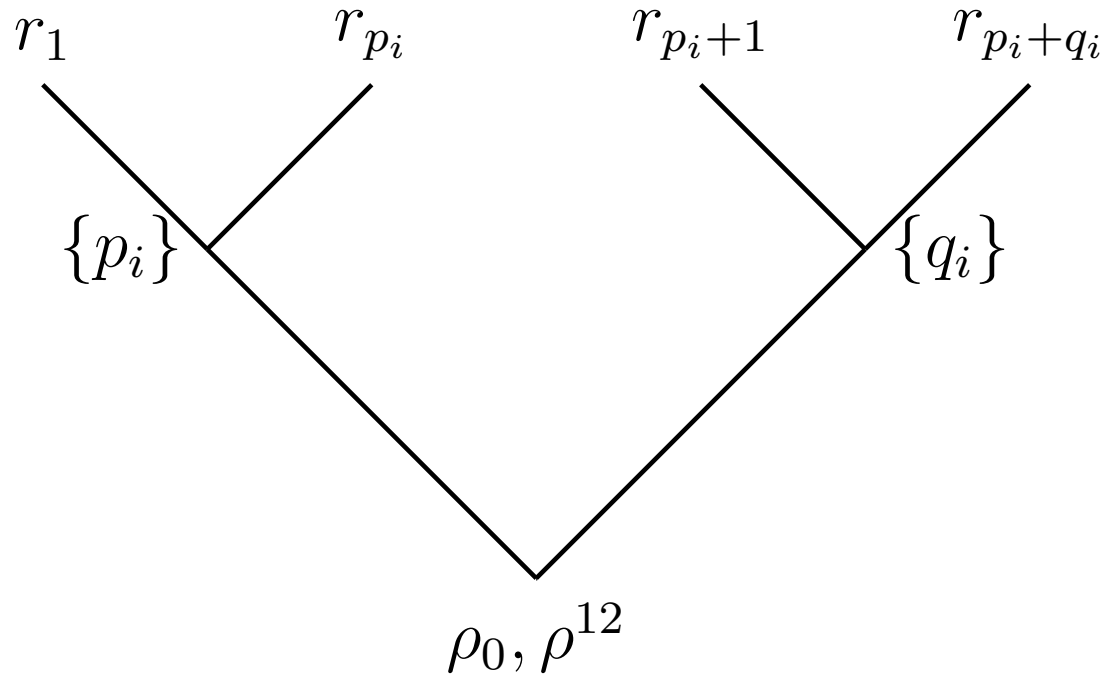


Figure: A generic Jacobi tree [4]

$$\boldsymbol{\rho}_i = \sqrt{\frac{p_i q_i}{p_i + q_i}} \left[\frac{1}{p_i} \sum_{j \in \{p_i\}} \mathbf{r}_j - \frac{1}{q_i} \sum_{j \in \{q_i\}} \mathbf{r}_j \right]. \tag{1}$$

$$\boldsymbol{\rho}_0 = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} \mathbf{r}_j. \tag{2}$$

Harmonic Oscillator basis

- The properly orthonormalized HO function for the wavefunction approximation is

$$\phi_{elm}(\boldsymbol{\rho}) = (-1)^n \left[\frac{2(n!)}{\Gamma(n+l+3/2)}\right]^{\frac{1}{2}} e^{\left(-\rho^2/2\right)} r^l L_n^{(l+1/2)}\left(\rho^2\right) Y_{lm}(\boldsymbol{\rho}/\rho). \tag{3}$$

- Jacobi coordinates in the J-scheme basis $|J^\pi T\rangle$.
- One particle coordinate transformations induce orthogonal transformations in the Jacobi basis.
- Talmi-Moshinsky transformation[5]

$$\begin{pmatrix} \sqrt{\frac{d}{1+d}} & \sqrt{\frac{1}{1+d}} \\ \sqrt{\frac{1}{1+d}} & -\sqrt{\frac{d}{1+d}} \end{pmatrix} \tag{4}$$

representation as HOB

$$\langle e_1 l_1, e_2 l_2 : L | e_1' l_1', e_2' l_2' : L \rangle_d \tag{5}$$

- Representations of this kind of transformations are finite.
- **Problem:** asymptotics of the HO functions $\propto e^{-\alpha r^2}$, while wavefunction asymptotics $\propto e^{-\alpha r}$.
- **Solution:** need to have high HO excitations for good approximation.

[5] G. P. Kamuntavičius et al.; Nucl. Phys. A 695, 191 (2001)

Formalism of the Reduced Hamiltonian in the harmonic oscillator basis

- **Isospin formalism:** the proton and the neutron as **two states of the same particle**- the nucleon.
- Two nucleon interactions:

$$H = \sum_{i=1<k}^{N} h(i,k). \tag{6}$$

- The reduced Hamiltonian[6]

$$h(i,k) = -\frac{\hbar^2}{2mN}(\nabla_i - \nabla_k)^2 + V\left(r_i - r_k, \sigma_i\tau_i\sigma_k'\tau_k'\right). \tag{7}$$

- Introducing the Jacobi coordinate

$$\rho = \frac{1}{\sqrt{2}b}\left(\mathbf{r} - \mathbf{r}'\right). \tag{8}$$

- Results in a Hamiltonian in HO basis

$$h = \frac{2}{N}\left[\frac{1}{2}\left(-\Delta_\rho + \rho^2\right)\right] + \left(\frac{1}{\hbar\omega}V\left(\sqrt{2}b\rho, \sigma\tau\sigma'\tau'\right) - \frac{1}{N}\rho^2\right). \tag{9}$$

[6] G. P. Kamuntavičius; Sov. J. Part. Nuclei 20, 261 (1989)

Construction of the antisymmetric subspace

- To ensure **Pauli principle** we must antisymmetrize the state vectors
- Slater determinants can be formalized as the **antisymmetrizer**

$$A_{1,\ldots,N} = \frac{1}{N!} \sum_{P \in S_N} \pi_P P. \tag{10}$$

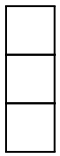
- Symmetric group chain for binary clusters

$$S_N \supset S_{N_1} \times S_{N_2}. \tag{11}$$

- Generating set of permutation operators [7]

$$\Lambda = \sum_{i<j=1}^{N} P_{ij}. \tag{12}$$

Irreps represented by Young Diagrams



$$[\lambda] = [1^3].$$

Figure: Young Diagram [111]

[7] V. Vanagas Algebraic Methods in Nuclear Theory, Mintis (1971)

The six nucleon system

Jacobi coordinates for the six nucleon system

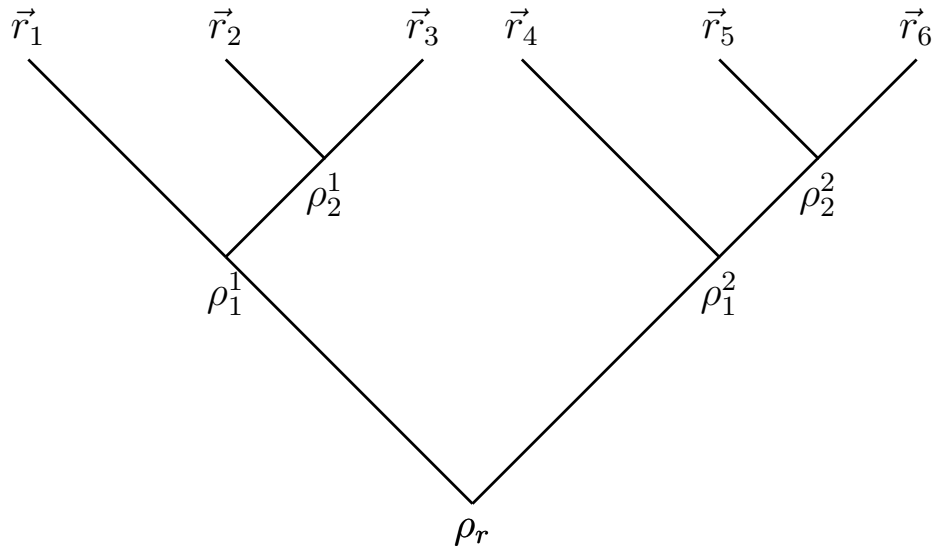


Figure: Jacobi tree for six nucleon system. ρ_y^x is the Jacobi coordinate, where the x is cluster number, y is the coordinate number, r- particle coordinate.

A case of three nucleons (Much simpler!)

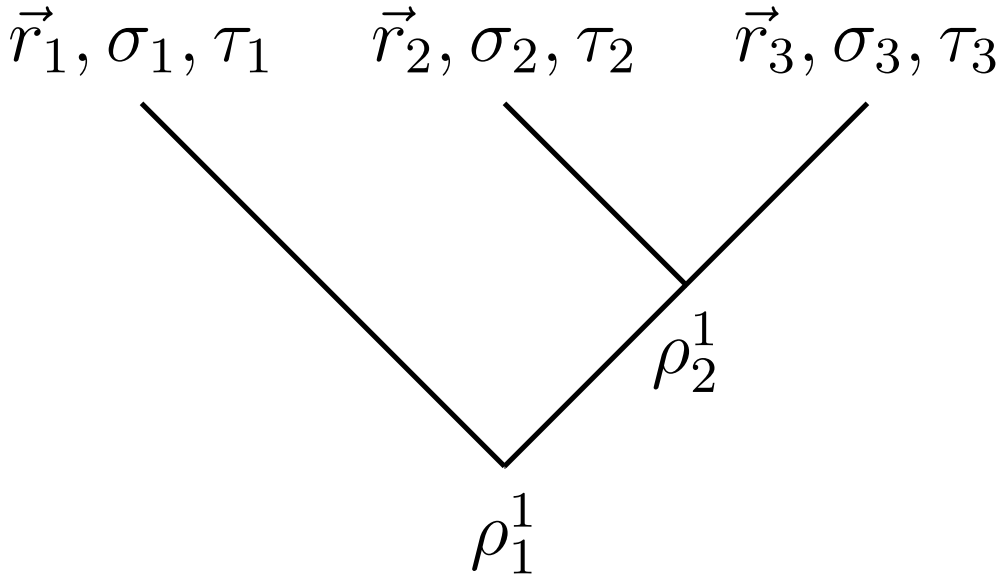


Figure: Jacobi tree for three-particle system. ρ_y^x is the Jacobi coordinate, where the x is cluster number, y is the coordinate number, r- particle coordinate,σ - the particle spin coordinate, τ - is the particle isospin coordinate.

This Jacobi tree corresponds to the following Jacobi coordinates

$$\boldsymbol{\rho}_1^1 = \sqrt{\frac{2}{3}}(\boldsymbol{r}_1 - \frac{1}{2}(\boldsymbol{r}_2 + \boldsymbol{r}_3)), \tag{13}$$

$$\boldsymbol{\rho}_2^1 = \frac{1}{\sqrt{2}}(\boldsymbol{r}_2 - \boldsymbol{r}_3).$$

A case of three nucleons

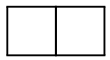
- Group chain for three particles

$$S_3 \supset S_1 \times S_2. \tag{14}$$

- Expression for the Λ operator

$$\Lambda = P_{12} + P_{13} + P_{23}. \tag{15}$$

- antisymmetric two particle subspace



$$a)[\lambda_1] = [1^2] \qquad\qquad b)[\lambda_2] = [2]$$

- The subcluster Λ operator

$$\Lambda = P_{12} + P_{13} + \overline{\Lambda}_2(\lambda_2). \tag{16}$$

- A simple algebra

$$\Lambda = \overline{\Lambda}_2\left(\left[1^2\right]\right) + 2P_{12}. \tag{17}$$

- Boils down to **diagonalization** of

$$P_{12} = \frac{1}{2}(\Lambda - \overline{\Lambda}_2(\lambda_2)). \tag{18}$$

Irreducible representation for three particles

$a)[\lambda_1] = [1^3]$ $\quad$ $b)[\lambda_2] = [21]$

Figure: The Young Diagrams corresponding to the irreps of S_3. a) corresponds to the totally antisymmetric irrep $[1^3]$ and b) corresponds to the irrep with lesser degree of antisymmetry [21].

HO representation

- A representation of the P_{13} in the HO basis

$$\langle(\left((e_1 l_1, \frac{1}{2})j_1, \left(\overline{E_1 L_1}, \overline{S}_1\right)\overline{J}_1\right); (\frac{1}{2}, \overline{T}_1)\left[1^2\right]\Big) E_1 J_1 T_1 | P_{13} \times$$
$$|(\left((e_1' l_1', \frac{1}{2})j_1', \left(\overline{E}_1' \overline{L}_1', \overline{S}_1'\right)\overline{J}_1'\right); (\frac{1}{2}, \overline{T}_1')\left[1^2\right]\Big) E_1 J_1 T_1\rangle$$
$$= (-1)^{L+\overline{L}'+\overline{S}+\overline{S}'+\overline{T}+\overline{T}'} \begin{bmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & \overline{T}_1' \\ \frac{1}{2} & \overline{T}_1 & T \end{bmatrix} \tag{19}$$
$$\times \sum_{LS} (-1)^L \begin{bmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & \overline{S}_1' \\ \frac{1}{2} & \overline{S}_1 & S \end{bmatrix} \begin{bmatrix} l_1 & \overline{L}_1 & L \\ \frac{1}{2} & \overline{S}_1 & S \\ j_1 & \overline{J}_1 & J \end{bmatrix} \begin{bmatrix} l_1' & \overline{L}_1' & L \\ \frac{1}{2} & \overline{S}_1' & S \\ j' & \overline{J}_1' & J \end{bmatrix}$$
$$\times \langle e_1 l_1, \overline{E}_1 \overline{L}_1 : L | \overline{E}_1' \overline{L}_1', e_1' l_1' : L \rangle_3 .$$

- The **eigenvectors**

$$\langle(\left((e_1 l_1, \frac{1}{2})j_1, \left(\overline{EL}, \overline{S}\right)\overline{J}\right); (\frac{1}{2}, \overline{T})\left[1^2\right]\Big) EJT | EJT\Delta \left[1^3\right]\rangle \tag{20}$$

are the CFPs! Coefficients for the transition to antisymmetric subspace.

The six nucleon system

Jacobi coordinates for six nucleon system

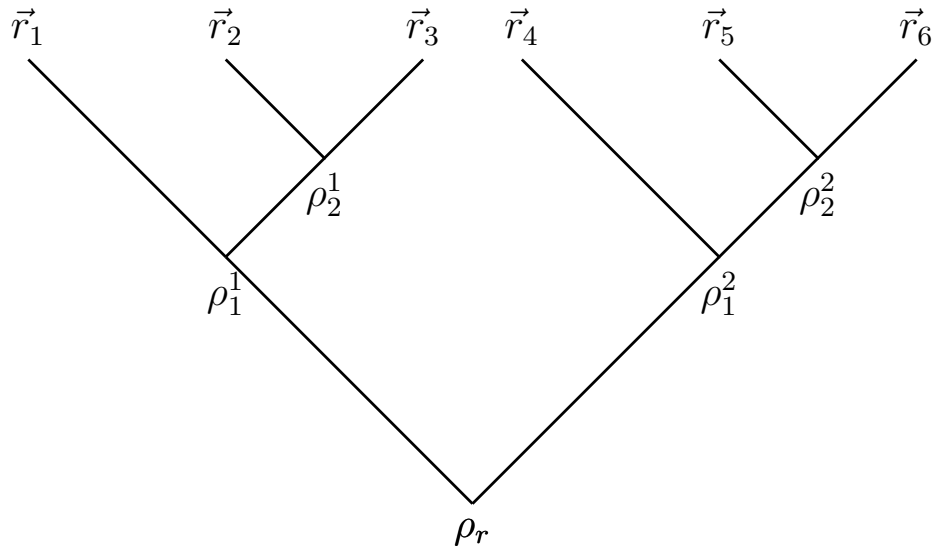


Figure: Jacobi tree for six nucleon system. ρ_y^x is the Jacobi coordinate, where the x is cluster number, y is the coordinate number, r- particle coordinate.

Coefficients of fractional parentage for the six nucleon system

- You need to **diagonalize** operator P_{14}!
- Like in the three-nucleon case, the expansion coefficients

$$\langle(\left(E_1 J_1 T_1 \Delta_1, E_2 J_2 T_2 \Delta_2\right)\overline{J}, el\right) E_6 J_6 T_6 \left[1^3\right] \left[1^3\right] | E_6 J_6 T_6 \Delta_6 \left[1^6\right] \left[1^3\right] \left[1^3\right]\rangle \qquad (21)$$

  are the **CFPs** for the six nucleon system.

Operator P_{14}

Factorization of the operator P_{14} of the S_6

$$\langle P_{14} \rangle = \langle P_{14}^{\sigma r} \rangle \langle P_{14}^{\tau} \rangle . \tag{22}$$

Further decoupling of the **spin-orbital** part

$$\langle P_{14}^{\sigma r} \rangle = \langle P_{14}^{\sigma} \rangle \langle P_{14}^{r} \rangle . \tag{23}$$

Operator P_{14}

The decoupling of L-S pretty complicated

$$\left\langle (l_r,((((l_1,s_1)j_1,(\overline{L}_1,\overline{S}_1)\overline{J}_1)J_1,((l_2,s_2)j_2,(\overline{L}_2,\overline{S}_2)\overline{J}_2)J_2)J_{12})J\right| P_{14}^{r\sigma} \tag{24}$$
$$\times \left|(l_r',((((l_1',s_1')j_1',(\overline{L}_1',\overline{S}_1')\overline{J}_1')J_1',((l_2',s_2')j_2',(\overline{L}_2',\overline{S}_2')\overline{J}_2')J_2')J_{12}')J\right\rangle$$
$$= \sum_{\substack{L_1S_1\\L_2S_2\\L_{12}S_{12}\\L}}\sum_{\substack{L_1'S_1'\\L_2'S_2'\\L_{12}'S_{12}'\\L'}} \begin{bmatrix} l_1 & s_1 & j_1\\ \overline{L}_1 & \overline{S}_1 & \overline{J}_1\\ L_1 & S_1 & J_1\end{bmatrix}\begin{bmatrix} l_2 & s_2 & j_2\\ \overline{L}_2 & \overline{S}_2 & \overline{J}_2\\ L_2 & S_2 & J_2\end{bmatrix}$$
$$\times \begin{bmatrix} L_1 & S_1 & J_1\\ L_2 & S_2 & J_2\\ L_{12} & S & J_{12}\end{bmatrix}\begin{bmatrix} L_{12} & S & J_{12}\\ l_r & 0 & l_r\\ L & S & J\end{bmatrix}$$
$$\times \left\langle ((l_1,\overline{L})L_1,(l_2,\overline{L}_2)L_2)L_{12},l_r)L\,|P_{14}^{r}|\,((l_1',\overline{L}')L_1',(l_2',\overline{L}_2')L_2')L_{12}',l_r')L\right\rangle$$
$$\times \left\langle ((s_1,\overline{S}_1)S_1,(s_2,\overline{S}_2)S_2)S\,|P_{14}^{\sigma}|\,((s_1',\overline{S}_1')S'_1,(s_2',\overline{S}_2')S'_2)S\right\rangle$$
$$\times \delta_{\overline{L}_1\overline{L}_2,\overline{L}_1'\overline{L}_2'};\delta_{\overline{S}_1\overline{S}_2,\overline{S}_1'\overline{S}_2'};\delta_{\overline{J}_1\overline{J}_2J,\overline{J}_1'\overline{J}_2'J'}\delta_{LS,L'S'}$$
$$\times \begin{bmatrix} L_{12}' & l_r' & L'\\ S' & 0 & S'\\ J_{12}' & l_r' & J\end{bmatrix}\begin{bmatrix} L_1' & L_2' & L_{12}'\\ S_1' & S_2' & S'\\ J_1' & J_2' & J_{12}'\end{bmatrix}\begin{bmatrix} l_1' & \overline{L}_1' & L_1'\\ s_1' & \overline{S}_1' & S_1'\\ j_1' & \overline{J}_1' & J_1'\end{bmatrix}\begin{bmatrix} l_2' & \overline{L}_2' & L_2'\\ s_2' & \overline{S}_2' & S_2'\\ j_2' & \overline{J}_2' & J_2'\end{bmatrix}.$$

Four particle harmonic oscillator brackets[8]

Action of the operator P_{14} on the orbital part boils down to:

$$\langle((e_1 l_1, e_2 l_2) l_{12}, e_3 l_3) l | T_{12}(d_1) T_{23}(d_2) T_{12}(d_1) | ((e_1' l_1', e_2' l_2') l_{12}', e_3' l_3') l \rangle_{d_1 d_2} = \tag{25}$$
$$\sum_{\substack{\varepsilon_1 \lambda_1, \varepsilon_2 \lambda_2, \Lambda_{23} \\ \varepsilon_2' \lambda_2'}} \langle e_1 l_1, e_2 l_2 : L_{12} | \varepsilon_1 \lambda_1, \varepsilon_2 \lambda_2 : L_{12} \rangle_{d_1} \delta_{L_{12} e_3 l_3, L_{12}' e_3' l_3'}$$
$$\times \begin{bmatrix} \lambda_1 & 0 & \lambda_1 \\ \lambda_2 & l_3 & \Lambda_{23} \\ L_{12} & l_3 & L \end{bmatrix} \left\langle \varepsilon_2 \lambda_2, e_3 l_3 : \Lambda_{23} | \varepsilon_2' \lambda_2', e_3' l_3' : \Lambda_{23} \right\rangle_{d_2}$$
$$\times \begin{bmatrix} \lambda_1 & \lambda_2' & L_{12}' \\ 0 & l_3' & l_3' \\ \lambda_1 & \Lambda_{23} & L \end{bmatrix} \langle \varepsilon_1 \lambda_1, \varepsilon_2' \lambda_2' : L_{12} | e_1' l_1', e_2' l_2' : L_{12}' \rangle_{d_1} \delta_{L_{12}, L_{12}'}.$$

$$T_{12}(d_1) T_{23}(d_2) T_{12}(d_1) = \tag{26}$$
$$\begin{pmatrix} \sqrt{\frac{d_1}{1+d_1}} & \sqrt{\frac{1}{1+d_1}} & 0 \\ \sqrt{\frac{1}{1+d_1}} & -\sqrt{\frac{d_1}{1+d_1}} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \sqrt{\frac{d_2}{1+d_2}} & \sqrt{\frac{1}{1+d_2}} \\ 0 & \sqrt{\frac{1}{1+d_2}} & -\sqrt{\frac{d_2}{1+d_2}} \end{pmatrix} \begin{pmatrix} \sqrt{\frac{d_1}{1+d_1}} & \sqrt{\frac{1}{1+d_1}} & 0 \\ \sqrt{\frac{1}{1+d_1}} & -\sqrt{\frac{d_1}{1+d_1}} & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

[8] D. Germanas et al, Comp. Phys. Commmun., **181**, 2, 420, (2010)

Irreducible representations for six nucleon system

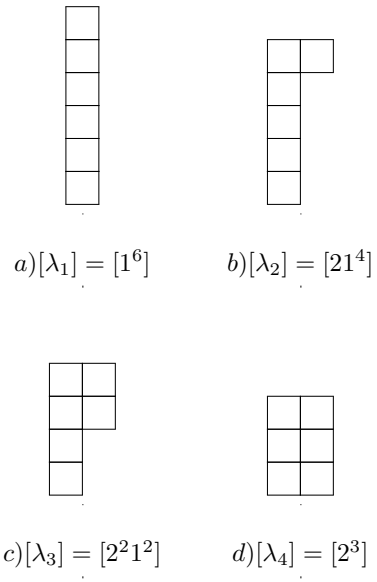


Figure: The Young Diagrams for the four configurations of irreps produced from the two antisymmetric subspaces of the three-particle subclusters. a) corresponds to the fully antisymmetric one- $[1^6]$. The configurations b),c),d) have lesser degree of antisymmetry.

Six nucleon antisymmetric states[9]

E	J	T	*Dimension*	-1	$-\frac{1}{3}$	$\frac{1}{9}$	$\frac{1}{3}$
0	1	0	1	0	0	1	0
1	1	0	10	0	2	5	3
2	1	0	63	3	12	33	15
3	1	0	282	11	63	132	76
4	1	0	1007	45	231	476	255
5	1	0	2035	86	472	947	530
6	1	0	8285	387	1988	3807	2103
0	0	1	1	0	0	1	0
1	0	1	7	0	1	4	2
2	0	1	44	2	8	24	10
3	0	1	192	7	41	93	51
4	0	1	679	29	151	326	173
5	0	1	2035	86	472	947	530
6	0	1	5434	244	1281	2518	1391

Table: Calculation of eigenvalues correspoding to the irreps for six body systems. E is HO energy quanta; J is total angular momentum; T is isospin; Dimension is size of calculated P_{14} matrix; Numbers are corresponding eigenvalues. J=0 and T=1 corresponds to ${}^{6}_{2}$He or ${}^{6}_{4}$Be ground states; J=1, T=0 corresponds to ${}^{3}_{3}$Li; Calculations were performed with supercomputer "HPC Sauletekis", using 3 nodes (36 cores). We used standard Double precision for calculation of the matrix and library "ScaLAPACK" and sparse matrix library "PeTSc" for parallelism of the calculation.

[9] S. Mickevičius et al. Phys. Atom. Nucl., **81**, 899, (2018)

Summary

1. **Jacobi coordinates are applicable** for the antisymmetric state vector construction for the six nucleon system in the harmonic oscillator basis
2. Coefficients of fractional parentage for the six nucleon systems can be constructed by **calculating only one transposition operator** of the generating set of the symmetric group S_6.
3. The ab-initio algebraic approach allows constructing the model space for the six nucleon system with **reasonable computational resources**.

Thank you!