An algebraic approach for the small systems of nucleons

A. Stepšys

Center For Physical Sciences and Technology

August 1, 2023

Together with: S. Mickevičius (VMU), D. Germanas (CPST), R. K. Kalinauskas (VMU)

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.
- 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 (spurious states!).
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**
  - Formulate **a systematic treatment of the transpositions of the Jacobi coordinates** and their representations in the coupled HO basis (Also 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:

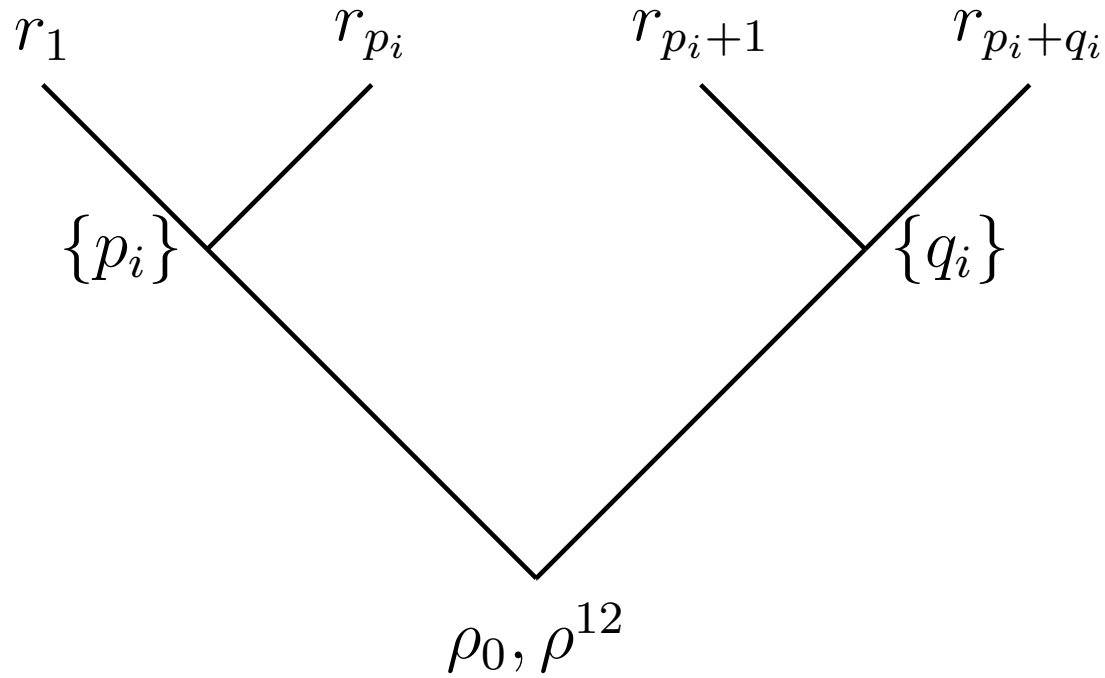


Figure: A generic Jacobi tree [4]

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

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

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 coordinates.
- 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**

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

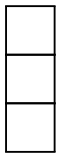
- Symmetric group chain for binary clusters

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

- 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)

A case of three nucleons

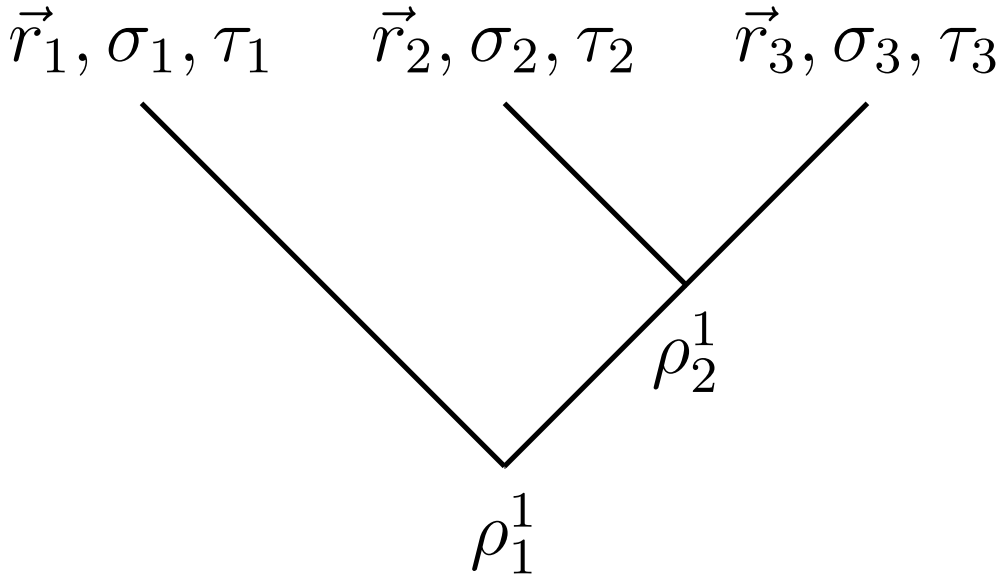


Figure: Jacobi tree for three-particle system. ρ_y^x is the Jacobi coordinate, where the x is cluster number, y is the coordinate number, r- particle coordinate,σ - the particle spin coordinate, τ - is the particle isospin coordinate.

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

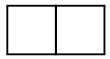
- Group chain for three particles

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

- 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 coupled 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 four nucleon system

Jacobi coordinates for the four nucleon system

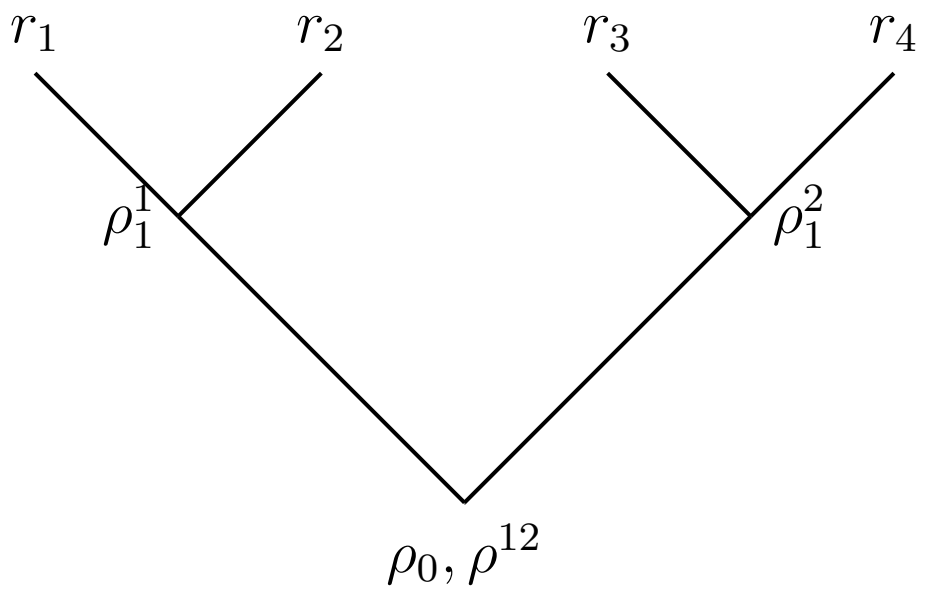


Figure: Jacobi tree for four nucleon system. ρ_y^x is the Jacobi coordinate, where the x is cluster number, y is the coordinate number, r- particle coordinate.

A case of four nucleons

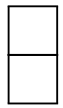
- Group chain for four particles

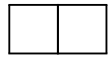
$$S_4 \supset S_2 \times S_2. \tag{21}$$

- Expression for the Λ operator

$$\Lambda = P_{12} + P_{13} + P_{23} + P_{14} + P_{24} + P_{34}. \tag{22}$$

- antisymmetric two particle subspace:





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

- The subcluster Λ operator

$$\Lambda = P_{13} + P_{14} + P_{23} + P_{24} + \overline{\Lambda}_1(\lambda_1) + \overline{\Lambda}_2(\lambda_2). \tag{23}$$

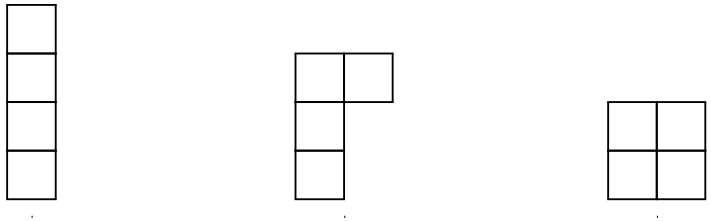
- A simple algebra

$$\Lambda = \overline{\Lambda}_1\left(\left[1^2\right]\right) + \overline{\Lambda}_2\left(\left[1^2\right]\right) + 4P_{13}. \tag{24}$$

- Boils down to **diagonalization** of

$$P_{13} = \frac{1}{4}(\Lambda - \overline{\Lambda}_1\left(\left[1^2\right]\right) - \overline{\Lambda}_2\left(\left[1^2\right]\right)). \tag{25}$$

Irreducible representation for four particles



$a)[\lambda_1] = [1^4] \quad b)[\lambda_2] = [21^2] \quad c)[\lambda_3] = [2^2]$

Figure: The Young Diagrams corresponding to the irreps of S_4. a) corresponds to the totally antisymmetric irrep $[1^4]$ and b) and c) corresponds to the irreps with a lesser degree of antisymmetry.

Coefficients of fractional parentage for the four nucleon system

- You need to **diagonalize** operator P_{13}!
- Like in the three-nucleon case, the expansion coefficients

$$\langle(\left(E_1 J_1 T_1 \Delta_1, E_2 J_2 T_2 \Delta_2\right)\overline{J}, el\right) E_4 J_4 T_4 \left[1^2\right] \left[1^2\right] | E_4 J_4 T_4 \Delta_4 \left[1^4\right] \left[1^2\right] \left[1^2\right]\rangle \tag{26}$$

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

Operator P_{13}

Factorization of the operator P_{13} of the S_4

$$\langle P_{13} \rangle = \langle P_{13}^{\sigma r} \rangle \langle P_{13}^{\tau} \rangle . \tag{27}$$

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

$$\langle P_{13}^{\sigma r} \rangle = \langle P_{13}^{\sigma} \rangle \langle P_{13}^{r} \rangle . \tag{28}$$

Operator P_{13}

The decoupling of L-S is

$$\langle(((e_1(l_1,s_1)j_1,e_2(l_2,s_2)j_2)J_{12},e_r l_r)J|\,P_{13}^{r\sigma}\,\big|((((e_1'(l_1',s_1')j_1',e_2'((l_2',s_2')j_2')J_{12}',e_r' l_r')J\Big\rangle$$

$$=\sum_{\substack{L_1 S_1\\ L_2 S_2\\ L_{12} S_{12}\\ L}}\sum_{\substack{L_1' S_1'\\ L_2' S_2'\\ L_{12}' S_{12}'\\ L'}}\begin{bmatrix} l_1 & s_1 & j_1\\ l_2 & s_2 & j_2\\ L_{12} & S & J_{12}\end{bmatrix}\begin{bmatrix} L_{12} & S & J_{12}\\ l_r & 0 & l_r\\ L & S & J\end{bmatrix}$$

$$\times\Big\langle((e_1 l_1,e_2 l_2)L_{12},e_r l_r)L\,|P_{13}^{r}|\,((e_1' l_1',e_2' l_2')L_{12}',e_r' l_r')L\Big\rangle$$

$$\Big\langle((\tfrac{1}{2},\tfrac{1}{2})s_1,(\tfrac{1}{2},\tfrac{1}{2})s_2)S\,|P_{13}^{\sigma}|\,((\tfrac{1}{2},\tfrac{1}{2})s_1',(\tfrac{1}{2},\tfrac{1}{2})s_2'))S\Big\rangle\,\delta_{LS,L'S'}$$

$$\times\begin{bmatrix} L_{12}' & l_r' & L'\\ S' & 0 & S'\\ J_{12}' & l_r' & J\end{bmatrix}\begin{bmatrix} l_1' & l_2' & L_{12}'\\ s_1' & s_2' & S'\\ j_1' & j_2' & J_{12}'\end{bmatrix}$$

Four particle harmonic oscillator brackets[8]

Action of the operator P_{13} on the orbital part boils down to:

$$\langle((e_1 l_1, e_2 l_2) l_{12}, e_3 l_3) l | T_{12}(d_1) T_{23}(d_2) T_{12}(d_1) | ((e_1' l_1', e_2' l_2') l_{12}', e_3' l_3') l \rangle_{d_1 d_2} = \tag{29}$$

$$\sum_{\substack{\varepsilon_1 \lambda_1, \varepsilon_2 \lambda_2, \Lambda_{23} \\ \varepsilon_2' \lambda_2'}} \langle e_1 l_1, e_2 l_2 : L_{12} | \varepsilon_1 \lambda_1, \varepsilon_2 \lambda_2 : L_{12} \rangle_{d_1} \delta_{L_{12} e_3 l_3, L_{12}' e_3' l_3'}$$

$$\times \begin{bmatrix} \lambda_1 & 0 & \lambda_1 \\ \lambda_2 & l_3 & \Lambda_{23} \\ L_{12} & l_3 & L \end{bmatrix} \left\langle \varepsilon_2 \lambda_2, e_3 l_3 : \Lambda_{23} | \varepsilon_2' \lambda_2', e_3' l_3' : \Lambda_{23} \right\rangle_{d_2}$$

$$\times \begin{bmatrix} \lambda_1 & \lambda_2' & L_{12}' \\ 0 & l_3' & l_3' \\ \lambda_1 & \Lambda_{23} & L \end{bmatrix} \langle \varepsilon_1 \lambda_1, \varepsilon_2' \lambda_2' : L_{12} | e_1' l_1', e_2' l_2' : L_{12}' \rangle_{d_1} \delta_{L_{12}, L_{12}'}.$$

$$T_{12}(d_1) T_{23}(d_2) T_{12}(d_1) = \tag{30}$$

$$\begin{pmatrix} \sqrt{\frac{d_1}{1+d_1}} & \sqrt{\frac{1}{1+d_1}} & 0 \\ \sqrt{\frac{1}{1+d_1}} & -\sqrt{\frac{d_1}{1+d_1}} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \sqrt{\frac{d_2}{1+d_2}} & \sqrt{\frac{1}{1+d_2}} \\ 0 & \sqrt{\frac{1}{1+d_2}} & -\sqrt{\frac{d_2}{1+d_2}} \end{pmatrix} \begin{pmatrix} \sqrt{\frac{d_1}{1+d_1}} & \sqrt{\frac{1}{1+d_1}} & 0 \\ \sqrt{\frac{1}{1+d_1}} & -\sqrt{\frac{d_1}{1+d_1}} & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

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

Benchmark calculations for 3He and 3H

3He	*Int.*	*b*	$g.s.E(MeV)$	$Abs(MeV)$
$E(HO) = 56$	*N3LO*	0.76	-8.0106	0.2926
$Dim = 11120$	$N3LO + e.m.$	0.88	-7.3542	0.3638
	*AV*18	0.82	-6.8665	0.8515
	*Reid*93	0.96	-7.6343	0.0837
	Exp.		**-7.718**	

Table: Calculation of ground state energy for 3He.

3H	*Int.*	*b*	$g.s.E(MeV)$	$Abs(MeV)$
$E(HO) = 56$	*N3LO*	0.86	-8.0520	0.4297
$Dim = 11120$	$N3LO + e.m.$	0.88	-8.0421	0.4396
	*AV*18	0.80	-7.5515	0.9302
	*Reid*93	0.96	-7.6130	0.8687
	Exp.		**-8.4817**	

Table: Calculation of ground state energy for 3H.

Benchmark calculations for 4He

4He	*Int.*	*b*	*g.s.E(MeV)*	*Abs(MeV)*
$E(HO) = 26$	*N3LO*	0.78	−26.9246	1.371
$Dim = 27803$	$N3LO + e.m.$	0.78	−26.1424	2.1532
	*AV*18	0.76	−23.5599	4.7357
	*Reid*93	0.74	−24.8145	3.4811
	Exp.		**-28.2956**	

Table: Calculation of ground state energy for 4He.

Summary

1. Coefficients of fractional parentage can be constructed by **calculating only one transposition operator** of the generating set of the symmetric group.
2. The ab-initio algebraic approach allows the construction of the model space for the observable calculation.
3. The algebraic approach is **extendable** for larger systems.