Calculation of Five Particle Harmonic-Oscillator Transformation Brackets

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August 28, 2016

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- Topic of Talk: **5HOB** - tool for calculation of permutation element $P_{n_1 n}$ for specific binary cluster models

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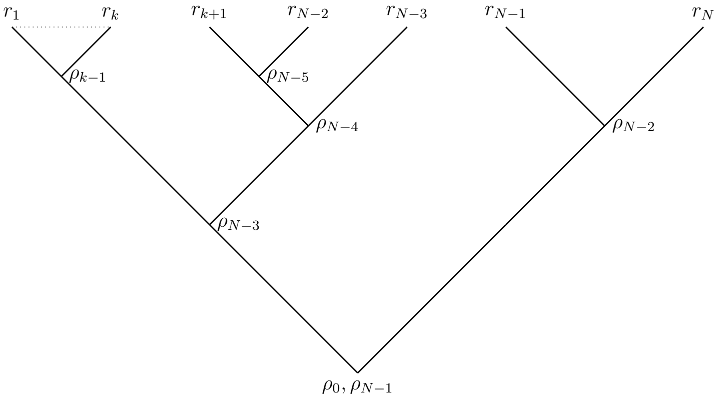
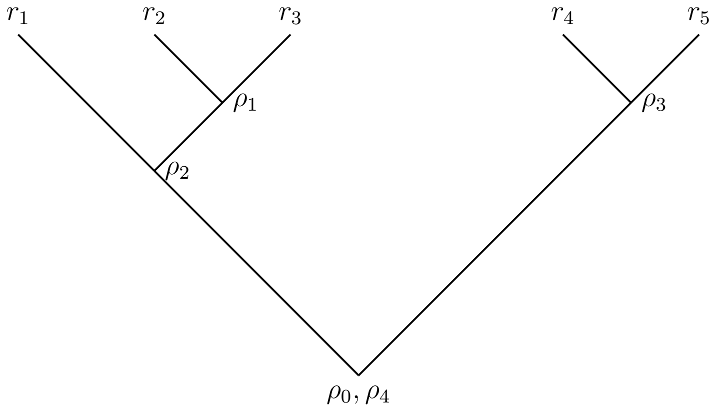
- Coupled cluster formalism, ensures that having antisymmetrized sub-clusters only two particle permutation operator $P_{n_1 n}$ is required to calculate.
- $P_{n_1 n}$ calculation for binary clusters $N = N_1 + N_2$:
  - System composed of N_1 and $N_2 = 2$;First cluster has two intrinsic K and $N - K - 2$ particle subclusters
  - System composed of N_1 and $N_2 = 1$ particle clusters;First cluster has its own clusterization of K and $N - K - 1$

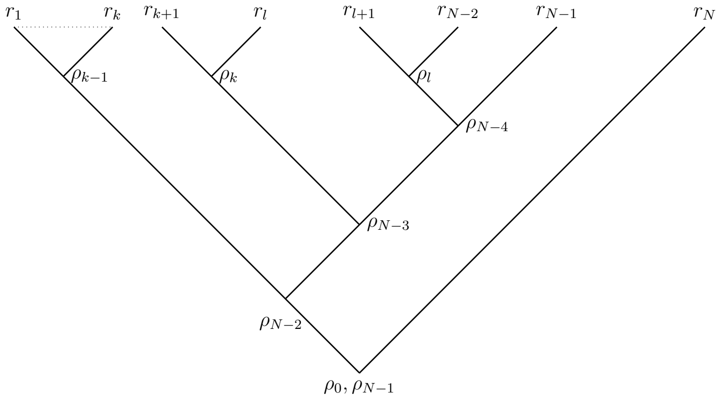
General Jacobi tree for N particle system, composed of N_1 and 2 particles, where the first cluster has two intrinsic K and $N-K-2$ particle subclusters



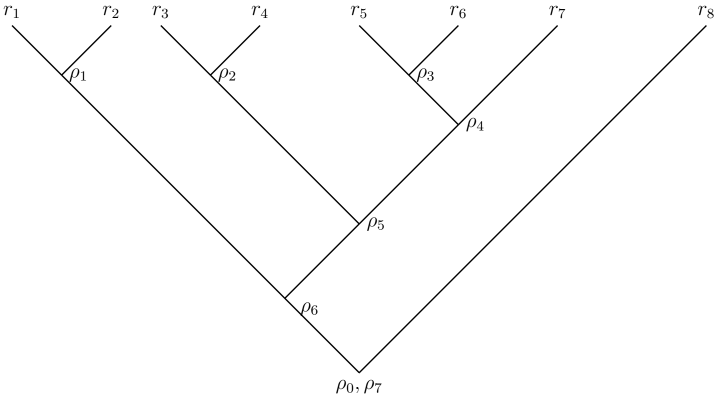
Jacobi tree for $N = 5$ particle system, composed of $N_1 = 3$ and $N_2 = 2$ particles.



General Jacobi tree for N particle system, composed of N_1 and 1 particles, where the N_1 cluster has two intrinsic K and $N-K-2$ particle subclusters.



Jacobi tree for $N = 8$ particle system, composed of $N_1 = 7$ and $N_2 = 1$ particles.



The coordinate transformation matrix of four Jacobi coordinates can be written as a product of five matrices in the following way:

$$\begin{pmatrix} \rho_1' \\ \rho_2' \\ \rho_3' \\ \rho_4' \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{d_1}{1+d_1}} & \sqrt{\frac{1}{1+d_1}} & 0 & 0 \\ \sqrt{\frac{1}{1+d_1}} & -\sqrt{\frac{d_1}{1+d_1}} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \sqrt{\frac{d_2}{1+d_2}} & \sqrt{\frac{1}{1+d2}} & 0 \\ 0 & \sqrt{\frac{1}{1+d_2}} & -\sqrt{\frac{d_2}{1+d_2}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\times \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \sqrt{\frac{d_3}{1+d_3}} & \sqrt{\frac{1}{1+d_3}} \\ 0 & 0 & \sqrt{\frac{1}{1+d_3}} & -\sqrt{\frac{d_3}{1+d_3}} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \sqrt{\frac{d_2}{1+d_2}} & \sqrt{\frac{1}{1+d_2}} & 0 \\ 0 & \sqrt{\frac{1}{1+d_2}} & -\sqrt{\frac{d_2}{1+d_2}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

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- Use of two-body Talmi-Moshinsky transformation

Middle matrix can be factorized like this:

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \sqrt{\frac{d_3}{1+d_3}} & \sqrt{\frac{1}{1+d_3}} \\ 0 & 0 & \sqrt{\frac{1}{1+d_3}} & -\sqrt{\frac{d_3}{1+d_3}} \end{pmatrix}$$

$$= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \sqrt{\frac{x}{1+x}} & \sqrt{\frac{1}{1+x}} \\ 0 & 0 & \sqrt{\frac{1}{1+x}} & -\sqrt{\frac{x}{1+x}} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \sqrt{\frac{x}{1+x}} & \sqrt{\frac{1}{1+x}} \\ 0 & 0 & \sqrt{\frac{1}{1+x}} & -\sqrt{\frac{x}{1+x}} \end{pmatrix}$$

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$$S = T_{12}(d_1)\,T_{23}(d_2)\,T_{34}(x)$$

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Coordinate transformation can be written in a following way:

$$\begin{pmatrix} \rho_1' \\ \rho_2' \\ \rho_3' \\ \rho_4' \end{pmatrix} = S \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} S^T \begin{pmatrix} \rho_1 \\ \rho_2 \\ \rho_3 \\ \rho_4 \end{pmatrix}.$$

- Basis construction using angular momentum algebra
  $|((e_1 l_1, e_2 l_2)L_{12}, e_3 l_3)L_{123}, e_4 l_4)L\rangle$

- Basis construction using angular momentum algebra $|((e_1 l_1, e_2 l_2)L_{12}, e_3 l_3)L_{123}, e_4 l_4)L\rangle$
- Bracket construction as sum through intermediate variables:

$$\begin{aligned}&\langle\alpha|T_{12}(d_1)T_{23}(d_2)|\alpha'\rangle\\ &=\sum_{\beta}\langle\alpha|T_{12}(d_1)|\beta\rangle\langle\beta|T_{23}(d_2)|\alpha'\rangle,\end{aligned}$$

where β denotes intermediate states.

Using this technique we can write the five particle wavefunction transformation M induced by the coordinate transformation S:

$$\langle(((e_1l_1, e_2l_2)L_{12}, e_3l_3)L_{123}, e_4l_4)L|M|(((e'_1l'_1, e'_2l'_2)L'_{12}, e'_3l'_3)L'_{123}, e'_4l'_4)L'\rangle =$$
$$\sum_{\varepsilon_2\lambda_2} \left\langle e_1l_1, e_2l_2 : L_{12} \left| e'_1l'_1, \varepsilon_2\lambda_2 : L_{12} \right.\right\rangle_{d_1}$$

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$$\langle(((e_1 l_1, e_2 l_2)L_{12}, e_3 l_3)L_{123}, e_4 l_4)L|M|(((e_1' l_1', e_2' l_2')L_{12}', e_3' l_3')L_{123}', e_4' l_4')L'\rangle =$$

$$\sum_{\varepsilon_2 \lambda_2} \langle e_1 l_1, e_2 l_2 : L_{12} \left| e_1' l_1', \varepsilon_2 \lambda_2 : L_{12} \right\rangle_{d_1}$$

$$\times \sum_{\Lambda_{23}} \left\langle ((l_1^{'}, \lambda_2)L_{12}, l_3)L_{123} | ((l_1^{'}, (\lambda_2, l_3)\Lambda_{23})L_{123} \right\rangle \langle \varepsilon_2 \lambda_2, e_3 l_3 : \Lambda_{23} \left| e_2' l_2', \varepsilon_3' \lambda_3' : \Lambda_{23} \right\rangle_{d_2}$$

$$\times \left\langle ((l_1^{'}, (l_2^{'}, \lambda_3^{'})\Lambda_{23})L_{123}^{'} | ((l_1^{'}, l_2^{'})L_{12}^{'}, \lambda_3^{'})L_{123}^{'} \right\rangle \delta_{L_{123} e_4 l_4 L, L_{123}' e_4' l_4' L'}$$

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$$\langle(((e_1 l_1, e_2 l_2)L_{12}, e_3 l_3)L_{123}, e_4 l_4)L|M|(((e'_1 l'_1, e'_2 l'_2)L'_{12}, e'_3 l'_3)L'_{123}, e'_4 l'_4)L'\rangle =$$

$$\sum_{\varepsilon_2\lambda_2} \langle e_1 l_1, e_2 l_2 : L_{12} \left| e'_1 l'_1, \varepsilon_2\lambda_2 : L_{12}\right\rangle_{d_1}$$

$$\times \sum_{\varepsilon'_3\lambda'_3\Lambda_{23}} \left\langle((l'_1, \lambda_2)L_{12}, l_3)L_{123}|((l'_1, (\lambda_2, l_3)\Lambda_{23})L_{123}\right\rangle \langle\varepsilon_2\lambda_2, e_3 l_3 : \Lambda_{23} \left| e'_2 l'_2, \varepsilon'_3\lambda'_3 : \Lambda_{23}\right\rangle_{d_2}$$

$$\times \left\langle((l'_1, (l'_2, \lambda'_3)\Lambda_{23})L'_{123}|((l'_1, l'_2)L'_{12}, \lambda'_3)L'_{123}\right\rangle \delta_{L_{123}e_4 l_4 L, L'_{123}e'_4 l'_4 L'}$$

$$\times\sum_{\Lambda'_{34}} \left\langle((L'_{12}, \lambda'_3)L'_{123}, l_4)L|((L'_{12}, (\lambda'_3, l_4)\Lambda'_{34})L\right\rangle \langle\varepsilon'_3\lambda'_3, e_4 l_4 : \Lambda'_{34}|e'_3 l'_3, e'_4 l'_4 : \Lambda'_{34}\rangle_x$$

$$\times \left\langle((L'_{12}, (l'_3, l'_4)\Lambda'_{34})L'|((L'_{12}, l'_3)L'_{123}, l'_4)L'\right\rangle \delta_{L,L'}$$

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$$\langle ((((e_1 l_1, e_2 l_2)L_{12}, e_3 l_3)L_{123}, e_4 l_4)L|M|((((e_1' l_1', e_2' l_2')L_{12}', e_3' l_3')L_{123}', e_4' l_4')L'\rangle =$$

$$\sum_{\varepsilon_2\lambda_2} \langle e_1 l_1, e_2 l_2 : L_{12} \left| e_1' l_1', \varepsilon_2\lambda_2 : L_{12} \right\rangle_{d_1}$$

$$\times \sum_{\varepsilon_3'\lambda_3'\Lambda_{23}} \left\langle ((l_1', \lambda_2)L_{12}, l_3)L_{123}|((l_1', (\lambda_2, l_3)\Lambda_{23})L_{123} \right\rangle \langle \varepsilon_2\lambda_2, e_3 l_3 : \Lambda_{23} \left| e_2' l_2', \varepsilon_3'\lambda_3' : \Lambda_{23} \right\rangle_{d_2}$$

$$\times \left\langle ((l_1', (l_2', \lambda_3')\Lambda_{23})L_{123}'|((l_1', l_2')L_{12}', \lambda_3')L_{123}' \right\rangle \delta_{L_{123}e_4 l_4 L, L_{123}' e_4' l_4' L'}$$

$$\times \sum_{\Lambda_{34}'} \left\langle ((L_{12}', \lambda_3')L_{123}', l_4)L|((L_{12}', (\lambda_3', l_4)\Lambda_{34}')L \right\rangle \langle \varepsilon_3'\lambda_3', e_4 l_4 : \Lambda_{34}'|e_3' l_3', e_4' l_4' : \Lambda_{34}'\rangle_x$$

$$\times \left\langle ((L_{12}', (l_3', l_4')\Lambda_{34}')L'|((L_{12}', l_3')L_{123}', l_4')L' \right\rangle \delta_{L,L'}$$

$$5HOB = M^T F M$$

E	Dim	$T(E_0)$	$\delta_{(E_0)}$	$\delta_{rel(E_0)}$
0	1	0.0005	0	0
1	4	0.0003	$1.1e-12$	$2.9e-13$
2	26	0.0009	$1.1e-11$	$4.2e-13$
3	84	0.013	$4.9e-11$	$5.9e-13$
4	295	0.038	$2.4e-10$	$8.2e-13$
5	776	6	$9.1e-10$	$1.2e-12$
6	2044	111	$3.7e-9$	$1.8e-12$
7	4616	1270	$1.3e-8$	$2.8e-12$
8	10234	13646	$4.6e-8$	$4.5e-12$
9	20640	111897	$1.5e-7$	$7.5e-12$

Figure: Calculation of 5HOB. Here E means HO energy quanta; Dimension is size of calculated transformation matrix; Calculation time is presented in seconds.The error $\delta(E_0)$ and relative error $\delta_{rel}(E_0)$ for the HO energy E_0 for the normalisation condition of the 5HOB transformation matrix. Calculations were performed with supercomputer "HPC Sauletekis", using 1 node (12 cores). We used standard double precision for calculation and library "MPI" for parallelism.

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- Need to compute Talmi - Moshinsky brackets - computationally expensive

Questions?