The Hyperspherical Harmonic method for a A-body system without permutation symmetry

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Motivations

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- Accurate solutions of Nuclear Hamiltonians – Model validation

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  - Simpler matrix-element calculations ☺
  - Simpler permutation-breaking calculations ☺

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  - Bigger basis set ☹

Outline

- Jacobi Coordinates

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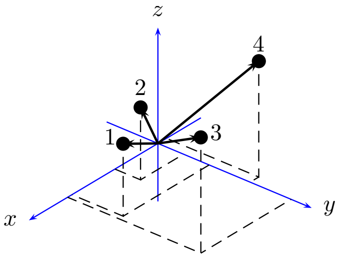
- Conclusions

Jacobi's coordinates

Kinetic Energy

$$T = -\sum_{i=1}^{A} \frac{\hbar^2}{2m_i} \nabla^2_{\mathbf{r}_i}$$



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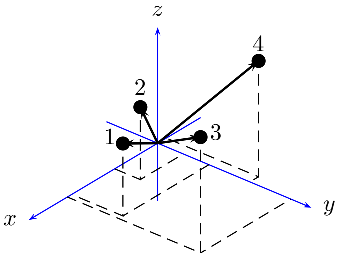

Center of Mass

$$\vec{X} = \frac{1}{M} \sum_{i=1}^{A} m_i \vec{r}_i \,, \quad M = \sum_{i=1}^{A} m_i$$

Jacobi's coordinates

$$\vec{x}_{N-j+1} = \sqrt{\frac{2m_{j+1} M_j}{(m_{j+1} + M_j) m}} \, (\vec{r}_{j+1} - \vec{X}_j)$$

$$j = 1, \ldots, N = A - 1$$

$$M_j = \sum_{i=1}^{j} m_j \,, \quad \vec{X}_j = \frac{1}{M_j} \sum_{i=1}^{j} m_i \vec{r}_i$$

Jacobi's coordinates

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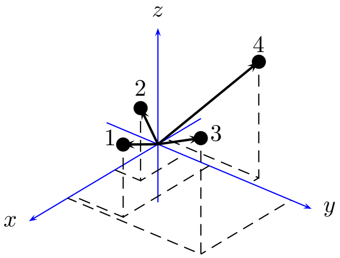
$$T = -\frac{\hbar^2}{2M}\nabla^2_{\mathbf{X}} - \frac{\hbar^2}{m}\sum_{i=1}^{N}\nabla^2_{\mathbf{x}_i}$$



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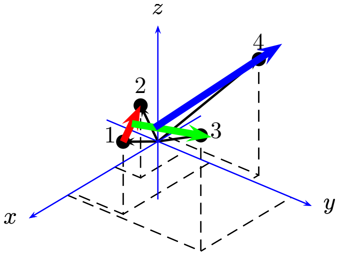

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Jacobi's coordinates

$$\vec{x}_3 = \vec{r}_2 - \vec{r}_1$$

$$\vec{x}_2 = \sqrt{\frac{4}{3}}\left(\vec{r}_3 - \frac{\vec{r}_1 + \vec{r}_2}{2}\right)$$

$$\vec{x}_1 = \sqrt{\frac{3}{2}}\left(\vec{r}_4 - \frac{\vec{r}_1 + \vec{r}_2 + \vec{r}_3}{3}\right)$$

Hyperspherical Coordinates

Hyperradius

$$\rho = \left(x_1^2 + x_2^2 + \cdots + x_N^2 \right)^{1/2}$$

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Hyperangles

$$\Omega_N = (\hat{x}_1, \ldots, \hat{x}_N, \varphi_2, \ldots, \varphi_N)$$

Where

$$\begin{aligned} x_N &= \rho \cos \varphi_N \\ x_{N-1} &= \rho \sin \varphi_N \cos \varphi_{N-1} \\ &\vdots \\ x_1 &= \rho \sin \varphi_N \cdots \sin \varphi_3 \sin \varphi_2 \end{aligned}$$

$$\cos \varphi_i = \frac{x_i}{\sqrt{x_1^2 + \cdots + x_j^2}}$$

$$j = 2, \ldots, N$$

Hyperspherical Coordinates

Laplacian Operator (Kinetic Energy)

$$\Delta = \sum_{i=1}^{N} \nabla_{\mathbf{x}_i}^2 = \left(\frac{\partial^2}{\partial \rho^2} + \frac{3N-1}{\rho} \frac{\partial}{\partial \rho} + \frac{\Lambda_N^2(\Omega_N)}{\rho^2} \right)$$

Hyperspherical Coordinates

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Grand-Angular operator momentum - recurrence equation

$$\Lambda_N^2(\Omega_N) = \frac{\partial^2}{\partial \varphi_N^2} + \left[3(N-2)\cot\varphi_N + 2(\cot\varphi_N - \tan\varphi_N) \right] \frac{\partial}{\partial \varphi_N} + \frac{L_N^2(\hat{x}_N)}{\cos^2\varphi_N} + \frac{\Lambda_{N-1}^2(\Omega_{N-1})}{\sin^2\varphi_N}$$

Hyperspherical Harmonics

Defining Equation

$$\left(\Lambda_N^2(\Omega_N) + K(K + 3N - 2)\right)\mathcal{Y}_{[K]}(\Omega_N) = 0$$

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Explicit form

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$$[K] = (l_1, m_1, \cdots, l_N, m_N$$

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Orthogonality

$$\int d\Omega_N \left(\mathcal{Y}_{[K']}(\Omega_N)\right)^* \mathcal{Y}_{[K]}(\Omega_N) = \delta_{[K],[K']}$$

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Completeness

$$\sum_{[K]}\left(\mathcal{Y}_{[K]}(\Omega_N)\right)^{*}\mathcal{Y}_{[K]}(\Omega'_N) = \delta^{3N-1}(\Omega'_N - \Omega_N)$$

Potential Basis

Basis set to develop one-side functions $f(\vec{r}_i - \vec{r}_j)$

$$f(\vec{r}_i - \vec{r}_j) = \sum_{n,l,m} f_{n,l,m} \mathcal{Y}^{PB}_{n,l,m}(\hat{x}_N, \varphi_N)$$

Jacobi coordinate $\vec{x}_N = \vec{r}_i - \vec{r}_j$

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Defined by

- Hyperspherical functions $K = 2n + l$

$$\Lambda^2_N(\Omega_N)\mathcal{Y}^{PB}_{n,l,m}(\hat{x}_N, \varphi_N) = -K(K + 3N - 2)\mathcal{Y}^{PB}_{n,l,m}(\hat{x}_N, \varphi_N)$$

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- Rotation invariance in $\{\vec{x}_1, \ldots, \vec{x}_{N-1}\}$

$$\Lambda^2_{N-1}(\Omega_{N-1})\mathcal{Y}^{PB}_{n,l,m}(\hat{x}_N, \varphi_N) = 0$$

Potential Basis

Basis set to develop one-side functions $f(\vec{r}_i - \vec{r}_j)$

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Explicitly

$$\mathcal{Y}^{PB}_{n,l,m}(\hat{x}_N, \varphi_N) = \mathcal{Y}_{[K]}(\Omega_N)\Big|_{\substack{l_1=\cdots=l_{N-1}=0 \\ m_1=\cdots=m_{N-1}=0 \\ n_2=\cdots=n_{N-1}=0}}$$

$$= \mathcal{N} Y_{l,m}(\hat{x}_N)(\cos\varphi_N)^l P_n^{3(N-1)/2-1,l+1/2}(\cos 2\varphi_N) \,,$$

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$$\mathcal{Y}^{PB}_n(\hat{x}_N, \varphi_N) = \left[\mathcal{Y}^{PB}_{n,l,m}(\hat{x}_N, \varphi_N)\right]_{L=0}$$

Potential Basis

Basis set to develop one-side functions $f(\vec{r}_i - \vec{r}_j)$

$$f(r_{ij}) = \sum_n f_n(\rho)\mathcal{Y}_n^{PB}(\Omega_{ij})$$

Jacobi coordinate $\vec{x}_N = \vec{r}_i - \vec{r}_j$

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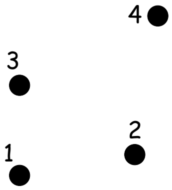
Potential Basis

Permutation properties



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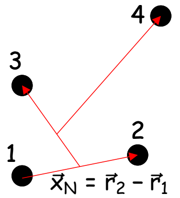

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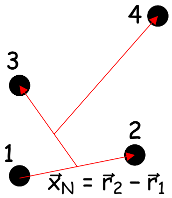

$$\mathcal{Y}^{PB}_{n,l,m}(\Omega_{12})$$

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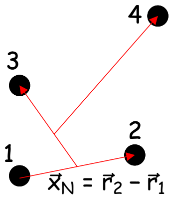

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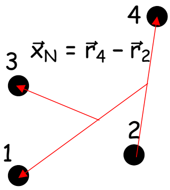

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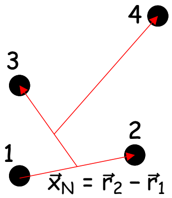

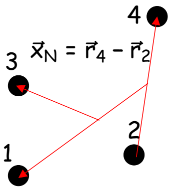

$\mathcal{Y}^{PB}_{n,l,m}(\Omega_{12})$ $\quad$ $\mathcal{Y}^{PB}_{n,l,m}(\Omega_{24})$

$$\mathcal{Y}^{PB}_{n,l,m}(\Omega_{ij}) = \sum_{[K'=2n+l]} {}^{(N)}\mathcal{C}^{n,l,m}_{[K']}(\psi^{ij})\,\mathcal{Y}_{[K']}(\Omega_{12})$$

Potential Basis

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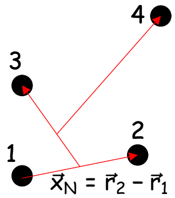

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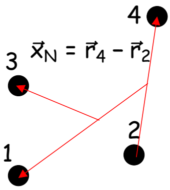

$\mathcal{Y}^{PB}_{n,l,m}(\Omega_{24})$

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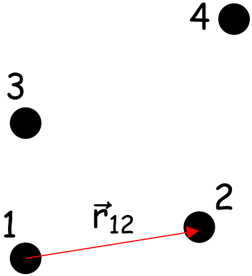
The coefficients of transformation are known

Potential Basis

(Central)-Potential on "One Side"



$$V(r_{12}) = \sum_n V_n(\rho)\mathcal{Y}_n^{PB}(\Omega_{12})$$

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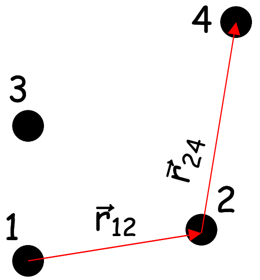

$$V(r_{12}) = \sum_n V_n(\rho)\mathcal{Y}_n^{PB}(\Omega_{12})$$

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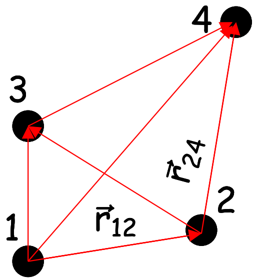
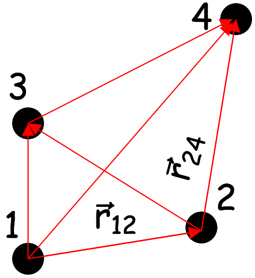


$$V(r_{12}) = \sum_{n} V_n(\rho)\mathcal{Y}_n^{PB}(\Omega_{12})$$

$$V = \sum_{i<j}^{A} V(r_{ij}) = \sum_{i<j}^{A}\sum_{n} V_n(\rho)\mathcal{Y}_n^{PB}(\Omega_{ij})$$

Potential Basis

(Central)-Potential on "One Side"



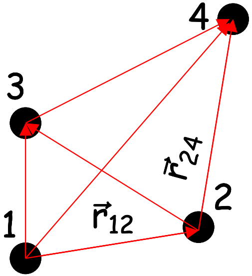
$$V(r_{12}) = \sum_n V_n(\rho)\mathcal{Y}_n^{PB}(\Omega_{12})$$

$$V = \sum_{i<j}^{A} V(r_{ij}) = \sum_{i<j}^{A}\sum_n V_n(\rho)\mathcal{Y}_n^{PB}(\Omega_{ij})$$

$$= \sum_{i<j}^{A}\sum_n V_n(\rho)\sum_{[K'=2n]}{}^{(N)}C_{[K']}^{n}(\psi^{ij})\left[\mathcal{Y}_{[K']}(\Omega_{12})\right]_{L=0}$$

Potential Basis

(Central)-Potential on "One Side"



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$$= \sum_n V_n(\rho)\, \mathcal{G}_n(\Omega_{12})$$

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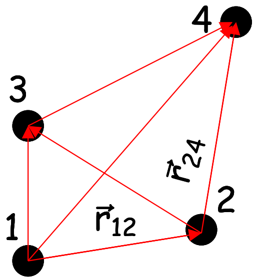

$$V(r_{12}) = \sum_{n} V_n(\rho)\mathcal{Y}_n^{PB}(\Omega_{12})$$

$$\begin{aligned} V &= \sum_{i<j}^{A} V(r_{ij}) = \sum_{i<j}^{A} \sum_{n} V_n(\rho)\mathcal{Y}_n^{PB}(\Omega_{ij}) \\ &= \sum_{i<j}^{A} \sum_{n} V_n(\rho) \sum_{[K'=2n]} {}^{(N)}\mathcal{C}^{n}_{[K']}(\psi^{ij}) \left[\mathcal{Y}_{[K']}(\Omega_{12})\right]_{L=0} \\ &= \sum_{n} V_n(\rho)\, \mathcal{G}_n(\Omega_{12}) \end{aligned}$$

$$\mathcal{G}_n(\Omega_{12}) = \sum_{[K''=2n]} \left(\sum_{i<j}^{A} {}^{(N)}\mathcal{C}^{n}_{[K'']}(\varphi^{ij}) \right) \left[\mathcal{Y}_{[K'']}(\Omega_{12})\right]_{L=0}$$

Hamiltonian

$$H = -\frac{\hbar^2}{m} \sum_{i=1}^{N} \nabla^2_{\mathbf{x}_i} + \sum_{i<j}^{A} V(r_{ij}) + H_{CM}$$

Hamiltonian

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Basis Set ($L = 0$)

$$\langle \rho\, \Omega \mid m\, [K] \rangle = \left(\beta^{3N/2} \sqrt{\frac{m!}{(3N-1+m)!}}\, L_m^{(3N-1)}(\beta\rho)\, e^{-\beta\rho/2} \right) \left[\mathcal{Y}_{[K]}(\Omega_N) \right]_{L=0}$$

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Matrix Elements

$$H_{m'[K'];\,m[K]} = \langle m'\,[K'] \mid H \mid m\,[K]\rangle = -\frac{\hbar^2\beta^2}{m}\delta_{[K],[K']}\,T^{K}_{m',m} + V_{m'[K'];\,m[K]}$$

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$$T^K_{m',m} = {}^{(1)}T_{m',m} - K(K + 3N - 2)\, {}^{(2)}T_{m',m}$$

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- Potential independent
- Simple-way dependency from A
- Triangular relation $K, K', K'' = 2n$

Diagonalization

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Drawback

Large basis set

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- Large matrix to storage

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Iterative Eigensolver Methods (ex. Lanczos)

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- Exploitation of the tensor-product structure of the Hamiltonian

$$H = {}^{(1)}T \otimes I + {}^{(2)}T \otimes D + \sum_n \mathcal{G}_n \otimes V_n$$

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- Ready for parallel implementation

Volkov's Potential testbed

Implementation of our strategy to the $A = 4$ case

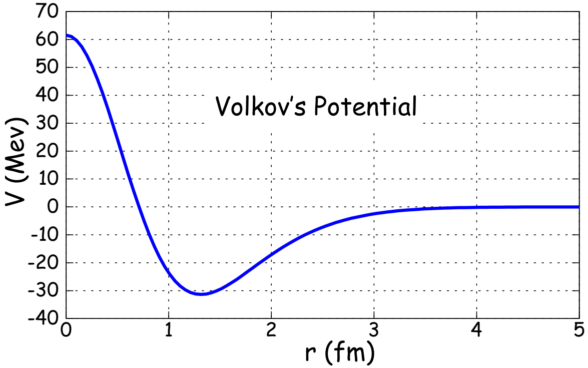
- Mass parameter

$$\hbar^2/m = 41.47 \text{ Mev fm}^{-2}$$

- Potential

$$V(r) = E_1\, e^{-r^2/R_1^2} + E_2\, e^{-r^2/R_2^2}$$

- $E_1 = 144.86$ Mev, $R_1 = 0.82$ fm, $E_2 = -83.34$ Mev, $R_2 = 1.6$ fm



Permutation Symmetries S_4

$m = 0, K = 6, \beta = 2$

Irreps		Eigen's (MeV)	Sym(1-2)	AntiSym(1-2)
[4]	1 2 3 4	-25.794	-25.794	
$[2^2]$	1 2 3 4	27.680 27.680	27.680	27.680
[3 1]	1 2 3 4	28.430 28.430 28.430	28.430 28.430	28.430
$[21^2]$	1 2 3 4	102.85 102.85 102.85	102.85	102.85 102.85
⋮	⋮	⋮	⋮	⋮
$[1^4]$	1 2 3 4	199.56		199.56

Results $N = 4$

Using 25 Laguerre's polynomials, and $\beta = 2$

K_{max}	N_{HH}	E_0 (MeV)	E_1 (MeV)
0	1	28.580	3.238
2	6	28.580	3.238
4	21	29.283	5.428
6	56	29.812	6.583
8	126	30.162	7.148
10	252	30.278	7.509
12	462	30.365	7.749
14	792	30.392	7.910
16	1287	30.407	8.040
18	2002	30.413	8.141
20	3003	30.416	8.223
22	4368	30.417	8.288

Results $N = 4$ with Coulomb interaction

Using 25 Laguerre's polynomials, and $\beta = 2$

K_{max}	N_{HH}	E_0 (MeV)	E_1 (MeV)
0	1	27.748	2.787
2	6	27.750	2.790
4	21	28.455	4.947
6	56	28.986	6.102
8	126	29.338	6.672
10	252	29.456	7.039
12	462	29.544	7.285
14	792	29.572	7.452
16	1287	29.587	7.587
18	2002	29.593	7.692
20	3003	29.596	7.778
22	4368	29.597	7.847

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