Hyperspherical harmonics approach: beyond the three-body system

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Introduction

Purpose

- Since many years the Pisa group has developed a hyperspherical-harmonics approach for an *ab initio* description of 3- and 4-body body systems (both bound states and reactions)
- Extend the approach for 5-, 6- (and more-?)body systems

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Applications

- $^4\mathrm{He}$+n scattering
- $d + t \to \alpha + n + (\gamma)$ "fusion"
- $\alpha + d \to ^6 \mathrm{Li} + \gamma$ radiative capture
- ...

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- Interessant *per se* and a good numerical test

Bound-state study

Schrödinger equation

$$H\Psi(1,\ldots,A) = \left(\sum_i \frac{p_i^2}{2m} + \sum_{i<j} v_{ij} + \sum_{i<j<k} v_{ijk} \right) \Psi(1,\ldots,A) = E\Psi(1,\ldots,A)$$

Variational approach

$$\Psi = \sum_i c_i \phi_i \Rightarrow \langle \phi_i | H - E | \phi_j \rangle = 0$$

Which choice for the variational basis $\{\phi_j\}$?

Variational basis

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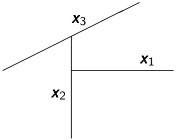
Hyperspherical coordinates (HH)

Jacobi coordinates

$$\boldsymbol{x}_{N-j+1} = \sqrt{\frac{2j}{j+1}} \left(\boldsymbol{r}_{j+1} - \frac{1}{j} \sum_{i=1}^{j} \boldsymbol{r}_i \right)$$



Hyperspherical coordinates (ρ, Ω_N)

- Hyperradius

$$\rho = \sqrt{\sum_{i=1}^{N} x_i^2} = \sqrt{\frac{2}{A} \sum_{j>i=1}^{A} (\boldsymbol{r}_i - \boldsymbol{r}_j)^2}$$

- Hyperangles $\Omega_N = (\hat{\boldsymbol{x}}_1, \ldots, \hat{\boldsymbol{x}}_N, \phi_2, \ldots, \phi_N)$

$$\cos \phi_i = \frac{x_i}{\sqrt{\sum_{j=1}^{i} x_j^2}}$$

Hyperspherical harmonics (HH)=Generalization of Y_{lm}

Kinetic energy

$$T = -\frac{\hbar^2}{m}\sum_{i=1}^{N}\Delta_{x_i} = -\frac{\hbar^2}{m}\left(\frac{\partial^2}{\partial\rho^2} + \frac{3N-1}{\rho}\frac{\partial}{\partial\rho} + \frac{\Lambda_N^2(\Omega_N)}{\rho^2}\right),$$

HH=Eigenvectors of grand angular operator Λ_N^2

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

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

HH=product of spherical harmonics and Jacobi polynomials

$$\mathcal{Y}^{KLM}_{[l_N L_{N-1} n_N]}(\Omega_N) = [\ldots[Y_{l_1}(\hat{x}_1)\otimes Y_{l_2}(\hat{x}_2)]_{L_2}\ldots\otimes Y_{l_{N-1}}(\hat{x}_{N-1})]_{L_{N-1}}\otimes Y_{l_N}(\hat{x}_N)]_{LM}$$
$$\times\prod_{j=2}^{N}\mathcal{N}_{n_j}^{\alpha_j^r\alpha_j^l}(\cos\phi_j)^{K_j^l}(\sin\phi_j)^{K_j^r}P_{n_j}^{\alpha_j^r,\alpha_j^l}(\cos 2\phi_j)$$

where $[l_N L_{N-1} n_N] = l_1,\ldots,l_N, L_2,\ldots,L_{N-1}, n_2,\ldots,n_N$ and $K=\sum_i(2n_i+l_i)$

System of identical bosons with spin 0

Variational basis

$$\phi_i = \mathcal{Y}^{KLM}_{[l^i_N L^i_{N-1} n^i_N]}(\Omega_N)\frac{f_j(\rho)}{\rho^{(3N-1)/2}}$$

- Good L and good π but not symmetric with respect to the particle-exchange

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$\Rightarrow$ Symmetrized HH

$$\mathcal{Y}^{KLM,\mathcal{S}}_{[l_N L_{N-1} n_N]}(\Omega_N) = \frac{2}{A!} \sum_{\text{even } p} \mathcal{Y}^{KLM}_{[l_N L_{N-1} n_N]}(\Omega^p_N),$$

- HH constitute a basis and Λ^2_N and $\boldsymbol{L}$ symmetric $\Rightarrow$

$$\mathcal{Y}^{KLM}_{[l_N L_{N-1} n_N]}(\Omega^p_N) = \sum_{[l'_N L'_{N-1} n'_N]} a^{KL,p}_{[l_N L_{N-1} n_N];[l'_N L'_{N-1} n'_N]} \mathcal{Y}^{KLM}_{[l'_N L'_{N-1} n'_N]}(\Omega_N)$$

Transformation coefficients

Recurrence relations

$$a^{K+2L,p}_{[l_N L_{N-1}],n_2,\ldots,n_i+1,0,\ldots,0;[l'_N L'_{N-1} n'_N]} = \sum_{k,q=1}^{N} \left[2b' \gamma^{(p)}_{ik} \gamma^{(p)}_{iq} + (b'-a') \sum_{j=i+1}^{N} \gamma^{(p)}_{jk} \gamma^{(p)}_{jq} \right]$$

$$\times \sum_{[l''_N L''_{N-1} n''_N]} a^{KL,p}_{[l_N L_{N-1}],n_2,\ldots,n_i,0,\ldots,0;[l''_N L''_{N-1} n''_N]}$$

$$\times \int d\Omega_N \left[\mathcal{Y}^{K+2LM}_{[l'_N L'_{N-1} n'_N]}(\Omega_N) \right]^* \frac{\boldsymbol{x}_k \cdot \boldsymbol{x}_q}{\rho^2} \mathcal{Y}^{KLM}_{[l''_N L''_{N-1} n''_N]}(\Omega_N)$$

$$+c' \sum_{k_1,\ldots k_{N-i}}{}' \eta^{(i)}_{k_1 \ldots k_{N-i}} a^{K+2L,p}_{[l_N L_{N-1}],n_2,\ldots,n_i-1,k_1,\ldots,k_{N-i};[l'_N L'_{N-1} n'_N]}.$$

- Generalization for an arbitrary number of particles of relations from [M. Viviani, Few-Body Systems 25, (1998) 177]

Orthonormal hyperspherical harmonics

Symmetrized HH $\mathcal{Y}^{KLM,\mathcal{S}}_{[l_N L_{N-1} n_N]}$

$$\mathcal{Y}^{KLM,\mathcal{S}}_{[l_N L_{N-1} n_N]}(\Omega_N) = \sum_{[l'_N L'_{N-1} n'_N]} a^{KL,\mathcal{S}}_{[l_N L_{N-1} n_N];[l'_N L'_{N-1} n'_N]} \mathcal{Y}^{KLM}_{[l'_N L'_{N-1} n'_N]}(\Omega_N),$$

- not orthonormal
- linearly dependent! (symmetric-function space $<$ full space)

Orthonormalization

- Gram-Schmidt: simple and recursive but round-off errors $\uparrow$ fast
- Singular value decomposition: more expensive but more robust

$$A^{(KL)} = U^{(KL)} \Sigma^{(KL)} (V^{(KL)})^T$$

System of identical bosons with spin 0

Variational basis

$$\phi_i = \mathcal{Y}^{KLM,S}_{[l_N^i L_{N-1}^i n_N^i]}(\Omega_N)\frac{f_j(\rho)}{\rho^{(3N-1)/2}}$$

- Good L and good π and symmetric with respect to the particle-exchange

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Symmetric basis

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- $\langle \phi_j | \sum_{pq} v_{pq} | phi_i \rangle \propto \langle \phi_j | v_{12} | phi_i \rangle$

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$$\phi_i = \mathcal{Y}^{KLM}_{[l^i_N L^i_{N-1} n^i_N, S]}(\Omega_N)\frac{f_j(\rho)}{\rho^{(3N-1)/2}}$$

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Which hyperradial basis?

Lagrange mesh

Mesh points

- Gauss-Laguerre-quadrature abscissae $\{h\rho_k\}$

$$\int_0^\infty d\rho g(\rho) = \sum_{k=1}^{N_\rho} h\lambda_k g(h\rho_k),$$

exact for $g(\rho) = P_{2N_\rho - 1}(\rho)\rho^\alpha \mathrm{e}^{-\rho/h}$.

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Lagrange condition

$$f_j(h\rho_i) = (h\lambda_i)^{-1/2}\delta_{ij}.$$

Each f_j vanishes at all mesh points but $h\rho_j$.

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Mesh approximation

$$\int_0^\infty d\rho f_{j'}(\rho)V(\rho)f_j(\rho) \approx V(h\rho_j)\delta_{jj'}$$

$\Rightarrow$ diagonal matrix

Lagrange mesh

Lagrange basis

$$f_j(\rho) \propto \frac{L_{N_\rho}^{(\alpha)}(\rho/h)}{\rho - h\rho_j} \rho^{\alpha/2} \mathrm{e}^{-\rho/2h}$$

with $\alpha = 3N - 1$

$\Rightarrow$ reproduces the origin behaviour of the wave function

Application

Systems of helium atoms = door to Efimov physics

Helium-Helium(-Helium) interactions

- Two-body soft-core potential

$$v_{12}[K] = -1.227\ \mathrm{e}^{-(r_{12}/10.03)^2}$$

Dimer

- Small binding energy (1.29589113343 mK)
- Huge radius (98.489 782 159 a0)

Trimer

$K_{\max}$	N_{HH}	E_0 [mK]	$\langle r_{ij} \rangle$ [a_0]	$\langle r_{i,\mathrm{cm}} \rangle$ [a_0]
20	14	-150.42107	16.343	9.4659
40	34	-150.426084	16.345618	9.467396
60	54	-150.42609324	16.34562900	9.46740228
80	74	-150.4260932945	16.3456290923	9.4674023347
100	94	-150.4260932951	16.34562909375	9.46740233562
120	114	-150.4260932951	16.34562909379	9.46740233564

Table: Ground-state properties ($L^{\pi} = 0^{+}$) of the $^4\mathrm{He}$ trimer ($l_{\max} = 4$, $N_{\rho} = 40$, and $h = 2$)

Trimer

$l_{\max}$	n_{K0}	E_0 [mK]	$\langle r_{ij} \rangle$ [a_0]	$\langle r_{i,\mathrm{cm}} \rangle$ [a_0]
0	60	-150.4260638	16.34562836	9.4674038
4	114	-150.4260932951	16.34562909379	9.46740233564
8	162	-150.4260932951	16.34562909379	9.46740233563

Table: Ground-state properties of the $^4\mathrm{He}$ trimer ($K_{\max} = 120$, $N_\rho = 40$, and $h = 2$)

Trimer

$K_{\max}$	n_{K0}	E_1 [mK]	$\langle r_{ij} \rangle$ [a_0]	$\langle r_{i,\mathrm{cm}} \rangle$ [a_0]
100	50	-2.35	134	79.7
200	100	-2.4640	145.4	86.9
300	150	-2.46822	146.95	87.93
400	200	-2.46846	147.13	88.04
Extrap.		-2.468476	147.153	88.057

Table: Excited-state properties of the $^4\mathrm{He}$ trimer ($l_{\max} = 0$, $N_\rho = 70$, $h = 10$)

Tetramer

K	N_{HH}	E_0 [mK]	$\langle r_{ij} \rangle$ [a_0]
$l_{\mathrm{max}} = 4$			
0	1	-726.0	11.64
10	18	-751.276	11.823
20	150	-751.377015	11.82732
30	445	-751.377359	11.8273516
40	890	-751.37736152	11.827352058
50	1485	-751.37736156	11.827352067

Table: Ground-state energy (in mK) and radius ($l_{\mathrm{max}} = 4$, $N = 30$, $h = 1.5$)

Tetramer

l_{max}	N_{HH}	E_0 [mK]	$\langle r_{ij} \rangle$ [a_0]
0	325	-751.363	11.8270
2	598	-751.37732	11.8273505
4	1485	-751.37736156	11.827352067
6	2193	-751.377361635	11.827352075

Table: Ground-state energy (in mK) and radius ($K = 50$, $N = 30$, $h = 1.5$)

Tetramer

K	E_1 [mK]	$\langle r_{ij} \rangle$ [a_0]
10	-136.94	26.36
20	-157.43	28.76
30	-161.54	30.52
40	-162.665	31.66
42	-162.7718	31.832
44	-162.8576	31.986
46	-162.9271	32.124
48	-162.9832	32.249
50	-163.0290	32.361
52	-163.0663	32.462
54	-163.0967	32.552
56	-163.1218	32.634
58	-163.1423	32.706
60	-163.1593	32.770
⋮		
∞	-163.23	33.4

Table: Excited-state energy (in mK) and radius

Pentamer

K	E_0 [mK]	E_1 [mK]
0	-1913	-642.84
8	-1945.0	-802.47
16	-1945.22	-827.22
24	-1945.22	-830.50

Table: Ground-state energy (in mK) and radius ($l_{\mathrm{max}} = 2$, $N = 25$, $h = 1.2$)

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- Next step: adding the spin and isospin (done) and applying to nuclear systems
- Develop an efficient parallelization

Collaborators

- Michele Viviani (INFN-Pisa)
- Alejandro Kievsky (INFN-Pisa)