A nonsymmetrized hyperspherical harmonics approach for few-nucleon bound and scattering states

Jérémy Dohet-Eraly

Physique Nucléaire et Physique Quantique, Université libre de Bruxelles (ULB)

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Motivation

The *ab initio* study of few-nucleon bound states and reactions is essential for

- assessing the validity of the inter-nucleon interactions currently on the market ;
- predicting reaction rates at energies of astrophysical interest.

Purpose

Developing a few-body approach based on **nonsymmetrized hyperspherical harmonics** for few-nucleon systems

Possible applications in nuclear physics

- α+N elastic scattering
- $d + t \to \alpha + n + (\gamma)$ transfer reaction ("fusion")
- $\alpha + d \to {}^6\mathrm{Li} + \gamma$ radiative capture
- study of the halo nucleus ${}^6\mathrm{He}$

Introduction

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Purpose

Developing a few-body approach based on **nonsymmetrized hyperspherical harmonics** for few-nucleon systems

Present applications (in this talk)

- Study of 3-, 4-, (5-), 6-nucleon bound systems using central potentials
- Study of $d + n$ elastic scattering using a central potential

Ab initio approach for an A-nucleon systems

Properties

- Degrees of freedom=nucleon
- Input=nucleon-nucleon (NN) interaction (+NNN interaction)
- Main task=solving accurately the **Schrödinger** equation

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

with **bound-state** or continuum-state asymptotic behaviour.

Bound-state study

Rayleigh-Ritz variational method

- Expansion of the wave function into some orthonormal square-integrable basis $\{\phi_i\}_{i=1,\dots,n}$

$$\Psi = \sum_{i=1}^{n} c_i \phi_i$$

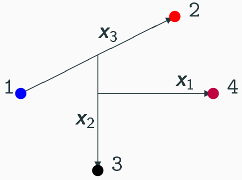
- Schrödinger equation $\rightarrow$ eigenvalue problem

$$\sum_{i=1}^{n} \langle \phi_j | H | \phi_i \rangle c_i = E c_i \qquad (j = 1, \dots, n)$$

Here, the basis functions are **hyperspherical harmonics** times Lagrange-Laguerre hyperradial functions.

Jacobi coordinates

$$\begin{cases} \mathbf{x}_1 &= \sqrt{\frac{3}{2}}\left(\mathbf{r}_4 - \frac{\mathbf{r}_1+\mathbf{r}_2+\mathbf{r}_3}{3}\right) \\ \mathbf{x}_2 &= \sqrt{\frac{4}{3}}\left(\mathbf{r}_3 - \frac{\mathbf{r}_1+\mathbf{r}_2}{2}\right) \\ \mathbf{x}_3 &= \mathbf{r}_2 - \mathbf{r}_1 \end{cases}$$



Hyperspherical coordinates (ρ, Ω_N)

Hyperradius

$$\rho^2 = x_1^2 + x_2^2 + x_3^2 = \frac{1}{2}\sum_{j>i=1}^{4}(\mathbf{r}_i - \mathbf{r}_j)^2$$

Hyperangles $\Omega = (\hat{\mathbf{x}}_1, \hat{\mathbf{x}}_2, \hat{\mathbf{x}}_3, \phi_2, \phi_3)$

$$\cos\phi_2 = \frac{x_1}{\sqrt{x_1^2 + x_2^2}}, \ \cos\phi_3 = \frac{x_2}{\rho}$$

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

Kinetic energy

$$T = -\frac{\hbar^2}{m}\left(\Delta_{x_1} + \Delta_{x_2} + \Delta_{x_3}\right) = -\frac{\hbar^2}{m}\left(\frac{\partial^2}{\partial\rho^2} + \frac{3N-1}{\rho}\frac{\partial}{\partial\rho} + \frac{\Lambda^2(\Omega)}{\rho^2}\right)$$

HH=Eigenvectors of grand angular operator Λ^2

$$\Lambda_N^2(\Omega_N)\mathscr{Y}_{[K]}(\Omega) = -K(K+7)\mathscr{Y}_{[K]}(\Omega),$$

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$$\Lambda^2_N(\Omega_N)\mathscr{Y}_{[K]}(\Omega) = -K(K+7)\mathscr{Y}_{[K]}(\Omega),$$

HH=functions of coupled spherical harmonics and Jacobi polynomials

$$\mathscr{Y}^{KLM}_{l_1 l_2 l_3 L_2 n_2 n_3}(\Omega) = [[Y_{l_1}(\hat{x}_1) \otimes Y_{l_2}(\hat{x}_2)]_{L_2} \otimes Y_{l_3}(\hat{x}_3)]_{LM}$$
$$\times \prod_{j=2}^{3} \mathscr{N}^{\alpha^r_j \alpha^l_j}_{n_j} (\cos\phi_j)^{K^l_j} (\sin\phi_j)^{K^r_j} P^{\alpha^r_j,\alpha^l_j}_{n_j}(\cos 2\phi_j)$$

where $K = \sum_i (2n_i + l_i)$.

Spin function

$$\chi_{S_2 S_3 S M_S} = [[\chi_s(1) \otimes \chi_s(2)]_{S_2} \otimes \chi_s(3)]_{S_3} \otimes \chi_s(4)]_{S M_S}$$

Isospin function

$$\zeta_{T_2 T_3 T M_T} = [[\zeta_t(1) \otimes \zeta_t(2)]_{T_2} \otimes \zeta_t(3)]_{T_3} \otimes \zeta_t(4)]_{T M_T}$$

Hyperspherical harmonics with spin and isospin functions

$$\mathbb{Y}^{KLSJM;TM_T}_{[KLST]} := \mathbb{Y}^{KLSJM;TM_T}_{l_1 l_2 l_3 L_2 n_2 n_3 S_2 S_3 T_2 T_3} = [\mathscr{Y}^{KL}_{l_1 l_2 l_3 L_2 n_2 n_3} \otimes \chi_{S_2 S_3 S}]_{JM} \; \zeta_{T_2 T_3 T M_T}$$

Basis function

$$\mathbb{Y}^{KLSJM;TM_T}_{[KLST]} \frac{f(\rho)}{\rho^4}$$

Hyperradial functions

Lagrange basis

- The hyperradial functions are expanded as sums of N_ρ Lagrange functions

$$f_j(\rho) \propto \frac{L_{N_\rho}^{(7)}(\rho/h)}{\rho - h\rho_j}\rho^4 \mathrm{e}^{-\rho/2h}$$

  where $L_{N_\rho}^{(7)}(\rho_j) = 0$.
- Reproduces the origin behavior of the wave function
- Asymptotic exponential decrease
- With the **Gauss-Laguerre quadrature** :

$$\begin{aligned}
\langle f_j | f_i \rangle_\rho &\approx \delta_{ij} \\
\langle f_j | V(\rho \cos\phi_N) | f_i \rangle_\rho &\approx V(\rho_i \cos\phi_N)\delta_{ij}
\end{aligned}$$

References

- D. Baye and P.-H. Heenen, J. Phys. A 19 (1986) 2041
- D. Baye, Phys. Rep. 565 (2015) 1

Pauli principle

Key facts

- The **wavefunction** is **antisymmetric** with respect to nucleon exchanges.
- The **HH basis functions** are (in general) **not antisymmetric** **but**...
- ... any **permuted HH** can be written as a linear combination of HH with same K, L, S, J, M, T, and M_T :

$$P\mathbb{Y}^{KLSJM;TM_T}{}_{[KLST]} = \sum_{[K'L'S'T']} a^{KLSJT}_{[KLST],[K'L'S'T']}\mathbb{Y}^{KLSJM;TM_T}{}_{[KLST]}.$$

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First strategy

1) Building **antisymmetric HH** basis functions as linear combinations of the original ones :

$$\mathscr{A}\mathbb{Y}^{KLSJM;TM_T}_{[KLST]} \frac{1}{A!}\sum_p (-1)^p P\mathbb{Y}^{KLSJM;TM_T}_{[KLST]}.$$

2) Removing **linearly dependent** antisymmetric HH basis functions.

[**JDE** and M. Viviani, Computer Physics Communications 253 (2020) 107183]

[L. E. Marcucci, **JDE**, L. Girlanda, A. Gnech, A. Kievsky, and M. Viviani, Frontiers in Physics 8 (2020) 69.]

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Second strategy

1) Solving the few-nuleon Schrödinger equation using a **non-symmetrized HH** basis.
2) Selecting the **antisymmetric eigenstates** among the solutions.

[M. Gattobigio, A. Kievsky, M. Viviani, and P. Barletta, Physical Review A 79 (2009) 032513.]
[M. Gattobigio, A. Kievsky, and M. Viviani, Physical Review C 83 (2011) 024001.]
[S. Deflorian, N. Barnea, W. Leidemann, and G. Orlandini, Few-Body Systems 54 (2013) 1879.]

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Present strategy

Searching the eigenvalues and eigenstates of $\mathscr{A}H\mathscr{A}$ using a **non-symmetrized HH** basis.

Searching the eigenvalues and eigenstates of $\mathscr{A} H \mathscr{A}$

Key points

- Search of the eigenvalues and eigenstates by using an **iterative approach** (Lanczos algorithm, for instance) $\Rightarrow$ requires to be able only to compute the **effect of $\mathscr{A} H \mathscr{A}$ on a linear combination of HH basis functions**.
- The operator $\mathscr{A} H \mathscr{A}$ can be written as

$$\begin{aligned} \mathscr{A} H \mathscr{A} &= \mathscr{A} \left(T + \sum_{i<j} v_{ij} + \sum_{i<j<k} v_{ijk} \right) \mathscr{A} \\ &= \mathscr{A} \left(T + \frac{A(A-1)}{2} v_{12} + \frac{A(A-1)(A-2)}{6} v_{123} \right) \mathscr{A} . \end{aligned}$$

- In the HH basis,
  - the matrix of T is **block diagonal** ;
  - the matrix of v_{12} is **sparse** (since $\boldsymbol{r}_{12}$ depends only on $\boldsymbol{x}_N$) ;
  - the matrix of v_{123} is **sparse** (since $\boldsymbol{r}_{12}$, $\boldsymbol{r}_{13}$, and $\boldsymbol{r}_{23}$ depend only on $\boldsymbol{x}_{N-1}$ and $\boldsymbol{x}_N$).

Computing the effect of $\mathscr{A}$

- 2-body systems

$$\mathscr{A}_2 = \frac{1}{2}(1 - P_{12})$$

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- 3-body systems

$$\begin{aligned}
\mathscr{A}_3 &= \frac{1}{3}(1 - P_{13} - P_{23})\mathscr{A}_2 \\
&= \mathscr{A}_2 \frac{1}{3}(1 - P_{13} - P_{23})\mathscr{A}_2 \\
&= \mathscr{A}_2 \frac{1}{3}(1 - 2P_{23})\mathscr{A}_2
\end{aligned}$$

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- 4-body systems

$$\begin{aligned}\mathscr{A}_4 &= \frac{1}{4}(1 - P_{14} - P_{24} - P_{34})\mathscr{A}_3 \\ &= \mathscr{A}_3 \frac{1}{4}(1 - P_{14} - P_{24} - P_{34})\mathscr{A}_3 \\ &= \mathscr{A}_3 \frac{1}{4}(1 - 3P_{34})\mathscr{A}_3\end{aligned}$$

Computing the effect of $\mathscr{A}$

A-body antisymmetrizer

$$\mathscr{A}_A = \mathscr{A}_{A-1}\frac{1}{A}[1-(A-1)P_{A-1\,A}]\mathscr{A}_{A-1}$$

$\Rightarrow$ The antisymmetrization requires $2^{A-1}-1$ **transpositions** (=permutation of type $P_{j\,j+1}$).

Transpositions

- Effect of P_{12} is **trivial** :

$$P_{12}\mathbb{Y}^{KLSJM;TM_T}_{[KLST]} = (-1)^{l_N+S_2+T_2}\mathbb{Y}^{KLSJM;TM_T}_{[KLST]}$$

- The matrix of $P_{j\,j+1}$ is a **sparse matrix** (since it involves only 2 Jacobi coordinates) obtained from **Raynal-Revai** and **Wigner** coefficients.

Computing the effect of $\mathscr{A}$

A-body antisymmetrizer

$$\mathscr{A}_A = \mathscr{A}_{A-1} \frac{1}{A} [1 - (A-1) P_{A-1\,A}] \mathscr{A}_{A-1}$$

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Conclusion

Applying $\mathscr{A} H \mathscr{A}$ to a linear combination of HH reduces to the **multiplication** of a **vector by** several **sparse matrices**.

NN interactions

- Volkov potential : central, spin-isospin independent
  [A. B. Volkov, Nuclear Physics 74 (1965) 33]
- Minnesota potential+Coulomb potential : central, spin-isospin dependent
  [D. .R. Thompson, M. LeMere, and Y. C. Tang, Nuclear Physics A 286 (1977) 53]

Nuclei

- ^{3}H, ^{3}He
- ^{3}H, ^{4}He
- ^{5}He (with Volkov)
- ^{6}Li

Test cases : ^{3}H and ^{3}He

K_{max}	Volkov (^{3}H/^{3}He)	Minnesota (^{3}H)	Minnesota (^{3}He)
0	-7.7075	-6.031	-5.290
10	-8.4157	-8.321	-7.642
20	-8.4623	-8.381	-7.705
30	-8.4647	-8.385	-7.710
40	-8.4649	-8.386	-7.710

Table 1 – Ground-state energy of ^{3}H and ^{3}He with the Volkov and Minnesota potentials in function of K_{max}. Quantum numbers $(L, S)J^{\pi}; T = (0, 1/2)1/2^{+}; 1/2$.

- Results in agreement with literature.

^{4}He

K_{max}	Volkov	Minnesota
0	-28.580	-25.609
10	-30.278	-29.787
20	-30.416	-29.943
30	-30.418	-29.947

Table 2 – Ground-state energy of ^{4}He with the Volkov and Minnesota potentials in function of K_{max}. Quantum numbers $(L, S)J^\pi; T = (0, 0)0^+; 0$.

- Results in agreement with literature.

K_{max}	Volkov
1	-39.635
3	-40.001
5	-41.022
7	-41.785
9	-42.384
11	-42.682
13	-42.868
15	-42.952
17	-42.996
19	-43.017

Table 3 – Unphysical ground-state energy of ^{5}He with the Volkov potential in function of K_{max}. Quantum numbers $(L, S)J^\pi; T = (1, 1/2)1/2^-; 1/2$.

- Results in agreement with literature.

$K_{\max}$	Volkov	Minnesota
2	61.142	-20.537
4	62.015	-26.128
6	63.377	-29.508
8	64.437	-31.288
10	65.354	-32.314
12	65.886	-33.020
14	66.201	-33.528

Table 4 – Ground-state energy of ^{6}Li with the Volkov and Minnesota potentials in function of $K_{\max}$. Quantum numbers $(L, S)J^\pi; T = (0, 1)1^+; 0$.

- Results in agreement with literature.

Bound state vs scattering state

Rayleigh-Ritz varional method	$><$	**Kohn** variational method
$\Psi = \sum_{ij} c_{ij} \mathbb{Y}_i \frac{f_j(\rho)}{\rho^{(3A-4)/2}}$	$><$	$\Psi = \sum_{ij} c_{ij} \mathbb{Y}_i \frac{f_j(\rho)}{\rho^{(3A-4)/2}} + \psi_F + K\psi_G$
Schrödinger eq.$\rightarrow$ eigenvalue problem	$><$	Schrödinger eq.$\rightarrow$ **linear systems**

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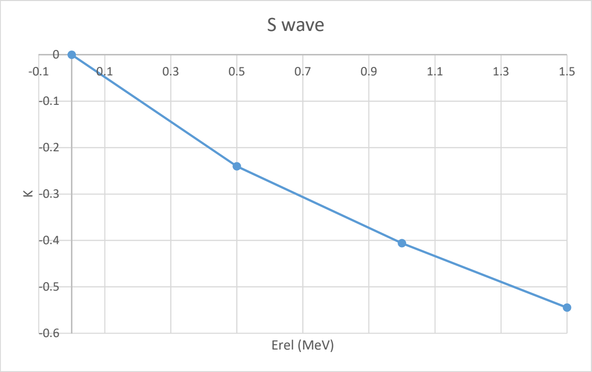
Extra need

- Computing the matrix elements

$$\langle \mathbb{Y}_i \frac{f_j(\rho)}{\rho^{(3A-4)/2}} | H - E | \psi_{F,G} \rangle \text{ and } \langle \psi_{F,G} | H - E | \psi_{F,G} \rangle$$

- Can be obtained approximately by projecting over the HH basis.

dn scattering



- Minnesota potential is used.

Conclusion

Summary

- A new implementation of the **hyperspherical harmonic** method for **few-nucleon bound** and **scattering** states has been presented.

Key features

- No need to build an antisymmetric hyperspherical harmonic basis but only **antisymmetric eigenstates** are found.
- The **Hamiltonian** and the **antisymmetrization** matrices are written as products of **sparse matrices**.

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- Groundstate energies for **3-, 4-, 5-, and 6-nucleon** systems using central potentials (Volkov and Minnesota).
- the $d+n$ S-wave phaseshifts using the Minnesota potential (as a proof of principle).

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Next steps

- Make the code faster (with more suitable numerical algorithms and parallelization)
- adapting the code for realistic potentials