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Calculation of the A = 6 bound states within the Hyperspherical Harmonic basis

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Solving the Schrödinger equation

$$H = \sum_{i} \frac{p_i^2}{2M} + \sum_{i < j} V(i, j) + \sum_{i < j < k} W(i, j, k) + \dots$$

Search for accurate solution of the Schrödinger equation

Variational approach (focus on bound state only)

$$H\Phi = E\Phi \qquad \Phi = \sum_{i=1}^{N} \frac{c_i}{\psi_i} \qquad (1)$$

• The ψ_i form a complete basis

$$\hat{O}\psi_i = O_i\psi_i \tag{2}$$

Transform the Schrödinger eq. in an eigenvalue problem

$$\sum_{j=1}^{N} \frac{c_{j} \langle \psi_{i} | \mathcal{H} | \psi_{j} \rangle = E(N) \sum_{j=1}^{N} \frac{c_{j} \langle \psi_{i} | \psi_{j} \rangle}{(3)}$$

• $E(N) \xrightarrow{N \to \infty} E \Rightarrow$ Check convergence

Hyperspherical Harmonics (HH)

- Reviews on A = 3 and 4 systems
 - A. Kievsky, et al., J. Phys. G, 35, 063101 (2008)
 - L.E. Marcucci, et al., Front. Phys. 8, 69 (2020)

- Articles on A = 6
 - AG, M. Viviani and L.E. Marcucci, Phys. Rev. C 102, 014001 (2020)
 - AG, L.E. Marcucci, R. Schiavilla, M. Viviani, arXiv:2106.07439 (2021)

Outline

- · The Hyperspherical Harmonics method
 - · General introduction
 - · Hands on
- The A = 6 bound state
 - · Convergence and spectrum
 - ⁶He beta decay
- Towards scattering states
 - $\alpha + d$ clusterization of ⁶Li
- Conclusions

The HH basis

•

• Jacobi vectors $\vec{\xi_1}, \dots, \vec{\xi_N} \Rightarrow \text{CoM}$ completely decoupled

$$T = -\frac{\hbar^2}{2m} \sum_{i=1}^{A} \nabla_{\vec{r}_i}^2 = T_{COM} - \frac{\hbar^2}{m} \sum_{i=1}^{A-1} \nabla_{\vec{\xi}_i}^2$$
Hyperangular variables $\rho = \sum_{k=1}^{5} (\xi_k)^2$, $\Omega = \{\hat{\xi}_i, \phi_i\}$, $\cos \phi_k = \frac{\xi_k}{\sqrt{\xi_1^2 + \dots + \xi_k^2}}$

$$T_0 = -rac{\hbar^2}{m} igg(rac{\partial^2}{\partial
ho^2} + rac{3A-4}{
ho} rac{\partial}{\partial
ho} - rac{L^2(\Omega)}{
ho^2} igg)$$

• Eigenbasis of $L^2(\Omega) \Rightarrow$ Hyperspherical Harmonics (HH)

$$L^{2}(\Omega)\mathcal{Y}_{[K]}(\Omega) = K(K + 3A - 5)\mathcal{Y}_{[K]}(\Omega)$$

· The variational wave function

$$\psi_{A}^{J^{\pi}} = \sum_{p} \sum_{l,[KST]} c_{l,[KST]} f_{l}(p) \underbrace{\left[\mathcal{Y}_{[K]}(\Omega_{A-1}^{p}) \left[\chi_{[S]}^{p} \otimes \chi_{[T]}^{p} \right] \right]_{J^{\pi}}}_{\phi_{[\alpha]}^{KLSTJ}(\Omega^{p})},$$

- Hyperradius \Rightarrow Laguerre polynomials $f_l(\rho)$
- Spin and Isospin degrees of freedom $\chi_{[S]}$ and $\chi_{[T]}$
- ho
 ightarrow even permutation of the particles
- CI, [KST] variational coefficients

- Antisymmetrization selecting quantum numbers \Rightarrow exploiting permutations
- Transformation Coefficients (TC)

$$\mathcal{Y}_{[K]}(\Omega^{p}) = \sum_{[K']}^{K=K'} a_{[K],[K']} \mathcal{Y}_{[K']}(\Omega)$$



Sum over the permutations rewritten in terms of the transformation coefficients

$$\sum_{\rho} \phi_{[\alpha]}^{\textit{KLSTJ}}(\Omega^{\rho}) = \sum_{[\alpha']} a_{[\alpha],[\alpha']}^{\textit{KLSTJ}} \phi_{[\alpha']}^{\textit{KLSTJ}}(\Omega)$$

Basis states are linear dependent ⇒orthogonalization

• Ground state of ⁶Li is $J^{\pi} = 1^+$ (mainly T = 0)



 $\frac{\#tot}{\#ind} \sim cost. = 370$

· Variational wave function

$$\Psi_{A} = \sum_{l,[\alpha]} c_{l,\alpha} \Phi_{l,\alpha} \qquad \Phi_{l,\alpha} = f_{l}(\rho) \sum_{\alpha'} a_{[\alpha],[\alpha']} \phi_{[\alpha']}(\Omega)$$

· Evaluation of the matrix elements

$$H_{l,\alpha,l',\beta} = \langle \Phi_{l,\alpha} | H | \Phi_{l',\beta} \rangle$$

- · Analytical for the kinetic energy
- · Potential matrix elements

$$\langle \Phi_{I,\alpha} | \sum_{i < j} V(i,j) | \Phi_{I',\beta} \rangle = \frac{A(A-1)}{2} \langle \Phi_{I,\alpha} | V(1,2) | \Phi_{I',\beta} \rangle$$

 \Rightarrow By using the sum over the permutations and the TC

Hands on

$$\langle \Phi_{I,\alpha} | V(1,2) | \Phi_{I',\beta} \rangle = \sum_{[\alpha'],[\beta']} a_{[\alpha],[\alpha']} a_{[\beta],[\beta']} \underbrace{V_{[I,\alpha'],[I',\beta']}(1,2)}_{\text{depend on } \mu \text{ only}}$$

 $\alpha, \beta = qn \text{ of 6-bodies}, \mu = qn \text{ of the couple (1,2)}$

$$\boldsymbol{V}_{[l,\alpha'],[l',\beta']}(1,2) = \int_{\rho,\Omega} f_l(\rho)\phi_{[\alpha']} V_{\mu}(\boldsymbol{r}_2 - \boldsymbol{r}_1)f_{l'}(\rho)\phi_{[\beta']}$$

To be notice that

- 1. The sum over $[\alpha'], [\beta']$ can run over millions of states
- 2. The potential involves only the particles (1,2) and so it depends on a small set μ of qn
- The sum over the qn which do not involve the couple (1,2) is independent of the particular potential model

qn= quantum numbers

Therefore, we can rewrite

$$\langle \Phi_{l,\alpha} | V(1,2) | \Phi_{l',\beta}
angle = \sum_{\mu} D^{[\alpha],[\beta]}_{\mu} V_{\mu,l,l'}(1,2)$$

- $D^{[\alpha],[\beta]}_{\mu}$ independent on the potential model \Rightarrow evaluated and stored only once
- Small number of combinations μ
 - small disc space required for saving $\sim 100 \text{GB}$
 - fast construction of potential matrix elements
- Extensible to 3N forces (in progress...)

Hands on

- Completely antisymmetrized
- Orthogonalization \Rightarrow relatively small basis Full calculation $N_{HH} \sim 7000$ Hamiltonian dimension $\sim 110000 \times 110000$
- · Easy computation of the matrix elements
- No need to save the matrix elements only the D coefficients
- ~ 3 hours for constructing and diagonalize the Hamiltonian
 ⇒ easy to test various potentials

Warning!

- We will use SRG evolved N³LO500 NN interaction [1-2]
 - SRG evolution parameter $\Lambda=1.2, 1.5, 1.8 \ \text{fm}^{-1}$
 - The Coulomb interaction is included as "bare" (not SRG evolved)
- Explorative study with NNLO^{*}_{sat} [3]
- No 3-body forces (for now)
- · We compute the mean values of "bare" operators

S.K. Bogner, R.J. Furnstahl, and R.J. Perry, PRC **75**, 061001(R) (2007)
 D.R. Entem and R. Machleidt, PRC **68**, 041001(R) (2003)
 A. Ekström, *et al.*, PRC **91**,051301 (2015)

- Include all the states up to a $K_{max} \Rightarrow FAIL!!$
- NOT all the states gives the same contribution ⇒ division by class [1]
 - Centrifugal barrier $\Rightarrow \ell_1 + \dots + \ell_5 \leq 4$
 - · two-body correlations are more important
- The ⁶Li ground state is a $J^{\pi} = 1^+$ state

wave	class	corr.	<i>K_{max}</i>
S	C1	two-body	14
	C3	many-body	10
D	C2	two-body	12
	C4	many-body	10
Р	C5	all	8
F-G	C6	all	8

[1] M. Viviani, et al., PRC 71,024006 (2005)



 $\Delta_i(K) = B_i(K) - B_i(K-2)$

Extrapolation to $K = \infty$

• Fit the quantity Δ_i with [1]

$$\Delta_i(K) = A_i e^{-b_i K} (1 - e^{-2b_i})$$

· Missing energy for class

$$\Delta_i(\infty) = \sum_{K=\overline{K}}^{\infty} \Delta_i(K) = A_i e^{-b_i \overline{K}}$$

where \overline{K} maximum K used for the class *i*

· Extrapolated energy

$$B(\infty) = B_{full} + \sum_i \Delta_i(\infty)$$

where B_{full} = binding energy with all the states

[1] S.K. Bogner et al., NPA 801, 21 (2008)

	"bare" Coul.		SRC		
	B_{full}	$B(\infty)$	B_{full}	$B(\infty)$	Ref. [1]
SRG1.2	31.75	31.78(1)	31.78	31.81(1)	31.85(5)
SRG1.5	32.75	32.87(2)	32.79	32.91(2)	33.00(5)
SRG1.8	32.21	32.64(9)	32.25	32.68(9)	32.8(1)
NNLO [*] _{sat}	29.77	30.71(15)			-

- · All the energies are in MeV
- · The errors come form the fit
- Results of Ref. [1] extrapolated from N_{max} = 10
- Experimental value B = 31.99 MeV

[1] E.D Jungerson, P. Navrátil and R.J. Furnstahl, PRC 83, 034301 (2011)



 $2^+, 1$

-27.47

- States (2⁺, 0) and (3⁺, 0) from K = 8.
- States $(0^+, 1)$ from K = 12.

A = 6 spectra with SRG1.5 (preliminary)



 $2^+, 1$

-27.47

- States (2⁺, 0) and (3⁺, 0) from K = 8.
- States $(0^+, 1)$ from K = 12.

- Pure Gamow-Teller transition (0^+ \rightarrow 1^+)

 $M_{fi} = \langle {}^{6}\text{Li} | J_{5}^{+} | {}^{6}\text{He} \rangle$

 $J_5^+ = -rac{g_a}{2}\sum_{i=1,A}\sigma_i au_i^+ + J^{RC}(1) + J^{OPE}(2) + J^{CT}(2) + \cdots$

- First accessible beta decay after ³He β -decay \Rightarrow first non trivial test of 2-body currents
- QMC calculations show a different sign for the two-body currents compare to NCSM [1,2]
- We used the N2LO450 EM potential [3] evolved with $\Lambda=1.2, 1.5, 1.8, 2.0, \infty$

P. Gysbers, *et al.* Nature Phys. **15**, 428 (2019)
 G.B. King, *et al.* Phys. Rev. C **102**, 025501 (2020)
 D.R. Entem, *et al.* Phys. Rev. C **91**, 024003 (2017)





	LO(GT)	NLO(RC)	N2LO(OPE)	N2LO(CT)	Tot.
SRG1.2	2.345(2)	-0.019	-0.038(1)	-0.018	2.272(3)
SRG1.5	2.342(3)	-0.021	-0.029(1)	-0.012	2.281(2)
SRG1.8	2.327(3)	-0.022	-0.019(1)	-0.009	2.280(4)
SRG2.0	2.338(3)	-0.022	-0.013(1)	-0.008	2.297(2)
bare	2.321(9)	-0.023	0.002(1)	-0.004	2.303(11)
Exp.					2.1609(40)

- · Errors come from the extrapolation
- Results pretty consistent with [1]
- Large dependence on SRG parameter of OPE

[1] P. Gysbers, et al. Nature Phys. 15, 428 (2019)

$\alpha + d$ cluster form factor of ⁶Li

• ⁶Li can be considered mainly as an $\alpha + d$ state

$$\Psi_{^{6}\mathsf{Li}} \simeq \sum_{L=0,2} \left[\left(\Psi_{\alpha} \otimes \Psi_{\sigma} \right)_{1} Y_{L}(\hat{r}) \right]_{1} \frac{f_{L}(r)}{r}$$

· The cluster form factor is defined as

$$\frac{f_{L}(r)}{r} = \langle \left[\left(\Psi_{\alpha} \otimes \Psi_{d} \right)_{1} Y_{L}(\hat{r}) \right]_{1} | \Psi_{6_{\text{Li}}} \rangle$$

Extract the Asymptotic Normalization Coefficients (ANCs)

$$C_L(r) = \frac{f_L(r)}{W_{-\eta,L+1/2}(2kr)} \xrightarrow{r \to \infty} C_L$$

$\alpha + d$ cluster form factor of ⁶Li

$$\frac{f_{L}(r)}{r} = \langle \left[(\Psi_{\alpha} \otimes \Psi_{d})_{S} Y_{L}(\hat{r}) \right]_{J} | \Psi_{^{6}\text{Li}} \rangle$$



Asymptotic Normalization Coefficient

$$C_L(r) = rac{f_L(r)}{W_{-\eta,L+1/2}(2kr)} \xrightarrow{r o \infty} C_L$$





A more precise approach for the ANC

- From the Schrödinger Equation \Rightarrow

$$\langle \Psi_{\alpha+d}^{(L)} | H_6 | \Psi_{^6\text{Li}} \rangle = \langle \Psi_{\alpha+d}^{(L)} | B_{^6\text{Li}} | \Psi_{^6\text{Li}} \rangle$$

• \Rightarrow An equation for the cluster form factor [1-2]

$$\left[-\frac{\hbar^2}{2\mu}\left(\frac{d^2}{dr^2}-\frac{L(L+1)}{r^2}\right)+\frac{2e^2}{r}+B_c\right]f_L(r)+g_L(r)=0$$

· Source term

$$g_{L}(r) = \langle \Psi_{lpha+d}^{(L)} | \left(\sum_{i \in lpha} \sum_{j \in d} V_{ij} - \frac{2e^2}{r}
ight) | \Psi_{^{6}Li}
angle |_{r ext{ fixed}}$$

- \Rightarrow Hard to compute in this form!
- ⇒ Same matrix elements needed for scattering!
- · Correct asymptotic behavior

$$g_L(r) \xrightarrow{r \to \infty} 0 \Rightarrow f_L(r) \xrightarrow{r \to \infty} W_{-\eta, L+1/2}(2kr)$$

[1] N.K. Timofeyuk, NPA 632,19 (1998)

^[2] M. Viviani, et al., PRC 71,024006 (2005)

The "projection" method

· A cluster wave function

$$\Psi_{\alpha+d}^{LSJ} = \left\{ \left[\Psi_{\alpha} \otimes \Psi_{d} \right]_{S} Y_{L}(\hat{r}) \right\}_{J} f(r)$$

- where f(r) intercluster wave function
- Expansion in term of the HH states $\phi_{[K]} =$ HH+spin+isospin

$$\Psi_{\alpha+d}^{LSJ} = \sum_{\bar{k}=0}^{\bar{k}_{max}} d_{[\bar{k}]}^{LSJ} \phi_{[\bar{k}]} \qquad d_{[\bar{k}]}^{LSJ} = \langle \phi_{[\bar{k}]} | \Psi_{\alpha+d} \rangle$$

- The equality holds only when $\bar{K}_{max}
 ightarrow \infty$
- · Advantages:
 - · Easy computation of the matrix elements
 - Control of the convergence \bar{K}



⁶Li wave function computed with K = 12



$$C_L(r) = \frac{f_L(r)}{W_{-\eta,L+1/2}(2kr)}$$

- Reproduced
 exactly the short
 range part
- Exact asymptotic behavior



	B_c [MeV]	<i>C</i> ₀ [fm ^{-1/2}]	$C_2 [\mathrm{fm}^{-1/2}]$
SRG1.2	3.00(1)	-4.19(12)	0.116(18)
SRG1.5	2.46(2)	-3.44(7)	0.072(15)
SRG1.8	2.02(9)	-3.01(7)	0.047(10)
Exp.	1.4743	-2.91(9)	0.077(18)

- · Extrapolated values of the ANC
- Errors from the convergence in K and \overline{K}
- Strong dependence on $B_c = E_{^{6}Li} E_{\alpha+d}$
- Same order of magnitude of the experiment!

- HH formalism
 - Extensible up to A = 8
 - Inclusion of three-body forces in progress
- Bound states of A = 6 nuclei
 - · Convergence for SRG potentials (similar to the NCSM)
 - ⁶He β -decay
- *α* + *d* clusterization
 - · Calculation of the Asymptotic Normalization Coefficients
 - Test of "projection" method to $A = 6 \Rightarrow$ Scattering

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Sparse

• $J^{\pi} = 1^+$ only LST = 010

Κ	This work	Ref. [1]
2	-61.142	-61.142
4	-62.015	-62.015
6	-63.377	-63.377
8	-64.437	-64.437
10	-65.354	-65.354
12	-65.884	-65.886

[1] M. Gattobigio et al., PRC 83, 024001 (2011)

Convergence (WRONG)



• Exponential behavior [1]

$$E(K) = E(\infty) + Ae^{-bK}$$

[1] S.K. Bogner et al., NPA 801, 21 (2008)

Extrapolation

		SRG1.2			SRG1.5		
i	K _{iM}	$\Delta_i(K_{iM})$	bi	$(\Delta B)_i$	$\Delta_i(K_{iM})$	bi	$(\Delta B)_i$
1	14	0.013	0.51	0.007(0)	0.023	0.49	0.014(0)
2	12	0.008	0.68	0.003(1)	0.042	0.58	0.019(0)
3	10	0.015	0.37	0.014(7)	0.022	0.32	0.024(12)
4	10	0.008	0.60	0.004(2)	0.022	0.49	0.013(6)
5	8	0.007	0.52	0.004(0)	0.023	0.37	0.021(0)
6	8	0.004	0.44	0.003(1)	0.018	0.26	0.026(13)
$(\Delta B)_T$			0.034(7)				0.117(19)
			SRG1.8		NNLO _{sat}		at
i	K _{iM}	$\Delta_i(K_{iM})$	bi	$(\Delta B)_i$	$\Delta_i(K_{iM})$	bi	$(\Delta B)_i$
1	14	0.035	0.46	0.023(0)	0.074	0.43	0.05(0)
2	12	0.144	0.50	0.084(11)	0.411	0.42	0.32(1)
3	10	0.024	0.30	0.029(15)	0.031	0.17	0.07(4)
4	10	0.045	0.38	0.039(20)	0.093	0.25	0.14(7)
5	8	0.049	0.26	0.070(1)	0.153	0.18	0.35(14)
6	8	0.048	0.11	0.19(9)	0.112	-	-
$(\Delta B)_T$				0.43(9)			0.93(20)



- $\bar{K} = 8$ in the "projection" of the cluster function
- Better convergence of ^{6}Li wf \Rightarrow better agreement with Method I and II



- $\bar{K} = 8$ in the "projection" of the cluster function
- Better convergence of ^{6}Li wf \Rightarrow better agreement with Method I and II

$\alpha + d$ cluster form factor of ⁶Li



Cluster form factor $\alpha + d$

$$\frac{f_{L}(r)}{r} = \langle \left[(\Psi_{\alpha} \otimes \Psi_{d})_{S} Y_{L}(\hat{r}) \right]_{J} | \Psi_{6_{Li}} \rangle$$



• For the NNLO^{*}_{sat} a node appears ⇒ strength of the tensor forces[1]

[1] V.I. Kukulin, et al. NPA 586,151 (1995)

Charge radius



• Extrapolation $r_c(K) = r_c(\infty) + Ae^{-bK}$

[1] CDB2k-SRG1.5 C. Forssén, E. Caurier, P. Navrátil, PRC 71, 021303 (2009)

$${}^{6}\text{Li} \simeq \alpha + d \Rightarrow \mu_{z}({}^{6}\text{Li}) \simeq \mu_{z}(d)$$

Experiment tells us $\mu_z(^6\text{Li}) < \mu_z(d)$

	$\mu_z(d)$	μ_z (⁶ Li)
SRG1.2	0.872	0.865(1)
SRG1.5	0.868	0.858(2)
SRG1.8	0.865	0.852(2)
NNLO [*] _{sat}	0.860	0.845(5)
Exp.	0.857	0.822

- Negative contribution only from the L = 2 S = 1 component \Rightarrow NOT SUFFICIENT
- We need two body currents contribution!! [1]

[1] R. Schiavilla, et al., PRC 99, 034005 (2019)

Electric quadrupole moment



• Large cancellations between different K

[1] CDB2k-SRG1.5 C. Forssén, E. Caurier, P. Navrátil, PRC 71, 021303 (2009)

Matrix elements between different waves

	S-D	D - D	P - P	P - D	remaining
SRG1.2	-0.187	-0.023	0.009	0.009	<0.001
SRG1.5	-0.102	-0.023	0.014	0.010	<0.001
SRG1.8	-0.058	-0.024	0.016	0.010	0.001
NNLO [*] _{sat}	0.049	-0.018	0.023	0.011	0.003

- · Direct connection with the strength of the tensor term in the potential
- Two-body currents contribution could be necessary!!

Towards "bare" chiral potential



D.R. Entem et al., PRC 91, 014002 (2015)



D.R. Entem et al., PRC 91, 014002 (2015)

- Increase the basis size up to K = 20From $\sim 30k$ h to $\sim 500 - 1000k$ h to compute *D* coefficients
- Better selection of the classes Only states with n_1 , n_2 , n_3 , n_4 , $n_5 = 0, 0, 0, 0, n$
- OpenMP \Rightarrow OpenMPI
- Use of accelerators (OpenACC, CUDA,...)