Quantified Gamow Shell Model interaction for *psd*-shell nuclei

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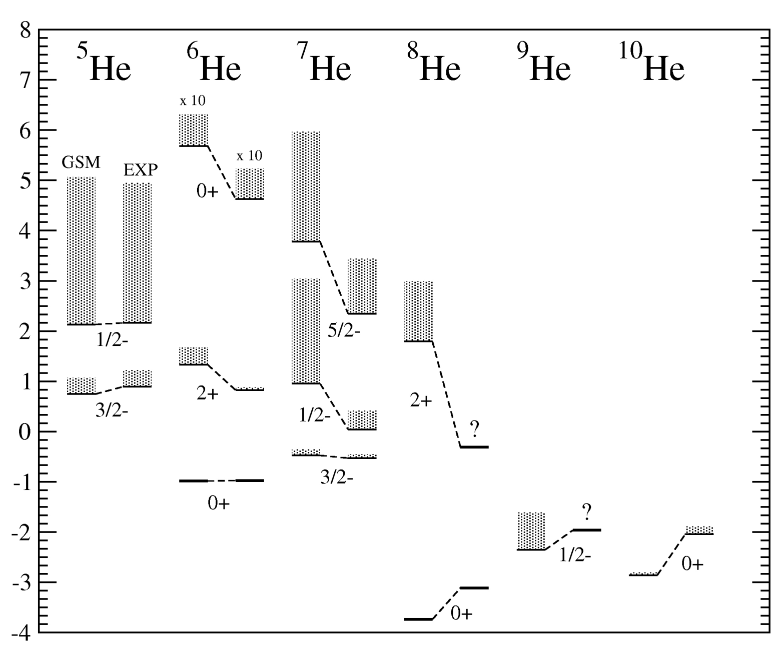
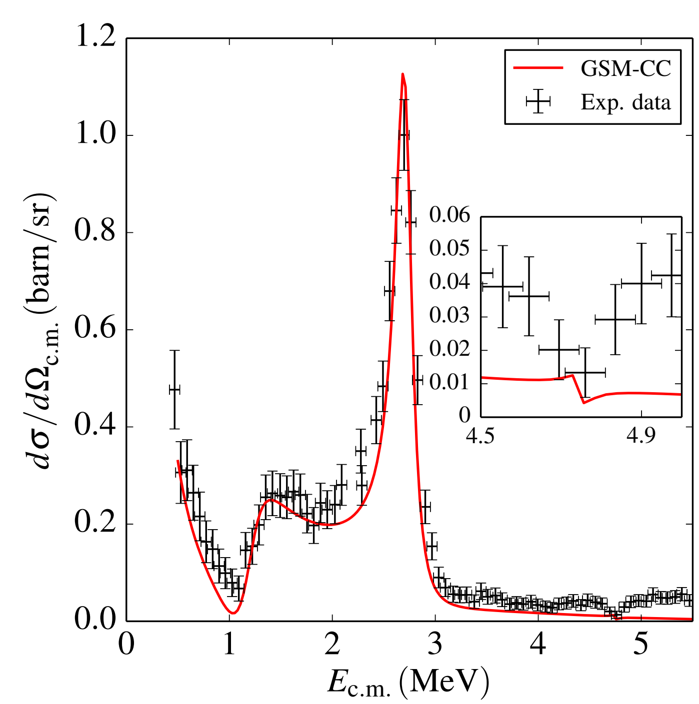
We have optimized an **effective N+NN potential** within the **Gamow Shell Model (GSM)** framework, designed to describe a variety of **structure** (**bound + unbound**) and **reaction** observables across the **psd-shell** nuclei (A ≃ 5 - 15)

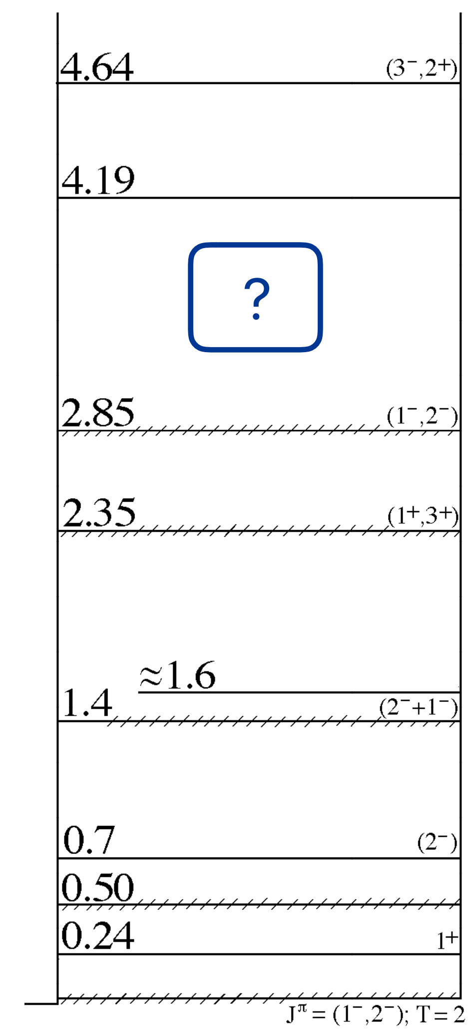
Statistical studies have been carried out to assess **statistical uncertainties and correlations** between parameters and/or predicted observables



GSM spectra of Helium isotopes obtained with a simple interaction



GSM-CC ^{14}O(p,p') excitation function



^{10}Li experimental spectrum

Outline

1. The framework
   - The Gamow Shell Model
   - Optimization and Uncertainty Quantification

2. The quantified GSM effective interaction
   - The core potential
   - The NN interaction

3. Applications
   - A=7 nuclei
   - Helium spectra

4. Conclusions

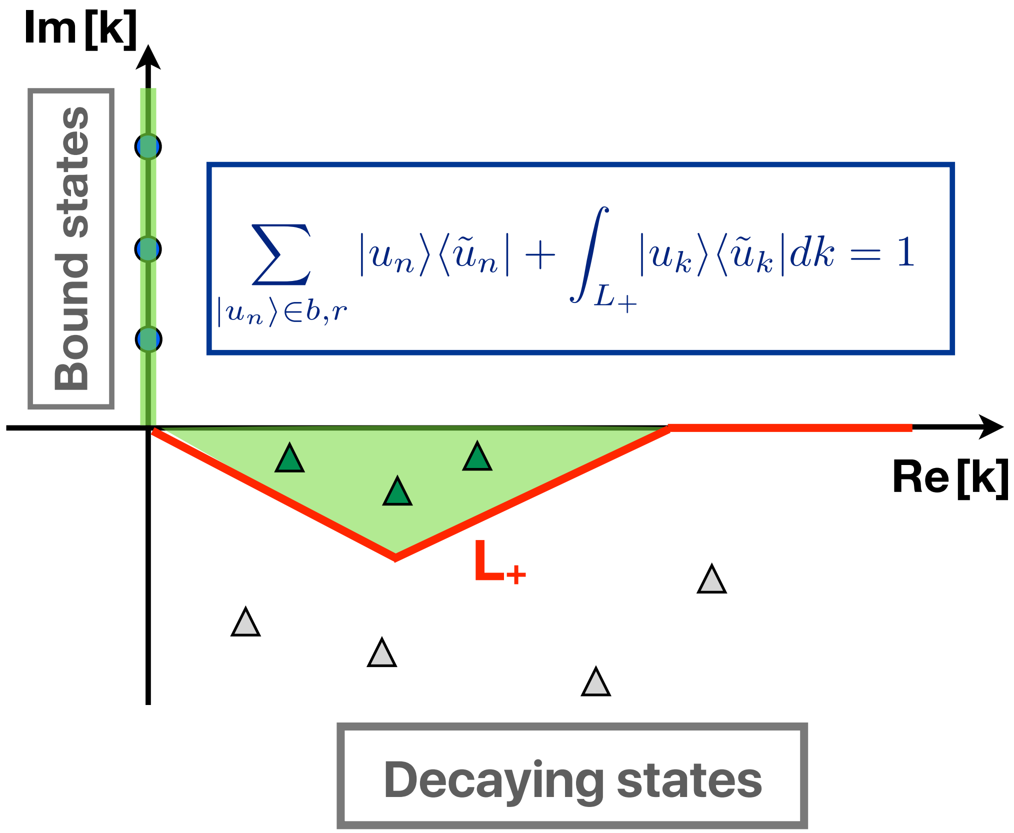
The Framework: The Gamow Shell Model

N. Michel, W. Nazarewicz, M. Płoszajczak, T. Vertse, J. Phys. G: Nucl. Part. Phys. 36, 013101 (2009)

- **Open-quantum system extension** of the traditional Shell Model
- Both **correlations** and **continuum effects** are treated on the same footing (**Berggren** ensemble)
- GSM-Cluster orbital shell model (COSM) Hamiltonian:

$$H = \sum_{i=1}^{N_v} \left[\frac{\vec{p}_i^{\,2}}{2\mu_i} + U(i) \right] + \sum_{i<j=1}^{N_v} \left[V_{res}(i,j) + \frac{\vec{p}_i \cdot \vec{p}_j}{M_c} \right]$$

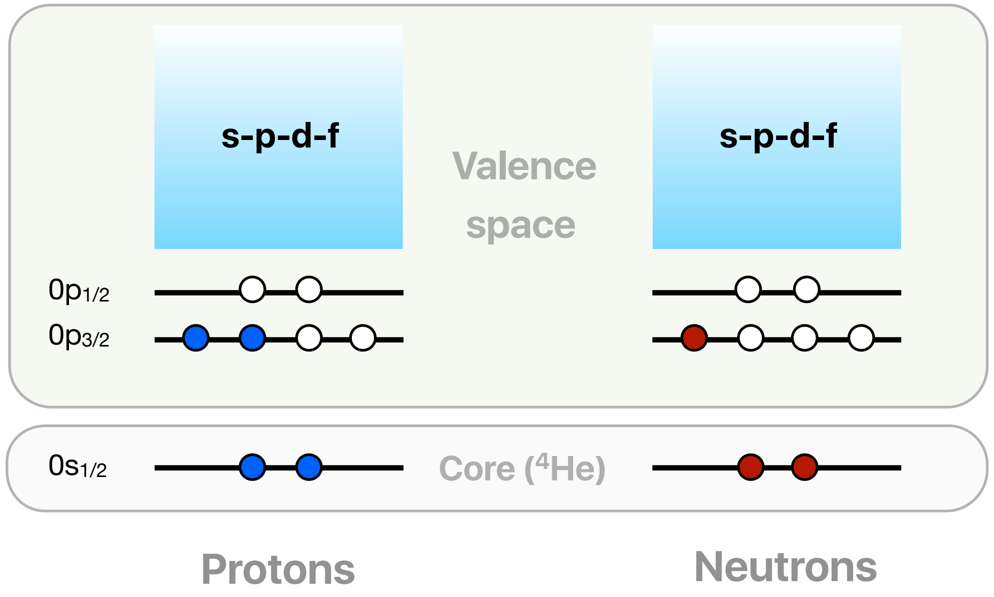
- Translational invariance
- Exact treatment of the Coulomb interaction



T. Berggren, Nucl. Phys. A 109, 265 (1968)

The Interaction

- ^{4}He core modeled by a Woods-Saxon + spin-orbit + Coulomb
- **Configuration space: psdf**
  - $0p_{3/2}$, $0p_{1/2}$ and/or $1s_{1/2}$, $0d_{5/2}$ resonances
  - s, p, d and f scattering continua, k_{max} = 2.0 fm^{-1}



- Effective finite-range NN potential
  - **Gaussian-like with central + spin-orbit + tensor + Coulomb channels**
  - Based on H. Furutani, H. Horiuchi, and R. Tamagaki, Prog. Theor. Phys. 62, 981 (1979)
  - **7 parameters** adjusted to the He, Li, Be chain ground-state energies + chosen excited states

- The calculations were made possible by the hybrid parallelization of the GSM code

The Optimization

- **Chi-square** minimization

  J. Dobaczewski, W. Nazarewicz, P.-G. Reinhard,
  J. Phys. G: Nucl. and Part. Phys. 41, 074001 (2014)

$$\chi^2(\mathbf{p}) = \sum_{i=1}^{N_d} \left(\frac{\mathcal{O}_i(\mathbf{p}) - \mathcal{O}_i^{\exp}}{\delta \mathcal{O}_i} \right)^2$$

- Part of the arbitrariness of the adopted errors is removed by requiring that

$$\frac{\chi^2(\mathbf{p}_0)}{N_{\mathrm{dof}}} \leftrightarrow 1$$

  at the minimum $\mathbf{p}_0$ (similarly to the case of a purely statistical distribution).

- In the case of a single type of data (and negligible experimental + numerical errors):
  $\Rightarrow$ **Global scaling of the adopted errors** (One single Birge factor)

The Optimization

- The minimization were performed using the **Gauss-Newton** algorithm augmented by the **Singular Value Decomposition (SVD)** technique:

- **Gauss-Newton method** (for the overdetermined case $N_{data} > N_{param}$)

$$P_{(s+1)} = P_{(s)} - \left(J_{(s)}^T J_{(s)} \right)^{-1} J_{(s)}^T F_{(s)}$$

s : step
P : parameter-vector
J : Jacobian
F : residual vector

- **Singular Value Decomposition (SVD)**: Moore-Penrose pseudoinverse to deal with sloppy parameters:

$$\cancel{M^{-1} = PD^{-1}P^{-1}} \rightarrow M_{MP}^{-1} = PD_{MP}^{-1}P^{-1}$$

$\Rightarrow$ $MX = B$ is solved in a restricted subspace of the space image of M.

The Statistical Uncertainty Quantification

- **Covariance matrix** (**linear regression**)

$$\mathcal{C} = (J^T J)^{-1} \, , \quad J_{i\alpha} = \frac{1}{\delta \mathcal{O}_i} \left. \frac{\partial \mathcal{O}_i}{\partial p_\alpha} \right|_{\mathbf{p}_0}$$

Uncertainties on **parameters**

$$\Delta p_\alpha = \sqrt{\mathcal{C}_{\alpha\alpha}}$$

Uncertainties on **observables**

$$\overline{\Delta A}^2 = \sum_{\alpha,\beta=1}^{N_p} \left. \frac{\partial A}{\partial p_\alpha} \right|_{\mathbf{p}_0} \mathcal{C}_{\alpha\beta} \left. \frac{\partial A}{\partial p_\beta} \right|_{\mathbf{p}_0}$$

Correlation coefficients between physical quantities

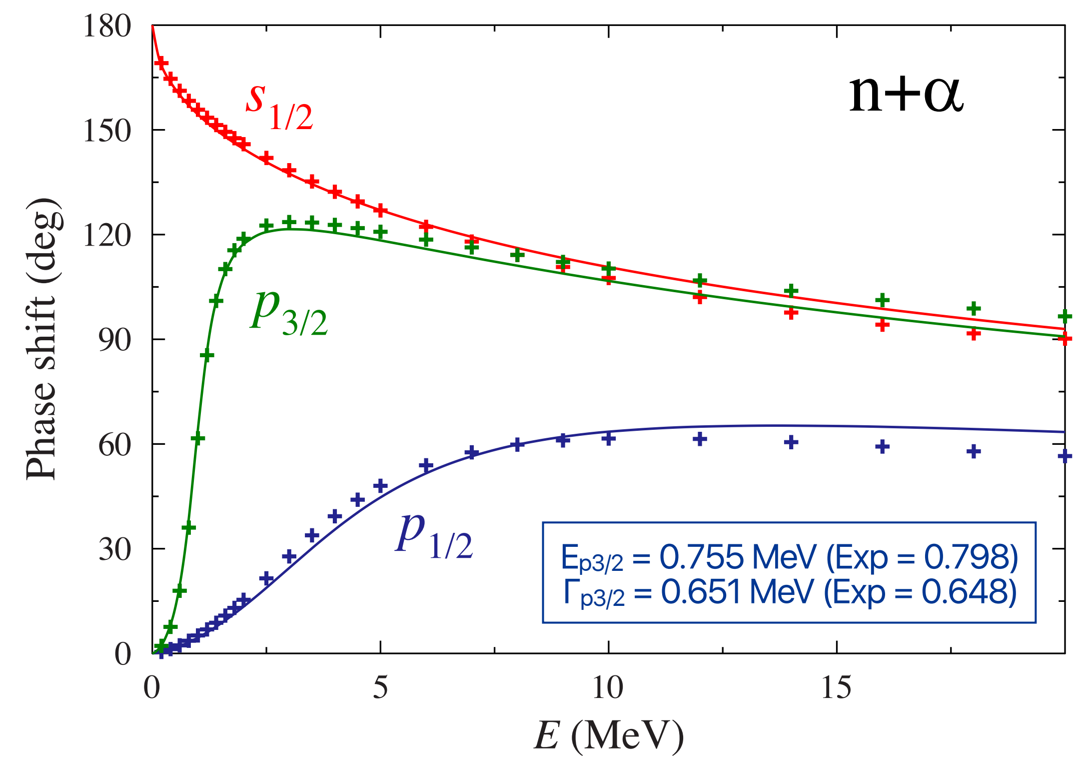
$$\overline{\Delta A \, \Delta B} = \sum_{\alpha,\beta=1}^{N_p} \left. \frac{\partial A}{\partial p_\alpha} \right|_{\mathbf{p}_0} \mathcal{C}_{\alpha\beta} \left. \frac{\partial B}{\partial p_\beta} \right|_{\mathbf{p}_0}$$

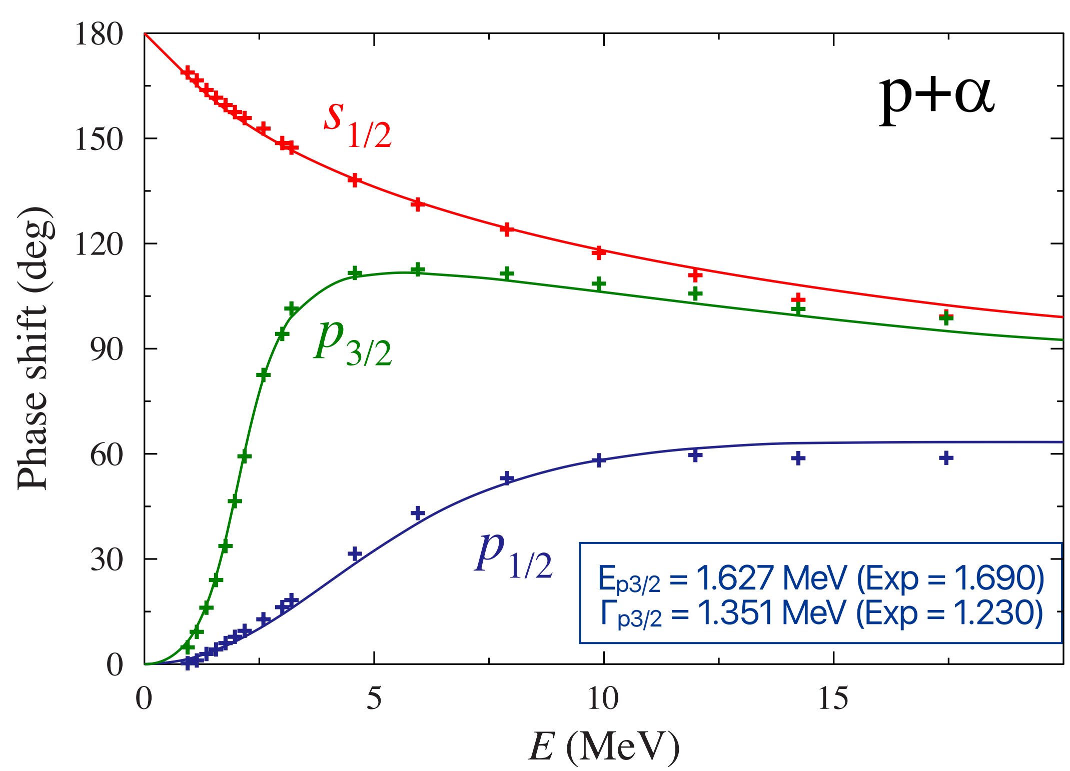
Uncertainties as in 'reasonable domain'

The Core Potential

- The Woods-Saxon + spin-orbit + Coulomb was adjusted to N - ^{4}He **phase shifts** up to E_{cm} = 20 MeV

Particle	R_0 [fm]	a [fm]	V_0 [MeV]	V_{so} [MeV fm^2]	R_{ch} [fm]
neutron	2.15 ± 0.04	0.63 ± 0.02	41.9 ± 1.0	7.21 ± 0.20	
proton	2.06 ± 0.04	0.64 ± 0.02	44.4 ± 1.1	7.24 ± 0.21	1.681

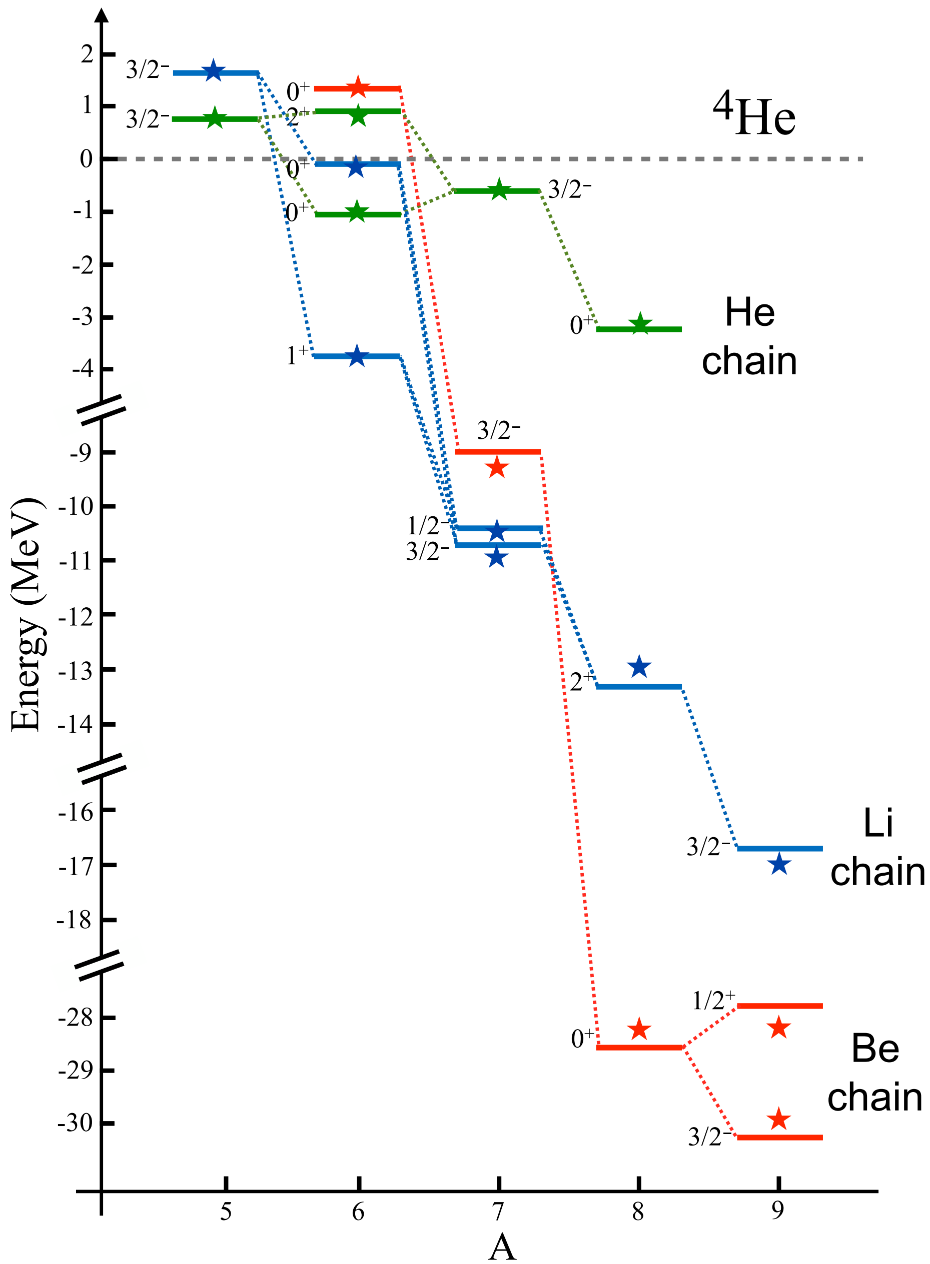




n\p	R_0	a	V_0	V_{so}
R_0	•	-0.81	**-0.94**	-0.78
a	-0.75	•	0.59	0.81
V_0	**-0.95**	0.51	•	0.62
V_{so}	-0.75	0.84	0.55	•

Correlation coefficients
(Normalized covariance matrix)

The zeroth order NN potential



Nucleus	State	E	E_{exp}	Γ	Γ_{exp}
^{6}He	0^+	-1.063	-0.973		
^{6}He	2^+	0.938	0.824	168	113(20)
^{7}He	$3/2^-$	-0.578	-0.528	178	150(20)
^{8}He	0^+	-3.225	-3.112		
^{6}Li	1^+	-3.724	-3.699		
^{6}Li	0^+	-0.054	-0.136		
^{7}Li	$3/2^-$	-10.688	-10.949		
^{7}Li	$1/2^-$	-10.359	-10.471		
^{8}Li	2^+	-13.350	-12.982		
^{9}Li	$3/2^-$	-16.677	-17.046		
^{6}Be	0^+	1.390	1.371	21	92(6)
^{7}Be	$3/2^-$	-8.977	-9.305		
^{8}Be	0^+	-28.572	-28.204	0	0.0056(3)
^{9}Be	$3/2^-$	-30.230	-29.870		
^{9}Be	$1/2^+$	-27.747	-28.186	0	217(10)

- 4 nucleons in the continuum (converged calculations)
- Could be used with other models (DMRG)

- r.m.s. deviation of 250 keV
- Good starting point for detailed structural and reaction studies

The zeroth order NN potential

- Parameters

Parameter		Value
central	S=1 , T=1	-3.2 ± 22.0
	S=1 , T=0	**-5.1 ± 1.0**
	S=0 , T=0	**-21.3 ± 6.6**
	S=0 , T=1	**-5.6 ± 0.5**
spin-orbit	S=1 , T=1	-540 ± 1240
tensor	S=1 , T=1	-12.1 ± 79.5
	S=1 , T=0	**-14.2 ± 7.1**

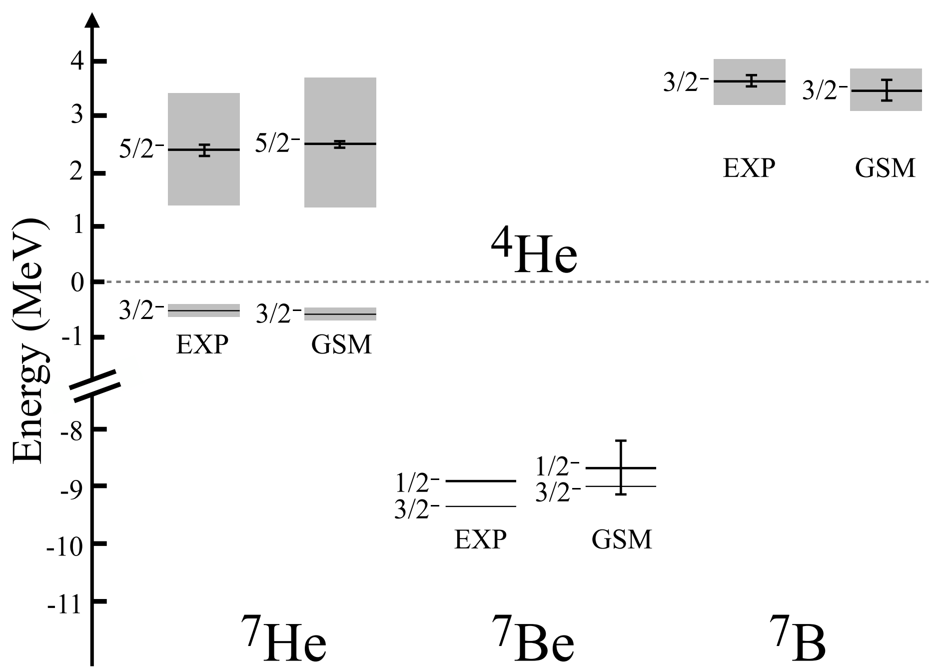
- Singular values (eigenvalues of the normalized Hessian matrix)

n	s_n	V_c^{11}	V_c^{10}	V_c^{00}	V_c^{01}	V_{LS}^{11}	V_T^{11}	V_T^{10}
1	243	0.00	**0.82**	−0.03	**0.53**	0.00	0.00	0.23
2	43.0	0.00	**−0.49**	−0.02	**0.85**	0.00	−0.01	−0.19
3	7.06	−0.04	−0.16	**0.79**	0.05	0.04	−0.07	**0.58**
4	3.94	0.02	−0.25	**−0.61**	0.01	−0.09	−0.04	**0.75**
5	0.57	−0.23	−0.02	−0.09	0.00	**0.97**	−0.01	0.04
6	0.20	**0.65**	−0.03	0.04	0.01	0.16	**0.74**	0.06
7	0.12	**0.73**	0.01	0.00	0.00	0.16	**−0.66**	−0.04

- Four parameters completely govern the optimization!
- The three remaining parameters are **sloppy**, i.e. unconstrained by the chosen set of experimental data
  - Can be constrained by experimental data of different kinds (charge/matter radii, EM moments)
  - Could be used to locally fine-tune the interaction

Predictions - Energy Spectra, A=7 nuclei

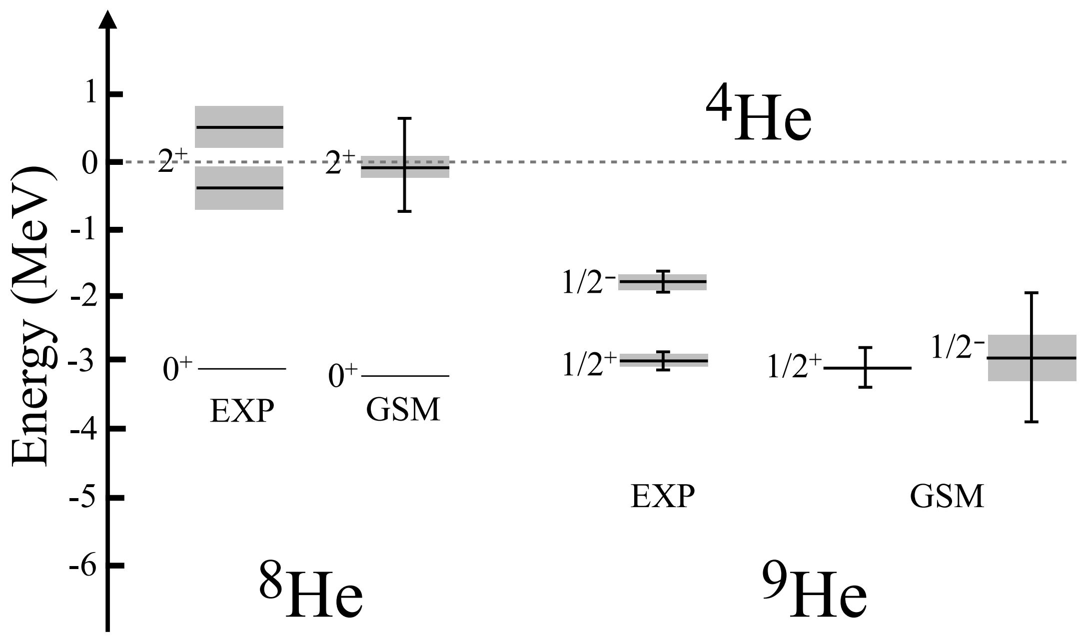
- Computed uncertainties have **two components**: $\Delta E = \sqrt{\Delta E_N^2 + \Delta E_{NN}^2}$
- **A=7 nuclei:**



State	E_{calc} (MeV)	E_{exp} (MeV)	Γ_{calc} (keV)	Γ_{exp} (keV)
^{7}He, 5/2-	+2.50 (2)	+2.39 (9)	2250 (280)	1990 (170)
^{7}Be, 1/2-	-8.67 (45)	-8.88		
^{7}B, 3/2-	+3.42 (21)	+3.58 (7)	740 (450)	801 (20)

- ΔE_N < 0.07 MeV (small compared to ΔE_{NN})
- **Good overall agreement** for the energies and the widths

Predictions - Energy Spectra, Heliums



State	E_{calc} (MeV)	E_{exp} (MeV)	Γ_{calc} (keV)	Γ_{exp} (keV)
^{8}He, 2+	-0.10 (75)	-0.41 / +0.49	290 (1010)	1990 (170)
^{9}He, 1/2+	-3.12 (31)	-2.93 (9)*	0	180 (160)*
^{9}He, 1/2-	-2.98 (102)	-1.88 (12)*	630 (330)	130 (170)*

[*] Al Kalanee et al., PRC 88, 034301 (2013)

- **^{8}He, 2^{+} :**
  - Uncertainty coming from the WS: ΔE_N = 0.07 MeV
  - Prediction with uncertainties does not favor any of the experimental scenario
- **^{9}He**: not resolved experimentally
  - ΔE_N (1/2^{+}) = 0.13 MeV, ΔE_N (1/2^{-}) = 0.59 MeV (s1/2 and p1/2 are less constrained in the WS)
  - **Shell inversion** observed (mean values)

Summary and Outlook

- The interaction is well optimized to the ground state + some excited state energies of the He, Li and Be chains

- The SVD analysis allowed to pinpoint the four interaction parameters which are **reasonably constrained** by the binding energies.
- The remaining three parameters are **sloppy**; hence new data are needed to limit them.

- With the covariance matrices calculated for the one and two-body potentials, we assessed **uncertainties** and **correlations** between physical quantities.

- In collaboration with the Department of Statistics and Probability at MSU, we have initiated a project to perform a **Bayesian study** of the interaction for a fully consistent statistical analysis (see Léo Neufcourt's talk this afternoon for a preliminary Bayesian study of the interaction).

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Thank you for your attention!

Back-up

$$V = V_c + V_{LS} + V_T + V_{\mathrm{Coul}}.$$

$$\tilde{V}_c(r) = \sum_{n=1}^{3} V_c^n \, (W_c^n + B_c^n P_\sigma - H_c^n P_\tau - M_c^n P_\sigma P_\tau) \, e^{-\beta_c^n r^2} \tag{5}$$

$$\tilde{V}_{LS}(r) = \boldsymbol{L} \cdot \boldsymbol{S} \sum_{n=1}^{2} V_{LS}^n \, (W_{LS}^n - H_{LS}^n P_\tau) \, e^{-\beta_{LS}^n r^2} \tag{6}$$

$$\tilde{V}_T(r) = S_{ij} \sum_{n=1}^{3} V_T^n \, (W_T^n - H_T^n P_\tau) \, r^2 e^{-\beta_T^n r^2}, \tag{7}$$

where $r \equiv r_{ij}$ stands for the distance between the nucleons i and j, $\boldsymbol{L}$ is the relative orbital angular momentum, $\boldsymbol{S} = (\boldsymbol{\sigma}_i + \boldsymbol{\sigma}_j)/2$, $S_{ij} = 3(\boldsymbol{\sigma}_i \cdot \hat{r})(\boldsymbol{\sigma}_j \cdot \hat{r}) - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j$, and P_σ and P_τ are spin and isospin exchange operators, respec-

In order to be applied in the present GSM formalism, the interaction is rewritten in terms of the spin-isospin projectors Π_{ST} [51, 52]:

$$V_c(r) = V_c^{11} f_c^{11}(r)\Pi_{11} + V_c^{10} f_c^{10}(r)\Pi_{10} + V_c^{00} f_c^{00}(r)\Pi_{00} + V_c^{01} f_c^{01}(r)\Pi_{01}, \tag{8}$$

$$V_{LS}(r) = (\boldsymbol{L} \cdot \boldsymbol{S}) \, V_{LS}^{11} f_{LS}^{11}(r)\Pi_{11}, \tag{9}$$

$$V_T(r) = S_{ij}\left[V_T^{11} f_T^{11}(r)\Pi_{11} + V_T^{10} f_T^{10}(r)\Pi_{10}\right], \tag{10}$$