

Ab initio reactions up to medium-mass nuclei with the symmetry-adapted resonating group method

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LSU



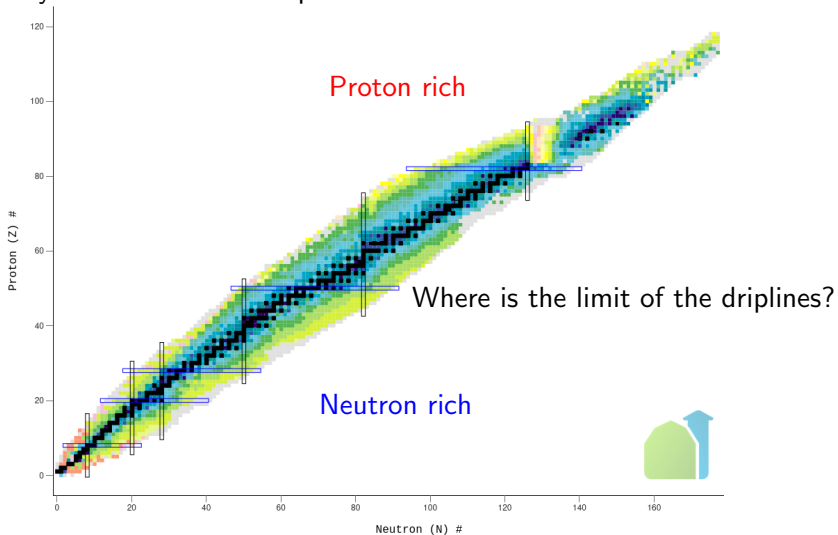
HPCC HIGH PERFORMANCE COMPUTING

Outline

- 1 Introduction
- 2 Unifying structure and reactions with RGM
- 3 RGM in the symmetry-adapted framework
- 4 Results
- 5 Conclusion

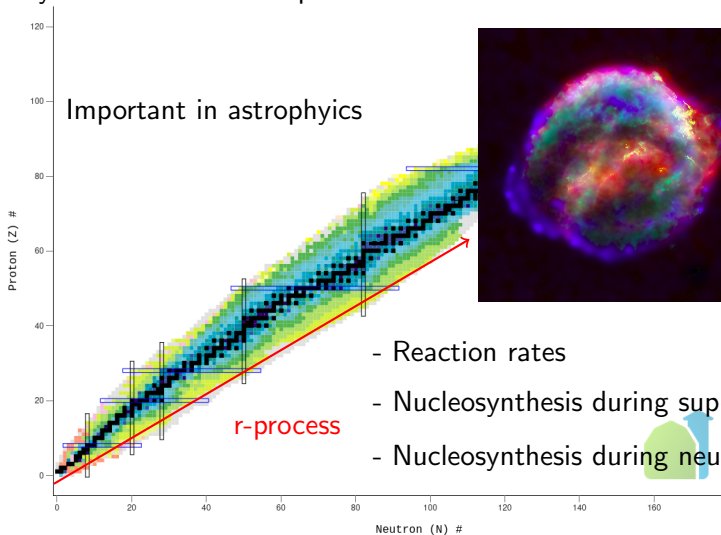
Exotic nuclei

Why are exotic nuclei important?



Exotic nuclei

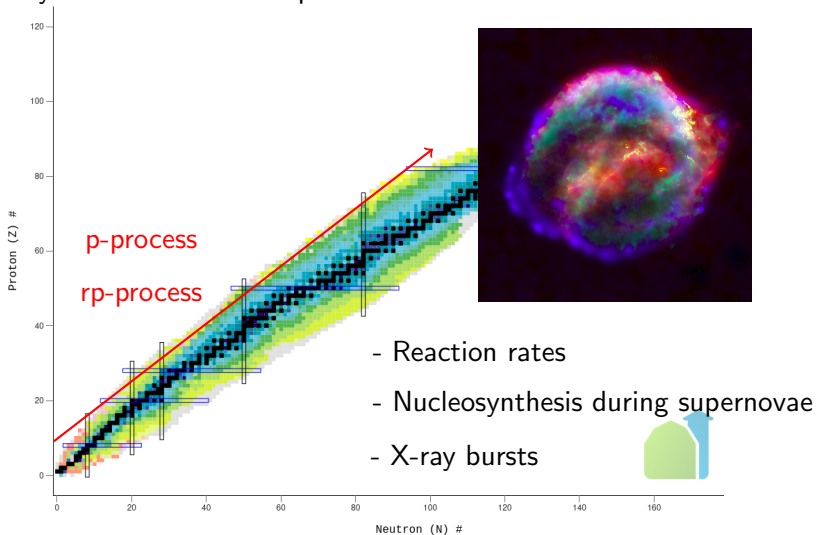
Why are exotic nuclei important?



- Reaction rates
- Nucleosynthesis during supernovae
- Nucleosynthesis during neutron star mergers

Exotic nuclei

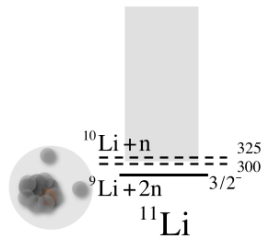
Why are exotic nuclei important?



Exotic nuclei

Exotic nuclei exhibit properties like:

- Short lifetimes
- Near threshold clustering
- Halo nuclei



These brings the following challenges:

Coupling to the continuum



Structure calculation cannot ignore the coupling to the continuum.

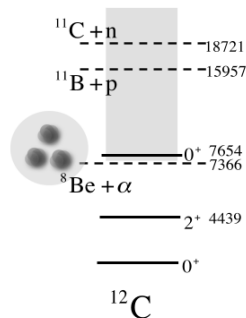
How do we address the low energy regime where individual resonances are important?

Towards a unified nuclear structure and nuclear reaction approaches!

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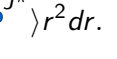
Towards a unified nuclear structure and nuclear reaction approaches!

Resonating group method (RGM)

We consider the ansatz:

$$|(c, r)^{J\pi}\rangle = \mathcal{A}_c \left\{ |\psi_T^{J\pi}\rangle \otimes |\psi_P^{J\pi}\rangle \right\}^{J\pi} = \mathcal{A}_c |\text{diagram}\rangle.$$

Antisymmetrized!



The wave functions are expanded in this basis

$$|\psi^{J\pi}\rangle = \sum_c \int_0^\infty \left(\frac{g_c^{J\pi}(r)}{r} \right) \mathcal{A}_c |\text{diagram}\rangle r^2 dr.$$

Relative motion between T and P.

Which lead to the coupled channel equation (Hills-Wheeler)

$$\sum_c \int_0^\infty \left[H_{cc'}^{J\pi}(r, r') - E N_{cc'}^{J\pi}(r, r') \right] \frac{g_c^{J\pi}(r)}{r} r^2 dr = 0.$$



Channels are not orthogonal!

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
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Asymptotics yield scattering information.



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Resonating group method (RGM)

First, we go from a generalized eigenvalue problem to the standard case by:

$$H|\Psi\rangle = EN|\Psi\rangle \rightarrow \bar{H}|\bar{\Psi}\rangle = E|\bar{\Psi}\rangle,$$

where we have defined and orthogonalized channel basis

$$\bar{H} = \hat{N}^{-1/2} \hat{H} \hat{N}^{-1/2} \quad |\bar{\Psi}\rangle = \hat{N}^{1/2} |\Psi\rangle.$$

This allows us to get the interaction between channels as a non-local potential:

$$\left(T_c(r) + E_{l_1^{\pi_1}} + E_{l_2^{\pi_2}} \right) \frac{u_c^{J\pi}(r)}{r} + \sum_{c'} \int dr' r'^2 W_{cc'}(r, r') \frac{u_{c'}^{J\pi}(r')}{r'} = 0,$$

which we can compute in matrix form as:

$$W = N^{-1/2} T_{\text{rel}} N^{1/2} - T_{\text{rel}} + N^{-1/2} V_{\text{rel}} \hat{N}^{-1/2}.$$

We compute scattering observables with a microscopic R-matrix calculation.

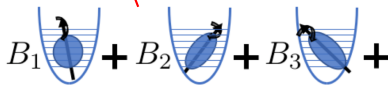
Resonating group method (RGM)

Let's use the wavefunctions from a microscopic model!

$$|\psi\rangle = \sum_c \int_0^\infty \left(\frac{g_c(r)}{r} \right) \mathcal{A} | \text{diagram} \rangle r^2 dr.$$

Symmetry-adapted No-core Shell Model

- All nucleons active.
- Chiral EFT interaction
- RGM version only nucleon projectiles (for now).



Symmetry-adapted no-core shell model

SA-NCSM is based on standard configuration interaction (CI) approach

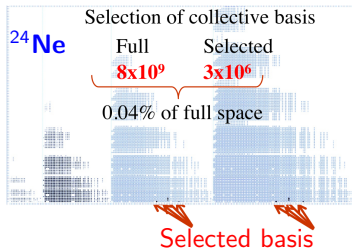
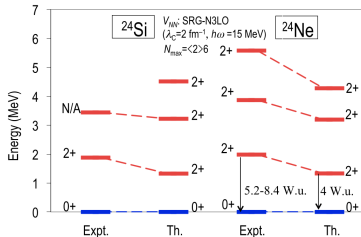
- Harmonic oscillator basis.
- Model space set by $N_{\max} \hbar\omega$
- Hamiltonian from first principles
 $V_{NN} = V_{\chi\text{EFT}}$.



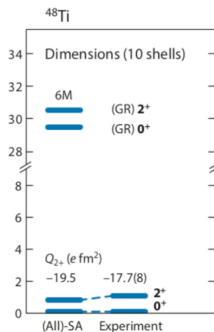
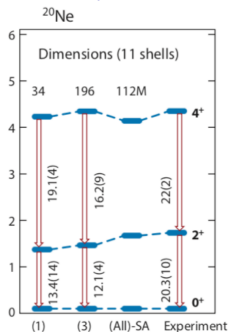
The SA-NCSM leverages near-exact symmetries

- Reorganization of the Slater determinant basis into $SU(3)$ coupled states.
- This allows the construction of model spaces containing only the most physically relevant configurations.
- This truncation still has exact CM factorization.
- In a complete model space equivalent to CI.

Symmetry-adapted no-core shell model



K. D. Launey et al., *Annu. Rev. Nucl. Part. Sci.* **71**, 253–277 (2021)



- Few basis states contribute and they capture relevant correlations.
- Practically exact calculations with selections.

Two important questions to address

- What do I mean by $SU(3)$ coupled states?
- How do we actually do the selection of the basis?

The $SU(3) \times SU(2)$ basis

$SU(2)$ coupling:

$$|j_1 j_2 JM\rangle = \sum_{m_1 m_2} \langle j_1 m_1 j_2 m_2 | JM \rangle |j_1 m_1 j_2 m_2\rangle$$

Clebsch–Gordan ($SU(2)$ coupling) coefficients

$SU(3)$ coupling:

$$|(\lambda_3 \mu_3) \alpha_3\rangle_\rho = \sum_{\alpha_1 \alpha_2} \langle (\lambda_1 \mu_1) \alpha_1; (\lambda_2 \mu_2) \alpha_2 | (\lambda_3 \mu_3) \alpha_3 \rangle |(\lambda_1 \mu_1) \alpha_1\rangle |(\lambda_2 \mu_2) \alpha_2\rangle$$

$SU(3)$ coupling coefficients

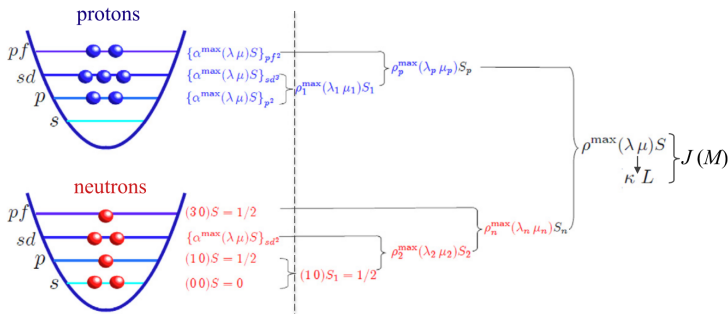
The $(\lambda \mu)$ projection convention
used is:

$$\alpha \rightarrow \kappa LM$$

Later we can couple in $SU(2)$:

$$\{LS\} \rightarrow \{j\}$$

The $SU(3) \times SU(2)$ basis



K. D. Launey et al., Prog. Part. Nuc. Phys. **89**, 101–136 (2016)

In the HO basis, we typically use:

$$N = 2n + \ell,$$

but we can also use Cartesian:

$$N = n_x + n_y + n_z$$

We can obtain (λ, μ) by:

$$\lambda = n_z - n_x \quad \mu = n_x - n_y$$

Physical interpretation of an SU(3) irrep

We have two quantum numbers (λ, μ)

$(\lambda, 0) \sim n_z - n_x \rightarrow$ prolate shape $(0, \mu) \sim n_x - n_y \rightarrow$ oblate shape



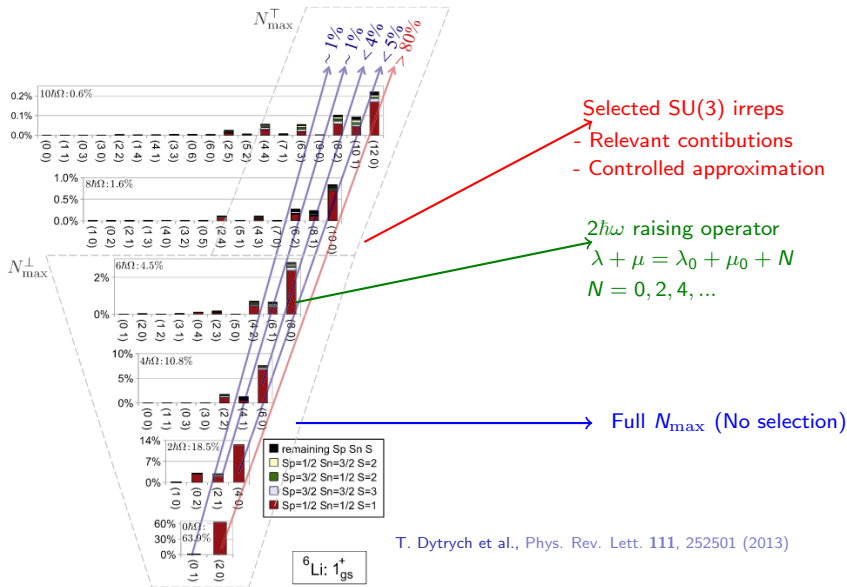
Specific superposition of (λ, μ)
creates triaxial shapes



We can relate them to β and γ too:


$$\beta^2 \propto \lambda^2 + \mu^2 + \lambda\mu + 3(\lambda + \mu)$$
$$\gamma = \arctan \left(\frac{\sqrt{3}\mu}{2\lambda + \mu} \right)$$

Model space selection



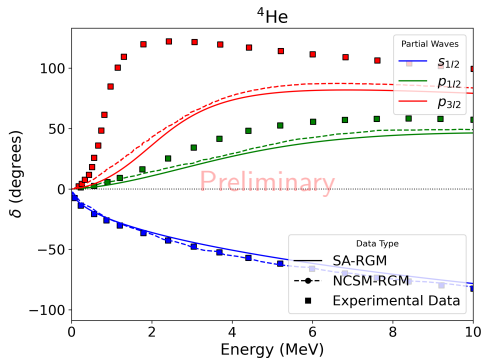
Validation against NCSM-RGM

$$|(c, r)\rangle = \mathcal{A} \left\{ |\Psi_T^{J_T}\rangle \otimes |\Psi_P^{J_P}\rangle \right\}_{M_A}^{J_A}$$


 $= \sum_i c_i | \text{state } i \rangle$ from SA-NCSM

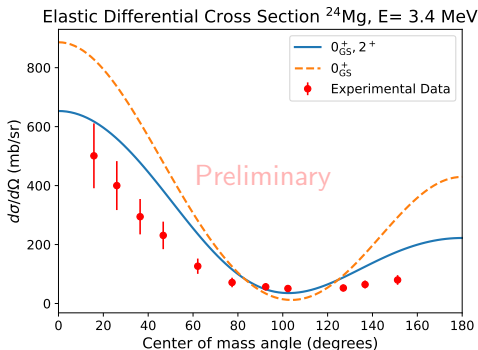
nucleon (for now)

- Interaction: NNLOOpt
- $N_{\max} = 14$
- Two target states:
Ground state 0^+ and
excited 2^-



We can compute cross-sections for intermediate nuclei

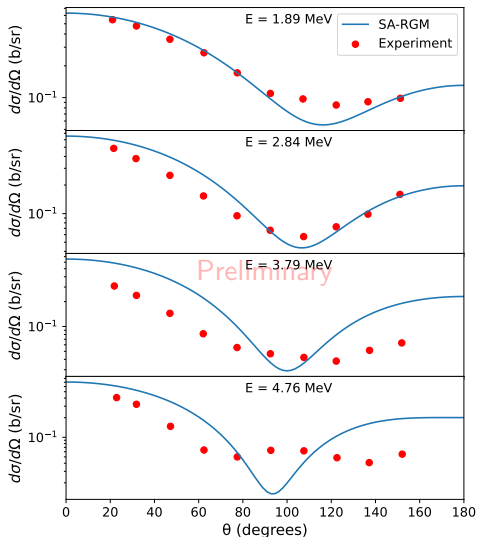
- Interaction: NNLOopt
- $N_{\text{max}} = \langle 2 \rangle 6$
- Two target states:
Ground state 0^+ , first excited 2^+ .
- Up to $\ell = 8$ partial waves.



$^{24}\text{Mg} + n$

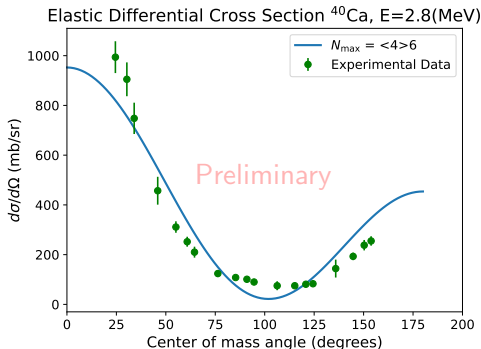
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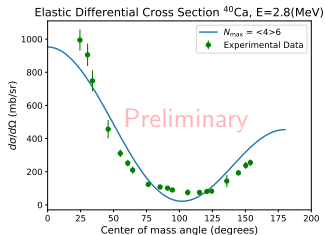
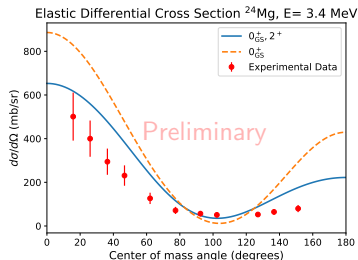
Let's push the model even more!

- Interaction: NNLOopt
- $N_{\text{max}} = \langle 4 \rangle 6$
- One target state:
Ground state 0^+
- Up to $\ell = 8$ partial waves.



Conclusions and outlook

- The resonating group method provides a powerful tool that can be applied to different nuclear models to unify nuclear structure and reactions.
- The SA-RGM is a powerful method that allows to do *ab initio* reaction calculations of intermediate nuclei at bigger N_{\max} spaces.
- Next step: radiative capture.



Acknowledgments

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