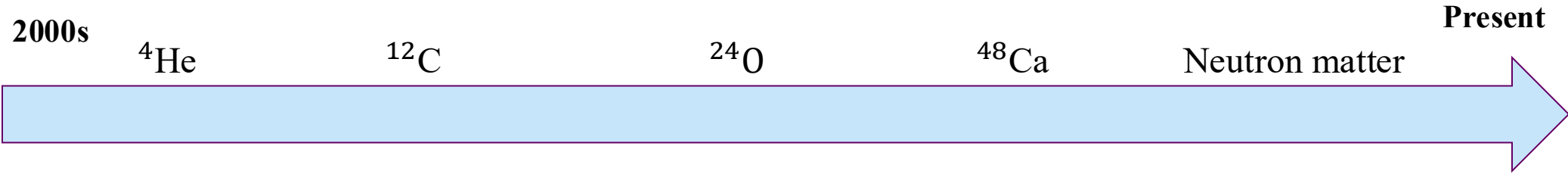


# Capturing Collectivity with a Symmetry-Adapted Basis for *ab initio* $\beta$ Decay and Reaction Studies

Alexis Mercenne



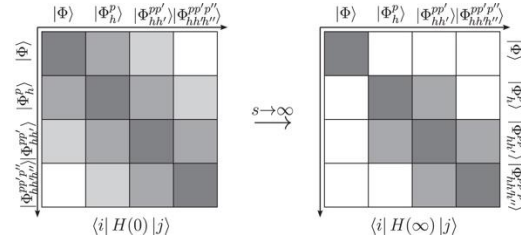
# From QCD to the Nucleus: Progress in Ab Initio Methods



**Forces**  
(phenomenological → chiral EFT)



**Renormalization**



**Methods**  
(GFMC, NCSM, CC, IMSRG, SCGF)

**Reactions**

- **Realistic Interactions:**

- Argonne  $V_{18}$ , Urbana IX → first realistic 2N+3N (late 90s)
- Chiral EFT → QCD-based, systematic expansion (2000s-)

- **Many-Body Methods:**

- Green's Function Monte Carlo (GFMC) for  $A \leq 12$  nuclei.
- No-core Shell Model (NCSM) & Symmetry-adapted NCSM
- Coupled-Cluster, In-Medium SRG, Self-Consistent Green's Functions

- **Unified Structure & Reactions**

- NCSM/RGM & NCSMC → low-energy scattering & astrophysics
- Microscopic optical potentials.

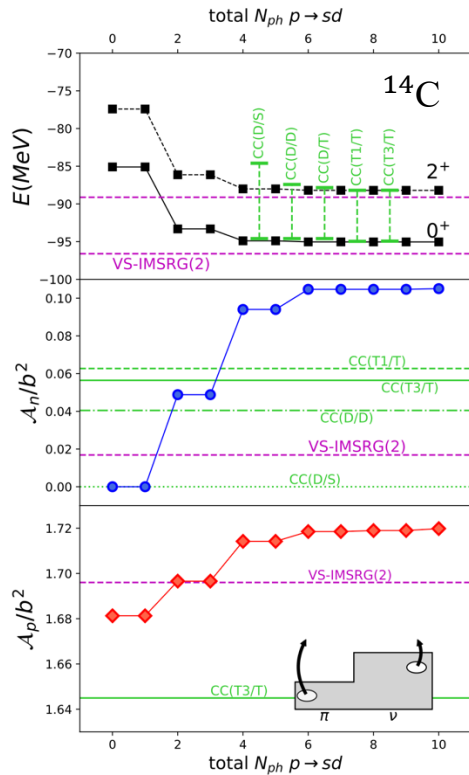
**Results:**

- Binding energies and spectra up to  $A \approx 12$ .
- Shell structure in  $^{24}\text{O}$ ,  $^{48}\text{Ca}$ ,  $^{78}\text{Ni}$
- Hoyle state in  $^{12}\text{C}$
- Solar neutrino rate:  $^7\text{Be}(p,\gamma)^8\text{B}$
- Neutron matter Eos from chiral EFT → neutron-star radii & GW170817

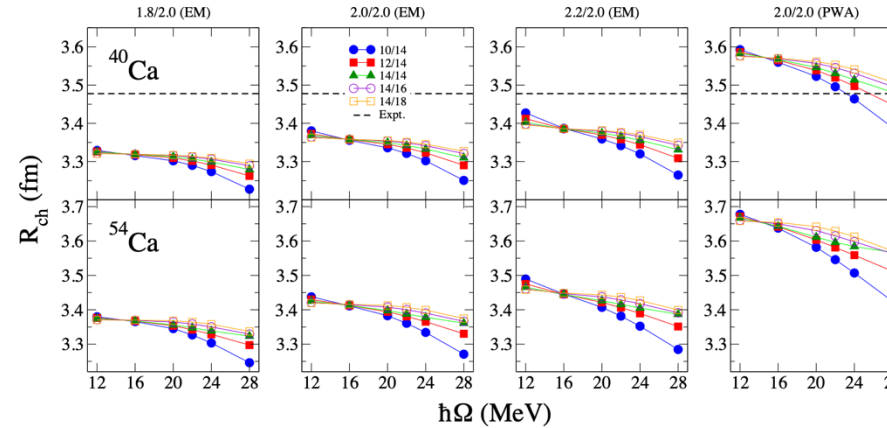
# On the Importance of Capturing Collective Excitations

- Many studies are pointing to the importance of including collective excitations:
  - E2 strengths systematically underestimated.
  - $^{14}\text{C}$  quadrupole moments needs 4p4h contributions.

Q2: Stroberg, PRC, 105, 034033 (2022)

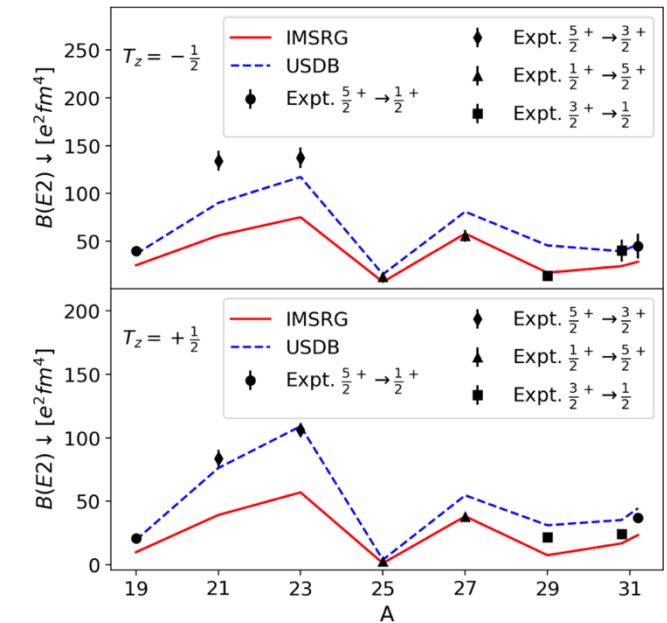


Charge radii: Simonis, PRC 96, 014303 (2017)

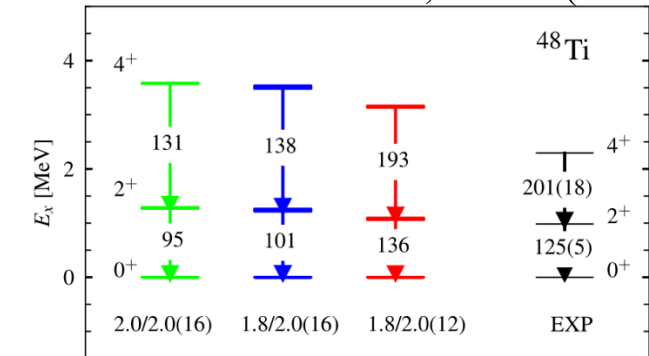


- Some remedies:
  - Use of effective charges/evolved operators.
  - Increase model space.
  - Interaction (3N) fitted to charge radii.
  - Mixing of deformation with GCM ...etc

B(E2): Stroberg, PRC, 105, 034033 (2022)

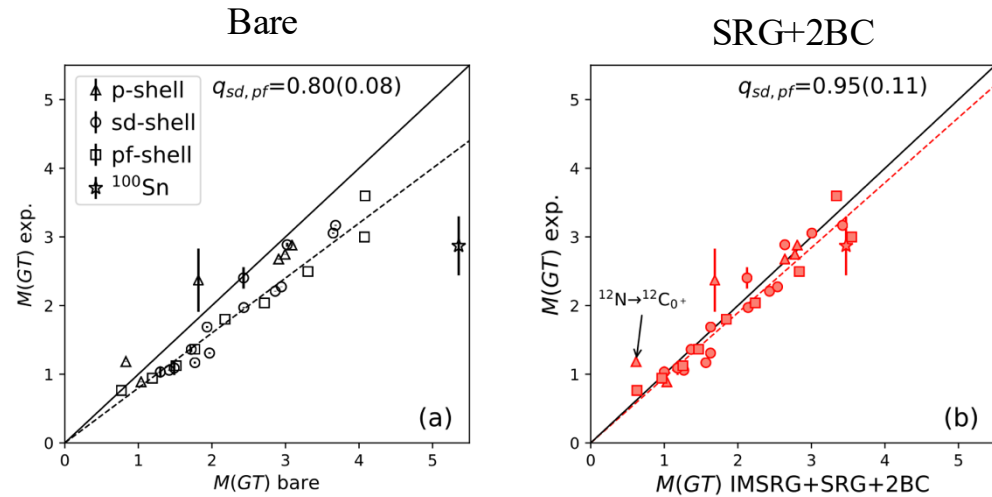


IMSRG+GCM: Yao PRL 124, 232501 (2020)

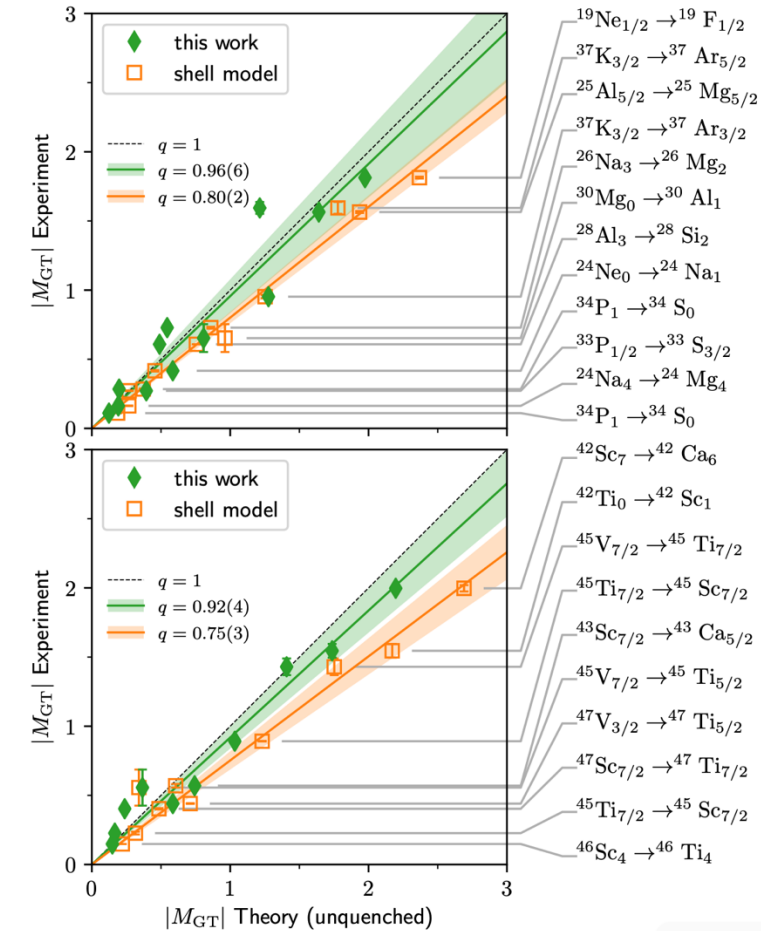
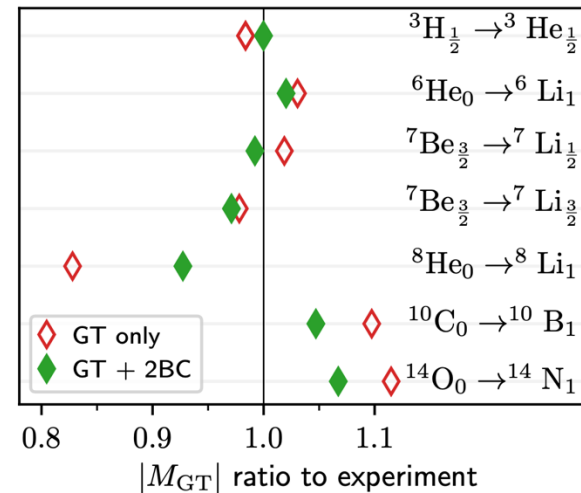


# On the Importance of Capturing Collective Excitations

- Same for  $\beta$ -decay studies:
  - Ab initio calculations typically overpredict GT strength.
  - Operator evolution + consistent (2B) currents largely removes quenching.



S. R. Stroberg, *Particles*, 4, 521 (2021)

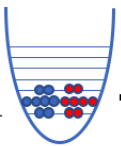
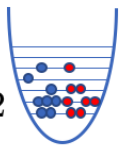
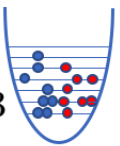


P. Gysberg et al., *Nat. Phys.*, 15, 428 (2019)

# The Symmetry-adapted No-core Shell Model

## Based on no-core shell model:

- HO basis with parameters  $\hbar\Omega$ ,  $N_{\max}$  ( $N\hbar\Omega$  truncation).
- Ab initio NN interactions: AV18, JISP16,  $\chi$ EFT (N2LO, N3LO ...)
- Exact center-of-mass factorization in  $N\hbar\Omega$  spaces.

NCSM  $C_1$    $+ C_2$    $+ C_3$    $+ \dots$

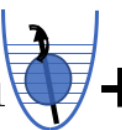
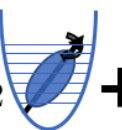
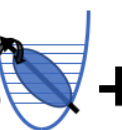
## Equipped with symmetry-adapted techniques:

- Recast basis into SU(3)/Sp(3,R) irreps that encode deformation and collective motion.
- Exploit emergent (quasi-dynamical) SU(3)/symplectic coherent mixing  $\rightarrow$  wave functions concentrate in few irreps.
- Using full space at given  $N_{\max}$  reproduces standard NCSM results.

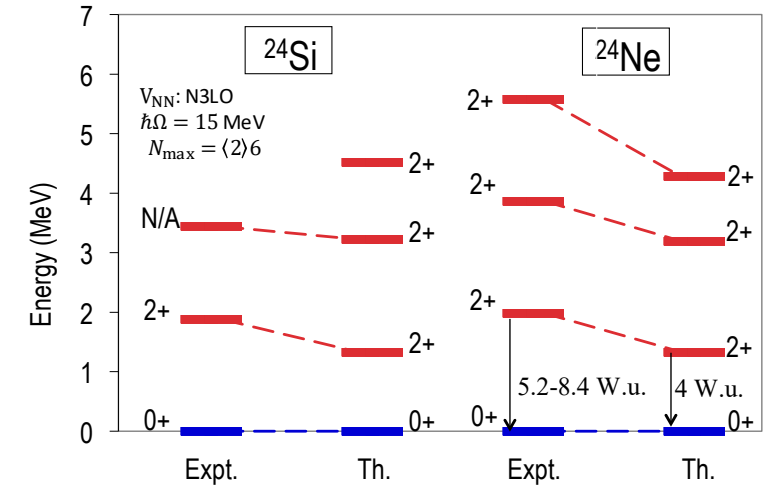
$$|\Psi_J\rangle \approx \sum_{\alpha} c_{\alpha} |(\lambda_{\alpha}\mu_{\alpha})b_{\alpha}J\rangle$$

$$N = N_x + N_y + N_z$$

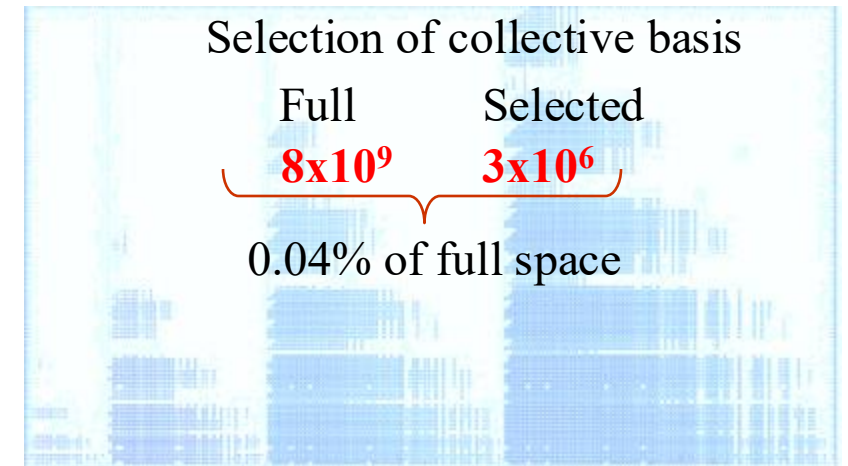
$$\lambda = N_z - N_x ; \mu = N_x - N_y$$

SA-NCSM  $B_1$    $+ B_2$    $+ B_3$    $+ \dots$

$$\left. \begin{array}{l} \text{Spherical: } (0\ 0) \\ \text{Prolate: } (\lambda\ 0) \\ \text{Oblate: } (0\ \mu) \end{array} \right\} \begin{array}{l} \beta(\lambda, \mu) \\ \gamma(\lambda, \mu) \end{array}$$

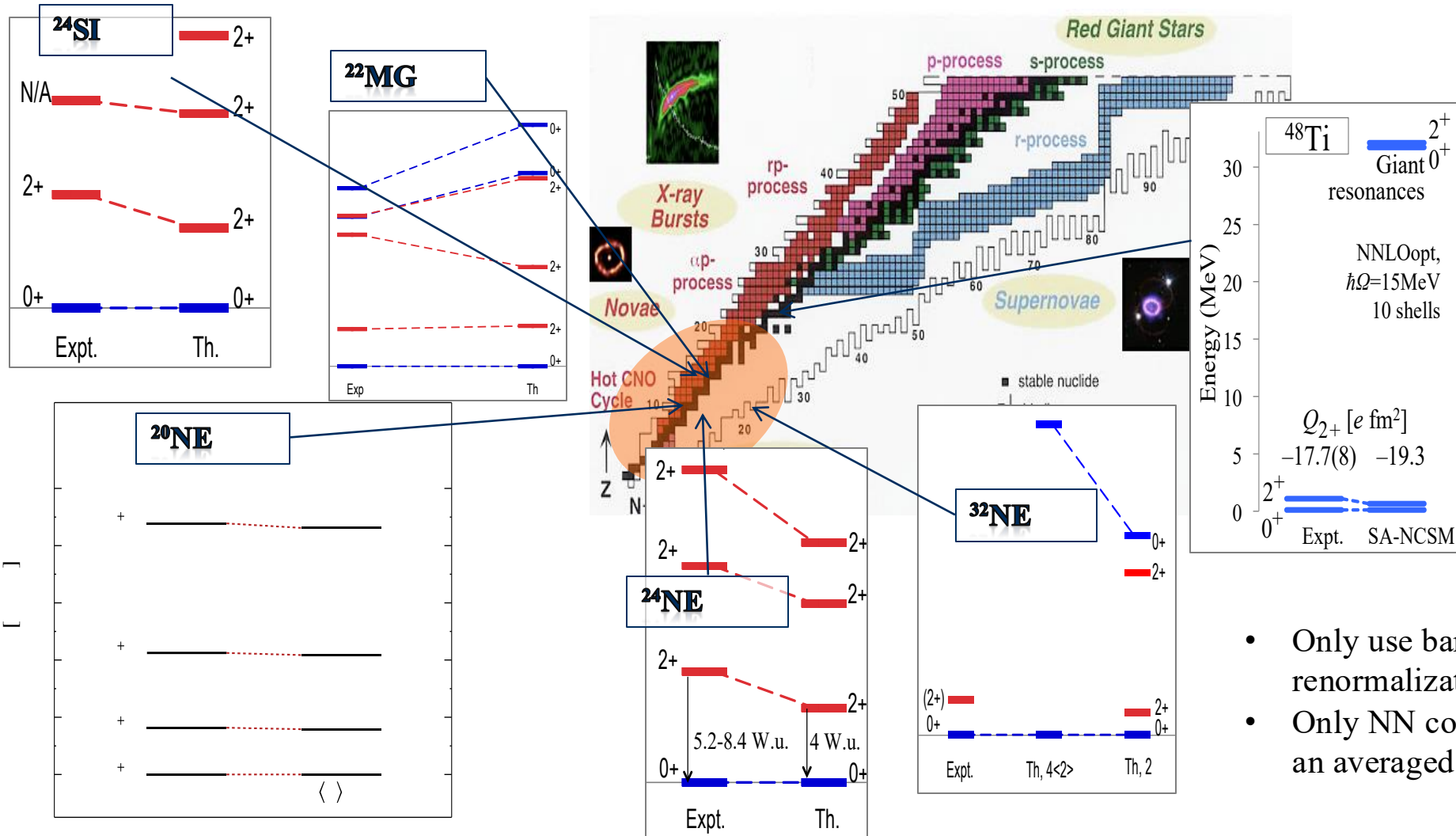


Dytrych et al., PRL (2020)



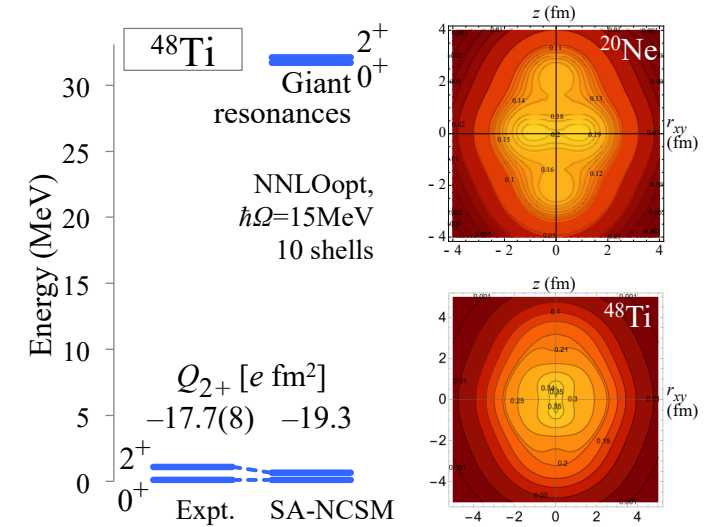
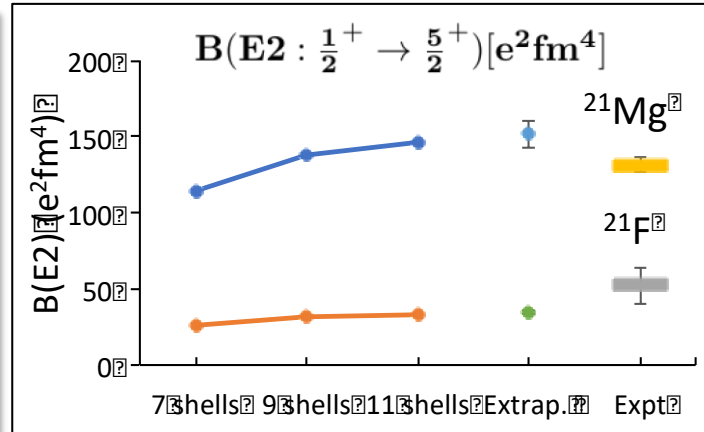
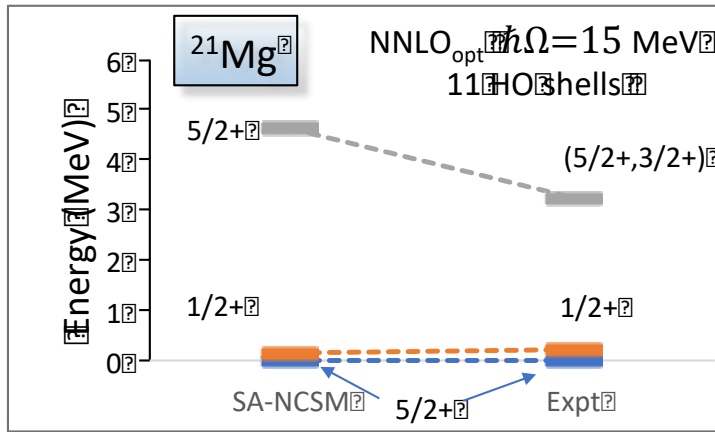
Launey et al., Annu. Rev. Nucl. Part. Sci. (2021)

# Pushing the Limits of Ab Initio Calculations

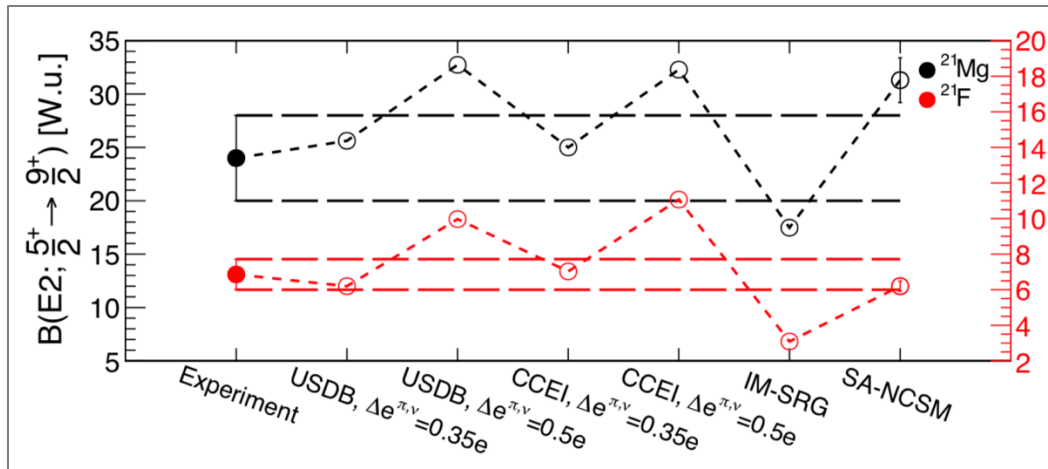


- Only use bare interactions (no SRG/LS renormalization).
- Only NN contribution (3N included as an averaged contribution  $\rightarrow$  NNLOsat)

# Ab Initio Description of Collectivity in Intermediate Mass Nuclei

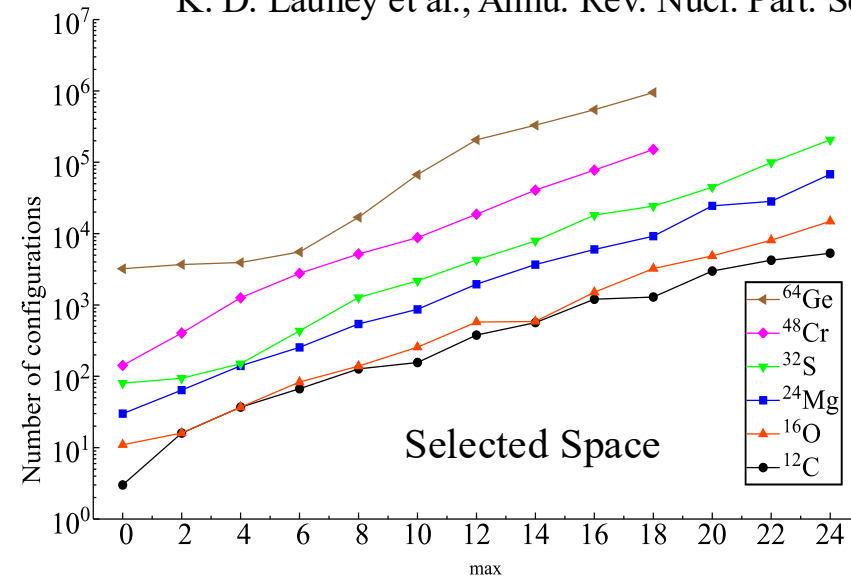


No effective charge

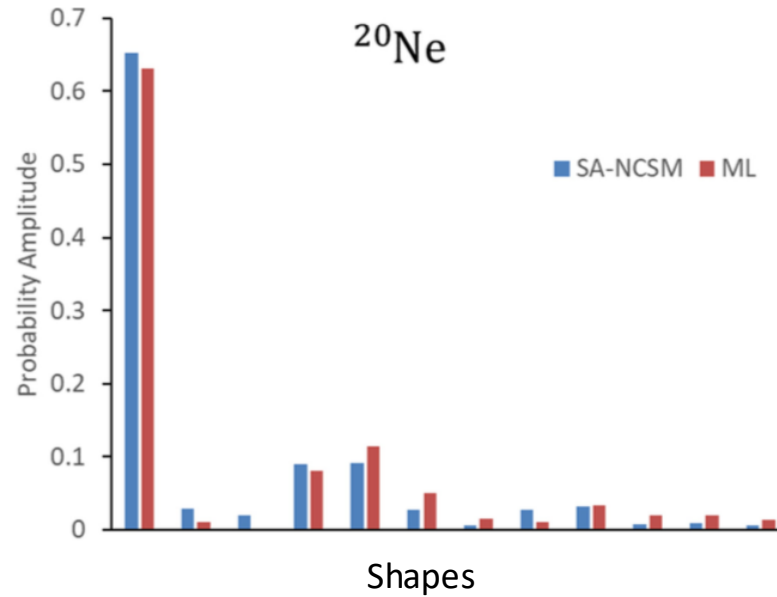
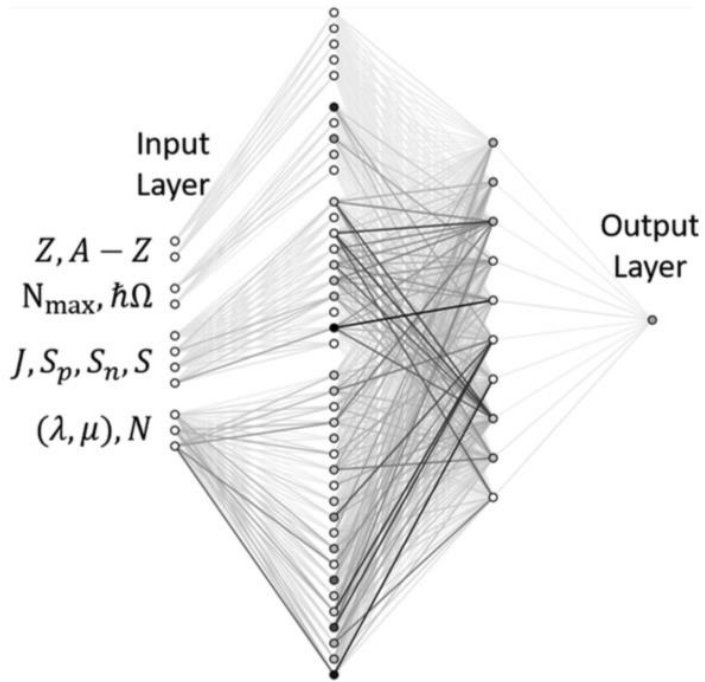


Ruotsalainen *et al.*, PRC **99**, 051301(R) (2019)

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

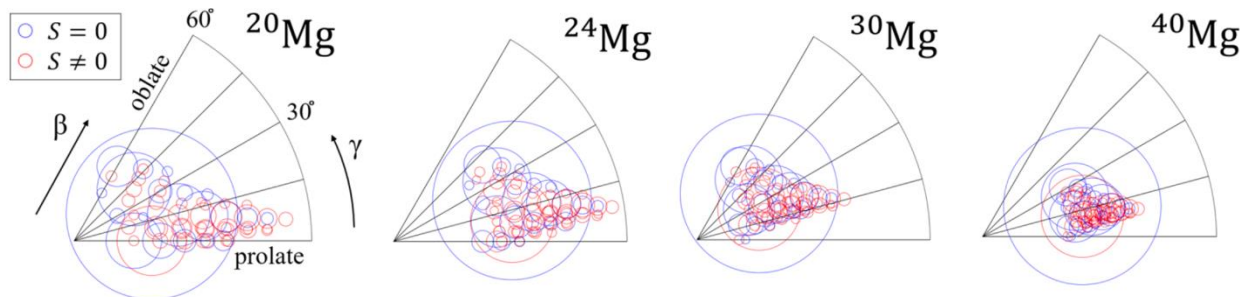


# Ubiquitous Patter – Ideal for Machine Learning

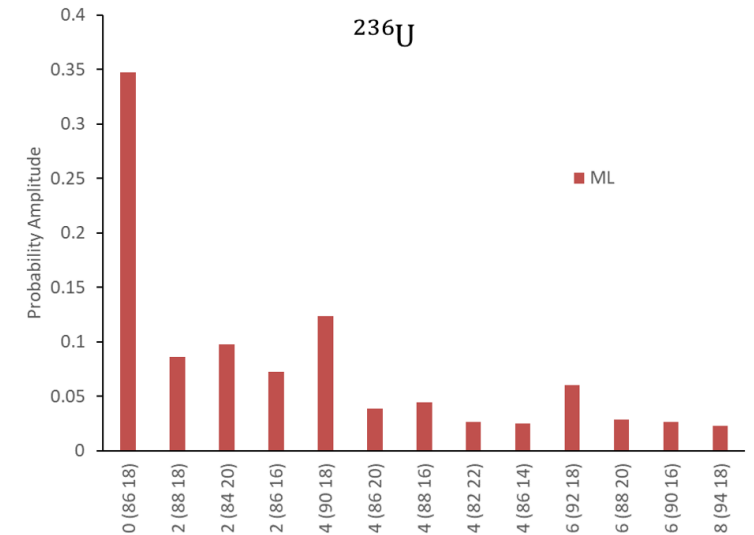


*O. M. Molchanov et al. PRC 105, 034306 (2022)*

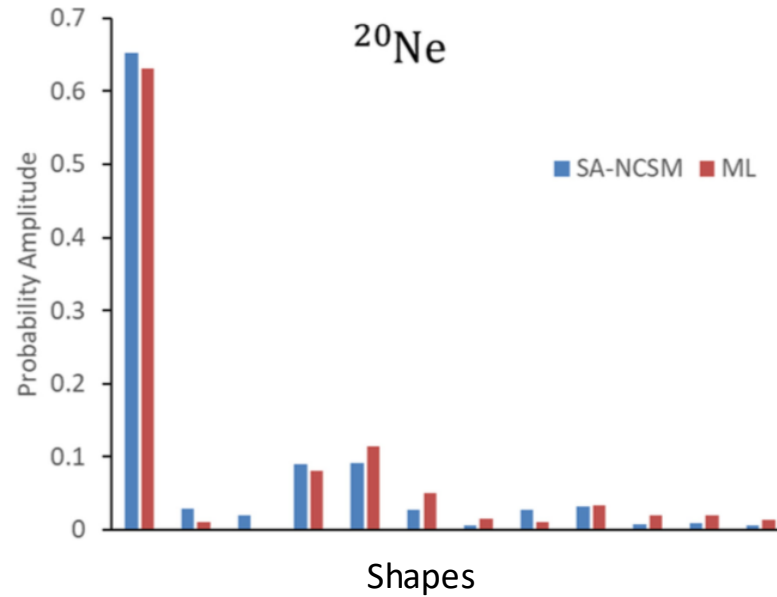
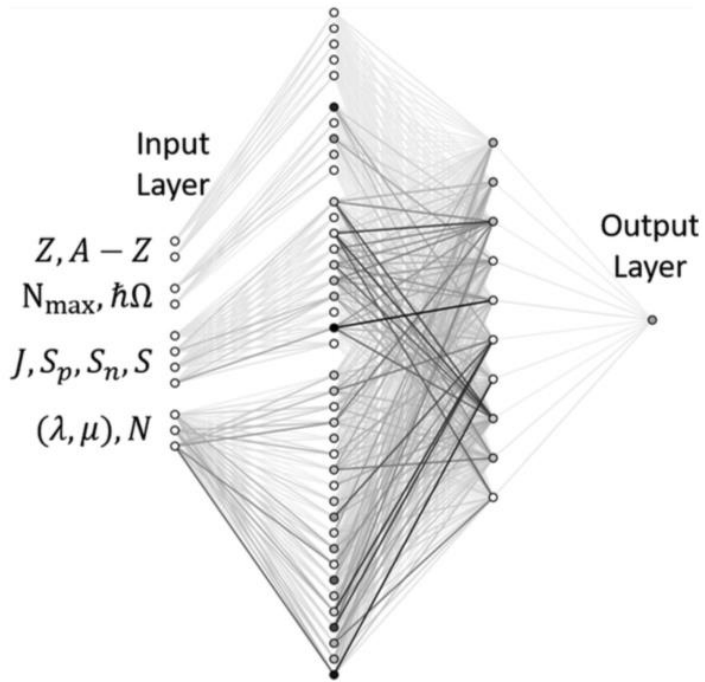
Mg isotopes



- Trained on  $^4\text{He}$ - $^{16}\text{O}$  (s- and p-shell,  $J=0$ ) wave functions.
- NNLOopt, with different  $\hbar\Omega$ , and  $N_{\max}$  values.
- **Goal:** predict important SU(3) subspace.

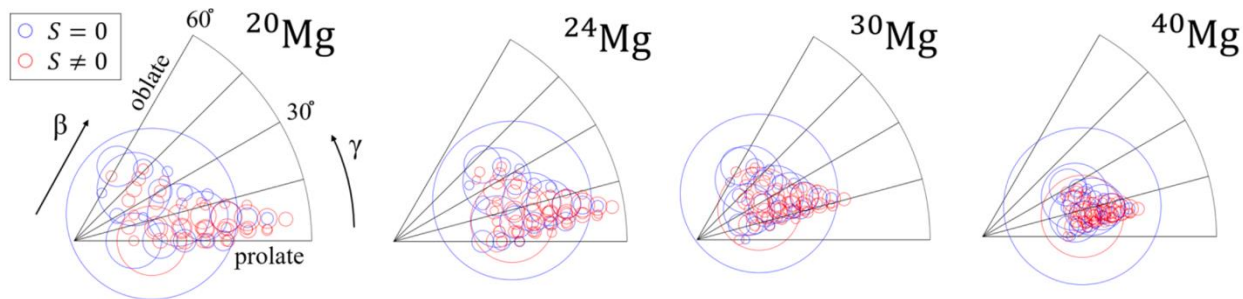


# Ubiquitous Patter – Ideal for Machine Learning



*O. M. Molchanov et al. PRC 105, 034306 (2022)*

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- Trained on  $^4\text{He}$ - $^{16}\text{O}$  (s- and p-shell,  $J=0$ ) wave functions.
- NNLOopt, with different  $\hbar\Omega$ , and  $N_{\max}$  values.
- **Goal:** predict important SU(3) subspace.

**Next step:** Use the network to help designing model space for challenging nuclei. Amplitudes will then be determined using SA-NCSM

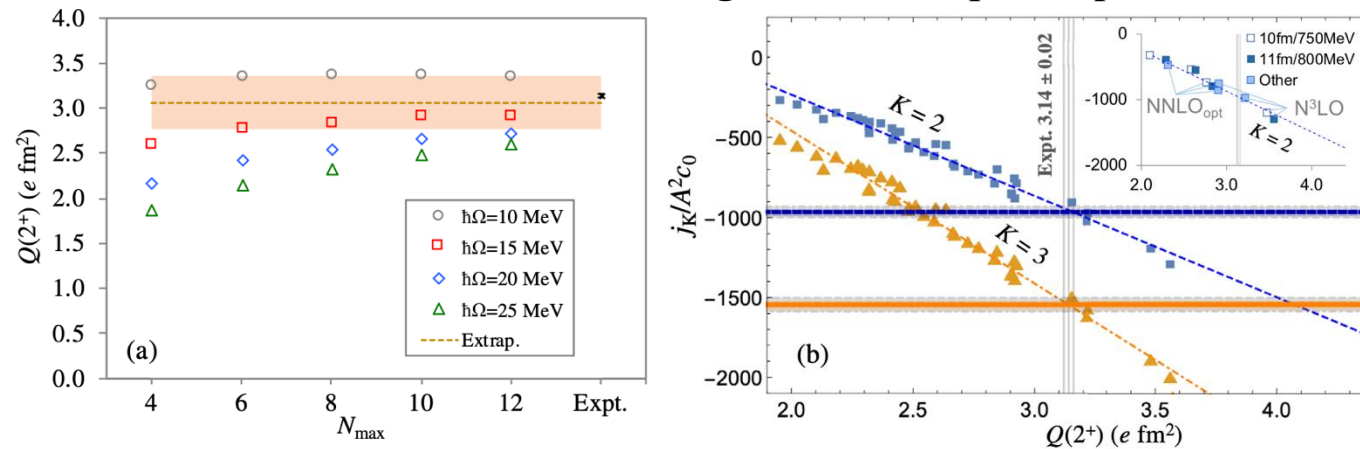
*N. C. Thompson, in preparation*

# Impact of Clustering on the $^8\text{Li}$ $\beta$ Decay and Recoil Form Factors

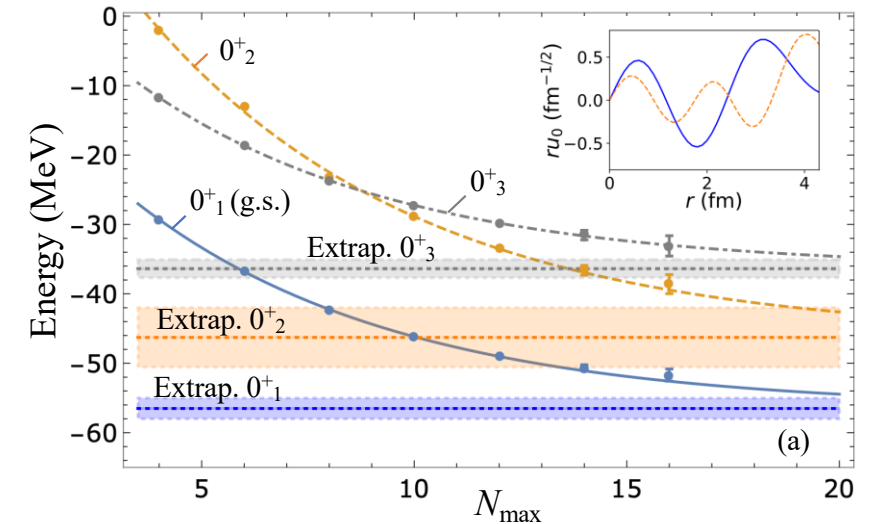
*Sargsyan et al., PRL 128, 202503 (2022)*

- SA-NCSM calculations for  $^8\text{Li} \rightarrow ^8\text{Be}$   $\beta$  decay in ultralarge, symmetry-adapted spaces.
- Chiral EFT interactions (NNLOopt, NNLOsat, N3LO) and JISP16.
- Computed recoil-order form factors  $j_2, j_3, d, b$

## Identified correlations with $^8\text{Li}$ ground-state quadrupole moment $Q$



## Intruder states



- Reduces the systematic uncertainty from recoil-order terms on searches for tensor currents by more than 50%

- Subsequent studies:

*Berkey et al., "Improved Limit on Tensor Currents in the Weak Interaction from  $^8\text{Li}$   $\beta$  Decay, PRL 2022*

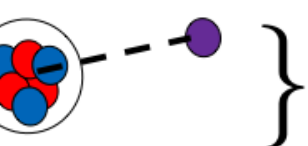
*Longfellow et al., "Improved Tensor Current Limit from  $^8\text{B}$   $\beta$  Decay Including New Recoil-Order Calculations, PRL 2024*

# Ab Initio Reactions: Symmetry-adapted Resonating Group Method (SA-RGM)

- $u_c(r)$  describes the relative motion between the two clusters.
- Asymptotic of  $u_c(r)$  gives cross section for specific channel.
- Requires internal wave functions and NN interaction.
- Microscopic: full antisymmetrization + cluster correlations.
- Can be generalized to any number of clusters.

$$c = \{A \ I_T; a \ I_p; n\ell j; J\}$$

$$|\Psi\rangle = \sum_c \int dr \frac{g_c(r)}{r} r^2 \mathcal{A} \left\{ \left( \text{cluster} \right) - \left( \text{particle} \right) \right\}$$





$$|\Phi\rangle = \sum_i c_i \left( \text{cluster} \right)$$



Main difficulty is to calculate:

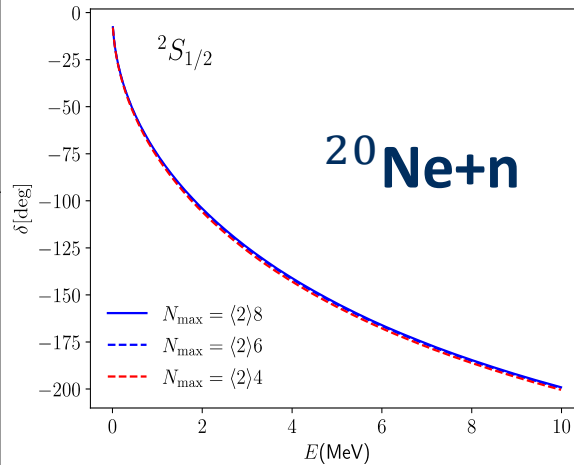
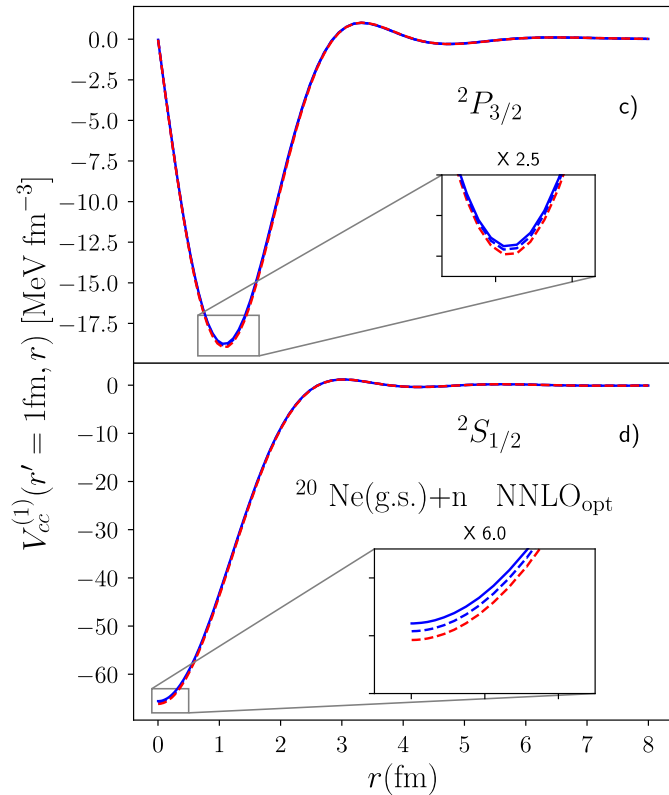
$$\mathcal{A} \left\{ \left( \text{cluster} \right)_{c'}^{\vec{r}'} \right\} \hat{H} \mathcal{A} \left\{ \left( \text{cluster} \right)_c^{\vec{r}} \right\}$$



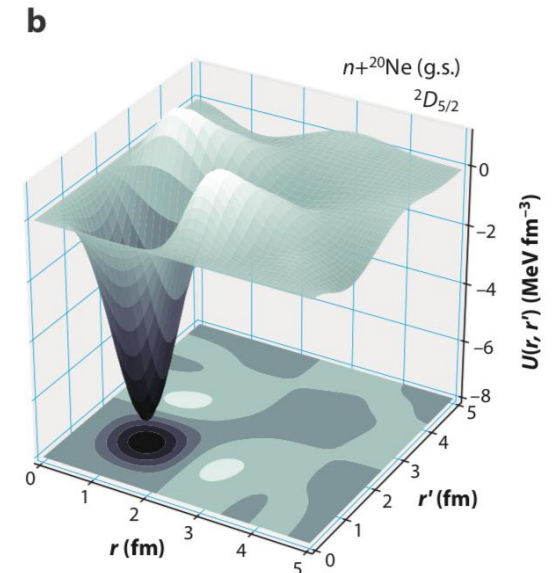
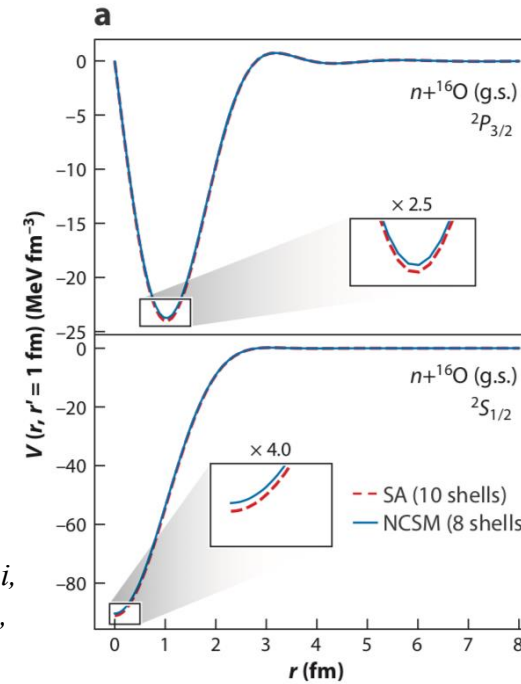
$$(T_c - (E - E_c))u_c(r) + \sum_{c'=1}^{N_c} \int dr' V_{cc'}(r', r) u_{c'}(r') = 0$$

# Symmetry-adapted Resonating Group Method (SA-RGM)

- *Ab initio* single-nucleon projectile reactions
- First results studied the influence of selected model space on non-local potentials.



Mercenne, Launey, Dytrych, Escher, Quaglioni, Sargsyan, Draayer *Comput. Phys. Comm.* **280**, 108476 (2022)



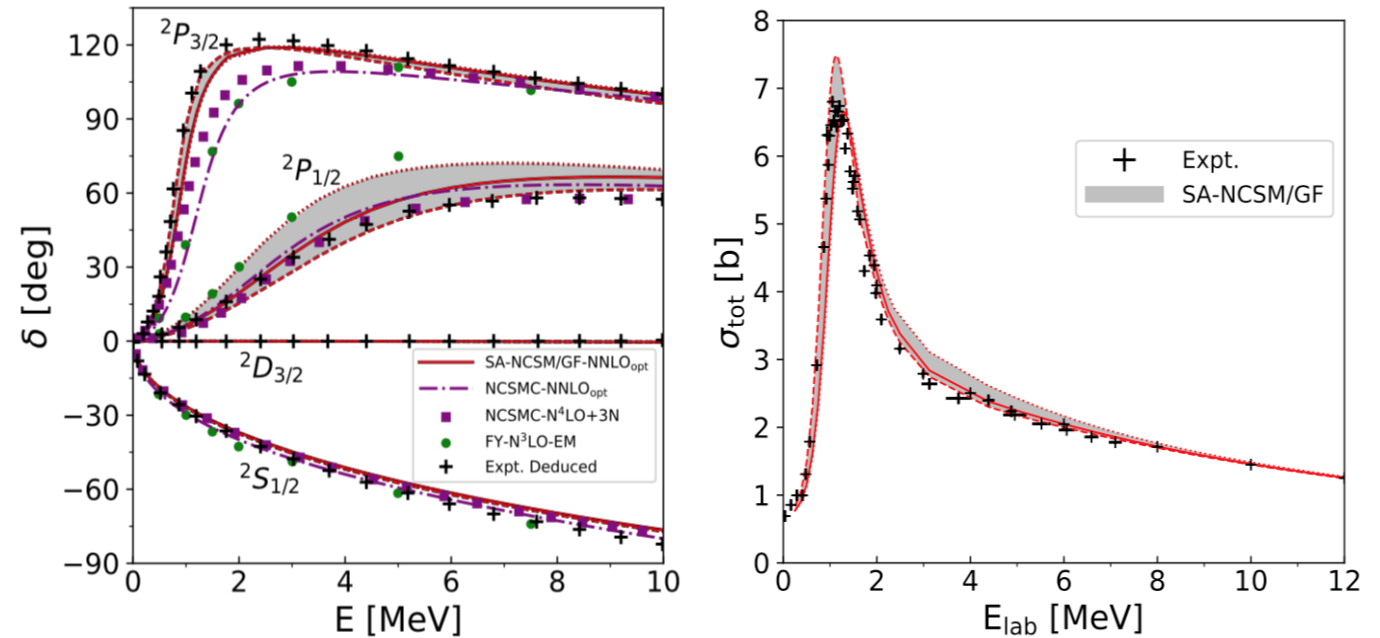
Launey, Mercenne, Dytrych *Ann. Rev. Nucl. Part. Sci.* **71**, 253 (2021)

# Ab Initio Optical Potential

- Novel approach: SA-NCSM-GF. Evaluate the single-particle time-ordered Green's function from SA-NCSM wave functions.
- Provides effective nucleon-nucleus potentials that contain the information about all near reaction channels.

$$G(\mathbf{r}, \mathbf{r}'; E) = \lim_{\epsilon \rightarrow 0} \langle \Psi_0^A | [a_{\mathbf{r}} + a_{\mathbf{r}'}^\dagger] \frac{1}{E - (\hat{H} - E_0^A - i\epsilon)(\hat{N} - A)} [a_{\mathbf{r}} + a_{\mathbf{r}'}^\dagger] | \Psi_0^A \rangle$$

$$V(\mathbf{r}, \mathbf{r}'; E) = (E - T_{\text{rel}}(\mathbf{r}))\delta(\mathbf{r} - \mathbf{r}') - G^{-1}(\mathbf{r}, \mathbf{r}'; E)$$

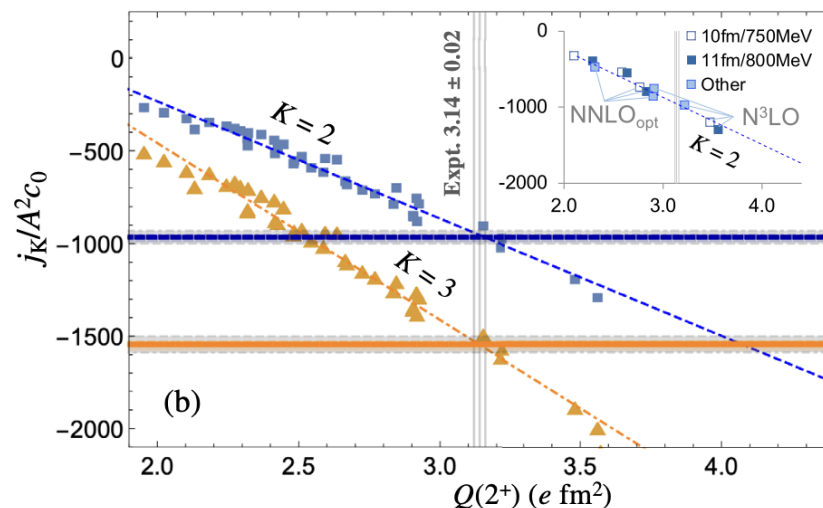
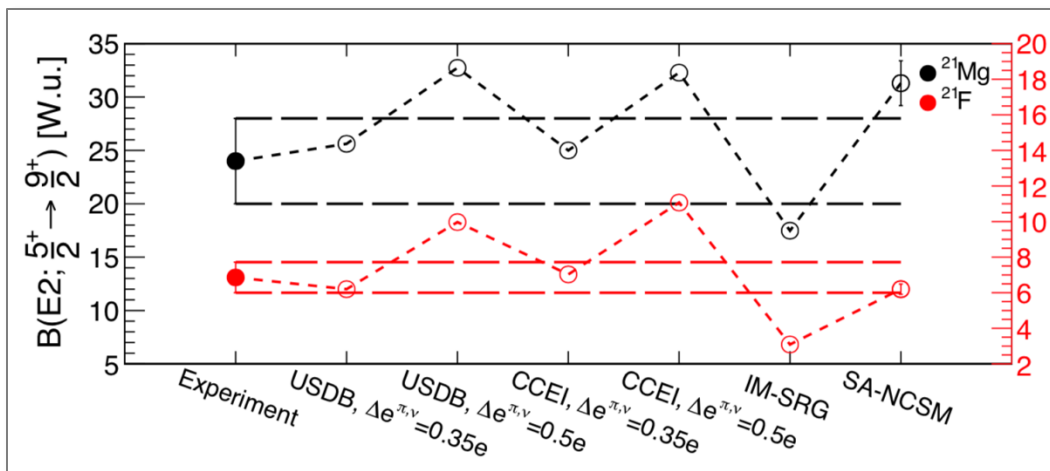
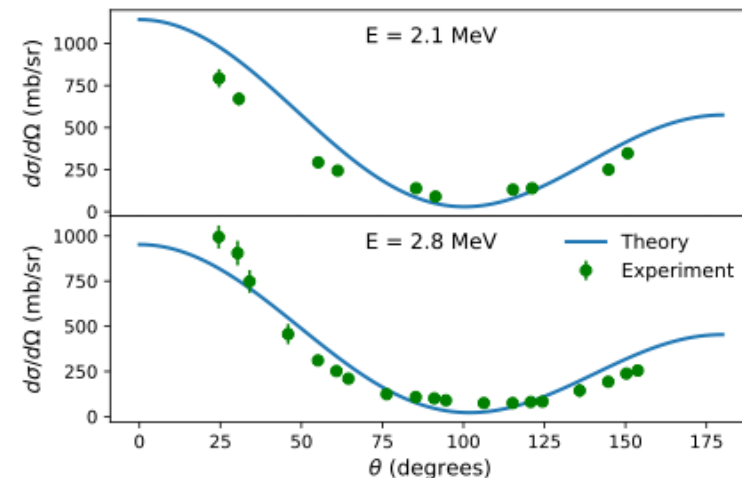


*M. Burrows et al., PRC 109 014616 (2024)*

# Summary

$$B_1 + B_2 + B_3 + \dots$$

- Long range correlations are important for capturing collectivity.
- The use of symmetry-adapted basis allows the good reproduction of  $B(E2)$  values without the use of effective charges.
- SA-NCSM calculations in  $8\text{Li}$  and  $8\text{Be}$  found a correlation between  $Q2$  and recoil terms, leading to unprecedented constraints on the ab initio estimation of these recoil terms.
- Prediction of intruder states in  $8\text{Be}$ .
- SA-RGM calculations of neutron elastic scattering up to  $40\text{Ca}$ . Next developments will include charge exchange reactions.



# Acknowledgements

## At LSU:

- Kristina Launey
- Jose Pablo Linares Fernandez
- Darin Mumma
- Kevin Becker
- Yu Kunita
- Noah Thompson

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- Grigor Sargsyan (MSU)
- Matt Burrows
- Jutta Escher (LLNL)
- Tomas Dytrych (Nuclear Physics Institute of the Czech Academy of Sciences)
- Daniel Langr (Czech Technical University in Prague)

TABLE I. Training and validation data sets. A data set for given  $N_{\max}$  and  $\hbar\Omega$  includes tens through hundreds to thousands of configurations. Complete model spaces are denoted by  $N_{\max}$ , whereas selected model spaces are denoted as  $\langle N \rangle N_{\max}$  (e.g., for  $^{20}\text{Ne}$ ,  $\langle 2 \rangle 10$  indicates the use of all basis states up to  $N = 2$  and selected basis states for  $N = 4, 6, 8$ , and  $10$ ). The number of inputs used in the training data set shows the total number of  $N(\lambda\mu)S_p S_n S$  configurations in all model spaces listed for each nucleus. Also shown is the dimension (number of all basis states) of the largest  $J = 0$  model space listed for each nucleus.

| Nucleus          | $N_{\max}$                                                             | $\hbar\Omega$ (MeV) | Number of inputs | Dimension             |
|------------------|------------------------------------------------------------------------|---------------------|------------------|-----------------------|
| Training data    |                                                                        |                     |                  |                       |
| $^4\text{He}$    | 6,8,10,12,14                                                           | 22                  | 696              | $5.80 \times 10^4$    |
| $^8\text{He}$    | 6                                                                      | 15                  | 218              | $3.18 \times 10^4$    |
| $^6\text{Li}$    | 8                                                                      | 15                  | 208              | $6.78 \times 10^4$    |
| $^8\text{Be}$    | 8,10,12, $\langle 8 \rangle$ 14                                        | 15                  | 3417             | $1.53 \times 10^8$    |
| $^{10}\text{C}$  | 8                                                                      | 15                  | 1037             | $4.44 \times 10^6$    |
| $^{12}\text{C}$  | 6, $\langle 6 \rangle$ 10, $\langle 6 \rangle$ 12                      | 15                  | 3211             | $1.90 \times 10^9$    |
| $^{14}\text{C}$  | 6, $\langle 6 \rangle$ 10                                              | 15                  | 2113             | $4.03 \times 10^8$    |
| $^{16}\text{O}$  | 8                                                                      | 20,25               | 4726             | $3.01 \times 10^7$    |
| Validation data  |                                                                        |                     |                  |                       |
| $^{20}\text{Ne}$ | $\langle 4 \rangle 6$ , $\langle 4 \rangle 8$ , $\langle 2 \rangle 10$ | 15                  |                  | $7.18 \times 10^{10}$ |
| $^{28}\text{Mg}$ | $\langle 0 \rangle 6$                                                  | 15                  |                  | $9.77 \times 10^9$    |
| $^{24}\text{Si}$ | 4                                                                      | 20                  |                  | $2.59 \times 10^7$    |