Ab initio structure input for scattering observables

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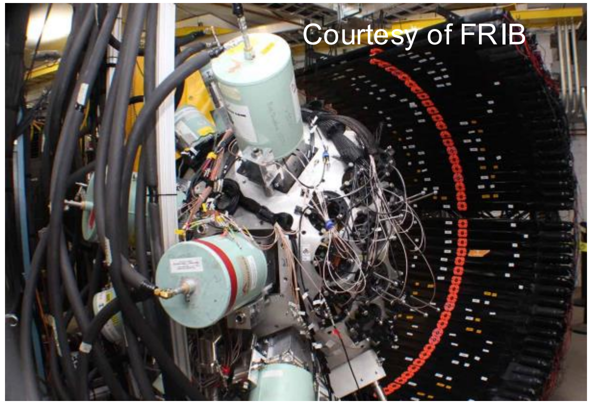
The era of rare isotope beams

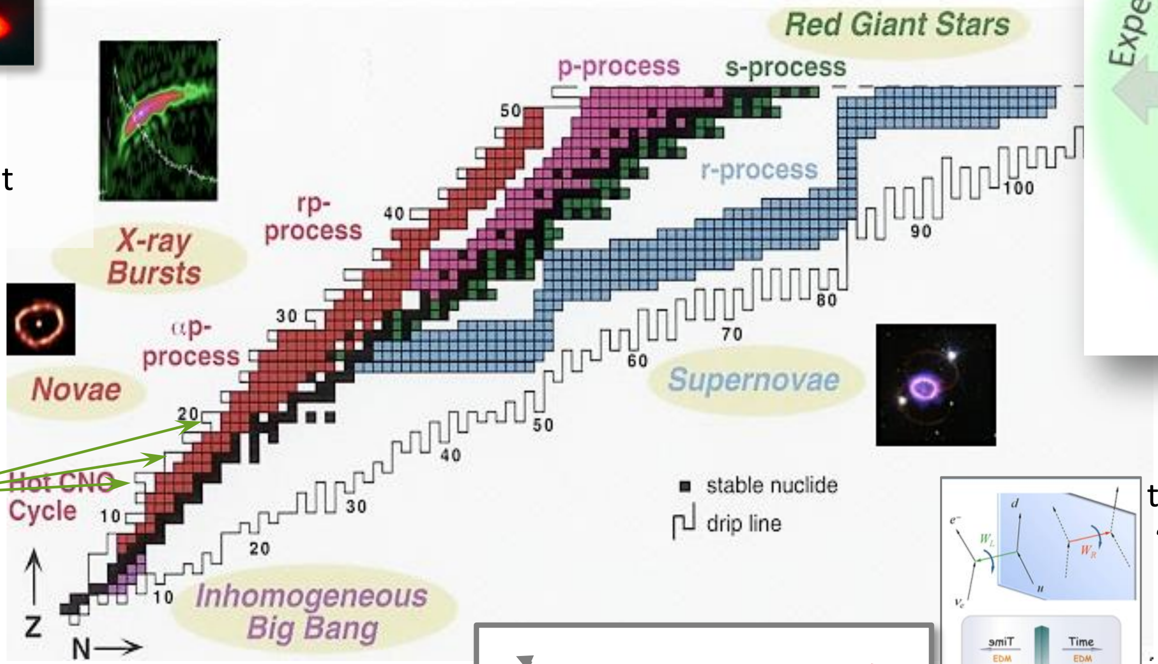


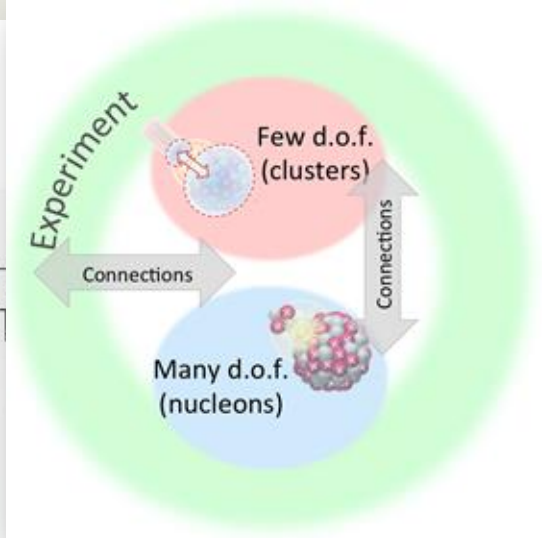
X-ray burst nucleosynthesis

Alpha widths

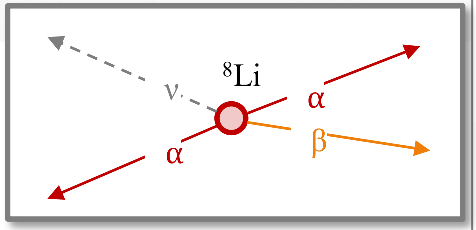
Reaction rates at low energies

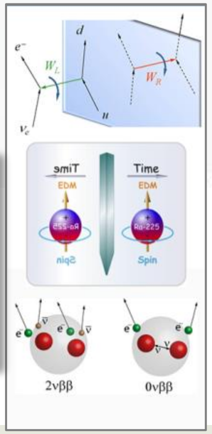
Close proximity of the drip lines





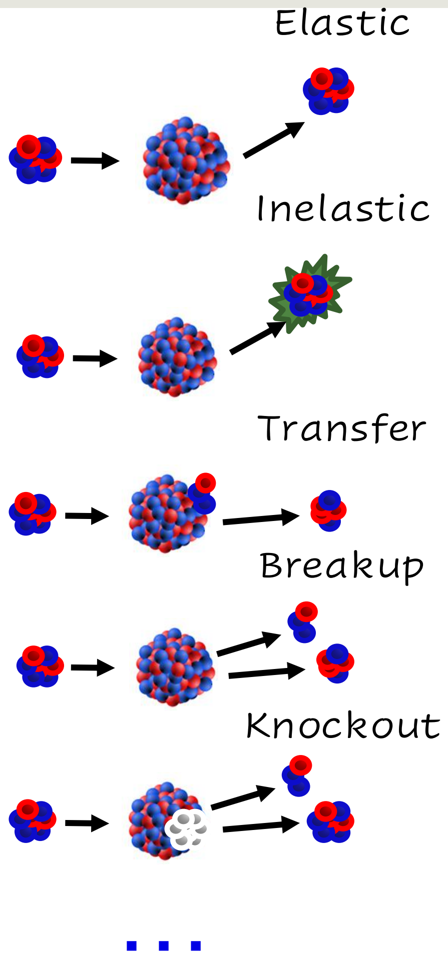
FRIB Theory Alliance topical program (2018) “From bound states to the continuum“ (C. Johnson et al.)





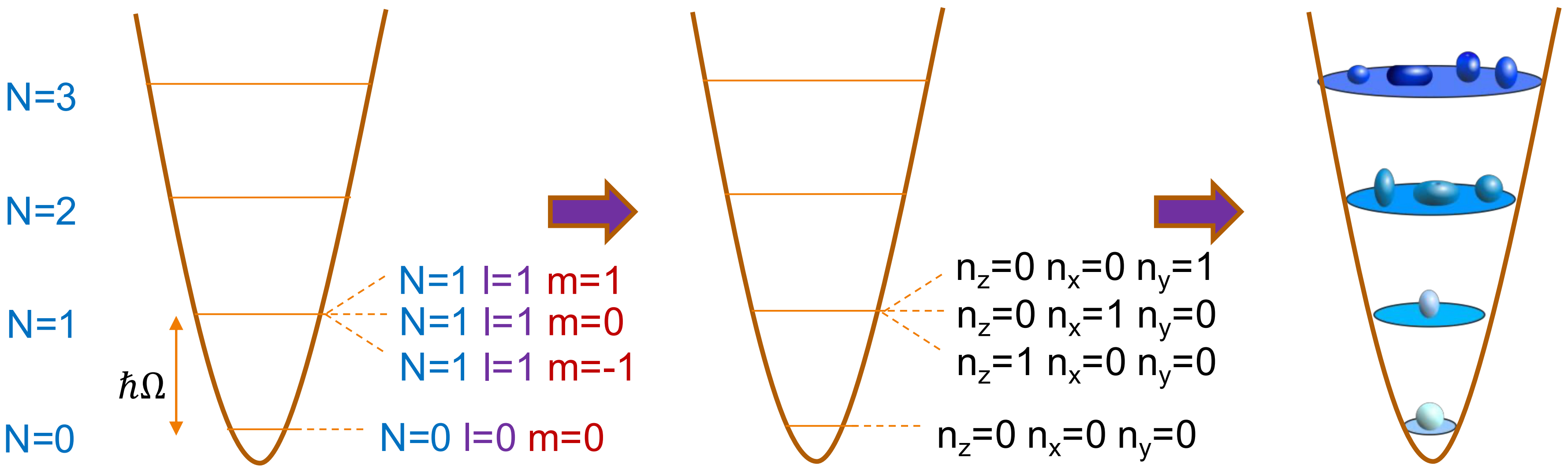
Fundamental symmetries

Reaction models need structure input



- Experiments need reaction models to interpret measured data
- Various reaction models require structure input (cluster wavefunctions, excitation spectrum, electromagnetic transitions, etc.)
- *Ab initio* structure methods can provide a reliable input especially for the tricky problems

Symmetry-adapted No-core Shell Model



Spherical harmonic oscillator (HO): basis states given by {N l m}

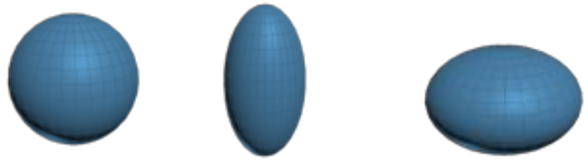
$N = n_z + n_x + n_y$

Basis states given by $\{n_x\ n_y\ n_z\}$

$\lambda = n_z - n_x$, $\mu = n_x - n_y$ (single particle)

Basis states given by $(\lambda\ \mu)$ quantum numbers

$$a^+_{Nlm} \equiv a^+_{(N\ 0)lm}$$

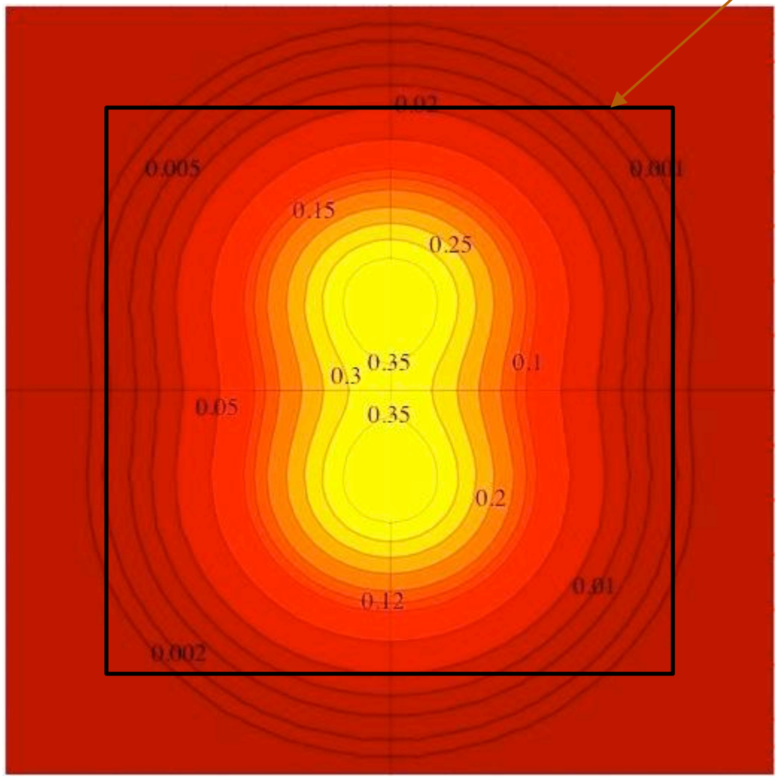


Sphere (0 0) Prolate (λ 0) Oblate (0 μ)

Symmetry-adapted basis helps reduce the models space size

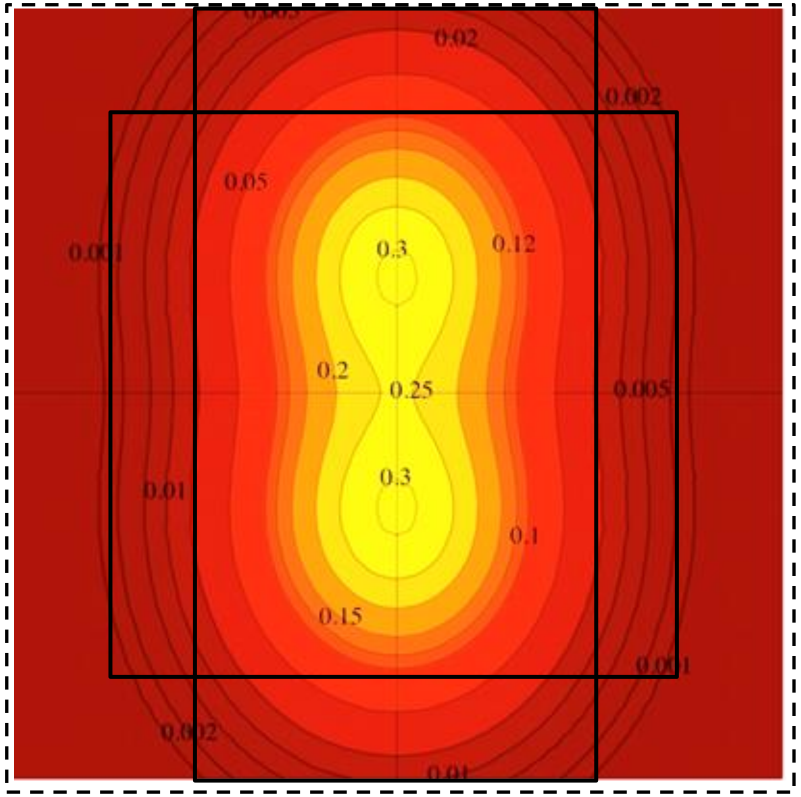
Conventional Shell Model

N_{max}



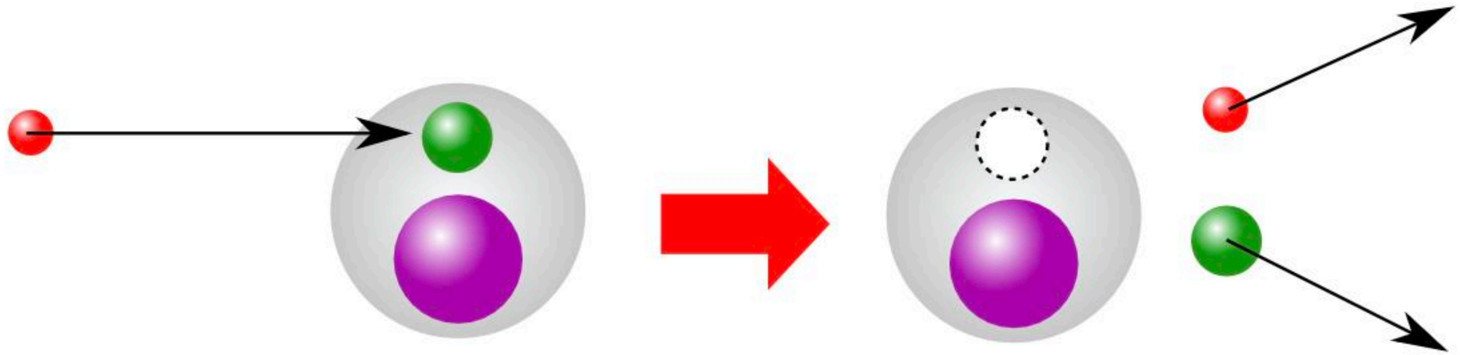
Nucleus in model space

***Ab initio* Symmetry-adapted No-core Shell Model (SA-NCSM)**



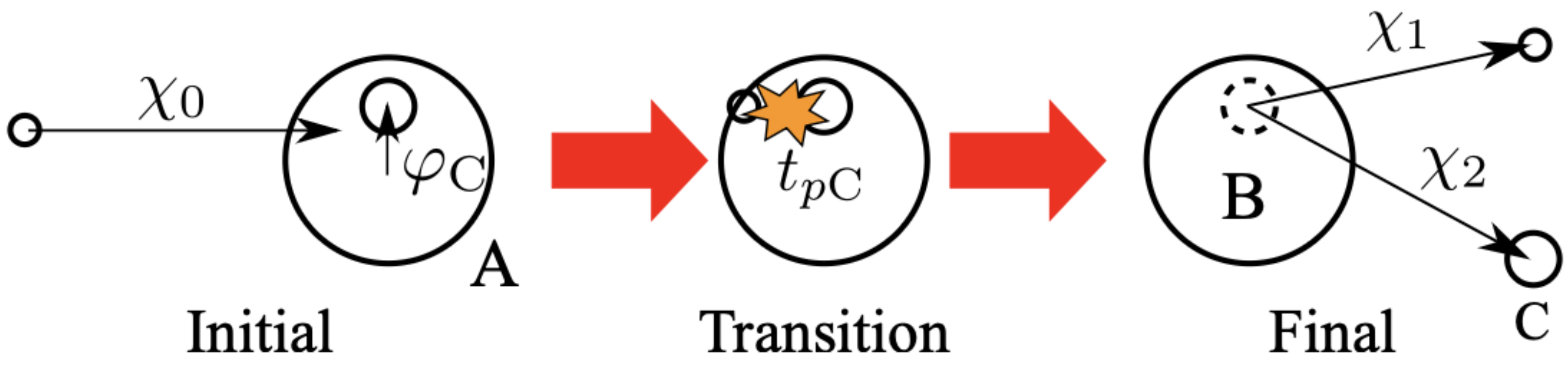
SU(3) and symplectic symmetry

Knockout reaction



- Typically >100 MeV/u incident energy
- Modeled as one-step direct reaction
- Probes mainly the ground state particle clustering in the target

Reaction model: Distorted Wave Impulse Approximation



Transition matrix

$$T = \langle \chi_1 \chi_2 \Phi_C \Phi_B \,|\, t_{pC} \,|\, \chi_0 \Phi_A \rangle = \langle \chi_1 \chi_2 \,|\, t_{pC} \,|\, \chi_0 \varphi_C \rangle$$

χ_i: Distorted waves under optical potentials

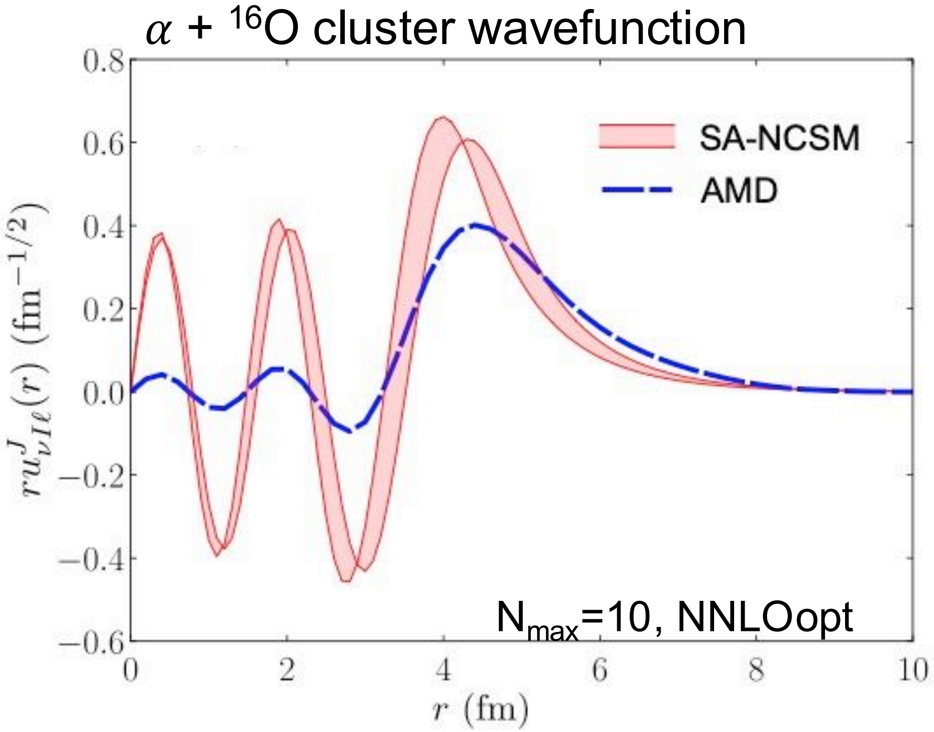
t_{pC}: p-C effective interaction in free space

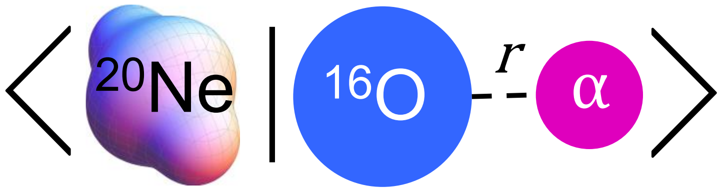
φ_C: Cluster wave function $\langle [\Phi_C \otimes \Phi_B] \,|\, \Phi_A \rangle$

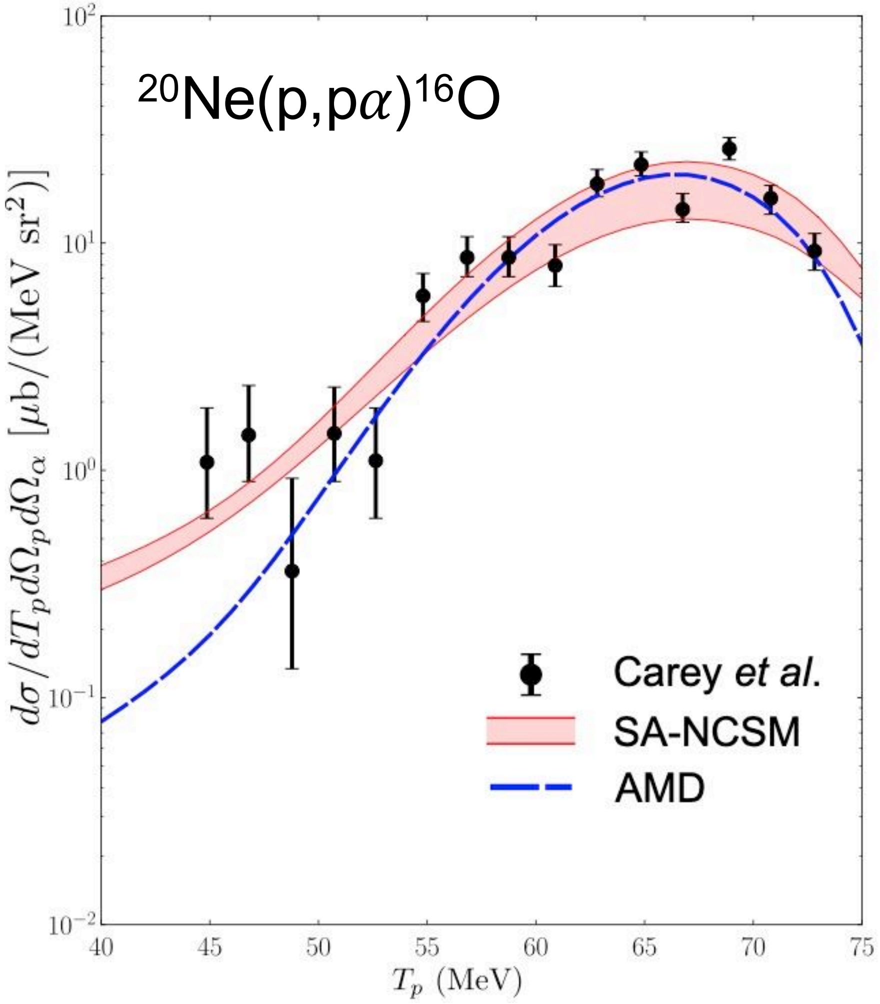
Knockout cross section (Triple differential cross section) $\frac{d^3\sigma}{dE_1 d\Omega_1 d\Omega_2} \propto |T|^2$

Slide credit: Kazuki Yoshida

Ab initio informed knockout elucidates α clustering in ^{20}Ne





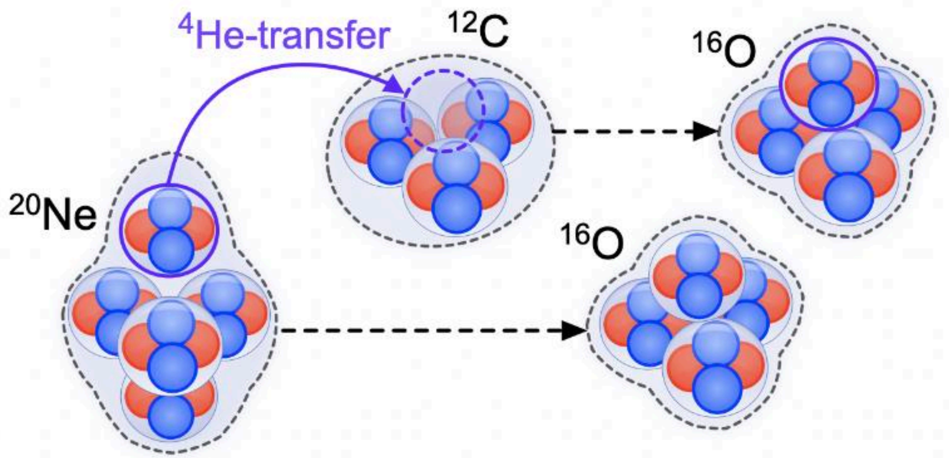


In collaboration with K. Yoshida (Osaka U.) and K. Ogata (Kyushu U.)

Sargsyan et al., PLB **866** 139563 (2025)

Quantifying α clustering in the ground states of ^{16}O and ^{20}Ne

$^{12}C(^{20}Ne,^{16}O)^{16}O$ α-transfer reaction



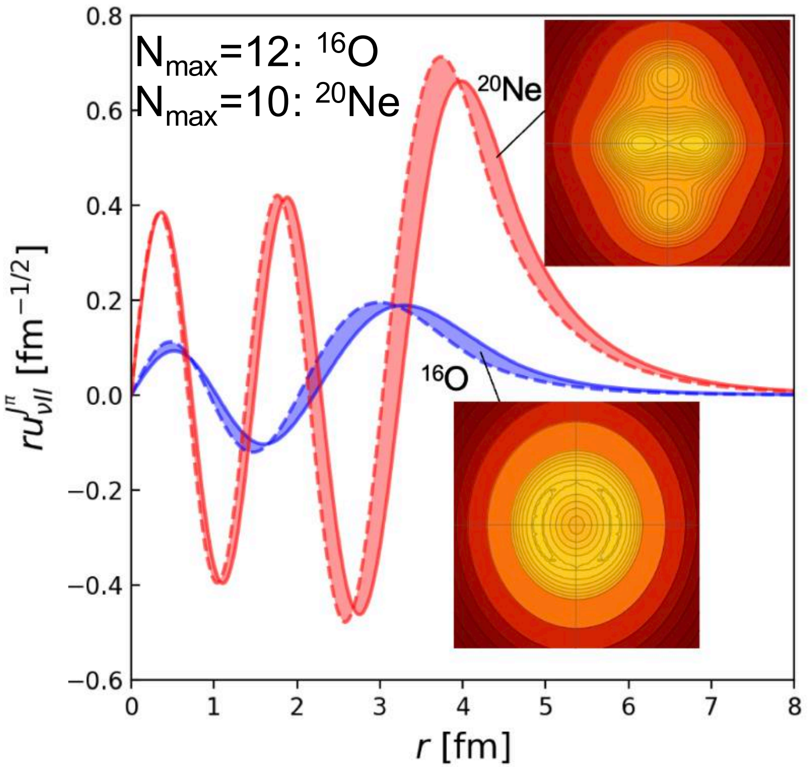
Experiment done at Texas A&M Cyclotron Institute

In collaboration with E. Harris and G. Rogachev (TAMU)

- Reaction model: distorted wave Born approximation (DWBA)
- Extracted product of ANCs $$C_{16O}C_{20Ne} \propto \left(\frac{d\sigma}{d\Omega}\right)_{transfer} / \left(\frac{d\sigma}{d\Omega}\right)_{elastic}$$

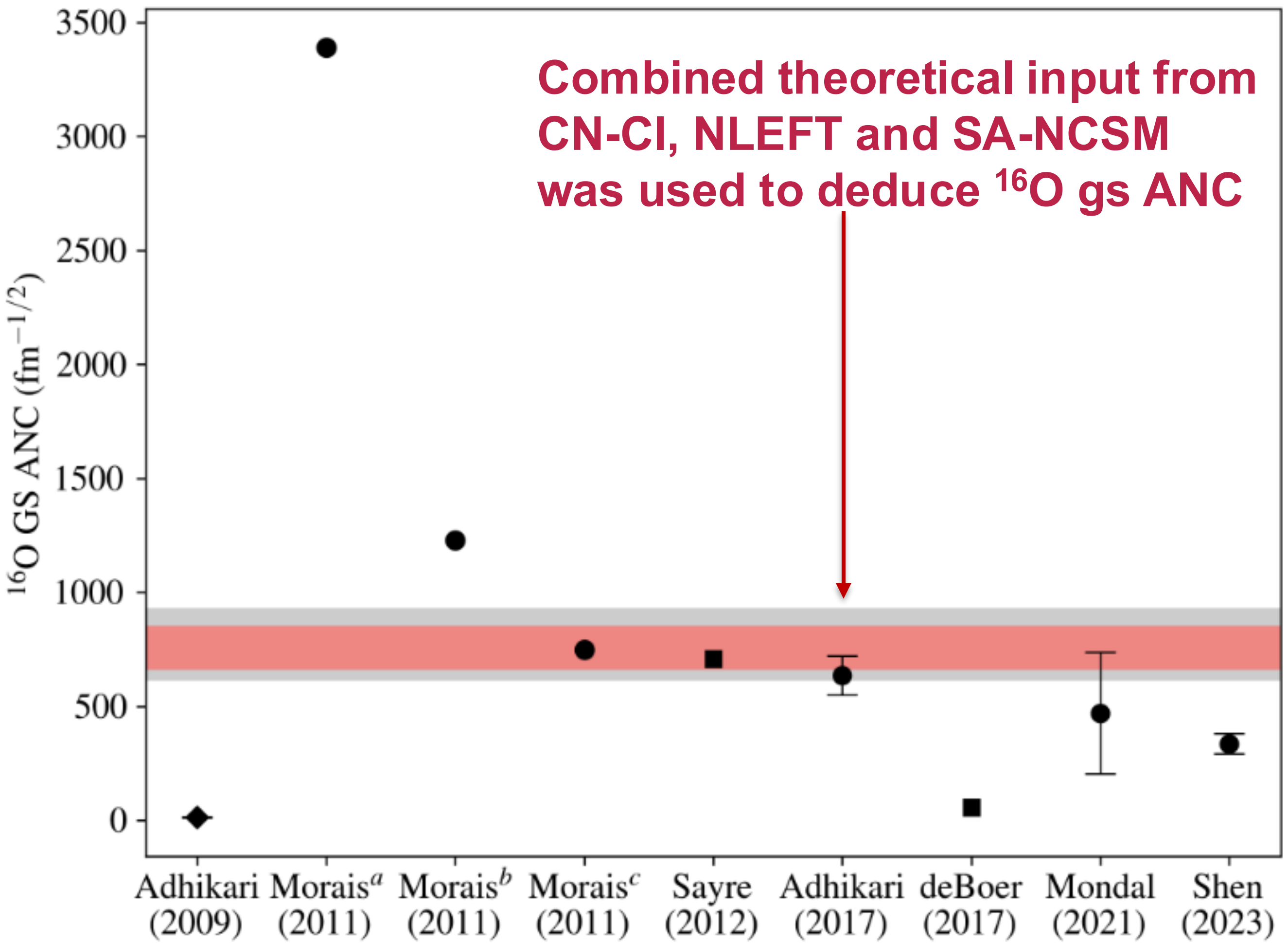
E. Harris et al., (incl. Sargsyan) arXiv:2507.17059

α asymptotic normalization coefficient for ^{16}O



α + ^{12}C and α + ^{16}O cluster wavefunctions from SA-NCSM using $NNLO_{opt}$

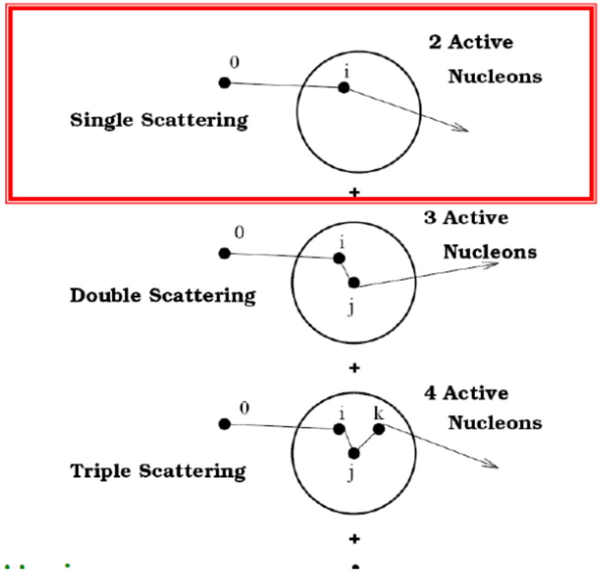
$$C_{16O} = (C_{16O}C_{20Ne})_{expt} / (C_{20Ne})_{theory}$$



E. Harris et al., (incl. Sargsyan) arXiv:2507.17059

Ab initio optical potentials for E > 65 MeV

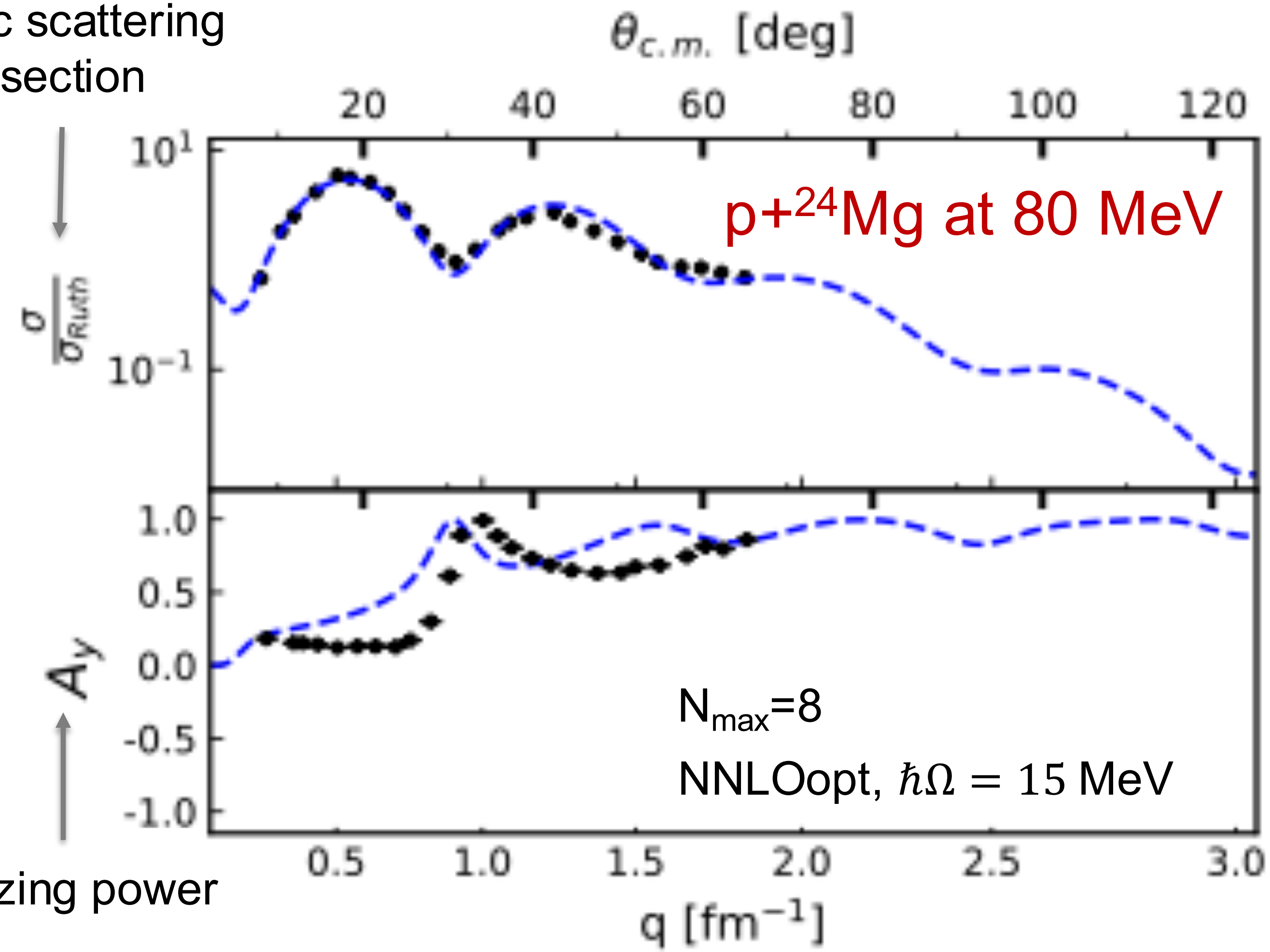
Multiple scattering expansion



In collaboration with C. Elster (OU)

See next talk!

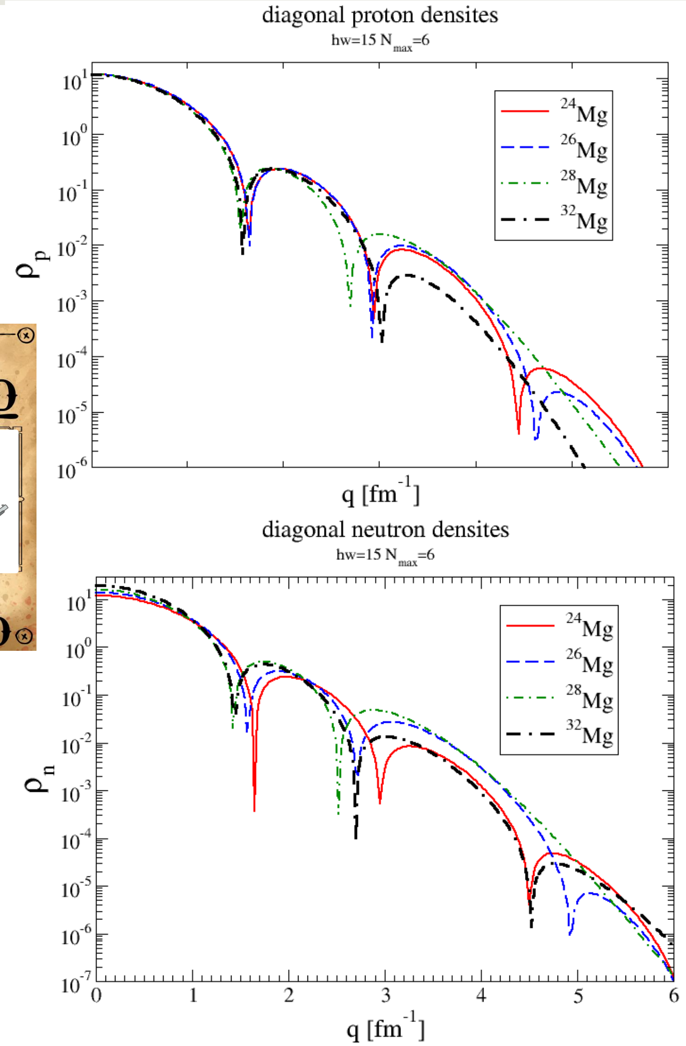
Elastic scattering cross section

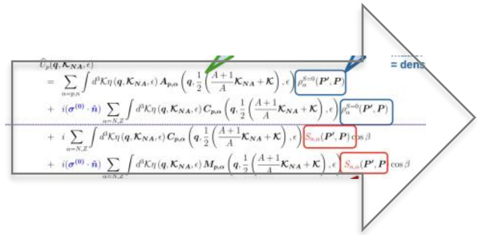


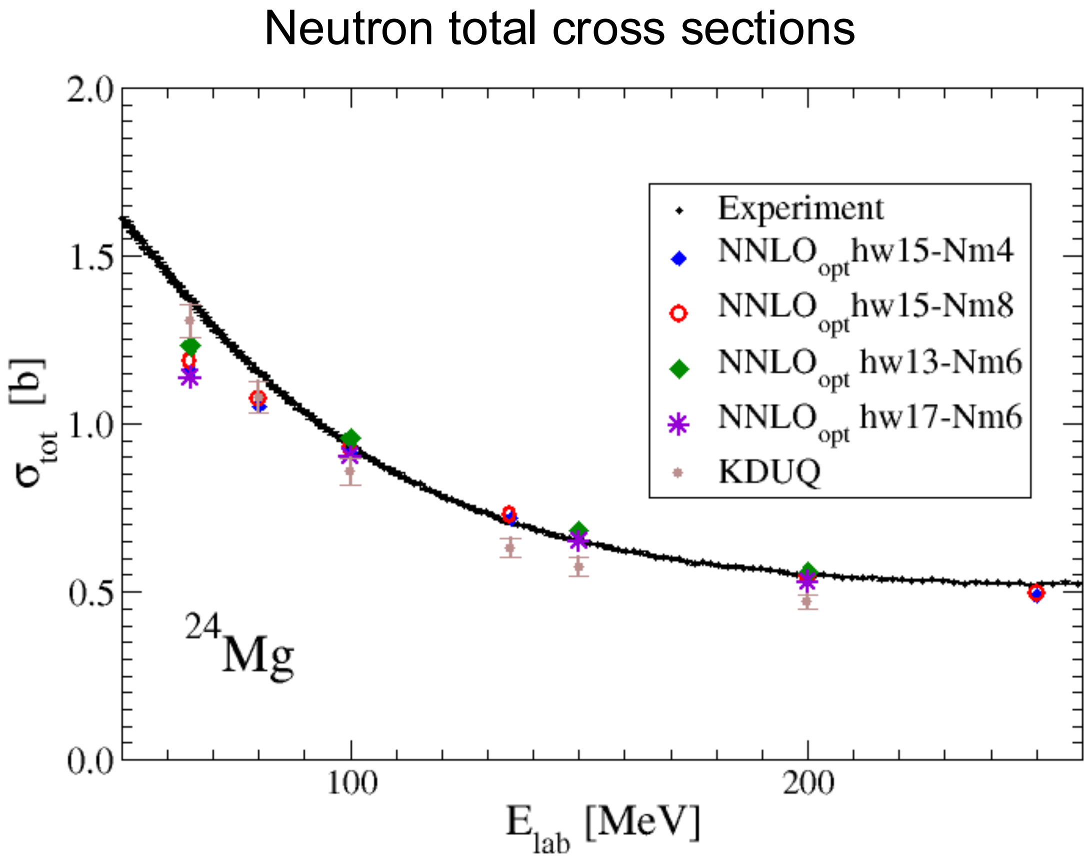
Analyzing power

Structure input from SA-NCSM

One-body densities of Mg isotopes from stable to N=20 lol





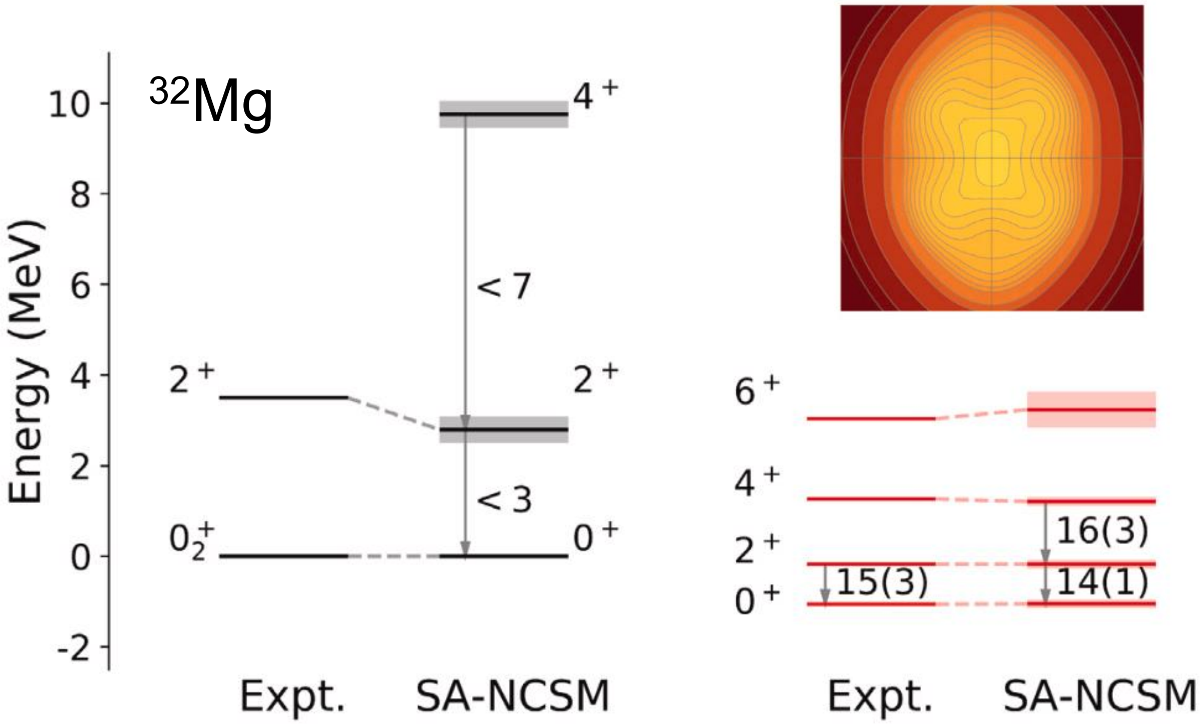


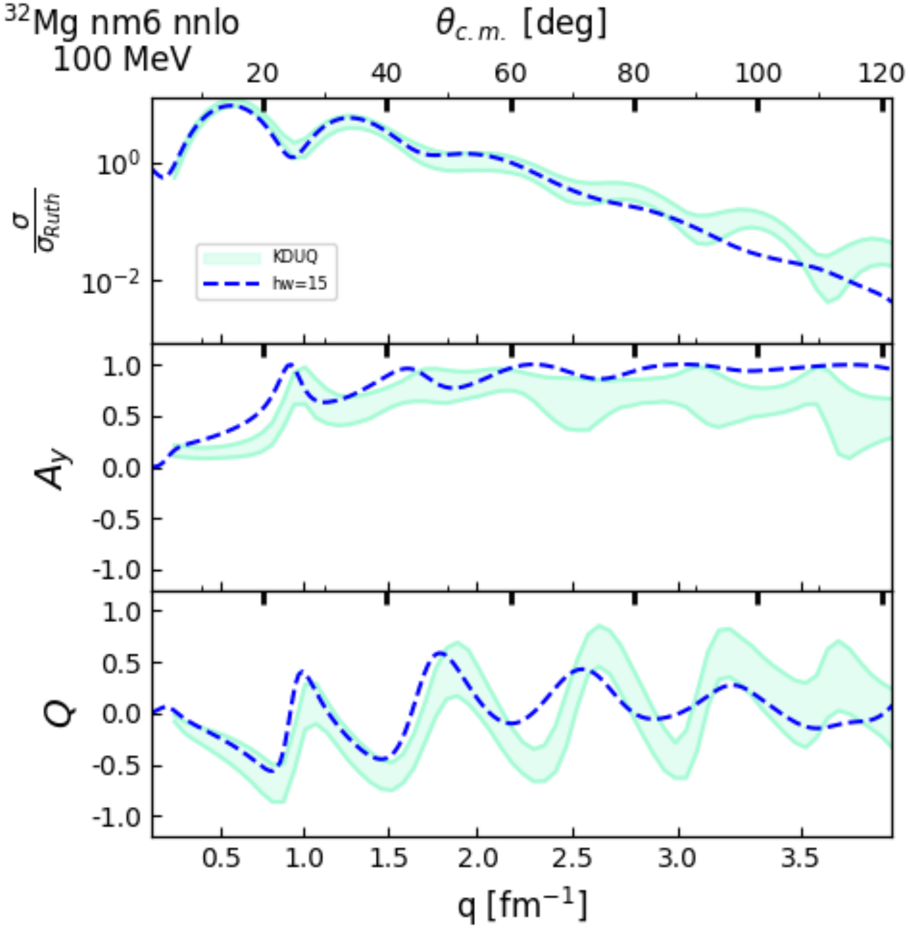
KDUQ: Pruitt et al., Phys. Rev. C **107**, 014602 (2023)

Sargsyan, Fuentealba-Bustamente, Beyer, Elster, in preparation

SA-NCSM structure input of ^{32}Mg for reactions calculations

7 PAC-approved FRIB experiments studying
N=20 island of inversion nuclei

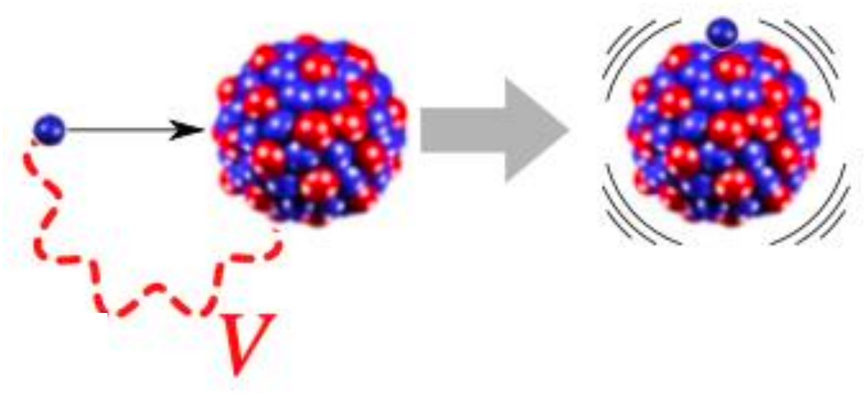




Launey, Sargsyan, et al., *Prog. Part. Nucl. Phys.* **148,** 104233 (2026)

Sargsyan, Fuentealba-Bustamente, Beyer, Elster, in preparation

Embedding nuclear structure information within OP



Feshbach formalism

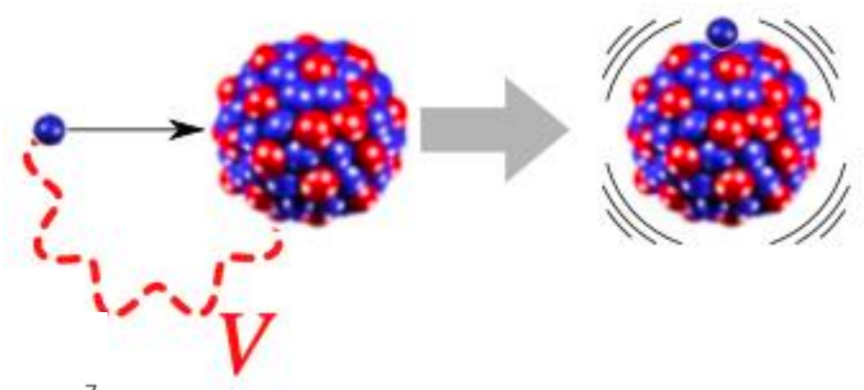
$$V(\boldsymbol{r},\boldsymbol{r}',E) = U_0(\boldsymbol{r}) + V_{PO}(\boldsymbol{r},\boldsymbol{r}',E-E_i)$$
$$= U_0(\boldsymbol{r}) + \sum_i U_{0i}(\boldsymbol{r}) G_i(\boldsymbol{r},\boldsymbol{r}',E-E_i) U_{0i}(\boldsymbol{r}')$$

Static, energy-independent potential

Polarization potential: Requires input from nuclear structure

Can be applied to any mass range if nuclear structure calculations are available

Embedding nuclear structure information within OP



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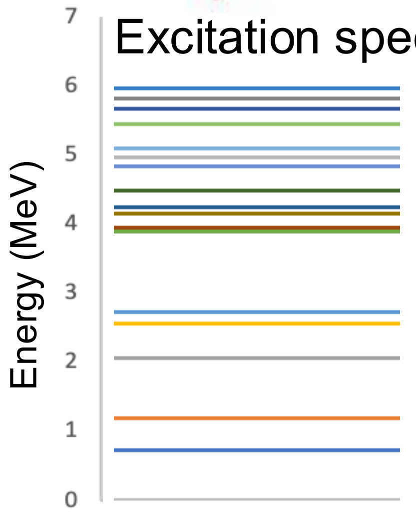
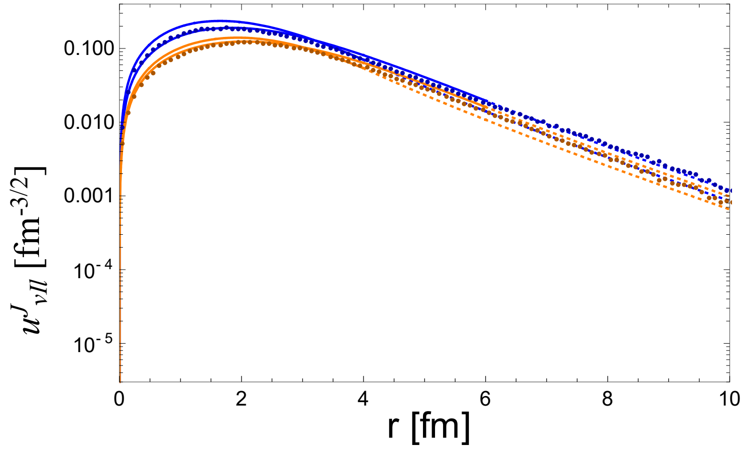
Polarization potential: Requires input from nuclear structure

Excitation spectrum



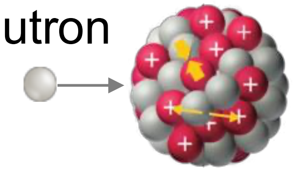
Single-nucleon overlaps

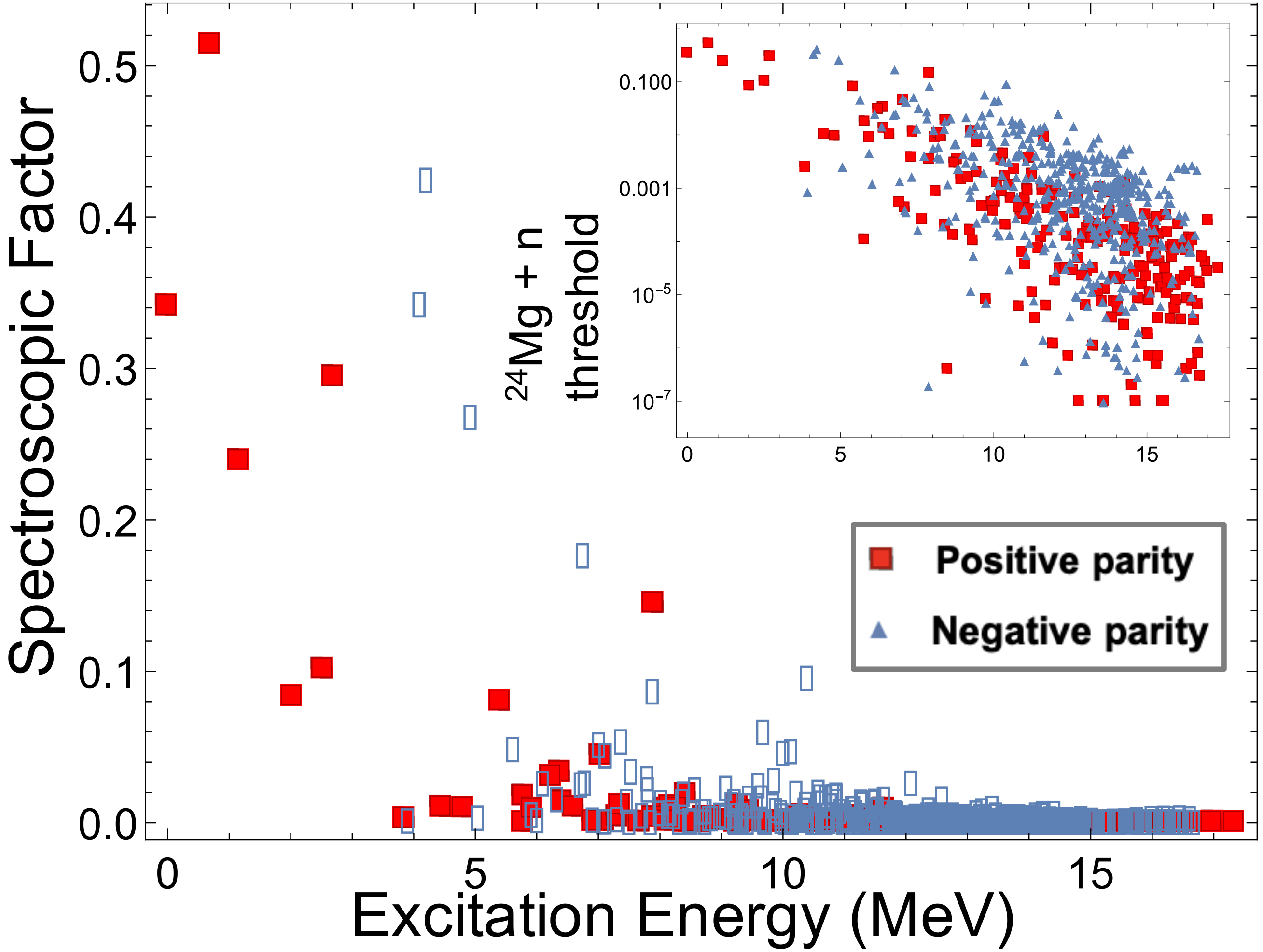


e.g., **shell model, RPA, ab initio models, ...**

Sargsyan, *et al.*, PRC 108, 054303 (2023)

1st ingredient for constructing OP: shell model input





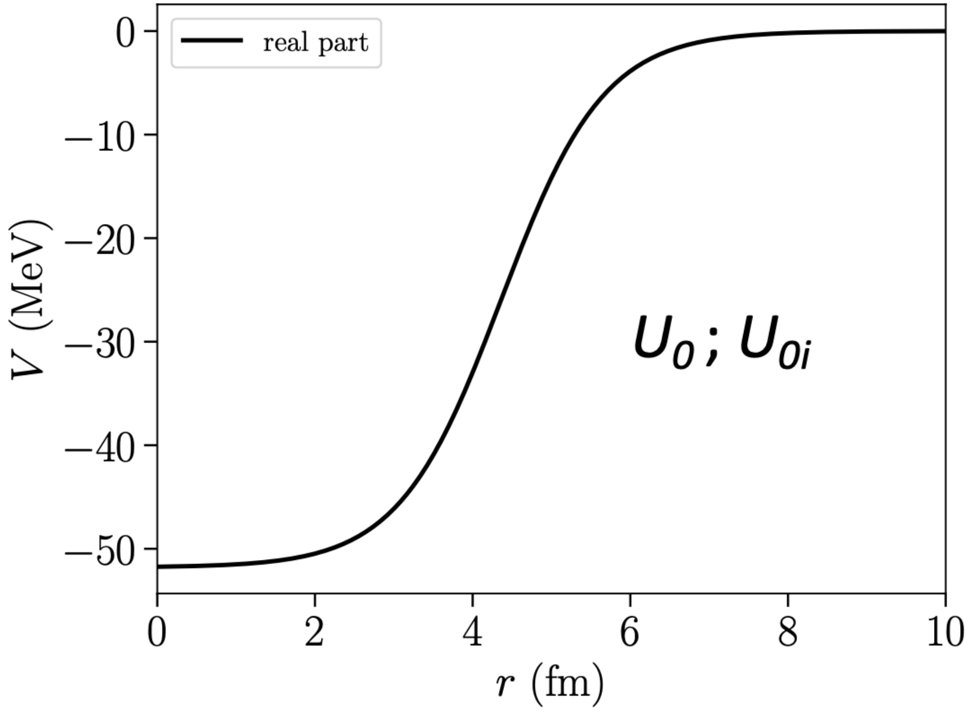
Around 600 intrinsic states

Shell model calculations done using **CoSMo**
PSDPF potential M Bouhelal, *et al.*, Nucl. Phys. A 864 (2011)

Sargsyan, *et al.,* Phys. Rev. C 112, 054606 (2025) [Editors' suggestion]

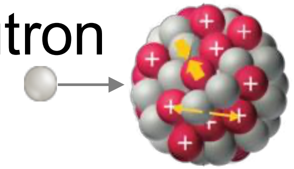
2nd ingredient: static potential and couplings

$$V(\boldsymbol{r},\boldsymbol{r}',E) = U_0(\boldsymbol{r}) + \sum_i U_{0i}(\boldsymbol{r}) G_i(\boldsymbol{r},\boldsymbol{r}',E-E_i) U_{0i}(\boldsymbol{r}')$$

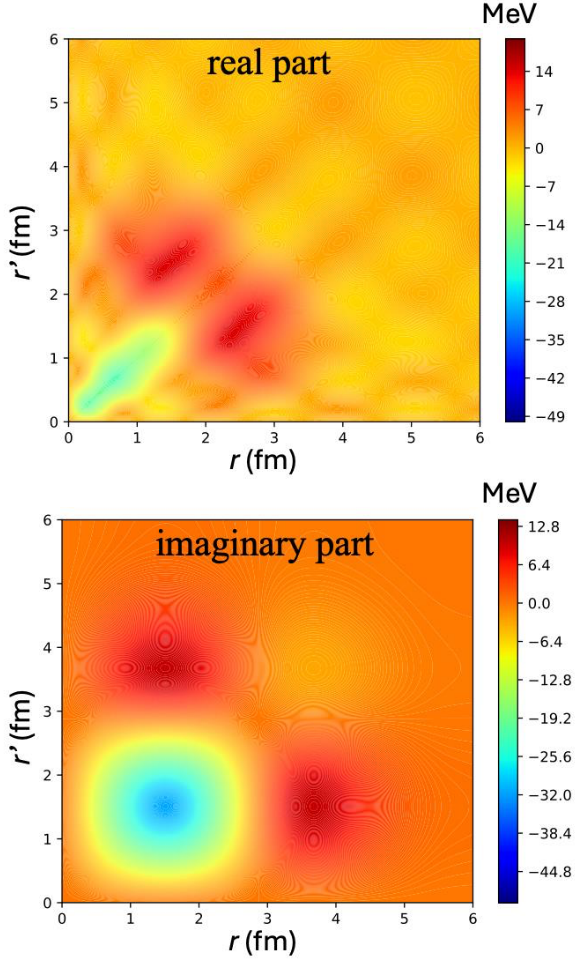


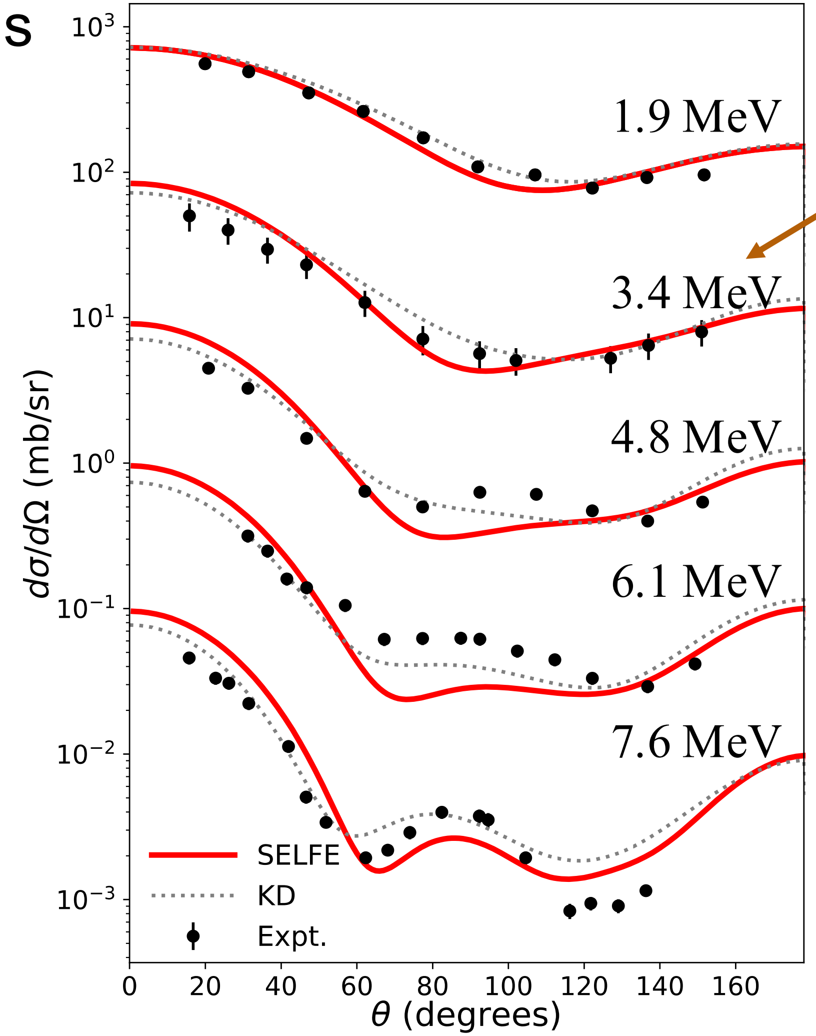
- static potential U_0 : real, local Woods-Saxon adjusted to reproduce binding energy of ^{25}Mg
- couplings U_{0i}: same real Woods-Saxon, but adjusted to each E_i and multiplied by spectroscopic factor *Si* from shell model

Accurate prediction without parameters fitted to experimental scattering data!



Optical potential for 3.4 MeV neutrons



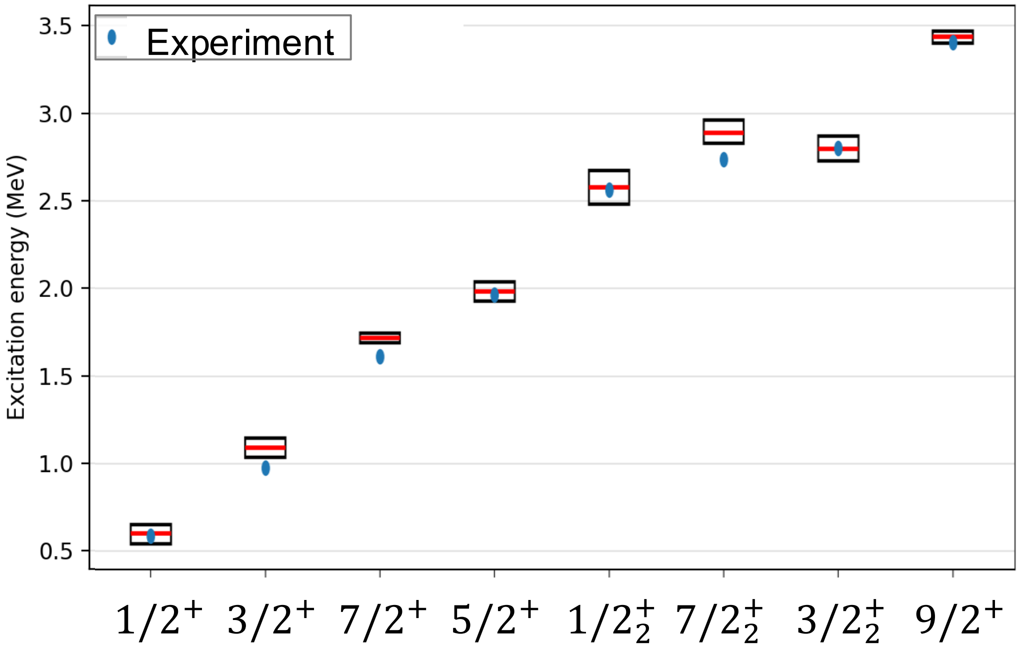


Sargsyan, *et al.*, Phys. Rev. C 112, 054606 (2025)
[Editors' suggestion]

Propagating structure uncertainties to reactions

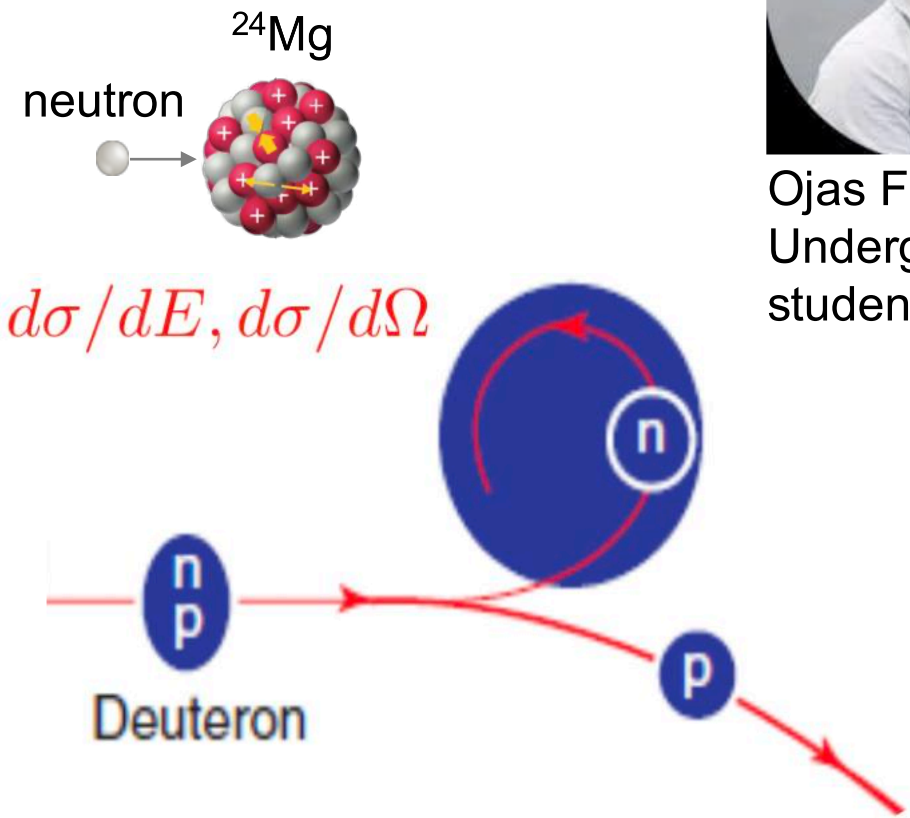
Uncertainty quantified shell model potential (USDBUQ)
O. Gorton, K. Kravvaris, Phys. Rev. C 112, 014302 (2025)

^{25}Mg spectrum



Calculations by O. Fernandes

UQ



Ojas Fernandes, Undergraduate student @MSU

Propagating structure uncertainties to reactions

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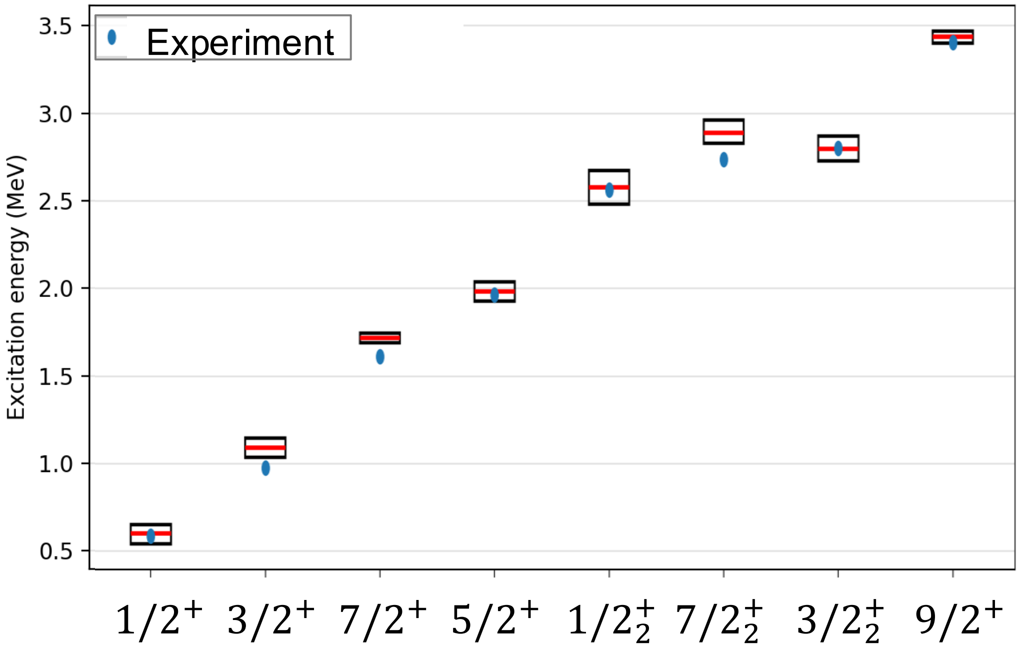

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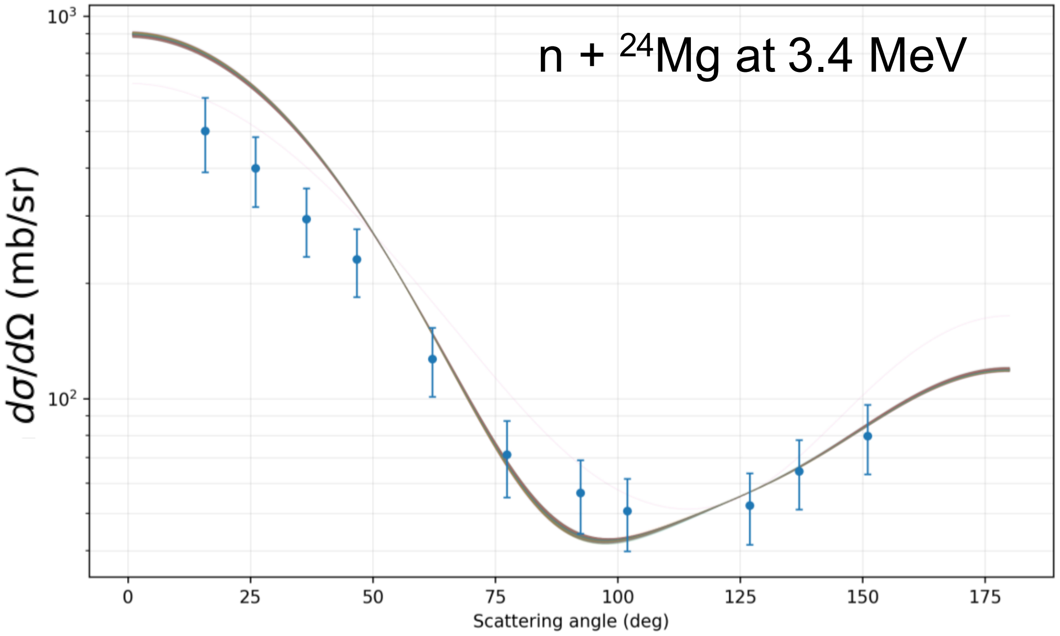
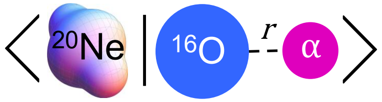
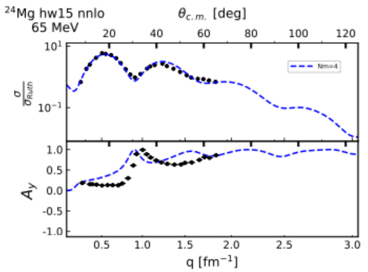


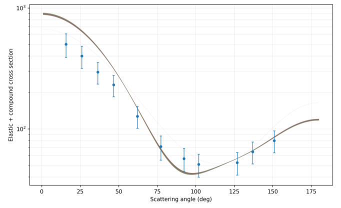
Calculations by O. Fernandes

Summary

- Nuclear reaction models need input from structure 

- Modern *ab initio* models can provide a reliable input with predictive capabilities
- We have used SA-NCSM to provide input to study alpha clustering in ^{16}O and ^{20}Ne via knockout and transfer reactions 

- Multiple scattering approach with SA-NCSM densities provides a good description of Mg scattering data for >65 MeV and predictions where no data exists 

- Our new approach for low-energy scattering uses spectroscopic factors and excitation energies to build an optical potential 
- This approach can propagate structure uncertainties to reaction observables

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UNIVERSIDAD DE SEVILLA

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U.S. DEPARTMENT OF ENERGY

Thank you!

Theory Alliance
FACILITY FOR RARE ISOTOPE BEAMS