PAINT26

# *Ab initio* optical potentials derived from SA-NCSM densities for elastic scattering from Magnesium isotopes

**Charlotte Elster**

Thanks to collaborators:

**G. Sargsyan, J. Fuentealba, K. Beyer**

Supported by

U.S. DEPARTMENT OF ENERGY Office of Science

NERSC National Energy Research Scientific Computing Center

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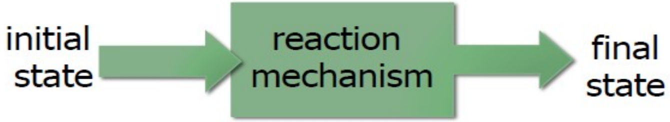
# Exploring Nuclei:
## Specifically Exotic nuclei are usually short lived

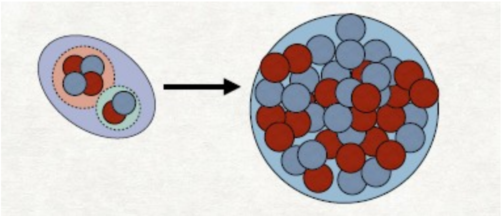
### Thus one can only study them through reactions:

*Have to be studied with reactions in inverse kinematics*

direct reaction:




Many-body
problem

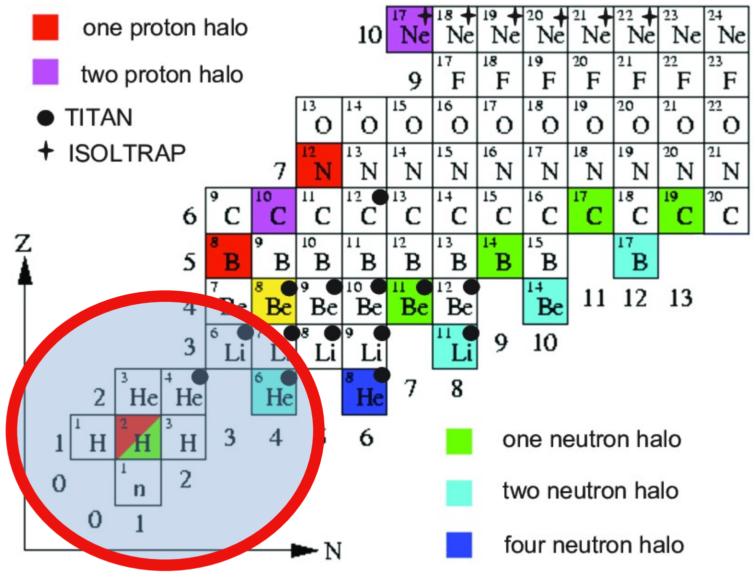


Quantum mechanical scattering problem

*"idealist" approach: Just do it!*

# Not so fast!

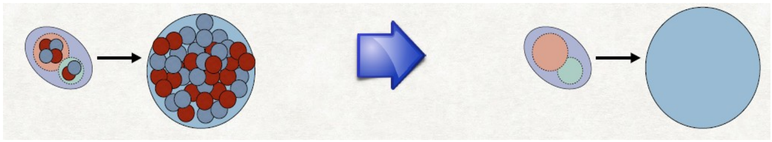
## Chart of light nuclei




"Idealists" current domain

## For heavier nuclei:

A more "pragmatic" approach is needed



**Reduce the Many-Body to a Few-Body Problem**

*Isolate relevant degrees of freedom*

*Solve the few-body problem with effective interactions*

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# Effective interactions from *ab initio* methods

Start from many-body Hamiltonian with 2 (and 3) body forces

**Theoretical foundations laid by Feshbach and Watson in the 1950s**

*Feshbach:*

effective nA interaction via Green's function from solution of many body problem using basis function expansion, e.g. SCGF, CCGF (current truncation to singles and doubles)

*energy ~ 10 MeV*

*Watson:*

► **Multiple scattering expansion, e.g. spectator expansion**

**(current truncation to two active particles)**

## Spectator Expansion:

Siciliano, Thaler (1977)

Picklesimer, Thaler (1981)

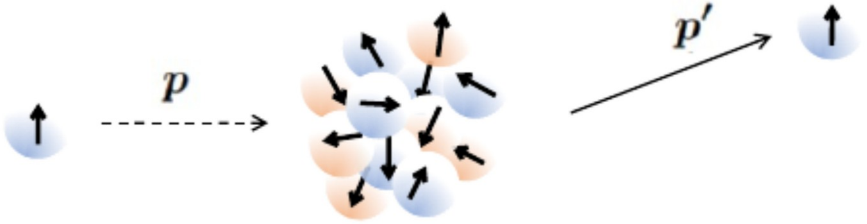
Chinn, Elster, Thaler, Weppner (1995)

*Expansion in:*

- *particles active in the reaction*
- *antisymmetrized in active particles*

*Intended for "fast reaction", i.e. ≳ 80 MeV*

# Building up an *ab initio* framework for elastic scattering from nuclei




**Ingredients:**

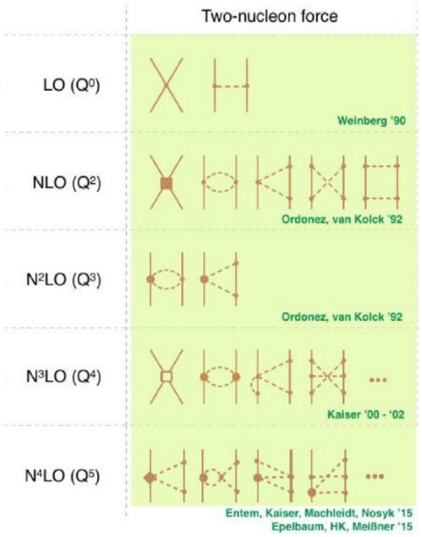
1) realistic nuclear interaction

must describe target and projectile

2) controllable structure framework

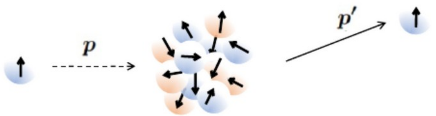
3) controllable reaction framework

4) a way to connect everything




Chiral NN Interaction

# Building up an *ab initio* framework




**Ingredients:**

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**must describe target and projectile**

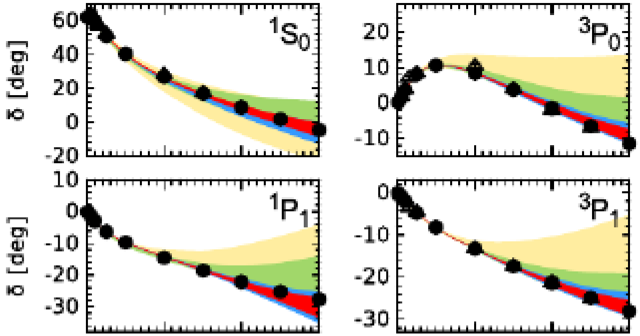
**2) controllable structure framework**

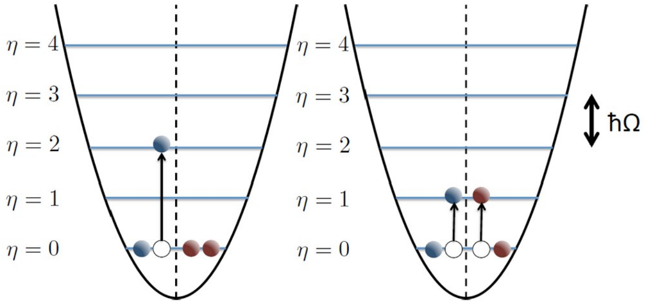
**here, no-core shell model (NCSM and SA-NCSM)**

**3) controllable reaction framework**

here, spectator expansion

**4) a way to connect everything**




| | $E(^3H)$ | $E(^3He)$ | $E(^4He)$ | $r_p(^4He)$ |
|---|---|---|---|---|
| NNLO | −8.249 | −7.501 | −27.759 | 1.43(8) |
| NNLO+NNN | −8.469 | −7.722 | −28.417 | 1.43(8) |
| Experiment | −8.482 | −7.717 | −28.296 | 1.467(13) |

Ekström et al., PRL 110, 192502 (2013)

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here, spectator expansion of

Watson multiple scattering series

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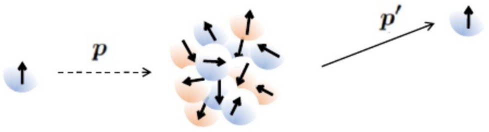


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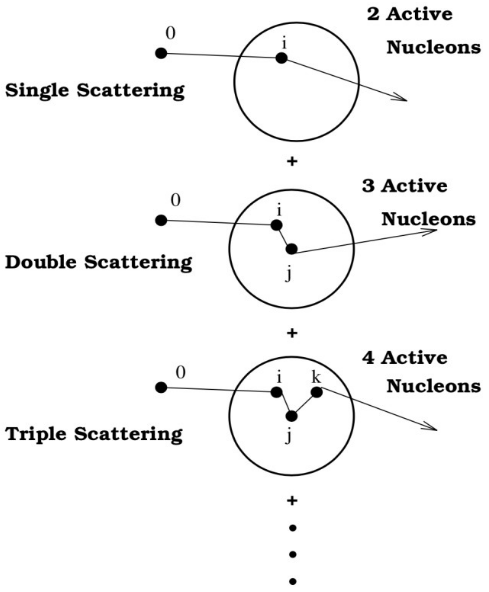


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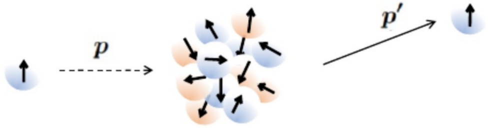
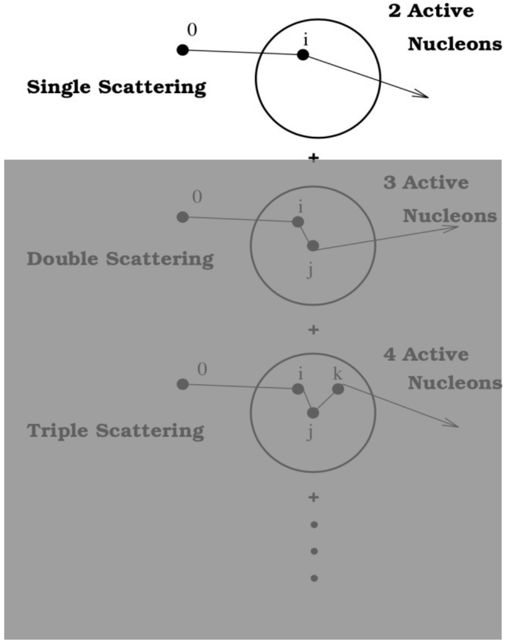
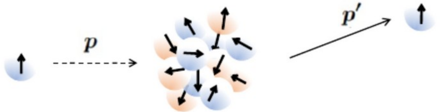



Leading order in spectator expansion can be computed *ab initio*

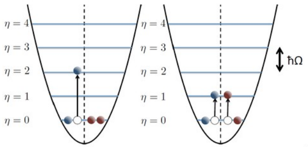
# Framework for *ab initio* Elastic Scattering

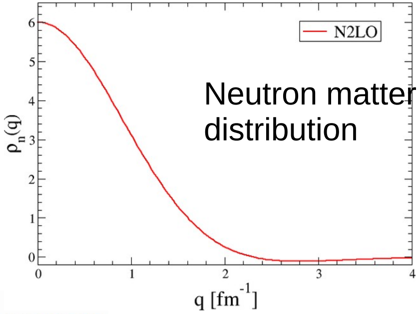


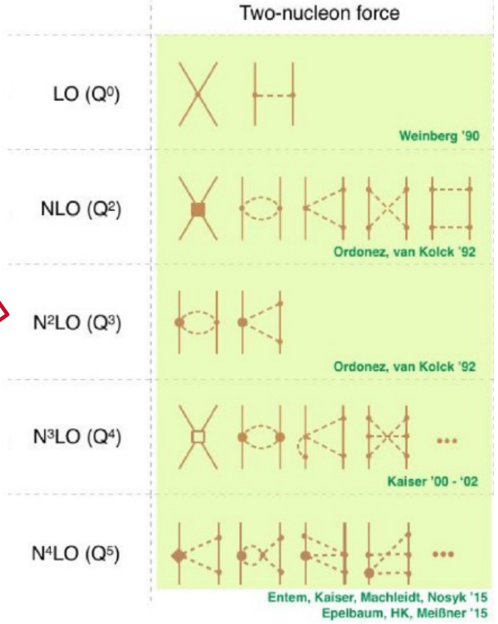

**Same NN force in all parts**

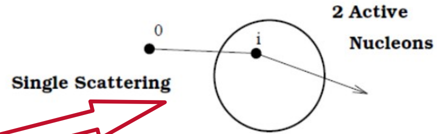
Reaction theory:
spectator expansion

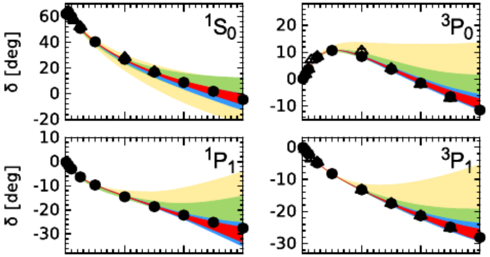
Structure theory:
No-Core Shell Model




Calculations shown with $NNLO_{opt}$ chiral interaction
A. Ekstrom et al. PRL 110, 192502 (2013)

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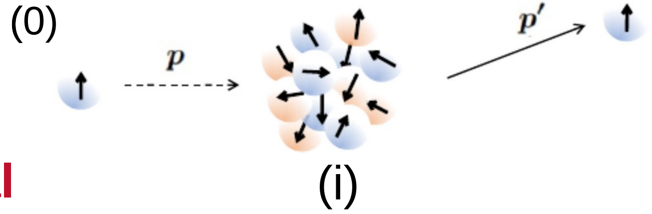
# Setting up the *ab initio* framework

$$\begin{pmatrix}\text{effective}\\ \text{interaction}\end{pmatrix} = \begin{pmatrix}\text{thing that puts}\\ \text{them together}\end{pmatrix} \times \begin{pmatrix}\text{reaction}\\ \text{information}\end{pmatrix} \times \begin{pmatrix}\text{structure}\\ \text{information}\end{pmatrix}$$

NN interaction represented by **Wolfenstein amplitudes**




$$\begin{aligned}\overline{M}(\boldsymbol{q},\boldsymbol{\mathcal{K}}_{NN},\epsilon) = {} & A(\boldsymbol{q},\boldsymbol{\mathcal{K}}_{NN},\epsilon)\mathbf{1}\otimes\mathbf{1}\\ & + iC(\boldsymbol{q},\boldsymbol{\mathcal{K}}_{NN},\epsilon)\left(\boldsymbol{\sigma}^{(0)}\cdot\hat{\boldsymbol{n}}\right)\otimes\mathbf{1}\\ & + iC(\boldsymbol{q},\boldsymbol{\mathcal{K}}_{NN},\epsilon)\,\mathbf{1}\otimes\left(\boldsymbol{\sigma}^{(i)}\cdot\hat{\boldsymbol{n}}\right)\\ & + M(\boldsymbol{q},\boldsymbol{\mathcal{K}}_{NN},\epsilon)(\boldsymbol{\sigma}^{(0)}\cdot\hat{\boldsymbol{n}})\otimes(\boldsymbol{\sigma}^{(i)}\cdot\hat{\boldsymbol{n}})\\ & + [G(\boldsymbol{q},\boldsymbol{\mathcal{K}}_{NN},\epsilon) - H(\boldsymbol{q},\boldsymbol{\mathcal{K}}_{NN},\epsilon)]\,(\boldsymbol{\sigma}^{(0)}\cdot\hat{\boldsymbol{q}})\otimes(\boldsymbol{\sigma}^{(i)}\cdot\hat{\boldsymbol{q}})\\ & + [G(\boldsymbol{q},\boldsymbol{\mathcal{K}}_{NN},\epsilon) + H(\boldsymbol{q},\boldsymbol{\mathcal{K}}_{NN},\epsilon)]\,(\boldsymbol{\sigma}^{(0)}\cdot\hat{\boldsymbol{\mathcal{K}}})\otimes(\boldsymbol{\sigma}^{(i)}\cdot\hat{\boldsymbol{\mathcal{K}}})\\ & + D(\boldsymbol{q},\boldsymbol{\mathcal{K}}_{NN},\epsilon)\left[(\boldsymbol{\sigma}^{(0)}\cdot\hat{\boldsymbol{q}})\otimes(\boldsymbol{\sigma}^{(i)}\cdot\hat{\boldsymbol{\mathcal{K}}}) + (\boldsymbol{\sigma}^{(0)}\cdot\hat{\boldsymbol{\mathcal{K}}})\otimes(\boldsymbol{\sigma}^{(i)}\cdot\hat{\boldsymbol{q}})\right]\end{aligned}$$

$$\boldsymbol{q} = \boldsymbol{p}' - \boldsymbol{p}$$

$$\boldsymbol{\mathcal{K}} = \frac{1}{2}(\boldsymbol{p}' + \boldsymbol{p})$$

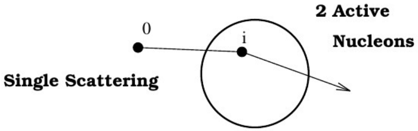
$$\hat{\boldsymbol{n}} = \frac{\boldsymbol{\mathcal{K}}\times\boldsymbol{q}}{|\boldsymbol{\mathcal{K}}\times\boldsymbol{q}|}$$

**A: central**
**C: spin-orbit**

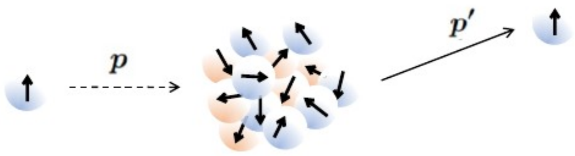
**M, G, H: tensor**

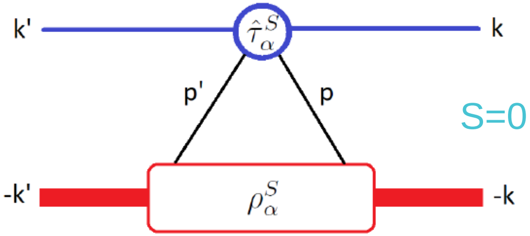
**Most general structure of NN amplitudes consistent with invariance principles**

# Computing the leading order effective potential




( **effective interaction** ) = ( thing that puts them together ) x ( reaction information ) x ( structure information )




S=0,1

scatter off nucleus with $0^+$ ground state

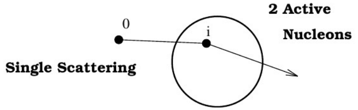
$$\widehat{U}_p(q,\mathcal{K}_{NA},\epsilon) = \sum_{\alpha=n,p}\sum_{S=0}^{1}\int d^3\mathcal{K}\quad \eta\left(q,\mathcal{K},\mathcal{K}_{NA}\right)\ \hat{\tau}^S_{p,\alpha}\left(q,\tfrac{1}{2}\left(\tfrac{A+1}{A}\mathcal{K}_{NA}-\mathcal{K}\right);\varepsilon\right)$$

$$\rho^S_\alpha\left(\mathcal{K}-\tfrac{A-1}{A}\tfrac{q}{2},\mathcal{K}+\tfrac{A-1}{A}\tfrac{q}{2}\right),$$

**Watson optical potential:** $U_{\rm p} = \widehat{U}_{\rm p} - \widehat{U}_{\rm p}G_0(E)PU_{\rm p},$

(N≠Z nuclei treated exactly)

# Computing the leading order effective potential




( effective interaction ) = ( thing that puts them together ) x ( reaction information ) x ( structure information )

matter distribution = density

$$
\begin{aligned}
\widehat{U}_p(\boldsymbol{q},\boldsymbol{\mathcal{K}_{NA}},\epsilon)
&= \sum_{\alpha=p,n}\int d^3\mathcal{K}\eta\left(\boldsymbol{q},\boldsymbol{\mathcal{K}_{NA}},\epsilon\right)\boldsymbol{A_{p,\alpha}}\left(\boldsymbol{q},\frac{1}{2}\left(\frac{A+1}{A}\boldsymbol{\mathcal{K}_{NA}}+\boldsymbol{\mathcal{K}}\right),\epsilon\right)\rho_{\alpha}^{S=0}(\boldsymbol{P'},\boldsymbol{P})\\
&+ i(\boldsymbol{\sigma}^{(0)}\cdot\hat{\boldsymbol{n}})\sum_{\alpha=N,Z}\int d^3\mathcal{K}\eta\left(\boldsymbol{q},\boldsymbol{\mathcal{K}_{NA}},\epsilon\right)\boldsymbol{C_{p,\alpha}}\left(\boldsymbol{q},\frac{1}{2}\left(\frac{A+1}{A}\boldsymbol{\mathcal{K}_{NA}}+\boldsymbol{\mathcal{K}}\right),\epsilon\right)\rho_{\alpha}^{S=0}(\boldsymbol{P'},\boldsymbol{P})\\
&+ i\sum_{\alpha=N,Z}\int d^3\mathcal{K}\eta\left(\boldsymbol{q},\boldsymbol{\mathcal{K}_{NA}},\epsilon\right)\boldsymbol{C_{p,\alpha}}\left(\boldsymbol{q},\frac{1}{2}\left(\frac{A+1}{A}\boldsymbol{\mathcal{K}_{NA}}+\boldsymbol{\mathcal{K}}\right),\epsilon\right)S_{n,\alpha}(\boldsymbol{P'},\boldsymbol{P})\cos\beta\\
&+ i(\boldsymbol{\sigma}^{(0)}\cdot\hat{\boldsymbol{n}})\sum_{\alpha=N,Z}\int d^3\mathcal{K}\eta\left(\boldsymbol{q},\boldsymbol{\mathcal{K}_{NA}},\epsilon\right)\boldsymbol{M_{p,\alpha}}\left(\boldsymbol{q},\frac{1}{2}\left(\frac{A+1}{A}\boldsymbol{\mathcal{K}_{NA}}+\boldsymbol{\mathcal{K}}\right),\epsilon\right)S_{n,\alpha}(\boldsymbol{P'},\boldsymbol{P})\cos\beta
\end{aligned}
$$

spin-projected momentum distribution

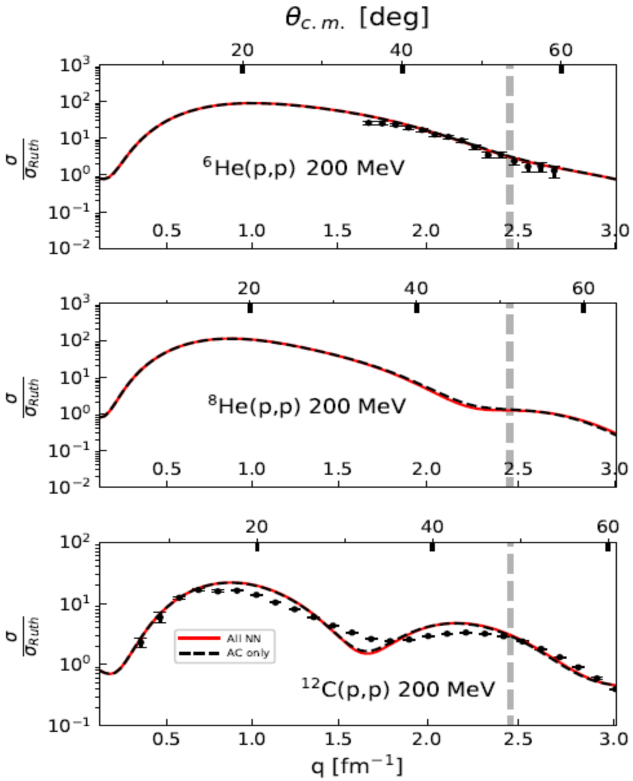
with $\mathcal{P}' = \left(\mathcal{K} - \frac{A-1}{A}\frac{q}{2}\right)$ and $\mathcal{P} = \left(\mathcal{K} + \frac{A-1}{A}\frac{q}{2}\right)$

# Observations for Open-shell nuclei

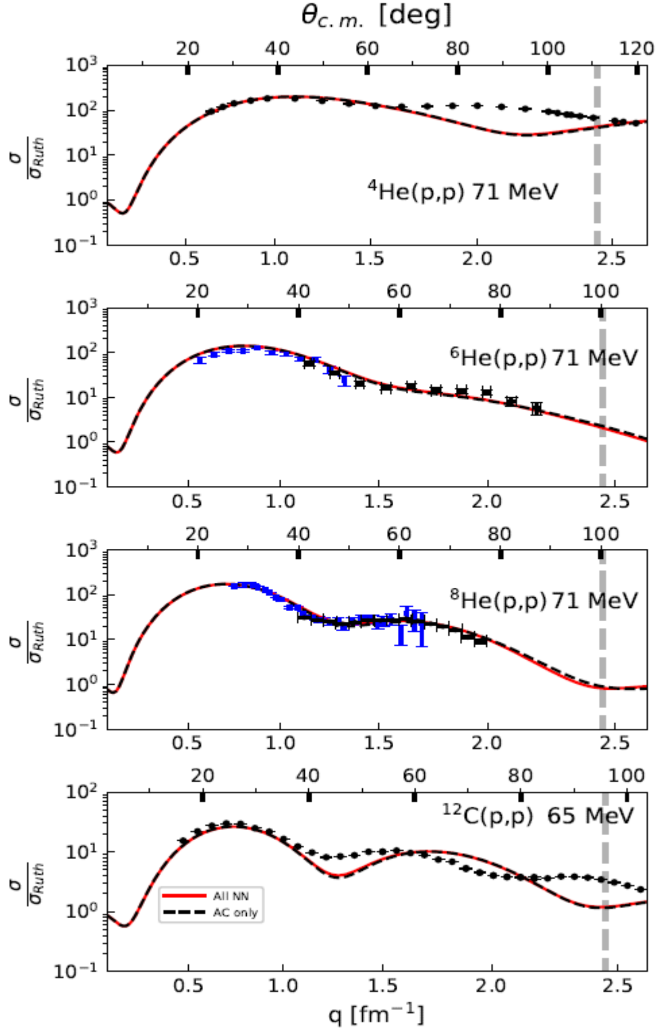
$NNLO_{opt}$
Chiral interaction

$N_{max}$=18

$N_{max}$=12




NCSM ħω=20 MeV




$N_{max}$=18

$N_{max}$=12

M. Burrows et al. PRC 102, 034606 (2020)

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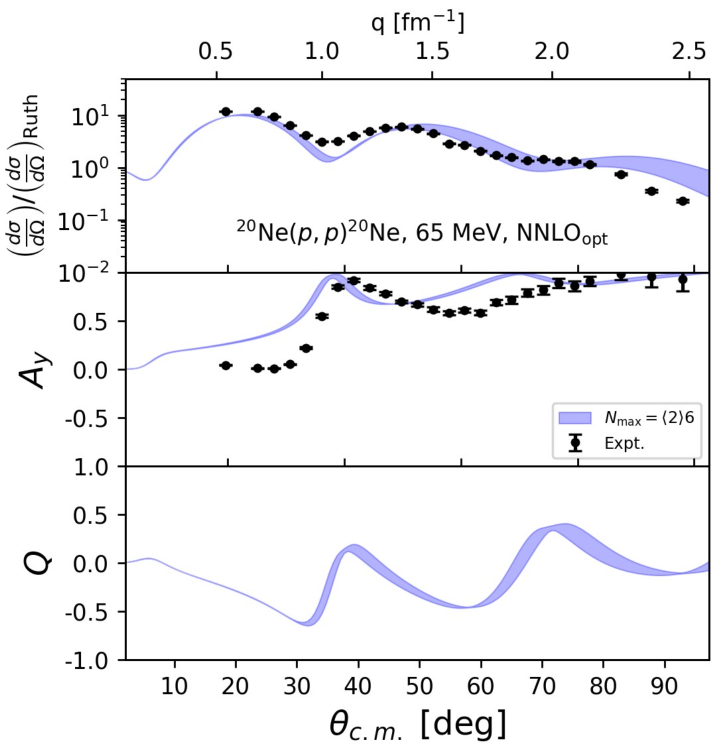
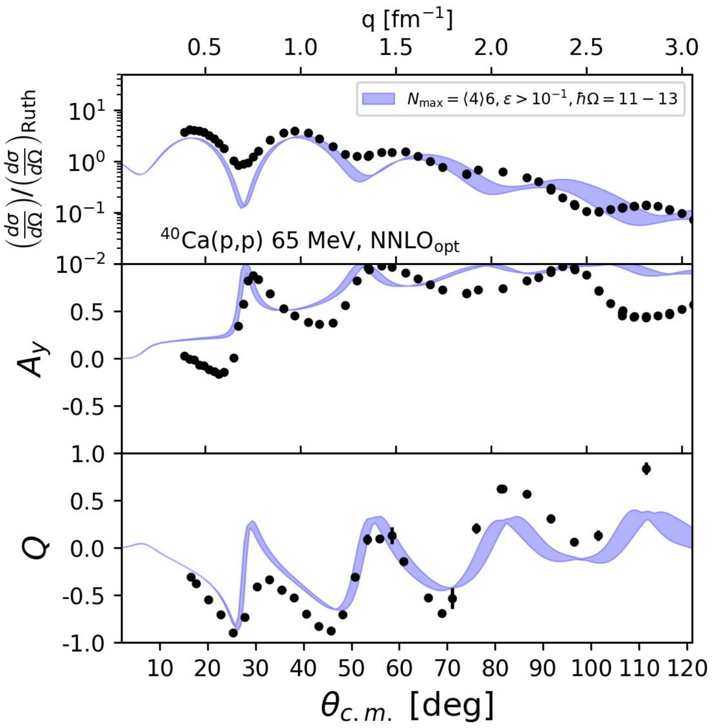
# Similar observation with SA-NCSM One-Body Densities

$NNLO_{opt}$ chiral potential

$\hbar\omega$=13-17 MeV




$\hbar\omega$=11-13 MeV

rms calc. 3.04 – 3.25 fm
rms exp. 3.48 fm

Baker, Elster, Dytrych, Launey, PRC 110, 034605 (2024)

*Ab initio leading order spectator seems to describe scattering data better for deformed nuclei*

# Why Magnesium Isotopes?

- Concentrate on Mg isotopes with $0^+$ ground states
- Those isotopes are all deformed
- There is considerable experimental information on scattering from $^{24}$Mg in our energy regime of interest
- $^{32}$Mg of special interest (island of inversion)
- SA-NCSM can provide off-shell one-body densities for $^{24}$Mg, $^{26}$Mg, $^{28}$Mg, $^{32}$Mg

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## New development for phenomenology:

**Uncertainty-quantified phenomenological optical potentials for single-nucleon scattering**

C. D. Pruitt,* J. E. Escher, and R. Rahman†
*Lawrence Livermore National Laboratory, Livermore, California 94550, USA*

PHYSICAL REVIEW C **107**, 014602 (2023)

- Phenomenological Woods-Saxon based optical potentials fitted to stable nuclei
- **Extrapolation of phenomenological optical potentials with uncertainty quantification**
- Ab initio is a theoretical well defined procedure for moving towards the drip-line with theory errors

jitR

VALIDATION

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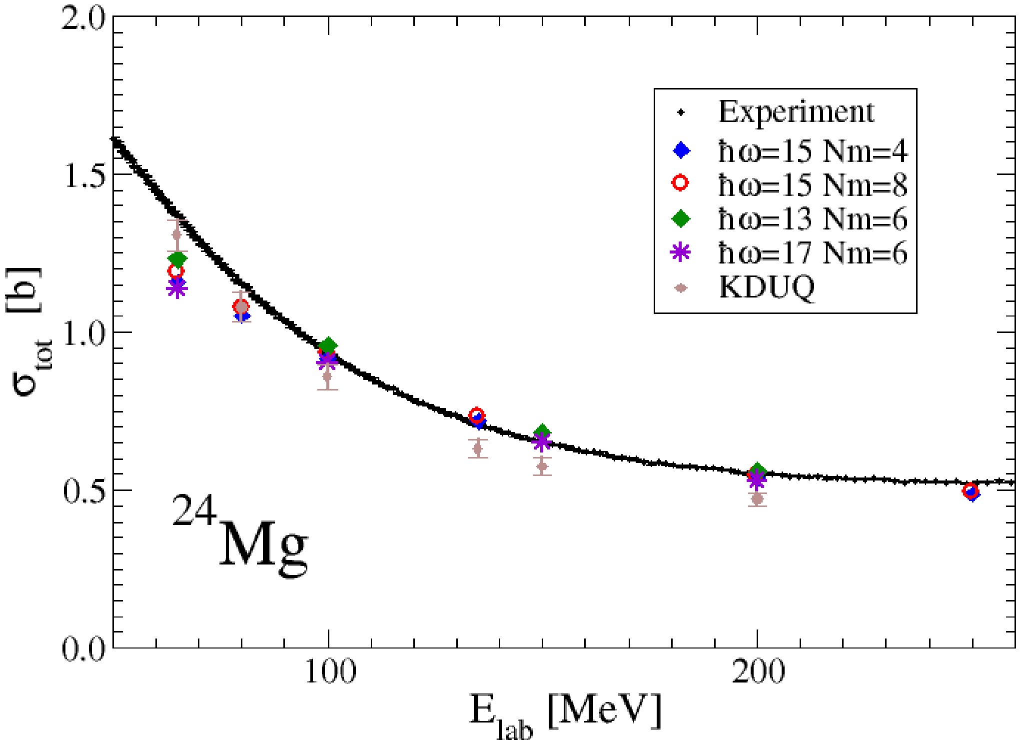
# Start and anchor on $^{24}$Mg (experiment availabe)

Neutron total cross section




*Ab initio* calculation employs **$NNLO_{opt}$ chiral potential**

**KDUQ**: Koning-Delaroche phenomenological optical potential with Uncertainty Quantification

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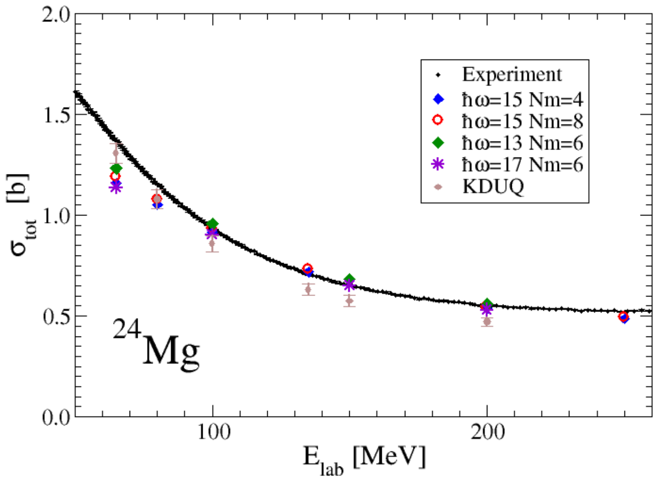
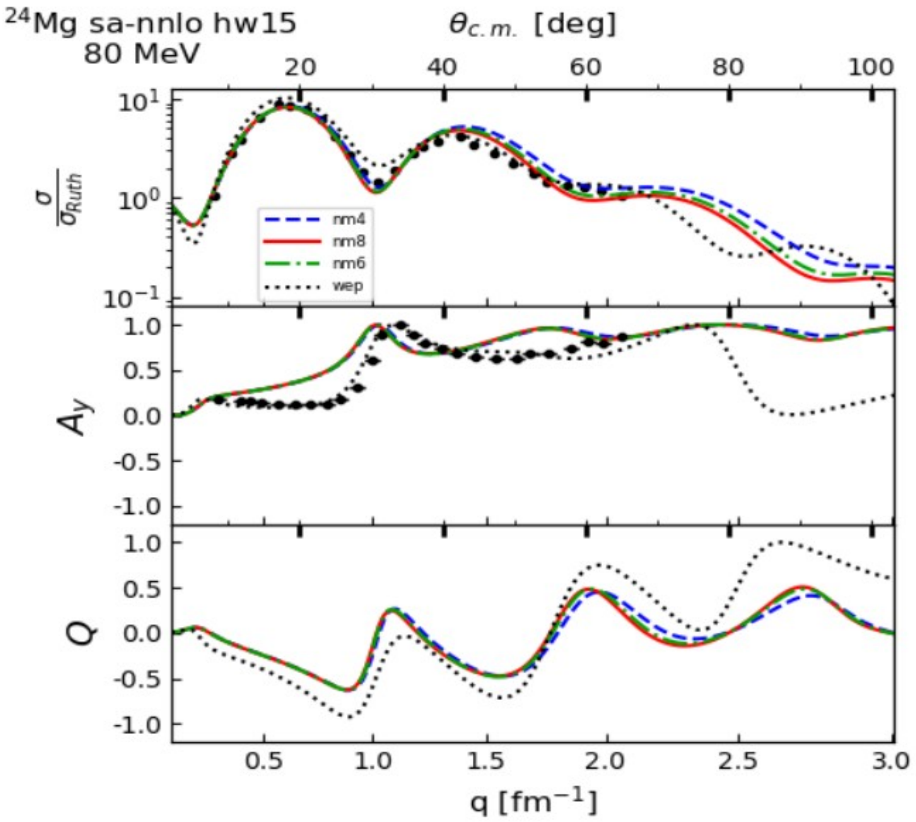
# Start and anchor on $^{24}$Mg

Neutron total cross section

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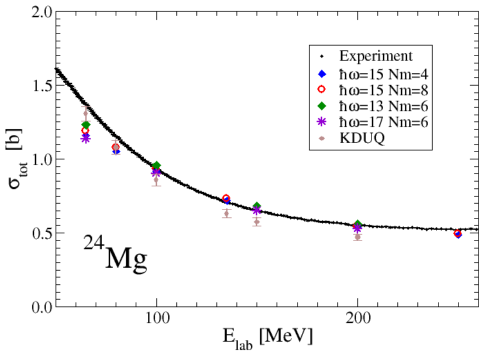
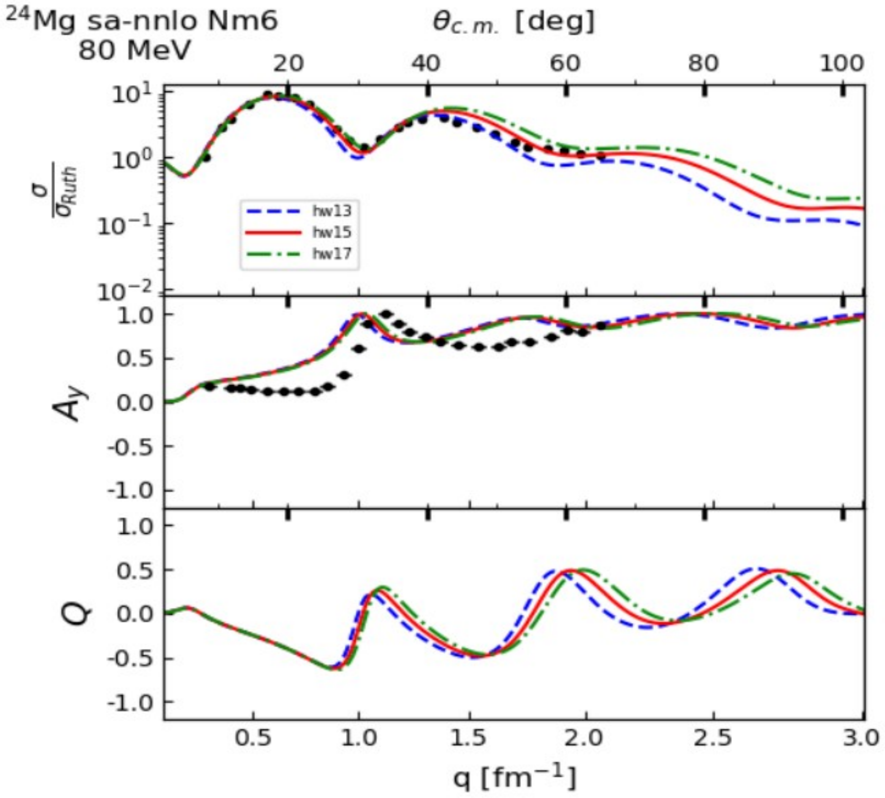
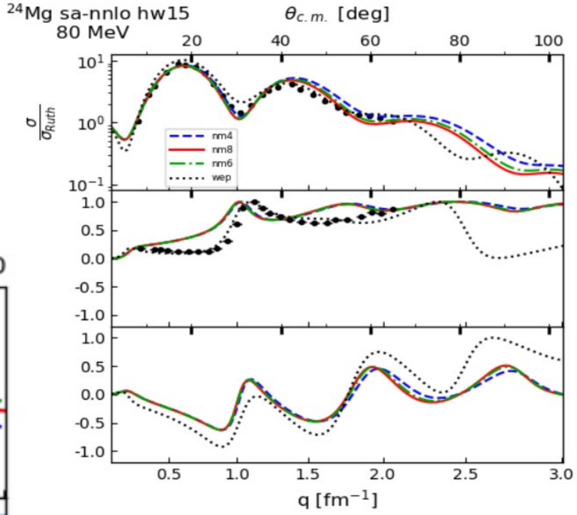
# Start and anchor on $^{24}$Mg

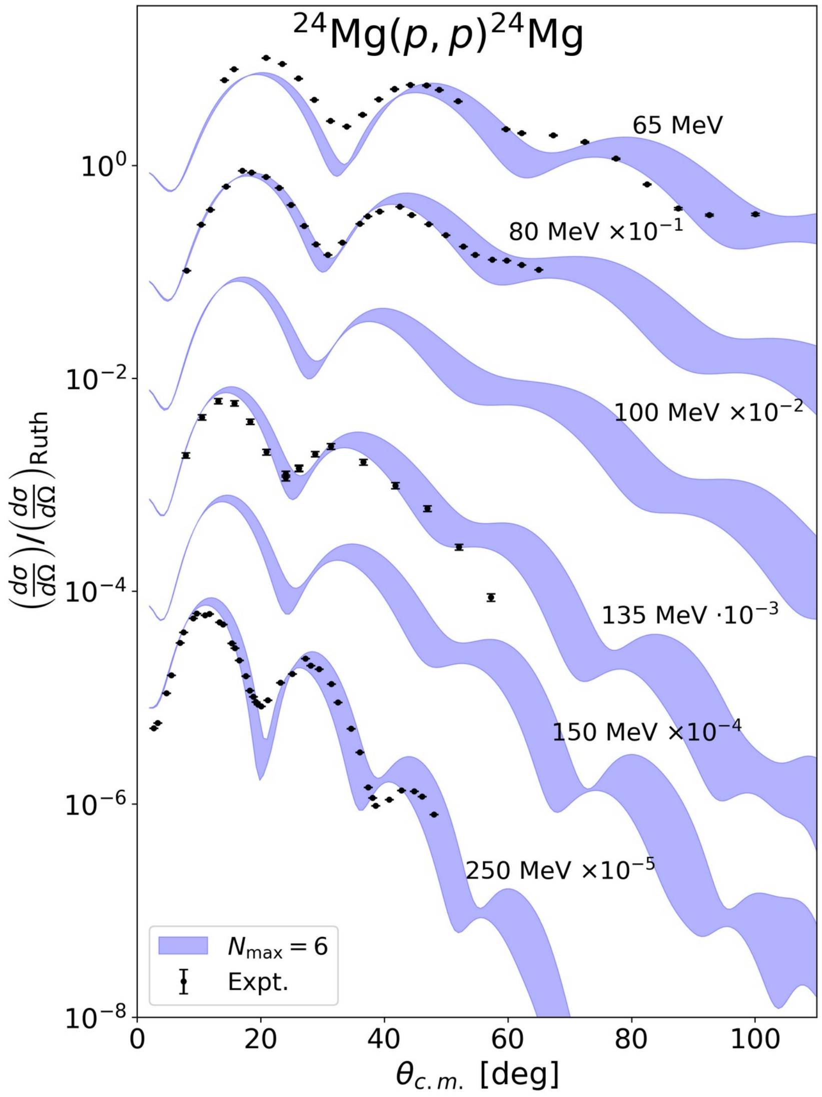
## Neutron total cross section



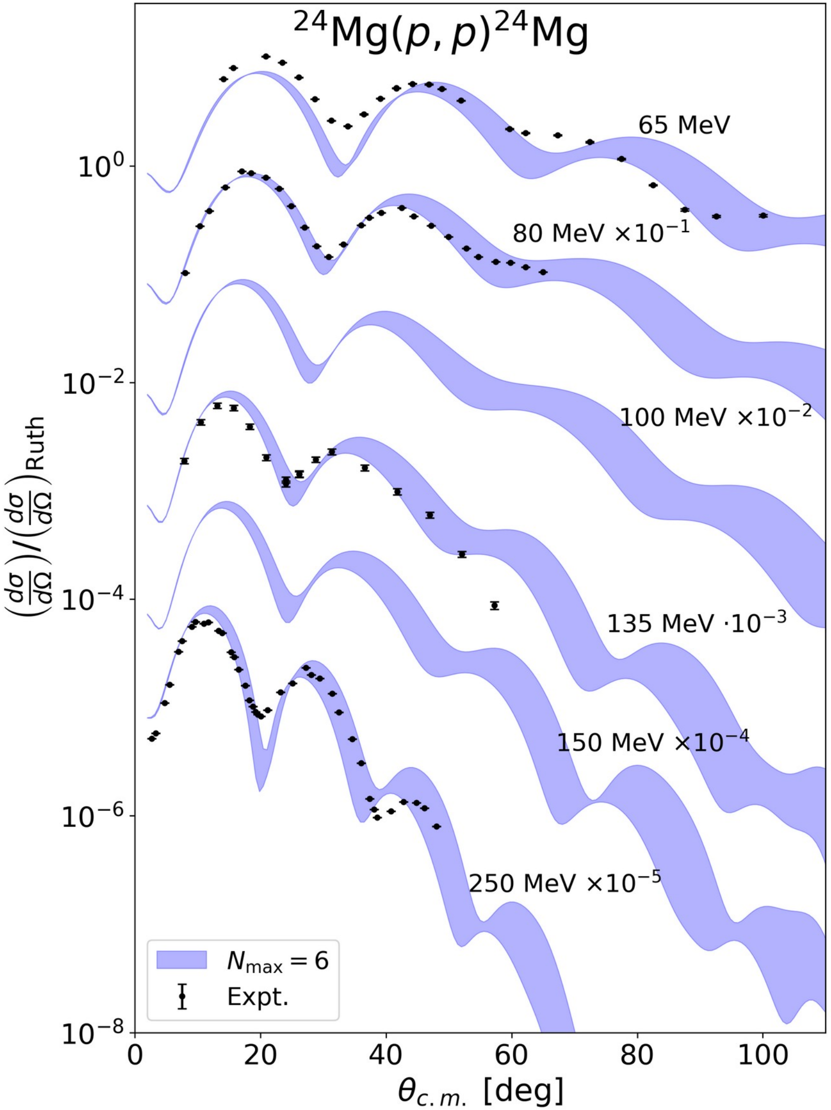



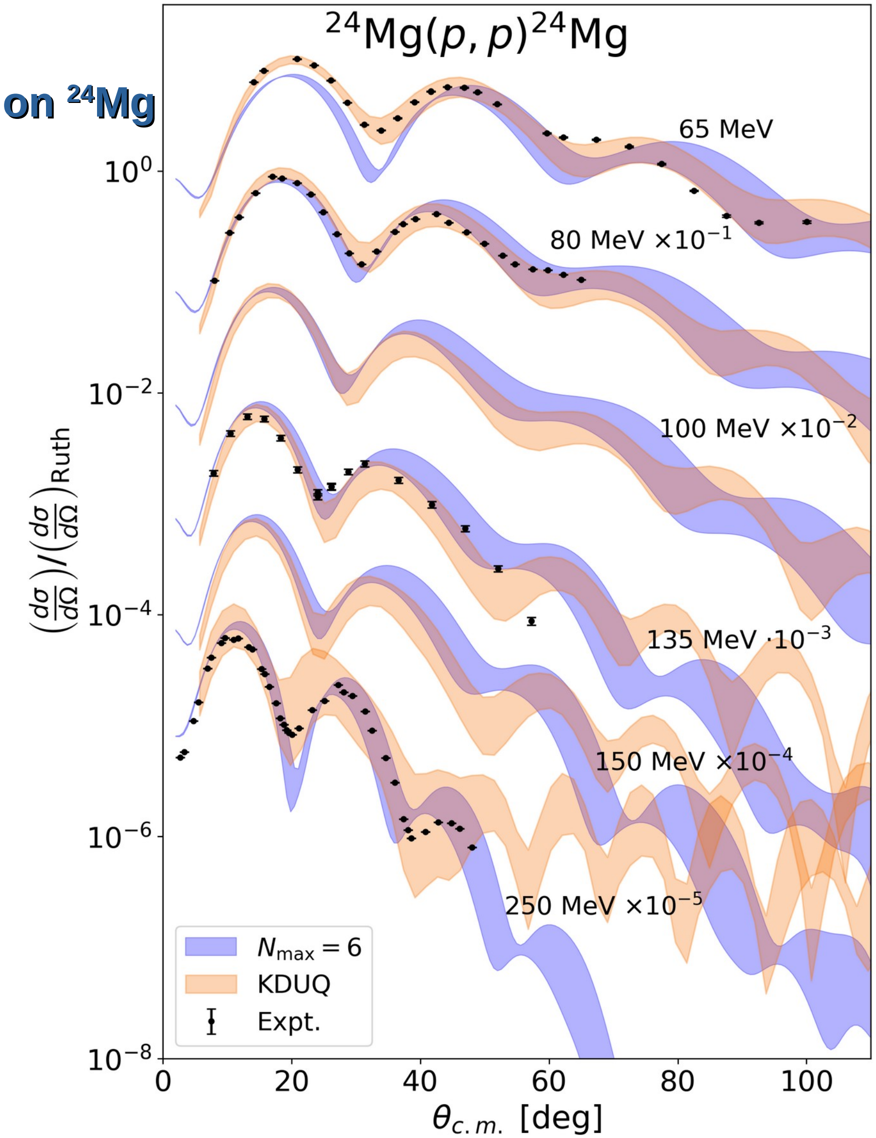



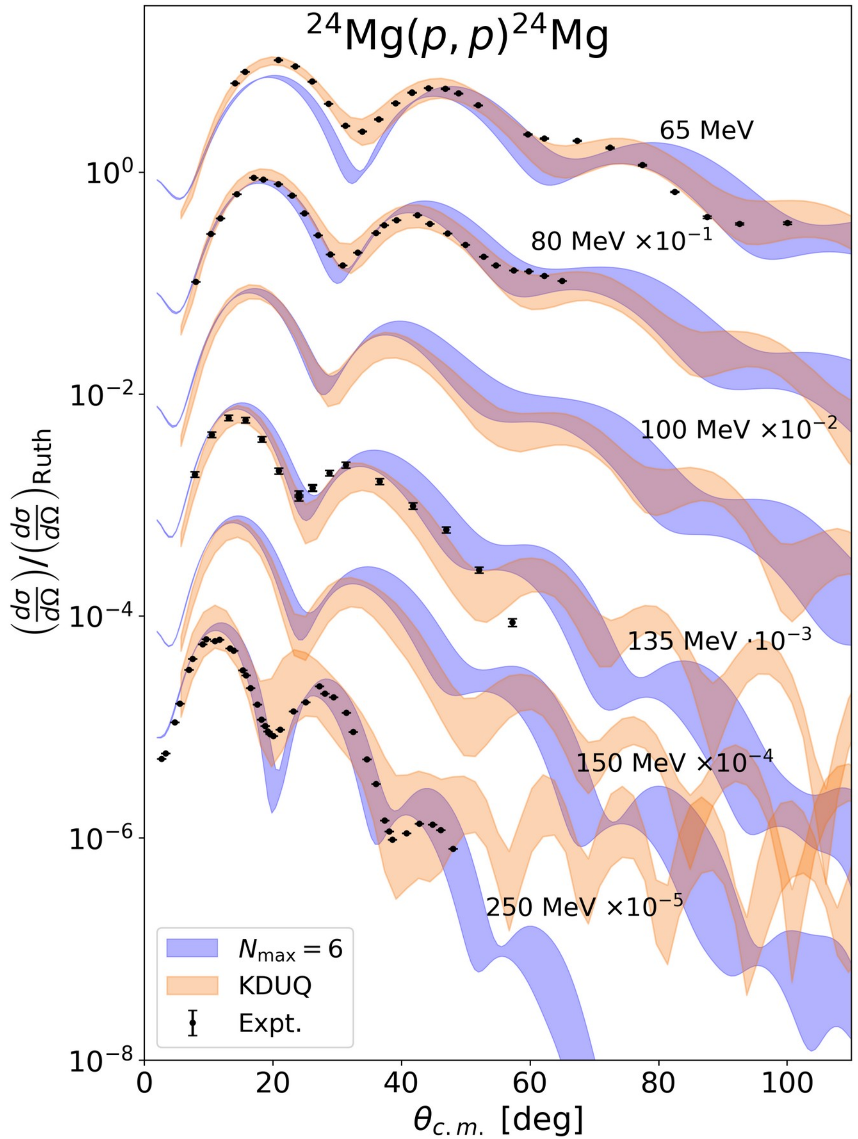
## Start and anchor on $^{24}$Mg



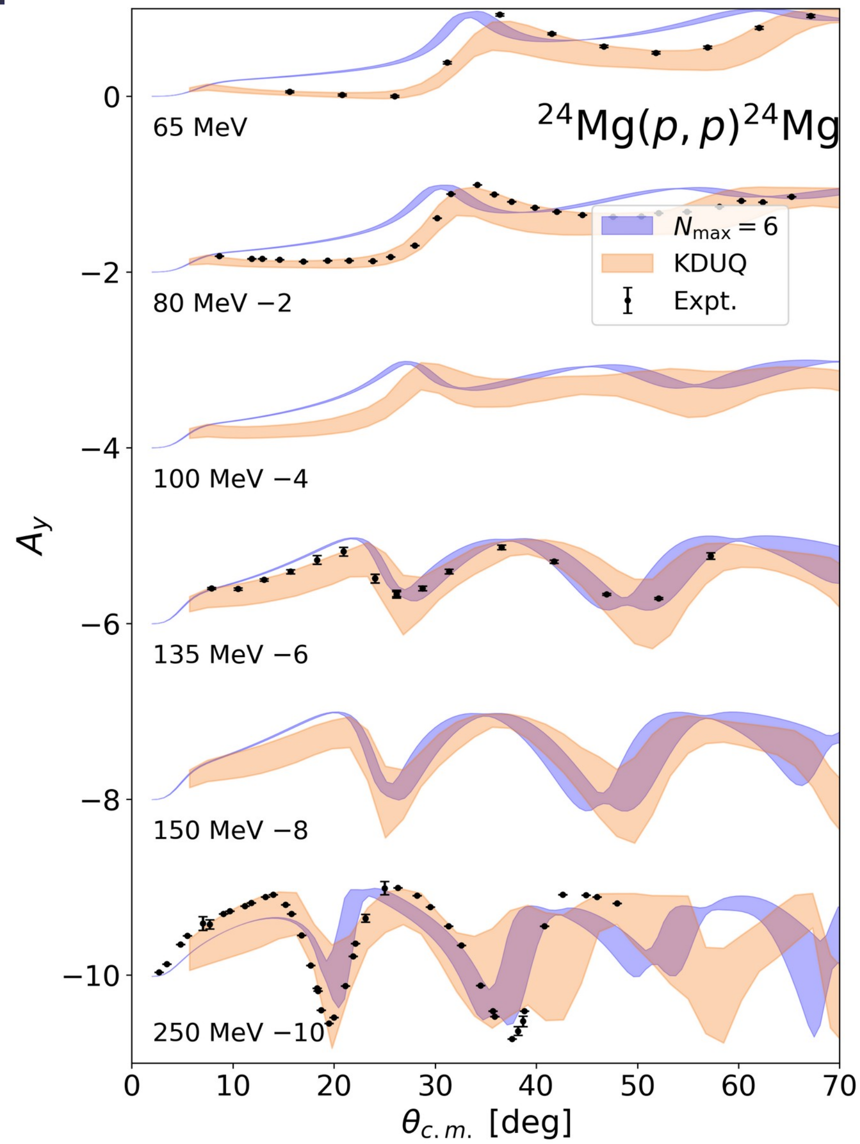
## Start and anchor on $^{24}Mg$



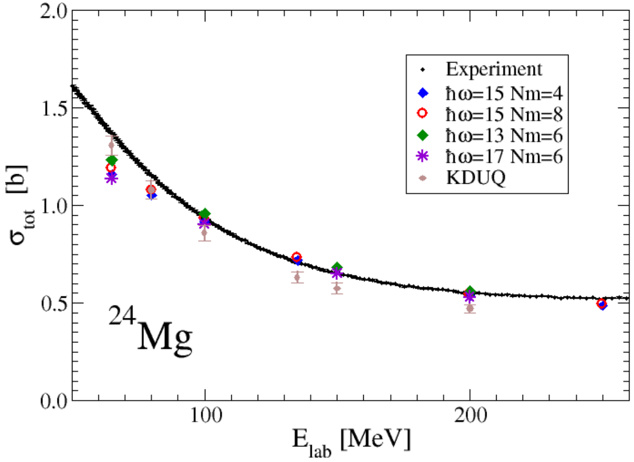


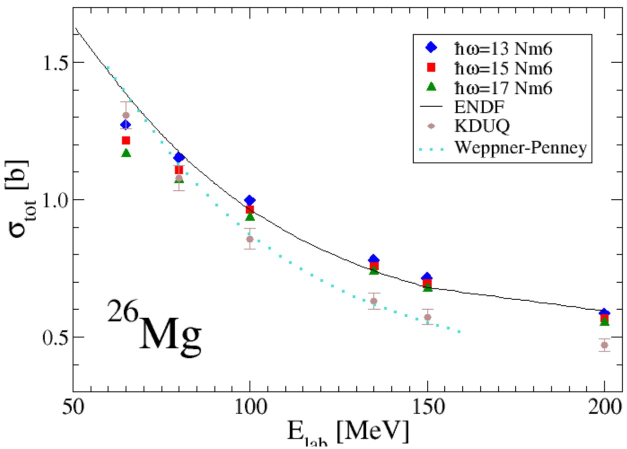
$^{24}Mg(p,p)^{24}Mg$
65 MeV
80 MeV ×10$^{-1}$
100 MeV ×10$^{-2}$
135 MeV ·10$^{-3}$
150 MeV ×10$^{-4}$
250 MeV ×10$^{-5}$
$N_{max} = 6$
KDUQ
Expt.
$(\frac{d\sigma}{d\Omega})/(\frac{d\sigma}{d\Omega})_{Ruth}$
$\theta_{c.m.}$ [deg]

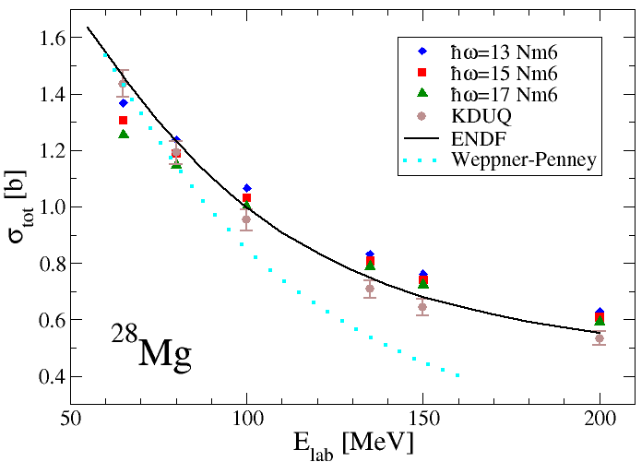



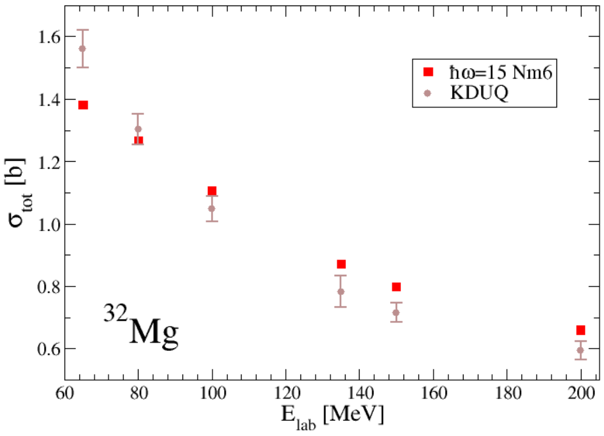
$^{24}Mg(p,p)^{24}Mg$
65 MeV
80 MeV −2
100 MeV −4
135 MeV −6
150 MeV −8
250 MeV −10
$N_{max} = 6$
KDUQ
Expt.
$A_y$
$\theta_{c.m.}$ [deg]

# Neutron total cross sections for Mg isotopes

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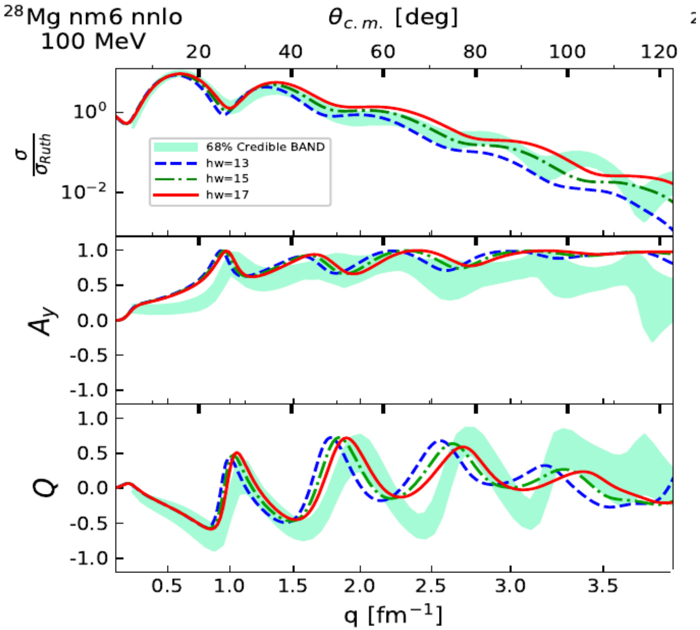
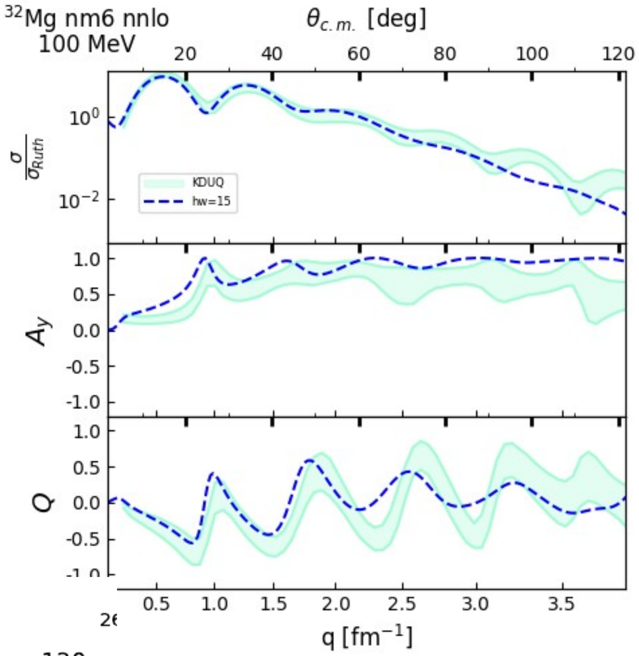
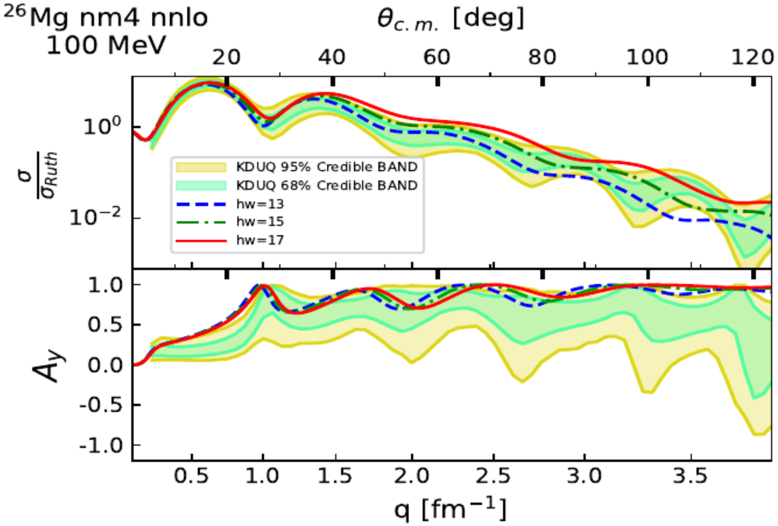


$^{28}$Mg nm6 nnlo
100 MeV
$\theta_{c.m.}$ [deg]
20 40 60 80 100 120
$\frac{\sigma}{\sigma_{Ruth}}$
$10^0$
$10^{-2}$
68% Credible BAND
hw=13
hw=15
hw=17
$A_y$
1.0 0.5 0.0 -0.5 -1.0
$Q$
1.0 0.5 0.0 -0.5 -1.0
0.5 1.0 1.5 2.0 2.5 3.0 3.5
q [fm$^{-1}$]

$^{32}$Mg nm6 nnlo
100 MeV
$\theta_{c.m.}$ [deg]
20 40 60 80 100 120
$\frac{\sigma}{\sigma_{Ruth}}$
$10^0$
$10^{-2}$
KDUQ
hw=15
$A_y$
1.0 0.5 0.0 -0.5 -1.0
$Q$
1.0 0.5 0.0 -0.5
0.5 1.0 1.5 2.0 2.5 3.0 3.5
q [fm$^{-1}$]

$^{26}$Mg nm4 nnlo
100 MeV
$\theta_{c.m.}$ [deg]
20 40 60 80 100 120
$\frac{\sigma}{\sigma_{Ruth}}$
$10^0$
$10^{-2}$
KDUQ 95% Credible BAND
KDUQ 68% Credible BAND
hw=13
hw=15
hw=17
$A_y$
1.0 0.5 0.0 -0.5 -1.0
0.5 1.0 1.5 2.0 2.5 3.0 3.5
q [fm$^{-1}$]

# What we learned so far:

- **Consistent approach to p+A effective interaction in leading order multiple scattering expansion is possible.**
  - **spin of projectile and struck target nucleon treated consistently**
  - **N≠Z effects for Watson potential treated exactly**

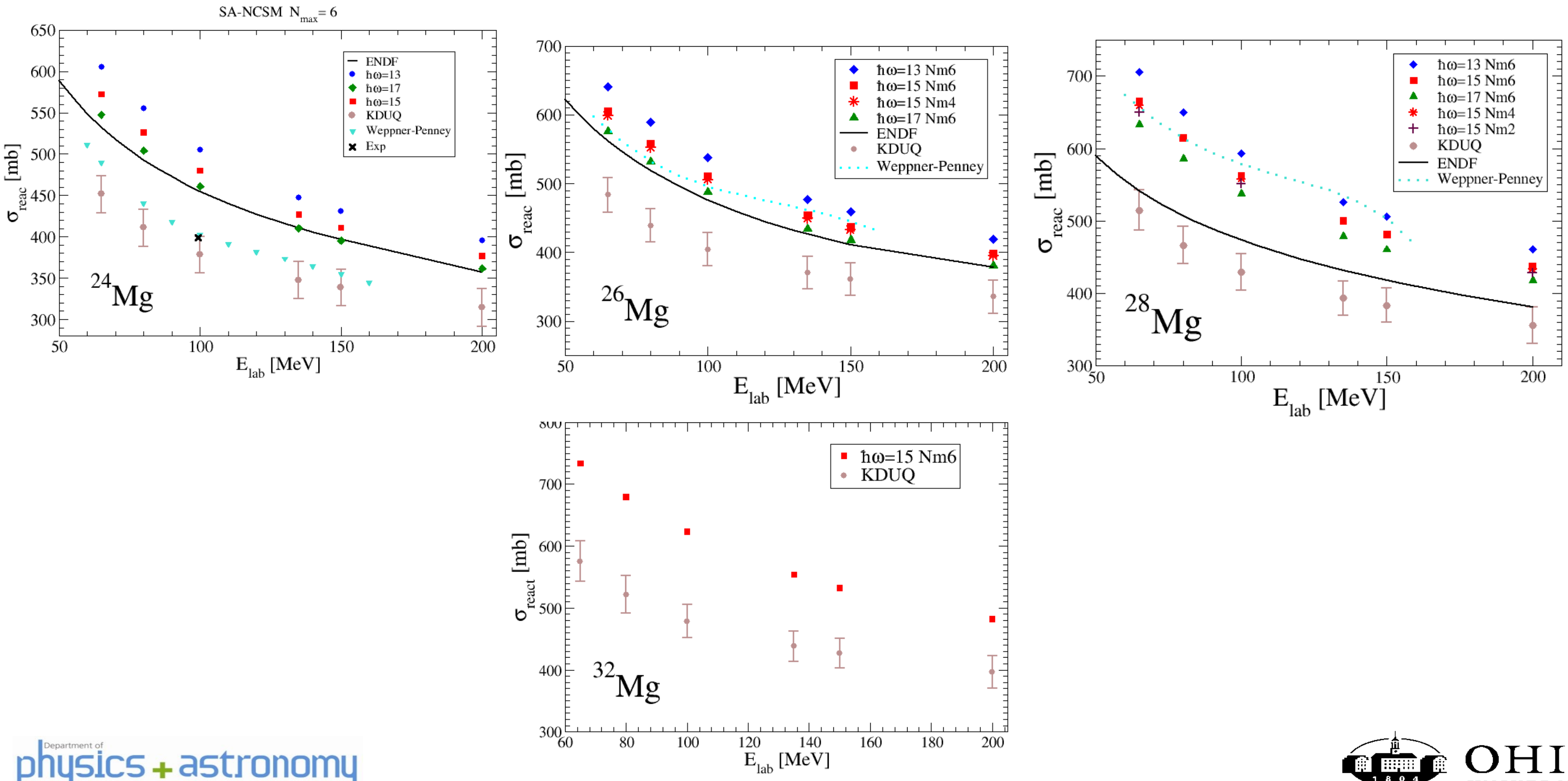
- **Some indication that the leading order the spectator expansion describes elastic scattering data better for open-shell (deformed) and exotic nuclei than closed shell nuclei**
  (good for providing predictions for optical potential fits in exotic regime)

- **Carried out study of Mg isotopes:**
  **Calculations for $^{24}$Mg compare favorably to experiment**
  **Confidence in predicting $^{26}$Mg, $^{28}$Mg, and $^{32}$Mg**

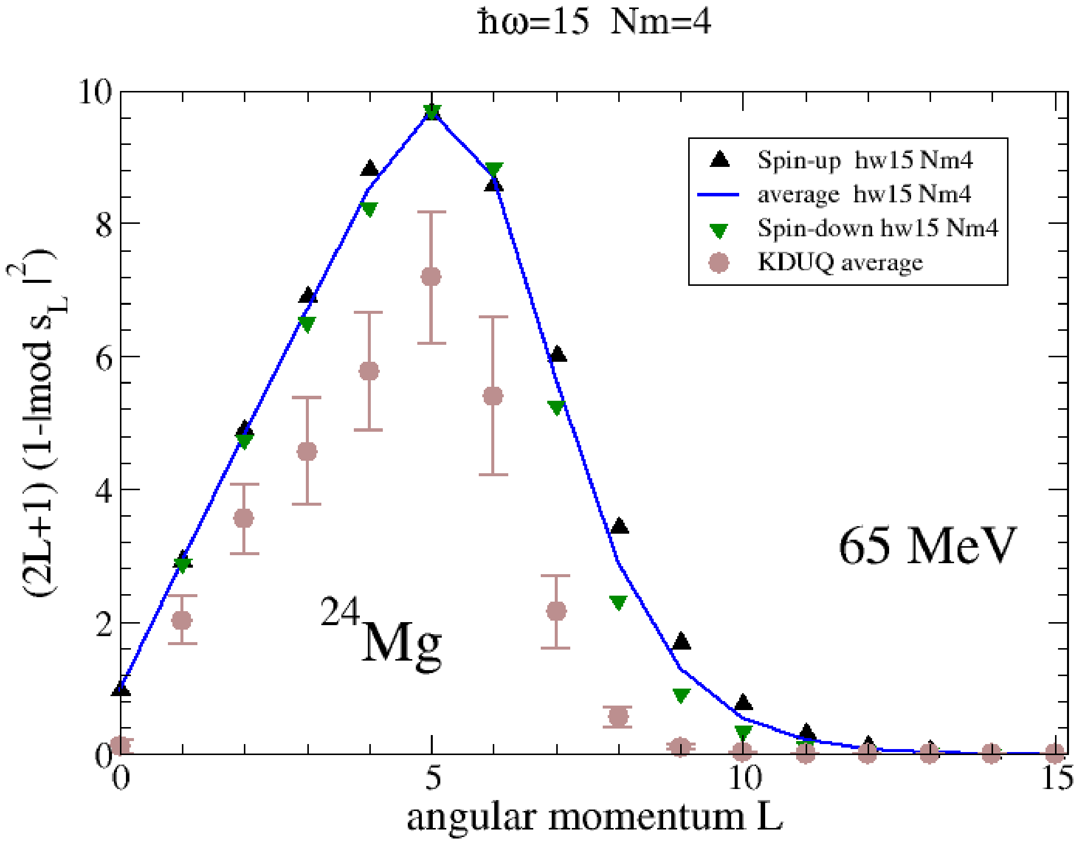

- Test of extrapolations of phenomenological optical potentials towards the dripline
  KDUQ extrapolates quite well (exept reaction cross sections)

Backup slides

# Proton reaction cross sections



# Proton partial reaction cross sections



# Diagonal densities (CoM)

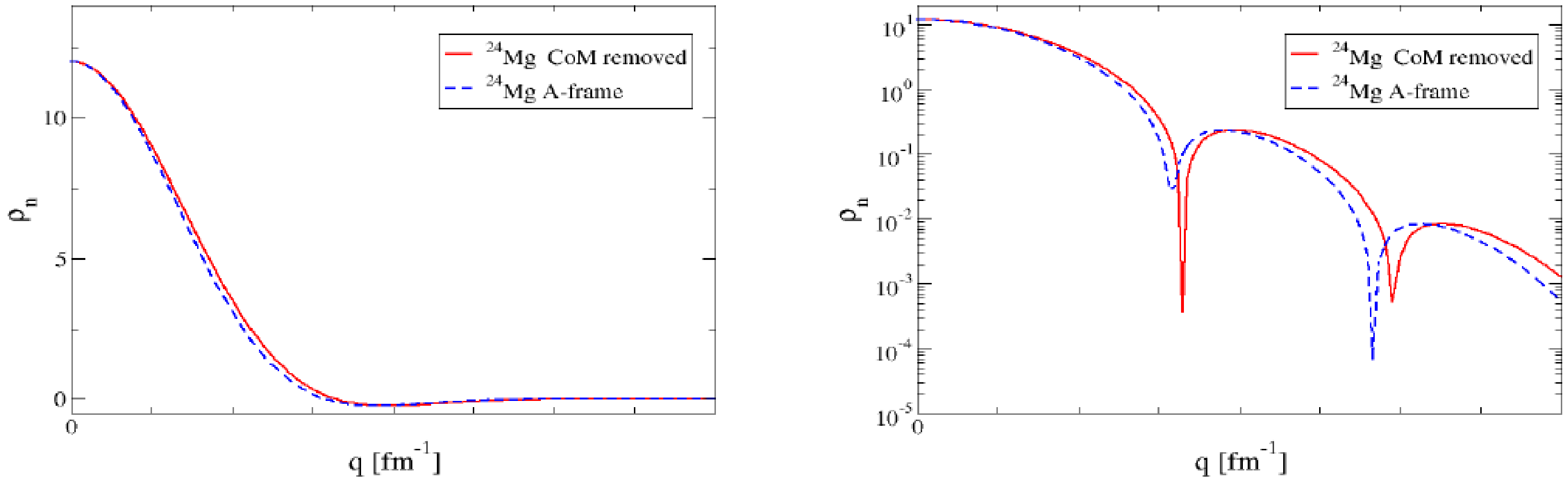



Figure 3: The diagonal one-body neutron densities for $^{24}$Mg for $\hbar\omega$=15 and $N_{max}$=6. Shown is the diagonal density for a calculation where the CoM is removed vs a calculation in the A-frame.

# Diagonal densities (neutron)

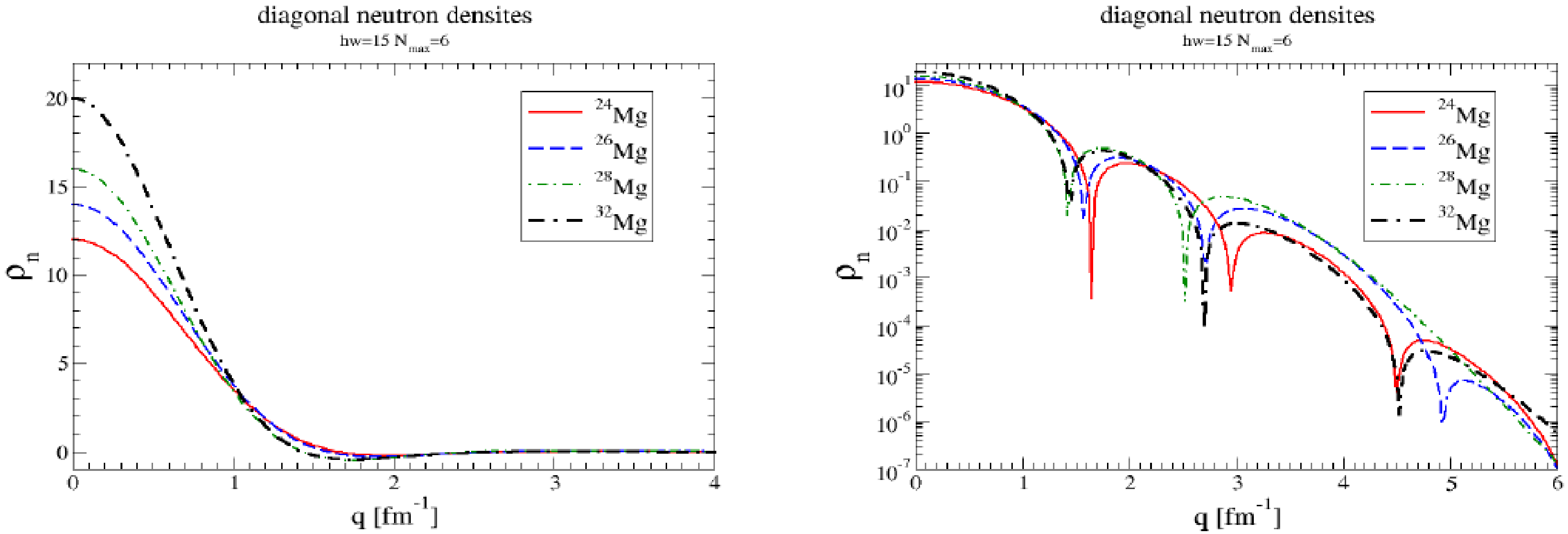



Figure 35: The diagonal neutron densities for $\hbar\omega$=15 and Nmax=6 for the Mg-isotopes we considered All calculations are based on the $\mathrm{NNLO_{opt}}$ potential and SA-NCSM densities They are plotted in linear as well as logarithmic scale.

# Diagonal densities (proton)

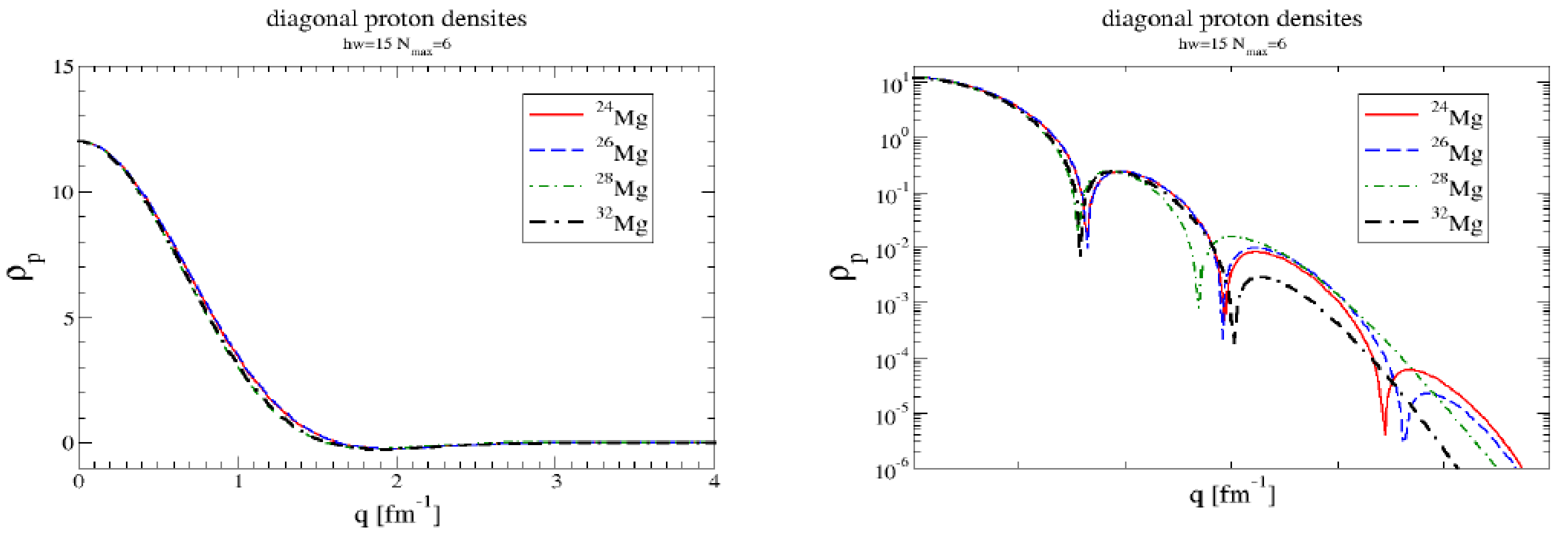



Figure 36: The diagonal neutron densities for $\hbar\omega$=15 and Nmax=6 for the Mg-isotopes we considered All calculations are based on the NNLO$_{opt}$ potential and SA-NCSM densities They are plotted in linear as well as logarithmic scale.