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INSTITUTE OF NUCLEAR & PARTICLE PHYSICS



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

Department of physics + astronomy

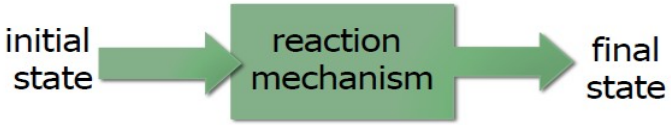
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Exploring Nuclei:
Specifically Exotic nuclei are usually short lived

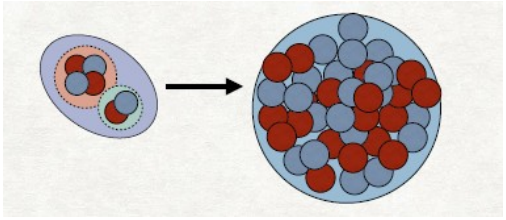
Thus one can only study them through reactions:

Have to be studied with reactions in inverse kinematics

direct reaction:



Many-body problem

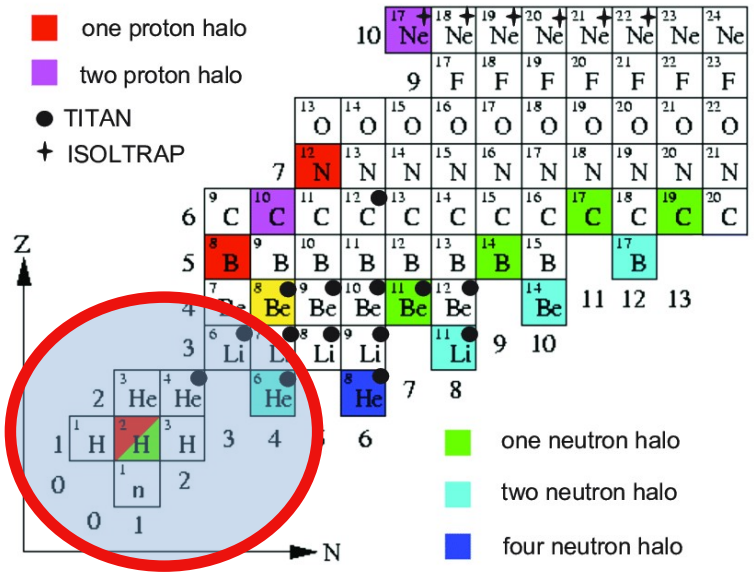


Quantum mechanical scattering problem

"idealist" approach: Just do it!

Not so fast!

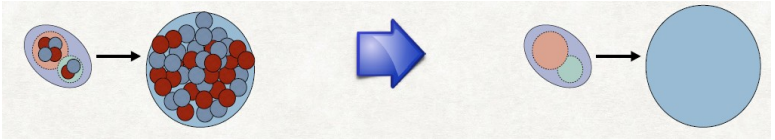
Chart of light nuclei



"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

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)

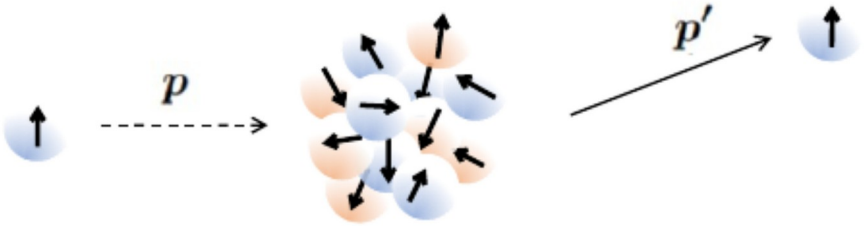
Chinn, Elster, Thaler, Weppner (1995)

Expansion in:

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

Intended for "fast reaction", i.e. ≳ 70 MeV

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



Ingredients:

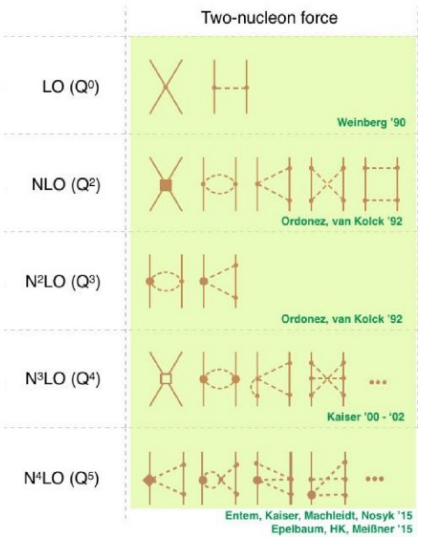
1) **realistic nuclear interaction**

must describe target and projectile

2) **controllable structure framework**

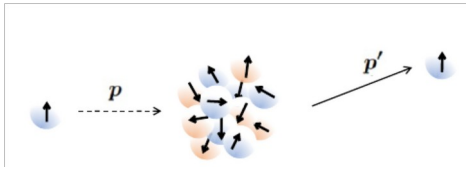
3) **controllable reaction framework**

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

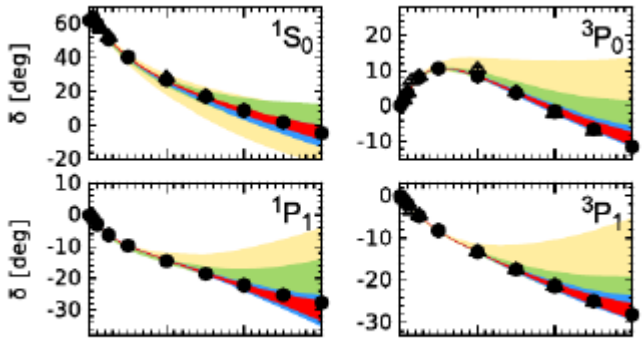
2) controllable structure framework

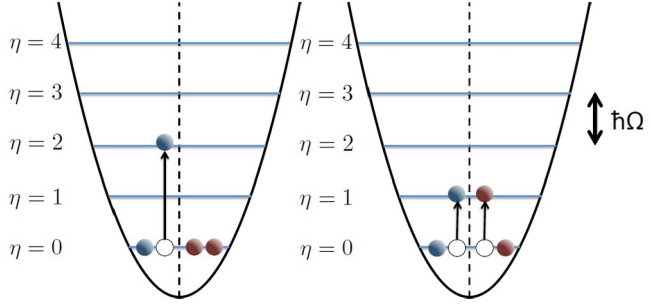
   here, no-core shell model (NCSM and SA-NCSM)

3) controllable reaction framework

   here, spectator expansion

4) a way to connect everything





	$E(^3\mathrm{H})$	$E(^3\mathrm{He})$	$E(^4\mathrm{He})$	$r_p(^4\mathrm{He})$
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)

Building up an *ab initio* framework

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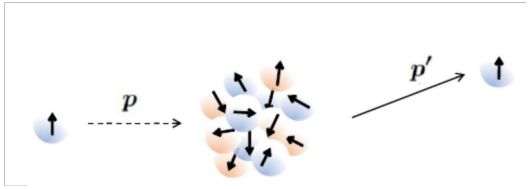
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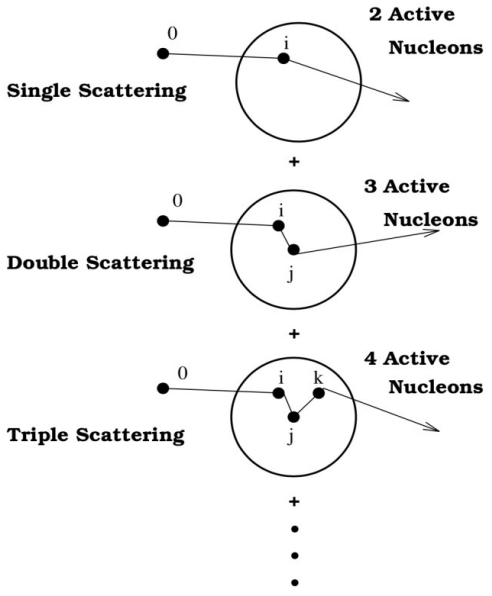
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here, spectator expansion of

Watson multiple scattering series

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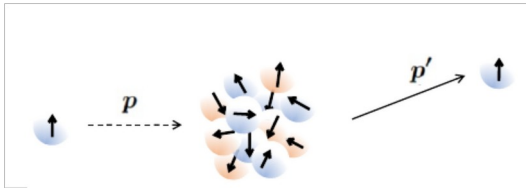
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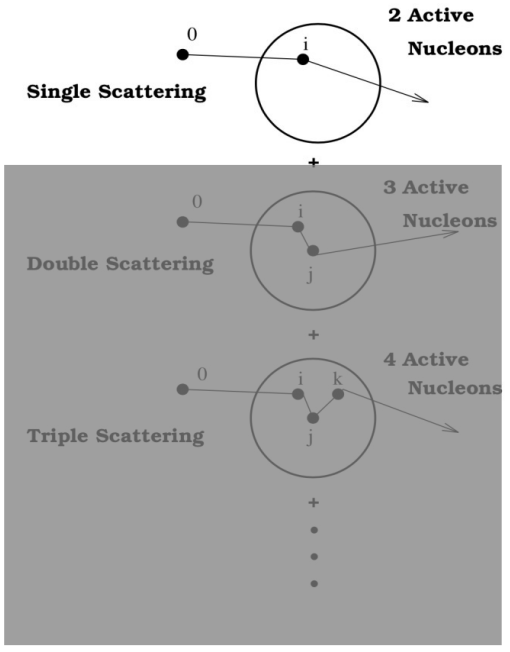
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Leading order in spectator expansion can be computed *ab initio*

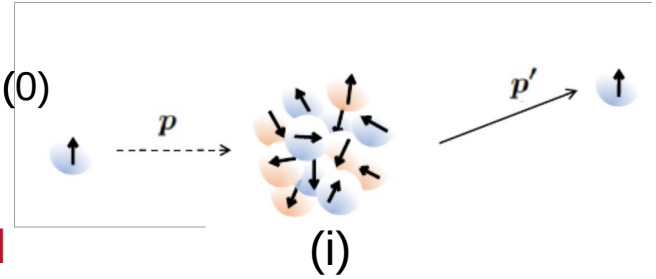
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Ekström et al., PRL 110, 192502 (2013)

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**



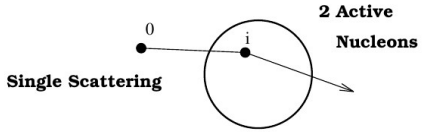
$$\begin{aligned}
\overline{M}(\boldsymbol{q},\boldsymbol{\mathcal{K}}_{NN},\epsilon) &= A(\boldsymbol{q},\boldsymbol{\mathcal{K}}_{NN},\epsilon)\mathbf{1}\otimes\mathbf{1}\\
&+ iC(\boldsymbol{q},\boldsymbol{\mathcal{K}}_{NN},\epsilon)\left(\boldsymbol{\sigma}^{(0)}\cdot\hat{\boldsymbol{n}}\right)\otimes\mathbf{1}\\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

$$\boldsymbol{q} = \boldsymbol{p}' - \boldsymbol{p}$$
$$\boldsymbol{\mathcal{K}} = \frac{1}{2}(\boldsymbol{p}' + \boldsymbol{p})$$
$$\hat{\boldsymbol{n}} = \frac{\boldsymbol{\mathcal{K}}\times\boldsymbol{q}}{|\boldsymbol{\mathcal{K}}\times\boldsymbol{q}|}$$

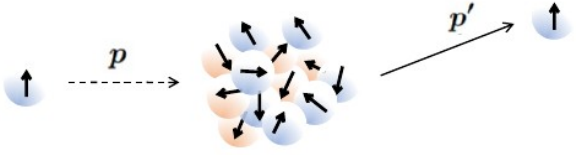
A: central
C: spin-orbit
M, G, H: tensor

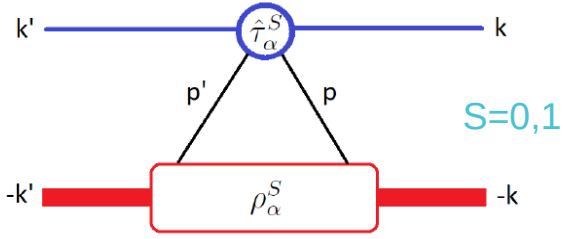
Most general structure of NN amplitudes consistent with invariance principles

Computing the leading order effective potential



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





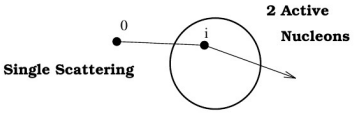
scatter off nucleus with 0^+ ground state

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

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)

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

matter distribution = density

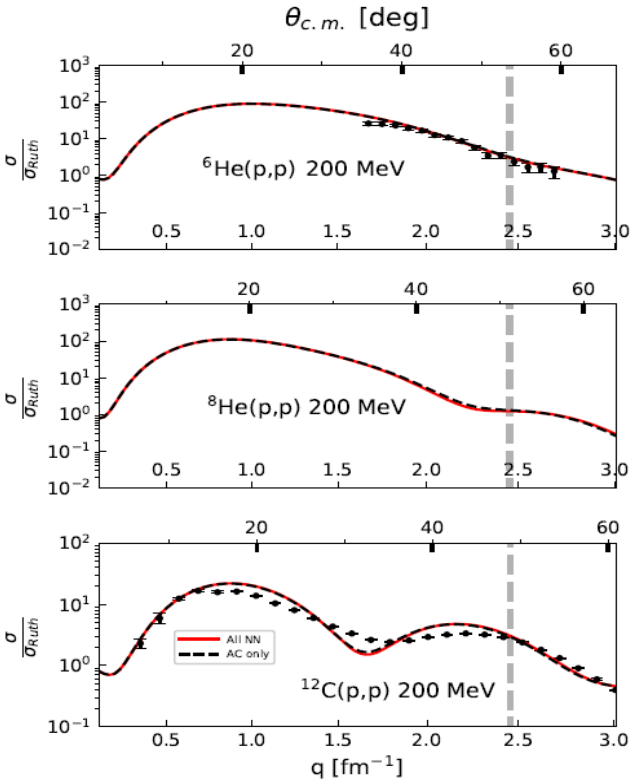
spin-projected momentum distribution

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

N_{max}=18

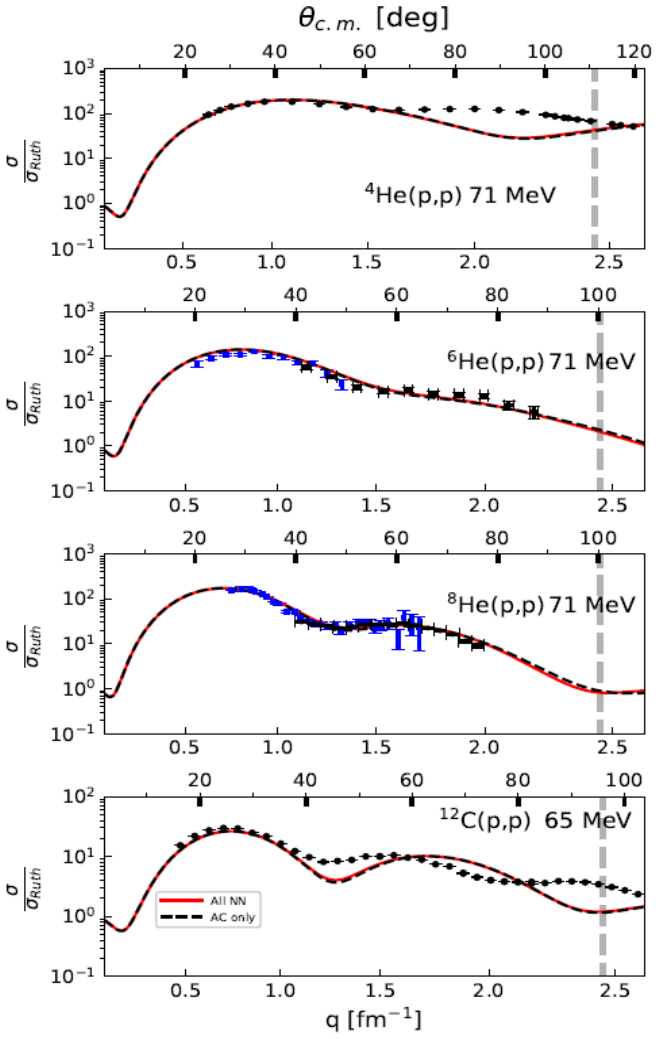
N_{max}=12



NCSM ħω=20 MeV

$NNLO_{opt}$

Chiral interaction



N_{max}=18

N_{max}=12

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

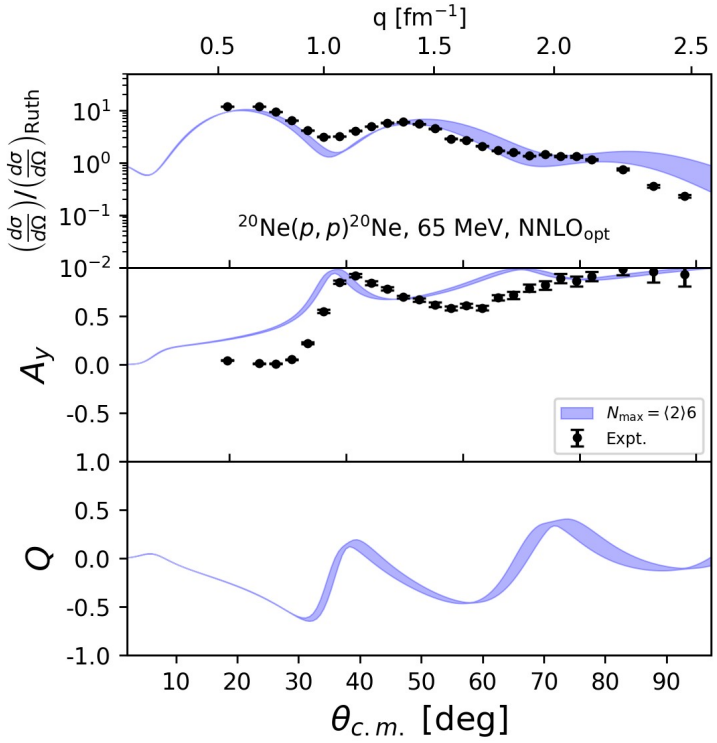
Department of physics + astronomy

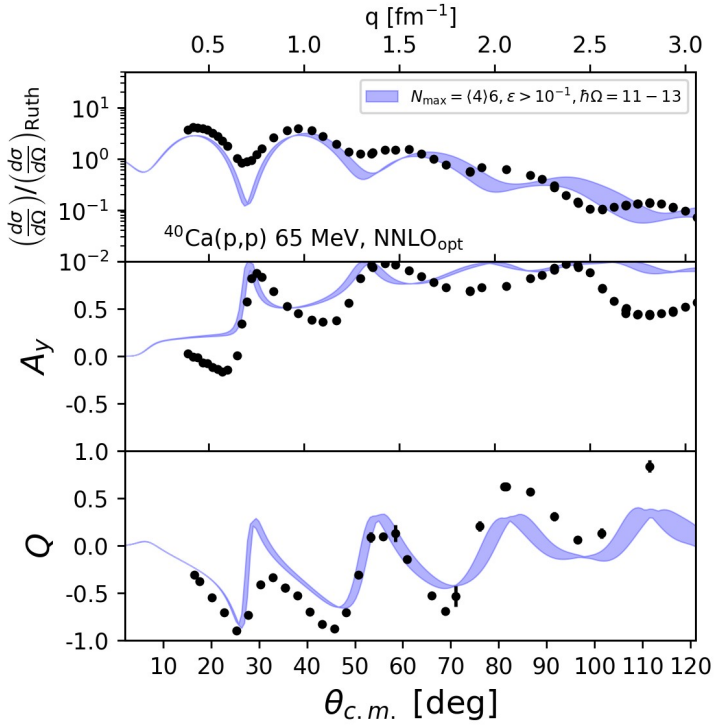
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Similar observation with SA-NCSM One-Body Densities

$NNLO_{opt}$ chiral potential

ħω=13-17 MeV





ħω=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

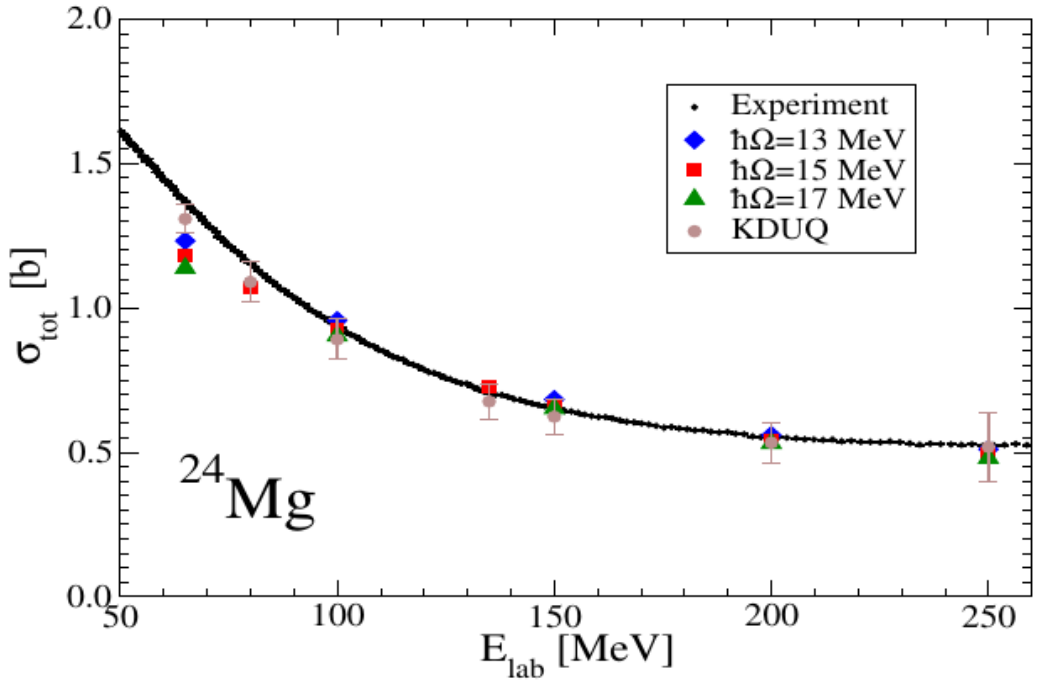
C. D. Pruitt,* J. E. Escher, and R. Rahman†
Lawrence Livermore National Laboratory, Livermore, California 94550, USA

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

VALIDATION

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



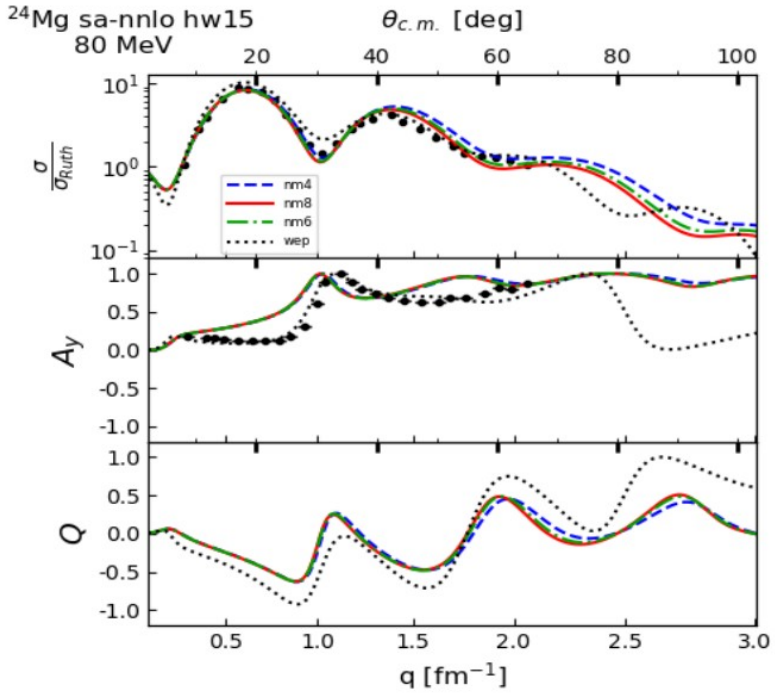
Ab initio calculation employs **NNLO$_{opt}$ chiral potential**

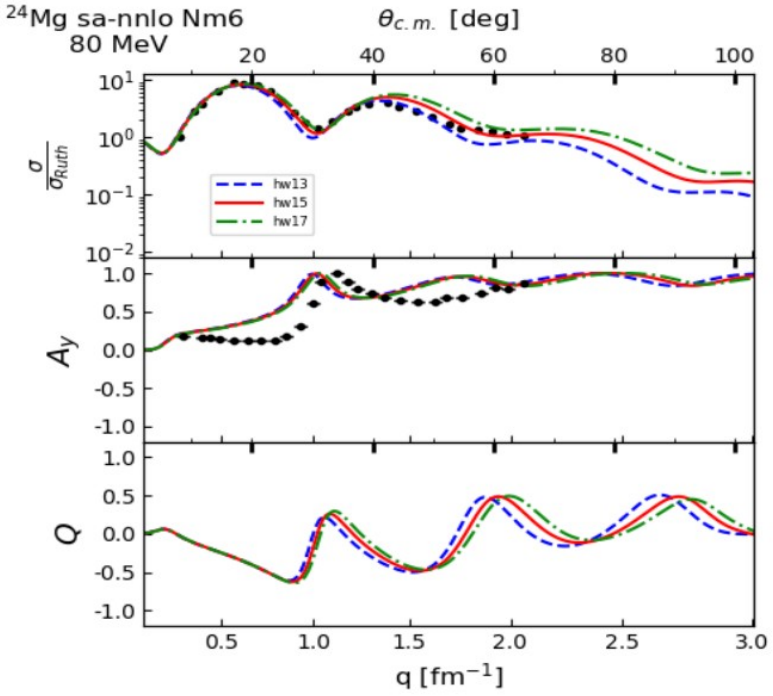
KDUQ: Koning-Delaroche phenomenological optical potential with Uncertainty Quantification

Experiment: W.P. Abfalterer et al.

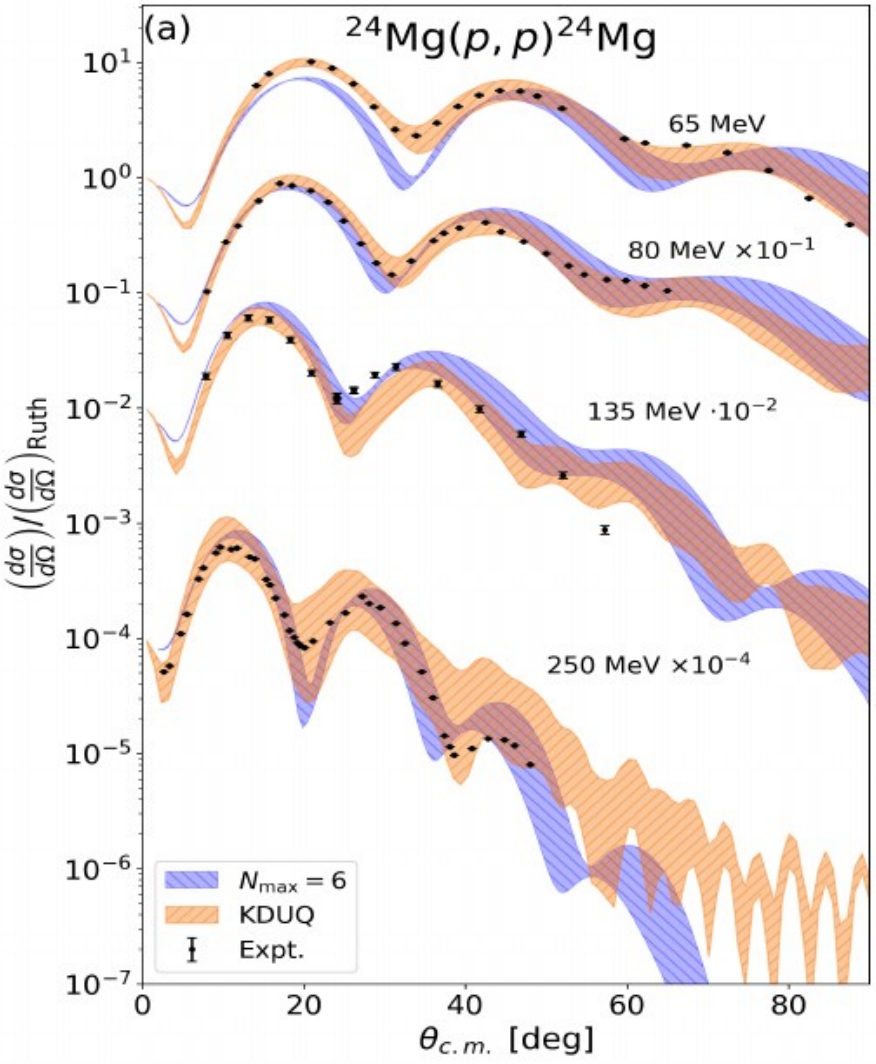
Phys.Rev.C 62 (2000) 064312

Start and anchor on ^{24}Mg

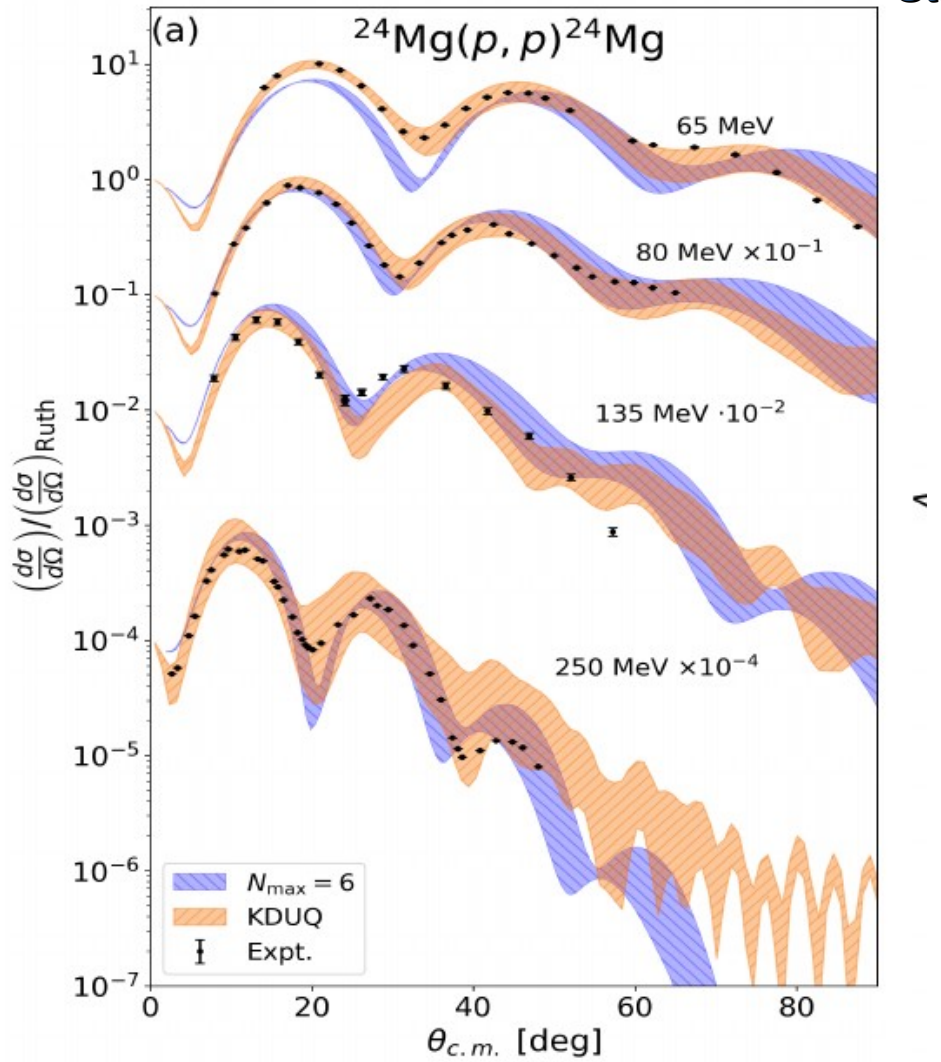


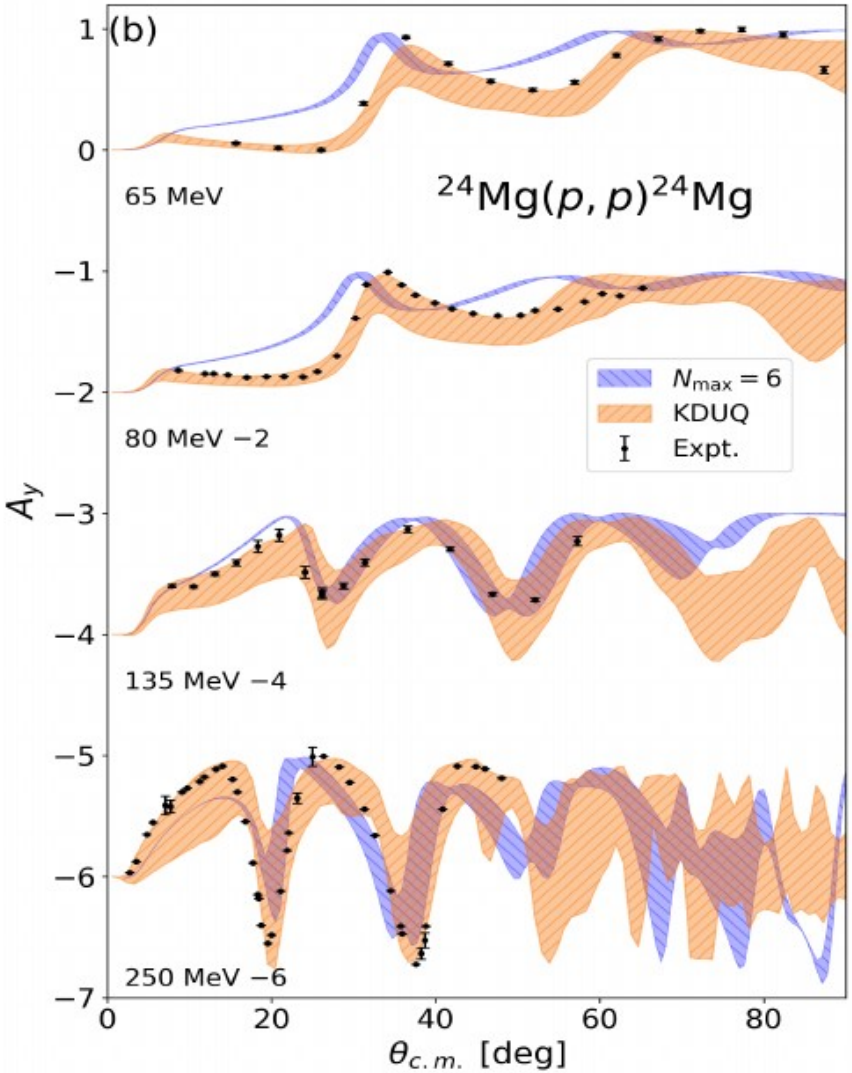


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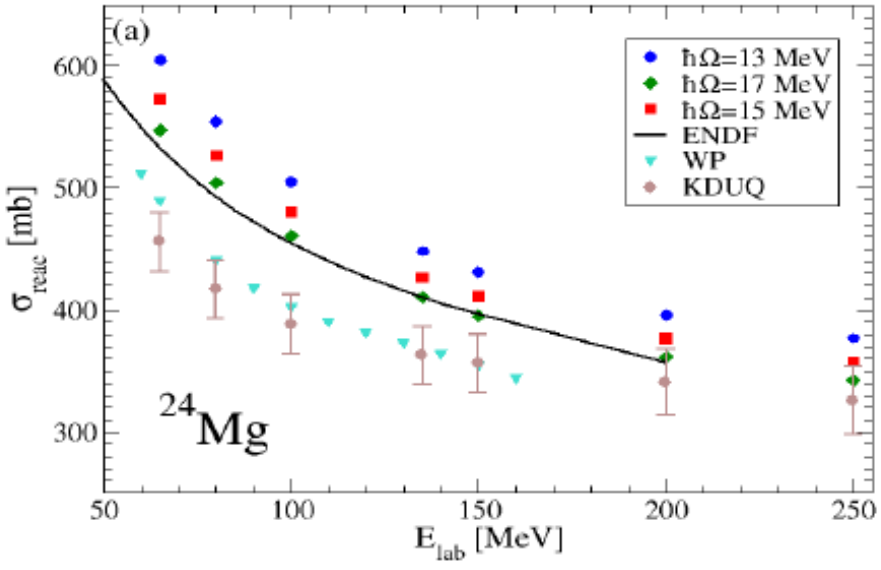


Start and ancho on ^{24}Mg

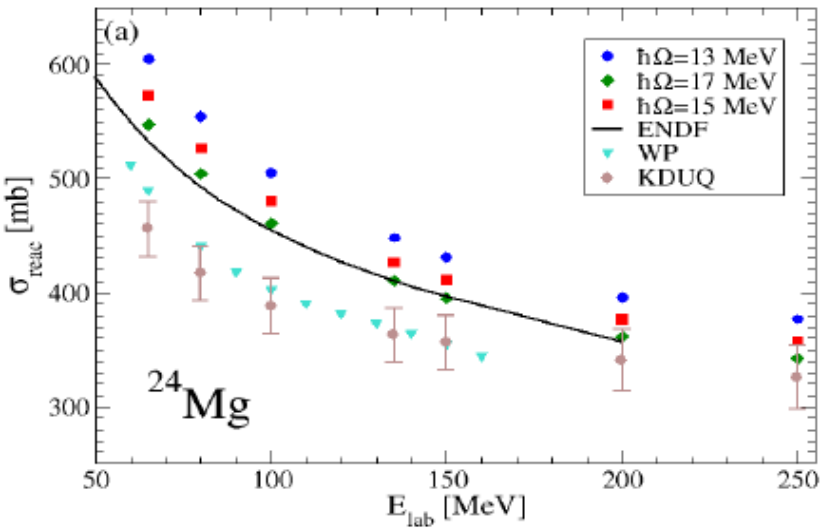


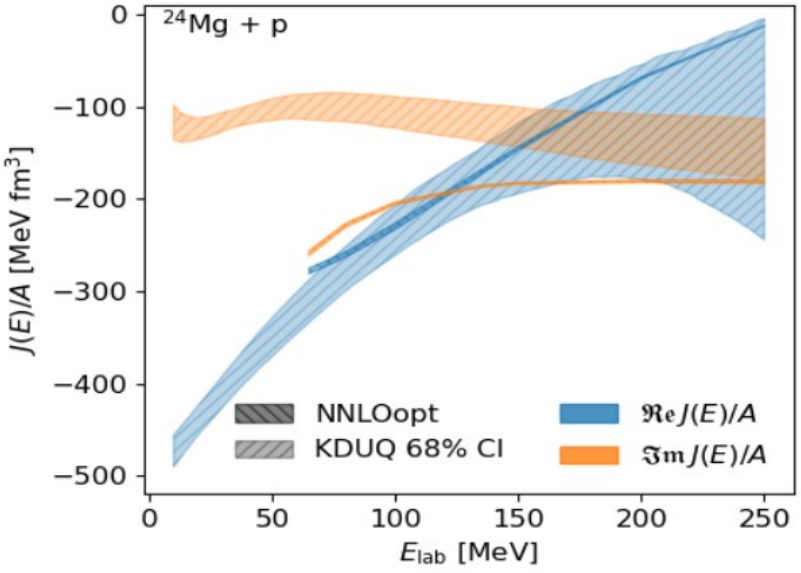


Reaction cross sections

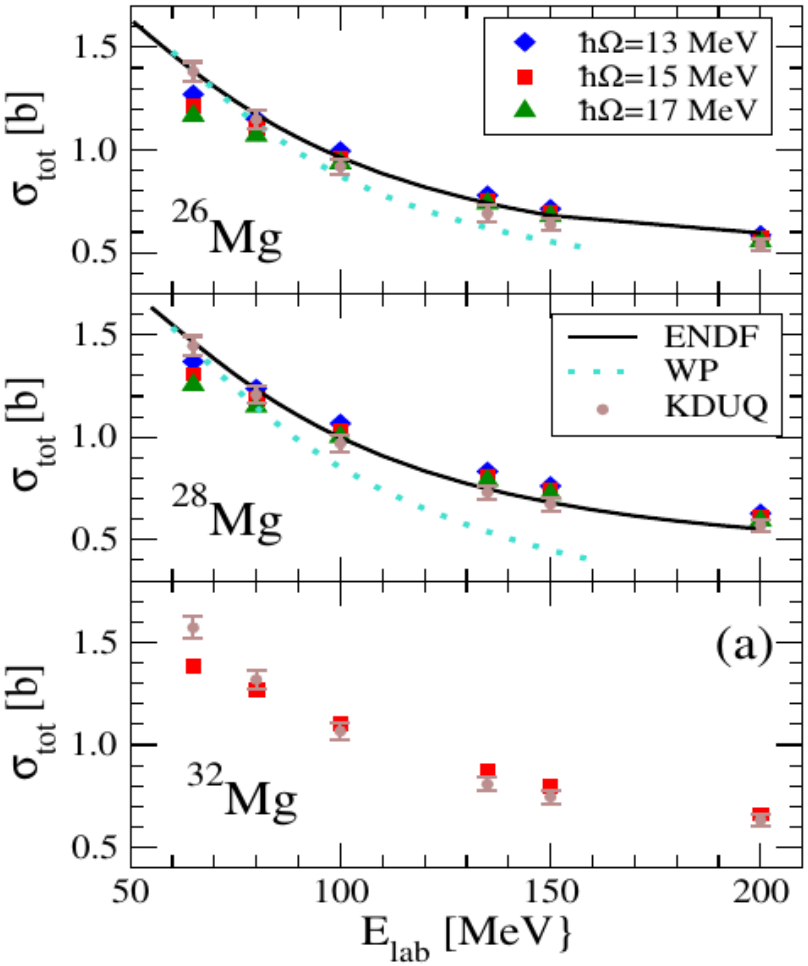


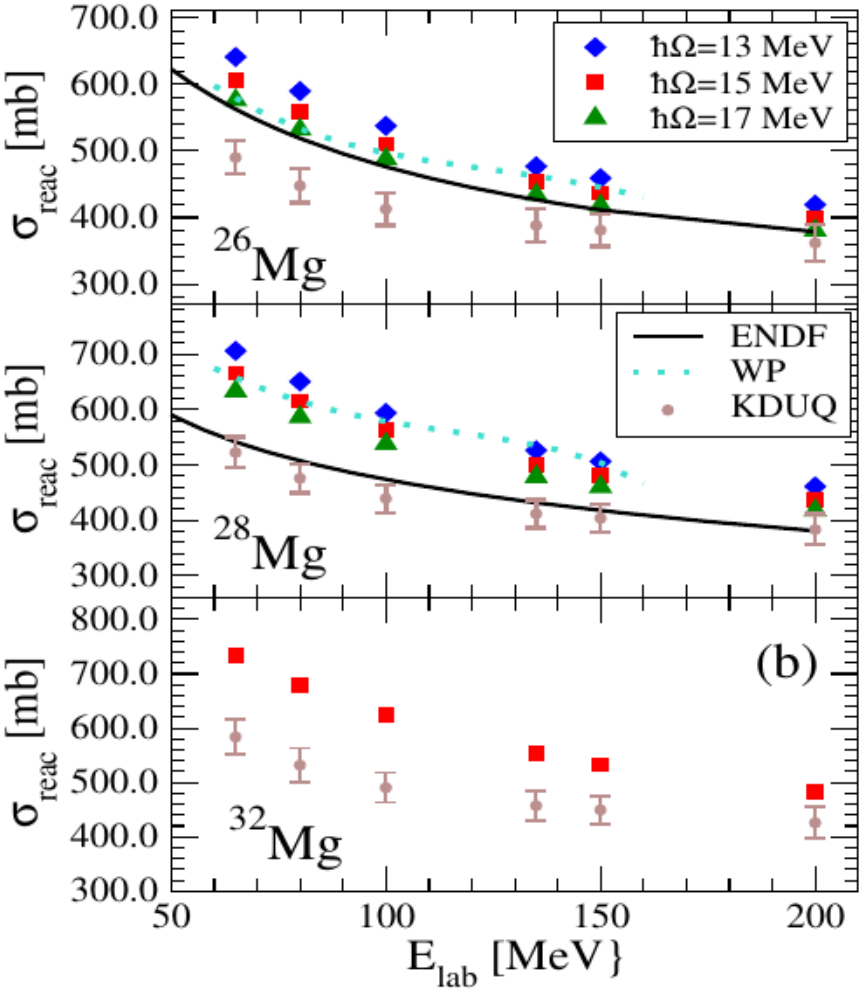
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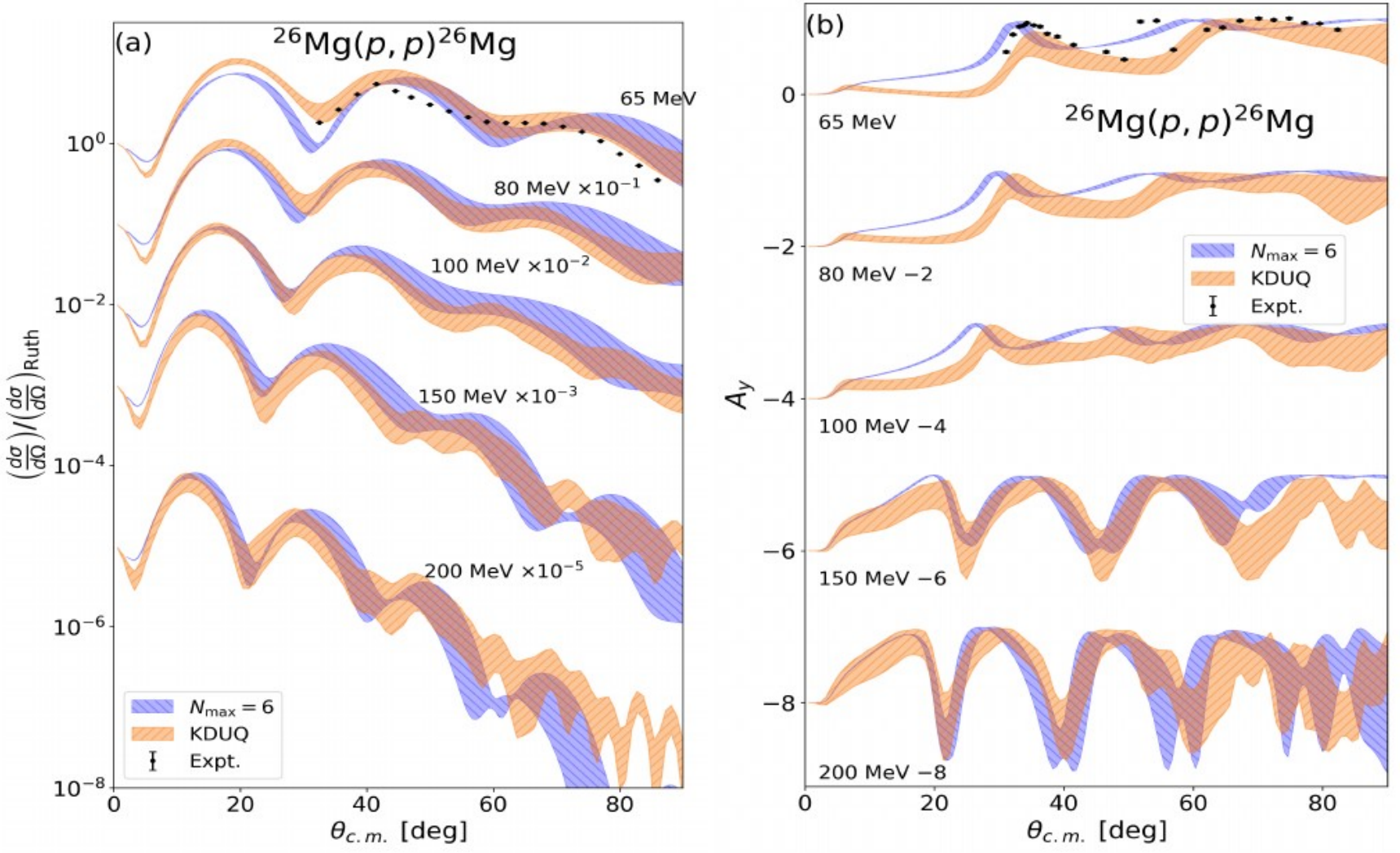


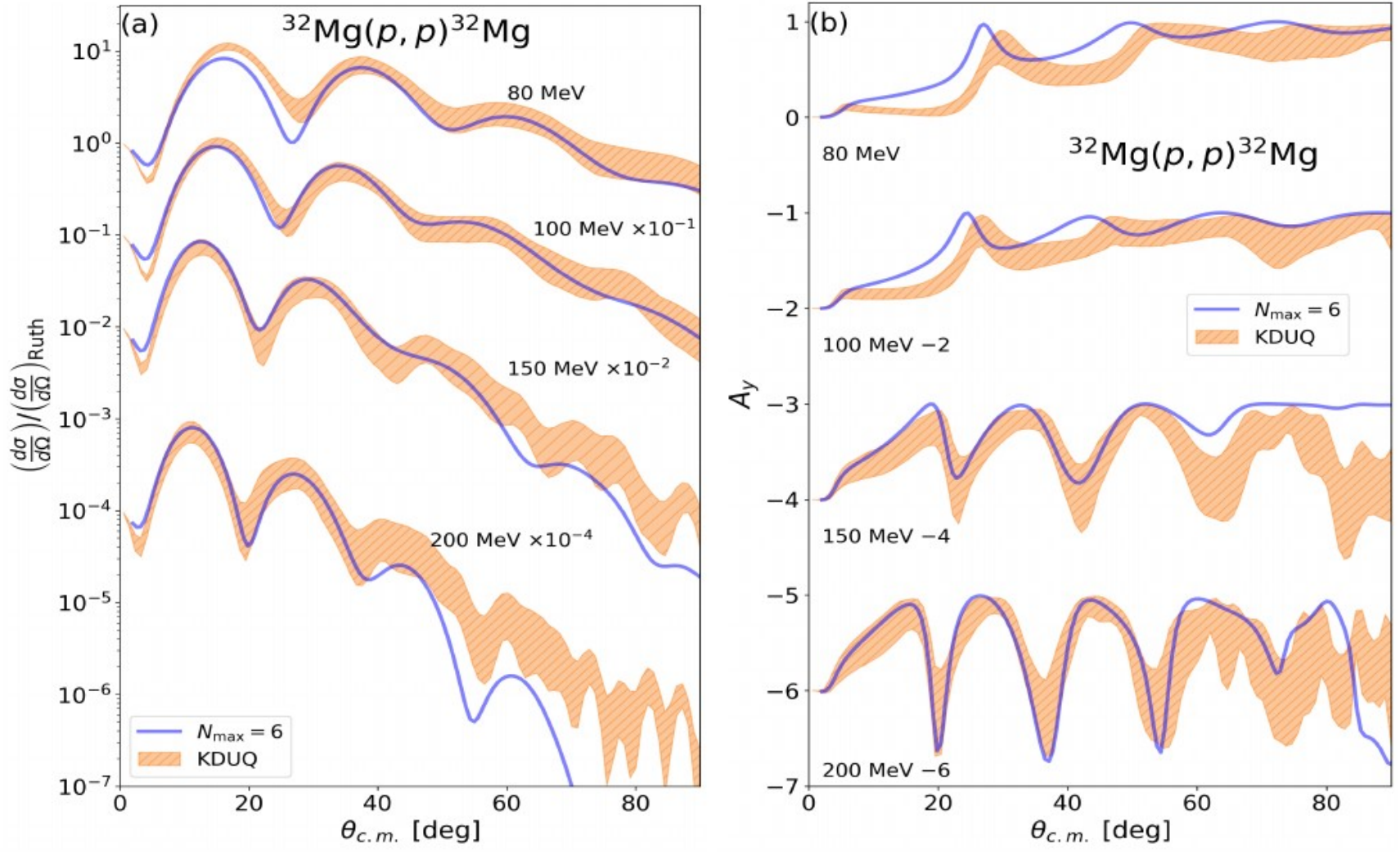


Neutron total cross and proton reaction cross sections for Mg isotopes






(a)
^{26}Mg$(p,p)^{26}$Mg
65 MeV
80 MeV ×10^{-1}
100 MeV ×10^{-2}
150 MeV ×10^{-3}
200 MeV ×10^{-5}
$N_{max} = 6$
KDUQ
Expt.
$\left(\frac{d\sigma}{d\Omega}\right)/\left(\frac{d\sigma}{d\Omega}\right)_{Ruth}$
$\theta_{c.m.}$ [deg]
(b)
^{26}Mg$(p,p)^{26}$Mg
65 MeV
80 MeV −2
100 MeV −4
150 MeV −6
200 MeV −8
$N_{max} = 6$
KDUQ
Expt.
A_y
$\theta_{c.m.}$ [deg]


(a)
^{32}Mg$(p,p)^{32}$Mg
80 MeV
100 MeV ×10^{-1}
150 MeV ×10^{-2}
200 MeV ×10^{-4}
$N_{max} = 6$
KDUQ
$\left(\frac{d\sigma}{d\Omega}\right)/\left(\frac{d\sigma}{d\Omega}\right)_{Ruth}$
$\theta_{c.m.}$ [deg]
(b)
^{32}Mg$(p,p)^{32}$Mg
80 MeV
100 MeV −2
150 MeV −4
200 MeV −6
$N_{max} = 6$
KDUQ
A_y
$\theta_{c.m.}$ [deg]

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)

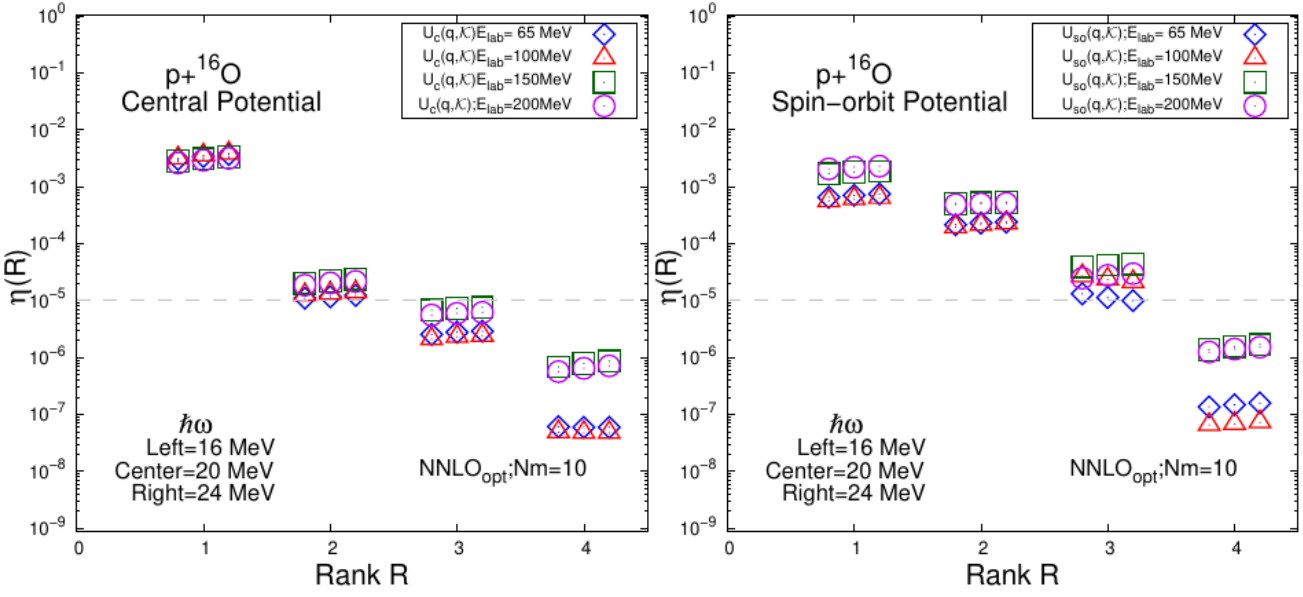
- **Carried out study of Mg isotopes:**
  Calculations for ^{24}Mg compare favorably to experiment
  Confidence in predicting ^{26}Mg, ^{28}Mg, and ^{32}Mg

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

Outlook: Opportunities for *ab initio* optical potentials in the era of ML

$\widehat{U}_{\rm p}(\boldsymbol{q}, \boldsymbol{\mathcal{K}}_{NA}; \epsilon)$ nearly independent of angle between q and $K_{\rm NA}$

Take 90° slice given by on-shell condition $q^2 + 4\mathcal{K}^2 = 4k_0^2$ and perform SVD



$$\eta(R) = 1 - \mathrm{PV}(R)$$

Preserved variance:

$$\mathrm{PV}(R) \equiv \frac{\sum_{i=1}^{R} \sigma_i^2}{\sum_{i=1}^{N} \sigma_i^2}$$

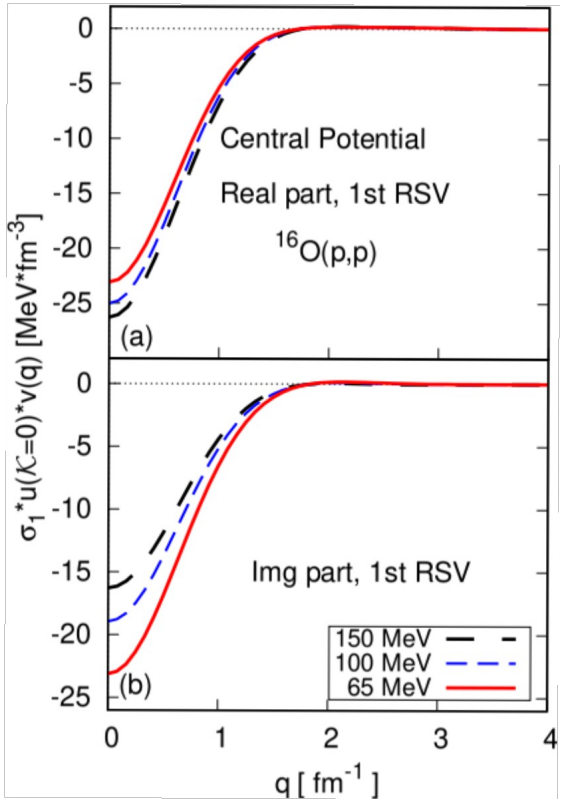
$\eta(R)$ does not depend on the scattering energy

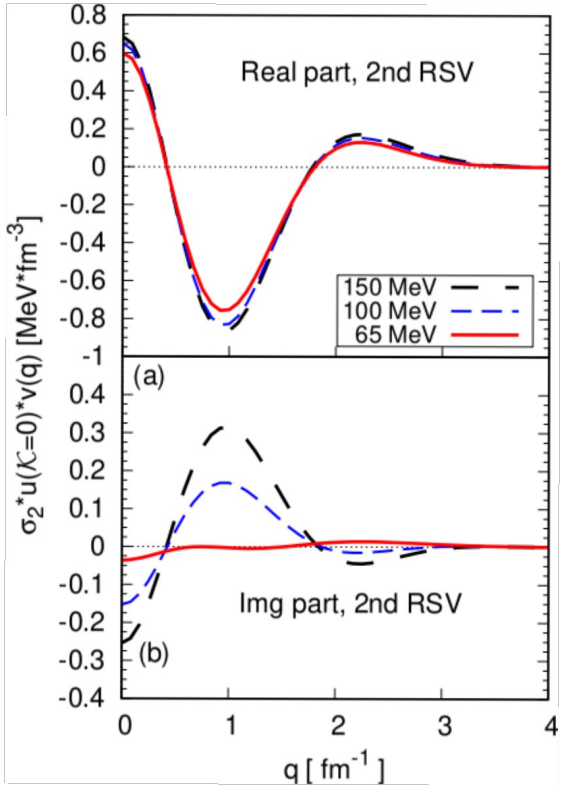
Department of physics + astronomy

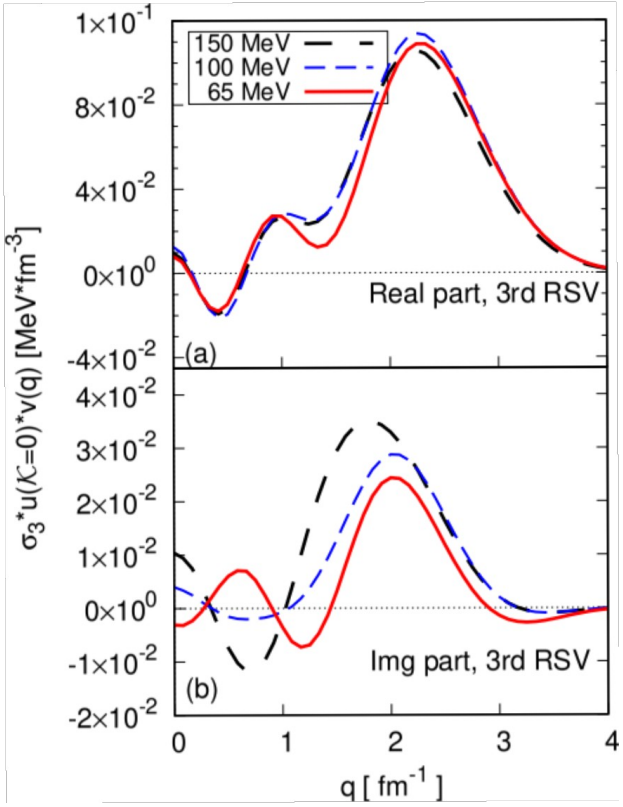
OHIO UNIVERSITY

Outlook: Opportunities for *ab initio* optical potentials in the era of ML

SVD eigenvectors as function of *q*:

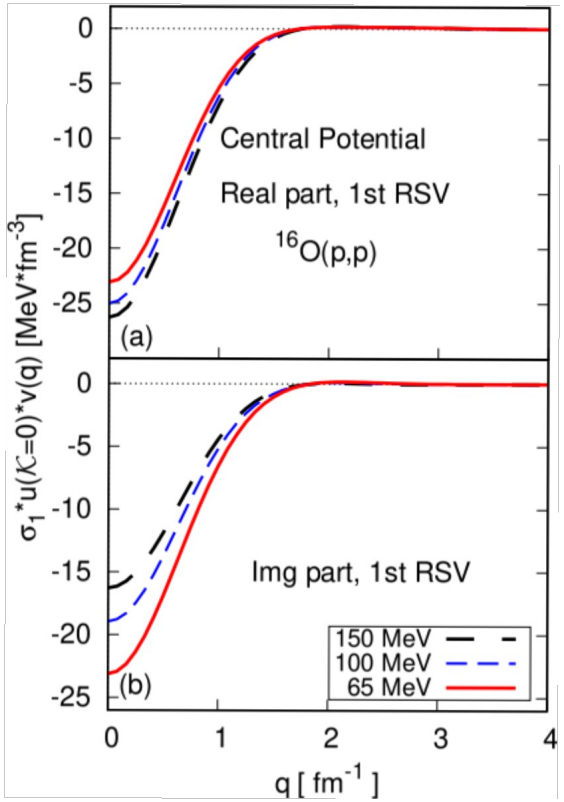


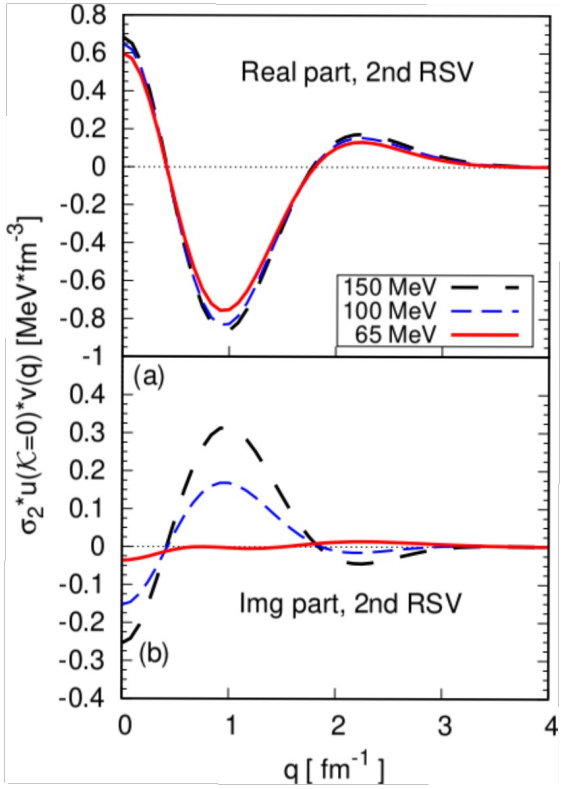


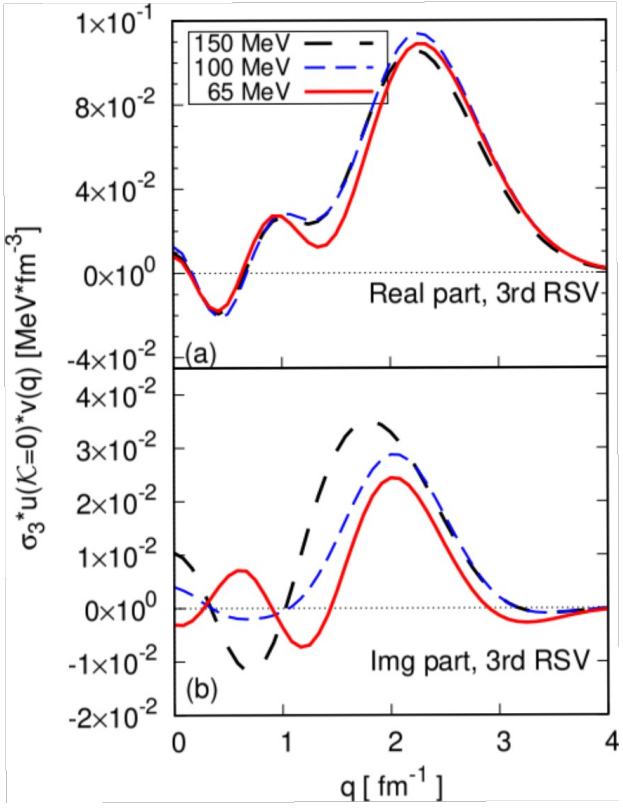


Outlook: Opportunities for *ab initio* optical potentials in the era of ML

SVD eigenvectors as function of *q*:

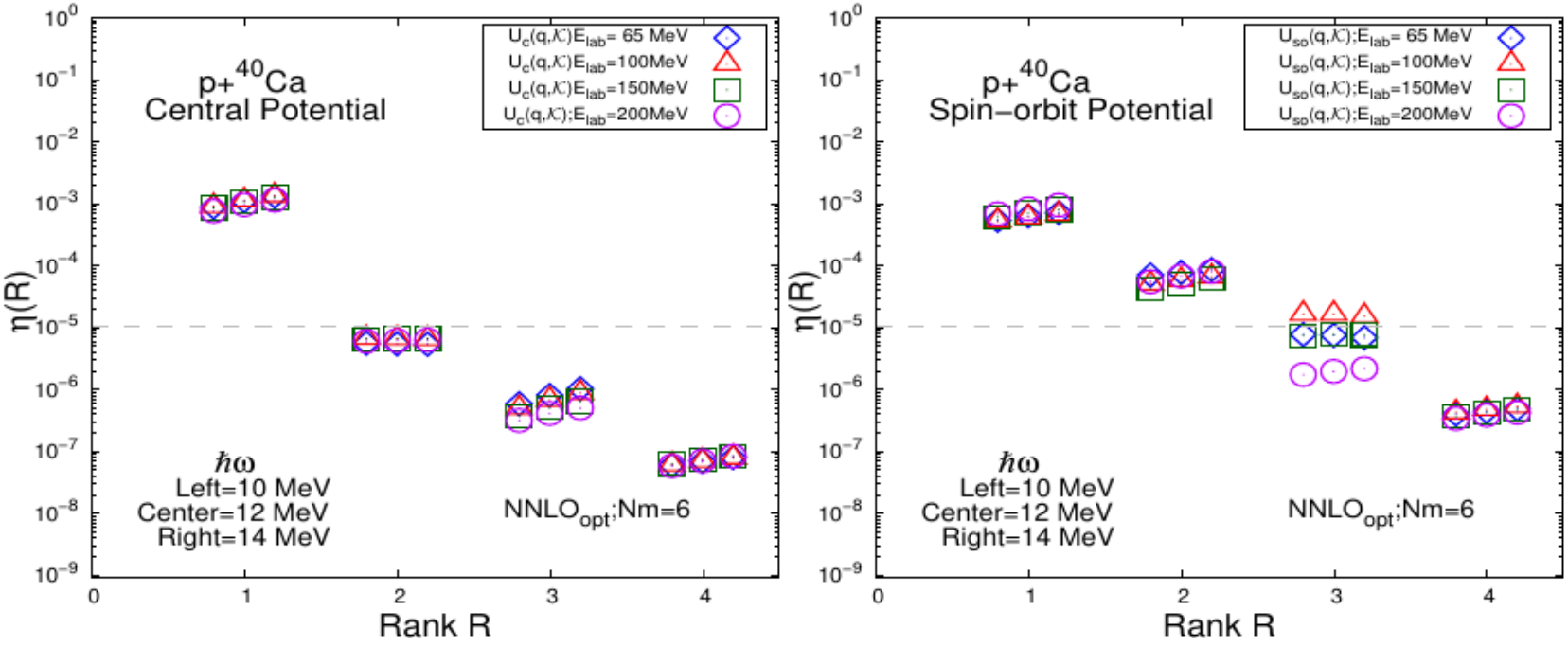






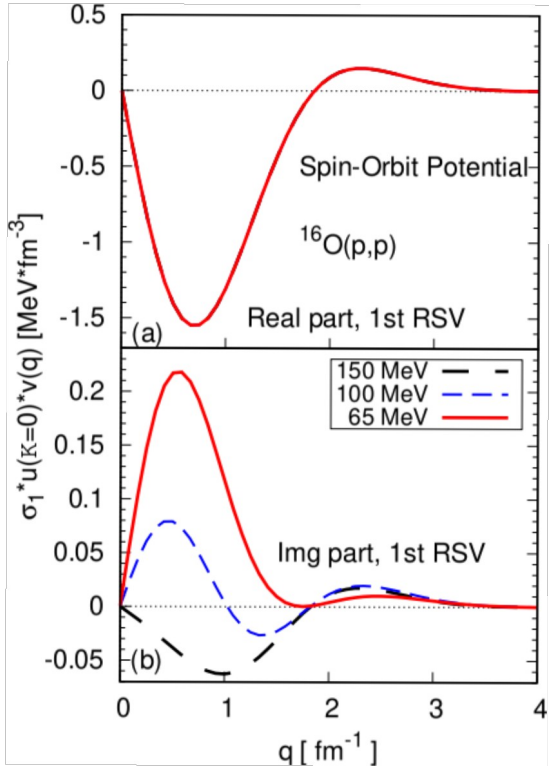
Backup slides

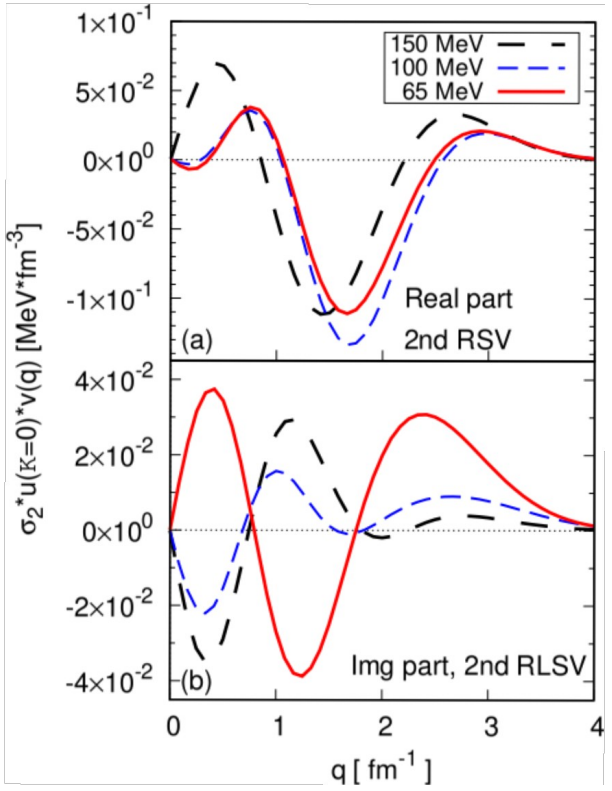
SVD decomposition of off-shell *ab initio* optical potential

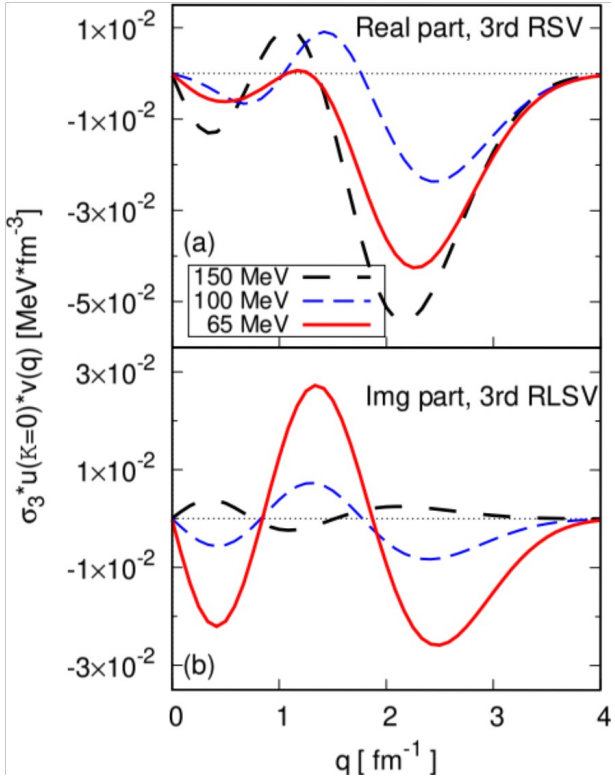


Outlook: Opportunities for *ab initio* optical potentials in the era of ML

SVD eigenvectors as function of *q*:

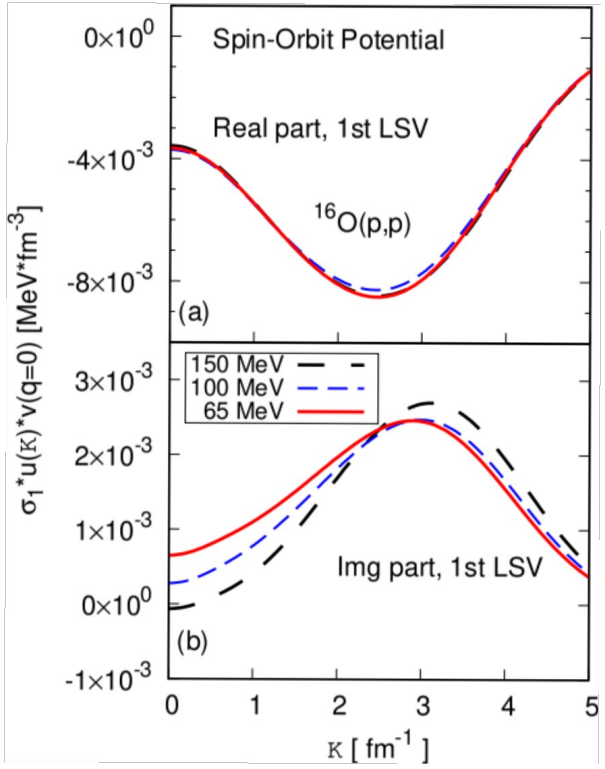


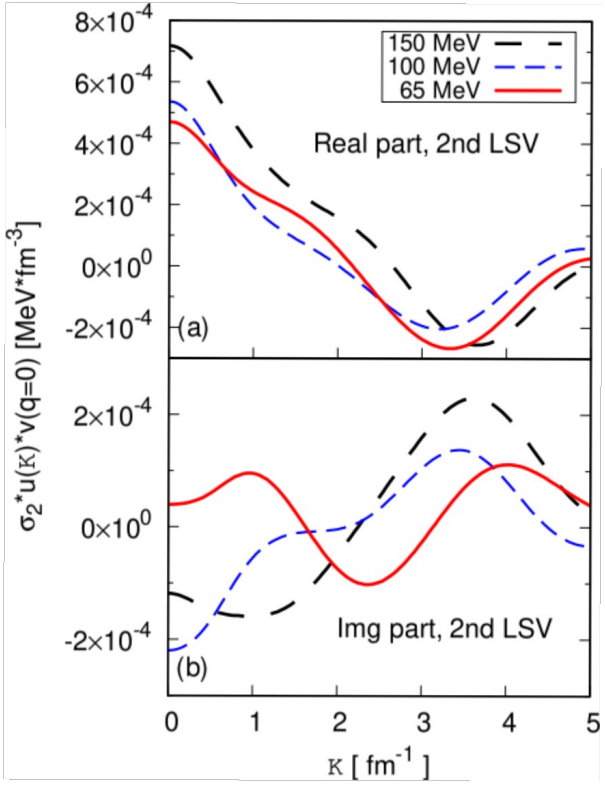


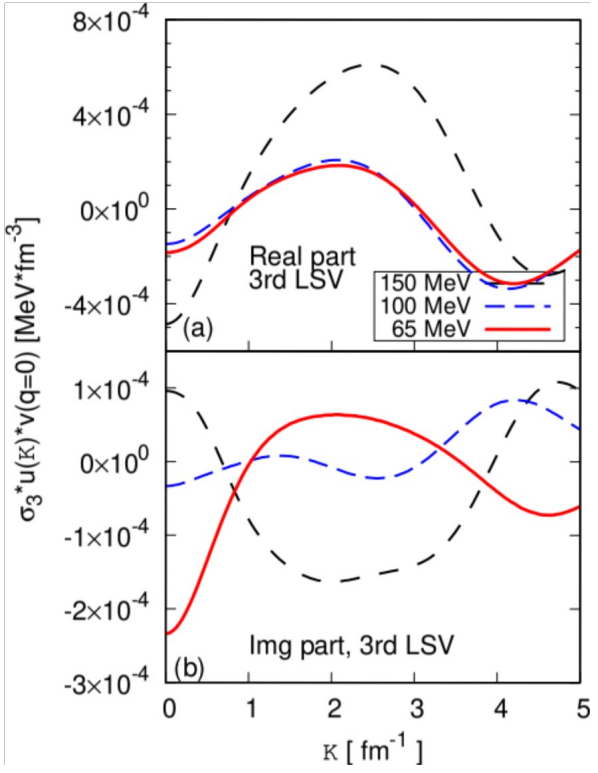


Outlook: Opportunities for *ab initio* optical potentials in the era of ML

SVD eigenvectors as function of *K*:







Diagonal densities (CoM)

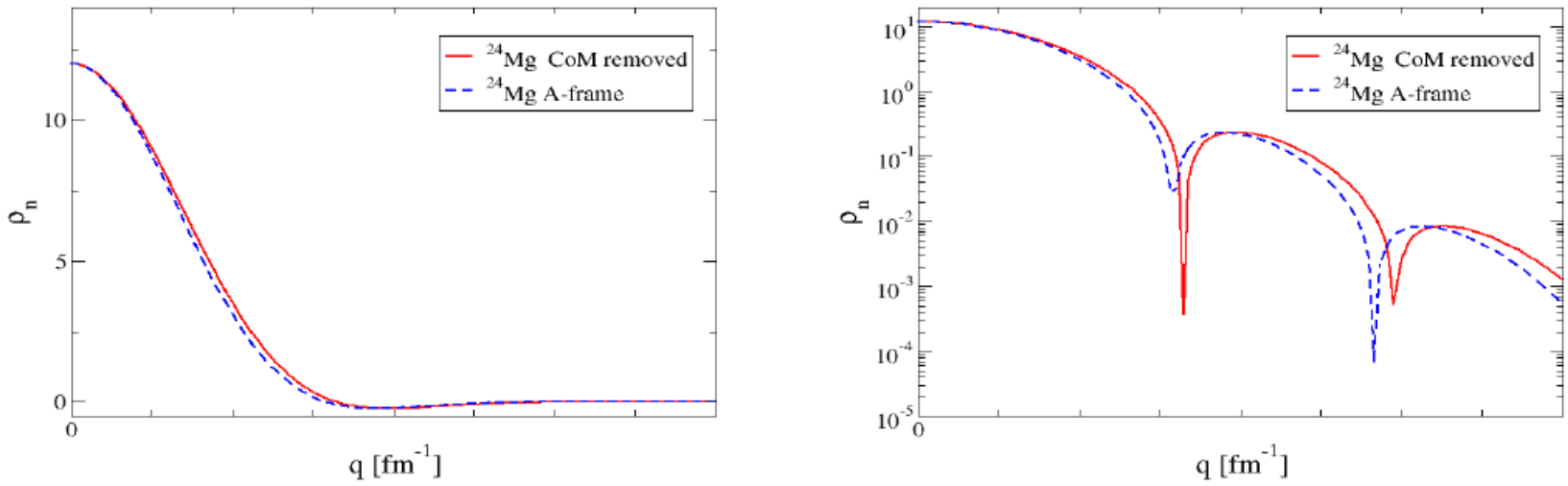


Figure 3: The diagonal one-body neutron densities for ^{24}Mg for $\hbar\omega$=15 and N_{max}=6. Shown is the diagonal density for a calculation where the CoM is removed vs a calculation in the A-frame.

Diagonal densities (CoM)

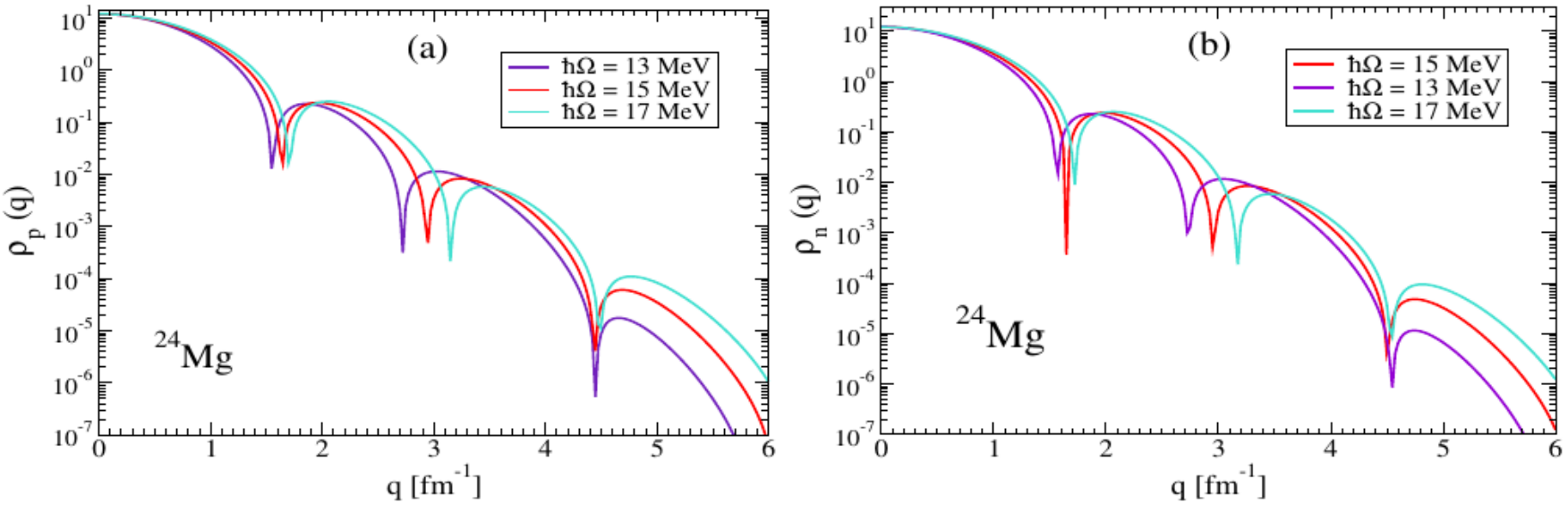


Figure 10. The diagonal one-body (a) proton and (b) neutron densities vs. momentum transfer for ^{24}Mg for $N_{\max}$=6 and $\hbar\Omega$=13, 15, and 17 MeV.

Diagonal densities (neutron)

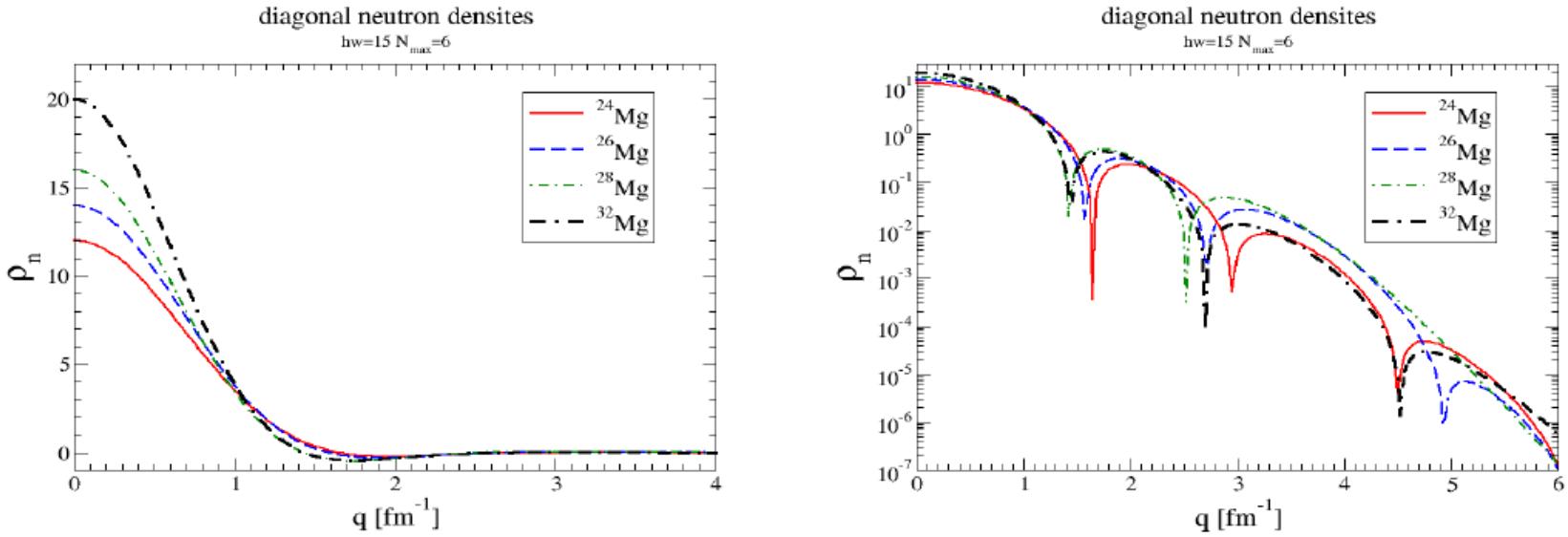


Figure 35: The diagonal neutron densities for $\hbar\omega$=15 and Nmax=6 for the Mg-isotopes we considered All calculations are based on the $\mathrm{NNLO_{opt}}$ potential and SA-NCSM densities They are plotted in linear as well as logarithmic scale.

Diagonal densities (proton)

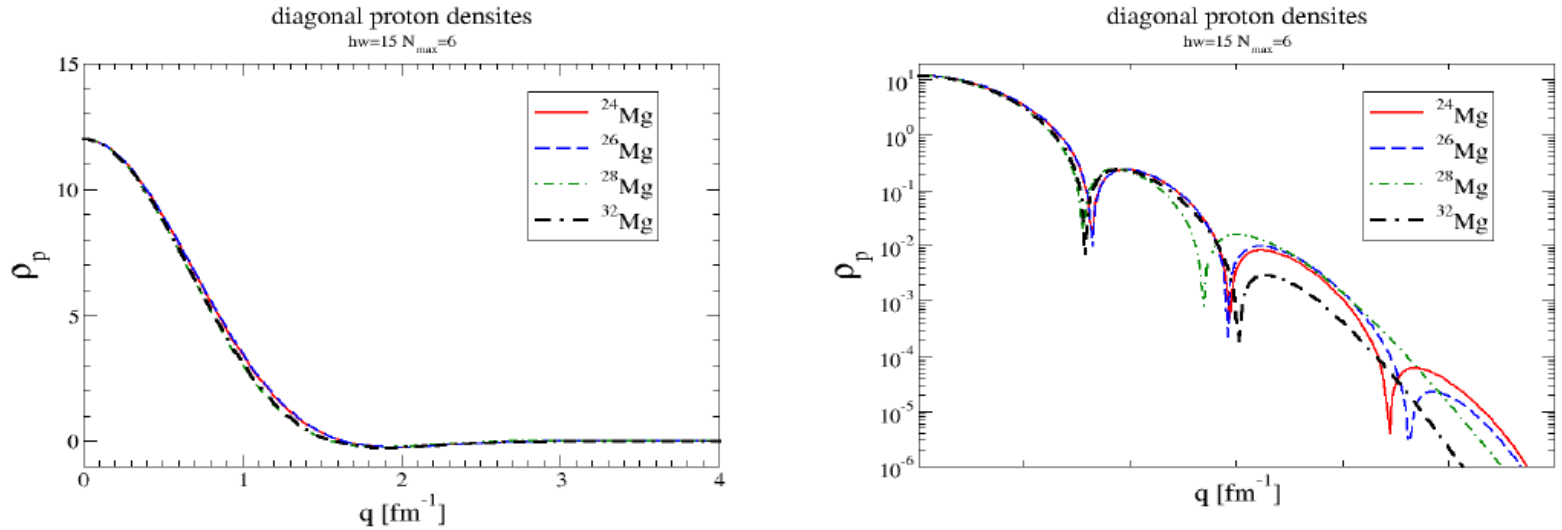


Figure 36: The diagonal neutron densities for $\hbar\omega$=15 and Nmax=6 for the Mg-isotopes we considered All calculations are based on the $\mathrm{NNLO_{opt}}$ potential and SA-NCSM densities They are plotted in linear as well as logarithmic scale.

Volume Integrals

