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INSTITUTE OF NUCLEAR & PARTICLE PHYSICS

No-Core Shell Model Densities and *ab initio* effective Potentials for elastic Nucleon-Nucleus Scattering

Charlotte Elster

Thanks to collaborators:

R.B. Baker, M. Burrows S.P. Weppner, K. Launey, P. Maris, G. Popa

Supported by

U.S. DEPARTMENT OF ENERGY
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NERSC National Energy Research Scientific Computing Center

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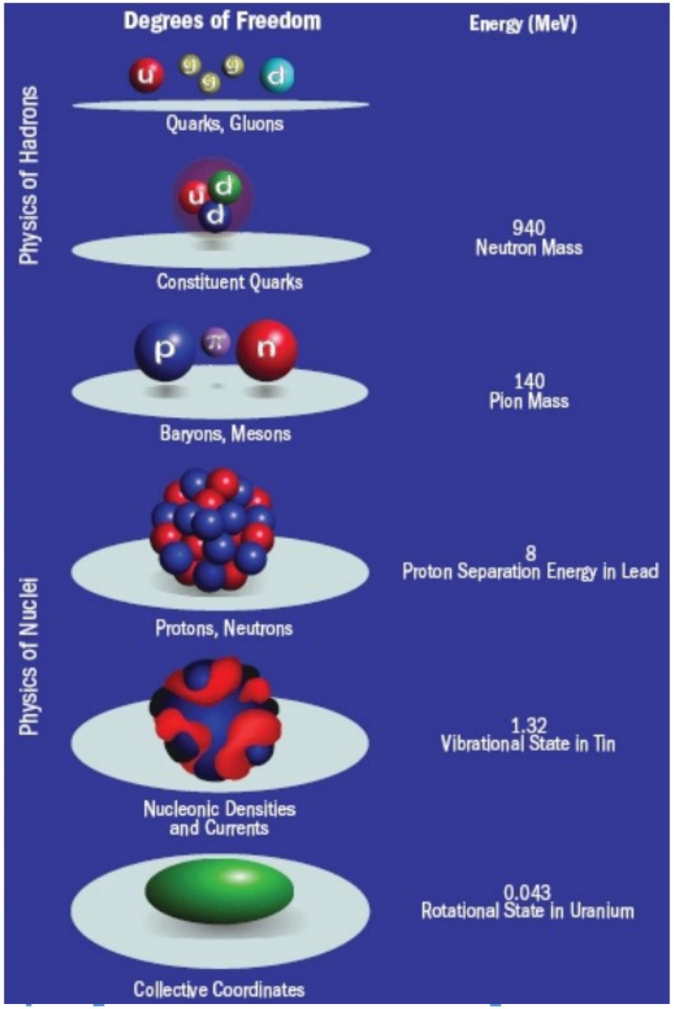
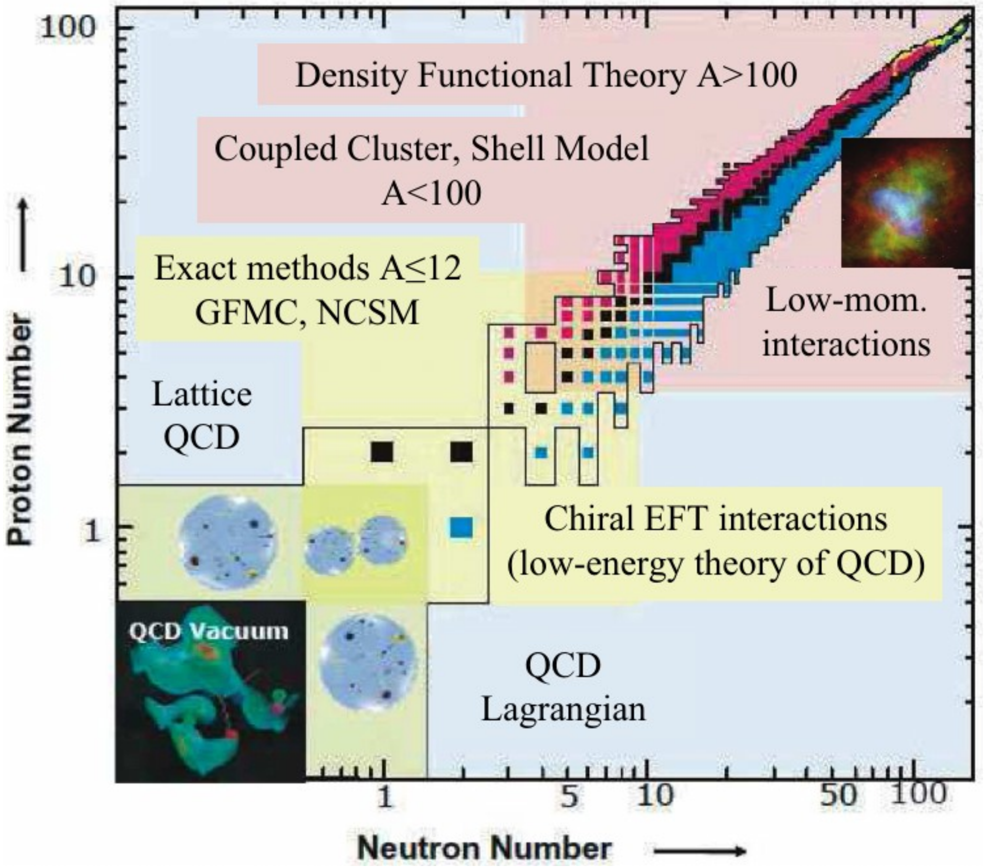
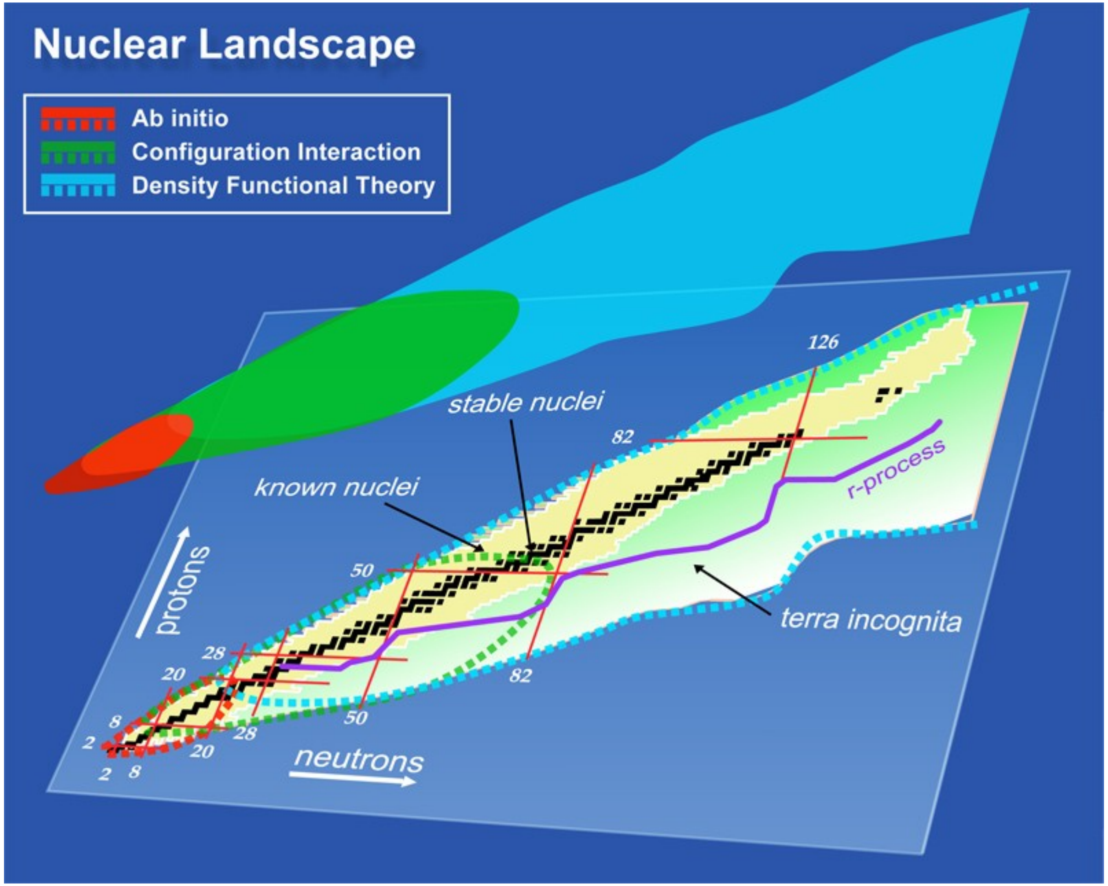
The big picture: from QCD to Nuclei







Goal:

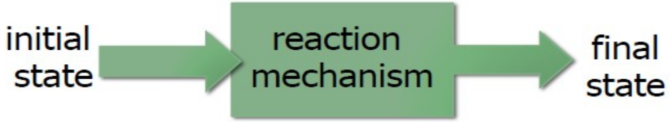
- Understand the richness of the nuclear landscape
- Most nuclei in this landscape are unstable
- Properties are experimentally mostly discovered/determined by nuclear reactions.
- Specifically, unstable nuclei can not be target material and must be studied in inverse kinematics.

Exploring Nuclei:
Specifically Exotic nuclei are usually short lived

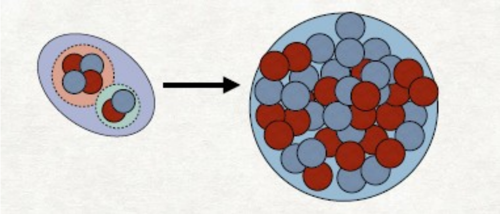
Thus one can only study them through reactions:

Have to be studied with reactions in inverse kinematics

direct reaction:



Many-body problem

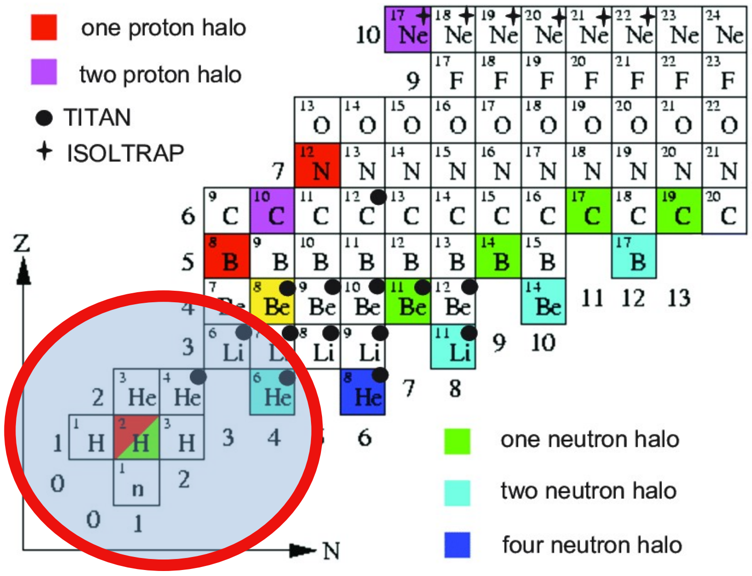


Quantum mechanical scattering problem

“idealist” approach: Just do it!

Not so fast!

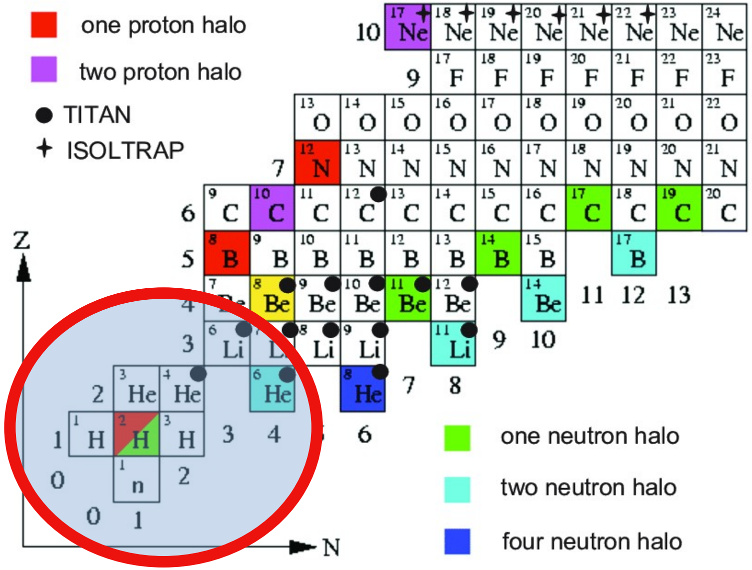
Chart of light nuclei



"Idealists" current domain

Not so fast!

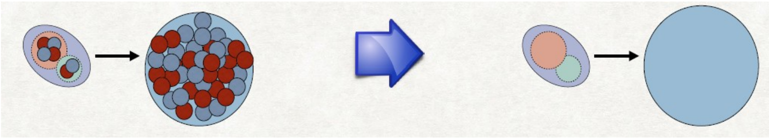
Chart of light nuclei



"Idealists" current domain

For heavier nuclei:

A more "pragmatic" approach is needed

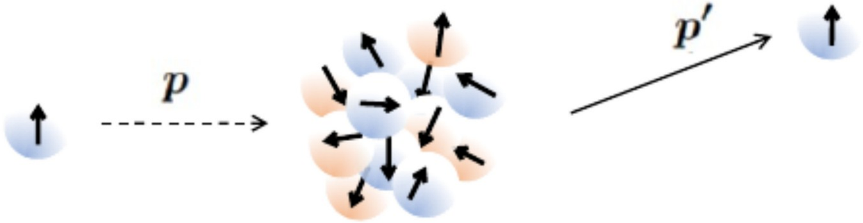


Reduce the Many-Body to a Few-Body Problem

Isolate relevant degrees of freedom

Solve the few-body problem with effective interactions

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



Ingredients:

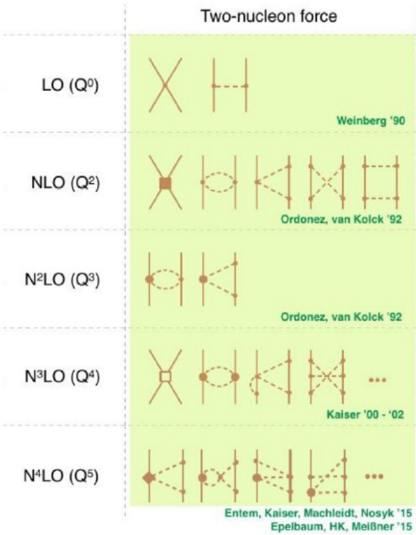
1) realistic nuclear interaction

must describe target and projectile

2) controllable structure framework

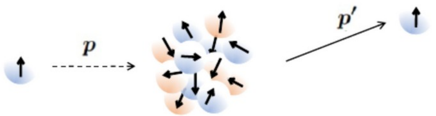
3) controllable reaction framework

4) a way to connect everything



Chiral NN Interaction

Building up an *ab initio* framework



Ingredients:

1) realistic nuclear interaction

must describe target and projectile

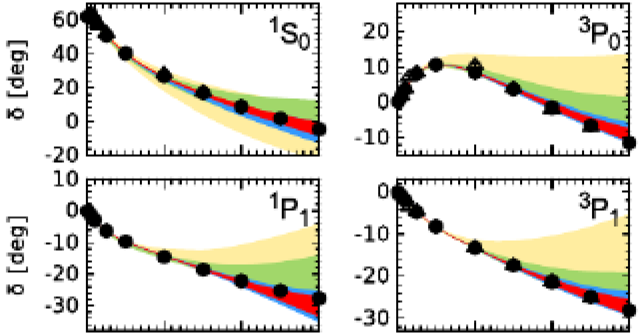
2) controllable structure framework

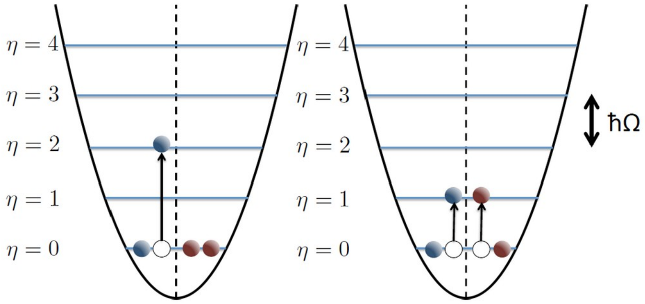
here, no-core shell model (NCSM and SA-NCSM)

3) controllable reaction framework

here, spectator expansion

4) a way to connect everything

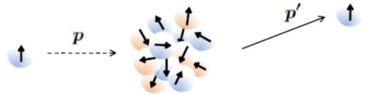




	$E(^3H)$	$E(^3He)$	$E(^4He)$	$r_p(^4He)$
NNLO	−8.249	−7.501	−27.759	1.43(8)
NNLO+NNN	−8.469	−7.722	−28.417	1.43(8)
Experiment	−8.482	−7.717	−28.296	1.467(13)

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

Building up an *ab initio* framework



Ingredients:

1) realistic nuclear interaction

   must describe target and projectile

2) controllable structure framework

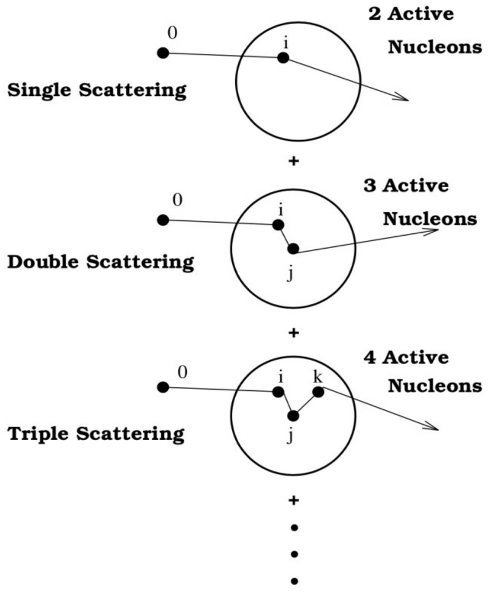
   here, no-core shell model (NCSM and SA-NCSM)

3) **controllable reaction framework**

   here, spectator expansion of

   Watson multiple scattering series

4) a way to connect everything



Spectator Expansion:

Siciliano, Thaler (1977)
Picklesimer, Thaler (1981)
Chinn, Elster, Thaler, Weppner (1995)
Baker, Burrows, Elster, *et.al* (2023)

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

Ingredients:

1) realistic nuclear interaction

   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 of

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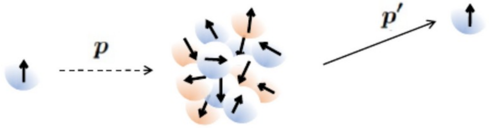
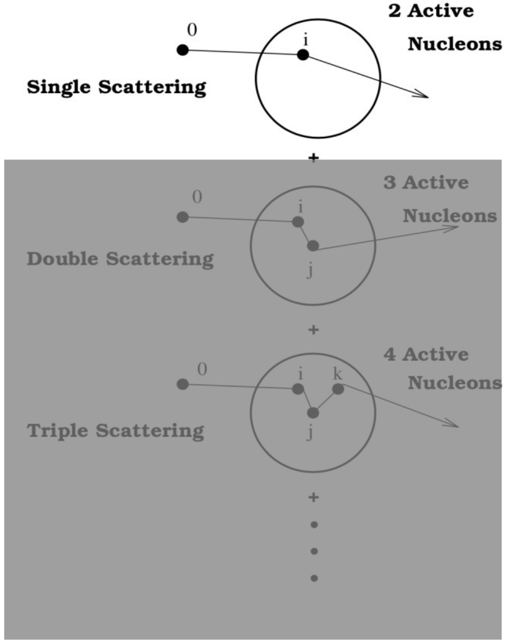
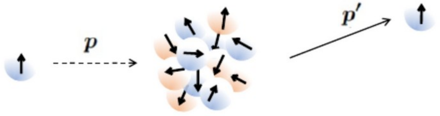
4) a way to connect everything





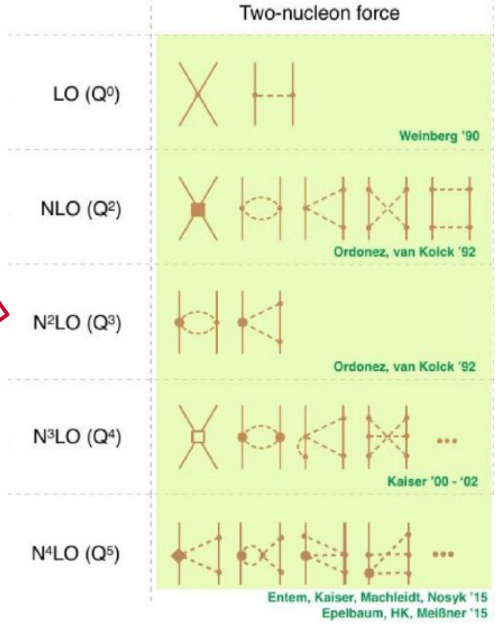
Leading order in spectator expansion can be computed *ab initio*

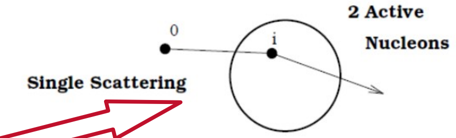
Framework for *ab initio* Elastic Scattering



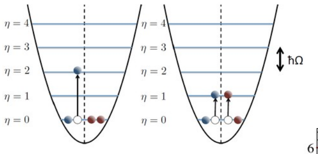
Same NN force in all parts

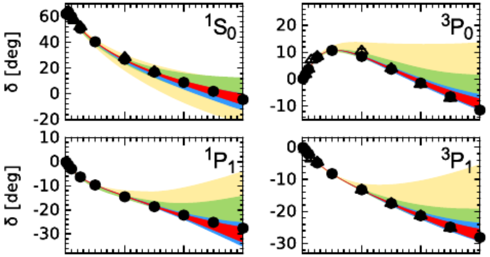
Reaction theory:
spectator expansion

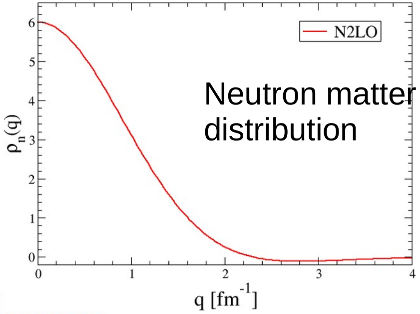




Structure theory:
No-Core Shell Model







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

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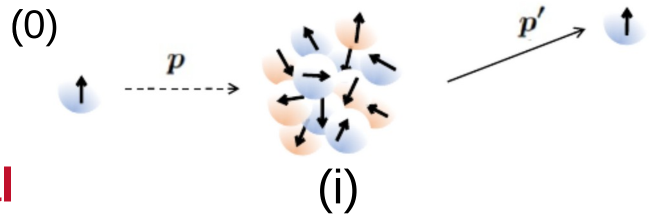
Setting up the *ab initio* framework

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

NN interaction represented by **Wolfenstein amplitudes**



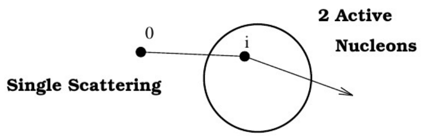
$$\overline{M}(\boldsymbol{q},\boldsymbol{\mathcal{K}}_{NN},\epsilon) = A(\boldsymbol{q},\boldsymbol{\mathcal{K}}_{NN},\epsilon)\mathbf{1}\otimes\mathbf{1}$$
$$+\, iC(\boldsymbol{q},\boldsymbol{\mathcal{K}}_{NN},\epsilon)\left(\boldsymbol{\sigma}^{(0)}\cdot\hat{\boldsymbol{n}}\right)\otimes\mathbf{1}$$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

A: central
C: spin-orbit

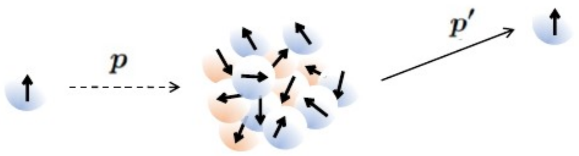
M, G, H: tensor

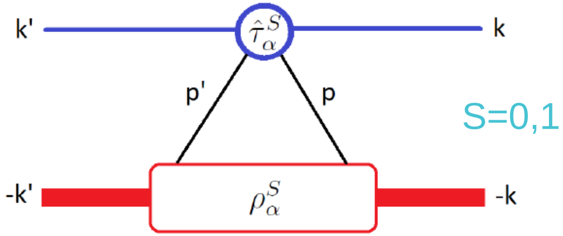
Most general structure of NN amplitudes consistent with invariance principles

Computing the leading order effective potential



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



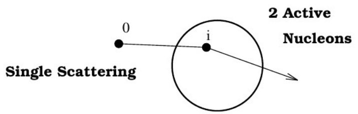


scatter off nucleus with 0^+ ground state

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

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

Computing the leading order effective potential



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

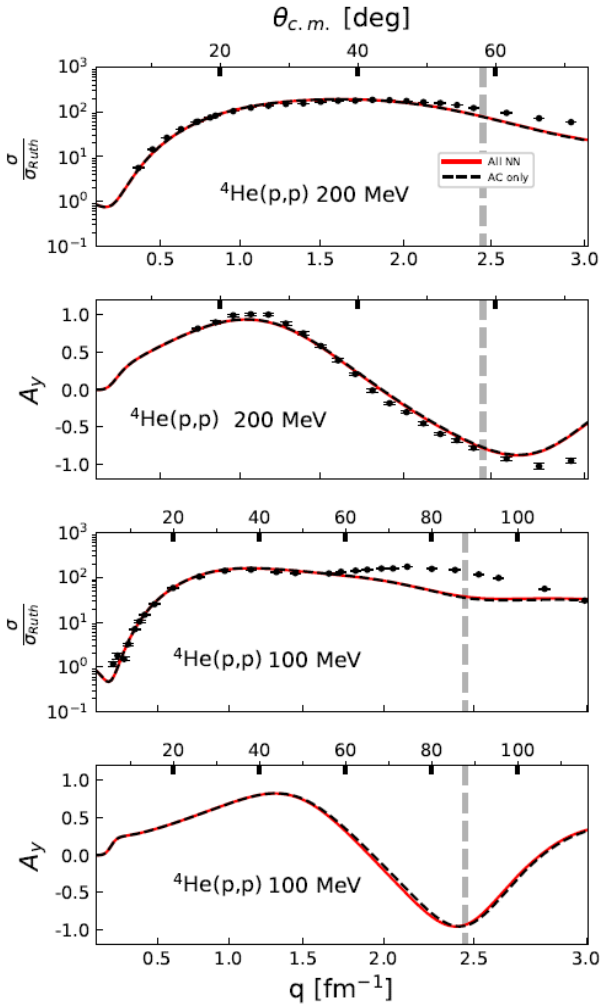
matter distribution = density

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

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

spin-projected momentum distribution

^{4}He N$_{max}$=18



$$\vec{q}_{nn} = \vec{q}_{nA} = \vec{q}$$

$$q \approx 480\ \text{MeV} = 2.45\ \text{fm}^{-1}$$

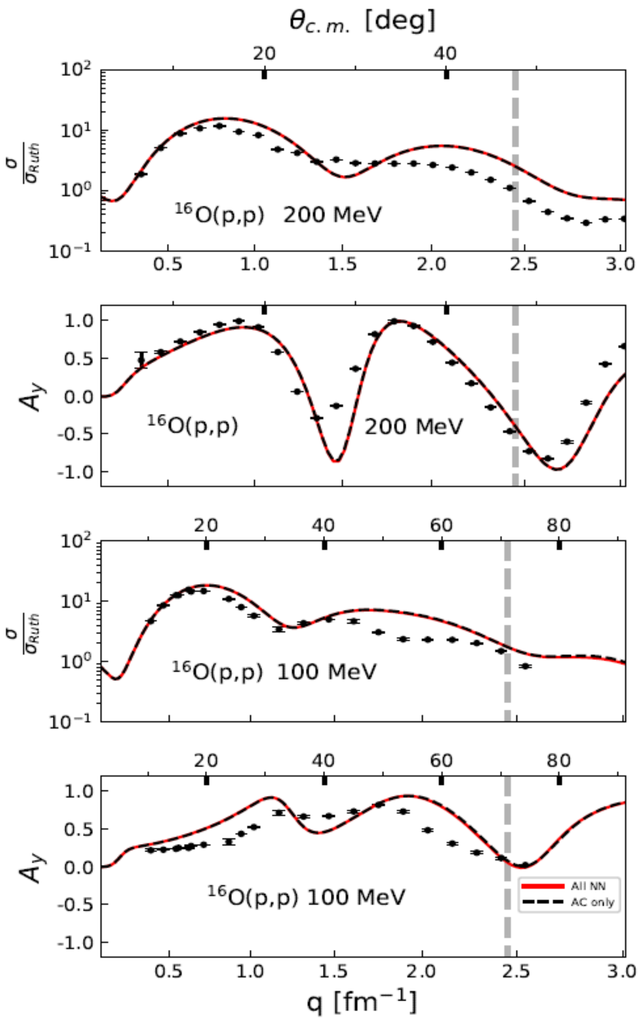
ħω=20 MeV

closed-shell nuclei

NNLO$_{opt}$
Chiral interaction

A. Ekstrom et al.
PRL 110, 192502 (2013)

N$_{max}$=10 ^{16}O

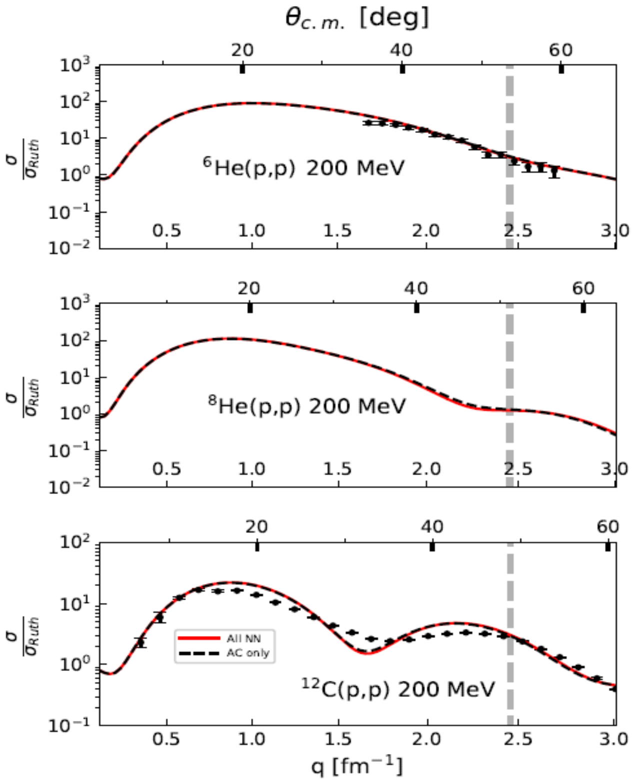


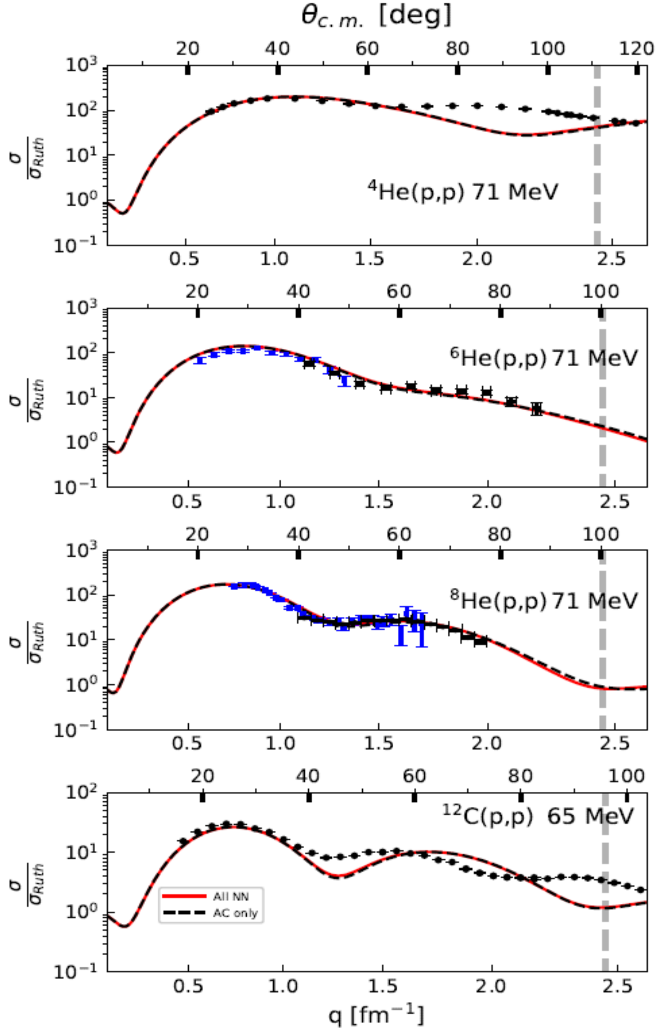
Open-shell nuclei

NNLO$_{opt}$
Chiral
interaction

N_{max}=18

N_{max}=12





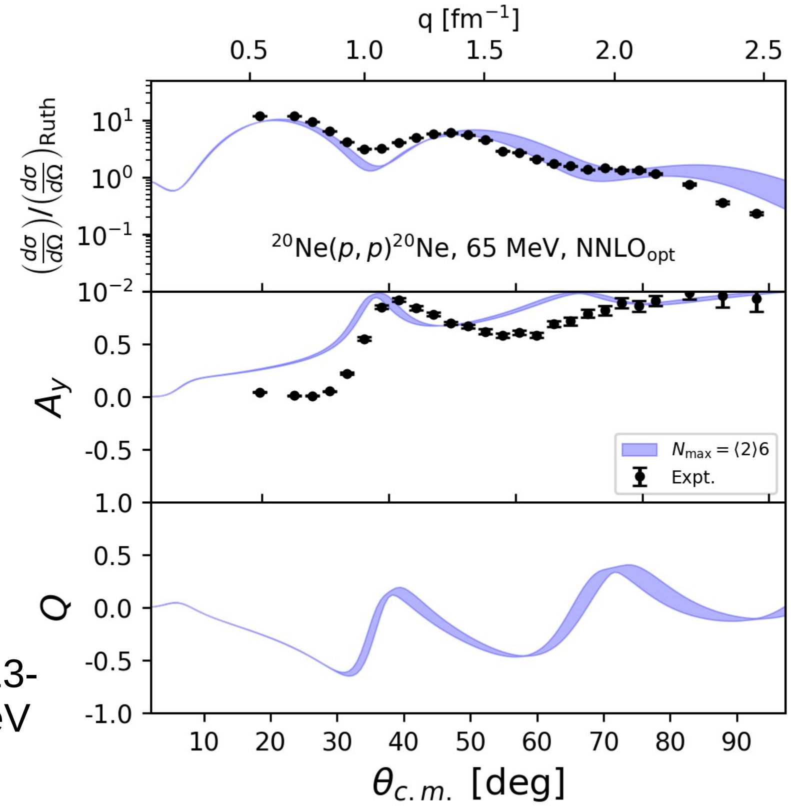
N_{max}=18

N_{max}=12

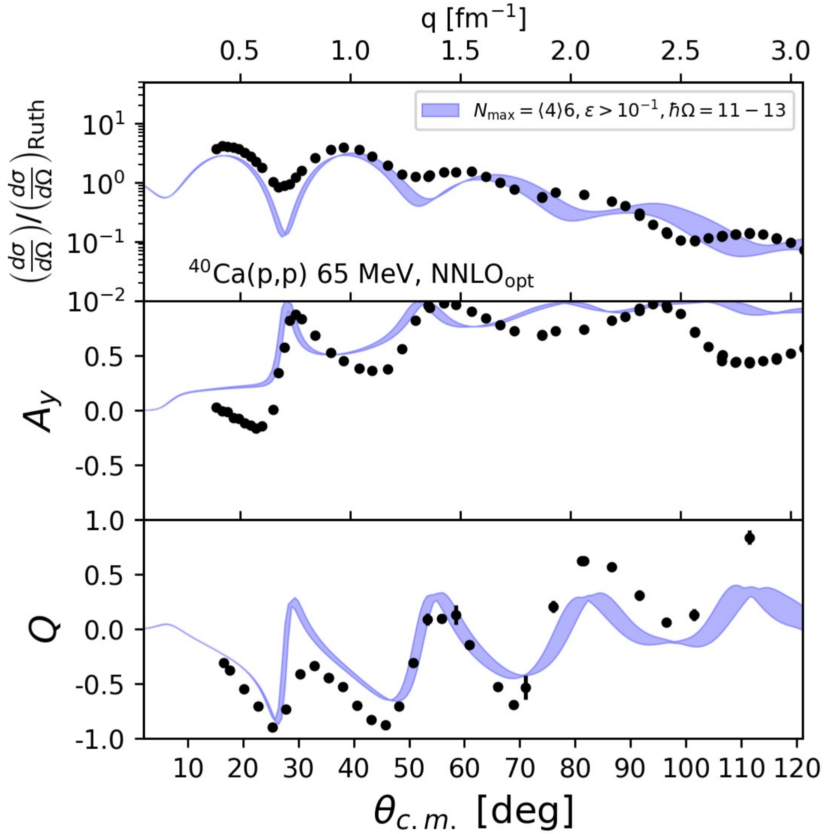
ħω=20 MeV

Beyond NCSM: SA-NCSM One-Body Densities

$NNLO_{opt}$ chiral potential



ħω=13-17 MeV



ħω=11-13 MeV

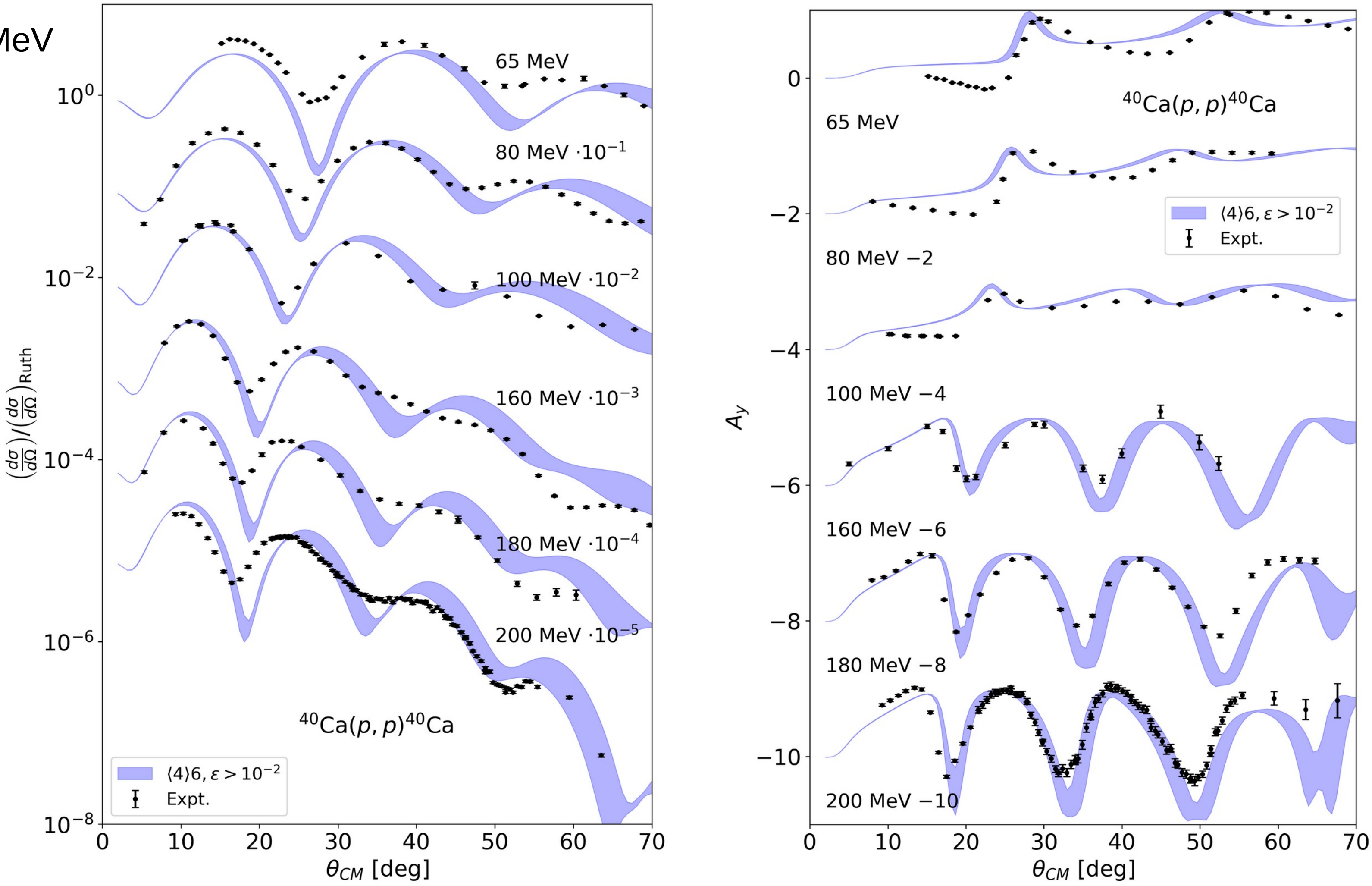
Baker, Elster, Dytrych, Launey arXiv 2404.03106 [nucl-th]

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

Beyond NCSM: SA-NCSM One-Body Densities

NNLO$_{opt}$ chiral potential

ħω=11- 13 MeV



physics + a

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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)

- **In the multiple scattering approach the leading order term can be calculated consistently *ab initio* for light nuclei based on NCSM**
  SA-NCSM is being explored for medium-mass nuclei

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

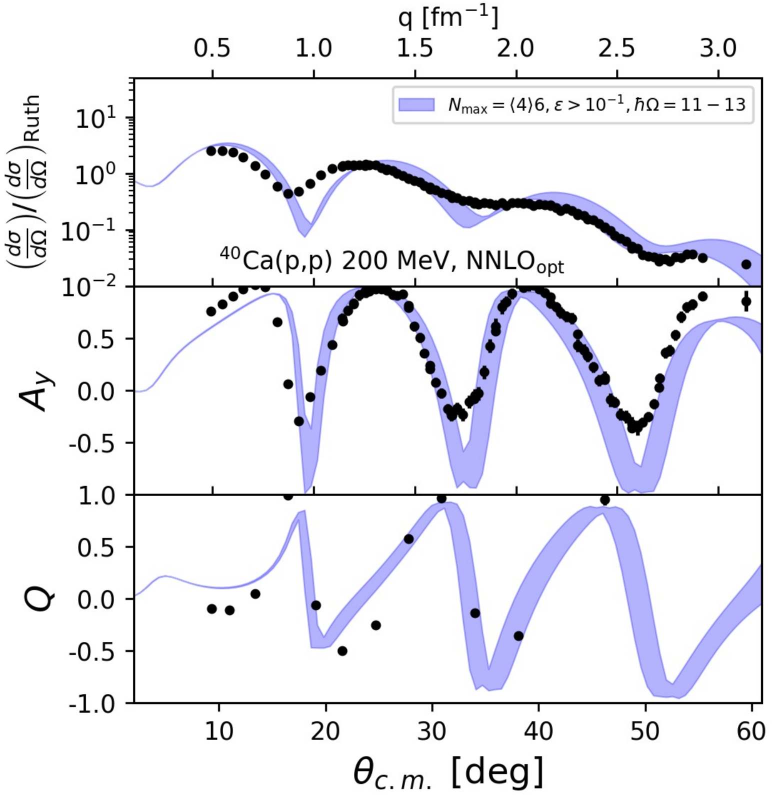
  We plan a study of Mg isotopes with the SA-NCSM – data at 65 MeV available

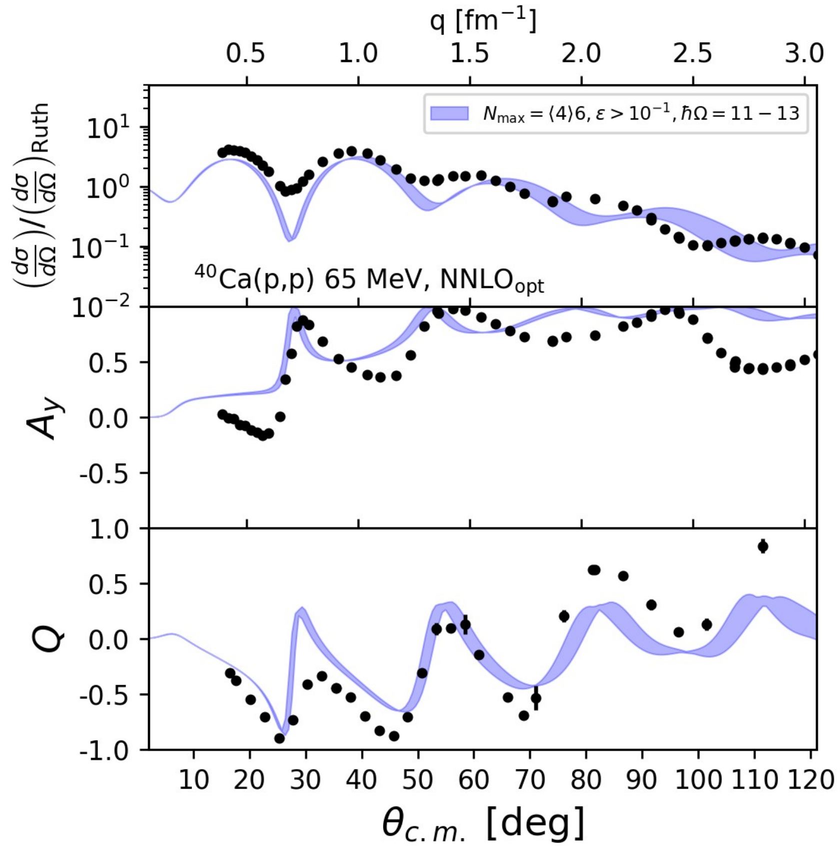
- **Ongoing work: move beyond nuclei with 0^+ ground states**
  Transition potentials for inelastic scattering

Backup slides

Beyond NCSM: SA-NCSM One-Body Densities

$NNLO_{opt}$ chiral potential





What about different chiral NN interactions ?

Description of NN data below ~ 130 MeV almost identical

$NNLO_{opt}$

Fitted to about 125 MeV NN E_{lab}

PRL **110,** 192502 (2013) PHYSICAL REVIEW LETTERS week ending 10 MAY 2013

Optimized Chiral Nucleon-Nucleon Interaction at Next-to-Next-to-Leading Order

A. Ekström,[1,2] G. Baardsen,[1] C. Forssén,[3] G. Hagen,[4,5] M. Hjorth-Jensen,[1,2,6] G. R. Jansen,[4,5] R. Machleidt,[7] W. Nazarewicz,[5,4,8] T. Papenbrock,[5,4] J. Sarich,[9] and S. M. Wild[9]

LENPIC – SCS

Semi-local coordinate space regulator R=1 fm
Sometimes referred to as EKM
(fitted up to about 300 MeV NN E_{lab})

PRL **115,** 122301 (2015) PHYSICAL REVIEW LETTERS week ending 18 SEPTEMBER 2015

Precision Nucleon-Nucleon Potential at Fifth Order in the Chiral Expansion

E. Epelbaum,[1] H. Krebs,[1] and U.-G. Meißner[2,3,4]

Physics Letters B 761 (2016) 87–91

Daejeon 16

N3LO *NN* interaction adjusted to light nuclei in *ab exitu* approach

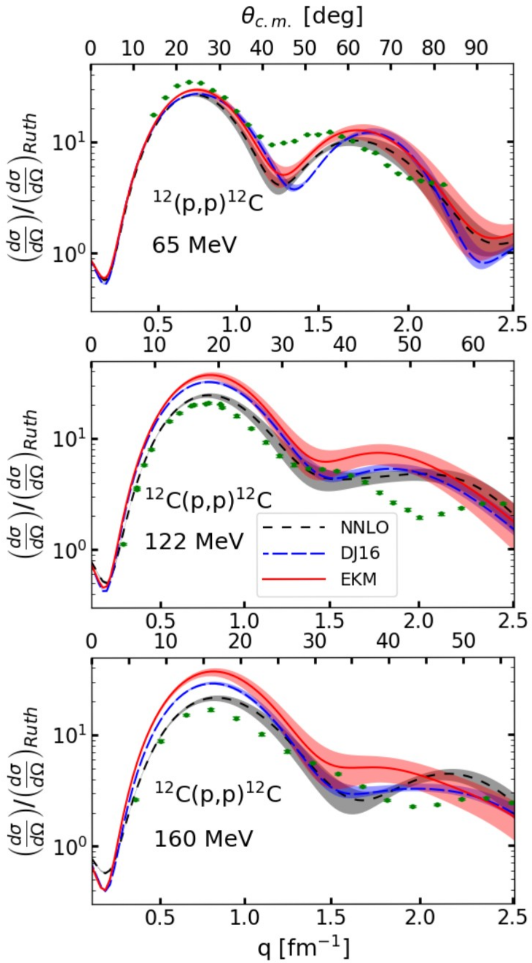
A.M. Shirokov[a,b,c,*], I.J. Shin[d], Y. Kim[d], M. Sosonkina[e], P. Maris[b], J.P. Vary[b]

Starts from Idaho N3LO, applies SRG transformation
And represents in HO basis
On-shell equivalent to Idaho N3LO (fitted to about 300 MeV NN E_{lab})

Baker, Burrows, Elster, Launey, Maris, Popa, Weppner, PRC 108, 044617 (2023)

Differential Cross Sections

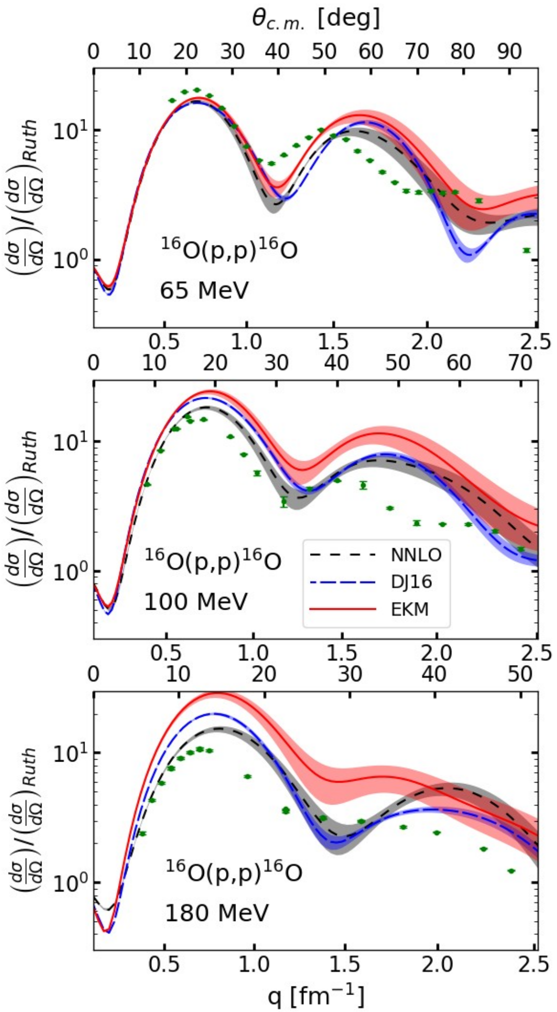
^{12}C



Bands indicate Dependence on Oscillator parameter

Energy dependence for small momentum transfer is different

^{16}O



Baker, Burrows, Elster, Maris, Popa, Weppner, PRC 108, 044617 (2023)

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