Ab initio nucleon-nucleus elastic scattering with chiral uncertainties

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Introduction Nucleon-Nucleus Scattering

- Spectator expansion of multiple scattering theory
  - ordering of the scattering process according to the number of active target nucleons interacting directly with the projectile nucleon
- Generally restricted to leading-order term:
  projectile interacts directly with only one target nucleon
  - believed to be applicable in the 50 $\sim$ 200 MeV projectile energies
  - need one-body density of target nucleus
- Note: unclear what the actual expansion parameter is
  (assuming the spectator expansion has a well-defined expansion parameter . . .)
- Until recently
  - use realistic NN potential
  - purely phenomenological, local, one-body density
- Recent development
  - use one-body density from ab initio nuclear structure calculation
  - use same NN interaction for structure and scattering
  - consistency:
    also restricted to NN-only interactions in structure calculation

Leading-order spectator expansion

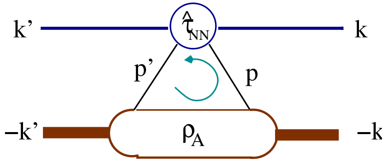
Effective (optical) potential

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

with $\eta(\ldots)$ the Moller factor, relating the NN frame to the NA frame
$\hat{\tau}_{n,p}^{K_s}$ the NN amplitude between projectile and target nucleon ($K_s = 0, 1$)
$\rho_{n,p}^{K_s}$ the (nonlocal) one-body density of the target ($K_s = 0, 1$) and

$$q = p' - p \qquad \mathcal{K} = \frac{1}{2}(p'+p)$$

$$\mathcal{K}_{NA} = \frac{A}{A+1}\left[(k'+k)+\frac{1}{2}(p'+p)\right]$$



Wolfenstein Amplitudes

NN amplitude can be parametrized in terms of Wolfenstein amplitudes

$$
\begin{aligned}
\overline{M}(q, \mathcal{K}_{NN}, \epsilon) \quad = \quad & A(q, \mathcal{K}_{NN}, \epsilon) \mathbf{1} \otimes \mathbf{1} \\
& + iC(q, \mathcal{K}_{NN}, \epsilon) \, \left(\sigma^{(0)} \cdot \hat{n} \right) \otimes \mathbf{1} \\
& + iC(q, \mathcal{K}_{NN}, \epsilon) \, \mathbf{1} \otimes \left(\sigma^{(i)} \cdot \hat{n} \right) \\
& + M(q, \mathcal{K}_{NN}, \epsilon) \, \left(\sigma^{(0)} \cdot \hat{n} \right) \otimes \left(\sigma^{(i)} \cdot \hat{n} \right) \\
& + \ldots
\end{aligned}
$$

with the ... representing terms that cannot contribute to elastic scattering in the leading-order spectator expansion, due to parity constraints, and

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

Leading-order potential for scattering on 0^+ states

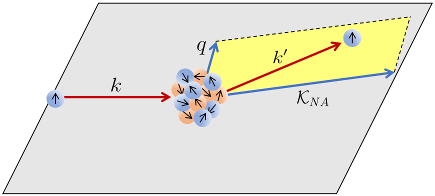
$$\widehat{U}_{\rm p}(q, \mathcal{K}_{NA}, \epsilon) =$$

$$\sum_{\alpha={\rm n,p}} \int d^3\mathcal{K}\, \eta\,(\ldots)\, A_{{\rm p}\alpha}\left(q, \frac{1}{2}\left(\frac{A+1}{A}\mathcal{K}_{NA} - \mathcal{K}\right); \epsilon\right) \rho_\alpha^{K_s=0}\,(\mathcal{P}', \mathcal{P})$$

$$+ \quad i(\sigma^{(0)} \cdot \hat{n}) \sum_{\alpha={\rm n,p}} \int d^3\mathcal{K}\, \eta\,(\ldots)\, C_{{\rm p}\alpha}\left(q, \frac{1}{2}\left(\frac{A+1}{A}\mathcal{K}_{NA} - \mathcal{K}\right); \epsilon\right) \rho_\alpha^{K_s=0}\,(\mathcal{P}', \mathcal{P})$$

$$+ \quad i \sum_{\alpha={\rm n,p}} \int d^3\mathcal{K}\, \eta\,(\ldots)\, C_{{\rm p}\alpha}\left(q, \frac{1}{2}\left(\frac{A+1}{A}\mathcal{K}_{NA} - \mathcal{K}\right); \epsilon\right) \rho_\alpha^{K_s=1}\,(\mathcal{P}', \mathcal{P}) \cdot \hat{n} \cos\beta$$

$$+ \quad (\sigma^{(0)} \cdot \hat{n}) \sum_{\alpha={\rm n,p}} \int d^3\mathcal{K}\, \eta\,(\ldots)\, M_{{\rm p}\alpha}\left(q, \frac{1}{2}\left(\frac{A+1}{A}\mathcal{K}_{NA} - \mathcal{K}\right); \epsilon\right) \rho_\alpha^{K_s=1}\,(\mathcal{P}', \mathcal{P}) \cdot \hat{n} \cos\beta$$



- nonlocal density $\rho_{p,n}^{K_s}$ function of

$$\mathcal{P} = \mathcal{K} + \frac{A-1}{A}\frac{q}{2}$$
$$\mathcal{P}' = \mathcal{K} - \frac{A-1}{A}\frac{q}{2}$$

- both $K_s = 0$ and $K_s = 1$ component

Ab Initio Nuclear Structure calculations

Given a Hamiltonian operator

$$\hat{\mathbf{H}} \quad = \quad \sum_{i<j} \frac{(\vec{p}_i - \vec{p}_j)^2}{2\,m\,A} + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \ldots$$

solve the eigenvalue problem for wave function of A nucleons

$$\hat{\mathbf{H}}\,\Psi(r_1,\ldots,r_A) \quad = \quad \lambda\,\Psi(r_1,\ldots,r_A)$$

- eigenvalues λ discrete (quantized) energy levels
  - total energies: $E_\Psi \;=\; \langle\Psi|\hat{\mathbf{H}}|\Psi\rangle \;=\; -E_\Psi^{\text{binding}}$
  - excitation energies: $E_{\rm exc} \;=\; E_\Psi - E_{\rm gs}$
- eigenvectors:
  - local One-Body Density: $|\Psi(r_1,\ldots,r_A)|^2$
    probability density for finding nucleons 1, ..., A at r_1, ..., r_A
    - can be used for ab initio calculations of NA scattering
  - static observables (radii, moments): $\langle\Psi_{JP}|\hat{\mathcal{O}}^K|\Psi_{JP}\rangle$
  - electroweak transition observables: $\langle\Psi'_{J'P'}|\hat{\mathcal{O}}^K|\Psi_{JP}\rangle$
    - one-body current easy but not consistent nor in agreement with data
    - two-body current operator work in progress

No-Core Configuration Interaction approach

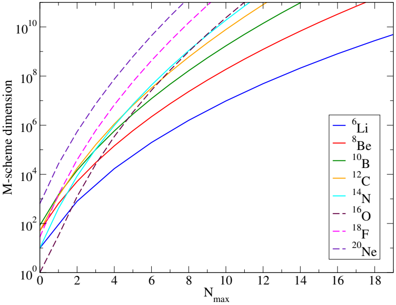
Barrett, Navrátil, Vary, *Ab initio no-core shell model*, PPNP69, 131 (2013)

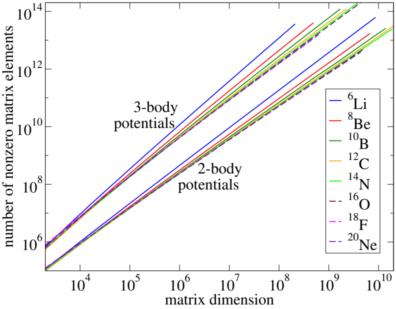
- Expand wavefunction in basis states $|\Psi\rangle = \sum a_i |\Phi_i\rangle$
- Express Hamiltonian in basis $\langle \Phi_j | \hat{\mathbf{H}} | \Phi_i \rangle = H_{ij}$
- Diagonalize Hamiltonian matrix H_{ij}
- No-Core: all A nucleons are treated the same
- Complete basis $\longrightarrow$ exact result
  - caveat: complete basis is infinite dimensional

- In practice
  - truncate basis
  - study behavior of observables as function of truncation

- Computational challenge
  - construct large ($10^{10} \times 10^{10}$) sparse symmetric matrix H_{ij}
  - obtain lowest eigenvalues & -vectors corresponding to low-lying spectrum and eigenstates

Main Computational Challenge





- Increase of basis space dimension with increasing A and N_{max}
  - need calculations up to at least $N_{\text{max}} = 8$, preferably $N_{\text{max}} = 10$
- More relevant measure for computational needs
  - number of nonzero matrix elements
  - current limit 10^{14} (Theta, Cori, Perlmutter)
- Initial scattering applications restricted to 0^+ ground states

One-Body Densities

One-Body Density for A-body wave function $|\Psi\rangle = |AJM\lambda\rangle$

$$\rho_{sf}(\vec{r},\vec{r'}) = \langle AJM\lambda|\sum_{i=1}^{A}\delta^3(\vec{r_i}-\vec{r})\delta^3(\vec{r_i'}-\vec{r'})|AJM\lambda\rangle$$

Expand One-Body Density in terms of tensors of rank $K \leq 2J$

$$\rho_{sf}(\vec{r},\vec{r'}) = \sum_{ll'K}(-1)^{J-M}\begin{pmatrix} J & K & J \\ -M & 0 & M \end{pmatrix} \mathcal{Y}^{*l'l}_{K0}(\hat{r},\hat{r}')\,\rho_{ll'K}(r,r')$$

$$\rho_{ll'K}(r,r') = \sum_{njn'j'}\hat{j}\hat{j}'(-1)^{l'+l+j+\frac{1}{2}+K}\left\{\begin{matrix} l' & l & K \\ j & j' & \frac{1}{2}\end{matrix}\right\} R_{n'l'}(r')R_{nl}(r)$$
$$\langle AJM\lambda||(a^\dagger_{nljm}\tilde{a}_{n'l'j'm})^{(K)}||AJM\lambda\rangle$$

with $(a^\dagger_{nljm}\tilde{a}_{n'l'j'm})^{(K)}$ one-body operator of rank K and $a_{nljm} = (-1)^{j-m}\,\tilde{a}_{nlj-m}$

- Reduced One-Body Density Matrix elements (OBDME) of rank K $\langle AJM\lambda||(a^\dagger_{nljm}\tilde{a}_{n'l'j'm})^{(K)}||AJM\lambda\rangle$ from ab initio NCSM calculations
- NCSM wavefunctions contain c.m. contributions ('space-fixed')

Translationally-Invariant Nonlocal Densities

- Use of HO basis and $N_{\max}$ truncation leads to exact factorization

$$|\Psi JM\rangle = |\Psi_{ti} JM\rangle \otimes |\phi_{c.m.} 0s\rangle$$

- Use relative and total momenta $\vec{q} = \vec{p'} - \vec{p}$ and $\vec{\mathcal{K}} = \frac{1}{2}(\vec{p'} + \vec{p})$, and corresponding coordinate space variables

$$\vec{\zeta} = \tfrac{1}{2}(\vec{r'} + \vec{r}) = \vec{\zeta}_{\text{rel}} + \vec{\zeta}_{\text{c.m.}} \qquad \vec{Z} = \vec{r'} - \vec{r}$$

- Use Talmi-Moshinsky transformations from $|n, l, n', l' : K\rangle$ to $|n_{\mathcal{K}}, l_{\mathcal{K}}, n_q, l_q : K\rangle$ to write $\rho_{sf}(\vec{p}, \vec{p'})$ as function of $\vec{q}$ and $\vec{\mathcal{K}}$
- One-Body Density in relative and total momenta

$$\begin{aligned}\rho_{sf}(\vec{q}, \vec{\mathcal{K}}) &= \langle \phi_{\text{c.m.}} 0s | \mathrm{e}^{-i\vec{q}\cdot\vec{\zeta}_{\text{c.m.}}} | \phi_{\text{c.m.}} 0s \rangle \\ &\quad \times \frac{1}{(2\pi)^3} \langle AJM\lambda | \sum_i \mathrm{e}^{-i\vec{q}\cdot\vec{\zeta}_{\text{rel},i}} \mathrm{e}^{-i\vec{\mathcal{K}}\cdot\vec{Z}_i} | AJM\lambda \rangle\end{aligned}$$

- Translationally-Invariant Nonlocal Density $\rho(\vec{q}, \vec{\mathcal{K}}) = \mathrm{e}^{\frac{b^2}{4}\frac{q^2}{A}} \rho_{sf}(\vec{q}, \vec{\mathcal{K}})$

Burrows, Elster, Popa, Launey, Nogga, PM, PRC97, 024325 (2018)

Spin-projected One-Body Densities

- Decouple orbital angular momentum l and spin s instead of using the total angular momentum j
- Scalar density ($K_s = 0$)
- Spin-orbit density ($K_s = 1$): $\rho^{K_s=1} \cdot \hat{n}$
- Explicitly, for $J = 0$ (ground) states

$$\rho^{K_s=1}(\vec{q}, \vec{\mathcal{K}}) \cdot \hat{n} \;=\; -i\sqrt{3} \sum_{nljn'l'j'} (-1)^{-l}\hat{j}\hat{j} \left\{ \begin{array}{ccc} l' & l & 1 \\ \frac{1}{2} & \frac{1}{2} & 1 \\ j & j & 0 \end{array} \right\} (-i)^{l+l'}$$

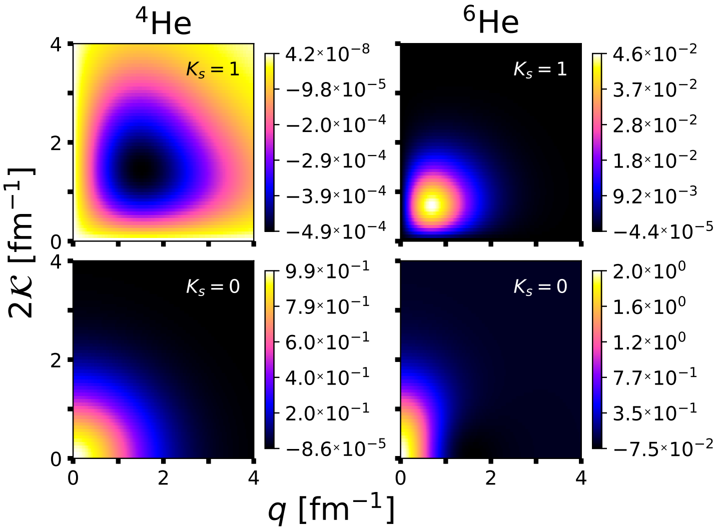
$$\sum_{n_q, n_{\mathcal{K}}, l_q, l_{\mathcal{K}}} \langle n_{\mathcal{K}} l_{\mathcal{K}}, n_q l_q : 1 | n' l', nl : 1 \rangle_{d=1} R_{n_{\mathcal{K}} l_{\mathcal{K}}}(\mathcal{K}) R_{n_q l_q}(q)$$

$$\sum_{q_s=-1,1} \mathcal{Y}^{*l_q l_{\mathcal{K}}}_{1-q_s}(\widehat{q}, \hat{\mathcal{K}}) \langle A\lambda 0 \left|\left| (a^{\dagger}_{n'l'j'} \tilde{a}_{nlj})^{(0)} \right|\right| A\lambda 0 \rangle e^{\frac{1}{4A} b^2 q^2}$$

Burrows, Baker, Elster, Webbner, Launey, PM, Popa, PRC102, 034606 (2020)

Spin-projected One-Body Densities with NNLO_opt

Popa, Burrows, Elster, Launey, PM, Weppner, arXiv:1910.00683



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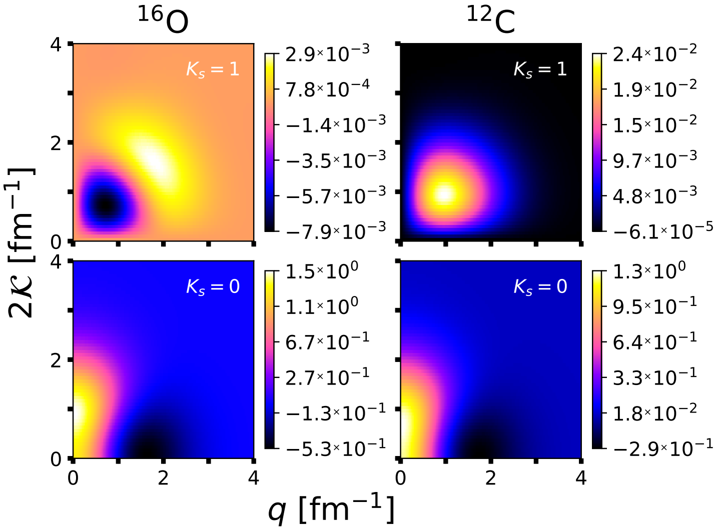


LENPIC SCS with chiral uncertainties

- Interaction
  - LENPIC SCS: LO, NLO, and N^2LO (NN-only)
- Same interaction in structure and scattering calculation
  - no SRG evolution, no 3NFs
- Results for ^4He, ^{12}C, ^{16}O
  - at energies for which data exist
- Pointwise chiral EFT uncertainty estimates for total cross-sections
- Correlated uncertainty estimates for differential cross-sections, analyzing power A_y, and spin rotation function Q
- Expansion parameter $Q = p/\Lambda_b$
  with $\Lambda_b = 600$ MeV for regulator $R = 1.0$ fm

Baker, McClung, Elster, PM, Weppner, Burrows, Poppa, arXiv:2112.02442
Baker, Burrows, Elster, Launey, PM, Popa, Weppner, in preparation (Frontiers UQ)

Expansion parameter

Dimensionless expansion parameter $Q = p/\Lambda_b$

- Here: c.m. momentum of NA system

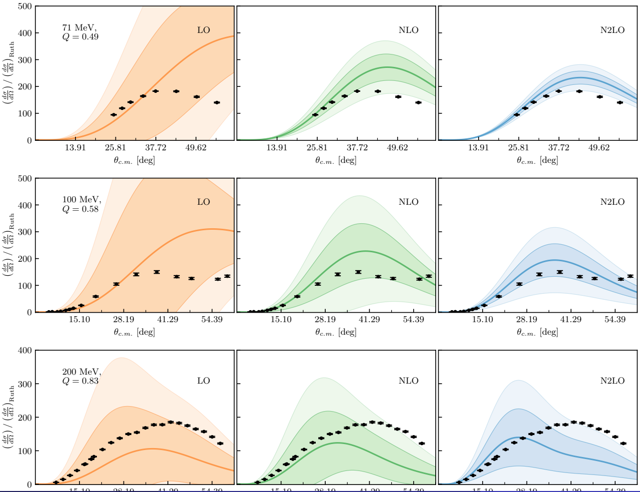
$$p_{NA}^2 = \frac{E_{\rm lab} A^2 m^2 (E_{\rm lab} + 2m)}{m^2 (A+1)^2 + 2AmE_{\rm lab}},$$

  - advantage: independent of scattering angle
  - assessed by evaluating posteriors for Q
- Probably better: max. of p_{NA} and momentum transfer q
  - this complicates posterior analysis for Q
  - $q = p_{NA}$ indicated by vertical grey bar
- Future: determined from order-by-order calculations?
  - need higher order(s)
  - challenge: 3NFs
    only in structure, or also in scattering calculation?

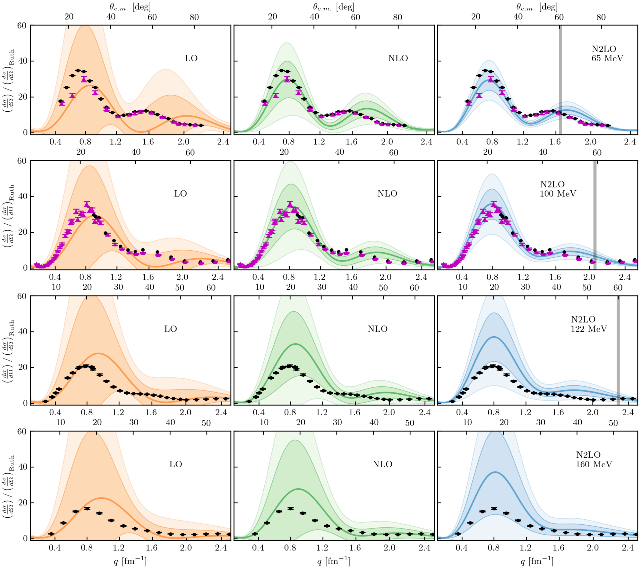
Differential cross section, $^4He(p,p)^4He$

Divided by Rutherford cross section

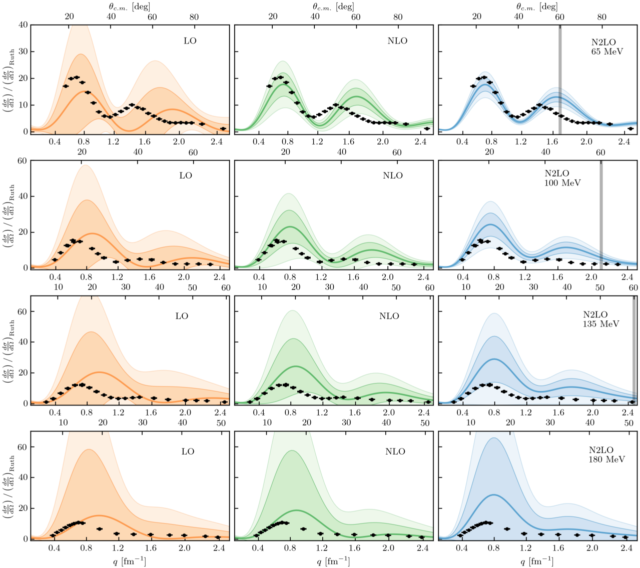
(we're interested in the nuclear interaction, not the electromagnetic scattering)



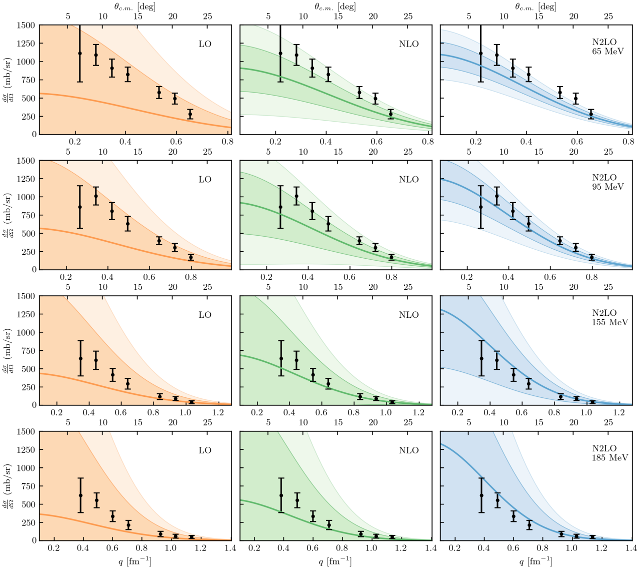
Differential cross section, $^{12}C(p,p)^{12}C$



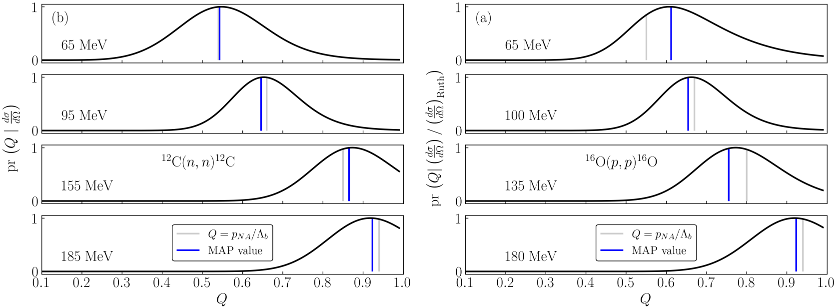
Differential cross section, $^{16}O(p,p)^{16}O$



Differential cross section, $^{12}C(n,n)^{12}C$

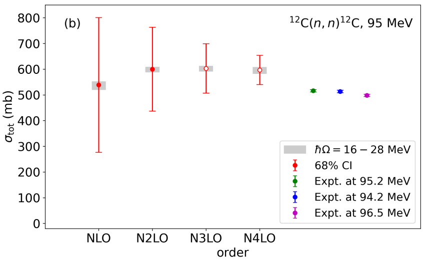


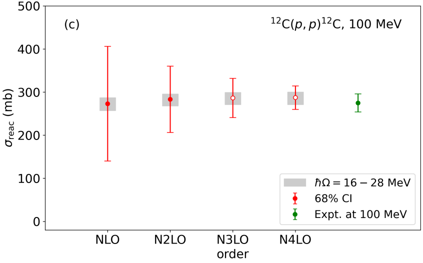
Posteriors on expansion parameter



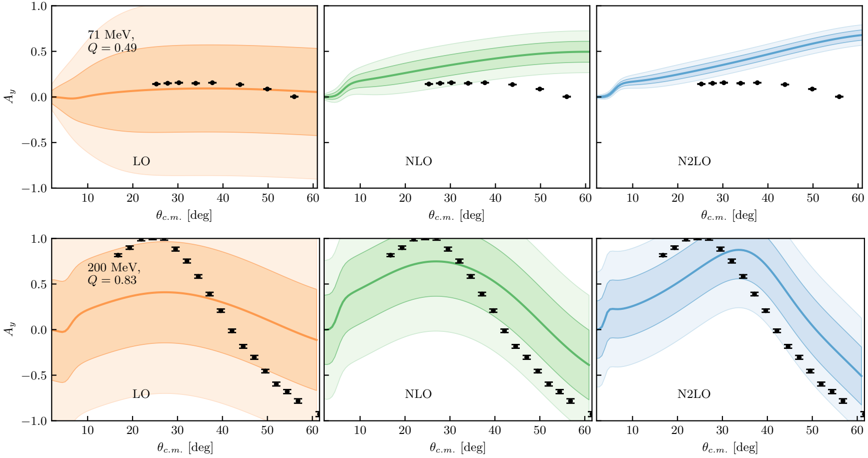
- Posteriors for Q for $^{12}C(n,n)^{12}C$ and $^{16}O(p,p)^{16}O$
- Extract maximum a posteriori (MAP)
  - in reasonable agreement with our choice $p_{NA}/Lambda_b$
- Note: only results for $q < p_{NA}$ included in posteriori analysis

Reaction cross section, ^{12}C, protons and neutrons

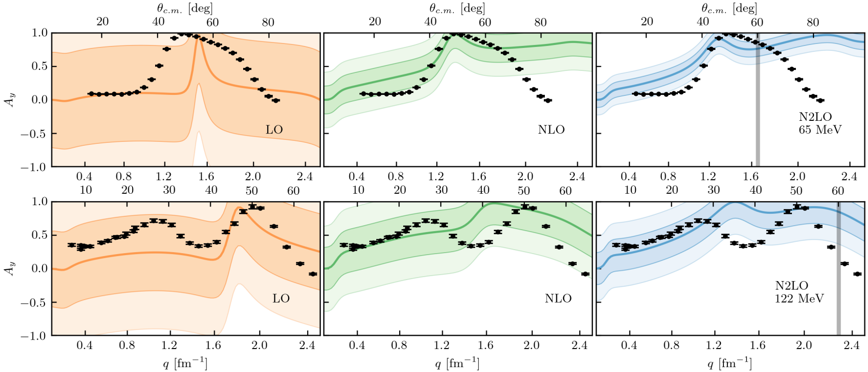




Analyzing power, $^4He(p,p)^4He$



Analyzing power, $^{12}C(p,p)^{12}C$



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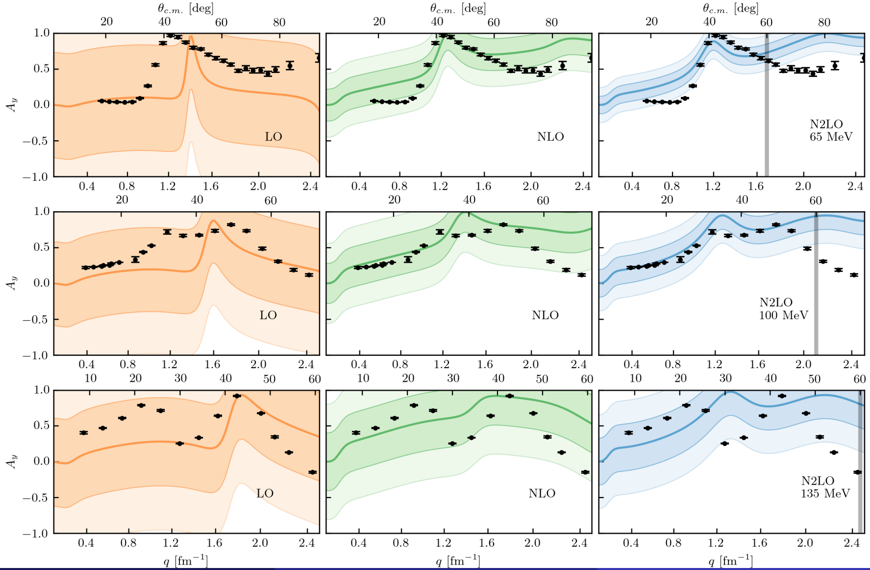
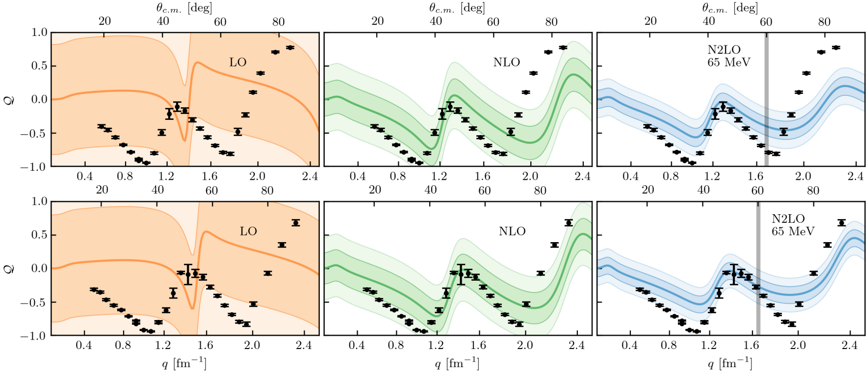


Spin rotation function Q

Top: $^{16}O(p,p)^{16}O$



Bottom: $^{12}C(p,p)^{12}C$

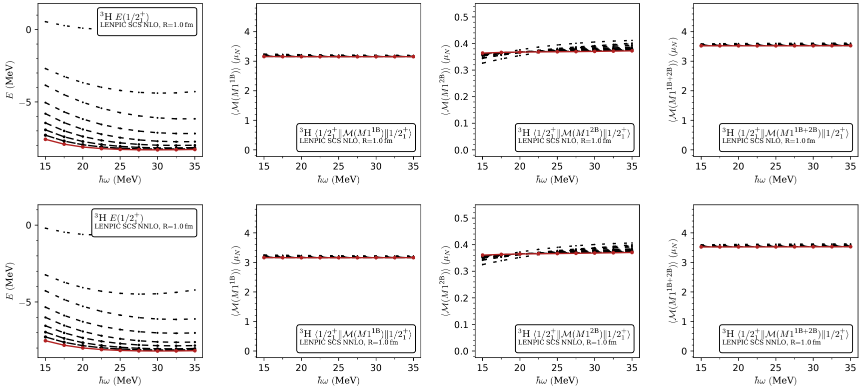
Conclusions / Challenges / Future work

- Can describe elastic nucleon-nucleus scattering data for $J = 0$ p-shell ground states within chiral EFT truncation uncertainties
  - Possible exception: A_y of ^{4}He
  - Breakdown of chiral expansion already at $\approx$ 180 MeV for $A = 16$
- Challenges
  - Consistent SRG evolution, including induced 3NFs
  - Explicit 3NFs in chiral expansion already at N^{2}LO
- Future work (not even planned yet . . .)
  Next-to-leading-order in spectator expansion:
  projectile interacting directly with two target nucleons
  - through 3-nucleon interactions (3NF)
  - need Two-Body Density of target nucleus
  - through two successive two-nucleon (NN-only) interactions
- Open question
  - Uncertainty quantification of spectator expansion

Status update: Magnetic moments

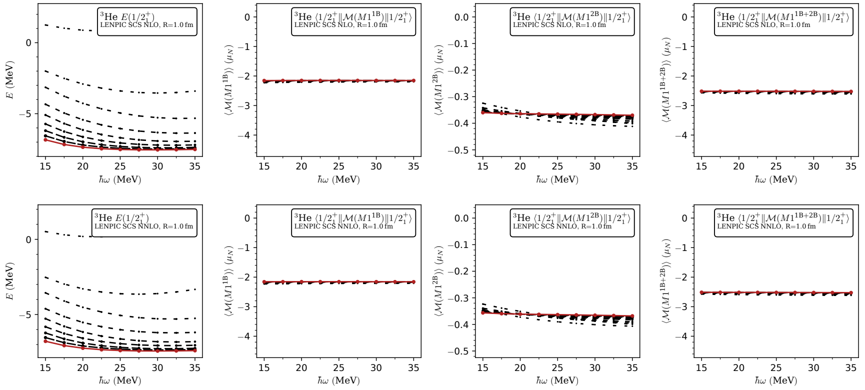
- LENPIC SCS, NLO and N^2LO (NN-only), no SRG
- Consistent NLO one-body and two-body current (no N^2LO contribution to M1 current)
- Work in progress
  - Soham Pal (ISU), PhD thesis May 2022 on $A = 3$ moments
  - Patrick Fasano (U. of Notre Dame), PhD thesis in preparation, select *p*-shell nuclei
  - paper(s) in preparation by (alphabetically) Caprio, Fasano, Maris, Pal, Sharker, Vary
- Future plans
  - LENPIC SMS current, two-body, SRG evolved
  - currently no plans for (induced) three-body currents
  - need to update interface with menj input files from Darmstadt for TBMEs of non-scalar operators

Magnetic moments for ^{3}H



Patrick Fasano (U. of Notre Dame), preliminary, PhD thesis in preparation

Magnetic moments for ^{3}He



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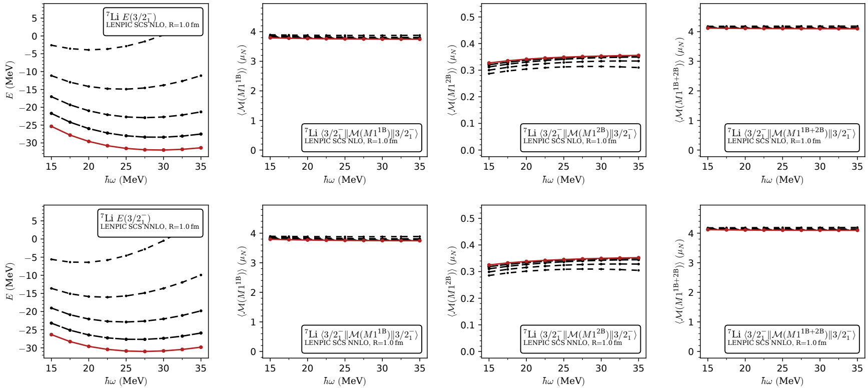
Magnetic moments for ^{7}Li



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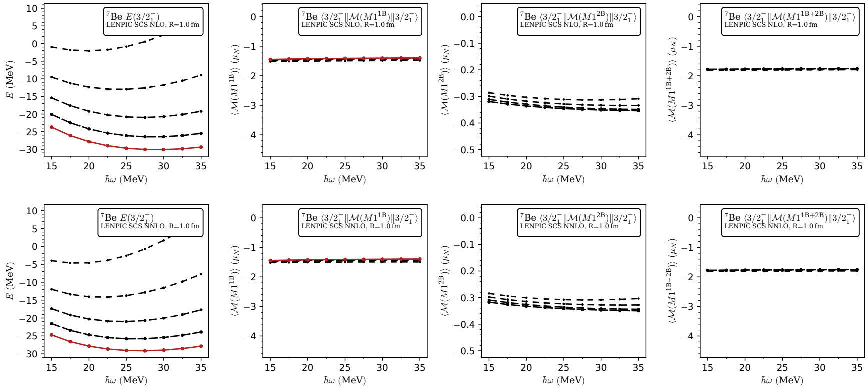
Magnetic moments for ^{7}Be



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