Quantum Monte Carlo and local chiral interactions: light and not-so-light nuclei

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SciDAC Scientific Discovery through Advanced Computing

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MICHIGAN STATE UNIVERSITY

NUCLEI Nuclear Computational Low-Energy Initiative

NERSC

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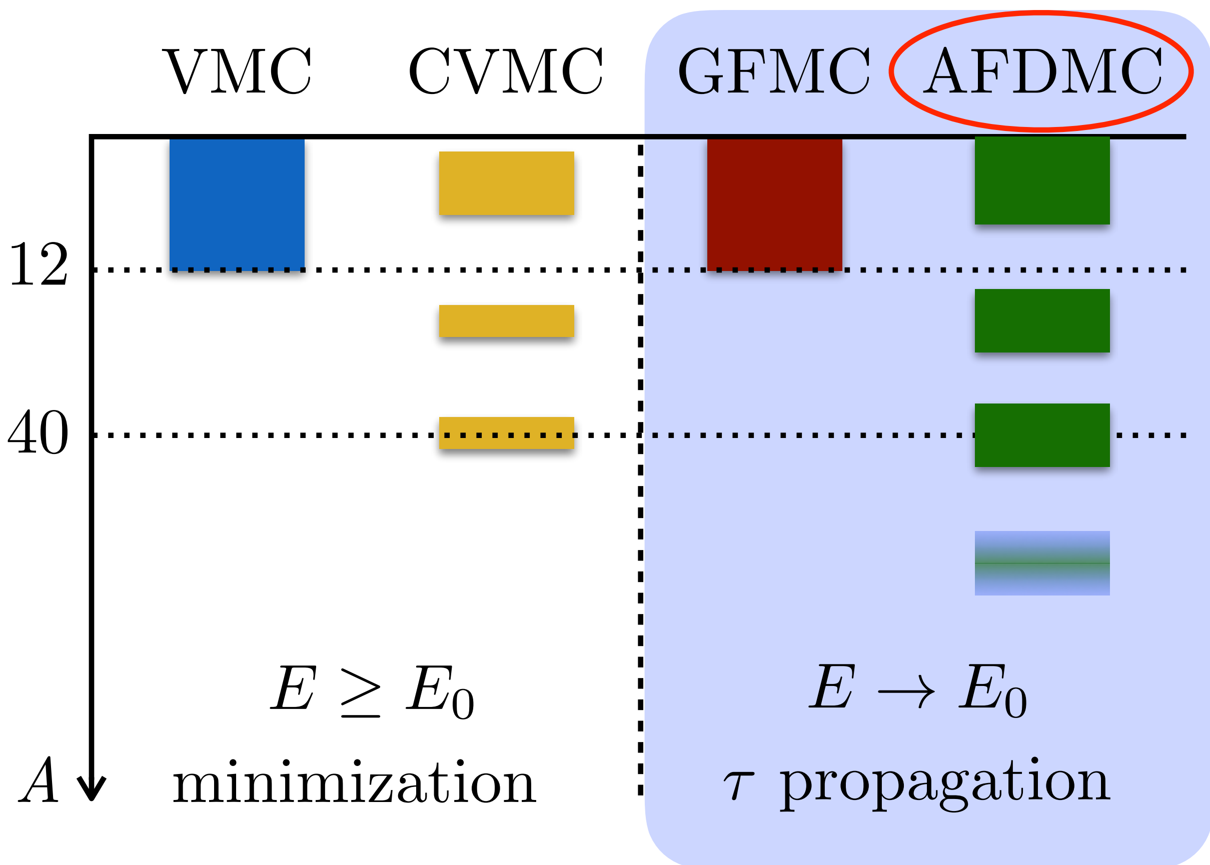
Outline

- ✓ Quantum Monte Carlo
  - AFDMC
- ✓ Nuclear Hamiltonians
  - Phenomenological potentials
  - Local chiral potentials
- ✓ AFDMC & local chiral potentials
  - Results
- ✓ Summary & Perspectives

Quantum Monte Carlo

Goal: solve the many-body problem for correlated systems in a non perturbative fashion



(C)VMC GFMC AFDMC	light systems	$A \leq 12$
CVMC AFDMC	light to medium-mass nuclei	$A \sim 50$
AFDMC	infinite matter	$A \to \infty$

Pros:

- Truly *ab-initio*: work with bare interactions.
- Good for strongly correlated systems.
- Stochastic method: errors quantifiable and systematically improvable. $\sigma \sim 1/\sqrt{\mathcal{N}}$

Cons:

- Limitations in the systems and/or in the interaction to be used.
- Can be computationally expensive.

Quantum Monte Carlo: AFDMC

Auxiliary Field Diffusion Monte Carlo (AFDMC)

$$|\Psi_V\rangle = \underbrace{\left[1+\sum_{i<j<k} U_{ijk}\right]}_{\text{3-body corr}} \underbrace{\left[1+\sum_{i<j} U_{ij}\right]\left[\prod_{i<j} f_c(r_{ij})\right]}_{\text{2-body corr (linear)}} \underbrace{\mathcal{A}\,|\Phi\rangle}_{\text{mean field}}$$

$\mathcal{A}\,|\Phi\rangle$ → $\mathcal{N}_{\rm det}$ determinants of single-particle orbtials + spinors: proper (J^π, T)

1. minimization: variational search of optimal parameters for $|\Psi_V\rangle$ $\longrightarrow$ SR, LM
2. propagation in imaginary time: $e^{-H\tau}|\Psi_V\rangle \xrightarrow{\tau\to\infty} |\Psi_0\rangle$ $\quad\tau = \mathcal{M}d\tau \quad \begin{array}{l}\mathcal{M}\gg 1\\ d\tau \ll 1\end{array}$

   - spatial degrees of freedom: diffusion of positions in coordinate space
   - spin-isospin degrees of freedom: Hubbard-Stratonovich transformation

$$e^{-\frac{1}{2}\lambda d\tau\mathcal{O}^2} = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} dx\, e^{-\frac{1}{2}x^2}\, e^{\sqrt{-\lambda d\tau}\,x\,\mathcal{O}}$$

Note: 2-body operators only — dx: auxiliary fields; $e^{\sqrt{-\lambda d\tau}\,x\,\mathcal{O}}$: spin-isospin rotations

   - sign problem: constrained path approximation + unconstrained evolution

ground-state energies within 1-2% with respect to GFMC

Nuclear Hamiltonians

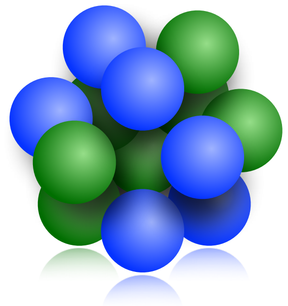
Model: non-relativistic nucleons interacting with an effective nucleon-nucleon (NN) force and three-nucleon interaction (NNN)

$$H = -\frac{\hbar^2}{2m_N}\sum_i \nabla_i^2 + \sum_{i<j} v_{ij} + \sum_{i<j<k} v_{ijk} + \ldots$$

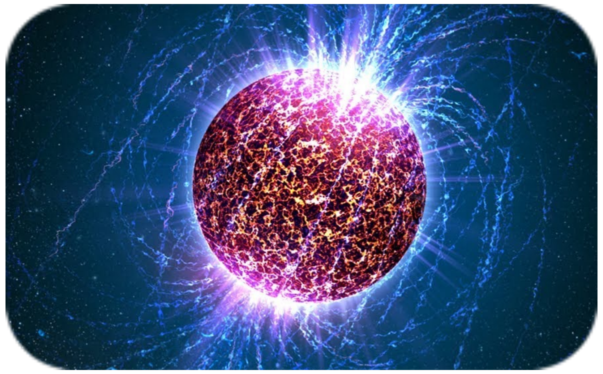
v_{ij} fit to NN scattering data & deuteron

v_{ijk} fit to properties of nuclei

Question: is it possible to describe nuclei and their global properties from microscopic nuclear Hamiltonians constructed to reproduce only few-body observables, while simultaneously predicting properties of matter?



nuclear potentials ?



$R \sim \text{fm} \sim 10^{-15}\,\text{m}$

$M \sim 10^{-27}\,\text{kg}$

$R \sim 10\,\text{km} \sim 10^{4}\,\text{m}$

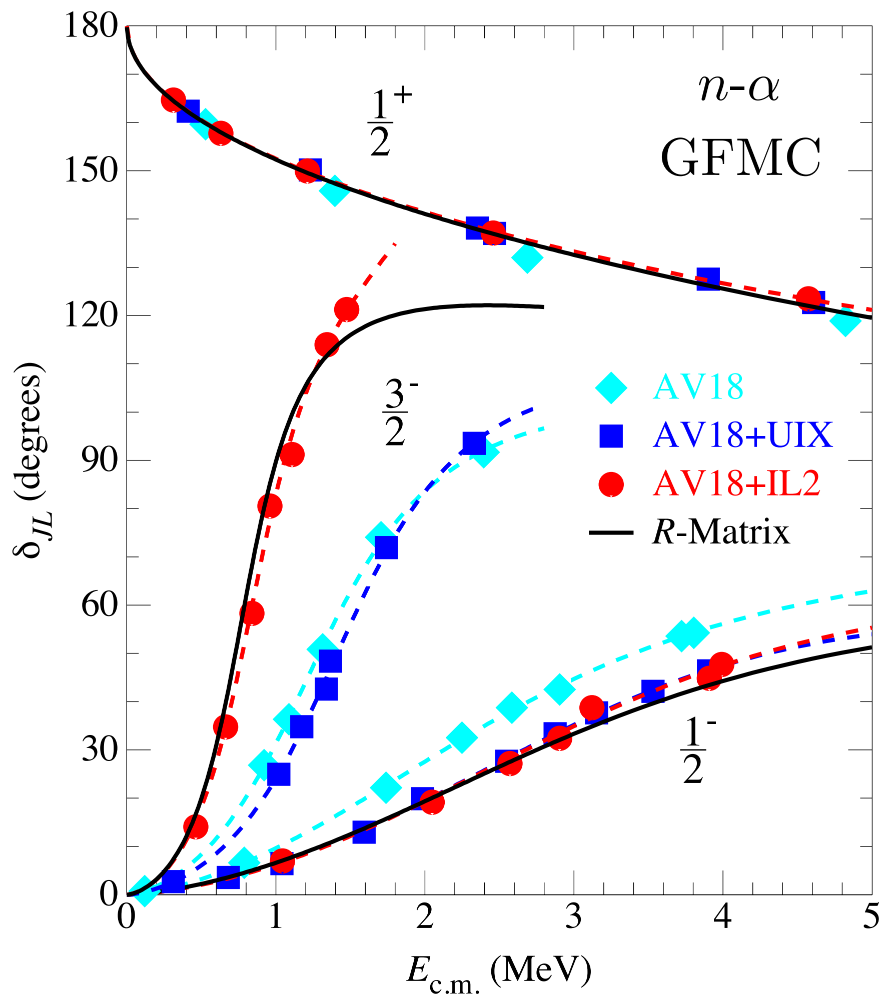
$M \sim 1.4\,M_\odot \sim 10^{30}\,\text{kg}$

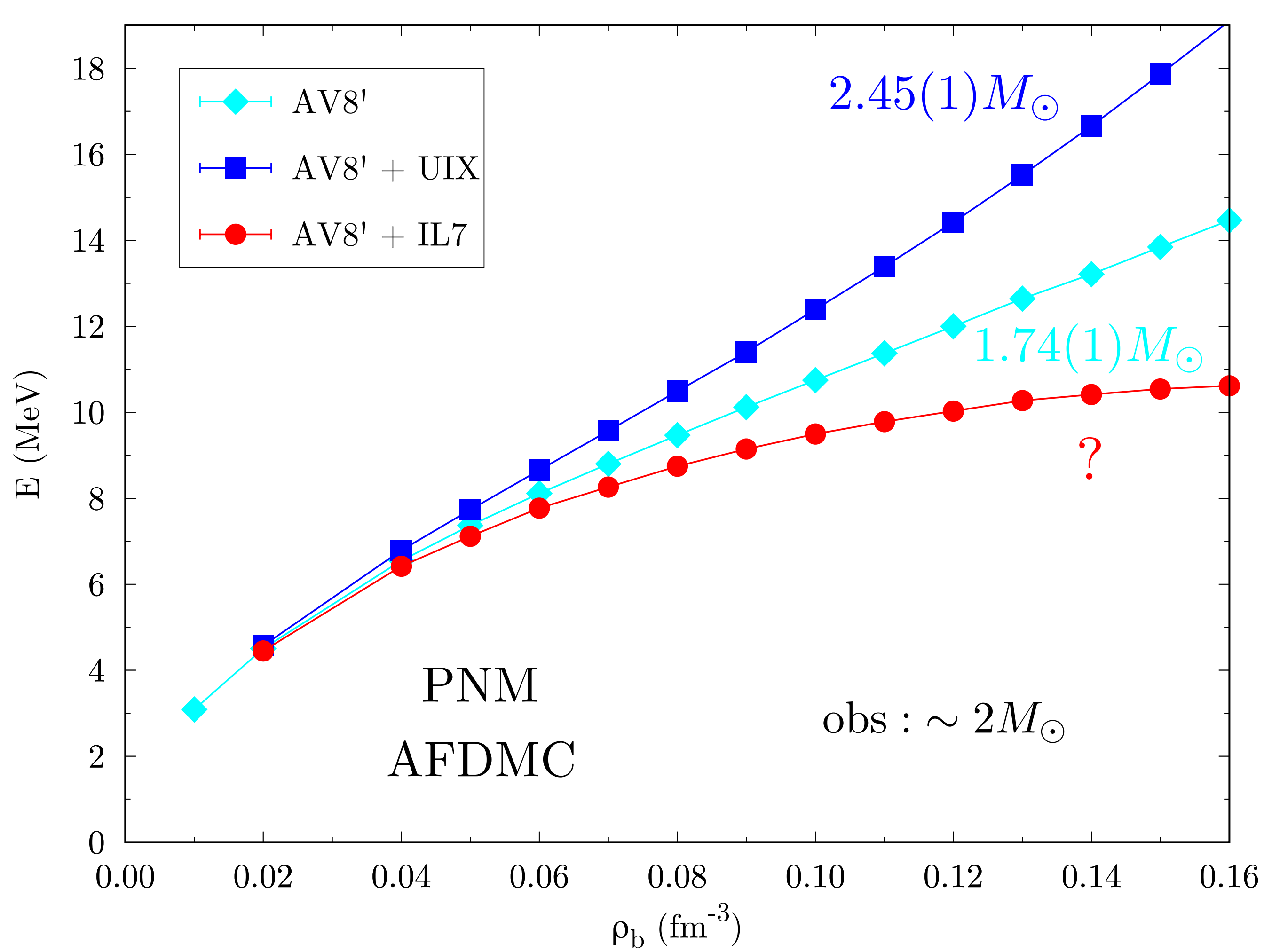
Nuclear Hamiltonians: phenomenological potentials

- ✓ remarkable description of the physics of light nuclei up to ^{12}C

  J. A. Carlson *et al.*, Rev. Mod. Phys. **87**, 1067 (2015)

- ✤ unrealistic description of pure neutron matter & neutron star structure

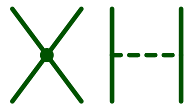
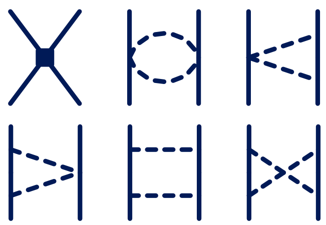
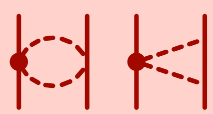
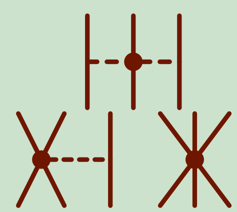




K. M. Nollett *et al.*, Phys. Rev. Lett. **99**, 022502 (2007)

P. Maris *et al.*, Phys. Rev. C **87**, 054318 (2013)

Nuclear Hamiltonians: local chiral potentials

	NN	NNN
LO $\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^0$		—
NLO $\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^2$		—
$\mathrm{N^2LO}$ $\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^3$		

local in coordinate space	AV7 operator structure	mostly 2-body operators
↓	↓	↓
good for QMC	ok in propagator	doable in propagator

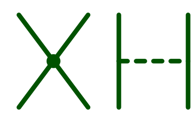
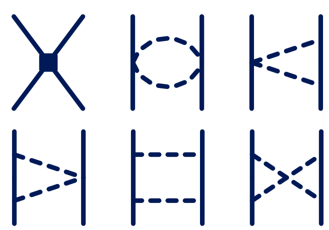
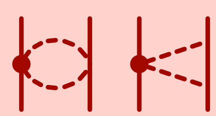
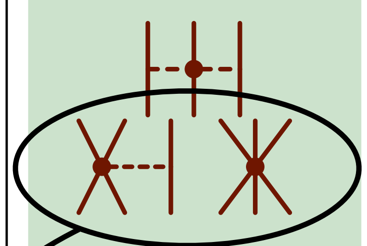
- χEFT: expansion in power of Q/Λ_b

  $Q \sim m_\pi \sim 140\,\mathrm{MeV}$ soft scale

  $\Lambda_b \sim m_\rho \sim 800\,\mathrm{MeV}$ hard scale

- Long-range physics: given explicitly (no parameters to fit) by pion-exchanges
- Short-range physics: parametrized through contact interactions with low-energy constants (LECs) fit to low-energy data
- Many-body forces enter systematically and are related via the same LECs
- Possibility for error quantification

Nuclear Hamiltonians: local chiral potentials

		NN	*NNN*
LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^0$		—
NLO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^2$		—
N^2LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^3$		

local in coordinate space

↓

good for QMC

c_D & c_E fit to:

- ✓ ^{4}He binding energy
- ✓ n-α scattering phase shifts

- χEFT: expansion in power of Q/Λ_b

  $Q \sim m_\pi \sim 140\,\text{MeV}$ soft scale

  $\Lambda_b \sim m_\rho \sim 800\,\text{MeV}$ hard scale

- Long-range physics: given explicitly (no parameters to fit) by pion-exchanges
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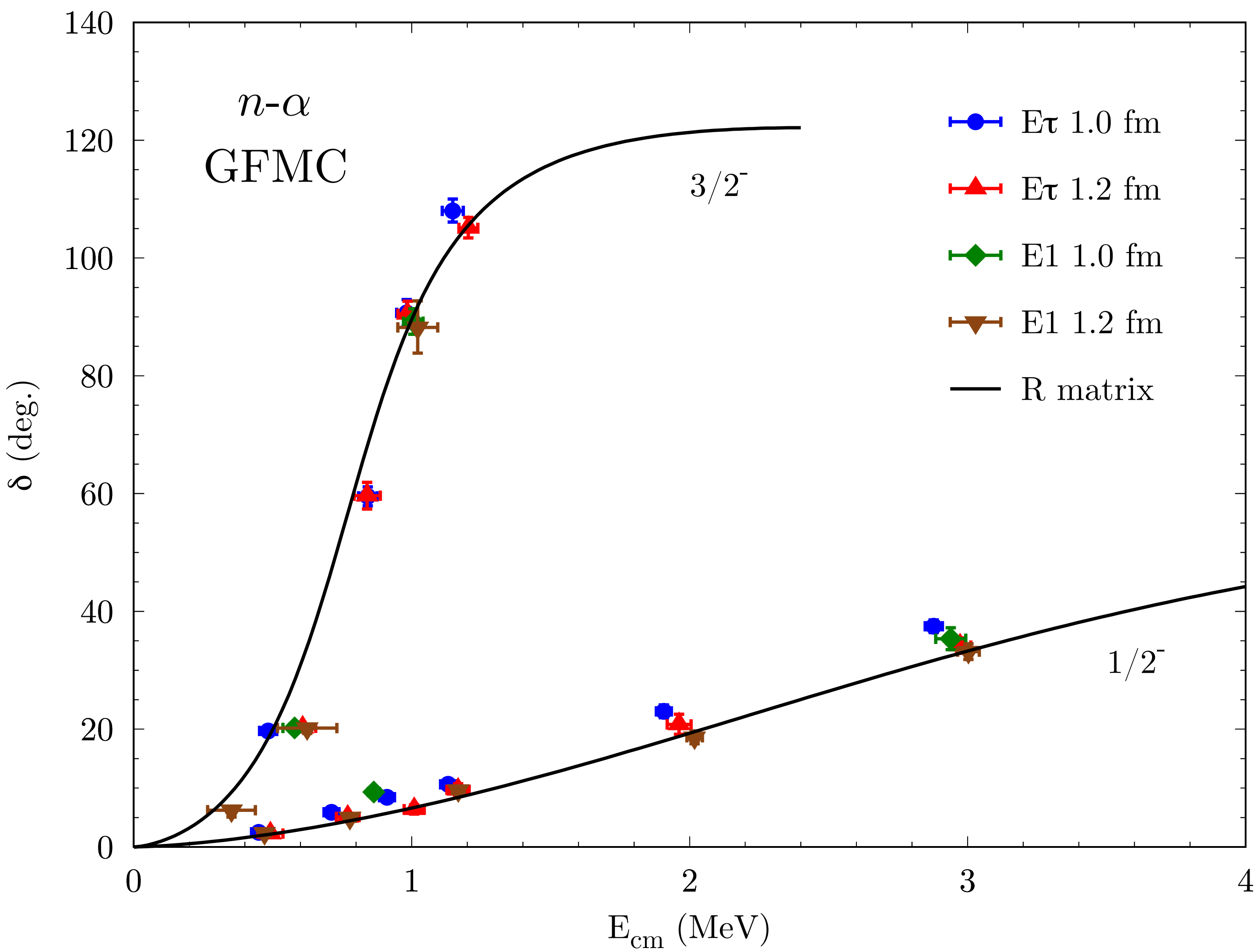
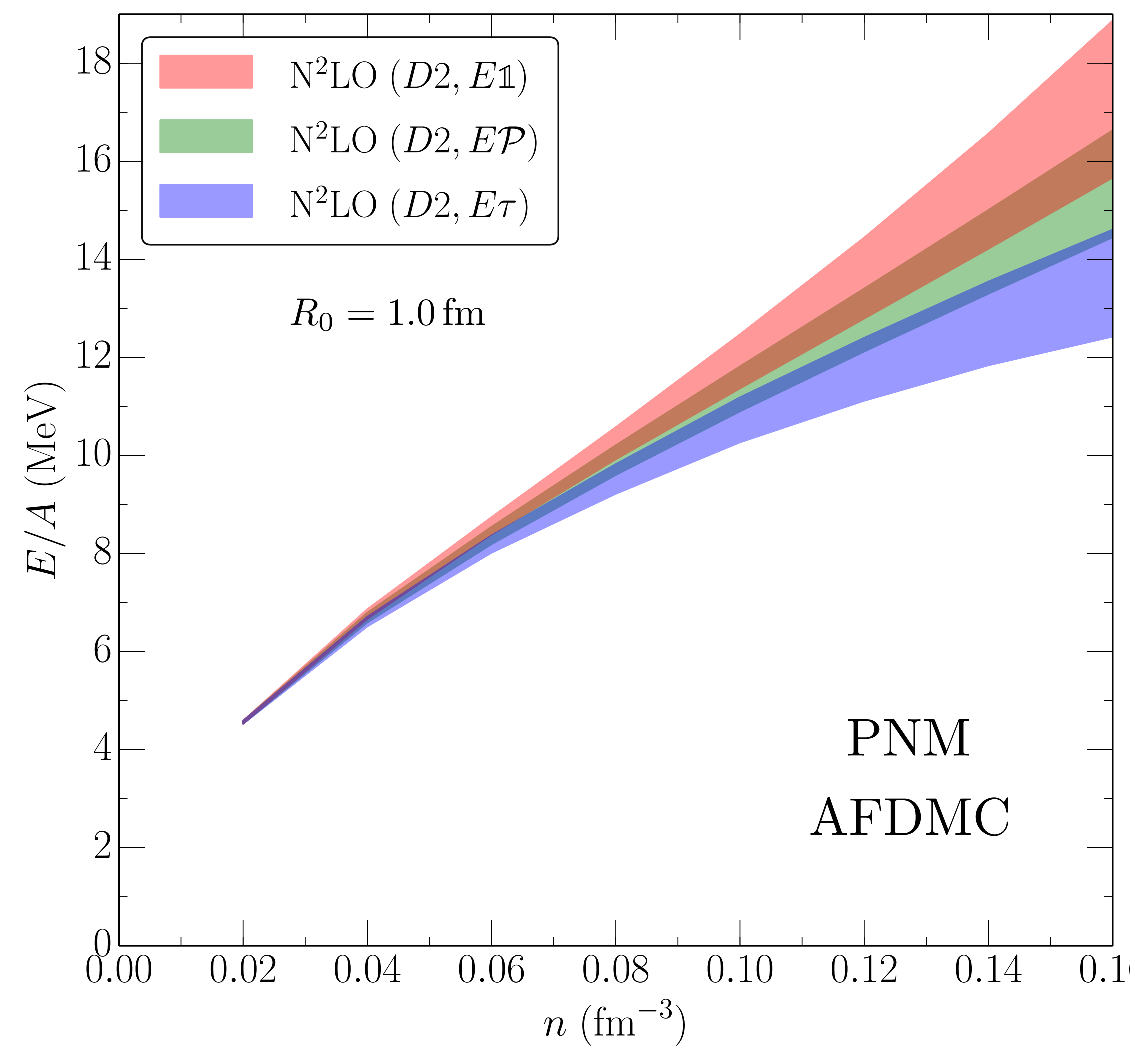
→ info on $T = \dfrac{3}{2}$ physics

Some details:

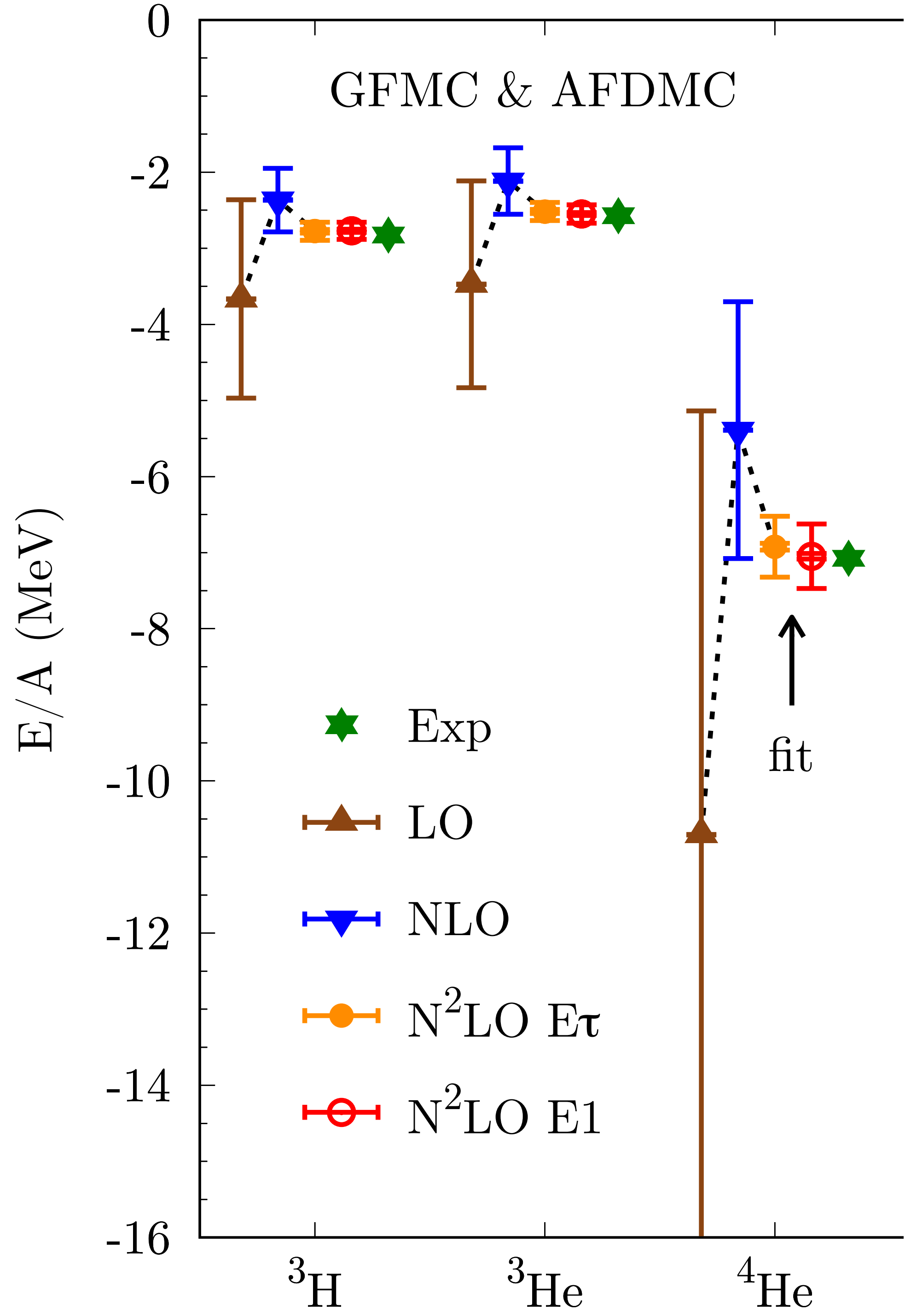
- ✓ coordinate-space cutoff: $R_0 = 1.0\,\text{fm}$ (harder) $R_0 = 1.2\,\text{fm}$ (softer)
- ✓ different possible operator structures: $V_D \longrightarrow D1,\ D2 \qquad V_E \longrightarrow E\tau,\ E\mathbb{1}$



D.L. *et al.*, Phys. Rev. C **97**, 044318 (2018)

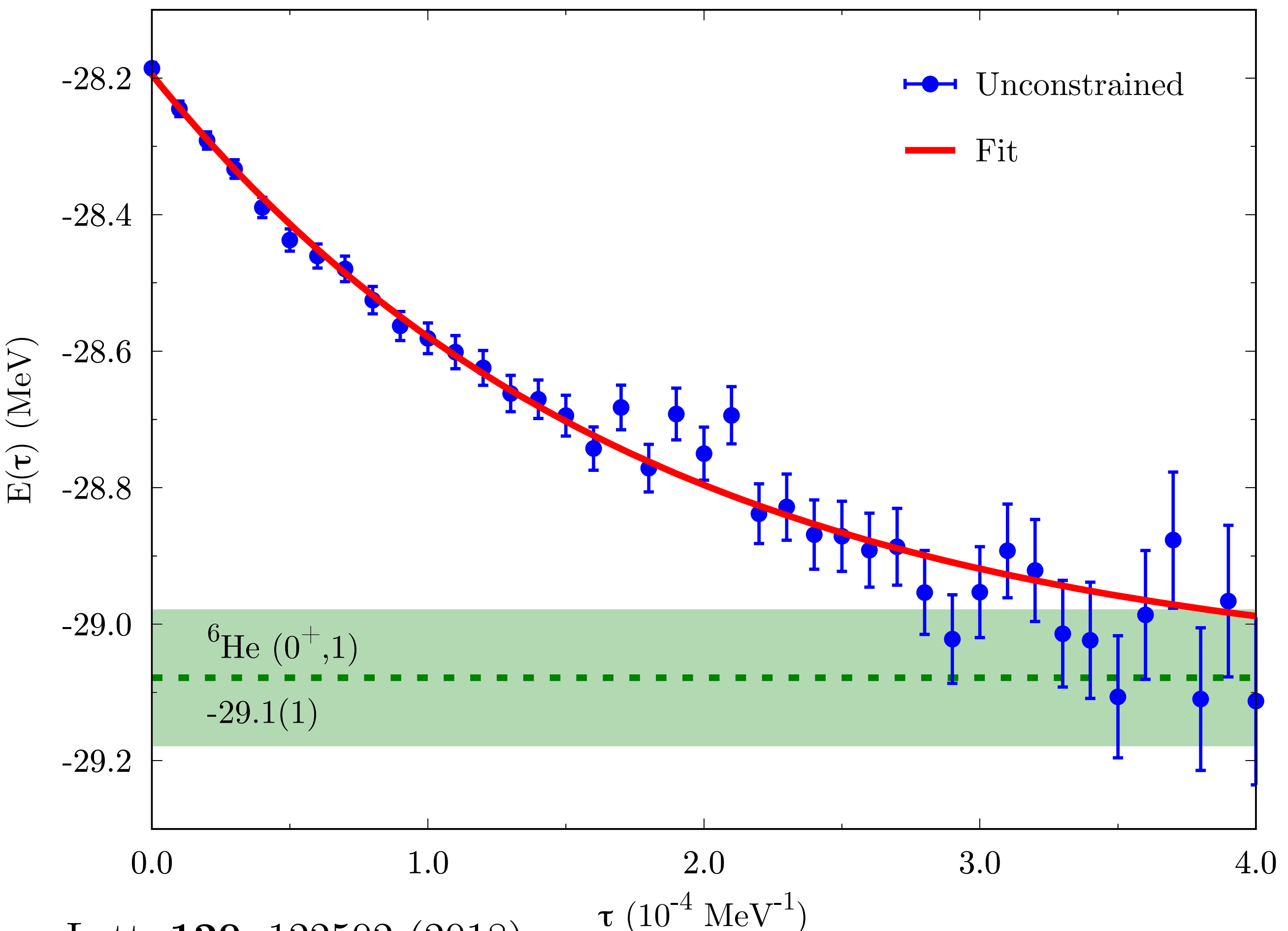


J. E. Lynn *et al.*, Phys. Rev. Lett. **116**, 062501 (2016) energies



first AFDMC calculations:

- ✓ full 2+3-body potentials & correlations
- ✓ closed- and open-shell systems
- ✓ unconstrained evolution
- ✓ statistical and theoretical error estimate



D.L. *et al.*, Phys. Rev. Lett. **120**, 122502 (2018)
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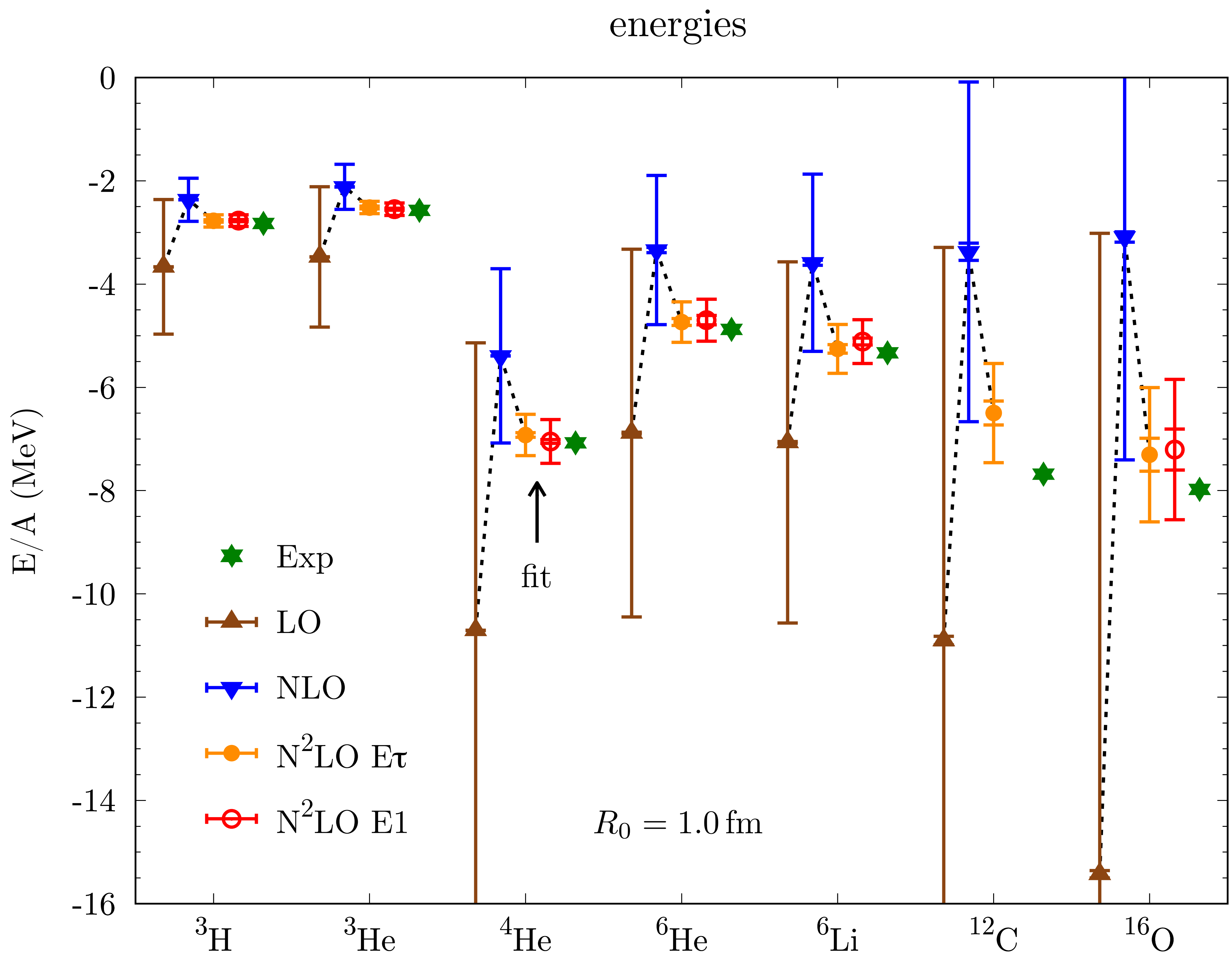

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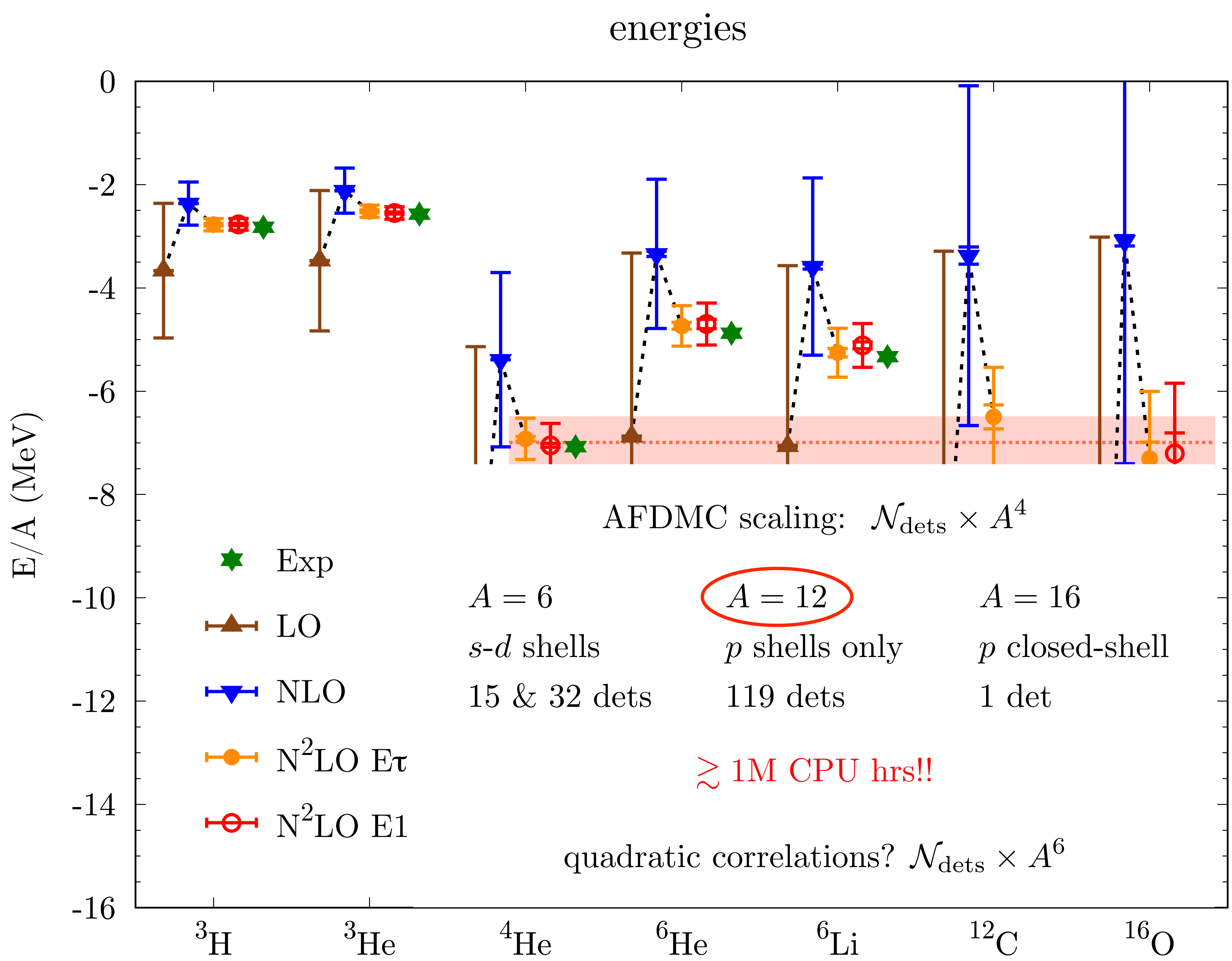
AFDMC & local chiral potentials: results



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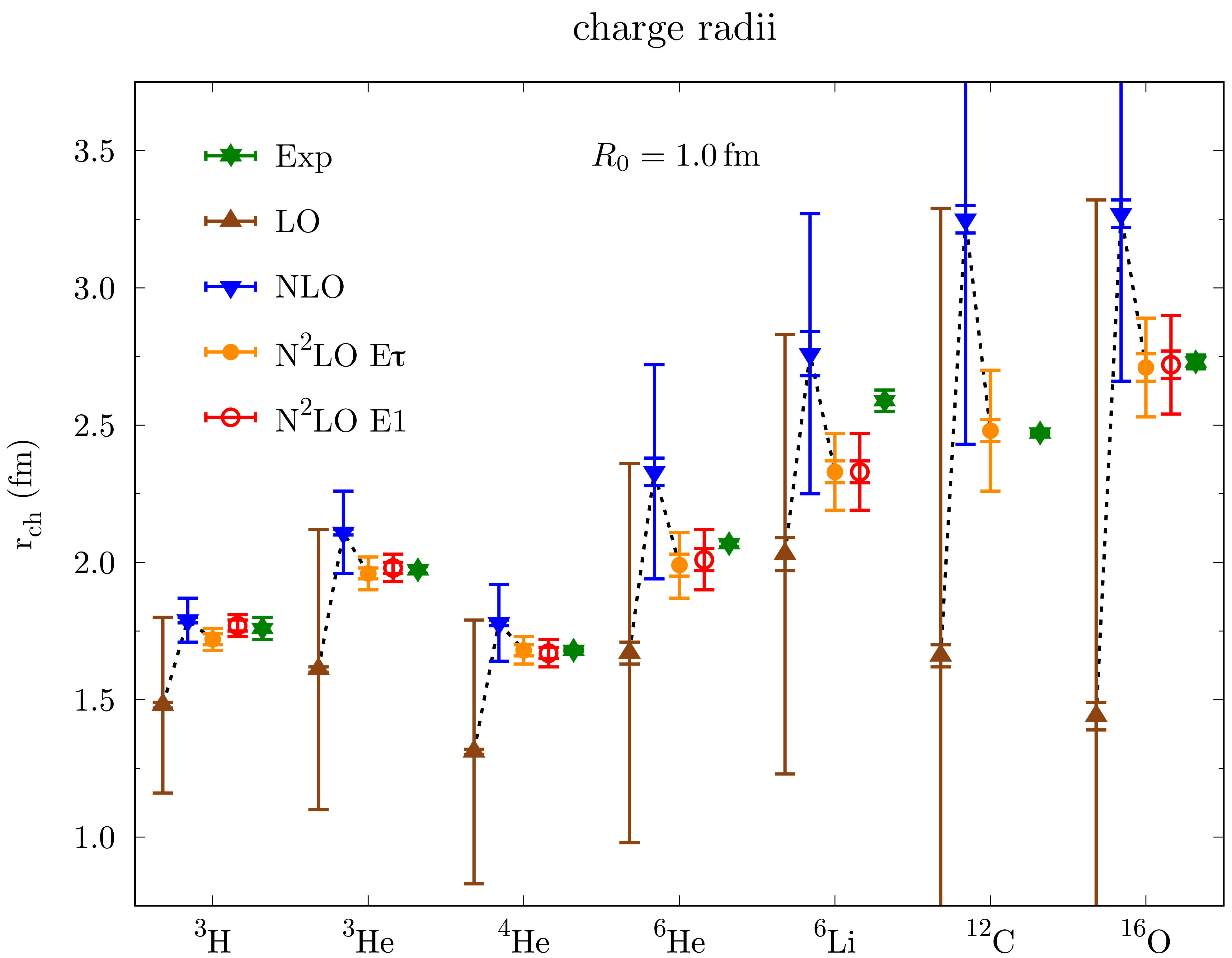

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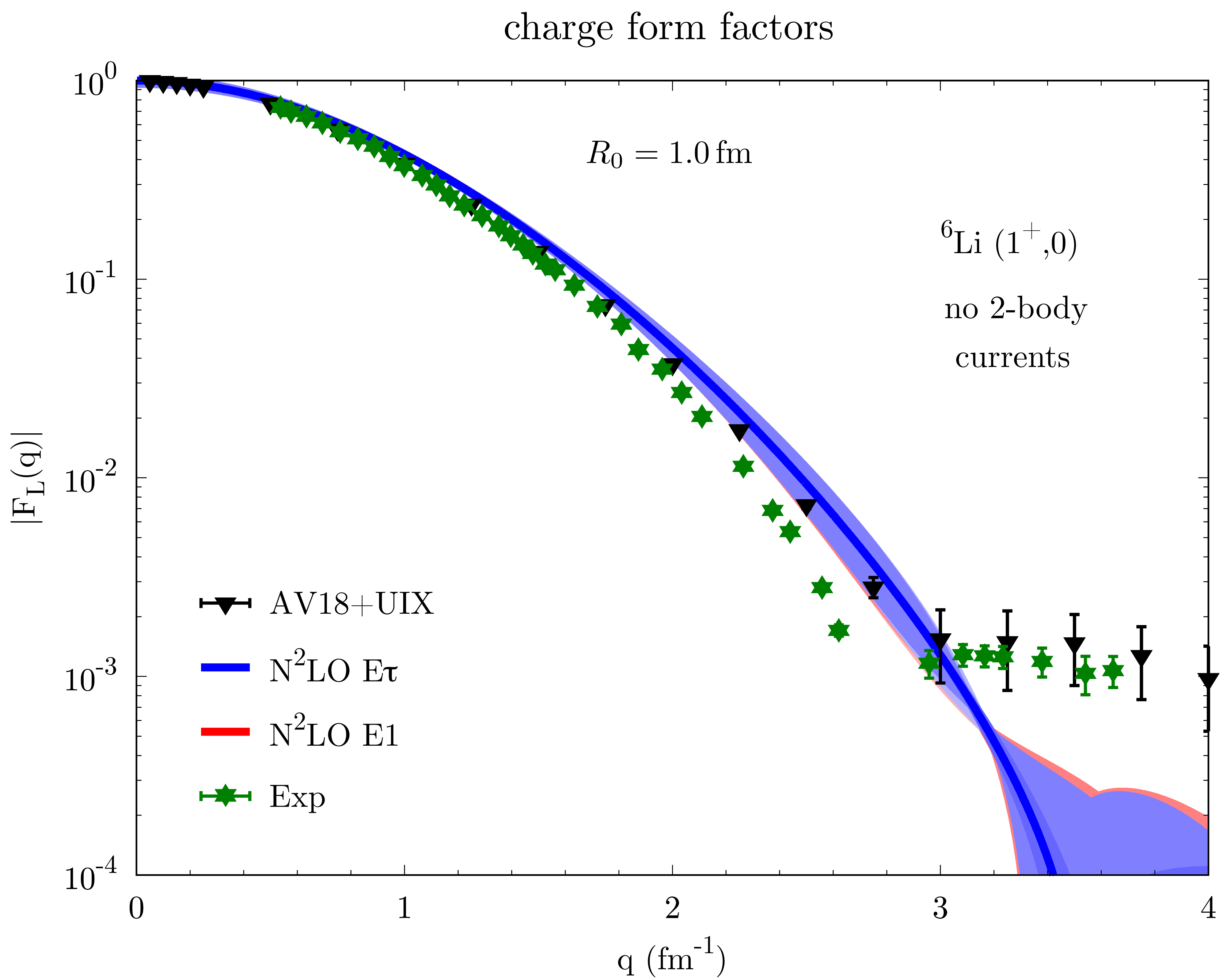

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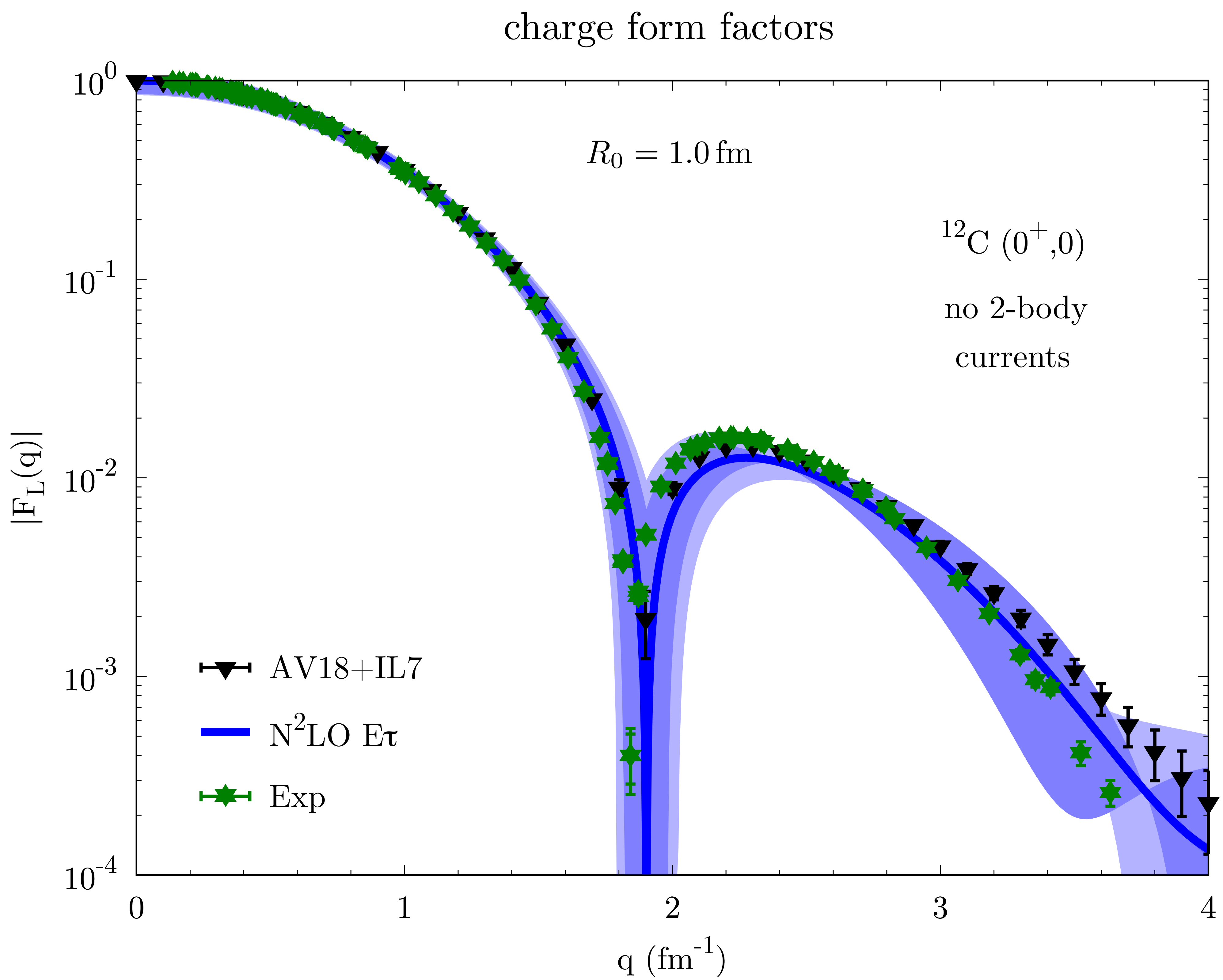

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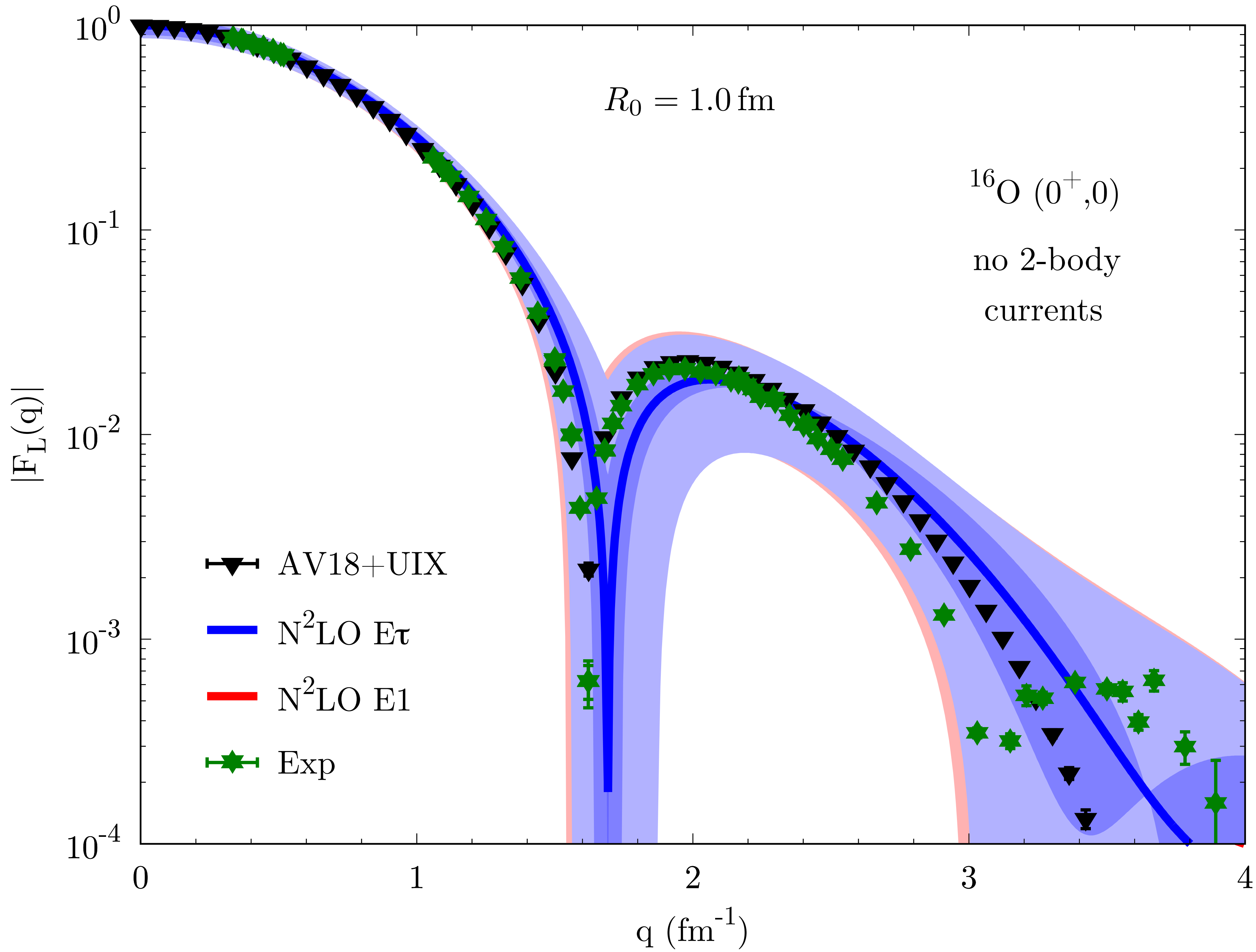
charge form factors



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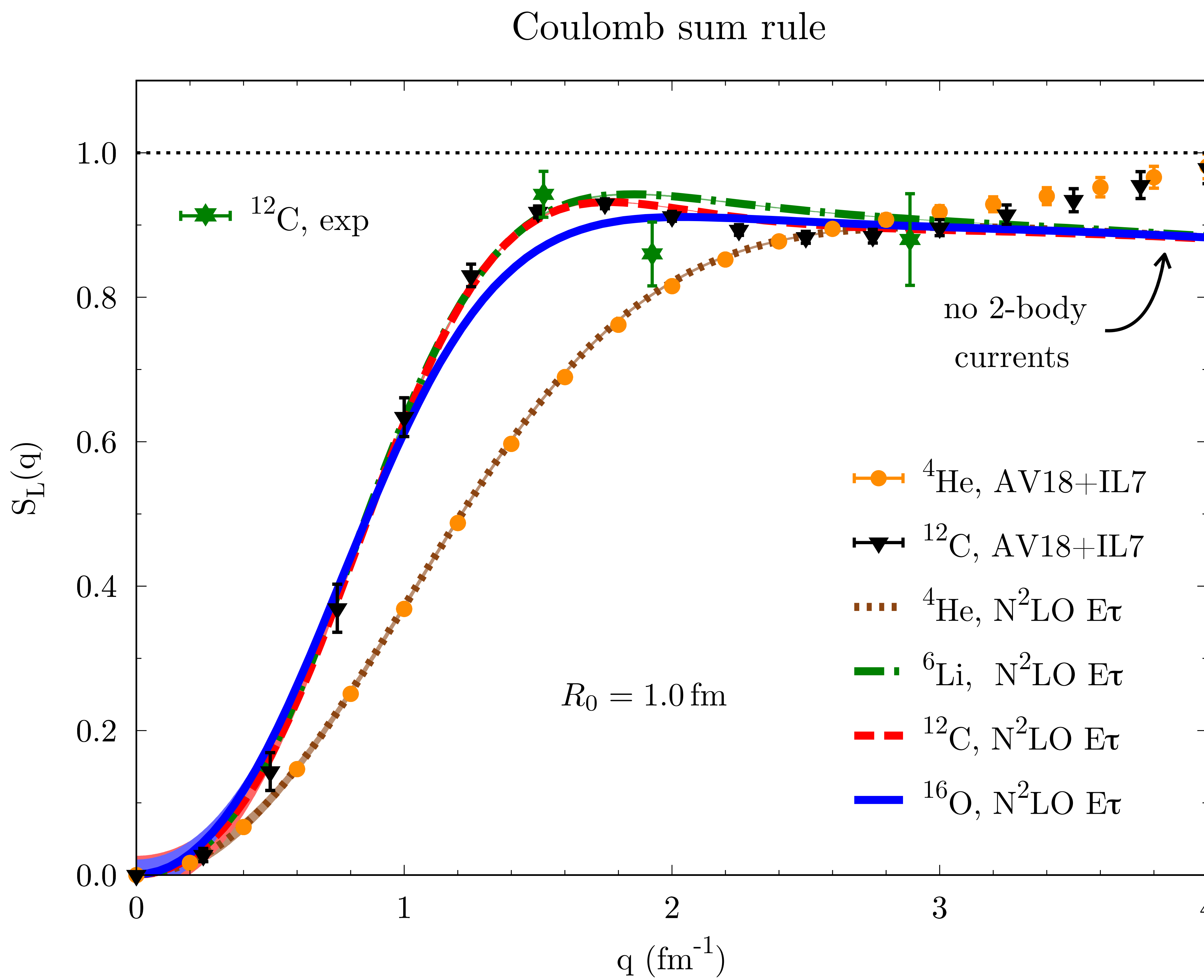

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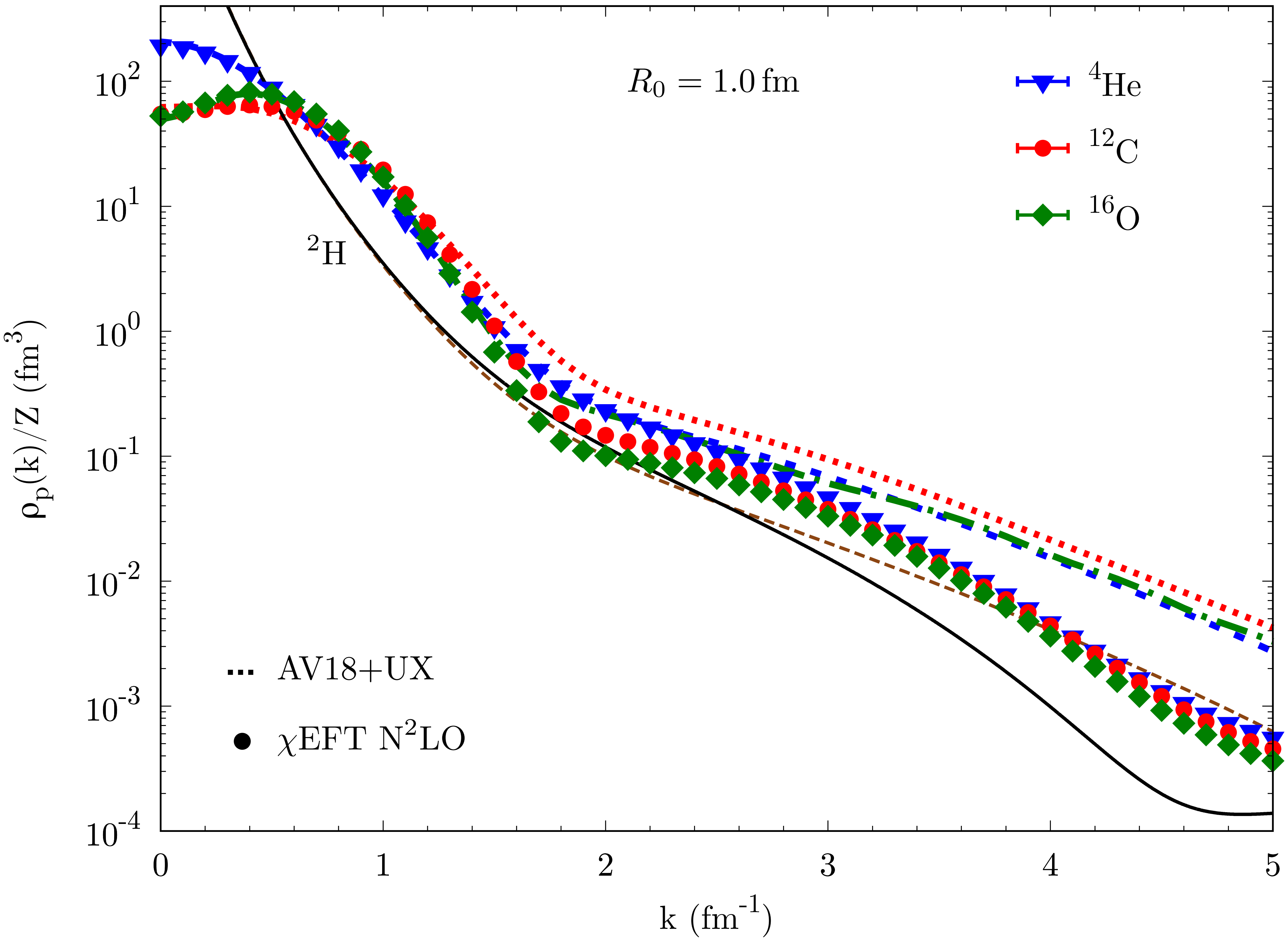
single-nucleon momentum distributions



D.L. *et al.*, Phys. Rev. C **98**, 014322 (2018)
(tables available as Supplemental Material)

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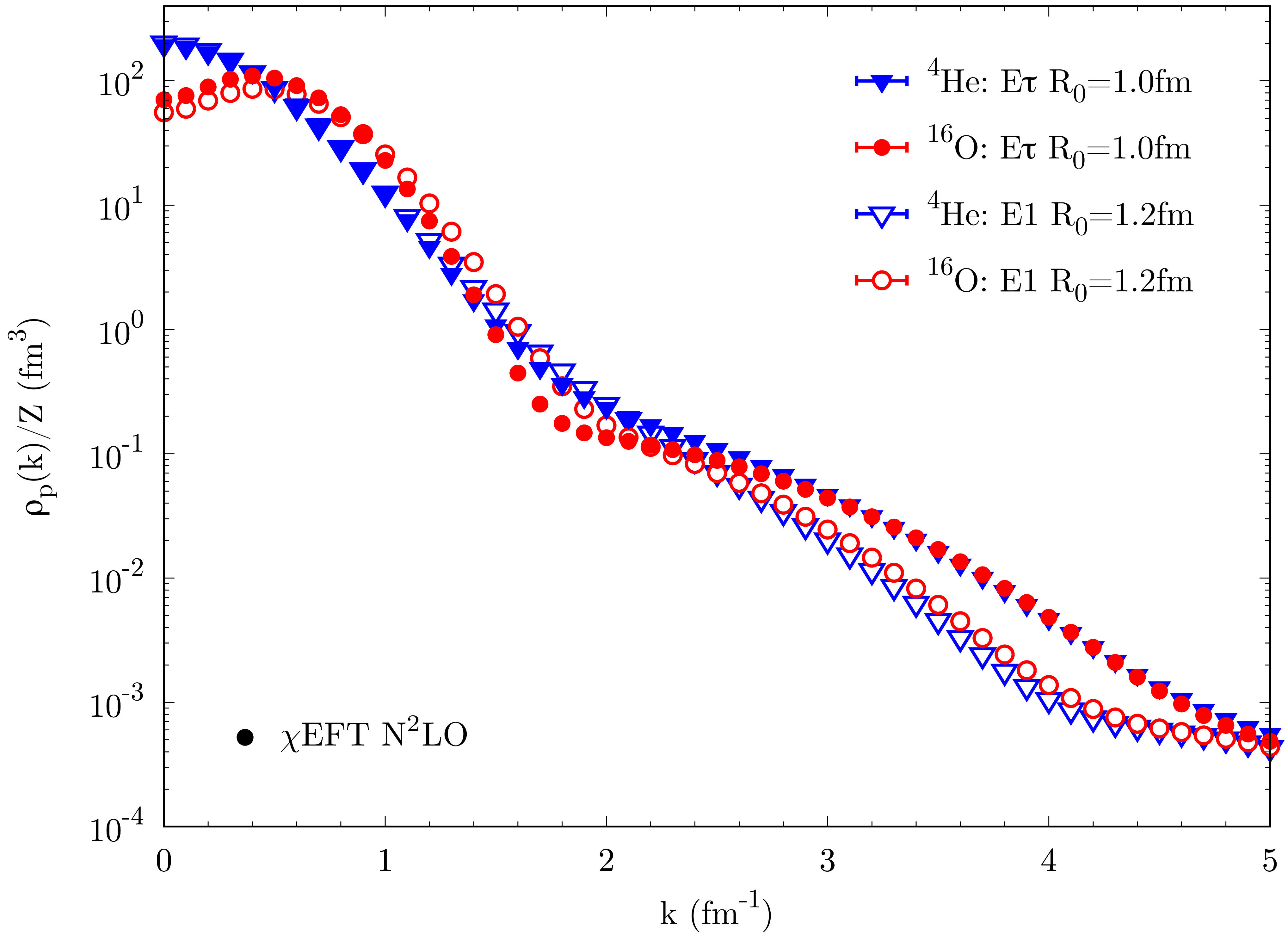

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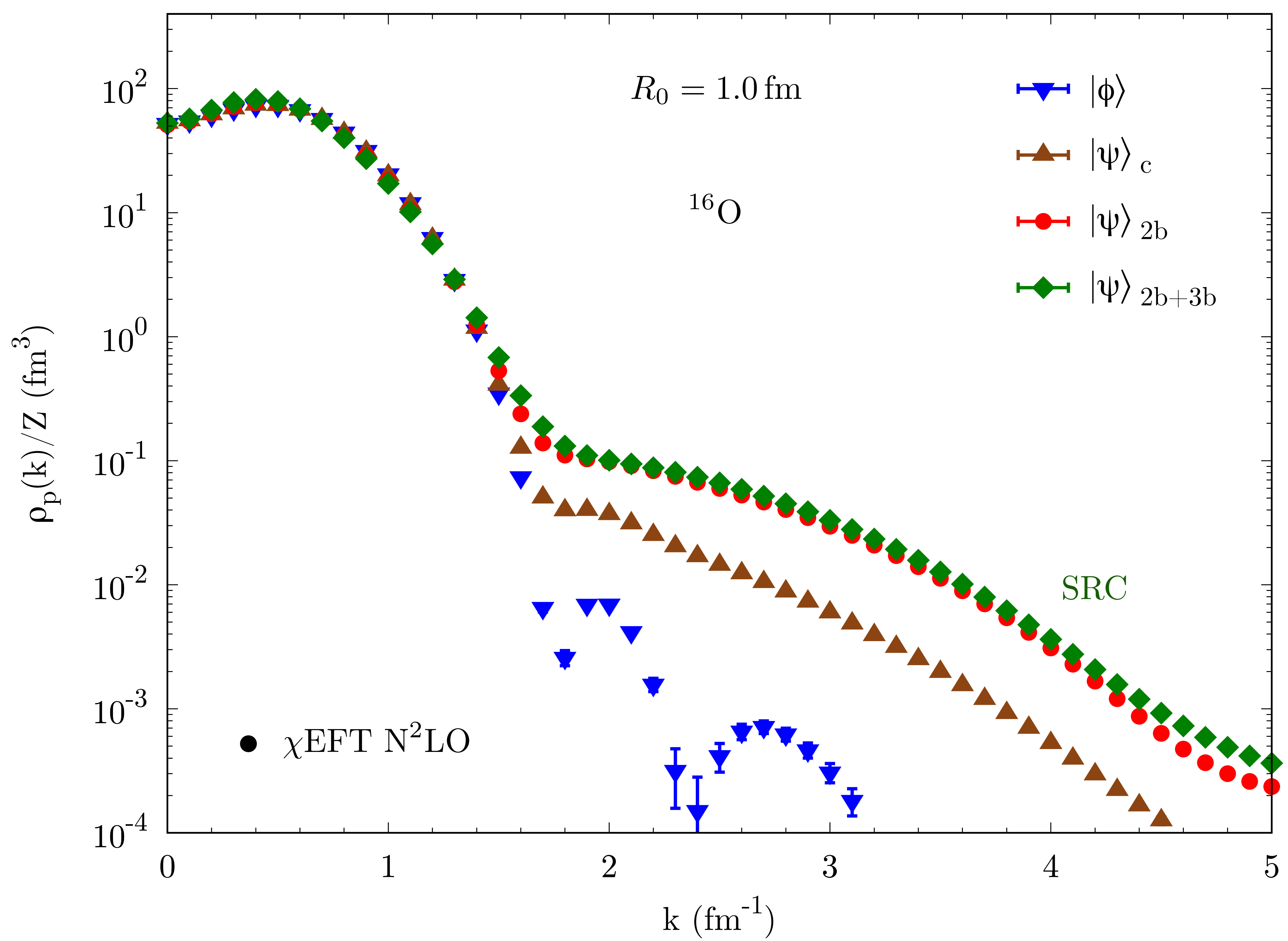

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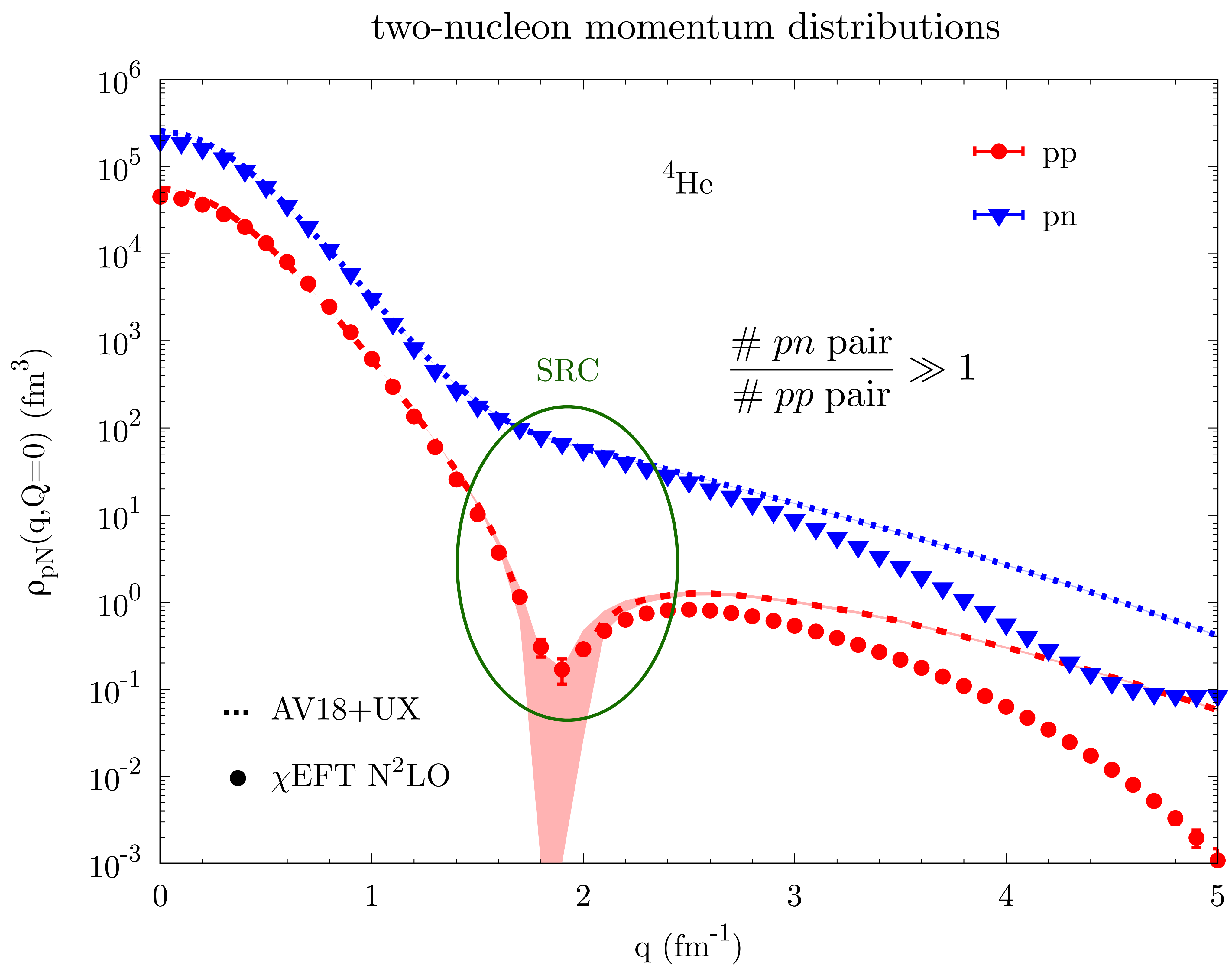

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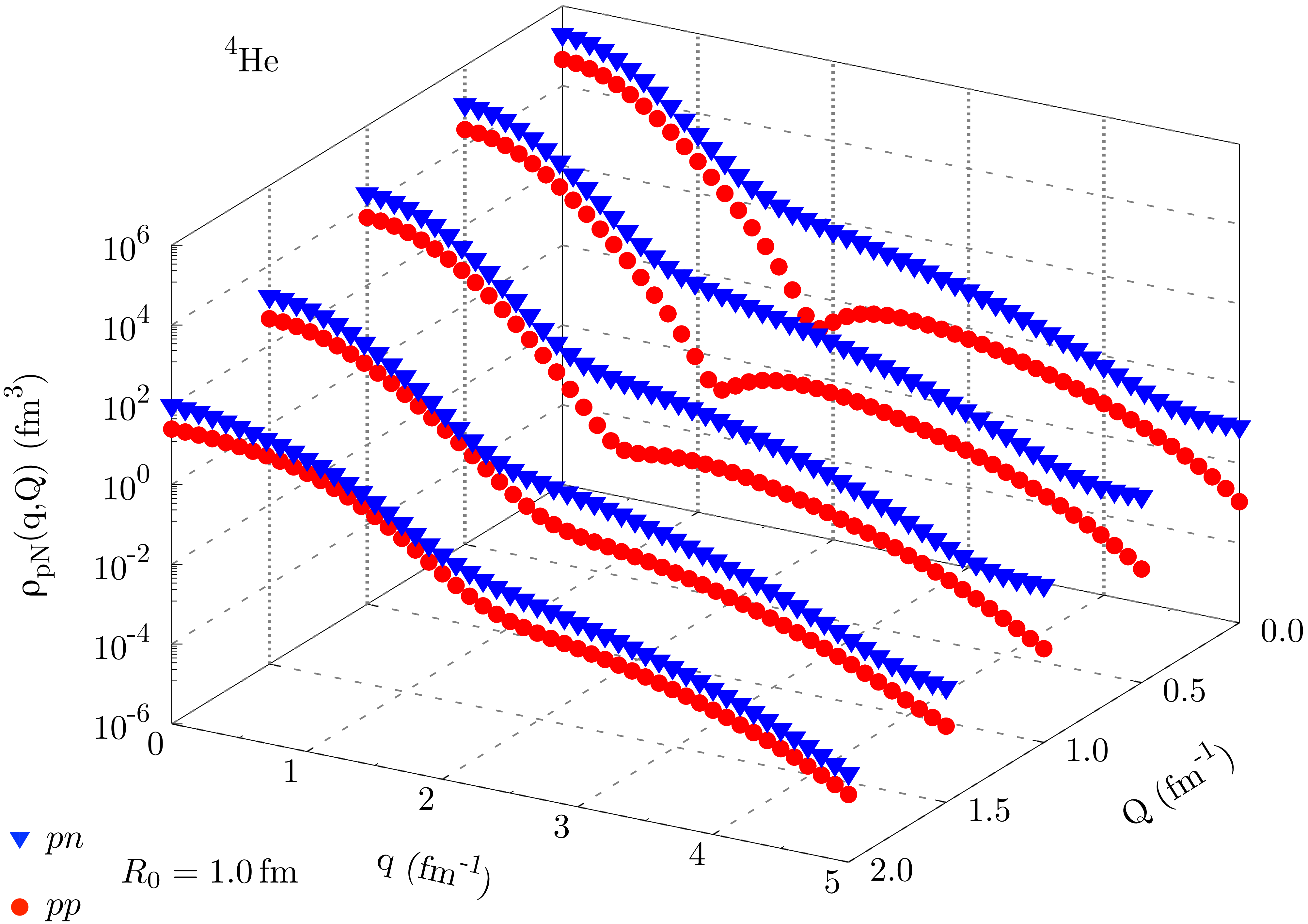
two-nucleon momentum distributions



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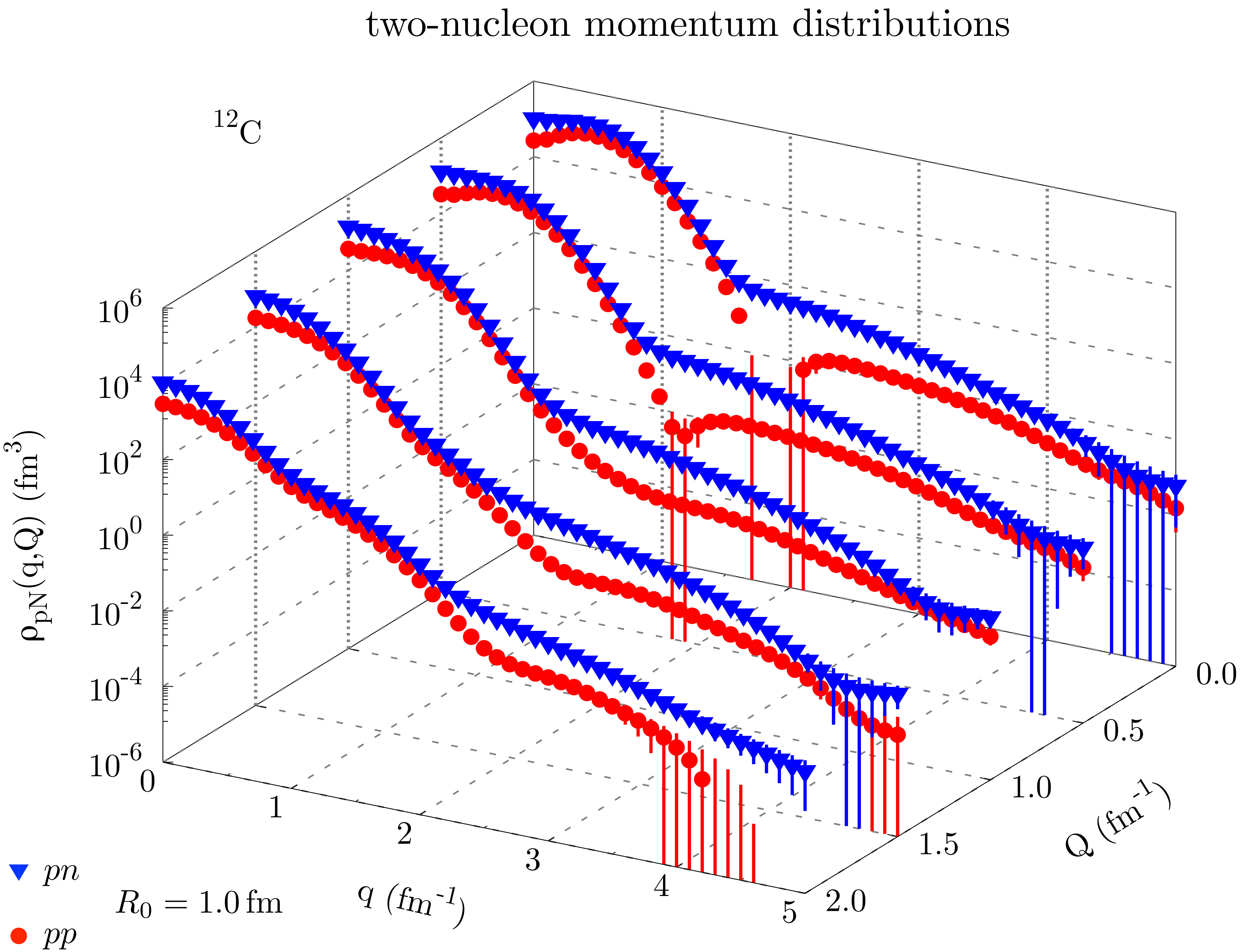

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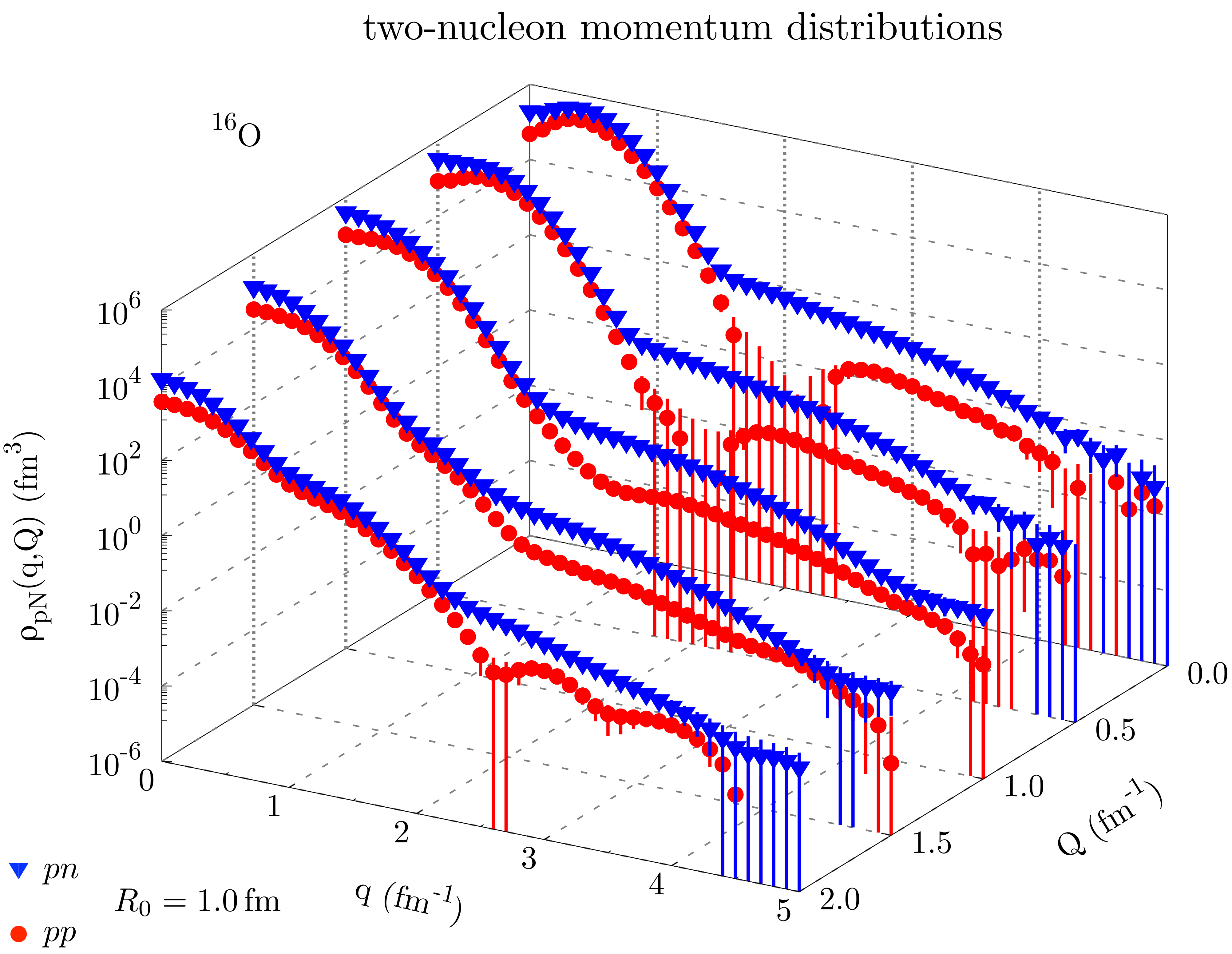

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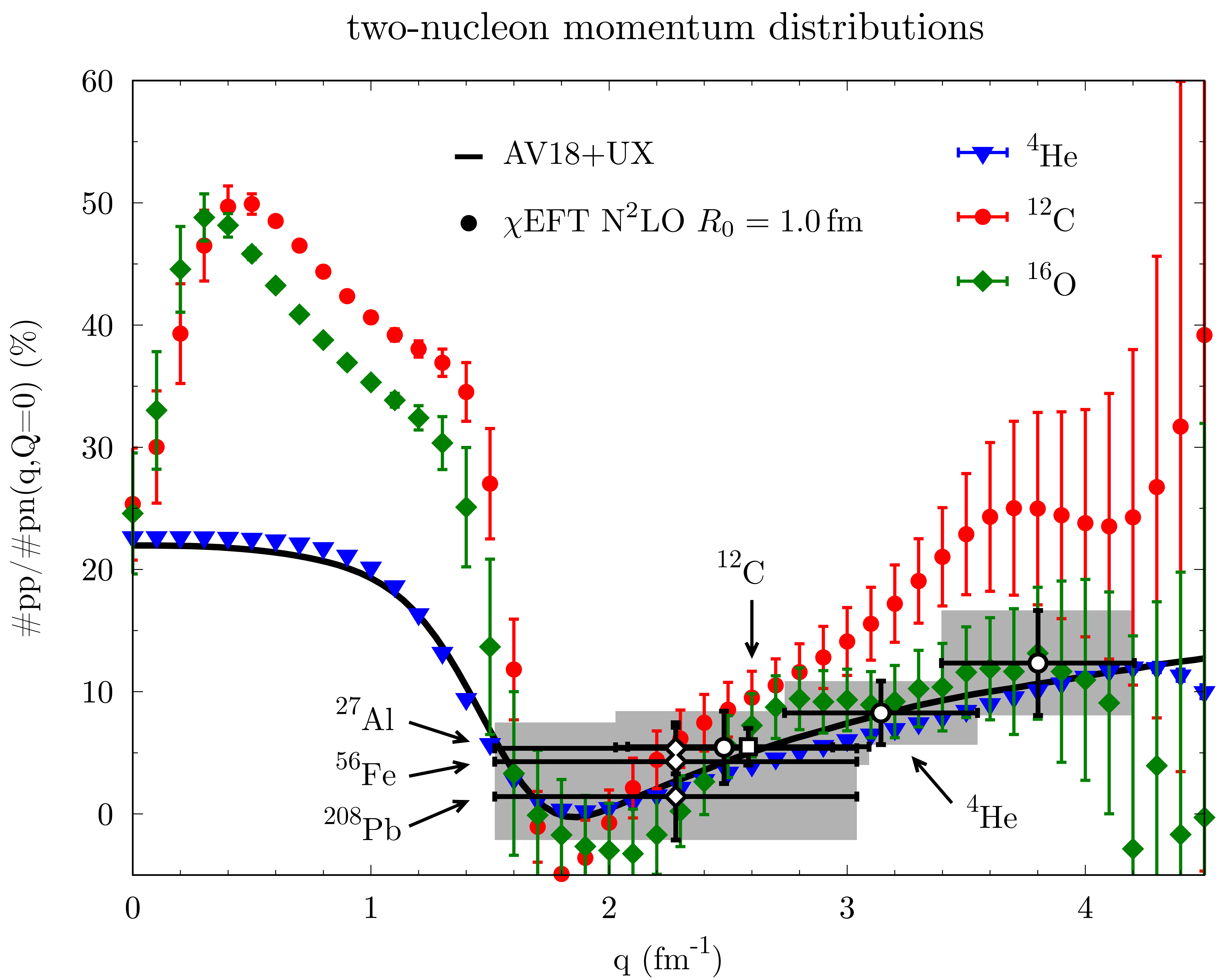

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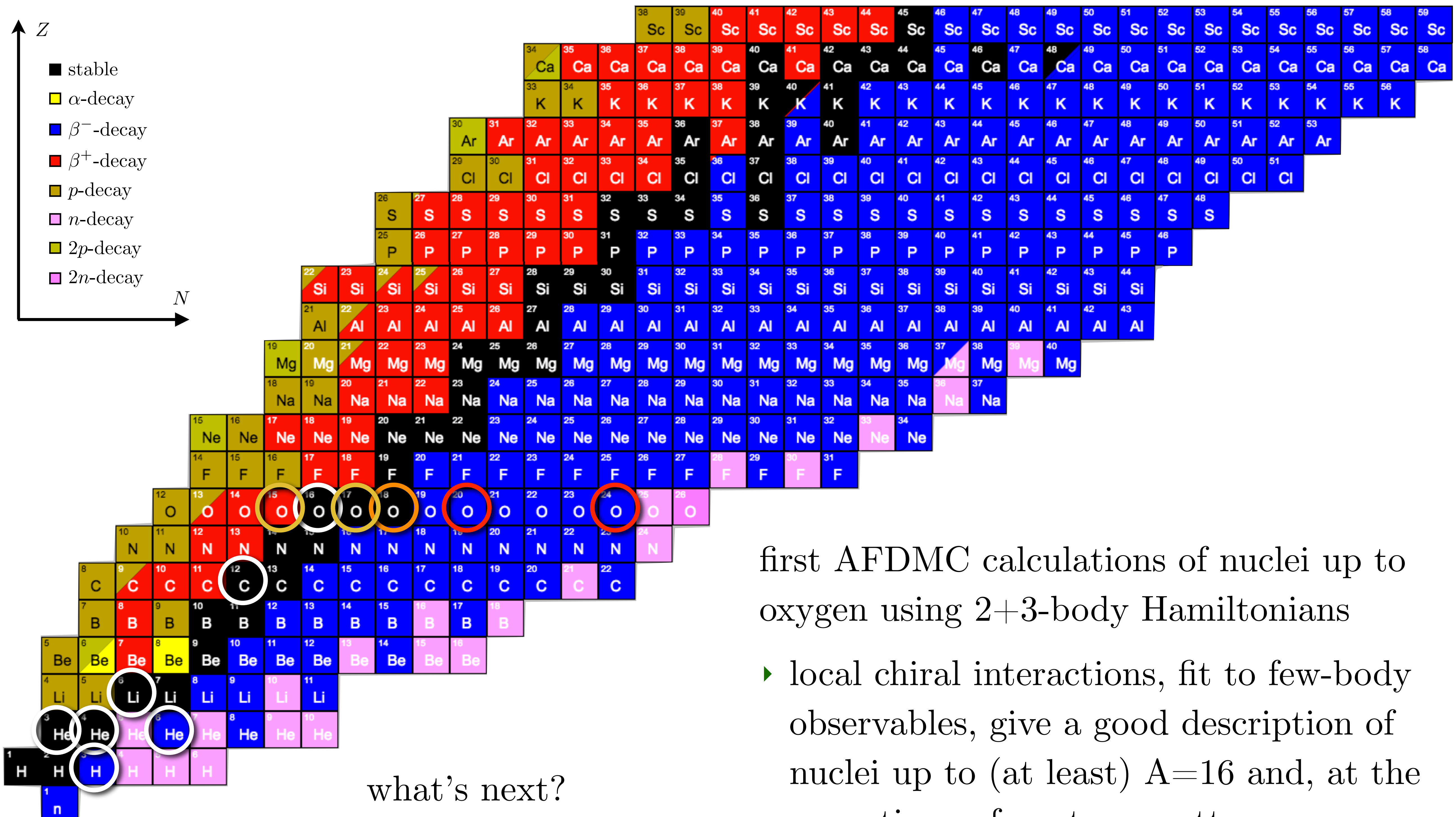
Summary & Perspectives

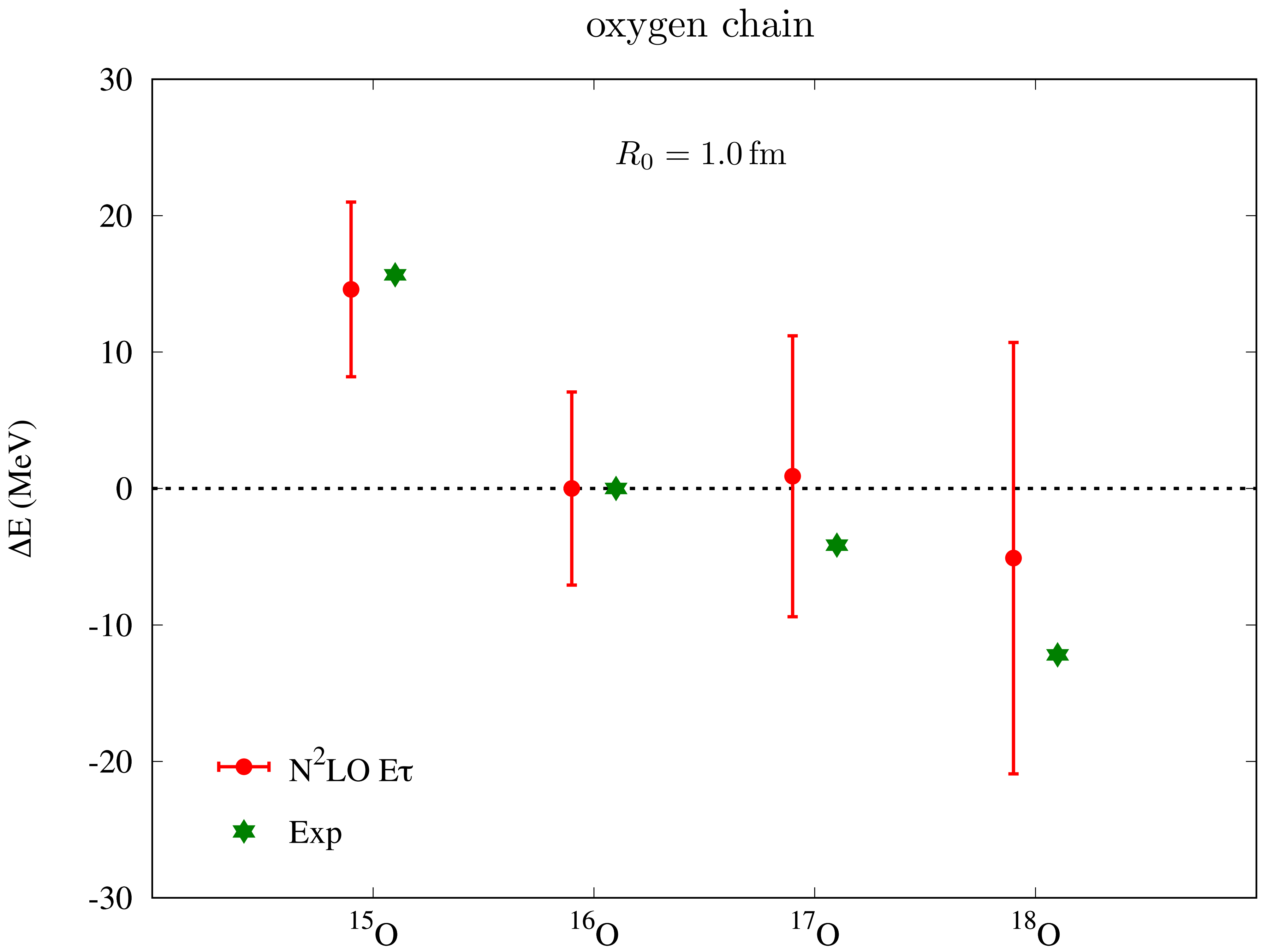


first AFDMC calculations of nuclei up to oxygen using 2+3-body Hamiltonians

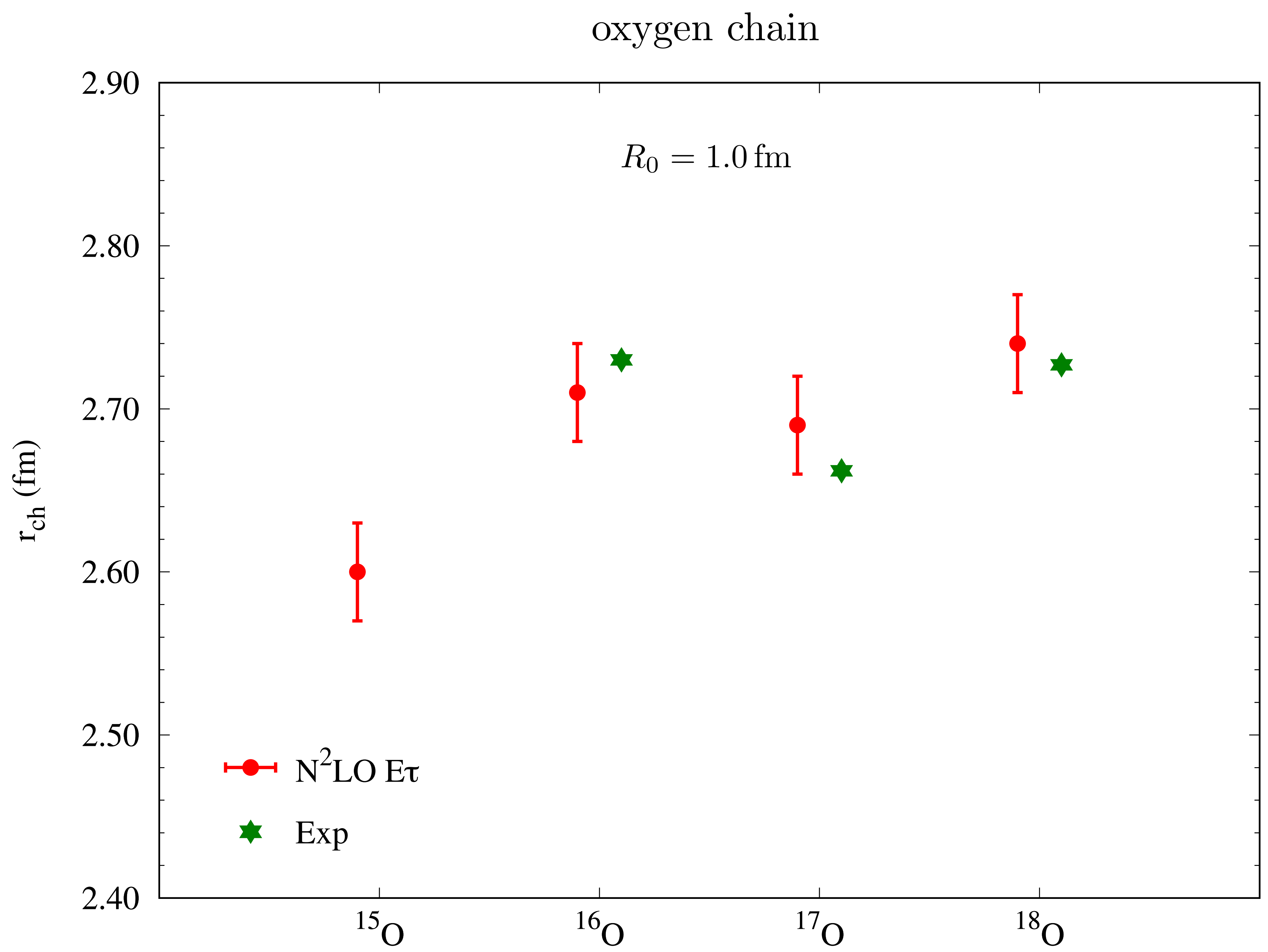
- local chiral interactions, fit to few-body observables, give a good description of nuclei up to (at least) A=16 and, at the same time, of neutron matter
- test of different parametrizations and cutoffs on several observables

what's next?
oxygen/other isotopic chains?
exotic nuclei?
symmetric nuclear matter?

Summary & Perspectives



preliminary!!



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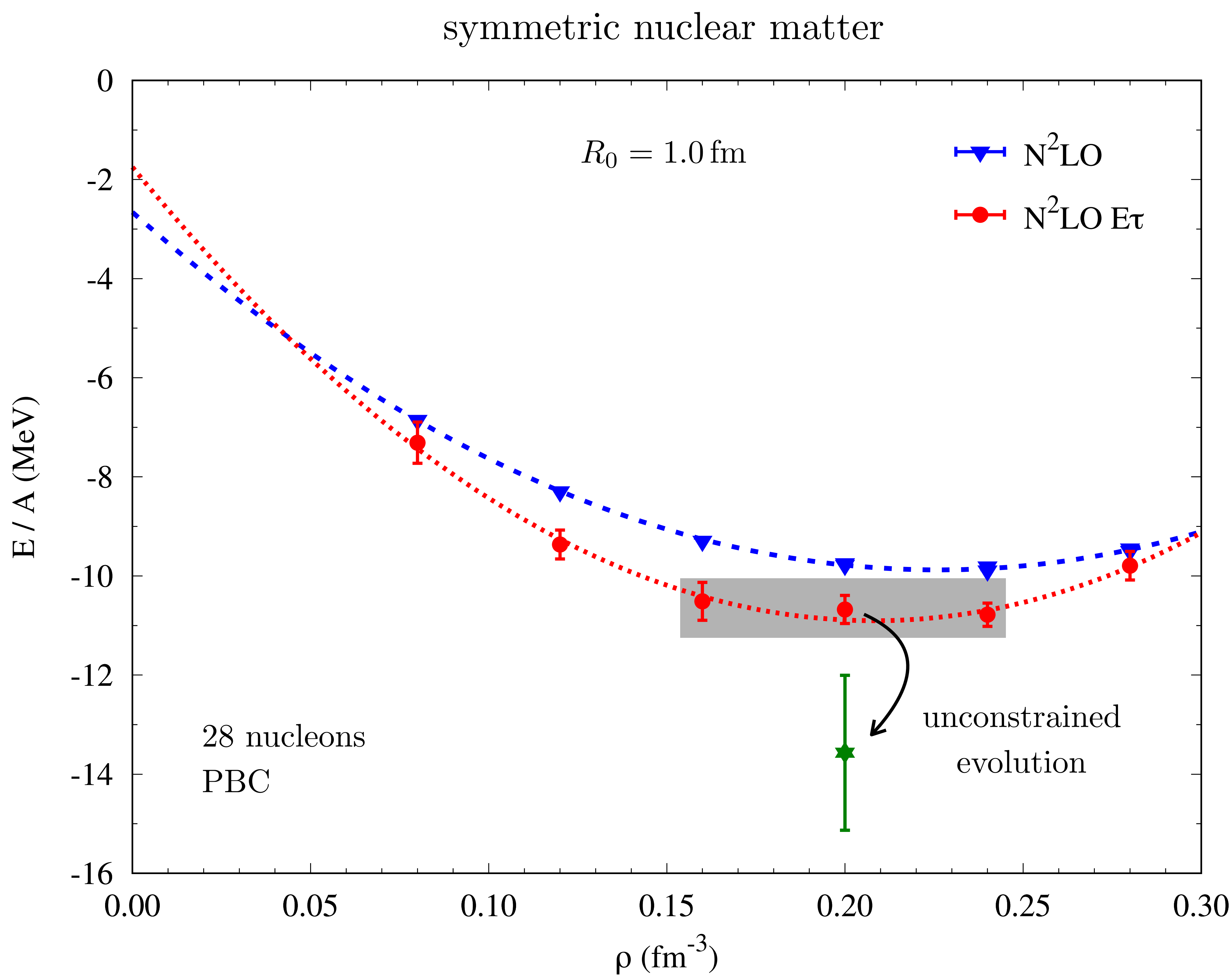

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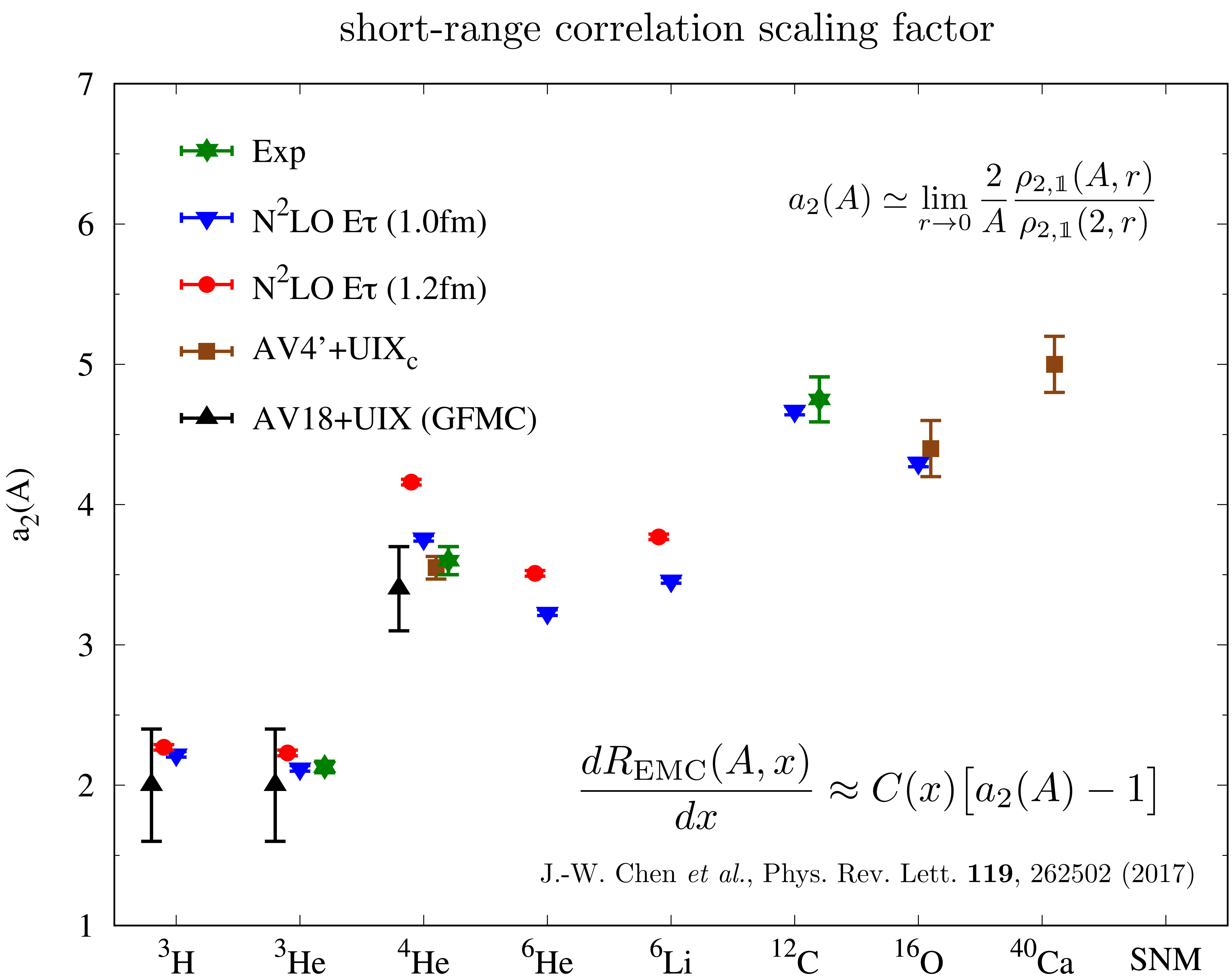

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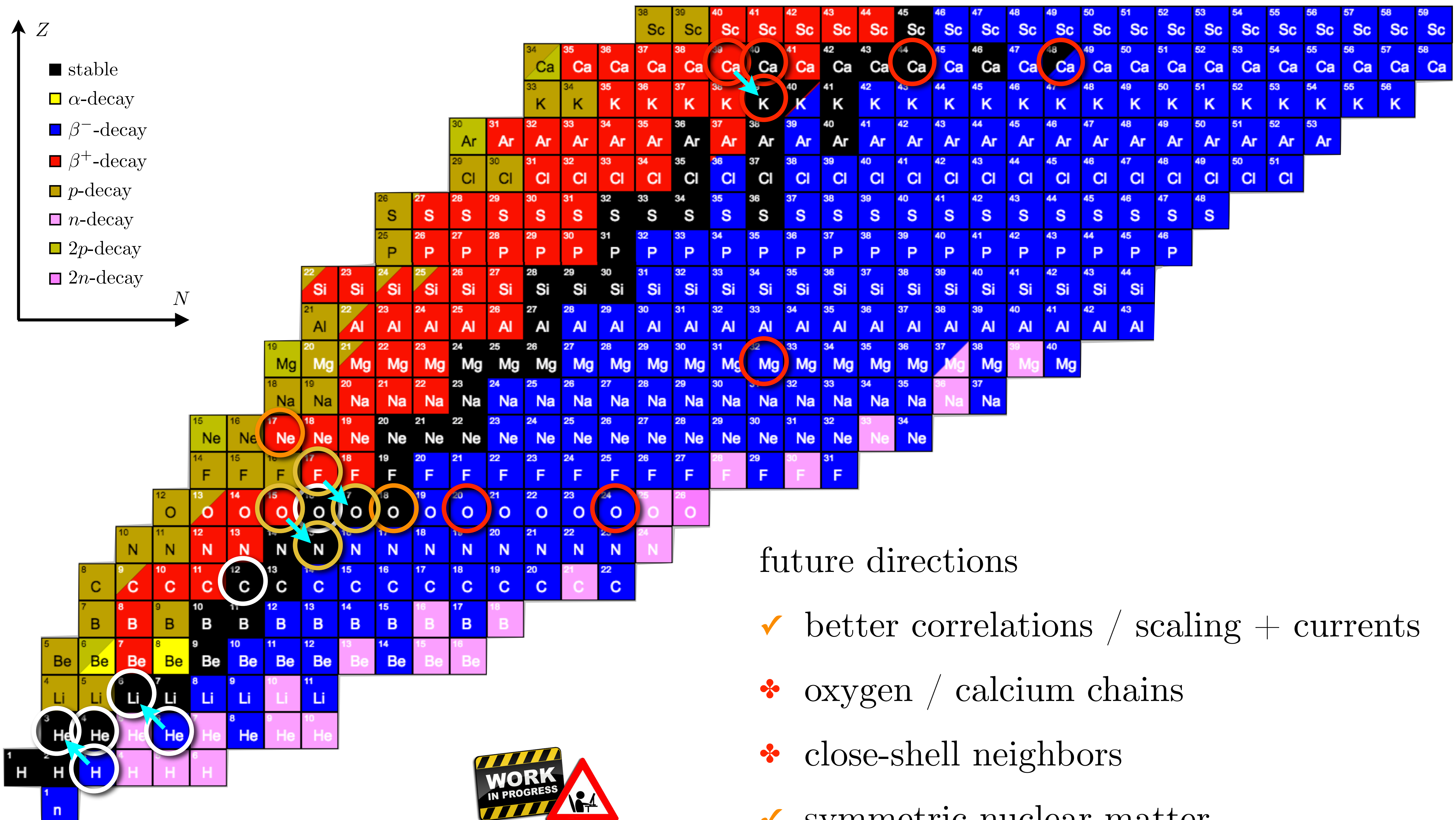

future directions

- ✓ better correlations / scaling + currents
- ✤ oxygen / calcium chains
- ✤ close-shell neighbors
- ✓ symmetric nuclear matter
- ✤ asymmetric nuclear matter
- ✤ beta-decay

Thank you!!