Exploring short-range correlation effects with quantum Monte Carlo

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- ✓ A. Schwenk @ TU Darmstadt
- ✓ X. B. Wang @ Huzhou University, China

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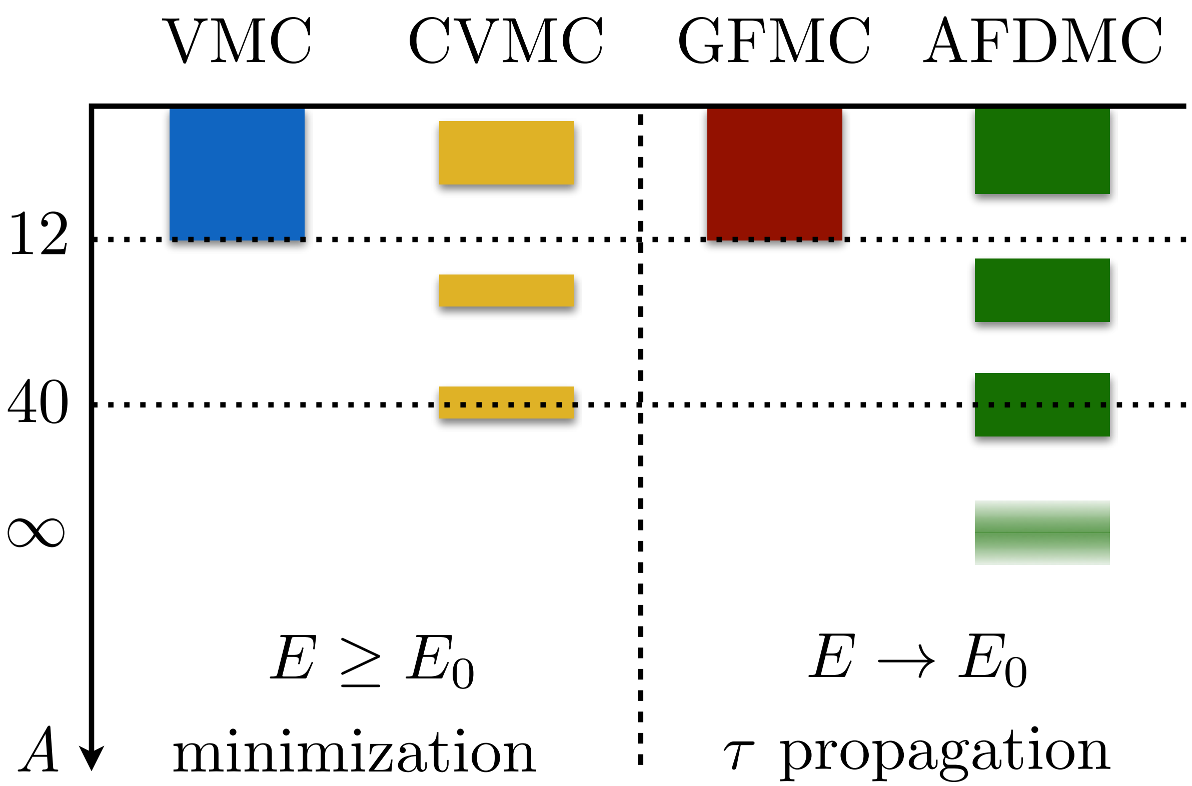
Quantum Monte Carlo

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:

- *Ab-initio*: microscopic approach, 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

$$|\Psi_V\rangle = \Big[F_3 \Big] \Big[F_2 \Big] \Big[F_c \Big] \mathcal{A}\,|\Phi\rangle$$

3-body corr — 2-body corr — mean field

$\mathcal{A}\,|\Phi\rangle$ → Slater determinants of single-particle orbitals + spinors: proper (J^π, T)

Quantum Monte Carlo

$$|\Psi_V\rangle = \left[1 + \sum_{i<j<k} U_{ijk}\right]\left[\mathcal{S}\prod_{i<j}\left(1+U_{ij}\right)\right]\left[\prod_{i<j} f_c(r_{ij})\right]\mathcal{A}\,|\Phi\rangle$$

3-body corr — 2-body corr — mean field

→ Slater determinants of single-particle orbitals + spinors: proper (J^π, T)

1. VMC: variational search of optimal parameters for $|\Psi_V\rangle$ ⟶ NLopt, SR, LM
   - A>12, CVMC: cluster expansion for the spin-isospin correlations (up to 5b cl.)

2. DMC: propagation in imaginary time: $e^{-H\tau}|\Psi_V\rangle \xrightarrow{\tau\to\infty} |\Psi_0\rangle \qquad \tau = \mathcal{M}d\tau \quad \mathcal{M} \gg 1,\ d\tau \ll 1$
   - spatial degrees of freedom: diffusion of positions in coordinate space
   - spin-isospin degrees of freedom: Hubbard-Stratonovich transformation

AFDMC

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

auxiliary fields — spin-isospin rotations

Note: 2-body operators only

   - sign problem: constrained path approximation + unconstrained evolution

ground-state of light nuclei within 1-2% with respect to GFMC

Nuclear Hamiltonians: phenomenological potentials

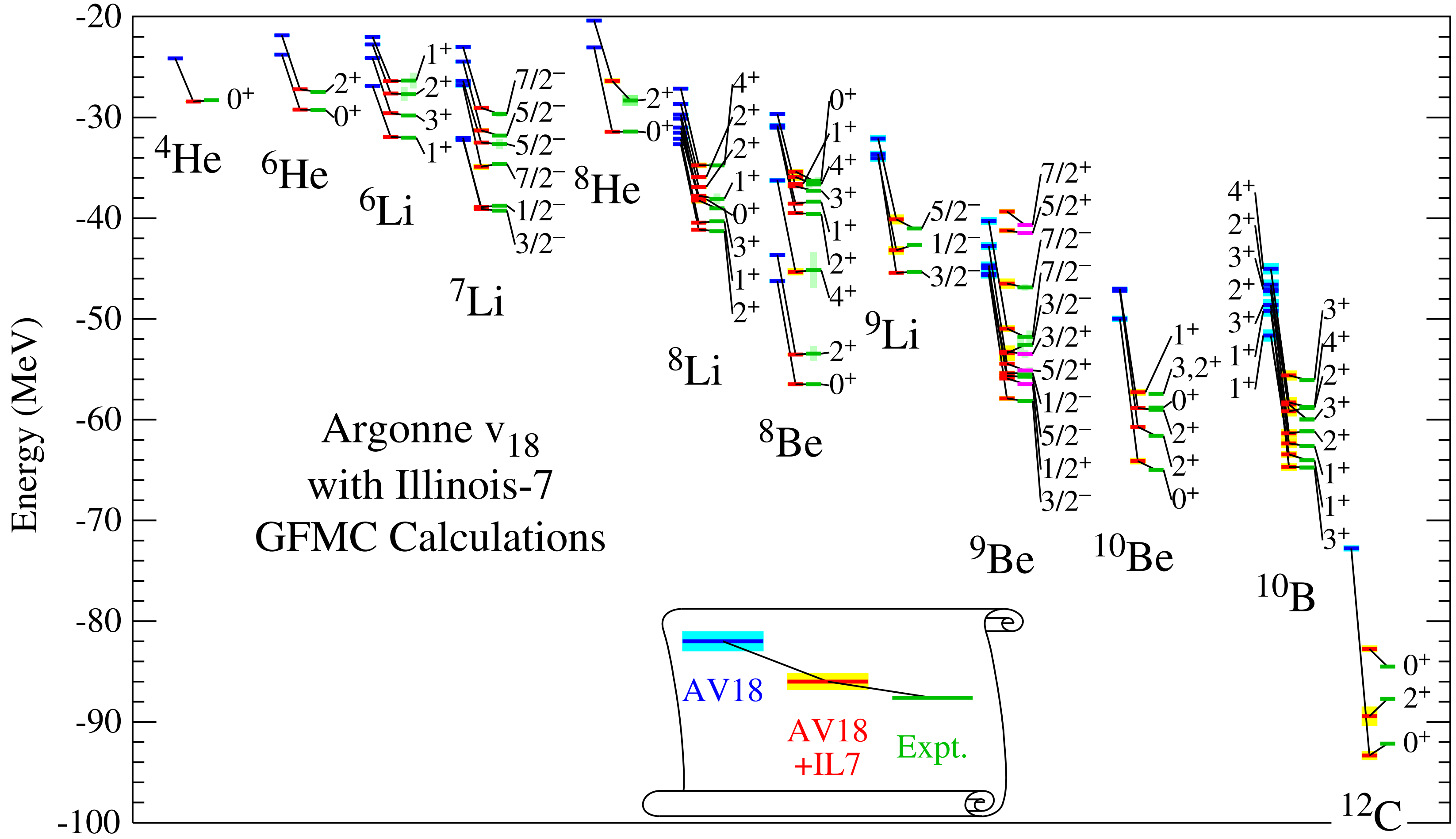
$$H = -\frac{\hbar^2}{2m_N}\sum_i \nabla_i^2 + \sum_{i<j} v_{ij} + \sum_{i<j<k} v_{ijk} + \dots$$

v_{ij} fit to NN scattering data & deuteron

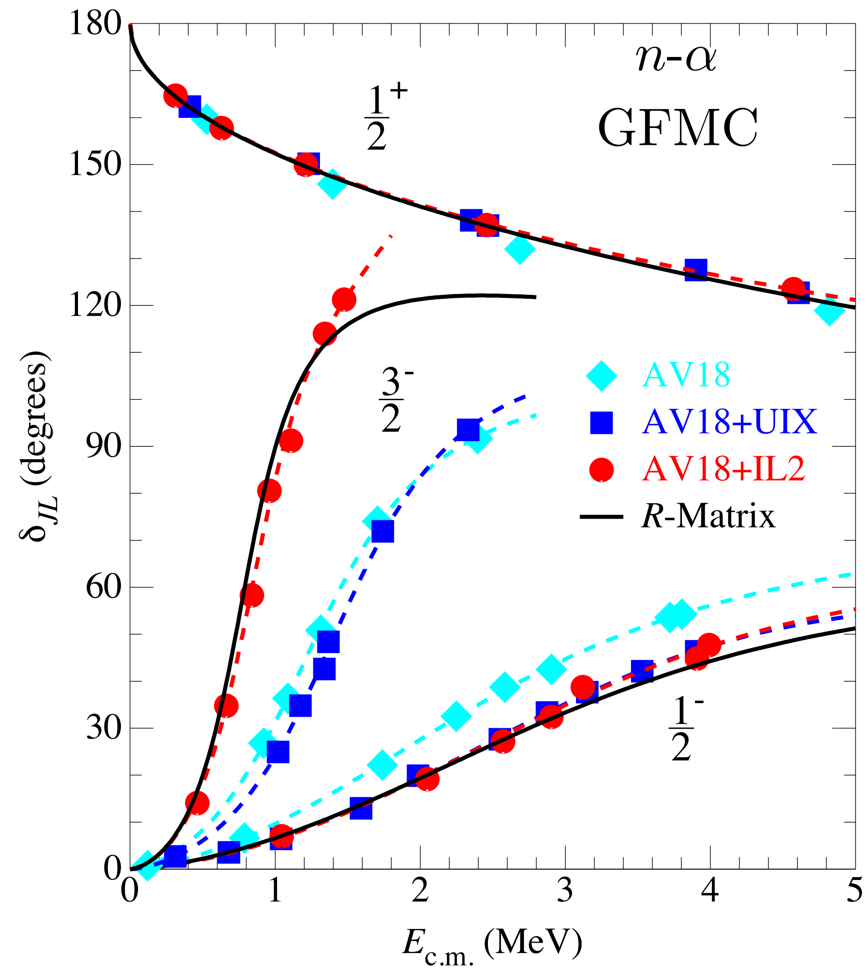
v_{ijk} fit to properties of nuclei

$$v_{ij} = \sum_{p=1,18} v_p(r_{ij})\,\mathcal{O}^p_{ij} \qquad \mathcal{O}^{p=1,8}_{ij} = \left\{\mathbb{1}, \sigma_{ij}, S_{ij}, (\mathbf{L}\cdot\mathbf{S})_{ij}\right\} \otimes \left\{\mathbb{1}, \tau_{ij}\right\}$$

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



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



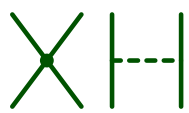
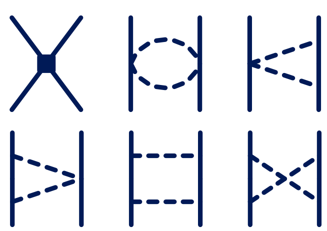
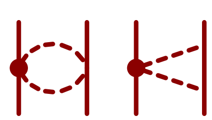
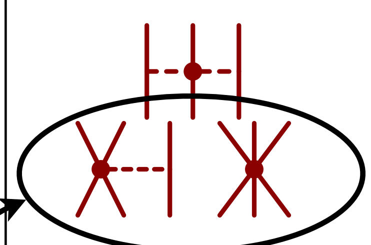
K. M. Nollett *et al.*, PRL **99**, 022502 (2007)

Nuclear Hamiltonians: local chiral potentials

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

v_{ij} fit to NN scattering data & deuteron

v_{ijk} fit to properties of nuclei

		NN	*NNN*
LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^0$		—
NLO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^2$		—
N^{2}LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^3$	 AV7 structure	

local: good for QMC

c_D & c_E fit to:

- ✓ ^{4}He binding energy
- ✓ n-α scattering phase shifts ⟶ info on $T = \frac{3}{2}$ physics

- χEFT: expansion in power of Q/Λ_b

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

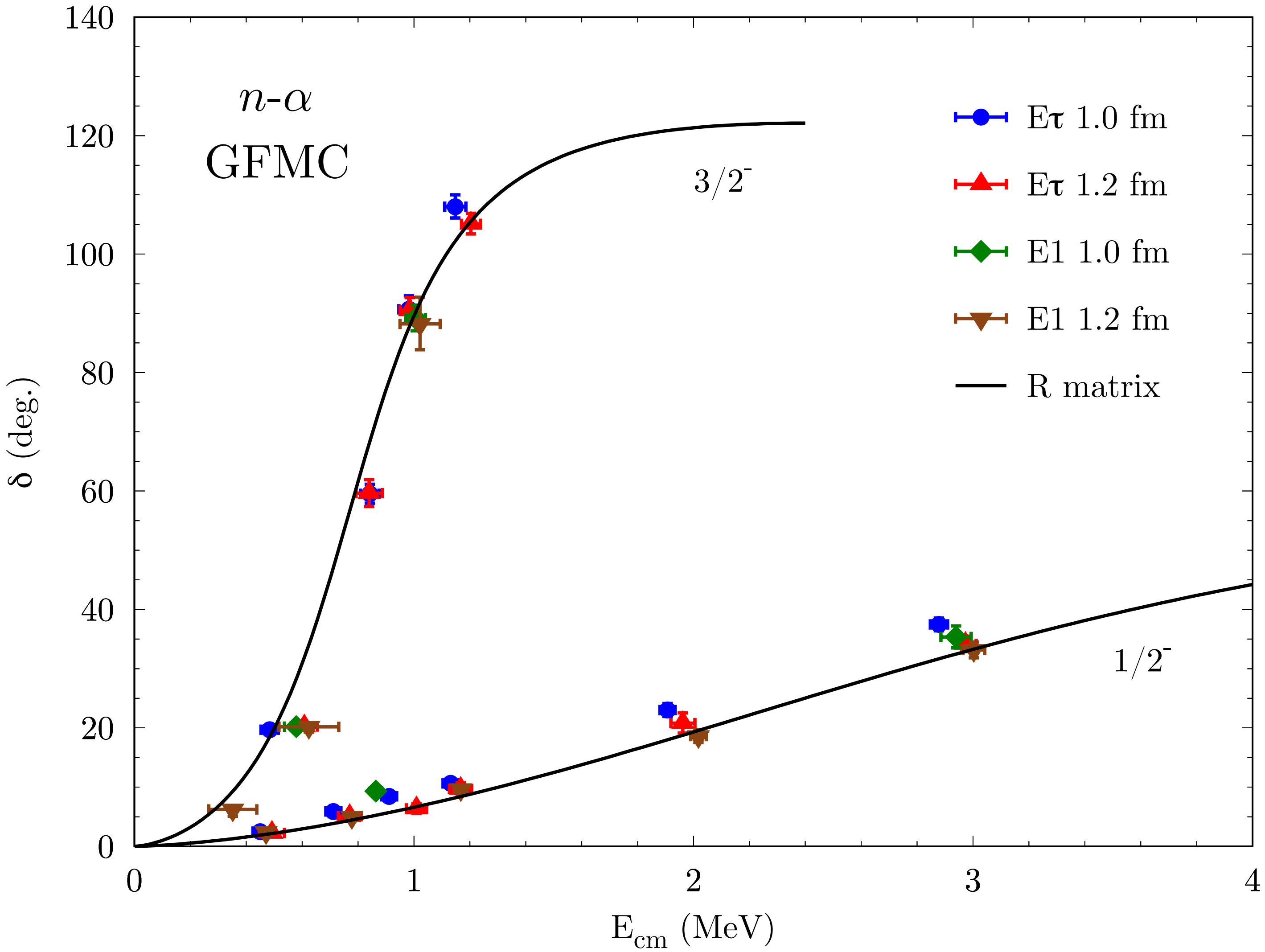
  $\Lambda_b \sim m_\rho \sim 800\,\text{MeV}$ hard scale

- Long-range physics: given explicitly (no parameters to fit) by pion-exchanges
- 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

Some details:

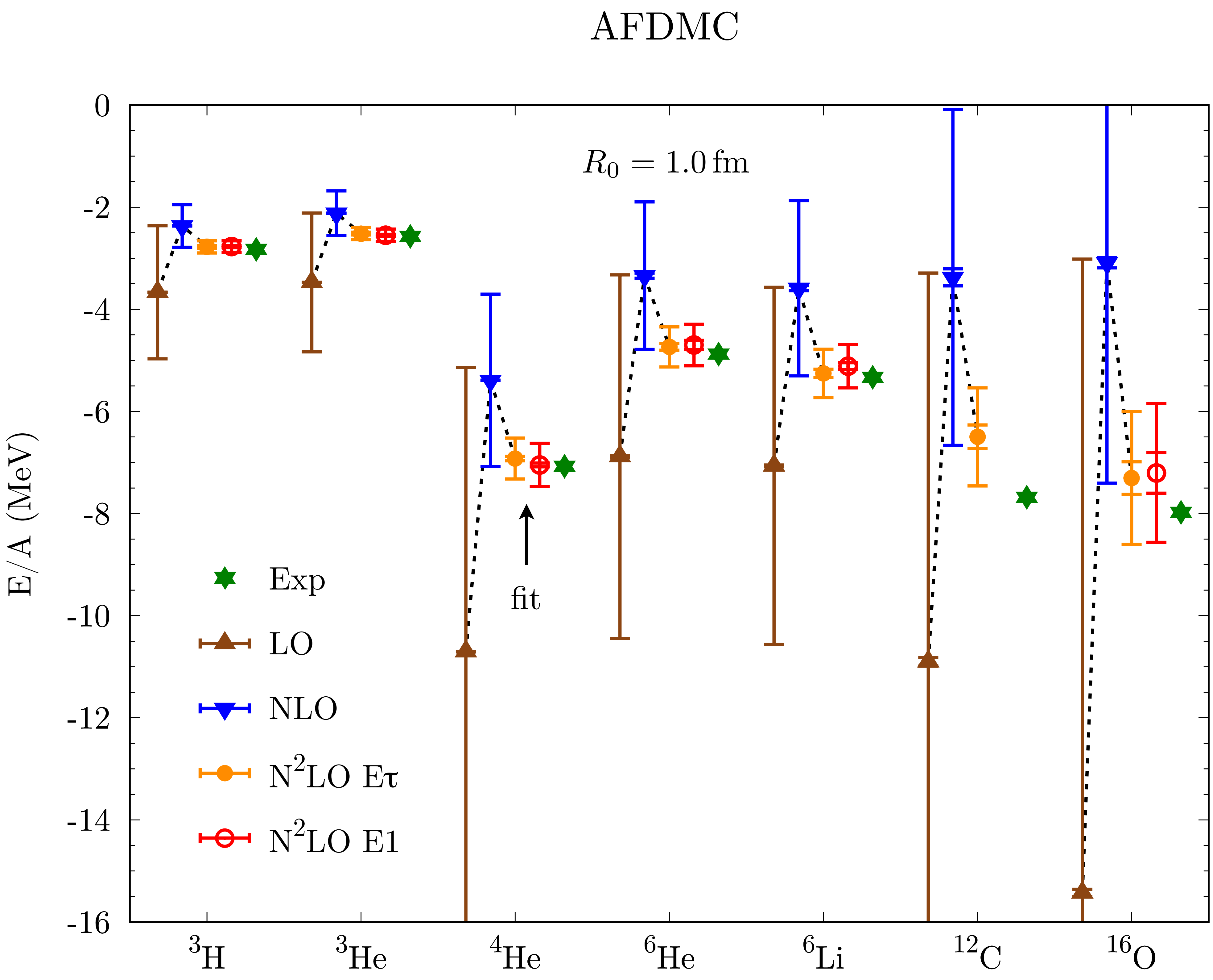
- ✓ coordinate-space regulators: $\sim e^{-(r/R_0)^4}$
- ✓ coordinate-space cutoffs: $R_0 = 1.0\,\text{fm}$ (harder) $R_0 = 1.2\,\text{fm}$ (softer)
- ✓ different 3-body operator structures: $V_D \longrightarrow D1,\, D2$ $V_E \longrightarrow E\tau,\, E\mathcal{P},\, E\mathbb{1}$



D.L. *et al.*, PRC **97**, 044318 (2018)

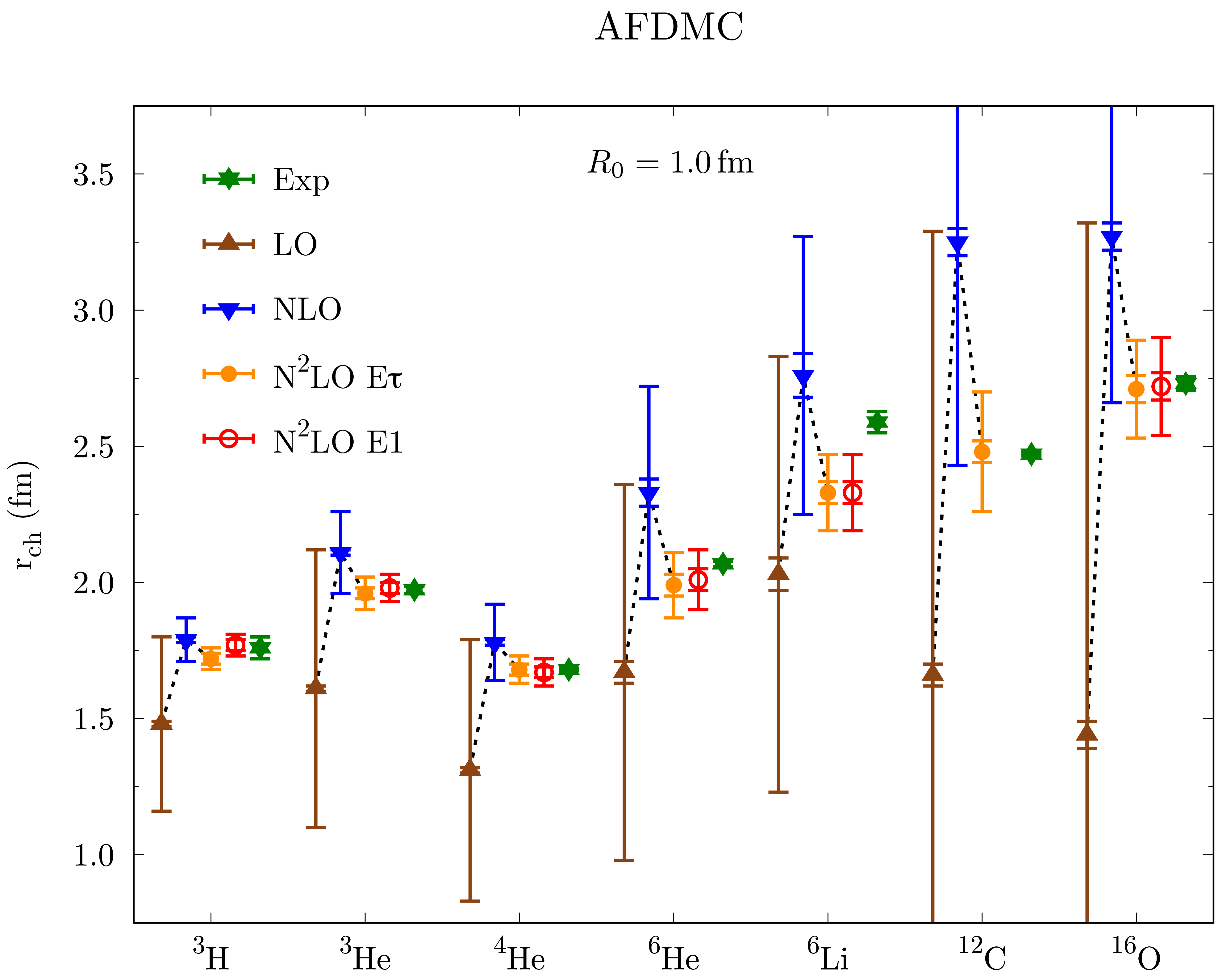
$3N$	R_0 (fm)	c_D	c_E
$E\tau$	1.0	0.0	−0.63
	1.2	3.5	0.09
$E\mathbb{1}$	1.0	0.5	0.62
	1.2	−0.75	0.025

Results: binding energies

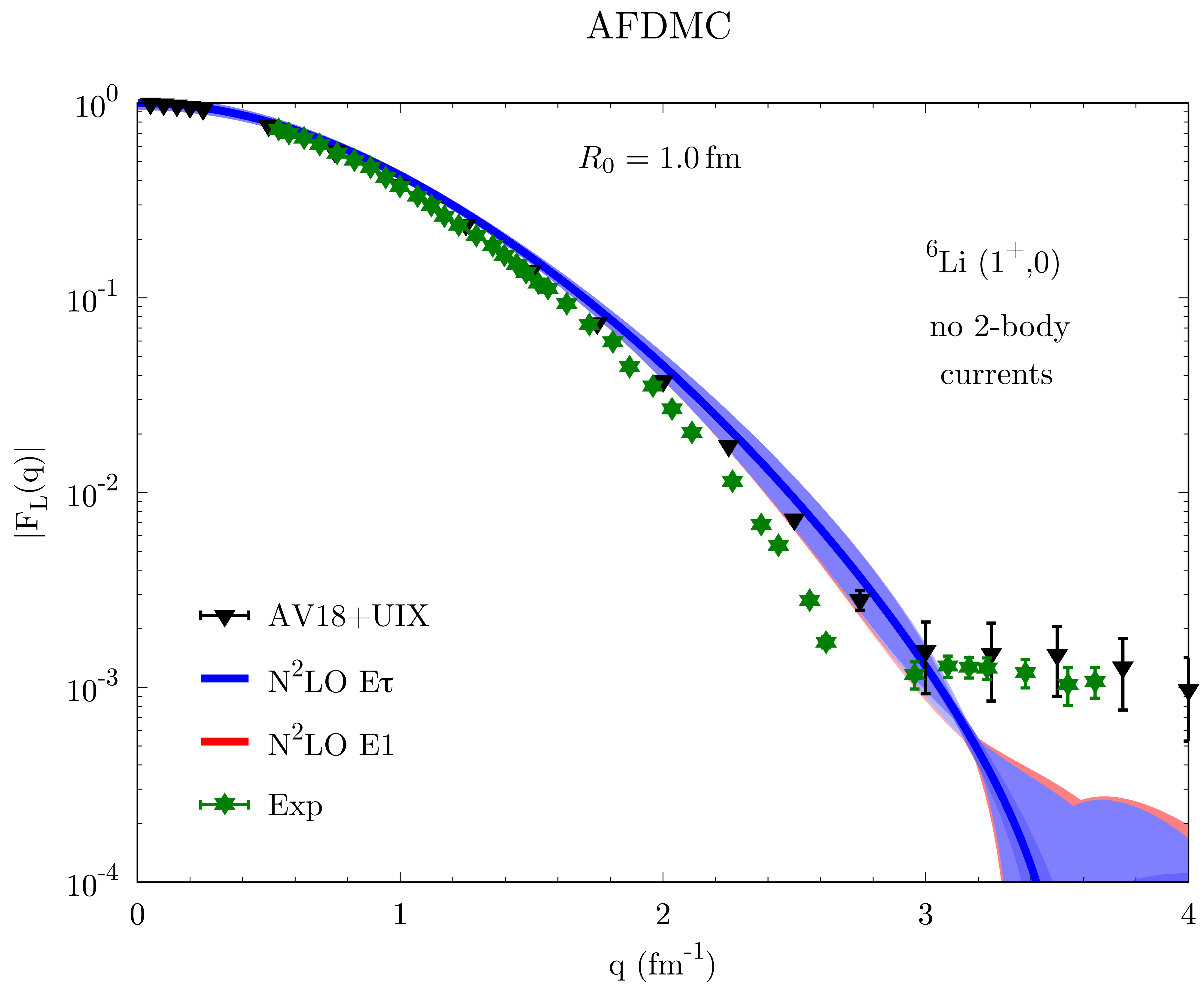


D.L. *et al.*, PRL **120**, 122502 (2018), D.L. *et al.*, PRC **97**, 044318 (2018)

Results: charge radii



D.L. *et al.*, PRL **120**, 122502 (2018), D.L. *et al.*, PRC **97**, 044318 (2018)



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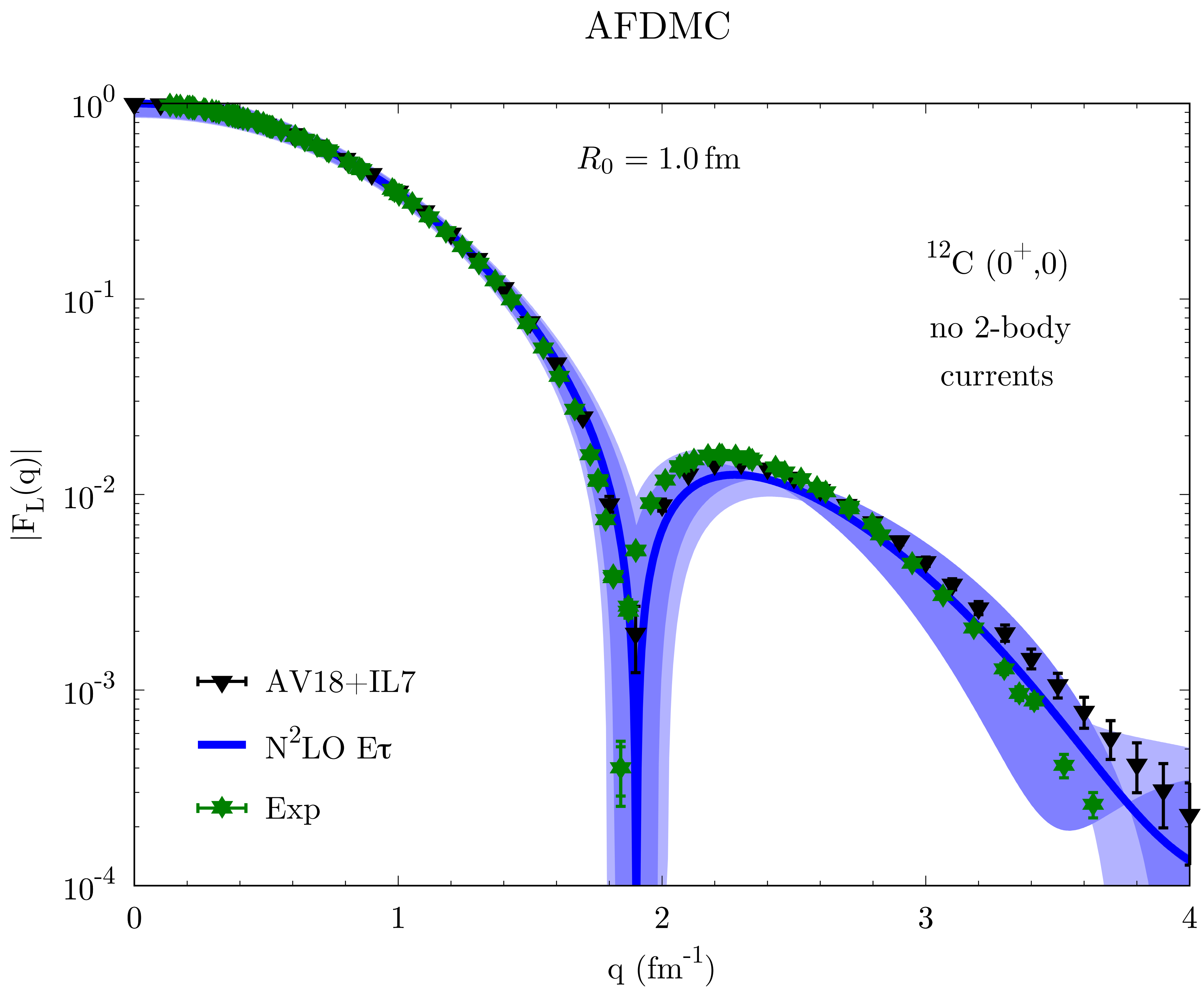
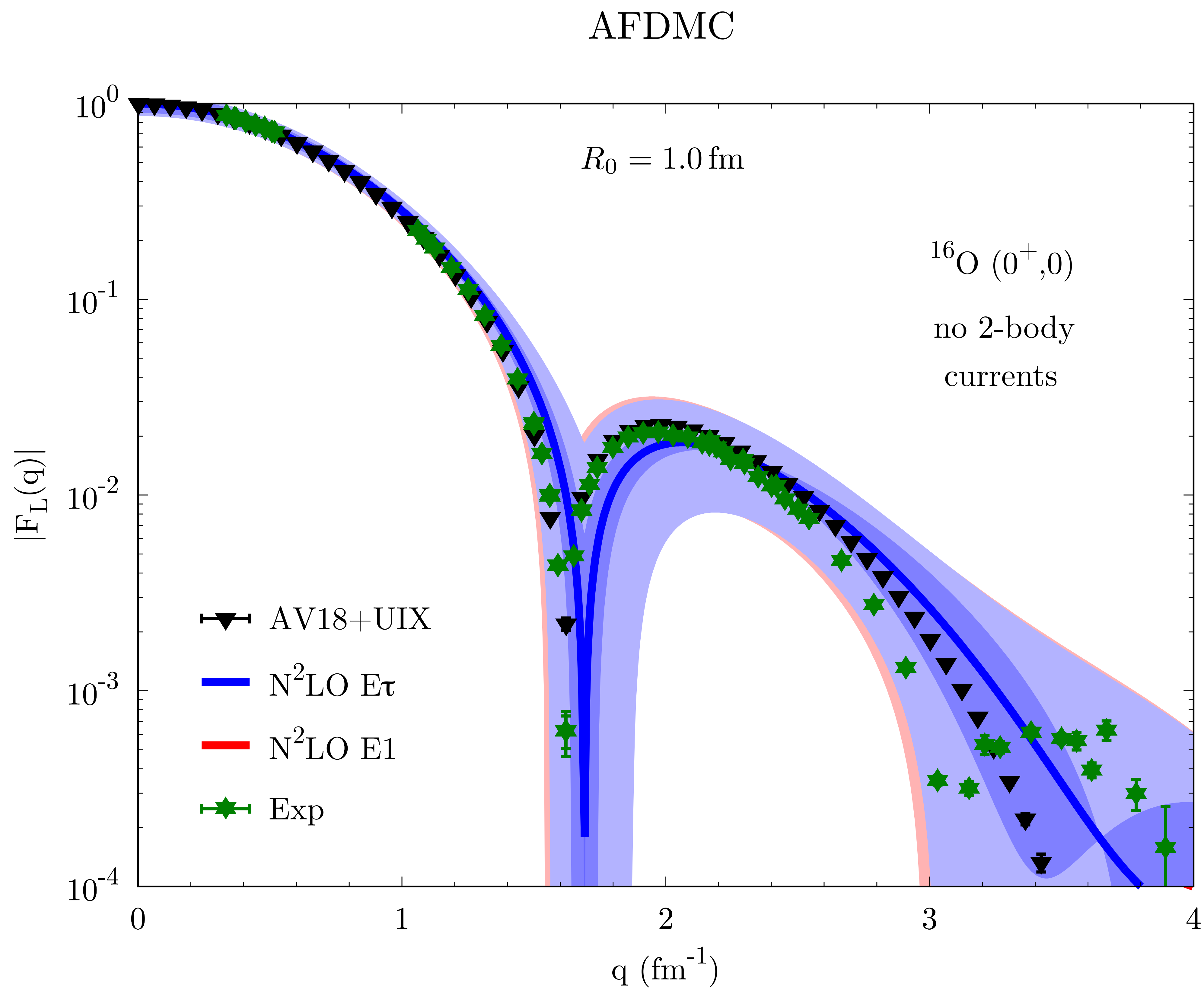


D.L. *et al.*, PRC **97**, 044318 (2018)

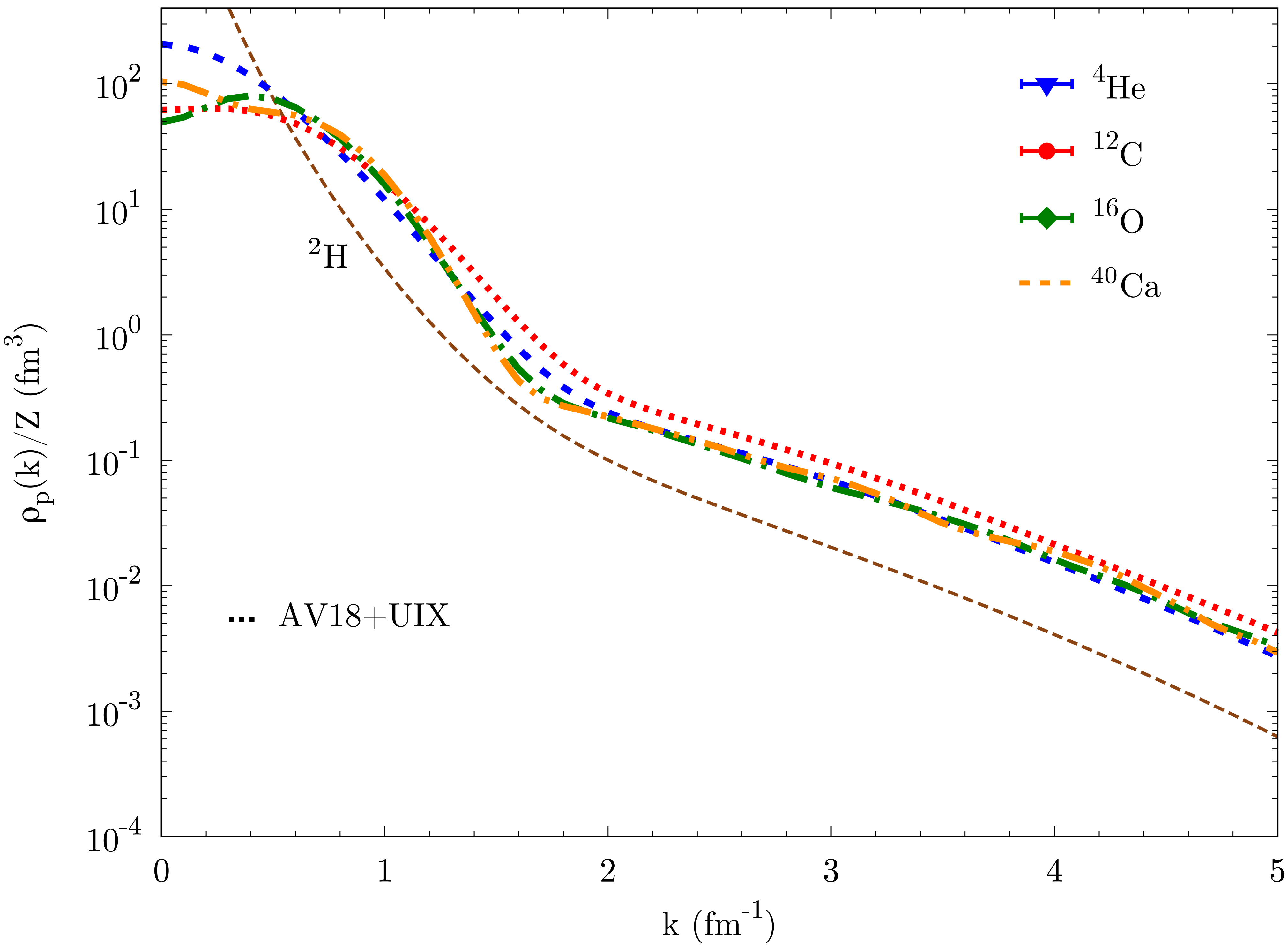
Results: charge form factors



D.L. *et al.*, PRC **97**, 044318 (2018), D.L. *et al.*, PRC **96**, 024326 (2017)

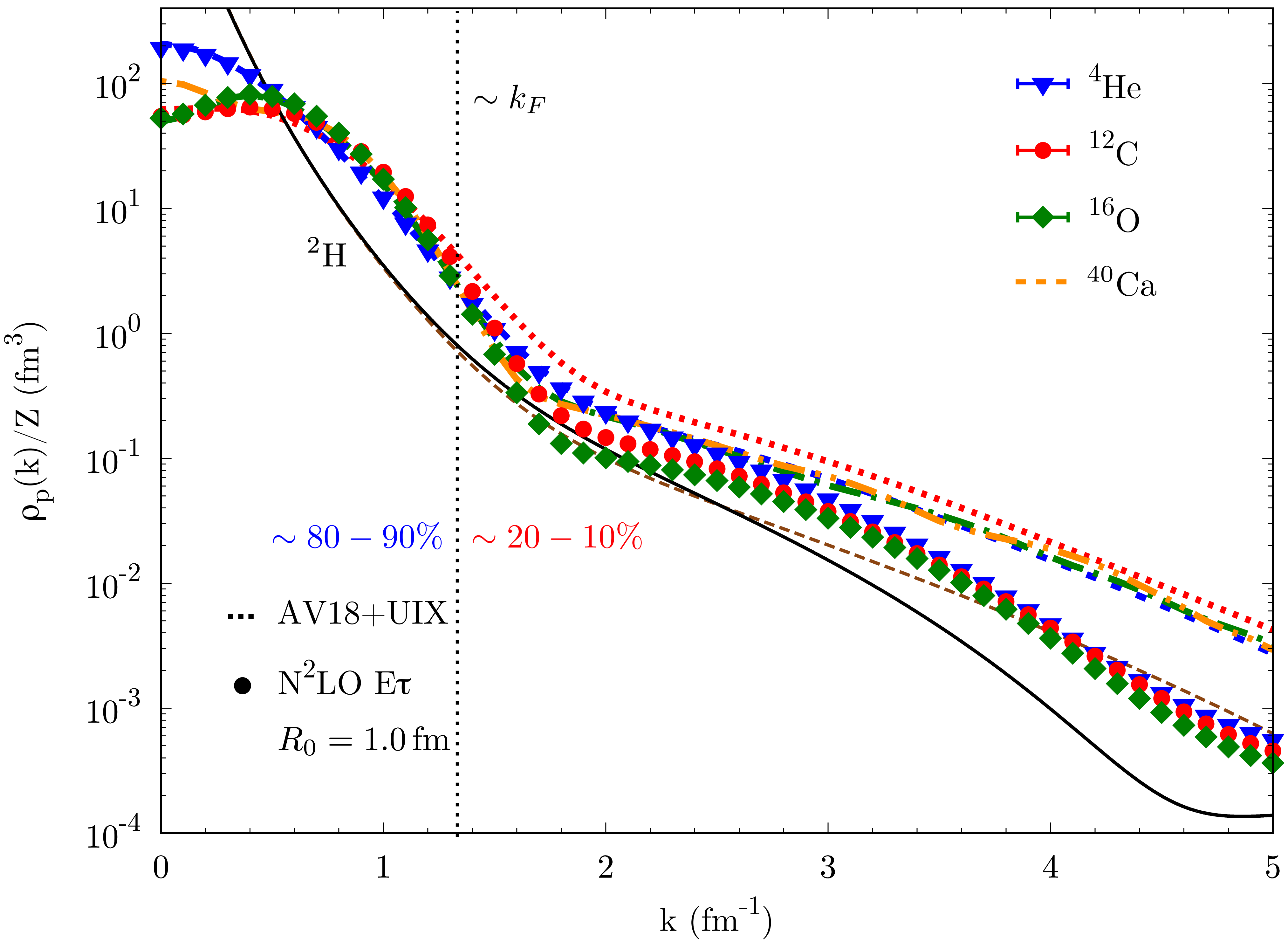
Results: single-nucleon momentum distributions

VMC with AFDMC wave function & CVMC



D.L. *et al.*, PRC **98**, 014322 (2018) (tables available as Supplemental Material), D.L. *et al.*, PRC **96**, 024326 (2017)

VMC with AFDMC wave function & CVMC



D.L. *et al.*, PRC **98**, 014322 (2018) (tables available as Supplemental Material), D.L. *et al.*, PRC **96**, 024326 (2017)

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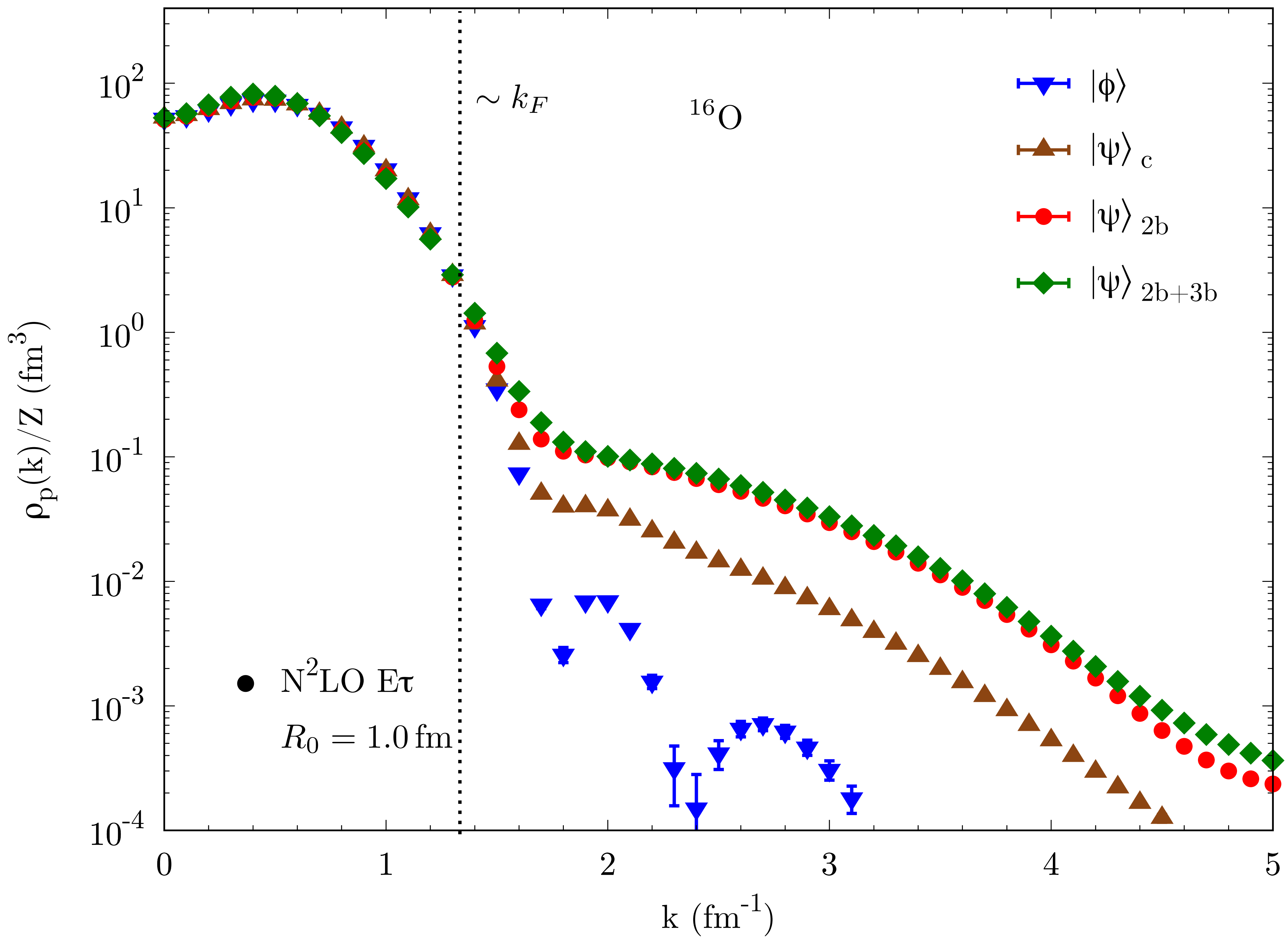

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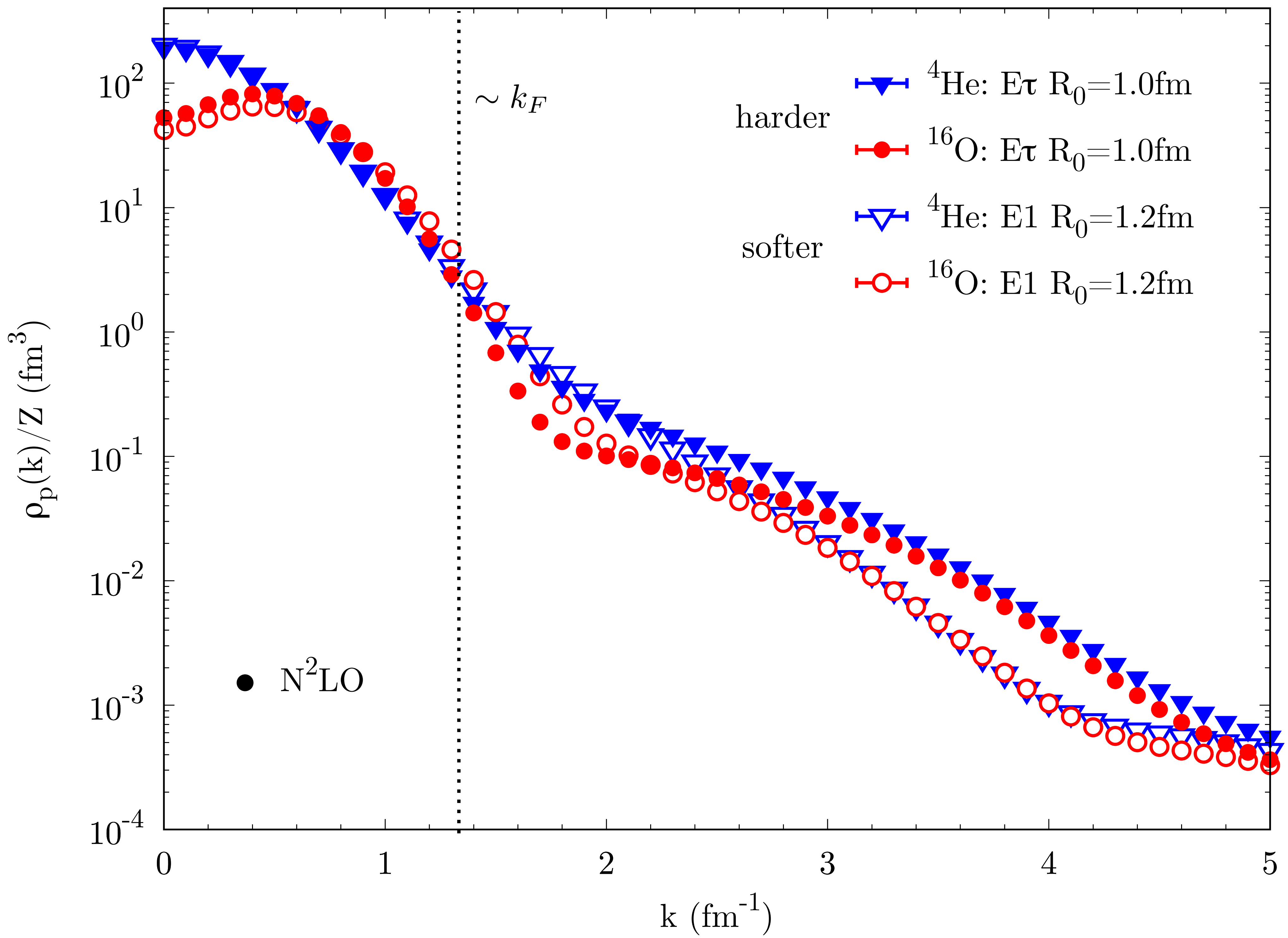
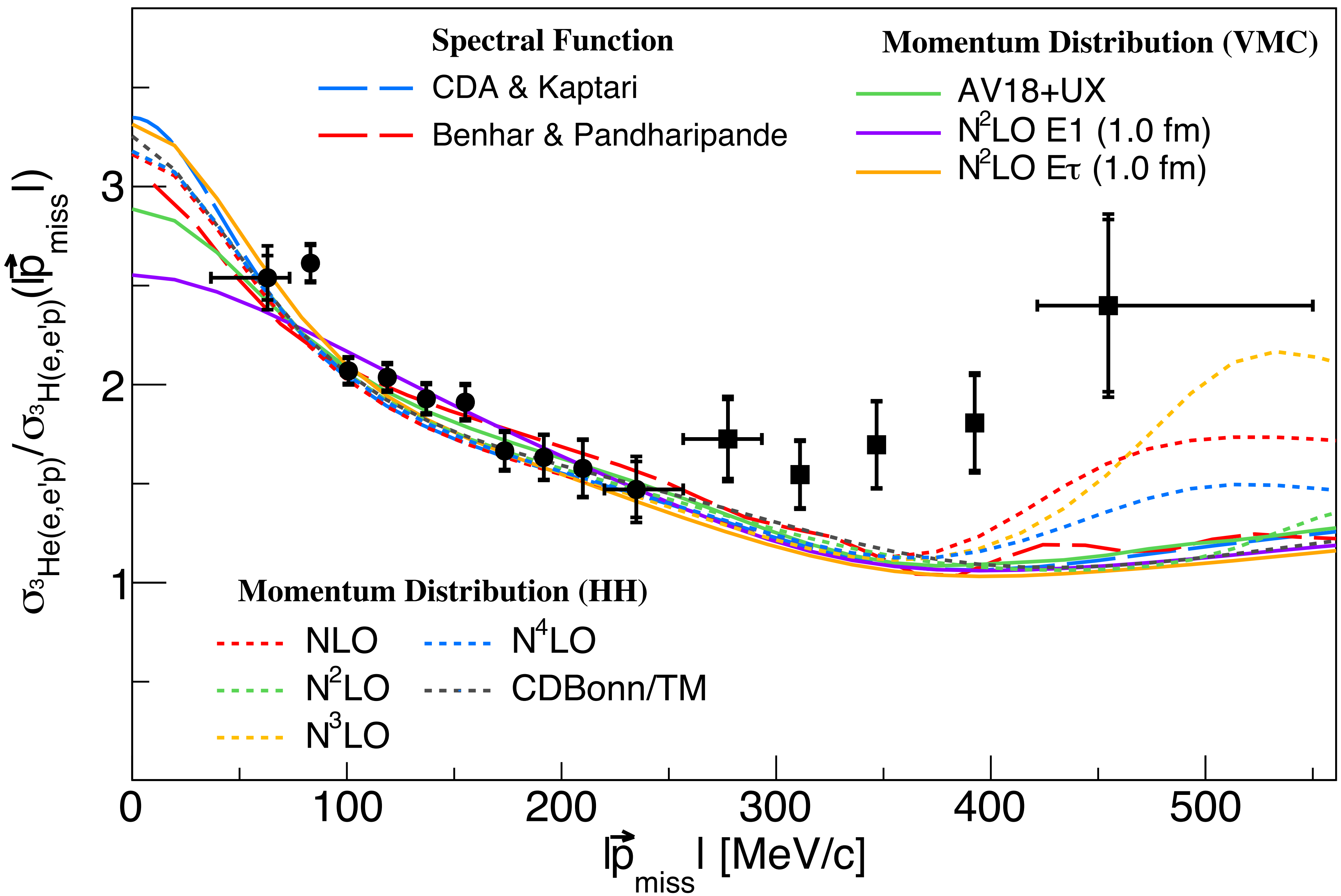
VMC with AFDMC wave function



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

VMC with AFDMC wave function

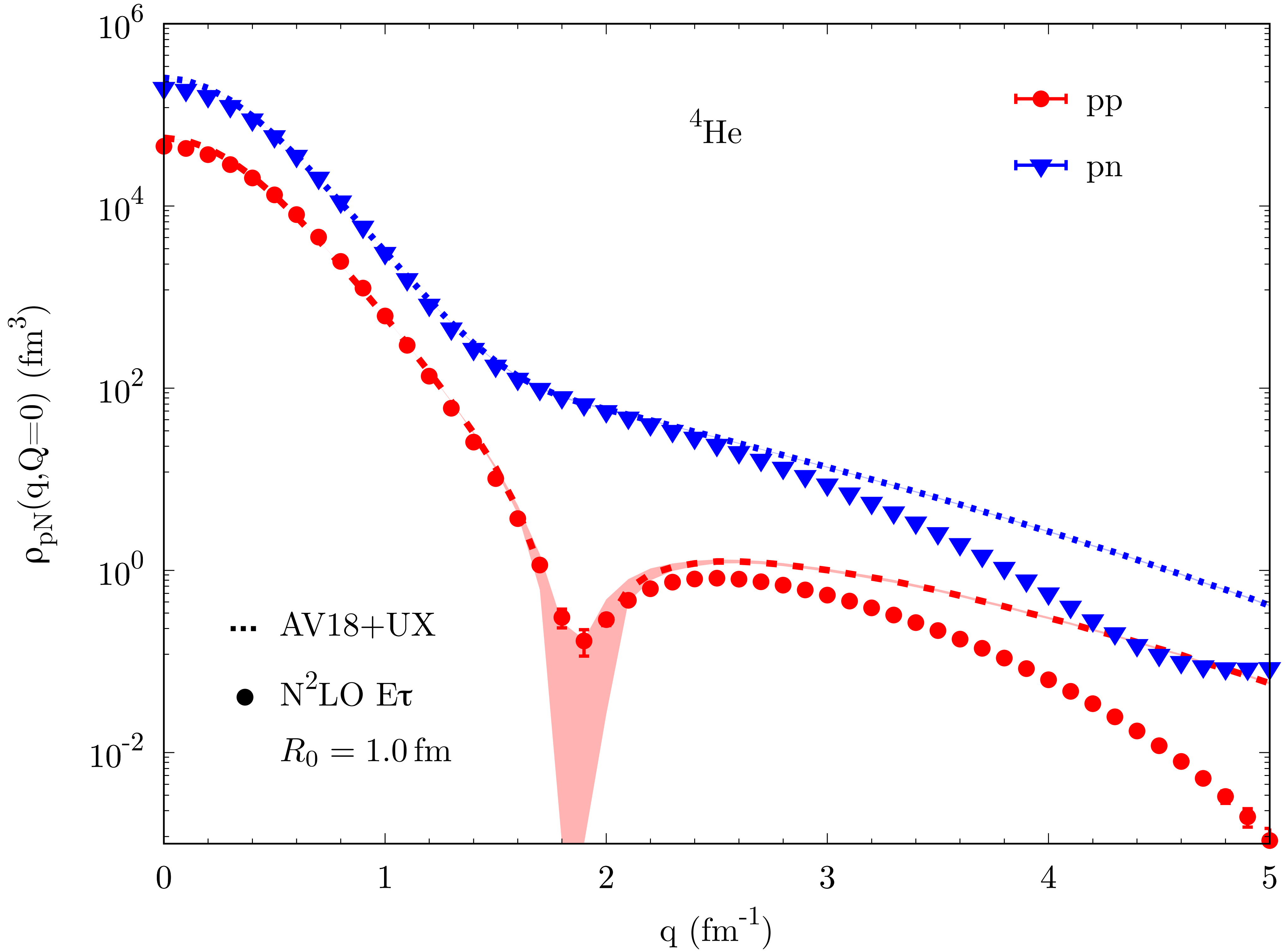
$A=3$



R. Cruz-Torres, D.L. *et al.*, arXiv:1902.06358 [nucl-ex]

Results: two-nucleon momentum distributions

VMC with AFDMC wave function



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

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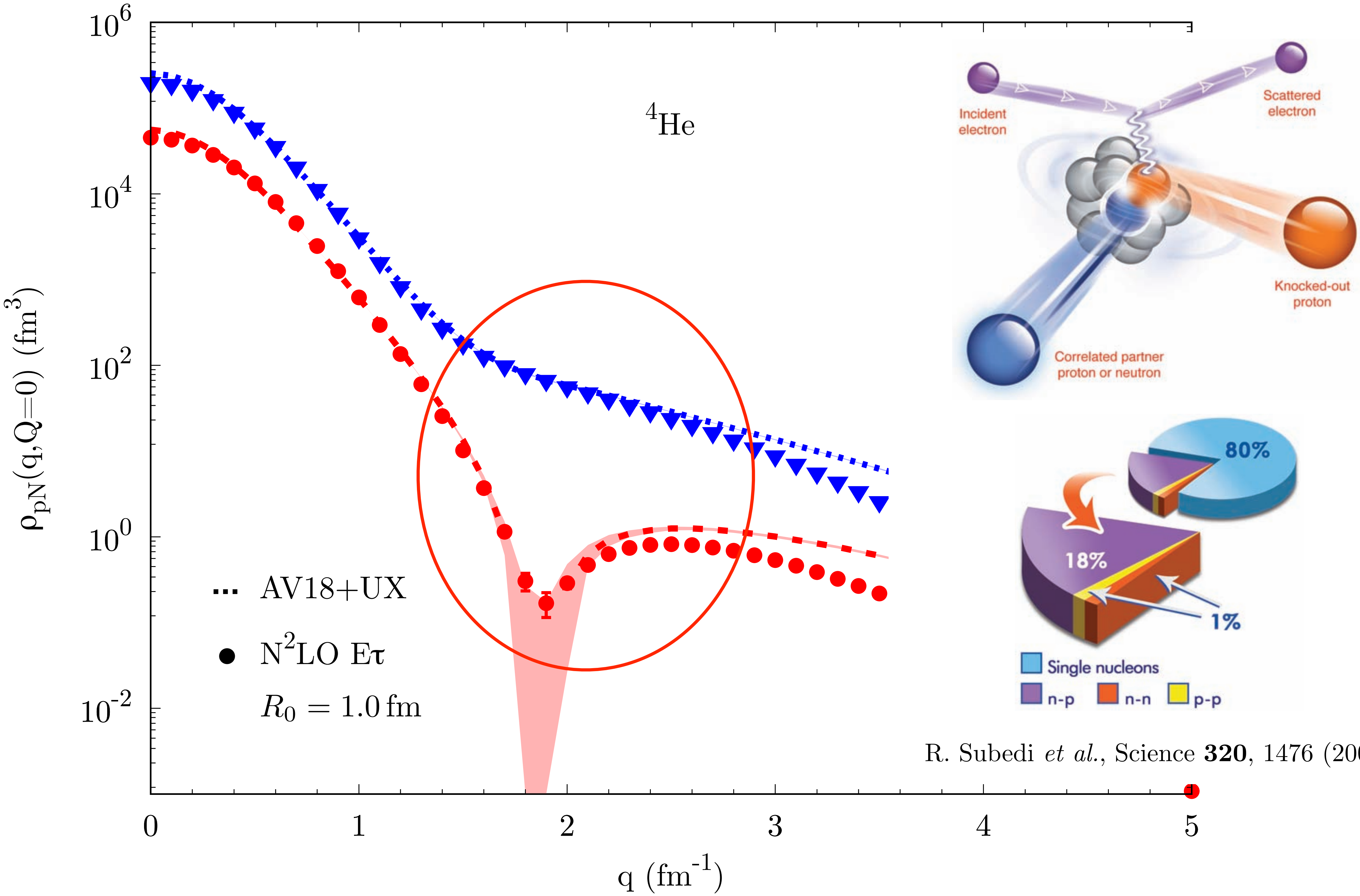
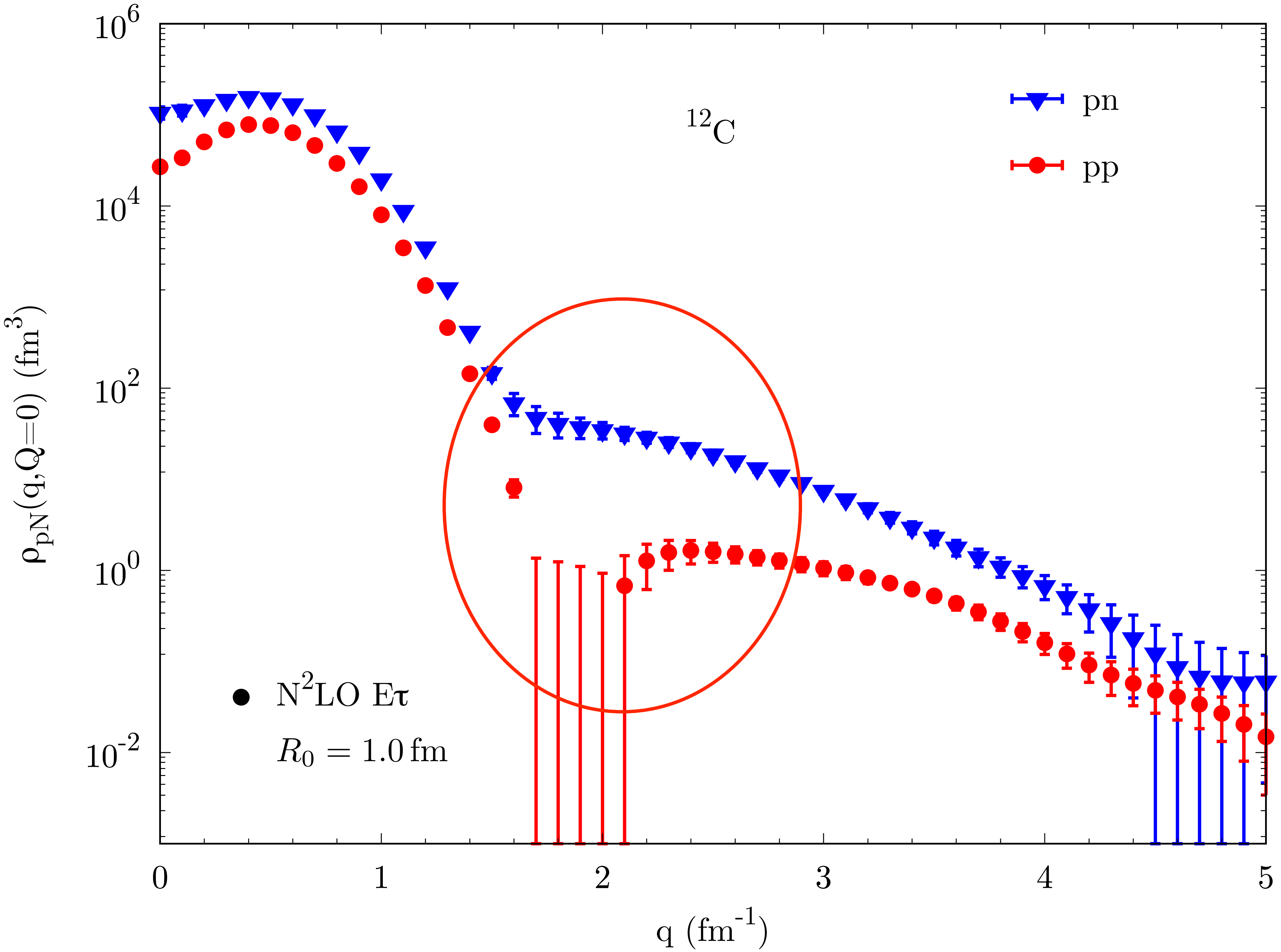


R. Subedi *et al.*, Science **320**, 1476 (2008)

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

VMC with AFDMC wave function



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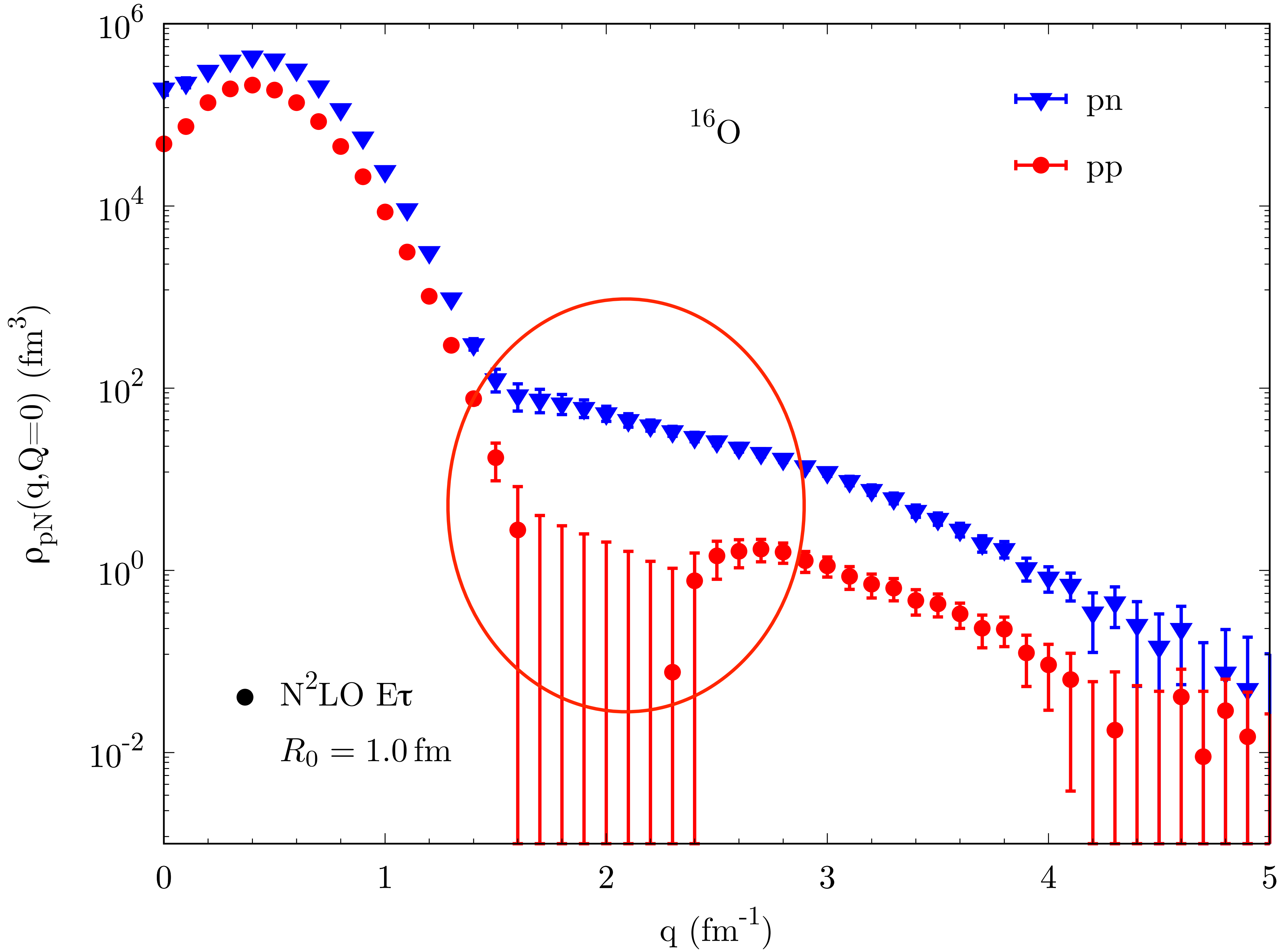

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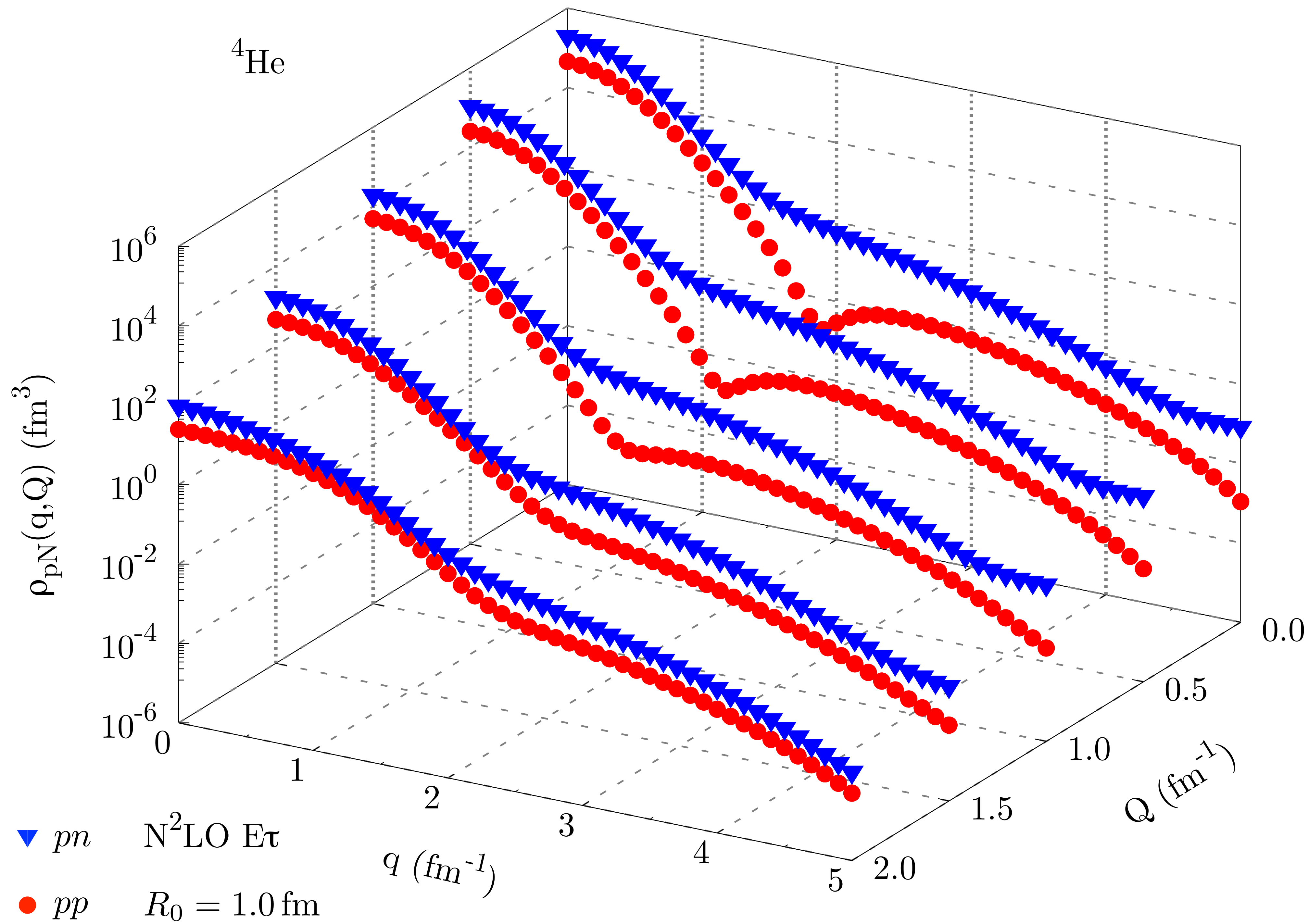

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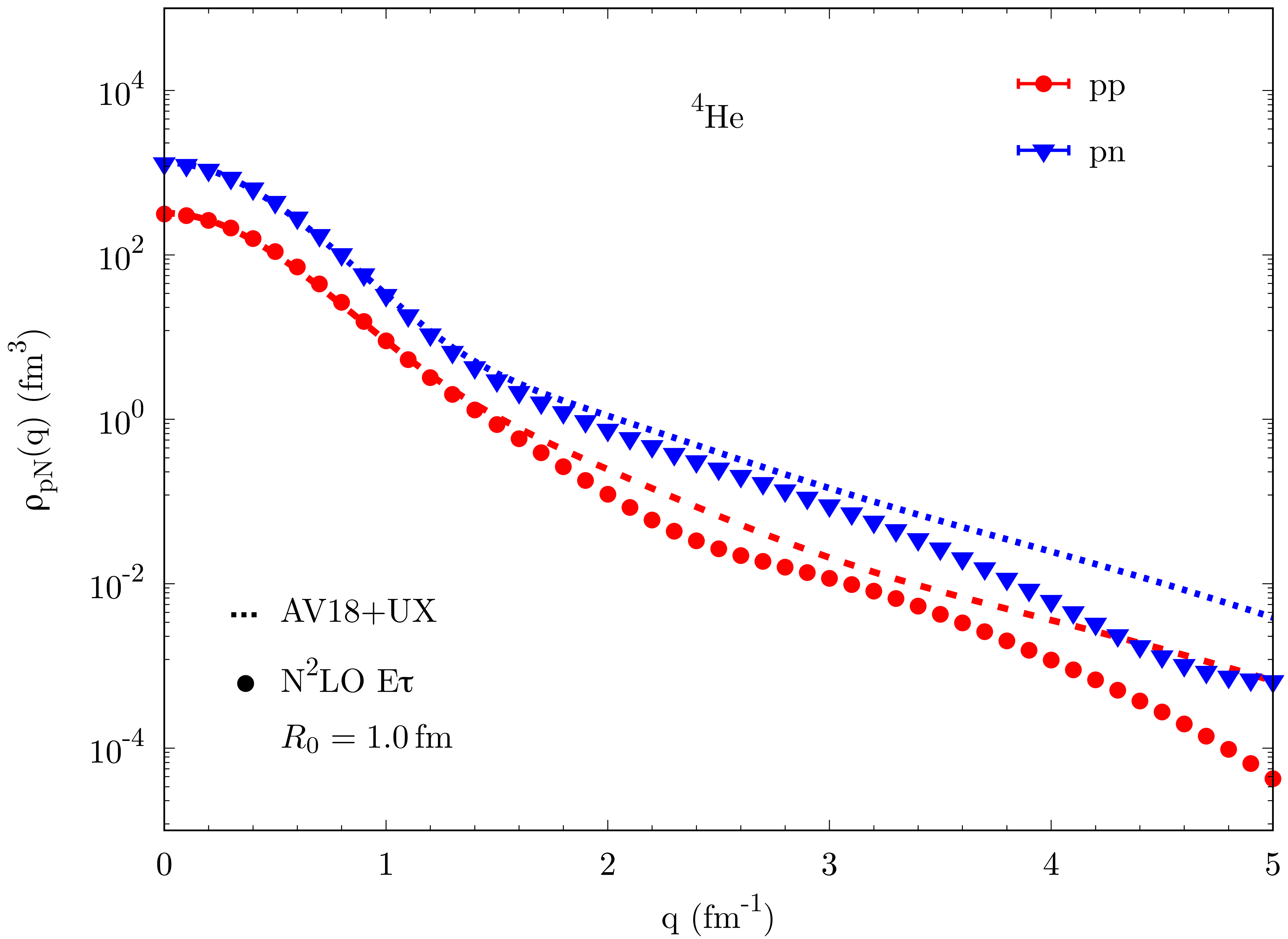
VMC with AFDMC wave function



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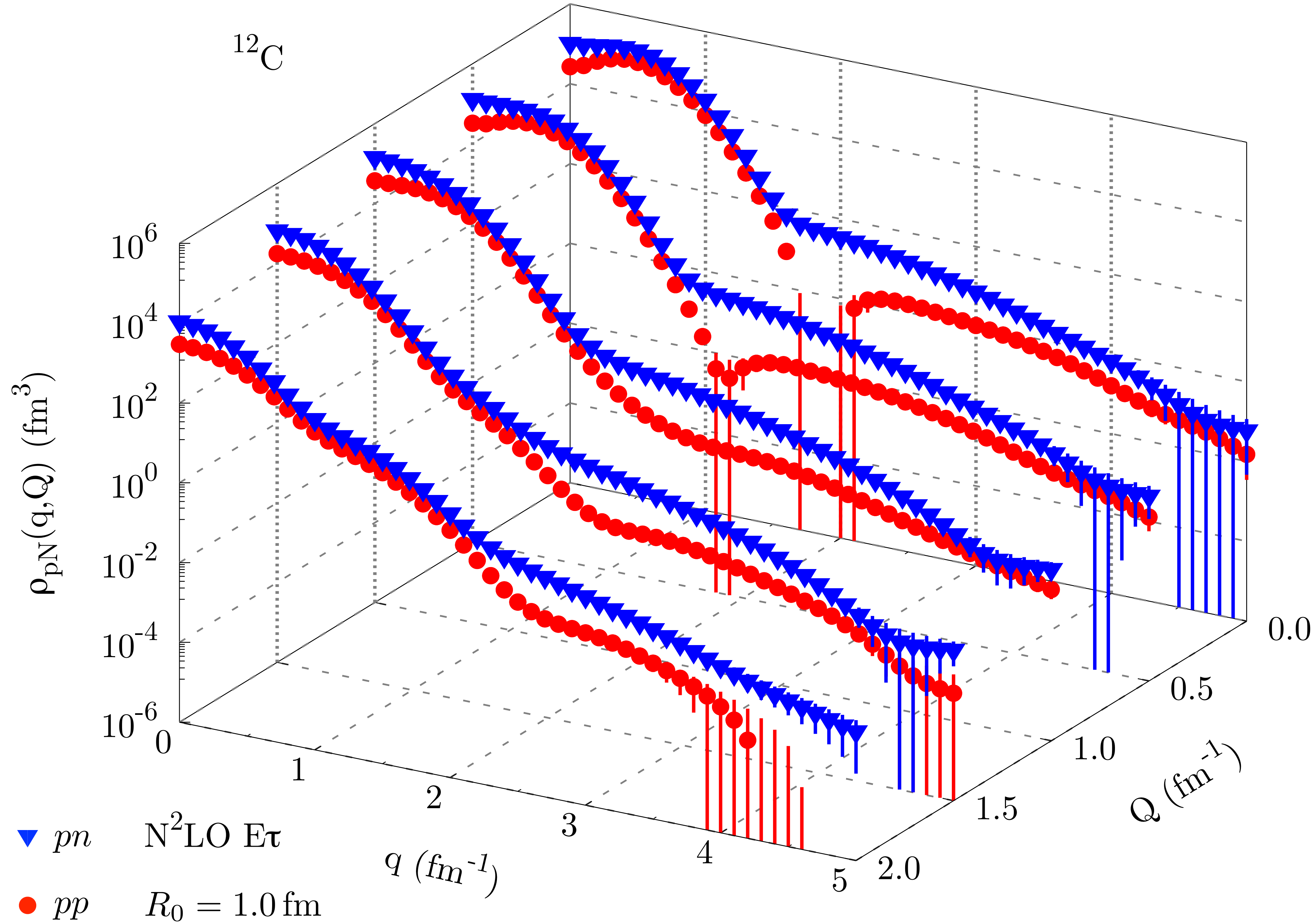

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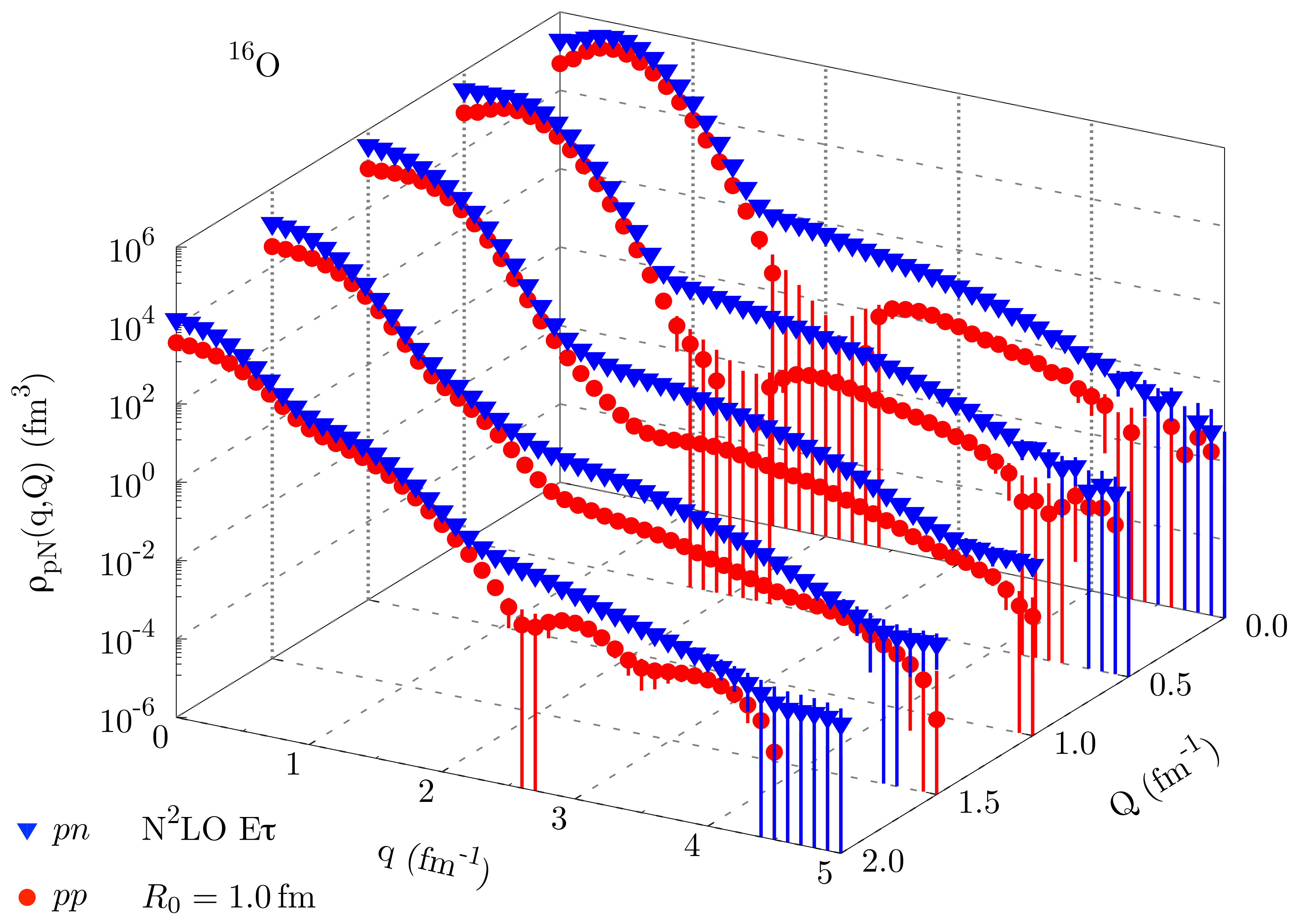

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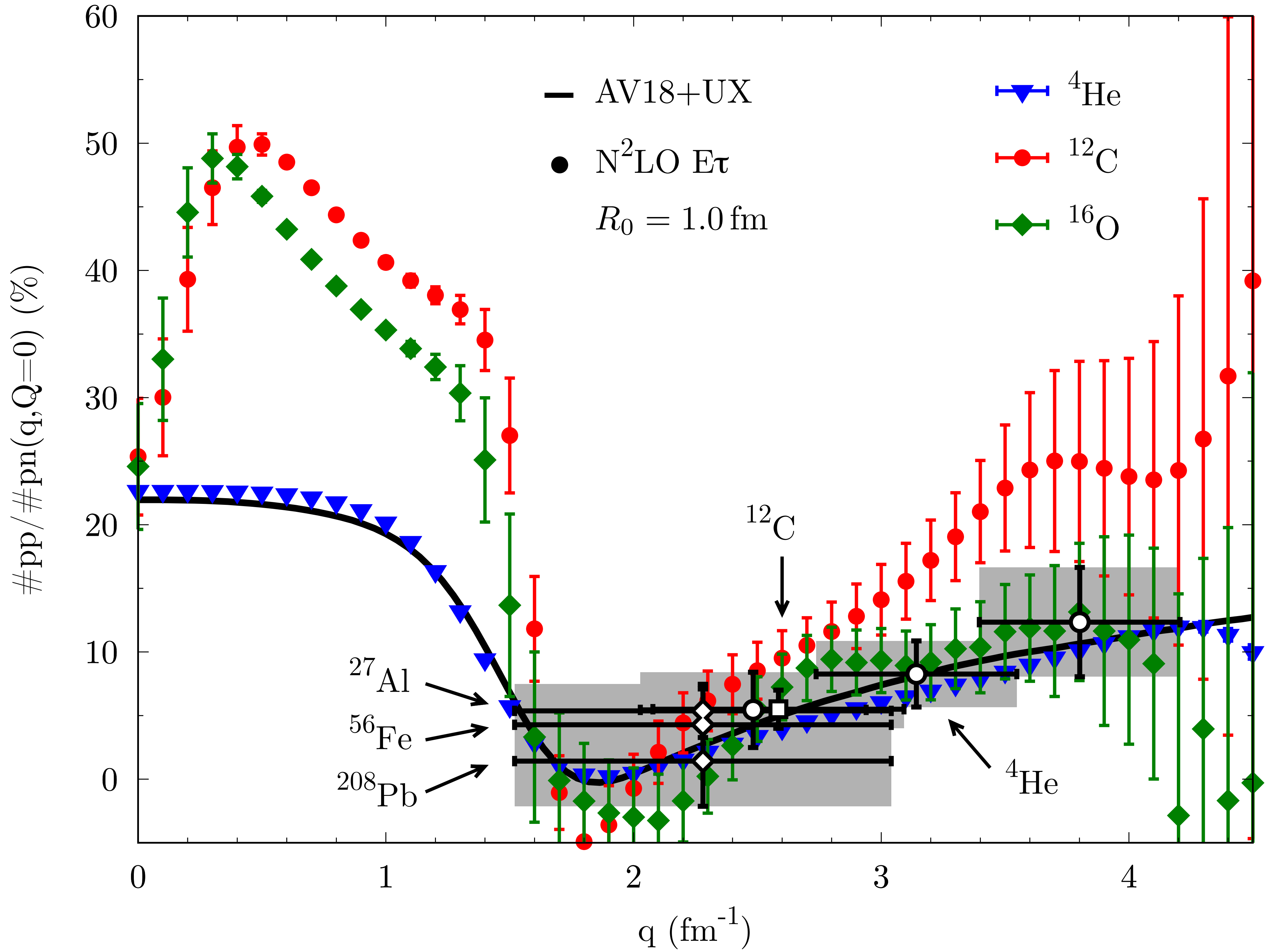
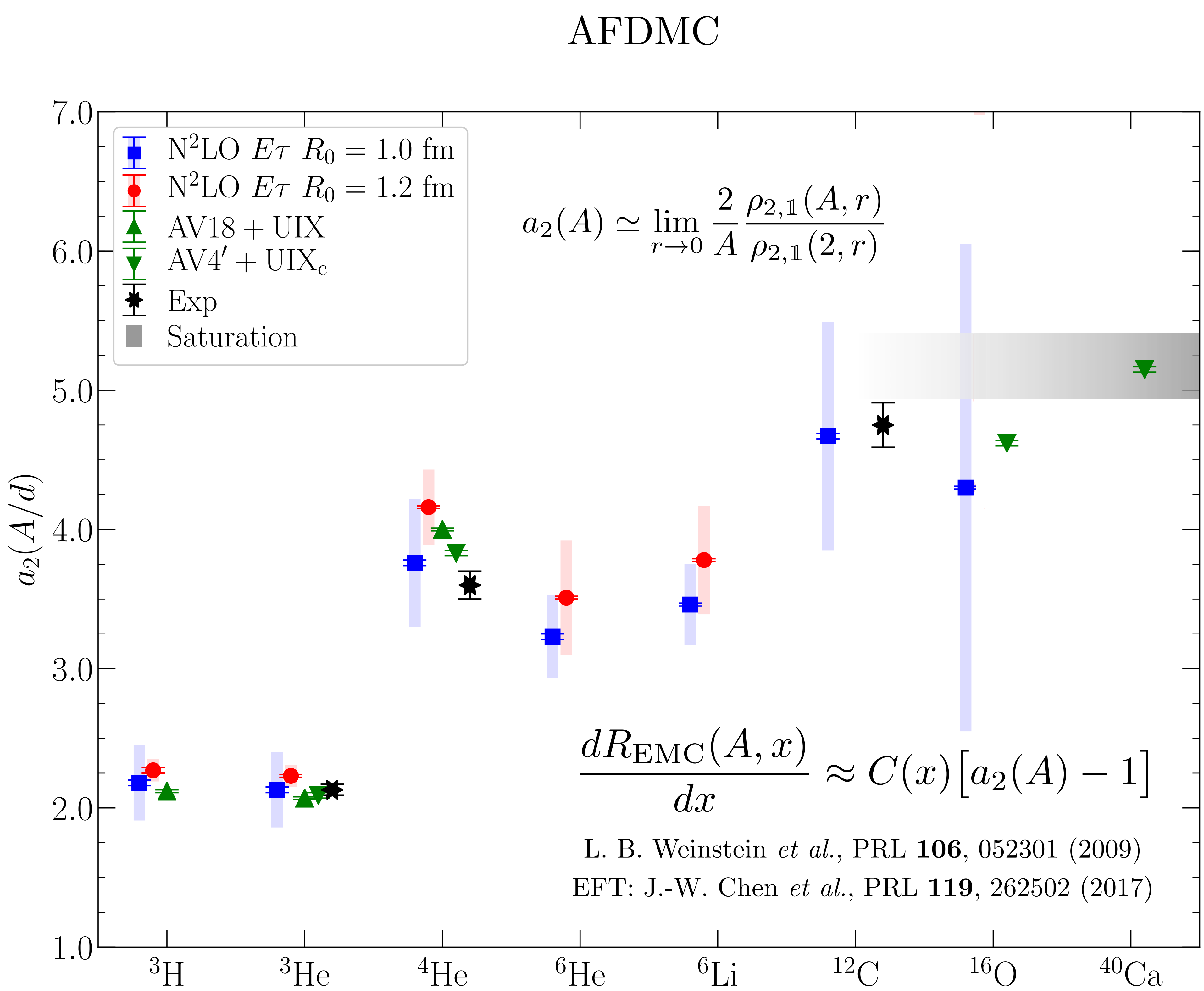


D.L. *et al.*, PRC **98**, 014322 (2018) (tables available as Supplemental Material)

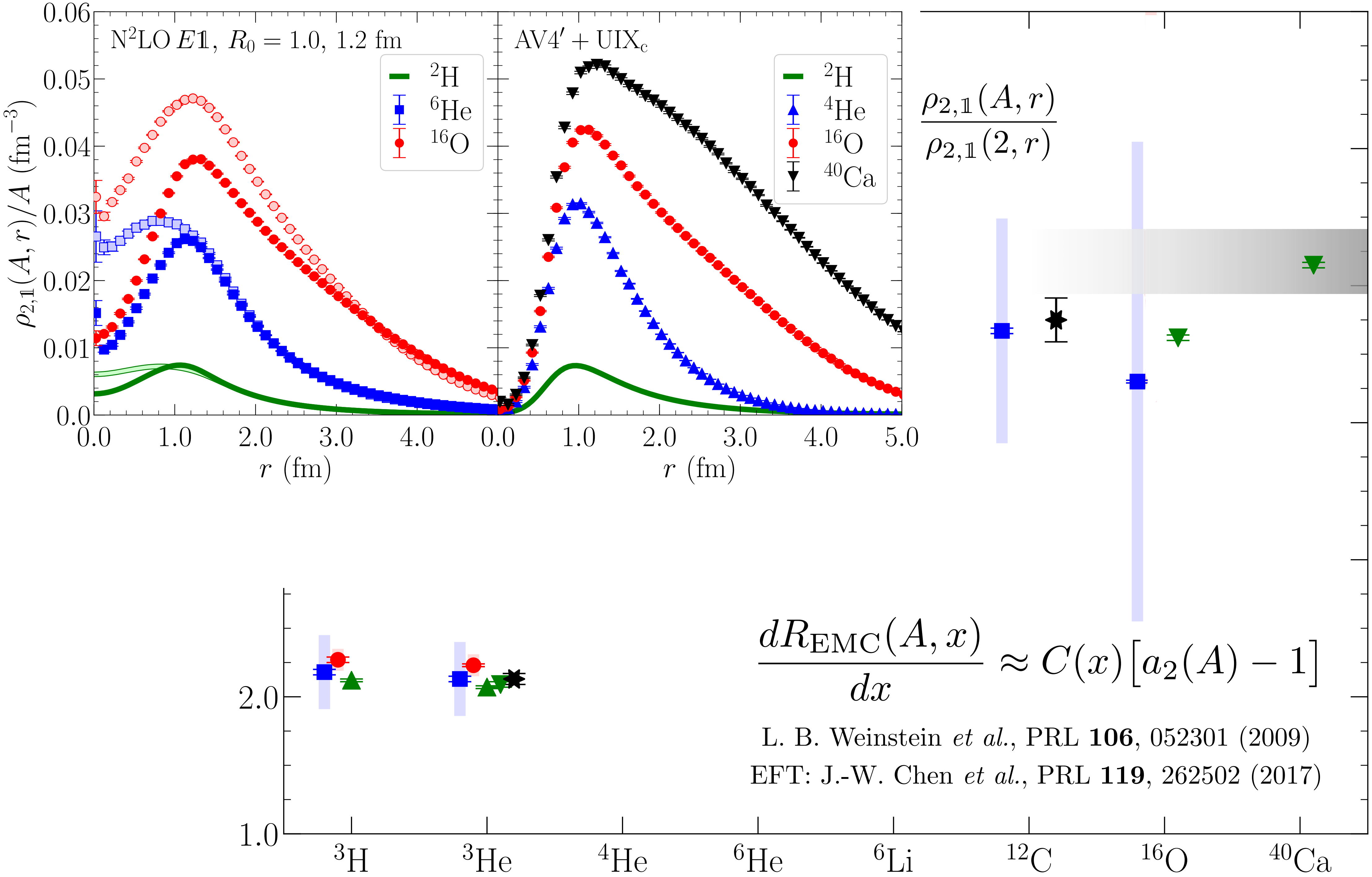
Results: short-range correlation scaling factor



J. E. Lynn, D.L. *et al.*, in preparation

Results: short-range correlation scaling factor

AFDMC



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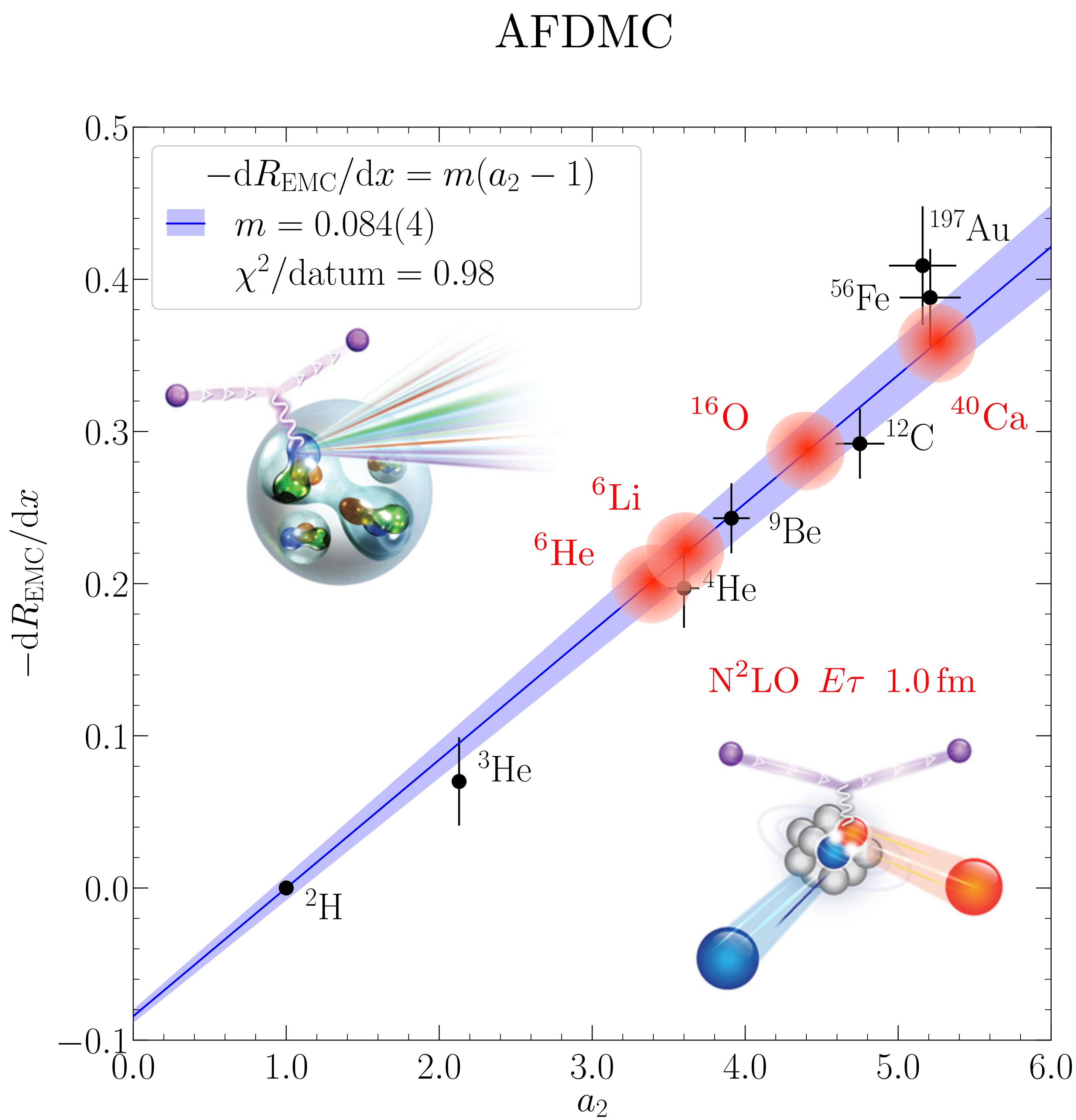
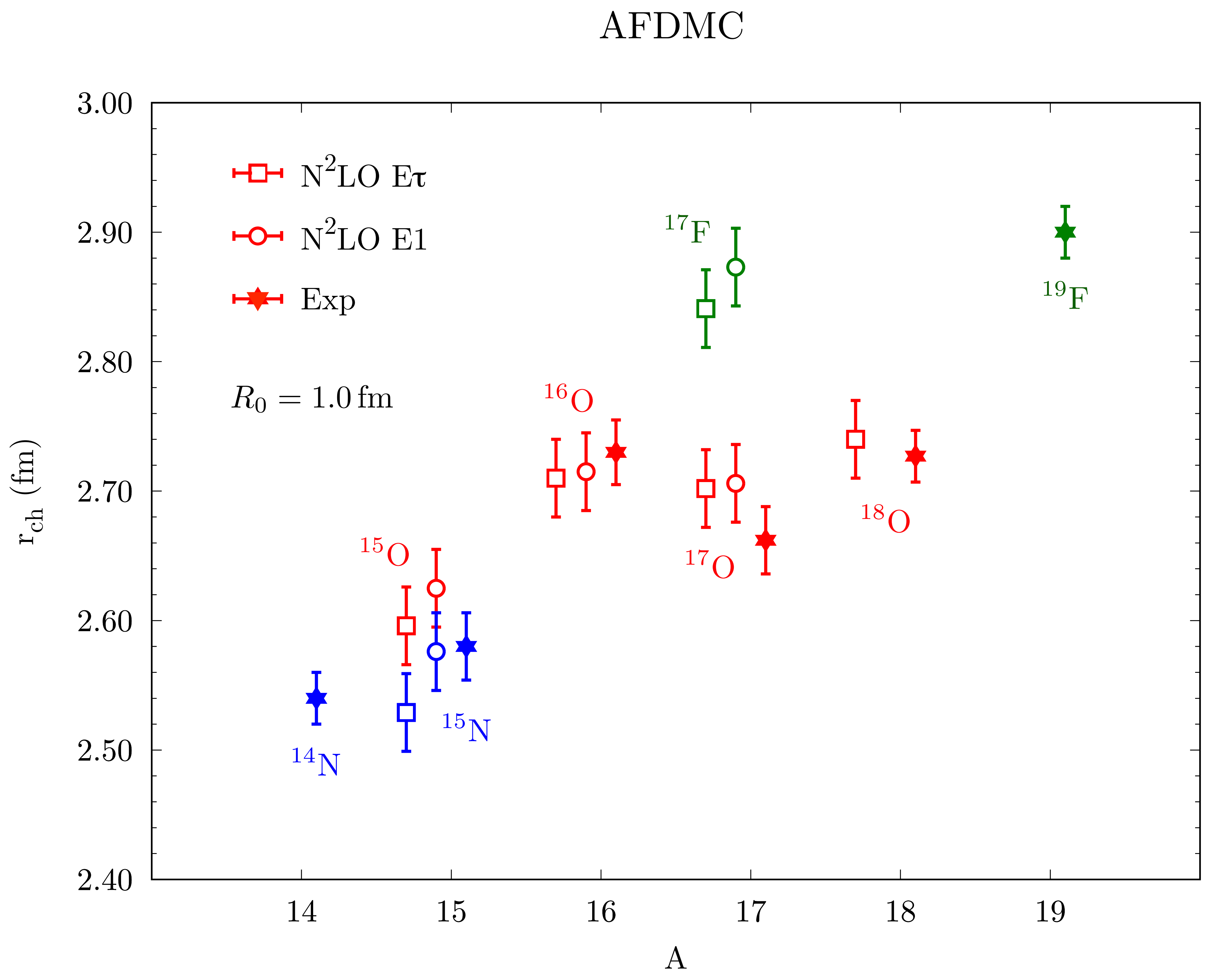


data from: O. Hen *et al.*, PRC **85**, 047301 (2012)

J. E. Lynn, D.L. *et al.*, in preparation

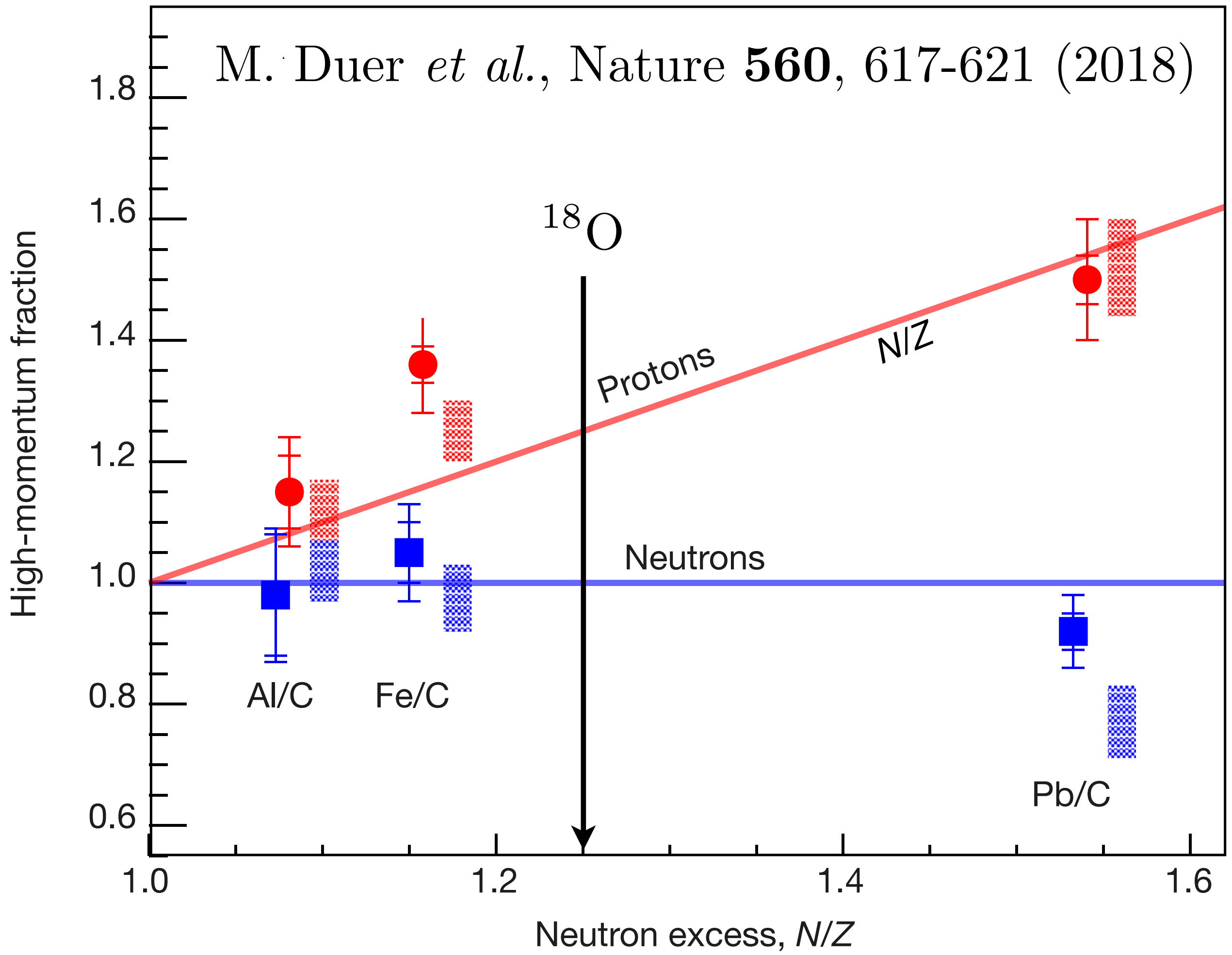
Results: neutron-rich nuclei

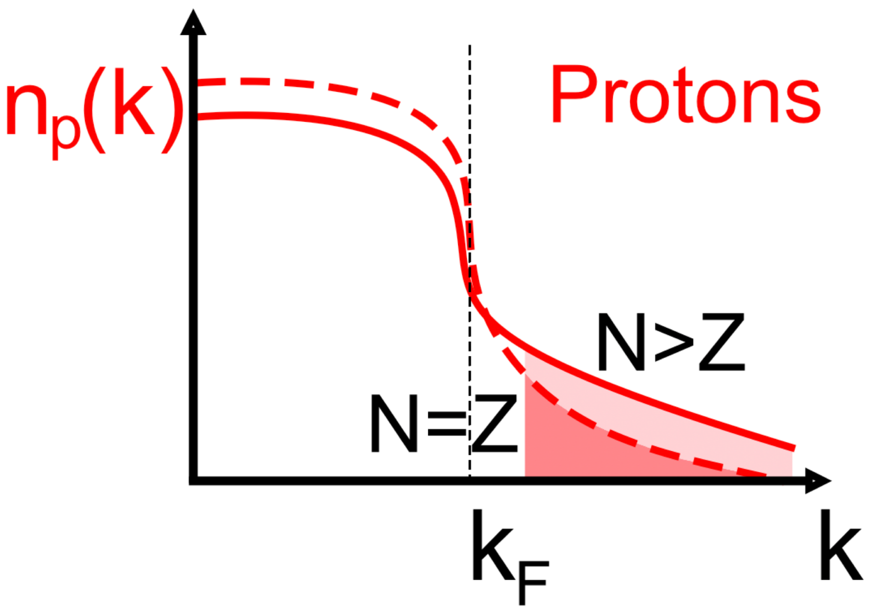


preliminary!!

Results: neutron-rich nuclei

AFDMC





increased proton kinetic energy for N>Z

AFDMC

N^{2}LO $E\tau$

$R_0 = 1.0\,\mathrm{fm}$

^{16}O : $\frac{E^p_{\rm kin}}{Z} = 23.1(5)\,\mathrm{MeV}$, $\frac{E^n_{\rm kin}}{N} = 23.1(5)\,\mathrm{MeV}$

^{18}O : $\frac{E^p_{\rm kin}}{Z} = 24.0(6)\,\mathrm{MeV}$, $\frac{E^n_{\rm kin}}{N} = 21.7(6)\,\mathrm{MeV}$

very preliminary!!

Summary

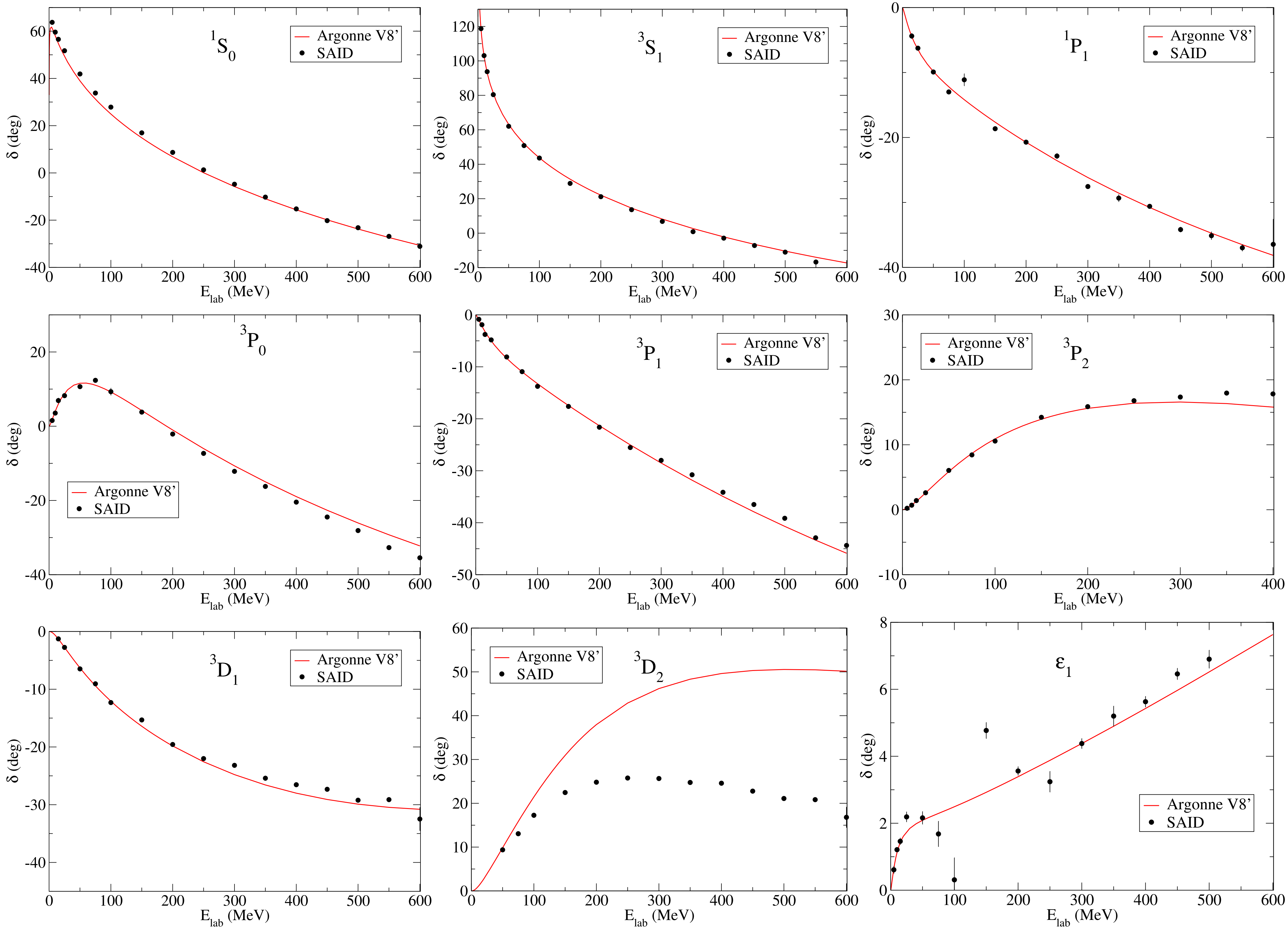
QMC study of nuclei up to Oxygen and Calcium is possible

- both phenomenological and local chiral interactions (delta-less & delta-full)
- full many-body correlated wave functions
- uncertainty quantification: many-body method and theoretical (for chiral potentials)

Short-range correlation effects

- single- and two-nucleon momentum distributions: universality of the tail for a given interaction model, 10-20% of the total strength from SRC
- single- and two-nucleon momentum distributions: scheme and scale dependent, but ratios are largely scheme and scale independent and consistent with data extracted from experiments
- short-range correlation scaling factor: two-body densities are scheme and scale dependent, but ratios are largely scheme and scale independent, and the resulting a_2 is consistent with data extracted from experiments
- neutron-rich nuclei: investigating SRC effects with QMC?

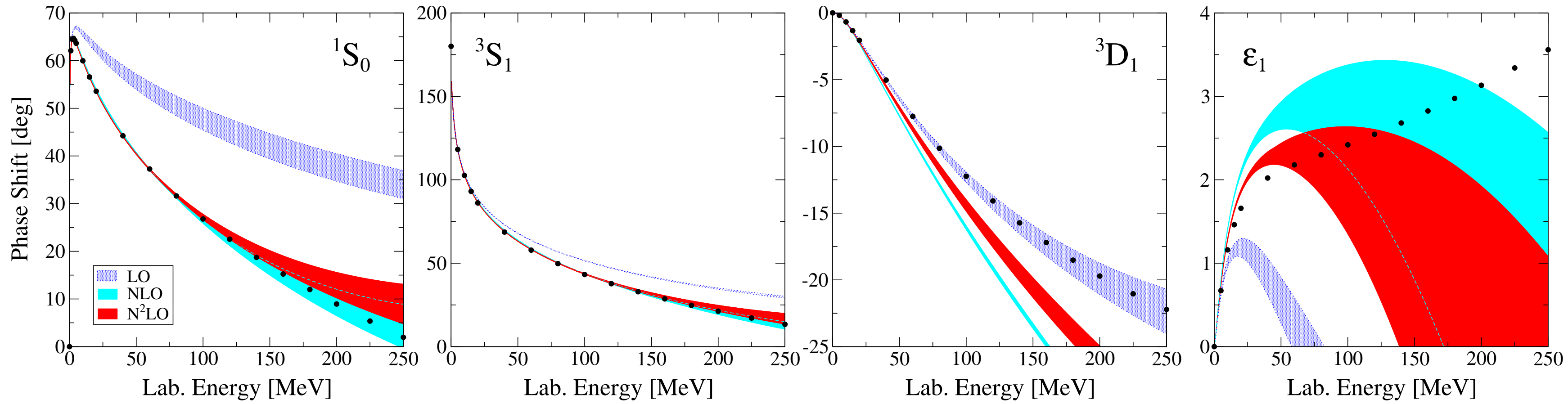
Backup: phenomenological potentials

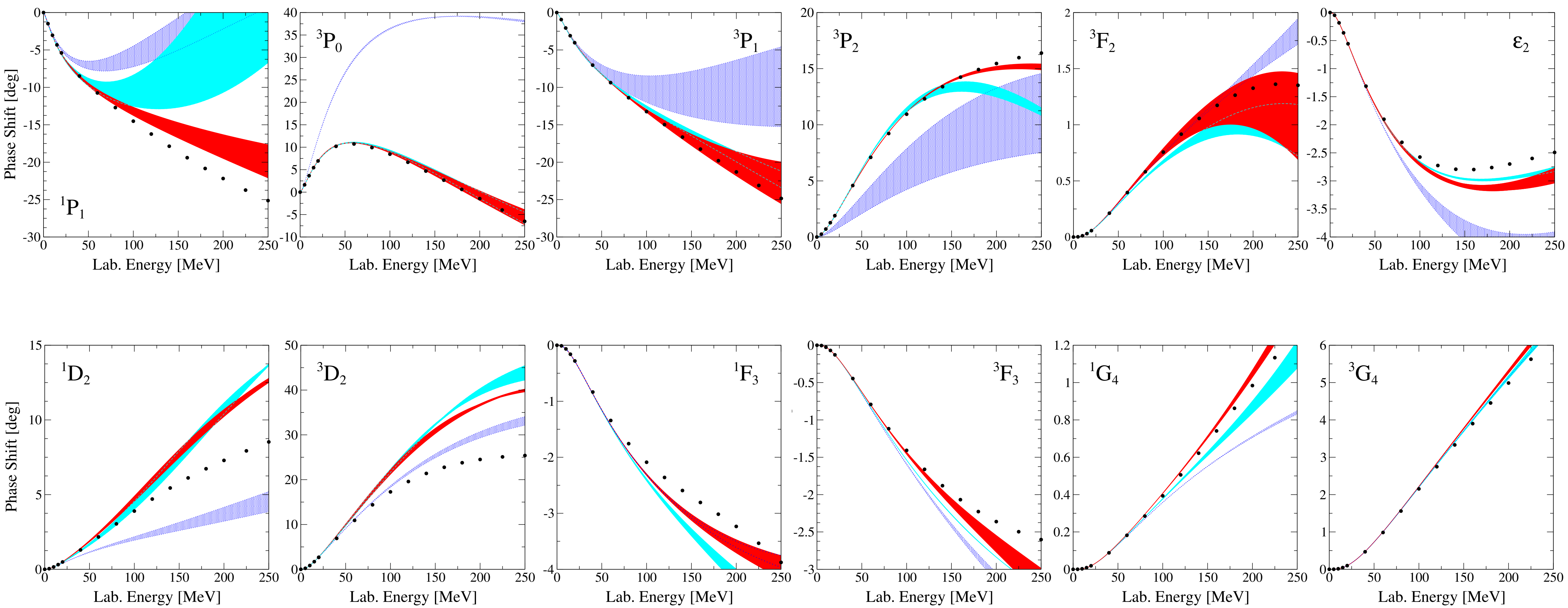


Backup: local chiral potentials

black dots:
Nijmegen PWA

bands:
cutoff variation
$R_0 = 1.0 - 1.2\,\mathrm{fm}$





A. Gexerlis *et al.*, PRC **90**, 054323 (2014)