Quantum Monte Carlo calculations of medium mass nuclei

Diego Lonardoni

FRIB Theory Fellow

In collaboration with:

- ✓ J. Carlson, LANL
- ✓ S. Gandolfi, LANL
- ✓ X. Wang, Huzhou University, China
- ✓ A. Lovato, ANL & UniTN
- ✓ S. C. Pieper, ANL
- ✓ R. B. Wiringa, ANL

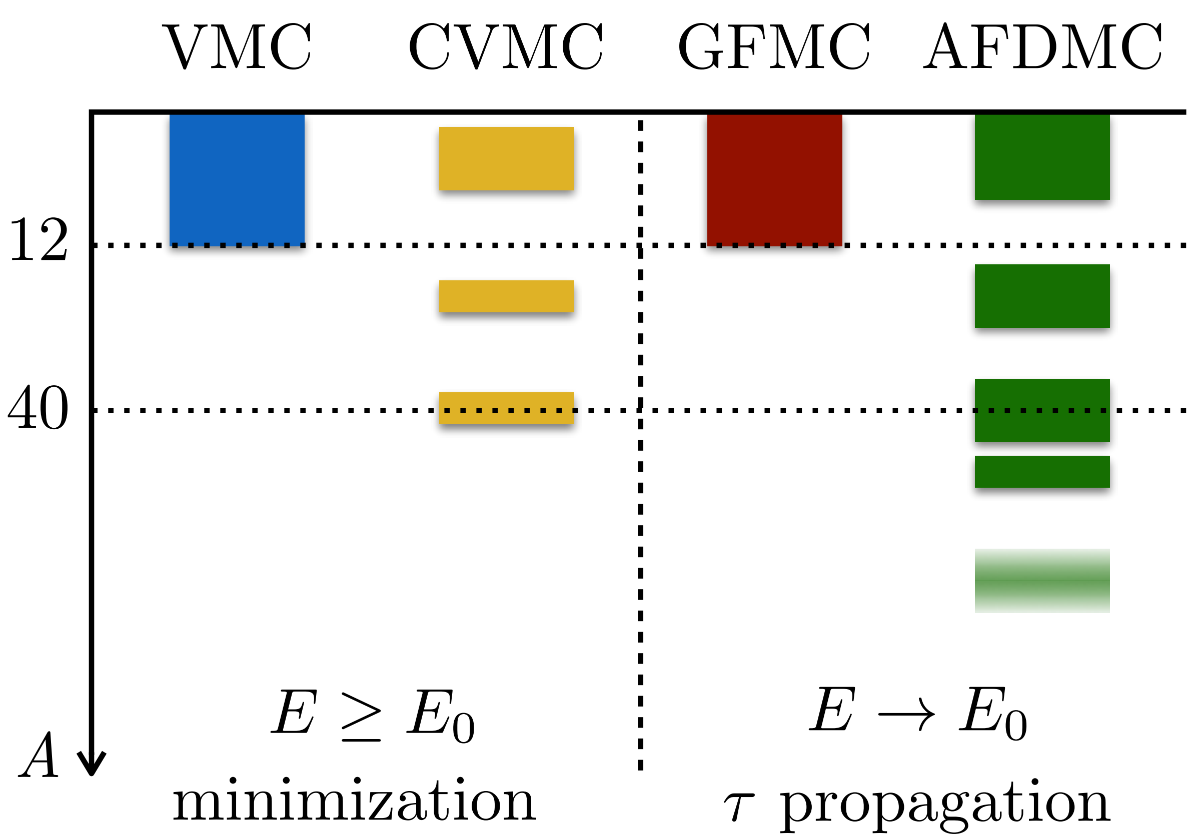
INT, Program INT 17-2a, June 26, 2017

Outline

- ✓ Introduction
  - Quantum Monte Carlo methods
  - Nuclear Hamiltonians
- ✓ Moving towards medium-mass nuclei
  - Phenomenological potentials & QMC
  - Chiral potentials & QMC
- ✓ Conclusions

Quantum Monte Carlo methods

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-heavy nuclei	$A \sim 50$
AFDMC	infinite matter	$A \to \infty$

Pros:

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

Cons:

- Some limitations in A and/or in the interaction to be used.

CVMC

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

→ 4 determinants: $D_{\tau\sigma}$

↓

closed-shell nuclei $A \leq 40$

minimization of $E_V = \frac{\langle\Psi_V|H|\Psi_V\rangle}{\langle\Psi_V|\Psi_V\rangle} \geq E_0$

→ cluster expansion for the spin-isospin dependent correlations

Example: one-body operator

$$\frac{\langle\Psi_V|\sum_i \mathcal{O}_i|\Psi_V\rangle}{\langle\Psi_V|\Psi_V\rangle} = \frac{\sum_i n_i + \sum_{i<j} n_{ij} + \sum_{i\neq j<k} n_{i,jk} + \sum_{i<j<k} n_{ijk} + \ldots}{1 + \sum_{i<j} d_{ij} + \sum_{i<j<k} d_{ijk} + \sum_{\substack{i<j\neq k<l \\ i<k}} d_{ij,kl} + \ldots}$$

$$n_i = \langle\mathcal{O}_i\rangle$$

$$n_{ij} = \left\langle\left(1+U_{ij}^\dagger\right)(\mathcal{O}_i+\mathcal{O}_j)\left(1+U_{ij}\right)\right\rangle - n_i - n_j$$

$f_c(r_{ij})$ included at every order in $\langle X\rangle$

Quantum Monte Carlo methods

CVMC

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

→ 4 determinants: $D_{\tau\sigma}$ → closed-shell nuclei $A \leq 40$

minimization of $$E_V = \frac{\langle\Psi_V|H|\Psi_V\rangle}{\langle\Psi_V|\Psi_V\rangle} \geq E_0$$

→ cluster expansion for the spin-isospin dependent correlations

Example: one-body operator

$$\frac{\langle\Psi_V|\sum_i \mathcal{O}_i|\Psi_V\rangle}{\langle\Psi_V|\Psi_V\rangle} = \frac{\sum_i n_i + \sum_{i<j} n_{ij} + \sum_{i\neq j<k} n_{i,jk} + \sum_{i<j<k} n_{ijk} + \ldots}{1 + \sum_{i<j} d_{ij} + \sum_{i<j<k} d_{ijk} + \sum_{\substack{i<j\neq k<l \\ i<k}} d_{ij,kl} + \ldots}$$

$$= \sum_i c_i + \sum_{i<j} c_{ij} + \sum_{i\neq j<k} c_{i,jk} + \sum_{i<j<k} c_{ijk} + \ldots$$

1b, 2b, 3b → up to 5b

AFDMC

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

$\downarrow$

nuclei $A \lesssim 48$

propagation in imaginary time: $e^{-H\tau}|\Psi_V\rangle \xrightarrow{\tau\to\infty} |\Psi_0\rangle$

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

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

$dx \downarrow$ auxiliary field

$\sqrt{-\lambda d\tau}\,x\mathcal{O} \downarrow$ rotation in spin-isospin space

- sign problem: constrained path approximation + release node

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)

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

v_{ij} fit to NN scattering data & deuteron

v_{ijk} fit to properties of (light?) nuclei + constraints

Focus on two families of nuclear interactions:

- ✓ Phenomenological potentials: Argonne V18 (NN) + Urbana / Illinois (NNN)
- ✓ χ-EFT potentials: N^{2}LO local

Note: local vs non-local

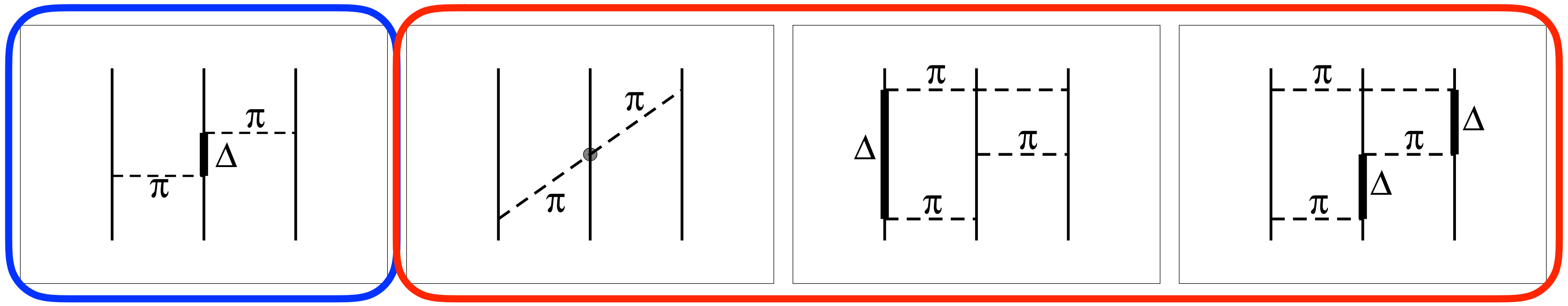
$$\begin{cases} \boldsymbol{p} = (\boldsymbol{p}_1 - \boldsymbol{p}_2)/2 \\ \boldsymbol{p}' = (\boldsymbol{p}'_1 - \boldsymbol{p}'_2)/2 \end{cases} \qquad \begin{cases} \boldsymbol{q} = \boldsymbol{p}' - \boldsymbol{p} \\ \boldsymbol{k} = (\boldsymbol{p}' + \boldsymbol{p})/2 \end{cases} \qquad \begin{matrix} \text{local} & \longrightarrow & \boldsymbol{r} \\ \text{non-local} & \longrightarrow & \boldsymbol{\nabla}_r \end{matrix}$$

Phenomenological potentials

NN: Argonne V18

$$v_{ij} = \sum_p \mathcal{O}^p_{ij}(r_{ij}) \qquad \mathcal{O}^{p=1,8}_{ij} = [\mathbb{1}, \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j, S_{ij}, \boldsymbol{L}_{ij} \cdot \boldsymbol{S}_{ij}] \otimes [\mathbb{1}, \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j]$$

NNN: Urbana / Illinois



+ short-range term

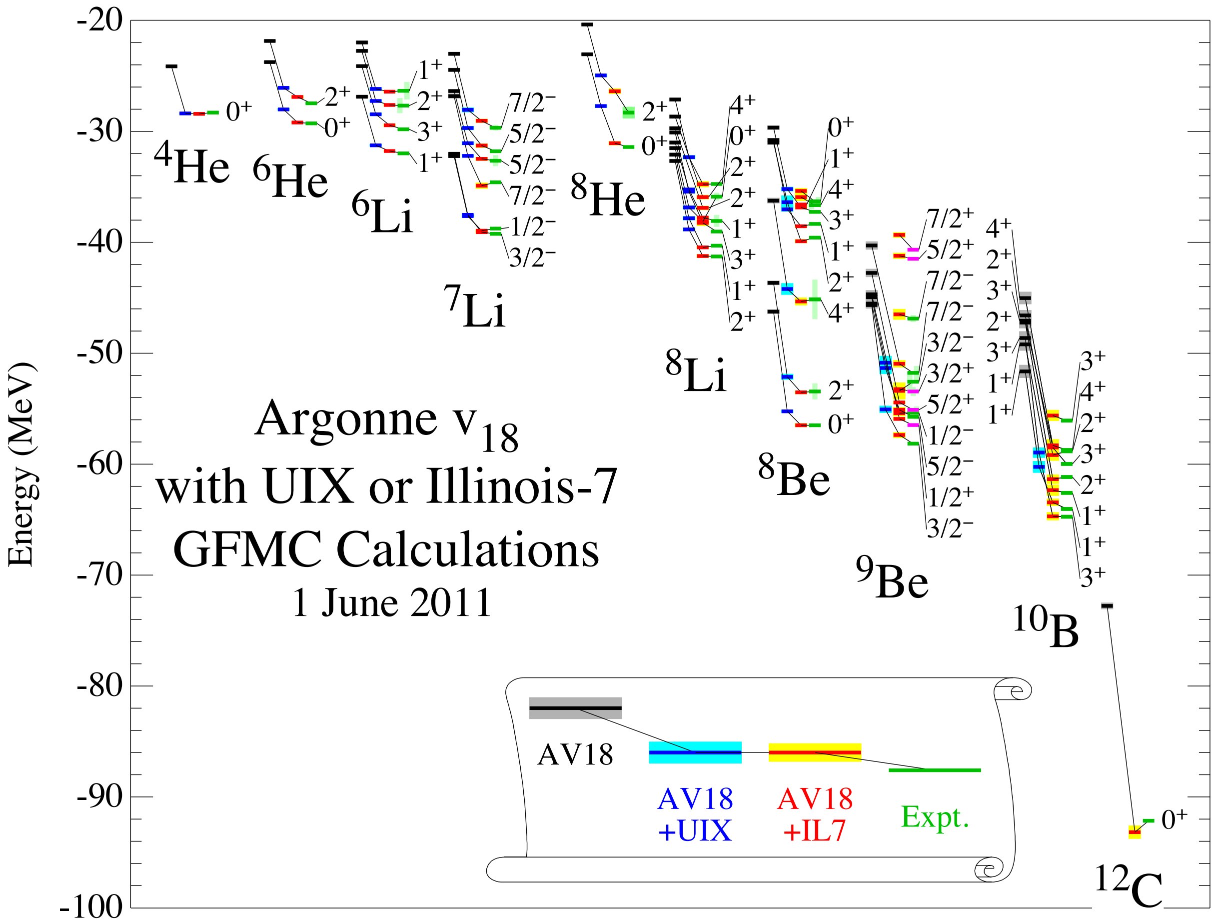
Pros:
- Argonne interactions fit phase shifts up to high energies. Accurate up to (at least) 2-3 saturation density.
- Suitable for QMC calculations. Very good description of several observables in light nuclei (GFMC ground-state energies: uncertainties within 1-2%).

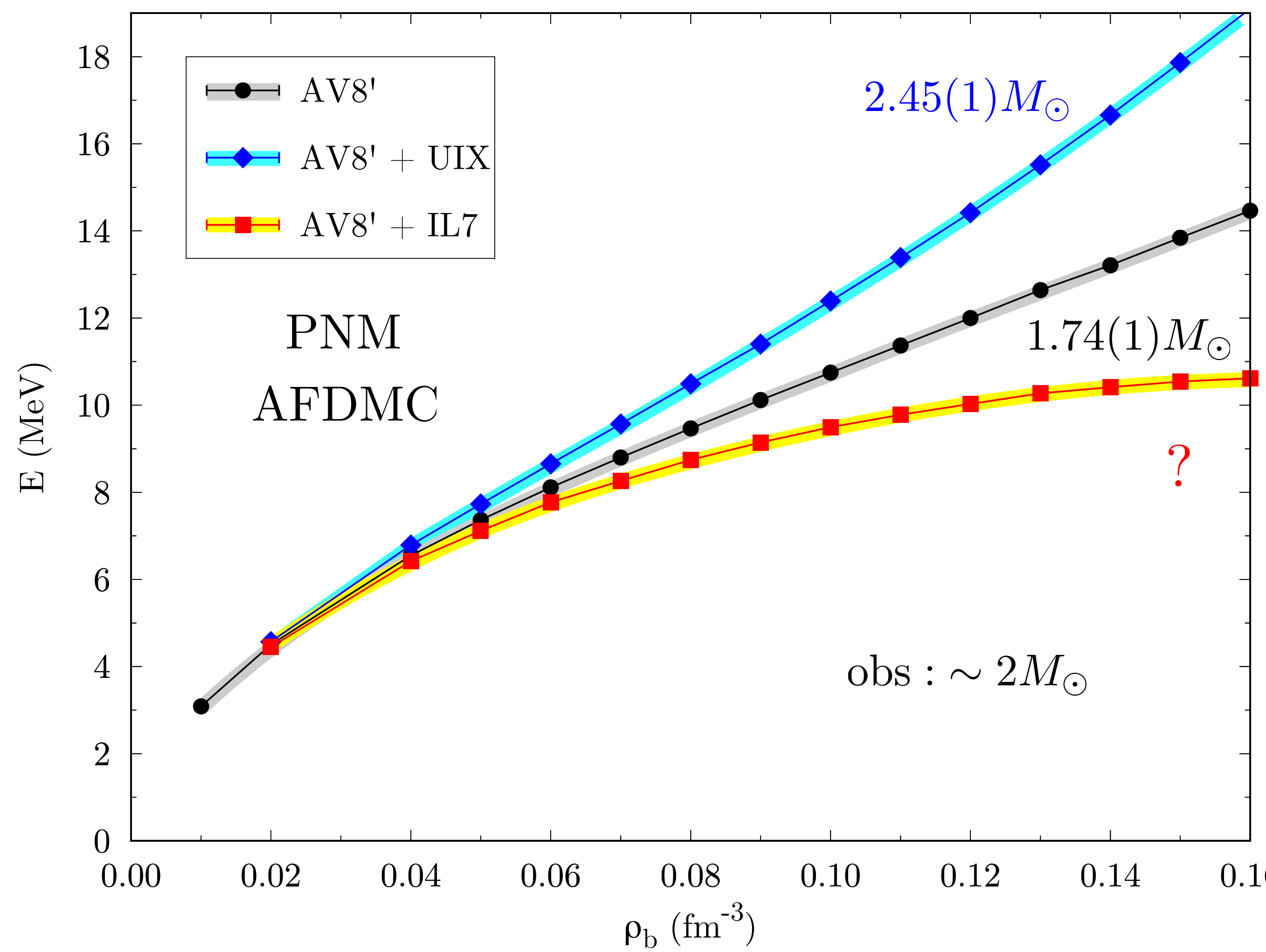
Cons:
- Phenomenological interactions are phenomenological, not clear how to improve their quality. Theoretical uncertainties hard to quantify.
- 3-body forces?

Phenomenological potentials & QMC

3-body forces:

- UIX: fit to H3 binding energy & saturation density of SNM
- IL7: fit to ground- and excited-state energies of light nuclei ($A<10$)



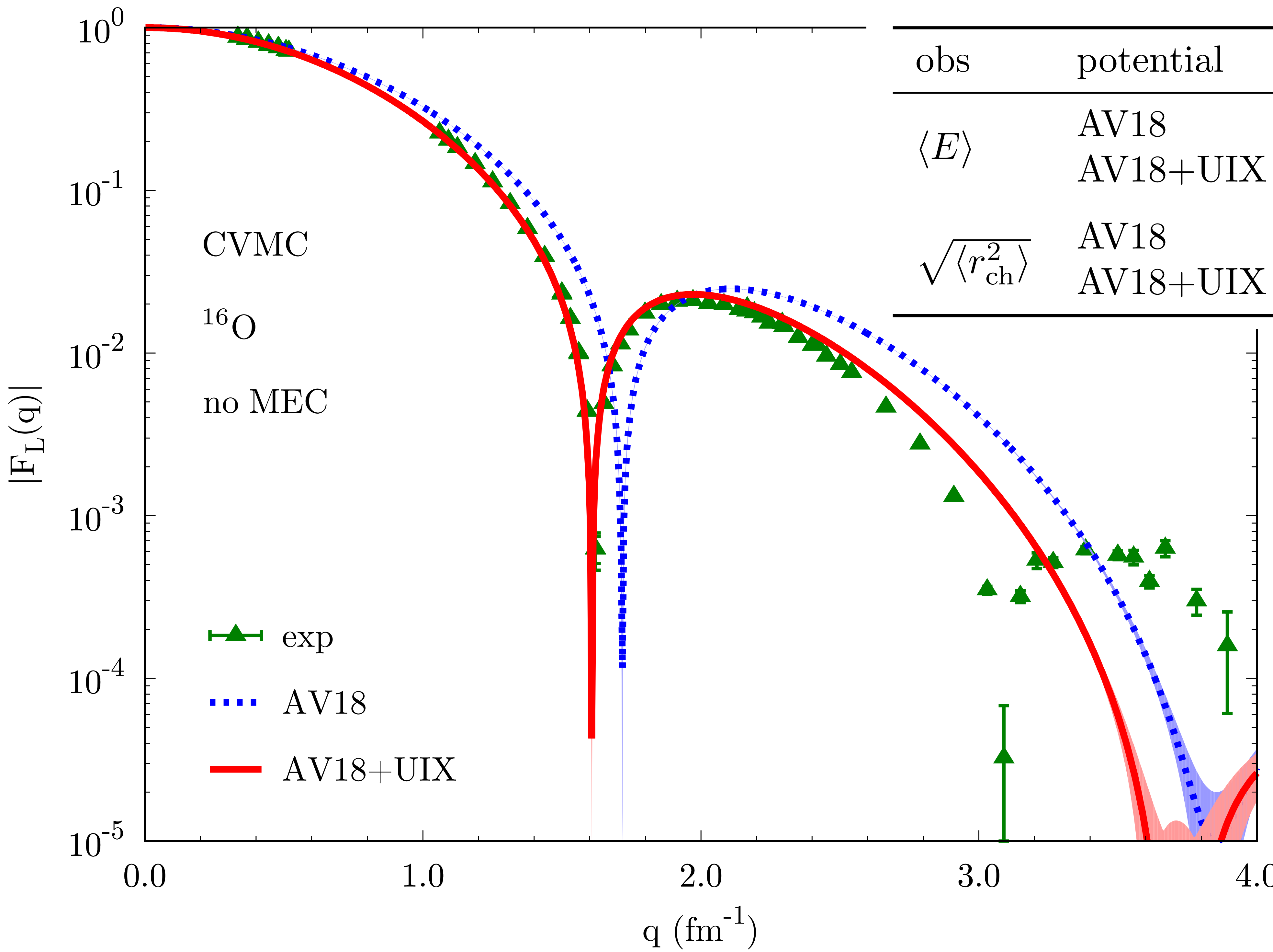


IL7 also needed to reproduce n-α scattering

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

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

^{16}O: variational energies, charge radii, charge form factors



obs	potential	CVMC	exp
$\langle E \rangle$	AV18 AV18+UIX	$-5.51(2)$ $-5.15(2)$	-7.98
$\sqrt{\langle r^2_{\rm ch} \rangle}$	AV18 AV18+UIX	2.538(2) 2.745(2)	2.699(5)

note: ^{12}C

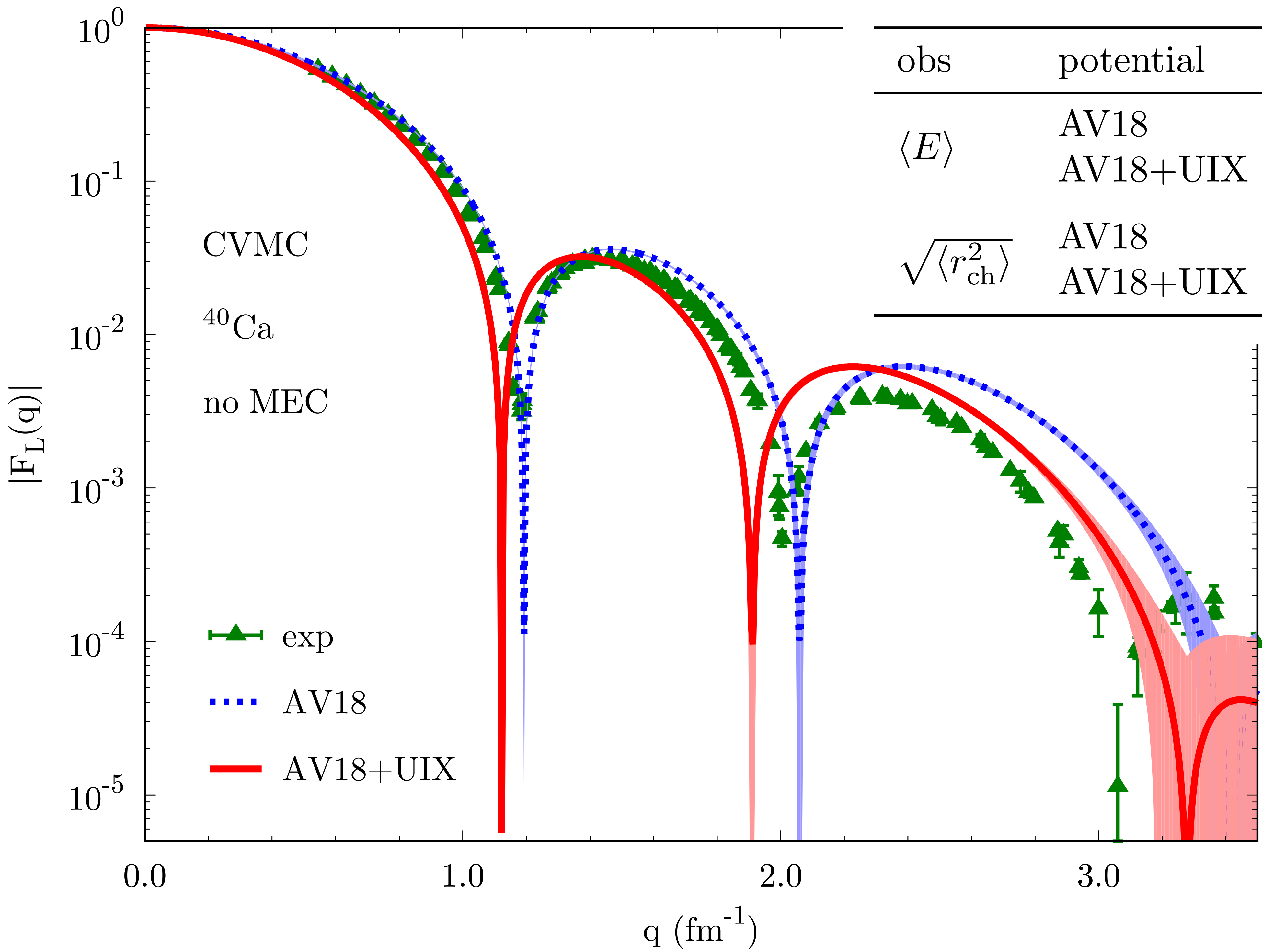
VMC : 2.484(2)

exp : 2.470(2)

credit to R. B. Wiringa

D.L., A. Lovato, S. C. Pieper, R. B. Wiringa, arXiv:1705.04337

^{40}Ca: variational energies, charge radii, charge form factors



obs	potential	CVMC	exp
$\langle E \rangle$	AV18 AV18+UIX	−5.88(10) −4.92(10)	−8.55
$\sqrt{\langle r^2_{ch} \rangle}$	AV18 AV18+UIX	3.361(2) 3.617(2)	3.478(1)

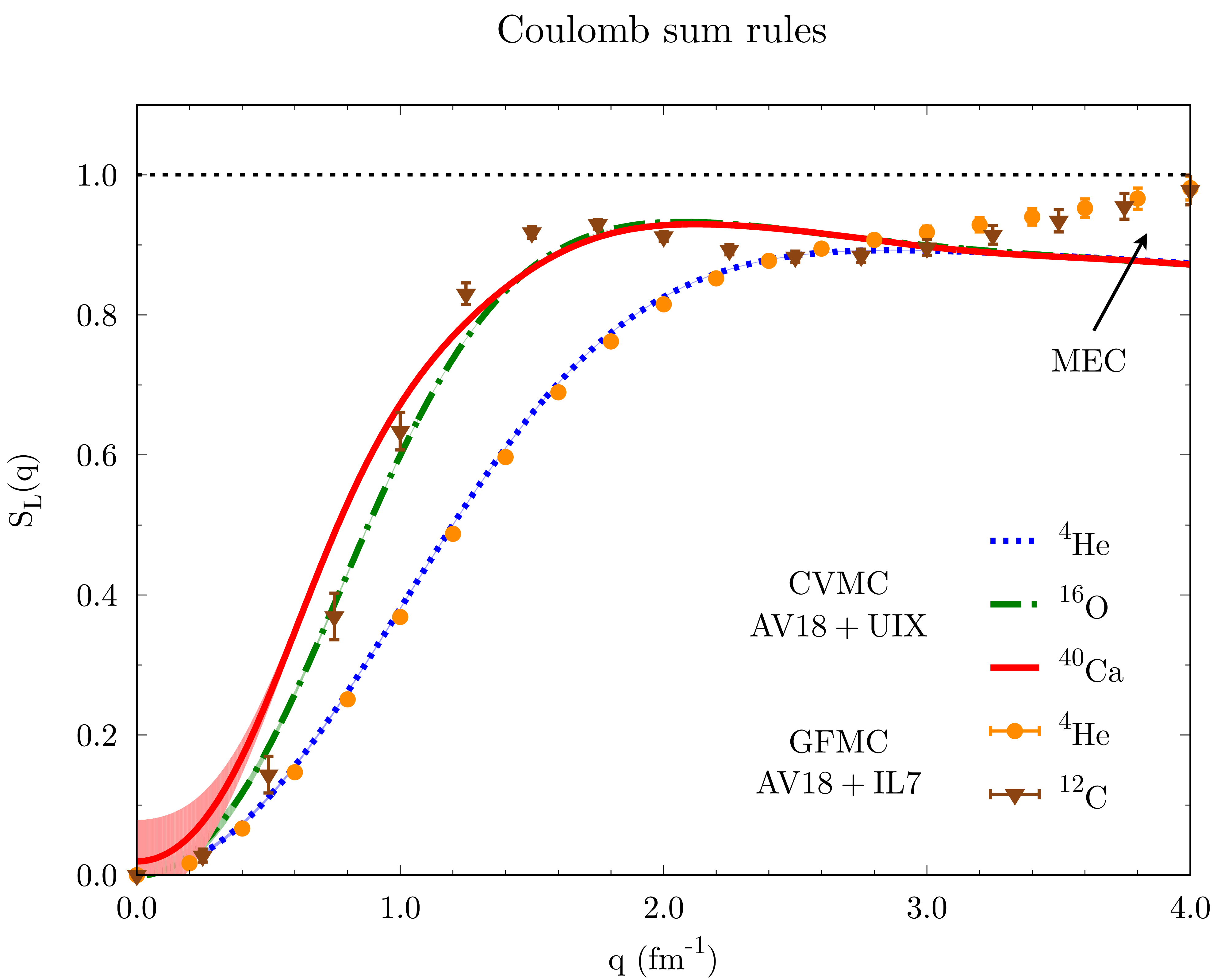
VMC SNM @ ρ_0

AV18 : − 14.59

AV18+UIX: − 11.85

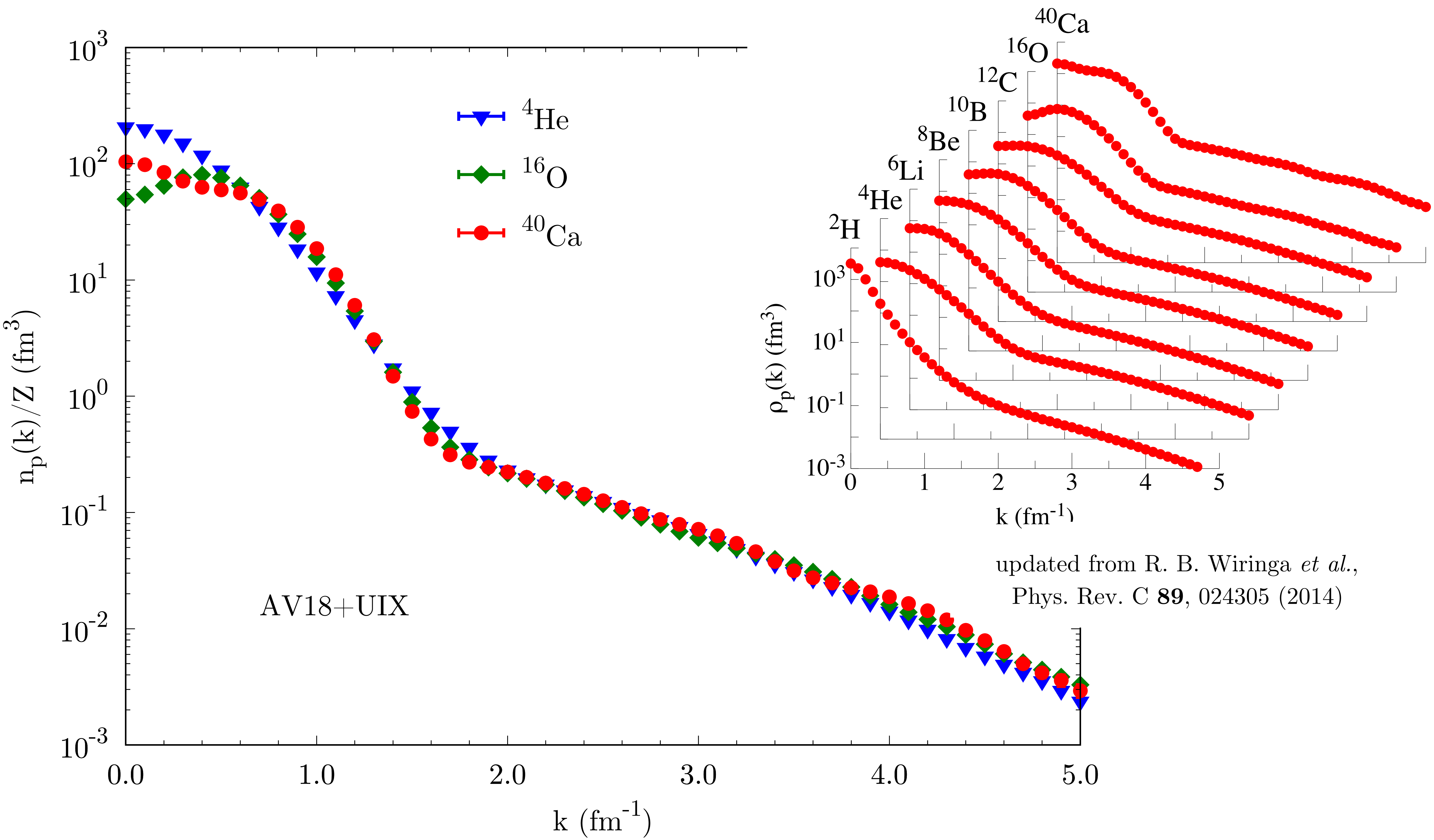
A. Akmal, *et al.*,
Phys. Rev. C **58**, 1804 (1998)

D.L., A. Lovato, S. C. Pieper, R. B. Wiringa, arXiv:1705.04337



D.L., A. Lovato, S. C. Pieper, R. B. Wiringa, arXiv:1705.04337

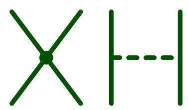
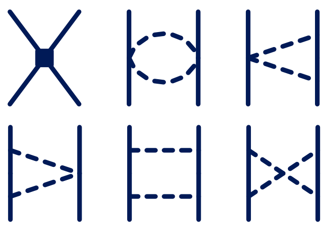
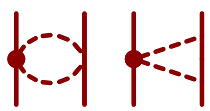
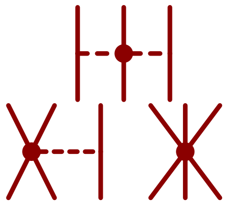
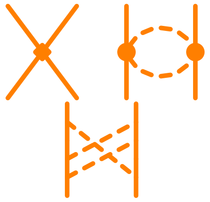
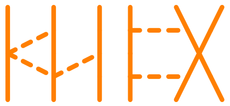
single-nucleon momentum distributions



updated from R. B. Wiringa *et al.*, Phys. Rev. C **89**, 024305 (2014)

D.L., A. Lovato, S. C. Pieper, R. B. Wiringa, arXiv:1705.04337

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^{2}LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^3$		
N^{3}LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^4$	 $+\cdots$	 $+\cdots$

- χEFT: expansion in power of Q/Λ_b

  $Q \sim m_\pi \sim 100\,\text{MeV}$ 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

Chiral potentials

Pros:

- Chiral interactions have a theoretical derivation and they can be systematically improved (if proper power counting...).
- They are typically softer than the phenomenological forces, making most of the calculations easier to converge.
- Many-body forces are naturally accounted for.

Cons:

- Standard formulation: momentum-space, non-local. Not suitable for QMC.

Chiral potentials

Pros:
- Chiral interactions have a theoretical derivation and they can be systematically improved (if proper power counting...).
- They are typically softer than the phenomenological forces, making most of the calculations easier to converge.
- Many-body forces are naturally accounted for.

Cons:
- ~~Standard formulation: momentum space, non local. Not suitable for QMC.~~

local chiral N^2LO potentials

2-body NN

A. Gezerlis *et al.*, Phys. Rev. Lett. **111**, 032501 (2013)
A. Gezerlis *et al.*, Phys. Rev. C **90**, 054323 (2014)
J. E. Lynn *et al.*, Phys. Rev. Lett. **113**, 192501 (2014)

3-body NNN

I. Tews *et al.*, Phys. Rev. C **93**, 024305 (2016)
J. E. Lynn *et al.*, Phys. Rev. Lett. **116**, 062501 (2016)

Δ-full local chiral N^3LO potentials

2-body NN

M. Piarulli *et al.*, Phys. Rev. C **91**, 024003 (2015)
M. Piarulli *et al.*, Phys. Rev. C **94**, 054007 (2016)

3-body NNN

in progress @ N^2LO

Local chiral potentials

✓ 2-body NN @ N^{2}LO

- pion exchanges up to N^{2}LO depend only on $\boldsymbol{p}$, $\boldsymbol{p}'$, $\boldsymbol{q}$

- contact terms: 2 LECs @ LO $\longrightarrow$ no momentum dependence

  7 LECs @ NLO - N^{2}LO $\longrightarrow$ depend on $\boldsymbol{q}$, $\boldsymbol{q}\times\boldsymbol{k}$

- local regulators in real space for both long and short range physics $\sim e^{-(r/R_0)^4}$

  coordinate cutoff: $R_0 = 1.0 - 1.2\,\mathrm{fm}$ $\longleftrightarrow$ momentum cutoff: $\sim 500 - 400\,\mathrm{MeV}$

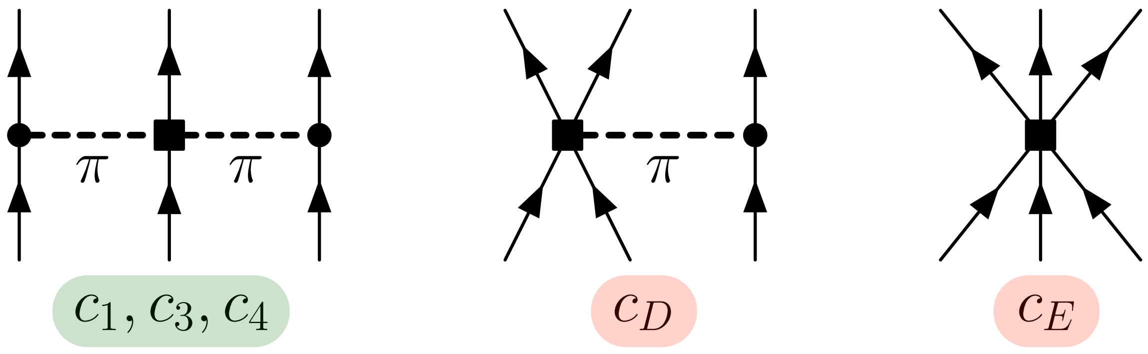
- Fierz freedom:

$$v_{ij} = \sum_p \mathcal{O}_{ij}^p(r_{ij}) \qquad \mathcal{O}_{ij}^{p=1,7} = \underbrace{\left[\mathbb{1}, \boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j, S_{ij}\right]\otimes\left[\mathbb{1}, \boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j\right]}_{\text{local (AV6)}} + \underbrace{\boldsymbol{L}_{ij}\cdot\boldsymbol{S}_{ij}}_{\downarrow\ \text{non-local}}$$

included in DMC propagators,
both GFMC and now AFDMC

Local chiral potentials

✓ 3-body NNN @ N^{2}LO



same as NN — need to be fit

fit to:

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

Note: regulator functions and finite cutoff in coordinate space

↓

different possible operator structures:

$$V_D \longrightarrow D1,\ D2$$

$$V_E \longrightarrow E\tau,\ E\mathbb{1},\ E\mathcal{P}$$

suitable for GFMC and now AFDMC:

light- to medium-heavy nuclei

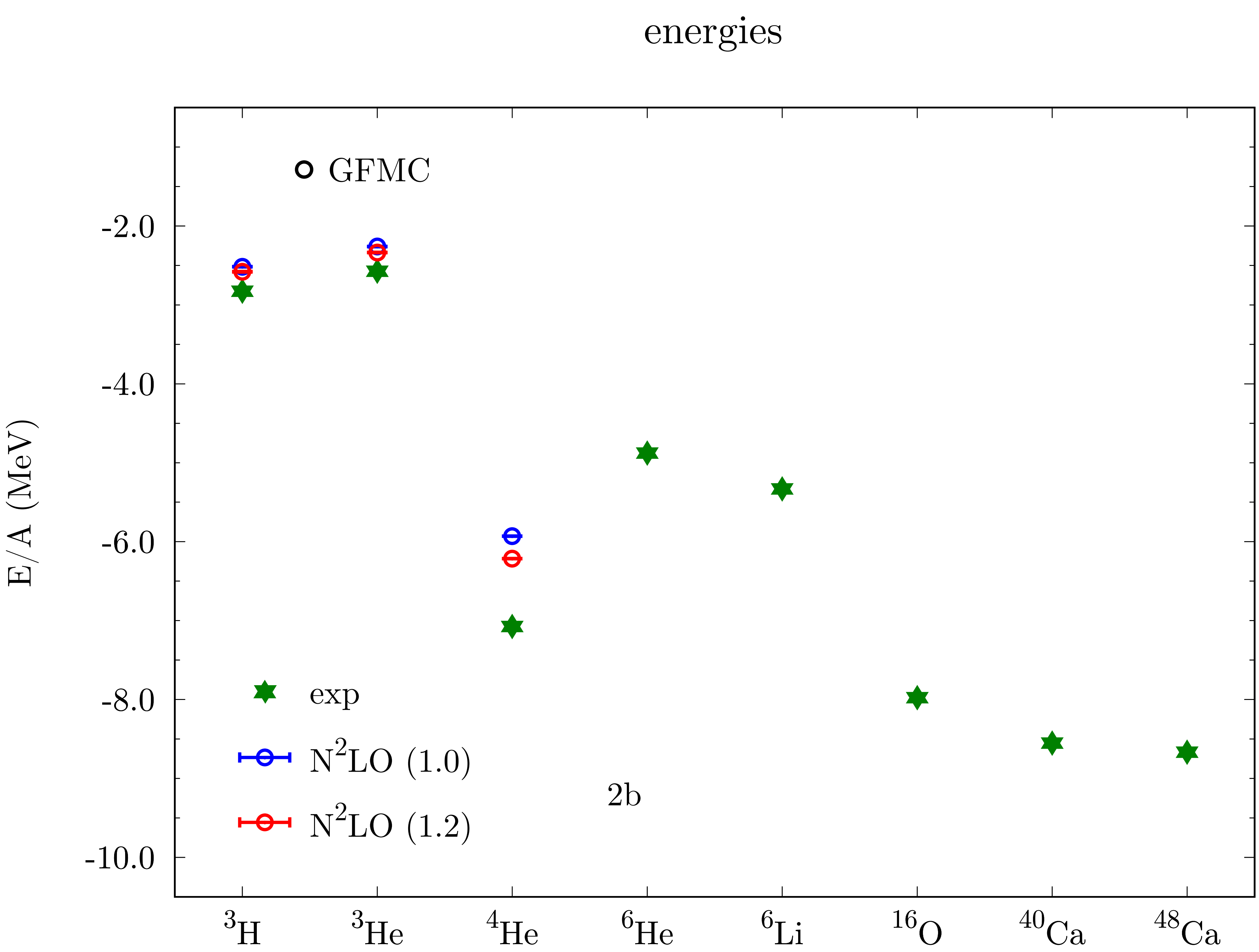
infinite matter

TABLE I. Fit values for the couplings c_D and c_E for different choices of 3N forces and cutoffs.

V_{3N}	R_0 (fm)	c_E	c_D
N^{2}LO $(D1, E\tau)$	1.0	−0.63	0.0
	1.2		
N^{2}LO $(D2, E\tau)$	1.0	−0.63	0.0
	1.2	0.09	3.5
N^{2}LO $(D2, E\mathbb{1})$	1.0	0.62	0.5
N^{2}LO $(D2, E\mathcal{P})$	1.0	0.59	0.0

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

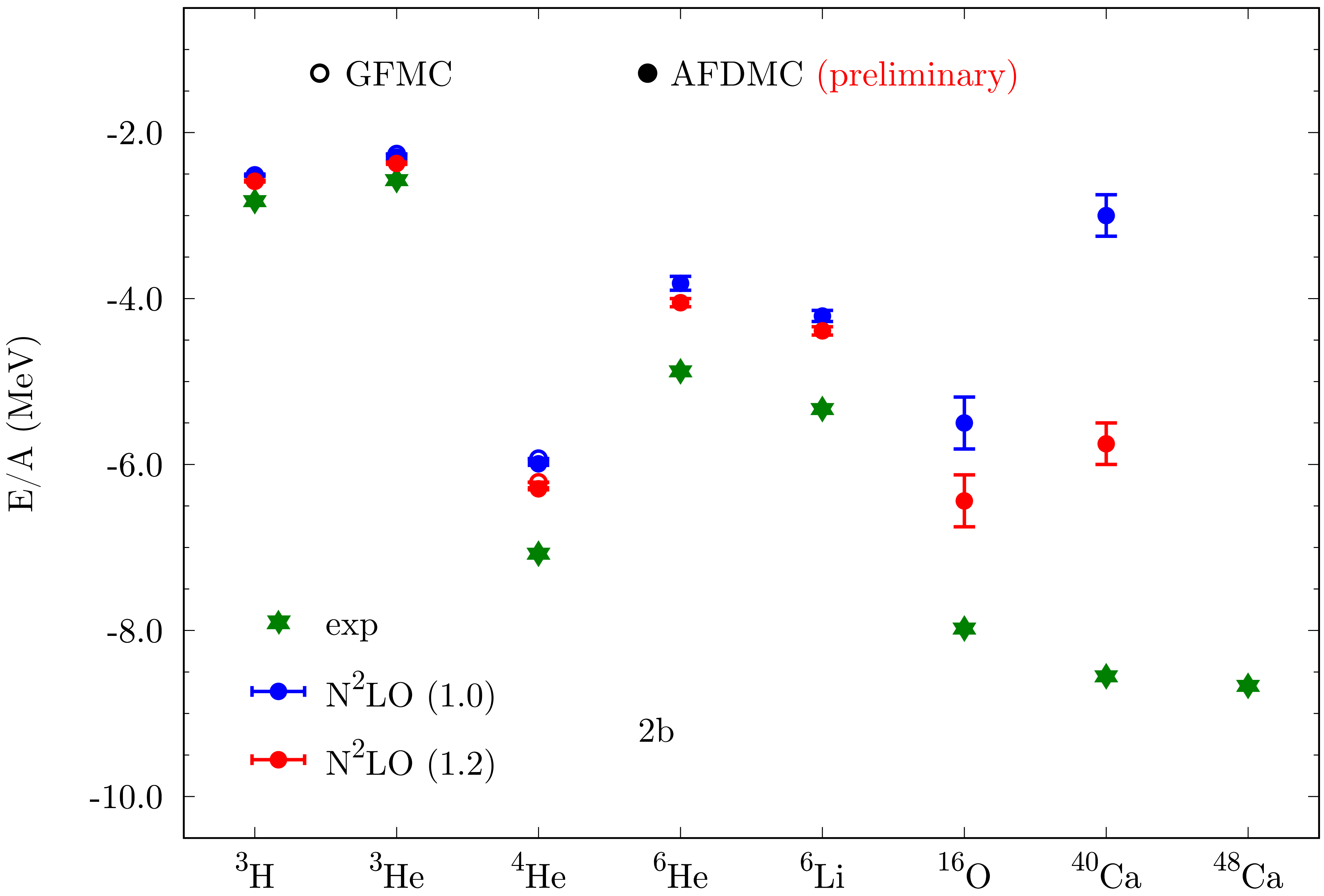
Local chiral potentials & QMC



GFMC: J. E. Lynn *et al.*, Phys. Rev. Lett. **113**, 192501 (2014) & Phys. Rev. Lett. **116**, 062501 (2016)

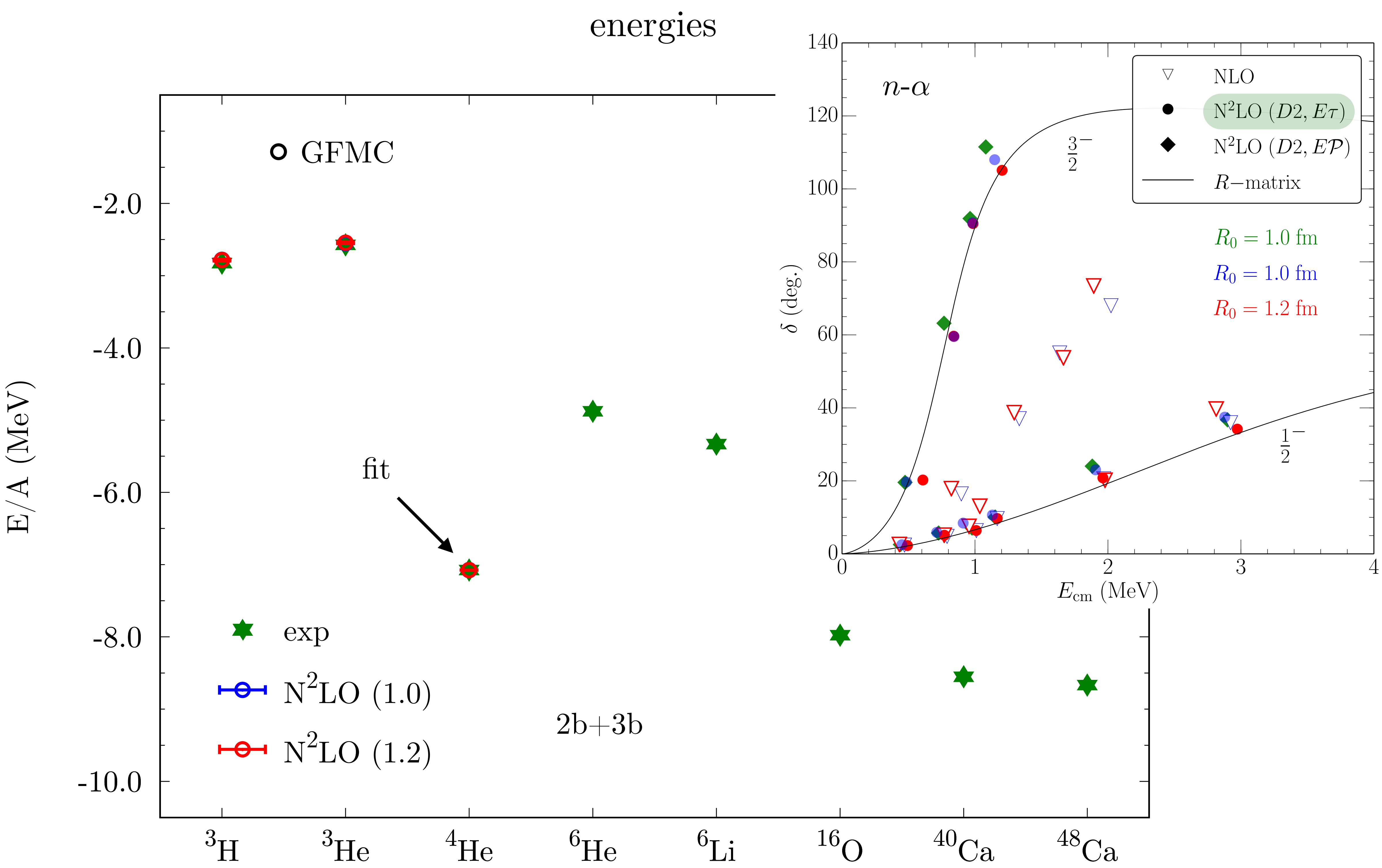
Local chiral potentials & QMC

energies

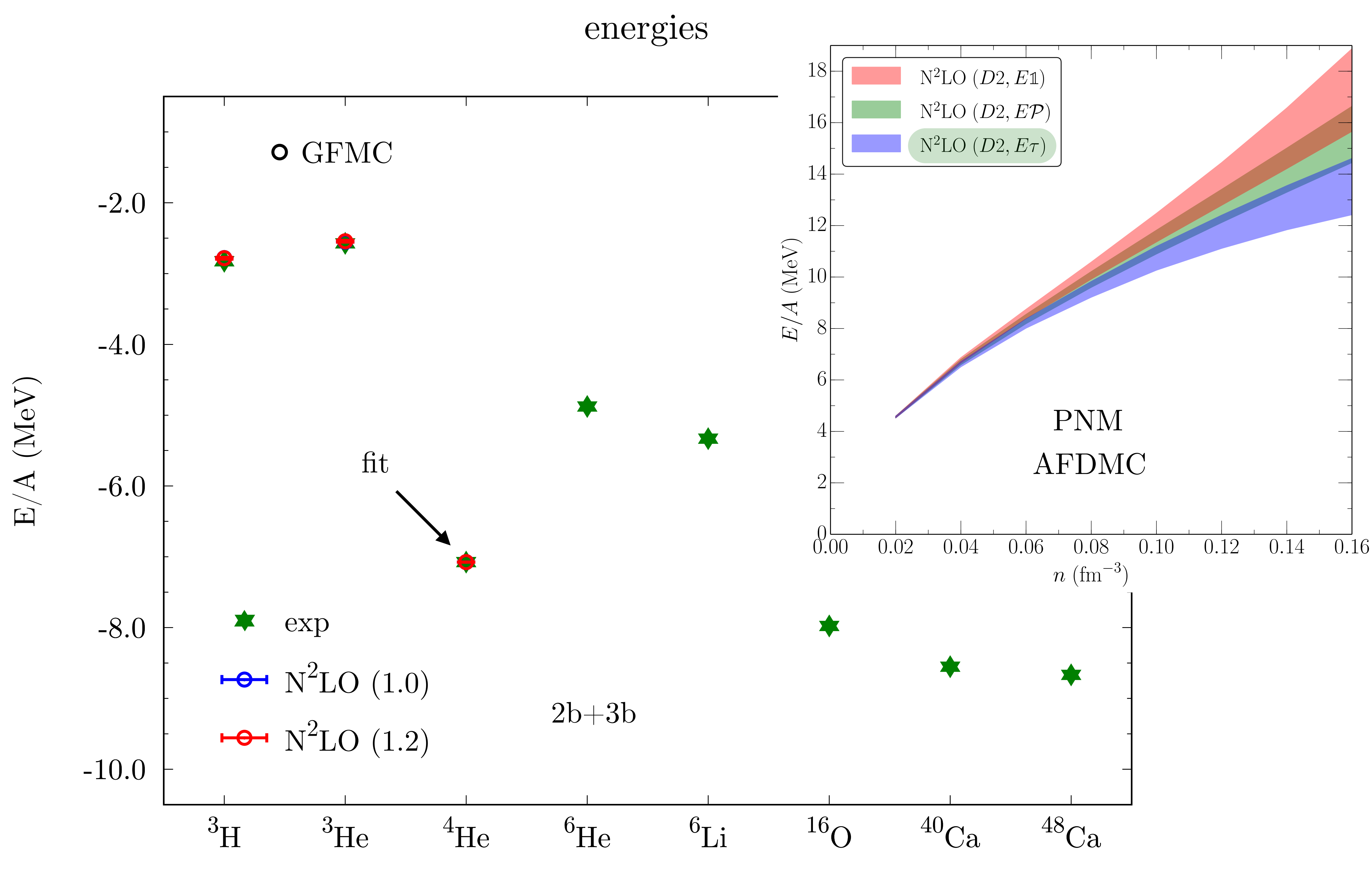


GFMC: J. E. Lynn *et al.*, Phys. Rev. Lett. **113**, 192501 (2014) & Phys. Rev. Lett. **116**, 062501 (2016)

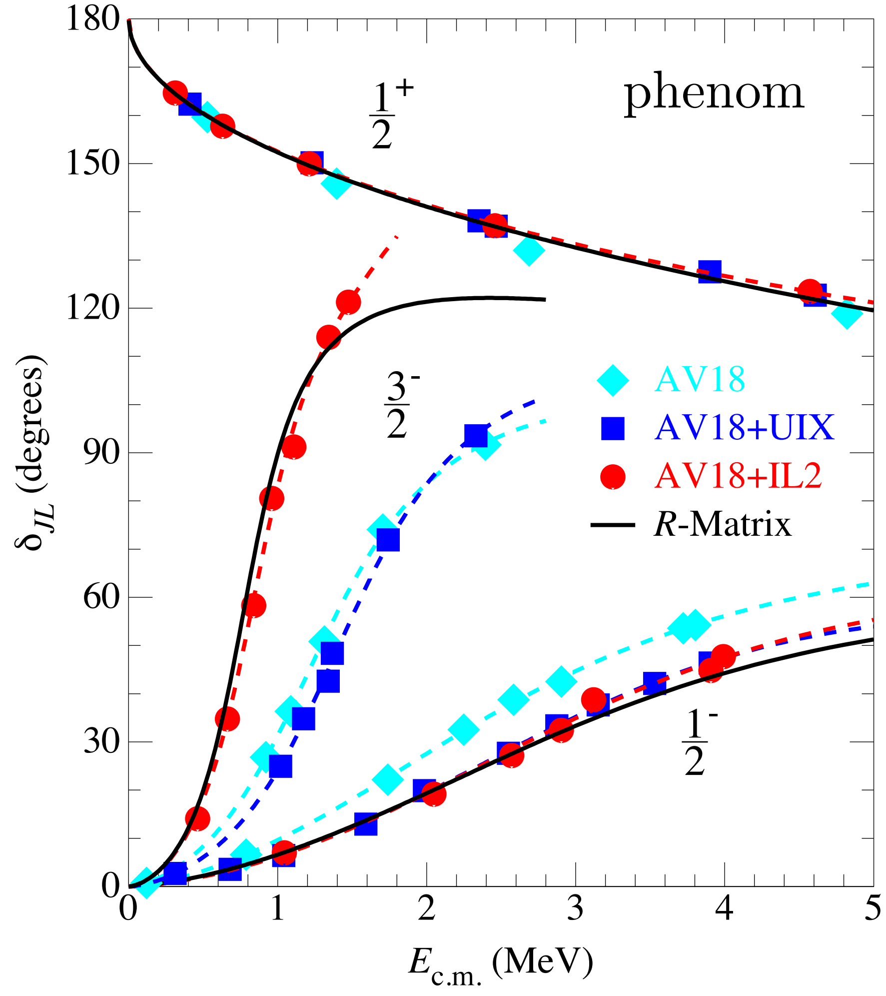
Local chiral potentials & QMC



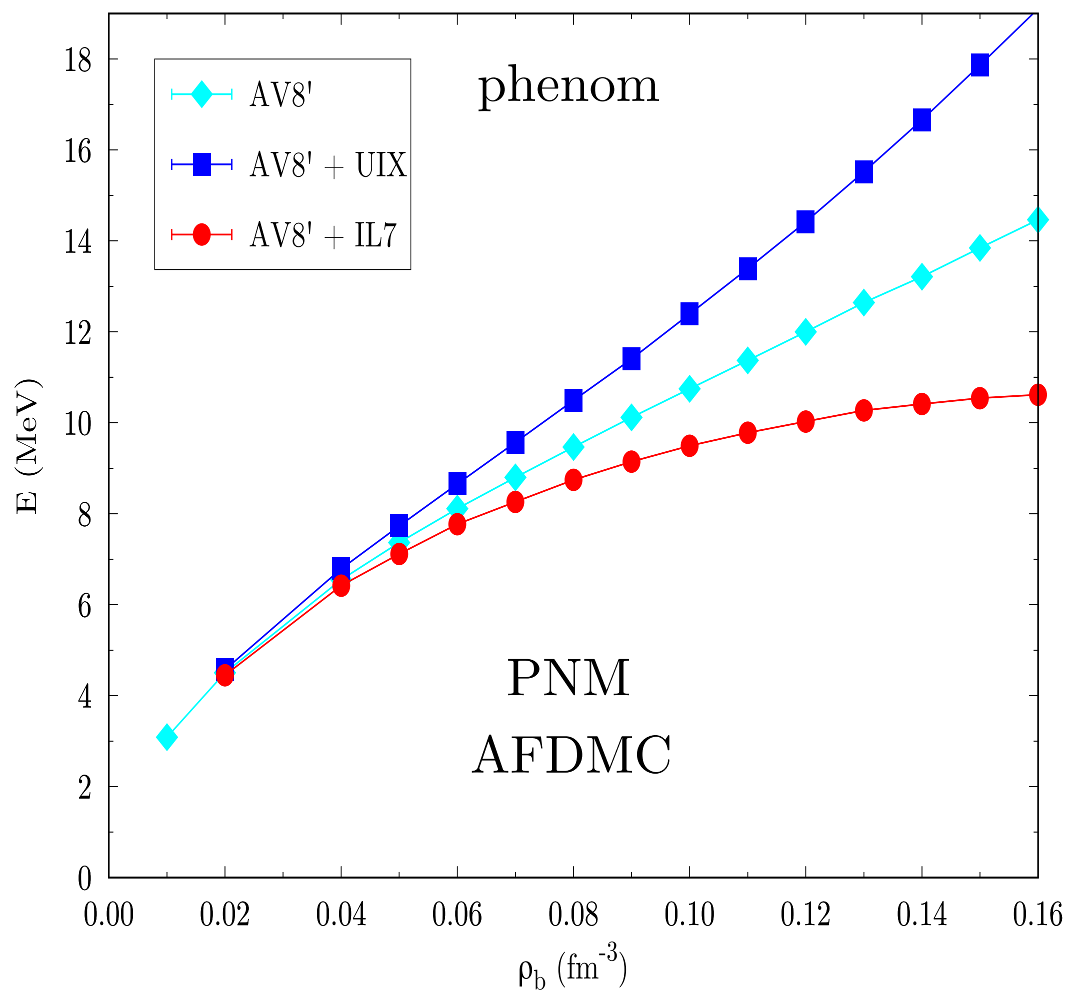
GFMC: J. E. Lynn *et al.*, Phys. Rev. Lett. **113**, 192501 (2014) & Phys. Rev. Lett. **116**, 062501 (2016)



GFMC: J. E. Lynn *et al.*, Phys. Rev. Lett. **113**, 192501 (2014) & Phys. Rev. Lett. **116**, 062501 (2016)



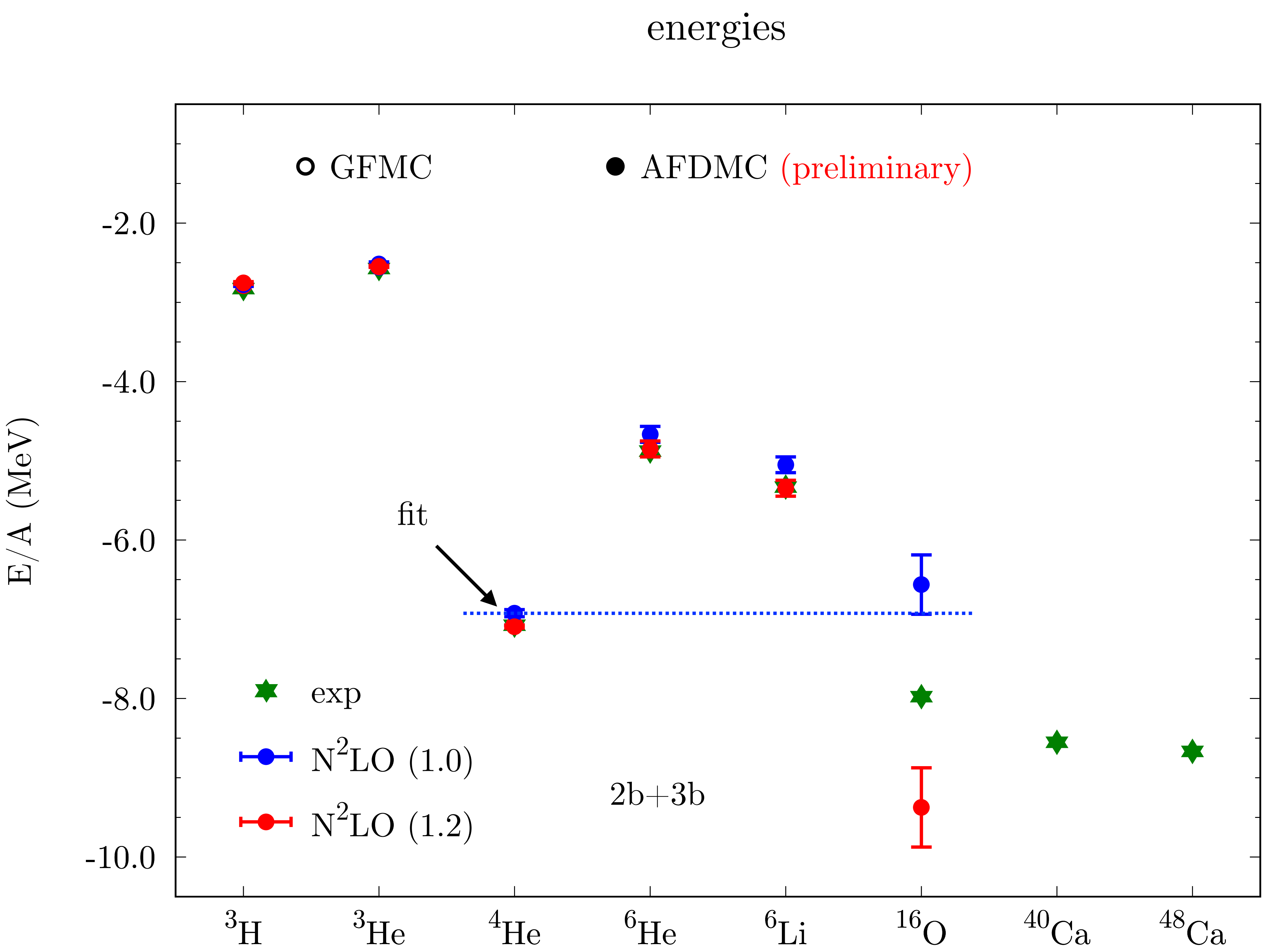
K. M. Nollett *et al.*, Phys. Rev. Lett. **99**, 022502 (2007)



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

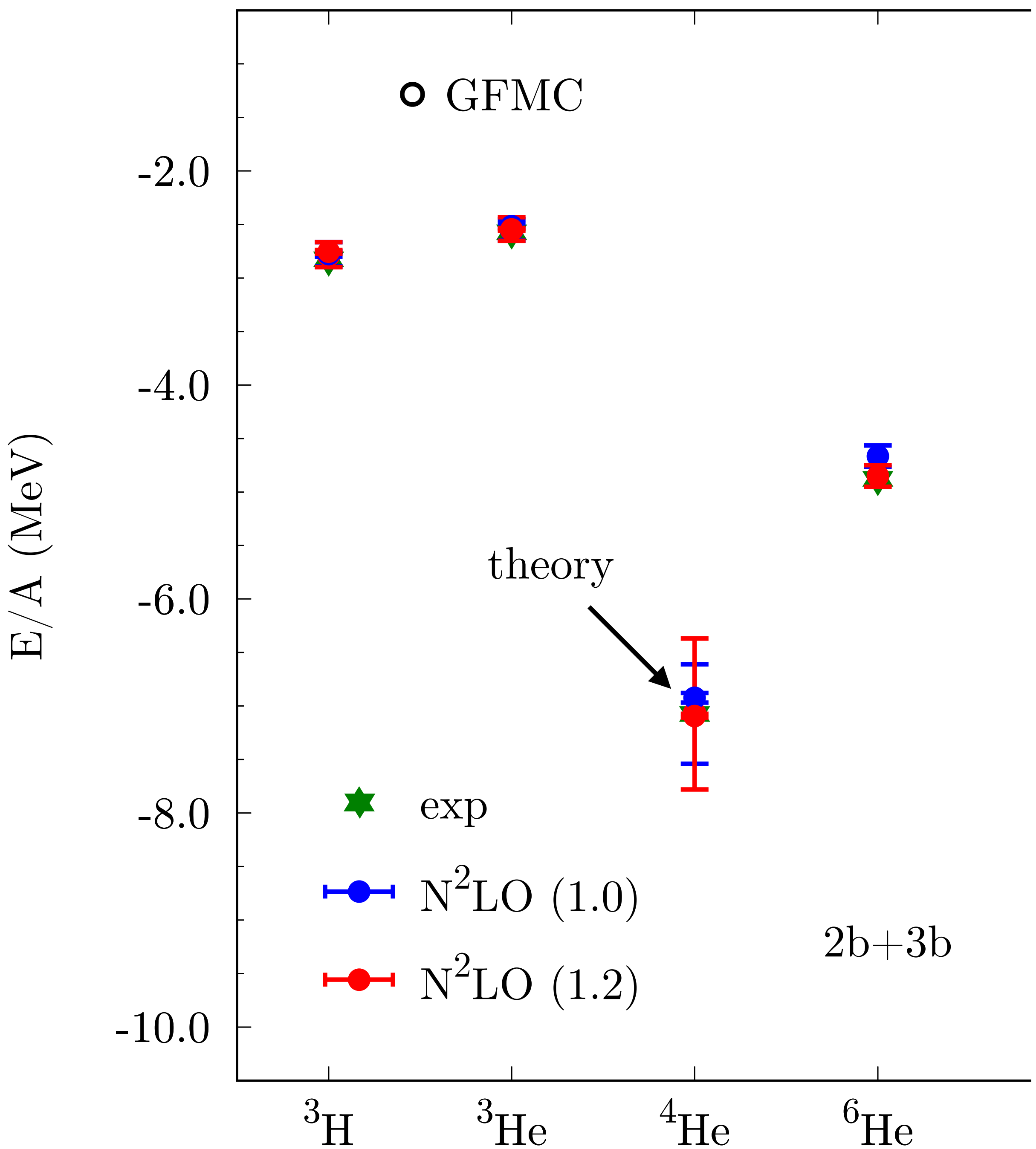
GFMC: J. E. Lynn *et al.*, Phys. Rev. Lett. **113**, 192501 (2014) & Phys. Rev. Lett. **116**, 062501 (2016)

Local chiral potentials & QMC

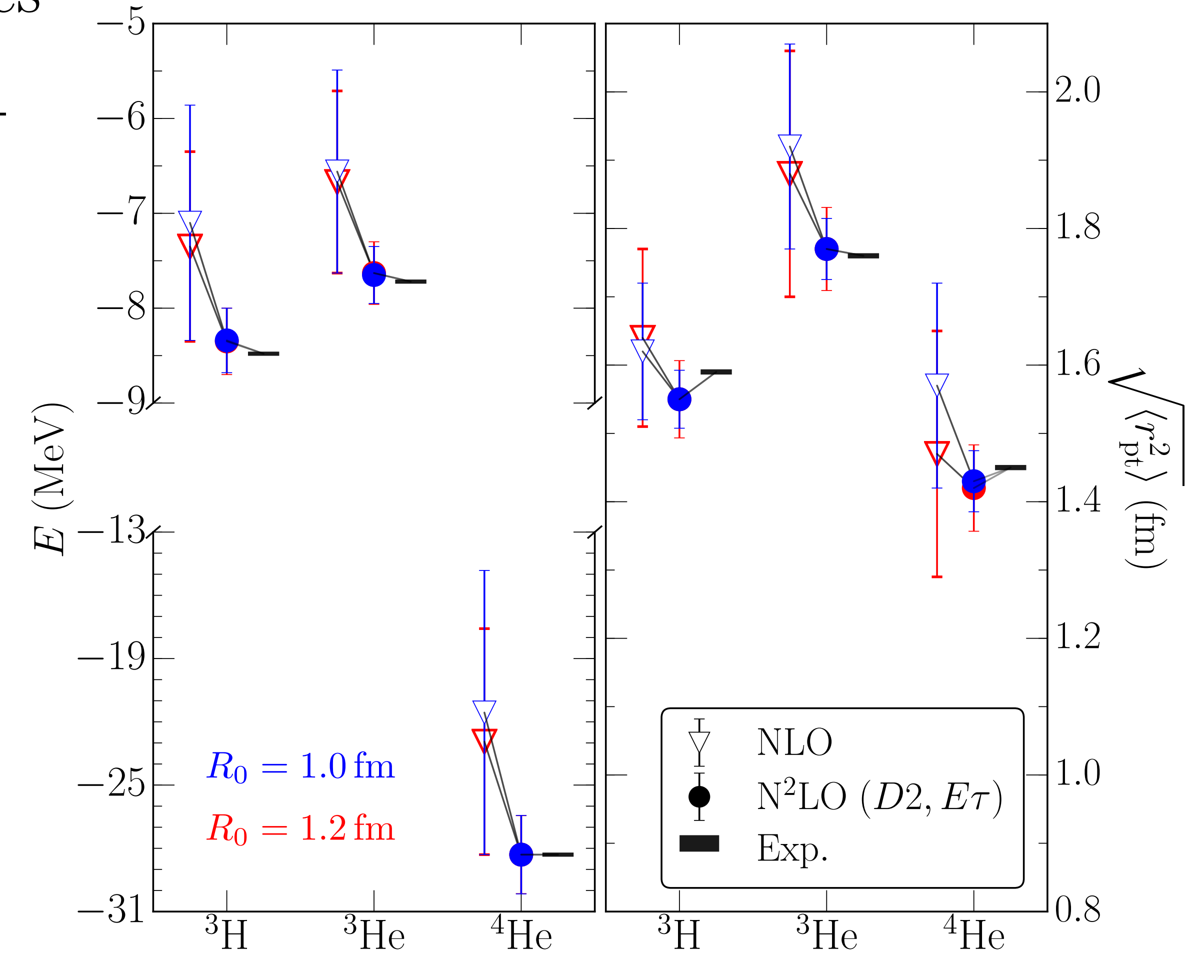


GFMC: J. E. Lynn *et al.*, Phys. Rev. Lett. **113**, 192501 (2014) & Phys. Rev. Lett. **116**, 062501 (2016)

Local chiral potentials & QMC



energies



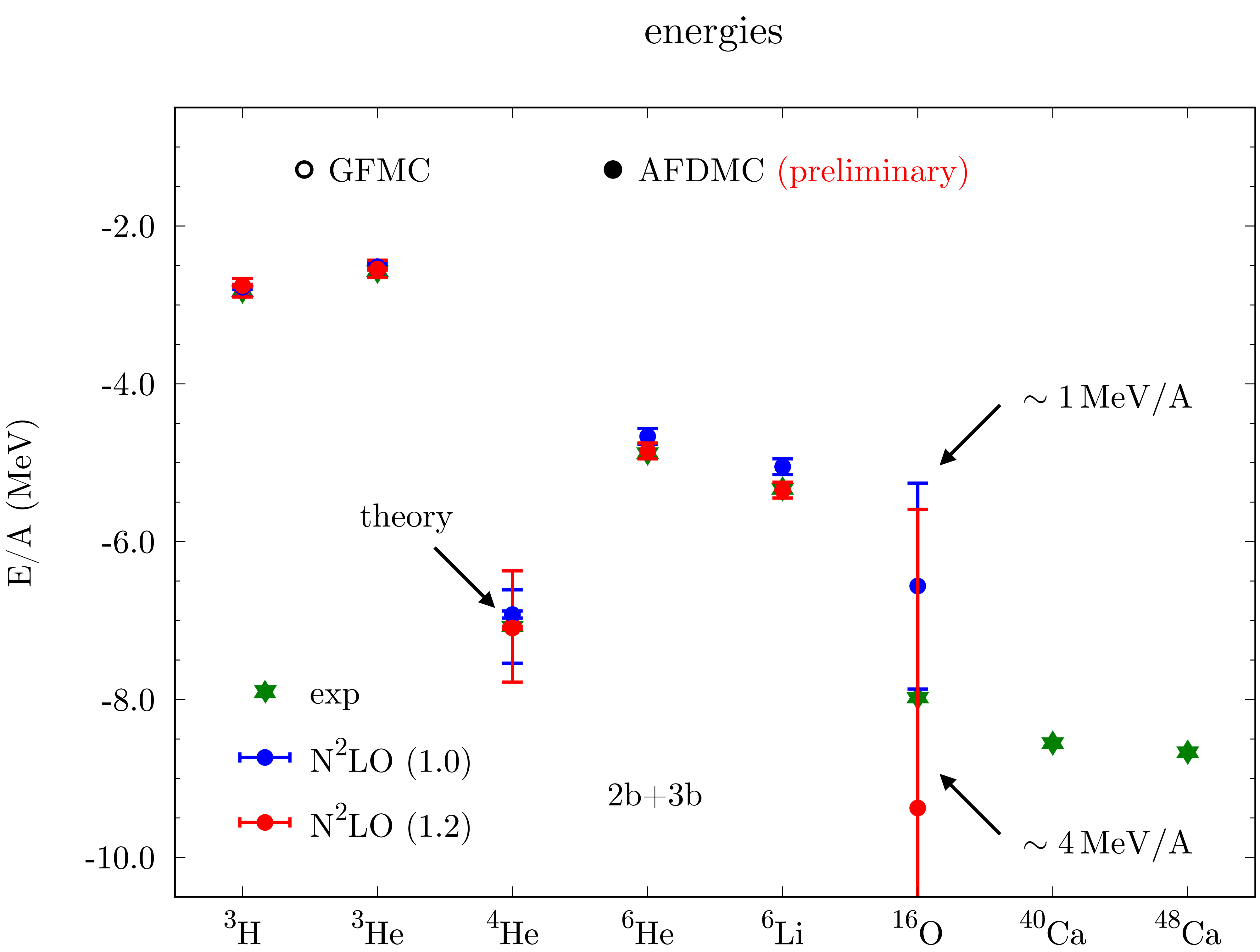
$$\Delta X^{\rm N^2LO} \sim \max\Big(Q^4 \cdot \left|X^{\rm LO}\right| ,\; Q^2 \cdot \left|X^{\rm LO} - X^{\rm NLO}\right| ,\; Q \cdot \left|X^{\rm NLO} - X^{\rm N^2LO}\right| \Big)$$

$$Q \sim \frac{m_\pi}{\Lambda_b}$$

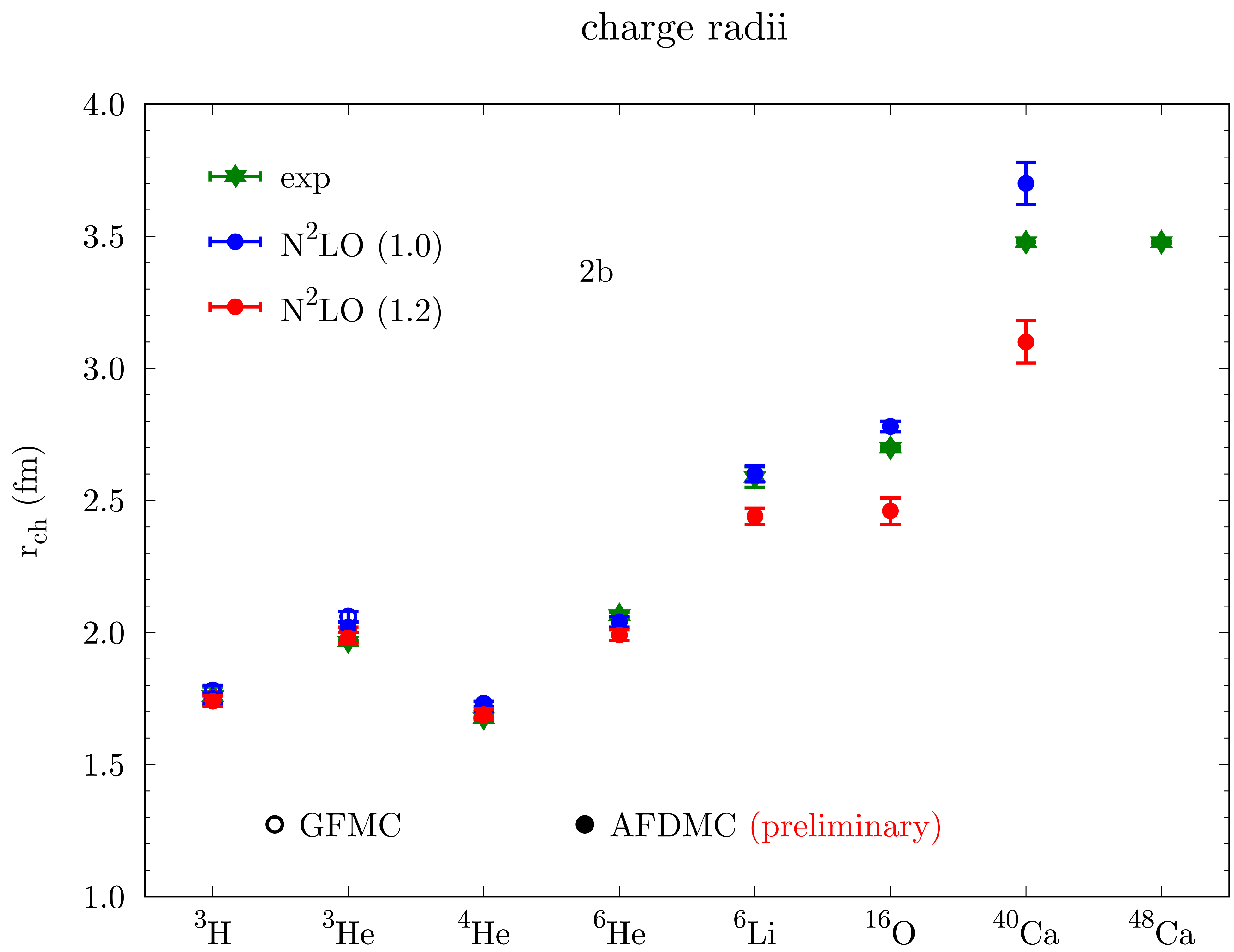
E. Epelbaum *et al.*, Eur. Phys. J. A **51** (2015)

GFMC: J. E. Lynn *et al.*, Phys. Rev. Lett. **113**, 192501 (2014) & Phys. Rev. Lett. **116**, 062501 (2016)

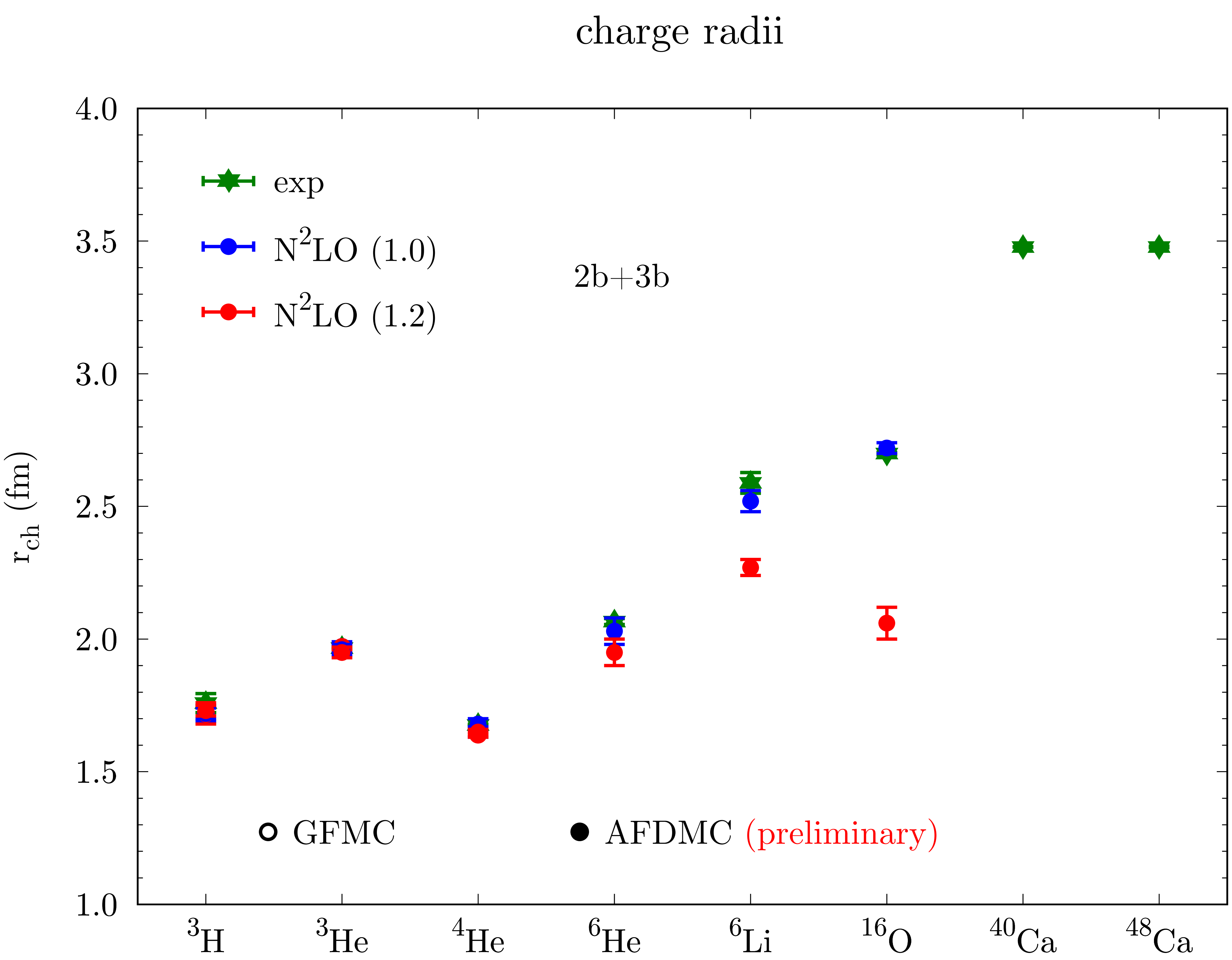
Local chiral potentials & QMC



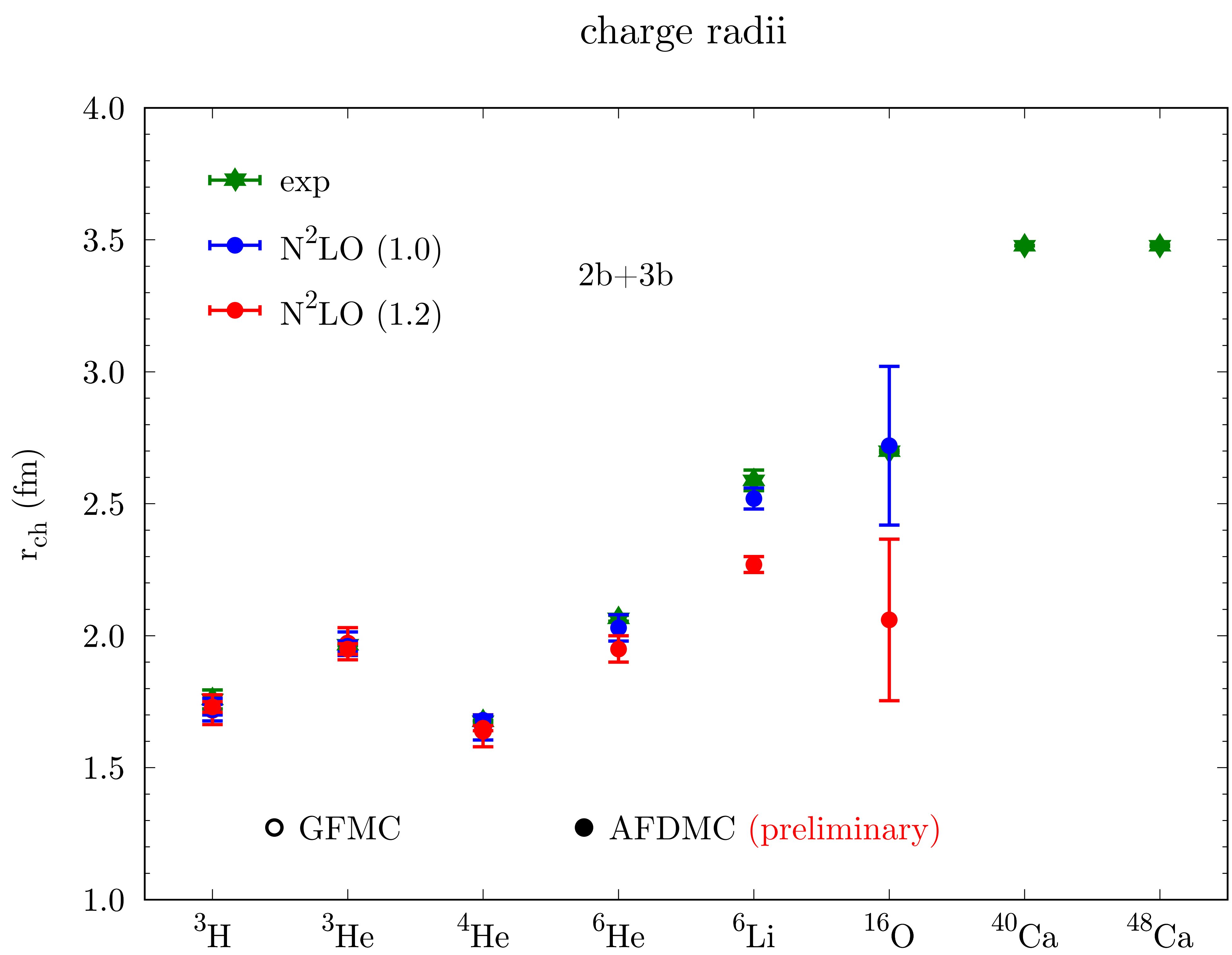
GFMC: J. E. Lynn *et al.*, Phys. Rev. Lett. **113**, 192501 (2014) & Phys. Rev. Lett. **116**, 062501 (2016)



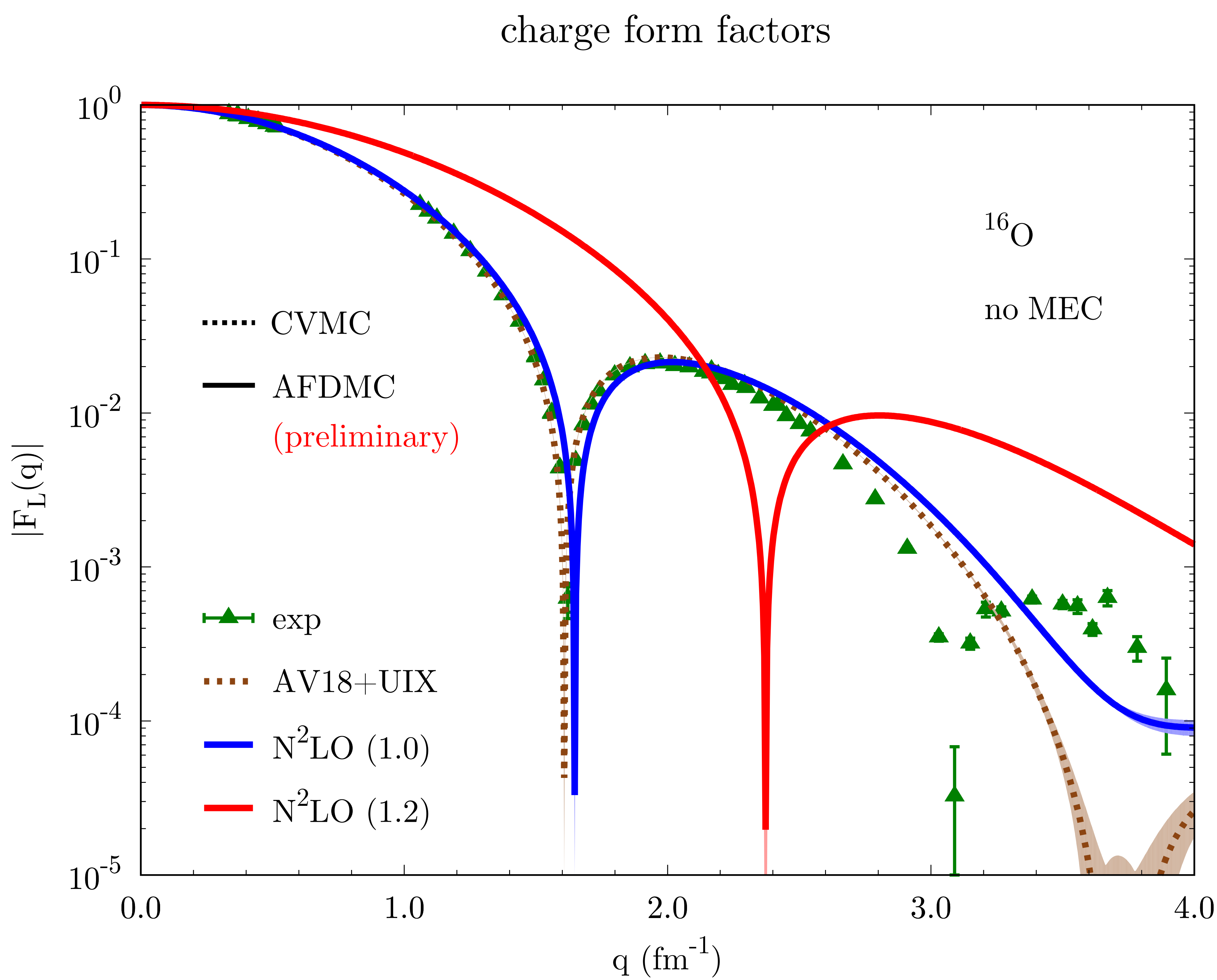
GFMC: J. E. Lynn *et al.*, Phys. Rev. Lett. **113**, 192501 (2014) & Phys. Rev. Lett. **116**, 062501 (2016)



GFMC: J. E. Lynn *et al.*, Phys. Rev. Lett. **113**, 192501 (2014) & Phys. Rev. Lett. **116**, 062501 (2016)

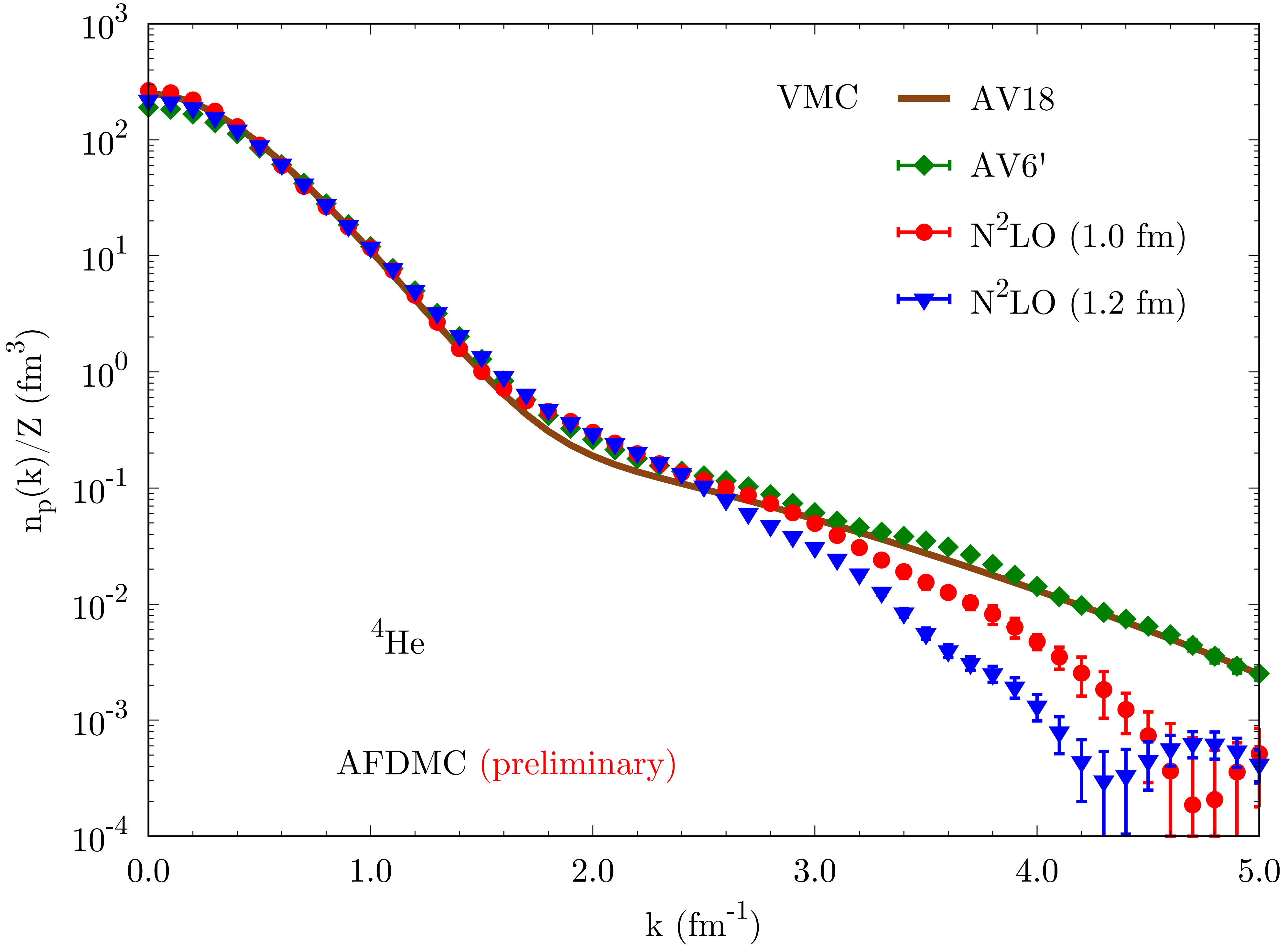


GFMC: J. E. Lynn *et al.*, Phys. Rev. Lett. **113**, 192501 (2014) & Phys. Rev. Lett. **116**, 062501 (2016)



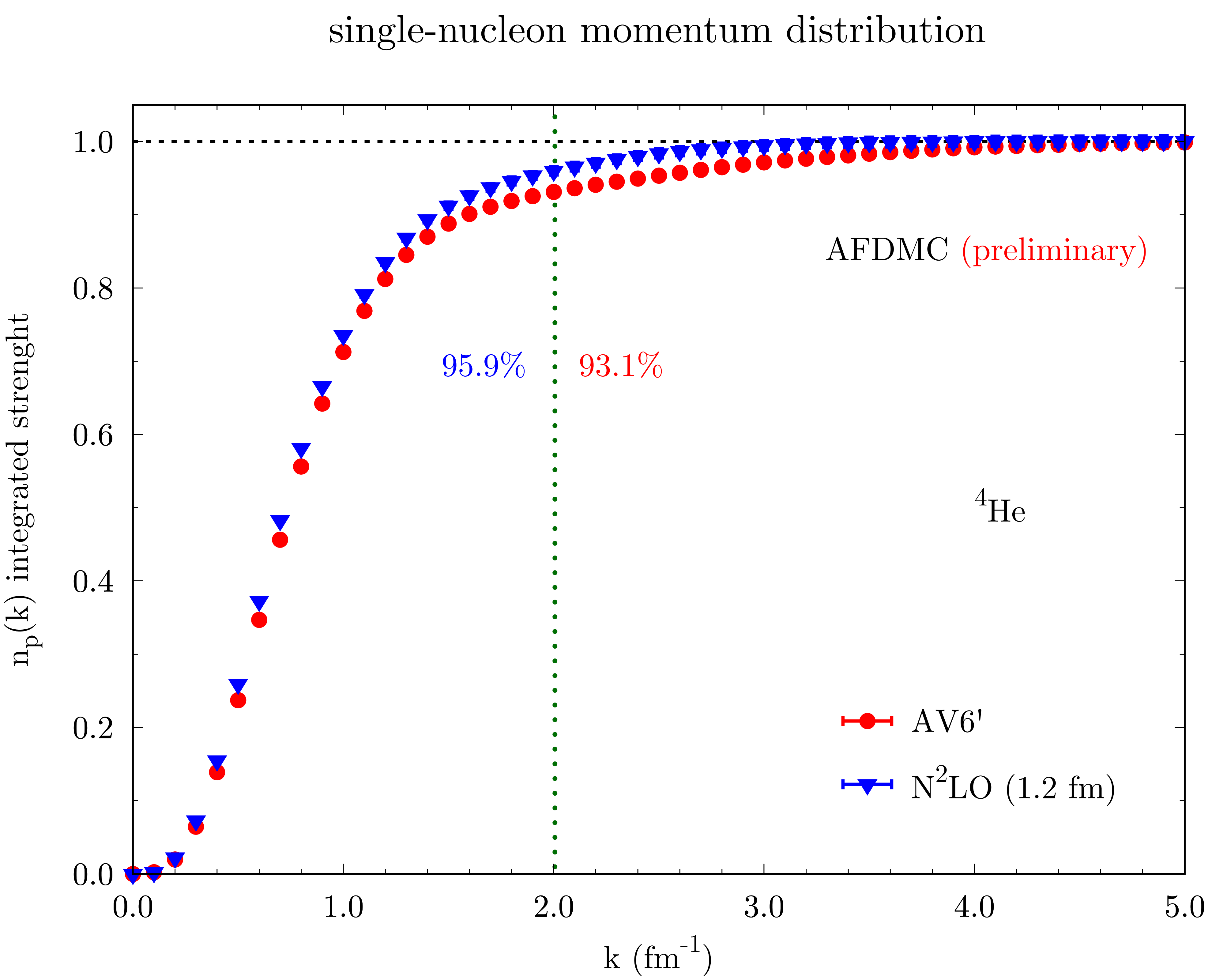
CVMC: D.L., A. Lovato, S. C. Pieper, R. B. Wiringa, arXiv:1705.04337

single-nucleon momentum distribution

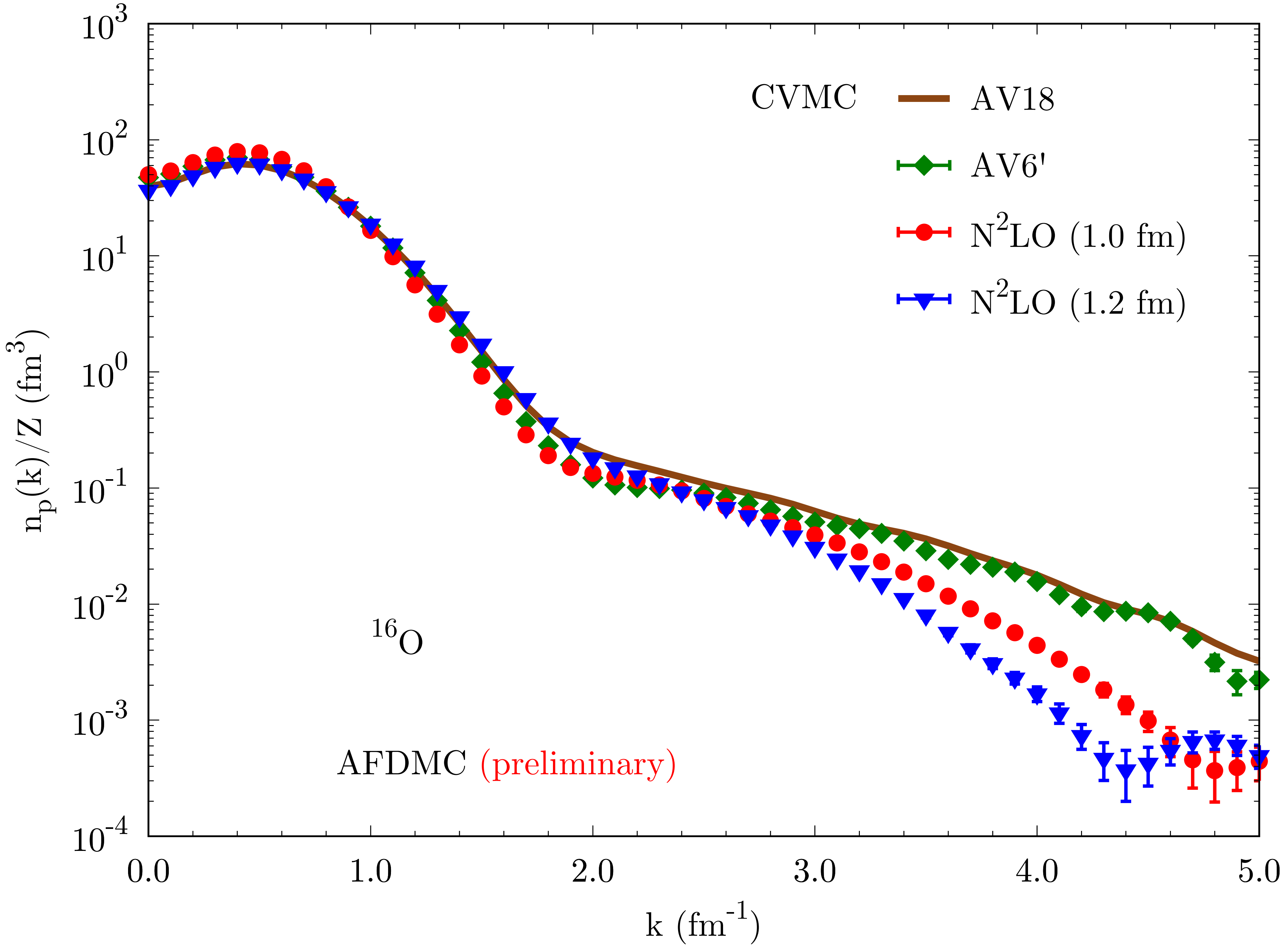


VMC: R. B. Wiringa *et al.*, Phys. Rev. C **89**, 024305 (2014)

Local chiral potentials & QMC



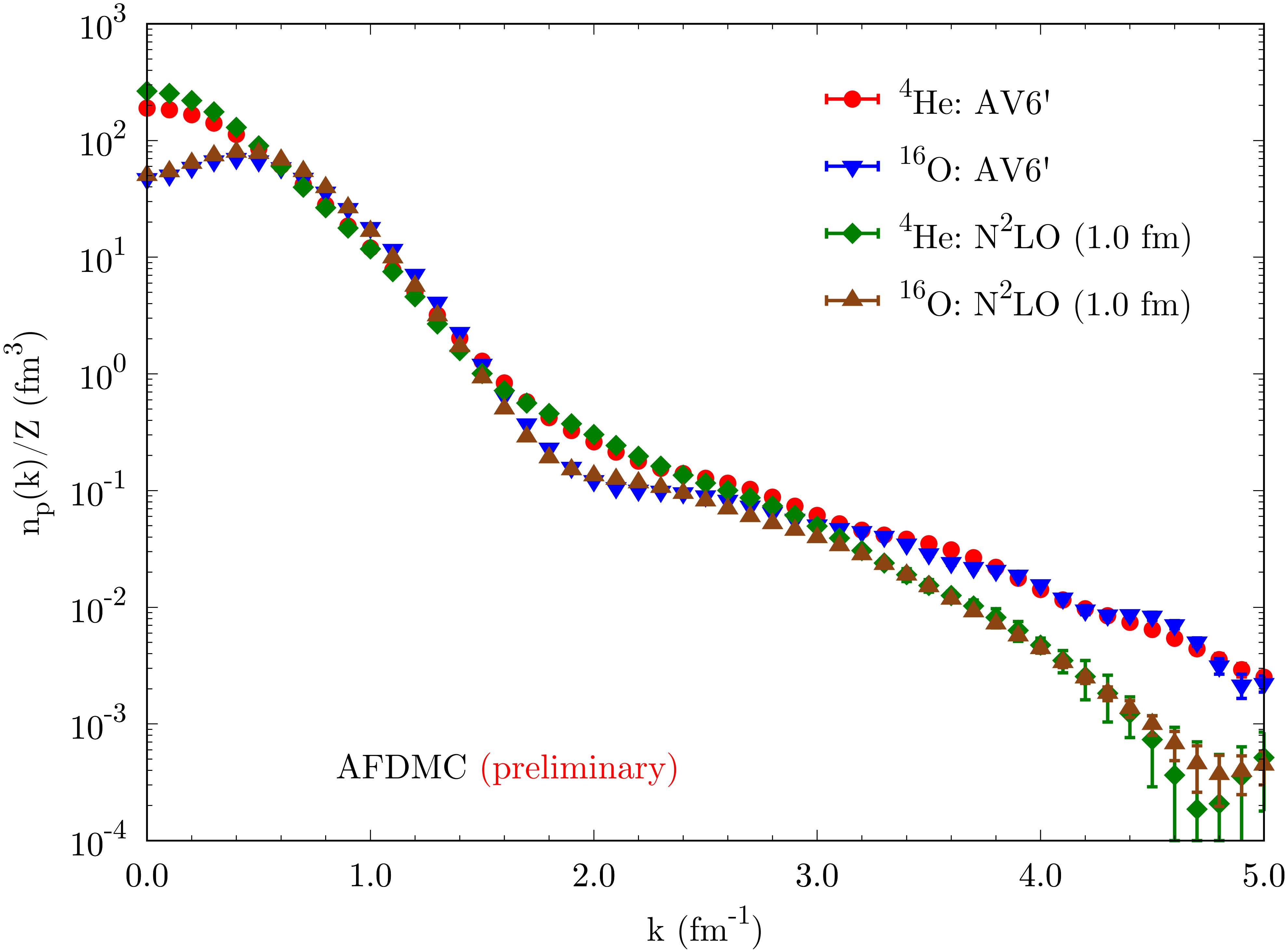
single-nucleon momentum distribution



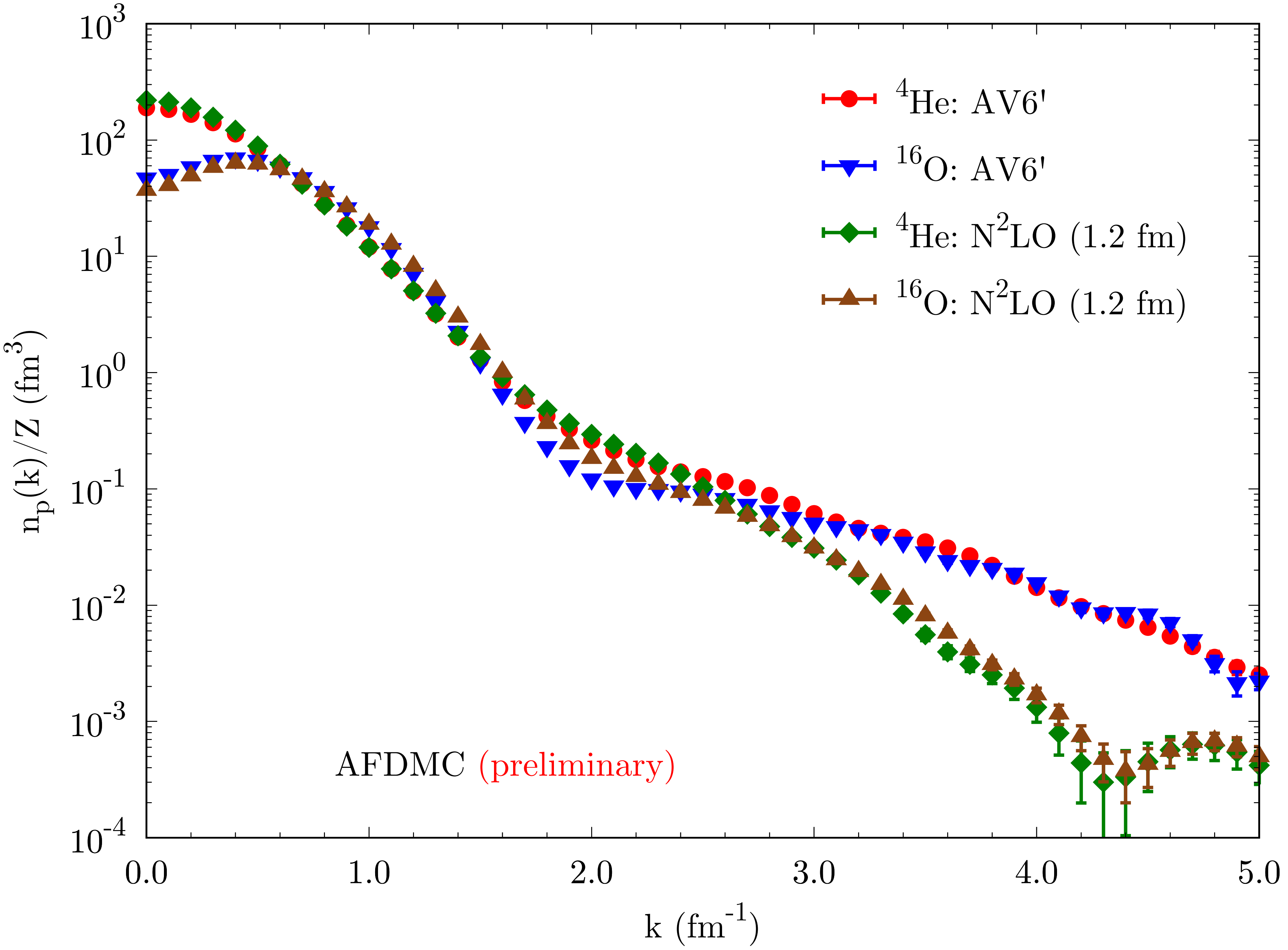
CVMC: D.L., A. Lovato, S. C. Pieper, R. B. Wiringa, arXiv:1705.04337

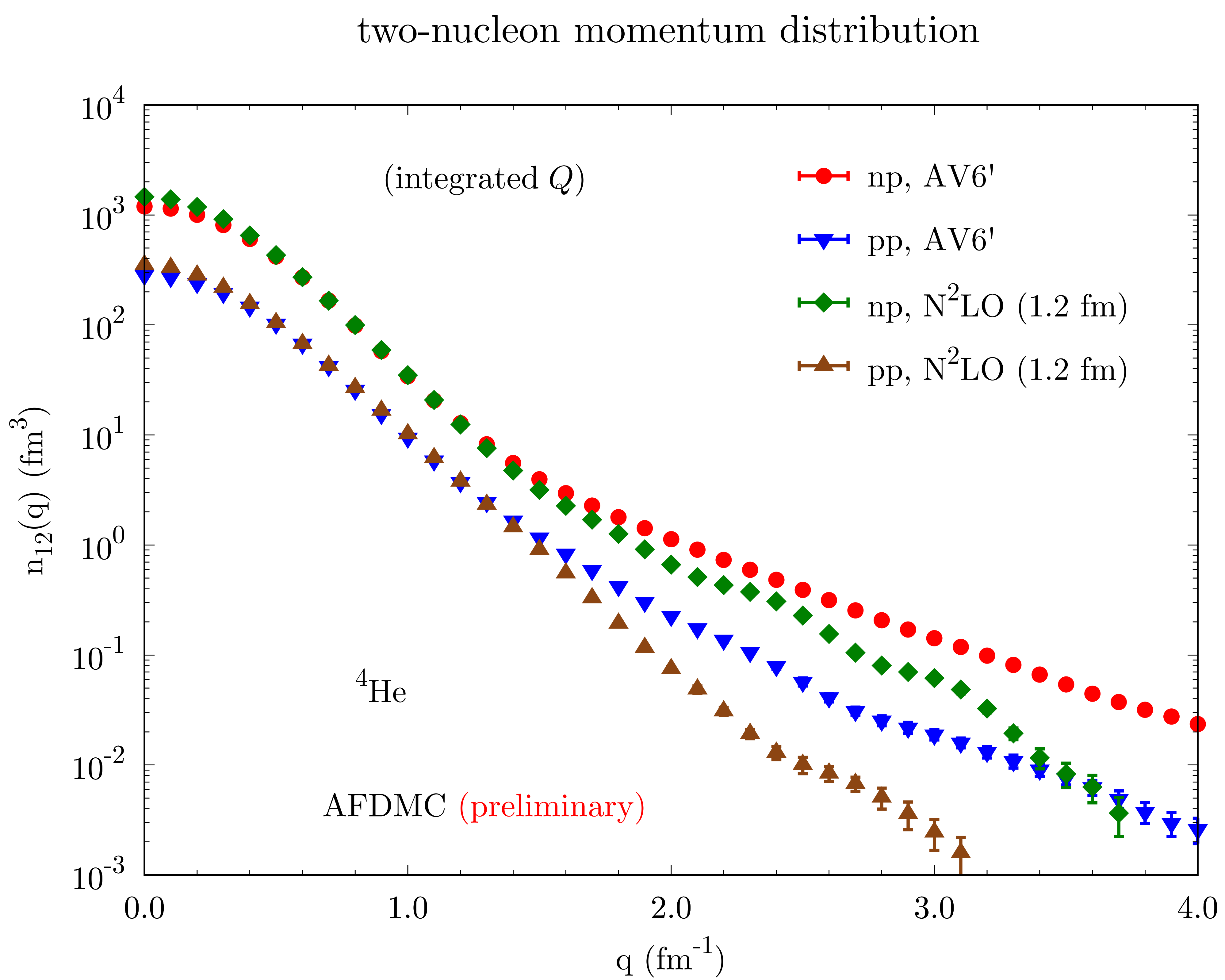
Local chiral potentials & QMC

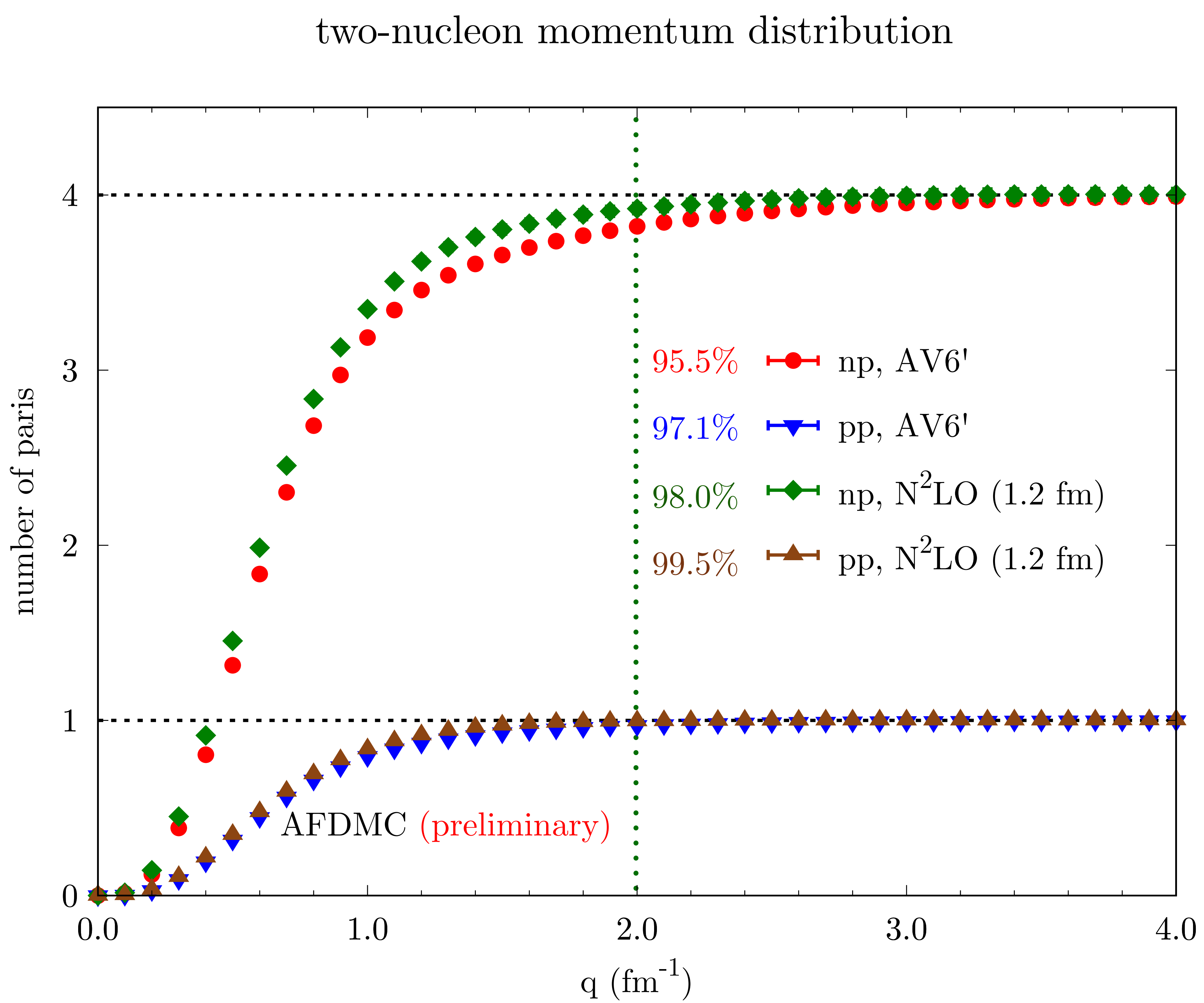
single-nucleon momentum distribution

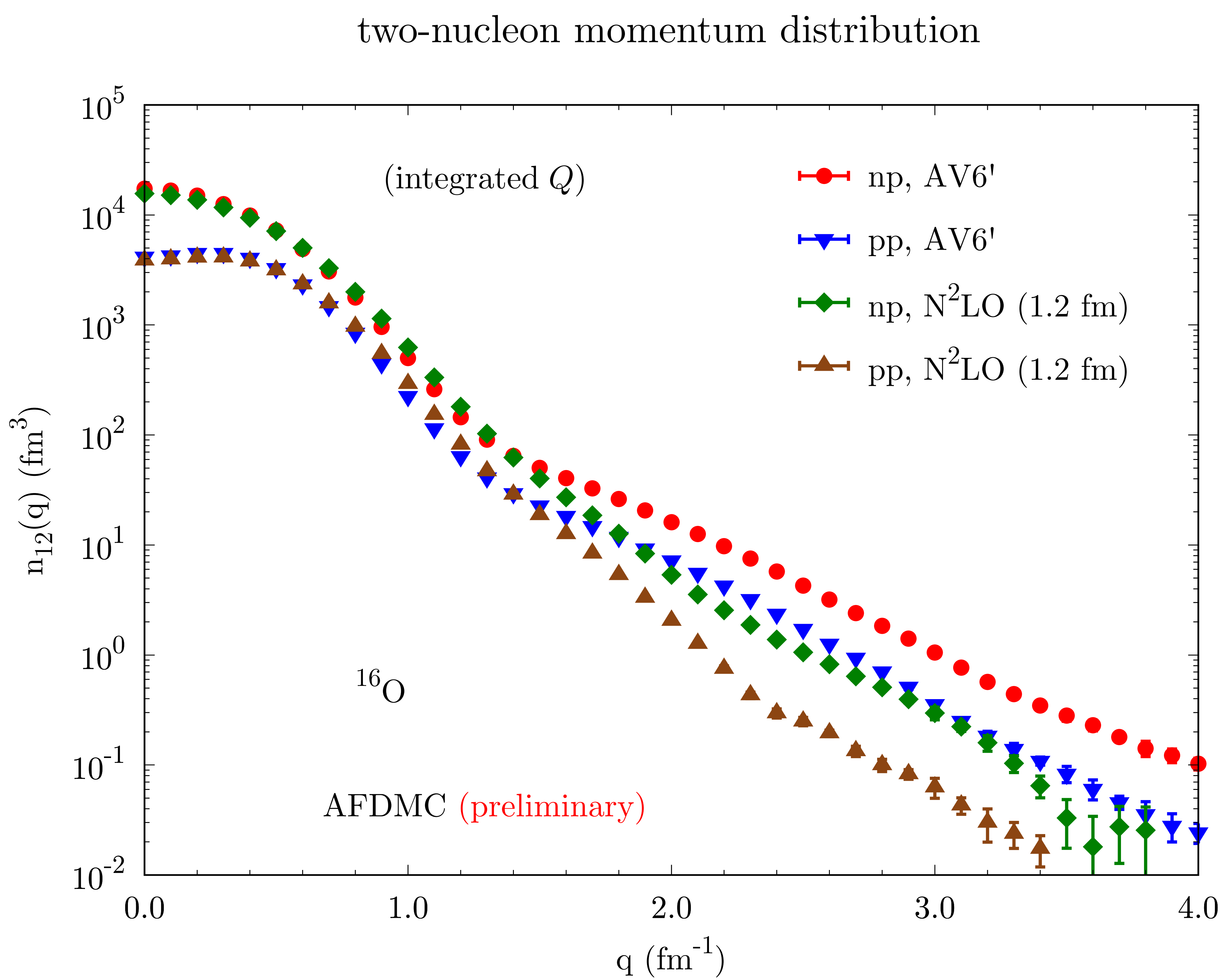


single-nucleon momentum distribution




two-nucleon momentum distribution
(integrated Q)
np, AV6'
pp, AV6'
np, N^{2}LO (1.2 fm)
pp, N^{2}LO (1.2 fm)
^{4}He
AFDMC (preliminary)
$n_{12}(q)$ (fm^3)
q (fm^{-1})
10^4
10^3
10^2
10^1
10^0
10^{-1}
10^{-2}
10^{-3}
0.0
1.0
2.0
3.0
4.0


two-nucleon momentum distribution
number of paris
q (fm-1)
95.5% np, AV6'
97.1% pp, AV6'
98.0% np, N2LO (1.2 fm)
99.5% pp, N2LO (1.2 fm)
AFDMC (preliminary)
0
1
2
3
4
0.0
1.0
2.0
3.0
4.0

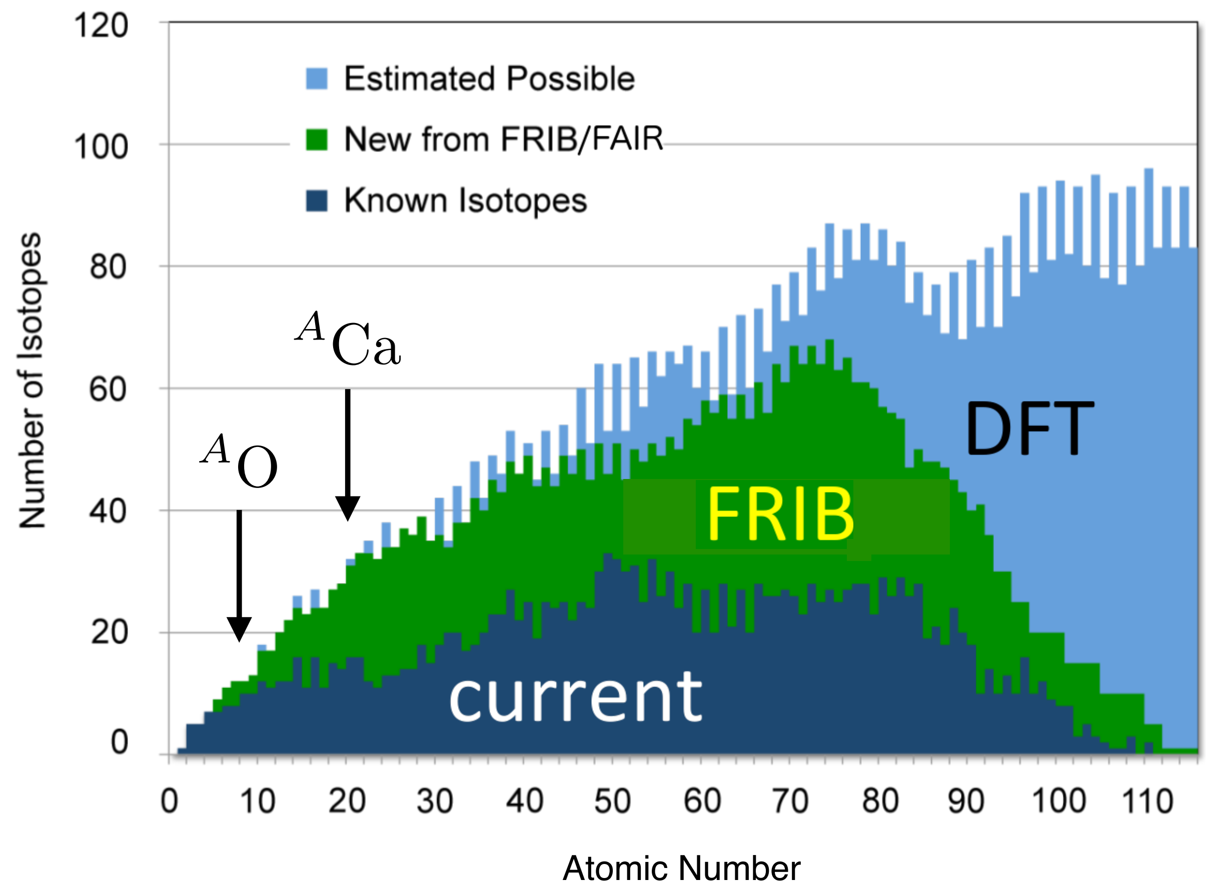

two-nucleon momentum distribution
(integrated Q)
np, AV6'
pp, AV6'
np, N2LO (1.2 fm)
pp, N2LO (1.2 fm)
16O
AFDMC (preliminary)
n12(q) (fm3)
q (fm-1)
10-2
10-1
100
101
102
103
104
105
0.0
1.0
2.0
3.0
4.0

Conclusions

progresses in QMC calculations → moving towards an "exact" description of the medium region of the nuclear chart

✓ CVMC
- ground state properties of closed-shell nuclei up to A=40
- investigation of phenomenological forces above A=16

✓ AFDMC
- ground state properties of light- and medium-heavy nuclei with delta-less local chiral potentials at N^2LO
- investigation of local chiral forces



adapted from A. B. Balantekin *et al.*, Mod. Phys. Lett. A **29**, 1430010 (2014)

Next:
- complete the study at N^2LO including truncation errors & other 3-body forms
- N^3LO? employ delta-full local chiral potentials?
- symmetric nuclear matter? neutron matter delta-full?
- currents? single- and double-beta decay?