Chiral forces and quantum Monte Carlo: from nuclei to neutron star matter

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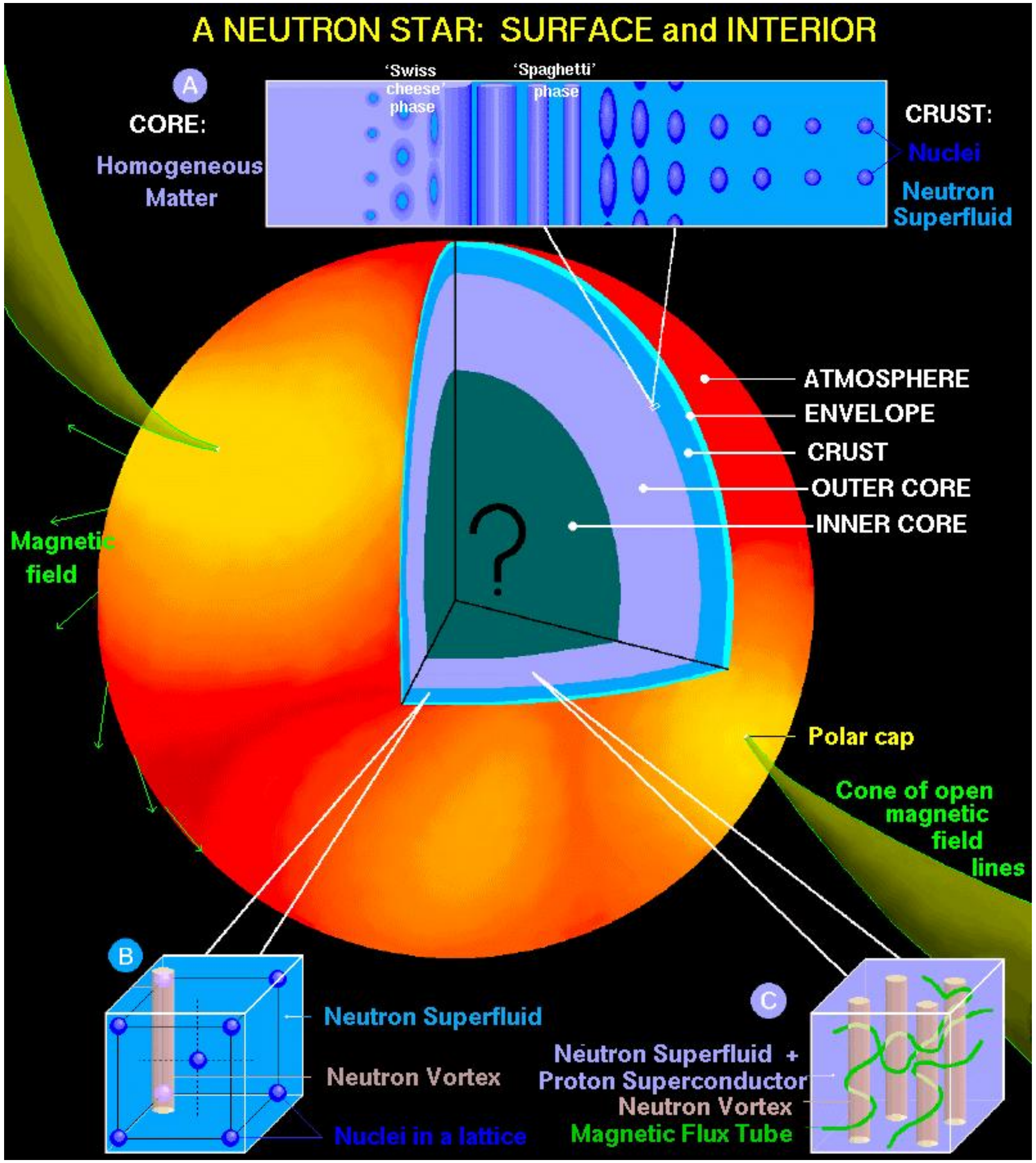
Introduction



curtesy of Dany Page

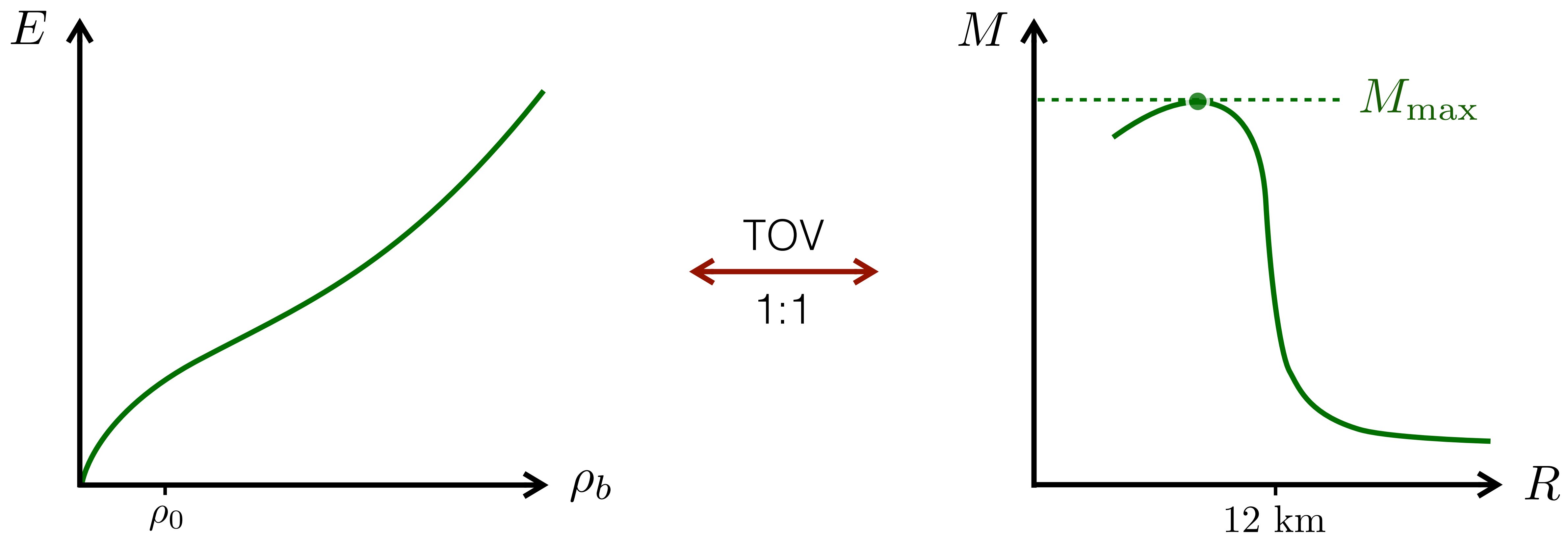
Neutron Star (NS): compact objects made mostly by neutrons

$$R \sim 12\,\mathrm{km}$$

$$M \sim 1.4\,M_\odot$$

- atmosphere: atomic and plasma physics
- outer crust: physics of superfluids (neutrons, vortex), solid state physics (nuclei)
- inner crust: deformed nuclei, pasta phase
- outer core: nuclear matter
- inner core: hyperons?? quark matter?? condensates (π, K)?? …?

The hydrostatic equilibrium of a static spherically symmetric star is given by the solution of Tolman-Oppenheimer-Volkoff equations (TOV): derivation of static properties of the stars like mass and radius



Note: for a given EOS the solution of the TOV is unique!! unique $M(R)$ relation!!

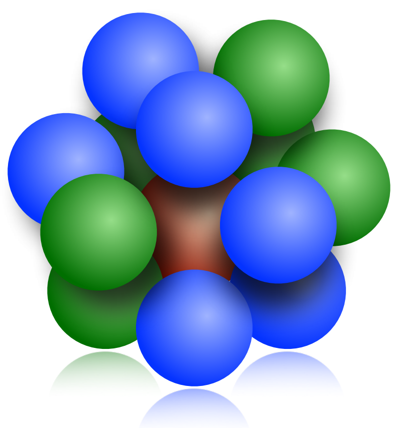
if you know the EOS you can predict the maximum mass and compare with observations

Problem: do we know the EOS?? not really…

but: EOS for NS: energy/pressure of a nuclear medium → nuclear interactions!!

Introduction

nuclei



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

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

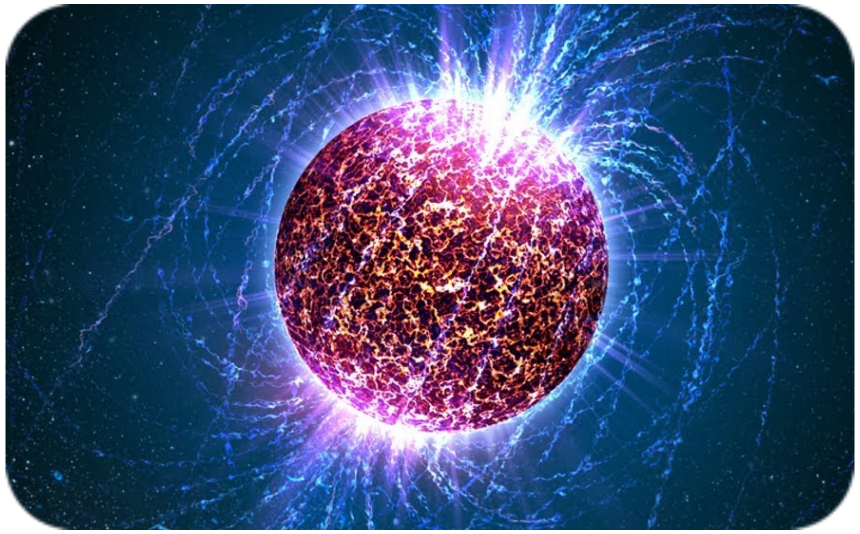
same underlying physics!!

$\longleftrightarrow$

nuclear interactions

look at experiments & observations

neutron stars



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

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

- ✓ Introduction
  - Quantum Monte Carlo methods & Nuclear Hamiltonians
- ✓ Moving towards medium-mass nuclei
  - AFDMC & chiral forces
  - Preliminary results: binding energies & radii
  - Preliminary results: single- & two-nucleon momentum distributions
- ✓ Future directions and conclusions

Quantum Monte Carlo methods

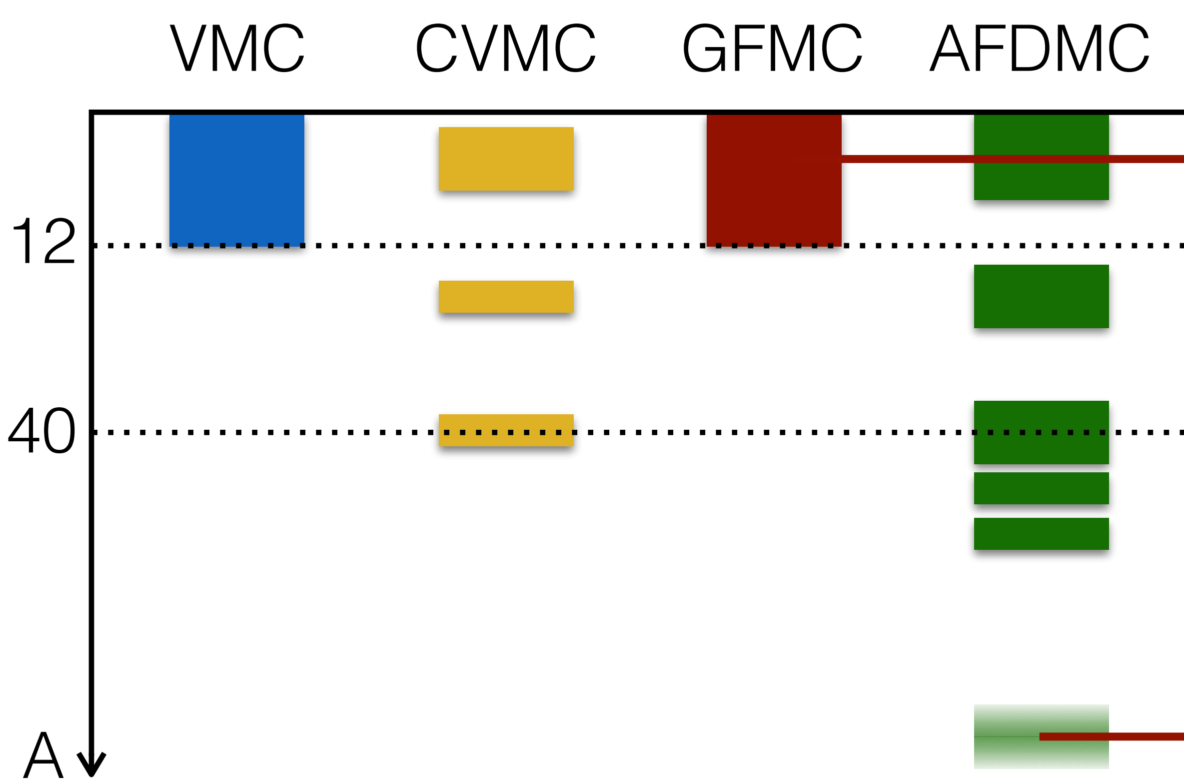
Goal: solve the many-body problem for correlated systems in a non-perturbative fashion

- ✓ **VMC, GFMC**: sampling in coordinate space
  - ⟶ reduced number of nucleons: A=12
- ✓ **CVMC**: sampling in coordinate space + cluster expansion
  - ⟶ closed shell nuclei (+/-1): A=40
- ✓ **AFDMC**: sampling in coordinate & spin-isospin space
  - ⟶ large number of nucleons

w.f. with 2-body & 3-body correlations

real-space (but not only)

local forces (possibly)



GFMC: light systems $A \leq 12$

AFDMC: light to medium-heavy nuclei $A \sim 50$

AFDMC: nuclear matter $A = \infty$

Nuclear Hamiltonians

Model: non-relativistic nucleons interacting with an effective nucleon-nucleon (NN) force and 3-nucleon interaction (NNN)

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

v_{ij} fitted on NN scattering data & deuteron

v_{ijk} fitted on properties of (light) nuclei (+constraints)

Focus on two families of nuclear interactions:

✓ Real-space, local (mostly), phenomenological: Argonne (NN) + Urbana-Illinois (NNN)

✓ Momentum-space, non-local, chiral effective field theory: X-EFT (NN+NNN+…)

Note: local vs non-local

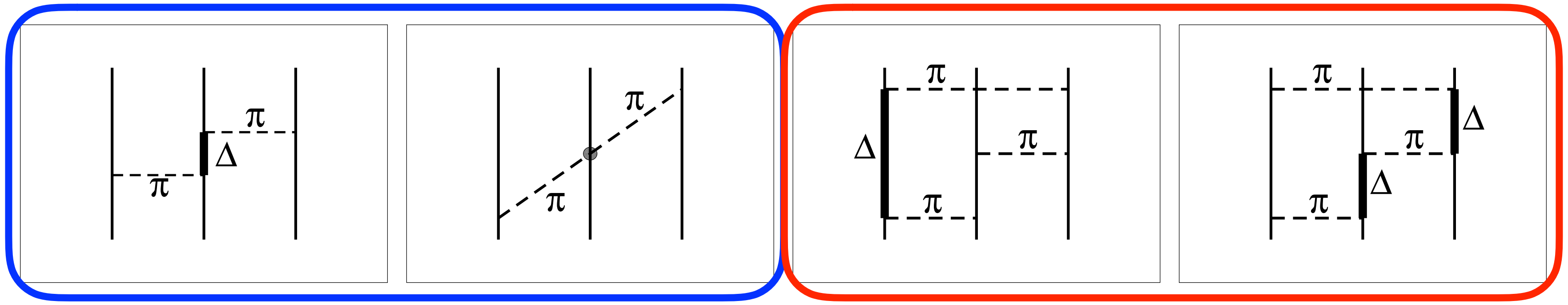
$$\begin{cases} \boldsymbol{p} = (\boldsymbol{p}_1 - \boldsymbol{p}_2)/2 \\ \boldsymbol{p}' = (\boldsymbol{p}'_1 - \boldsymbol{p}'_2)/2 \end{cases} \qquad \begin{cases} \boldsymbol{q} = \boldsymbol{p}' - \boldsymbol{p} & \text{local} \longrightarrow \boldsymbol{r} \\ \boldsymbol{k} = (\boldsymbol{p}'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

Nuclear Hamiltonians: phenomenological potentials

NN: Argonne AV18 (AV8')

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

NNN: Urbana-Illinois



+ short-range term

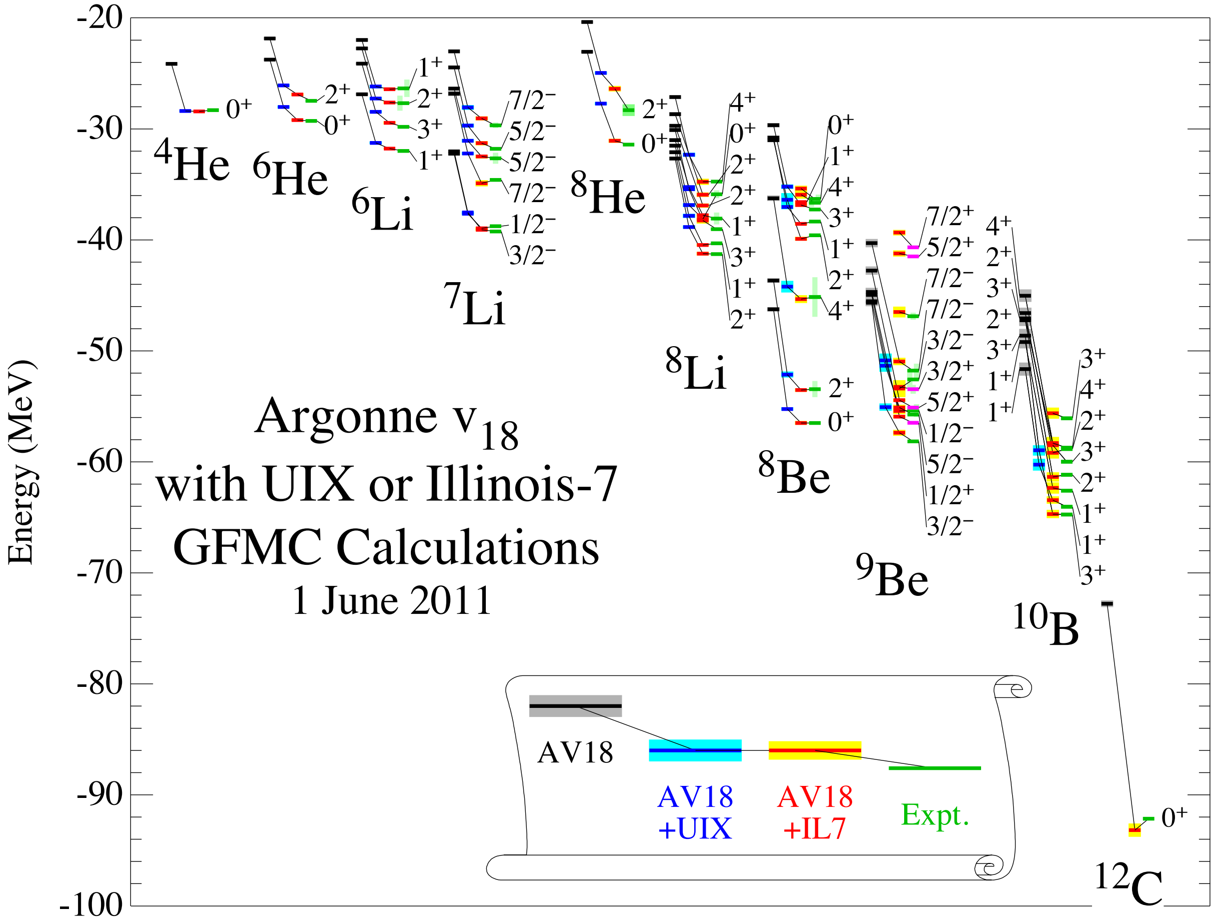
Pros:

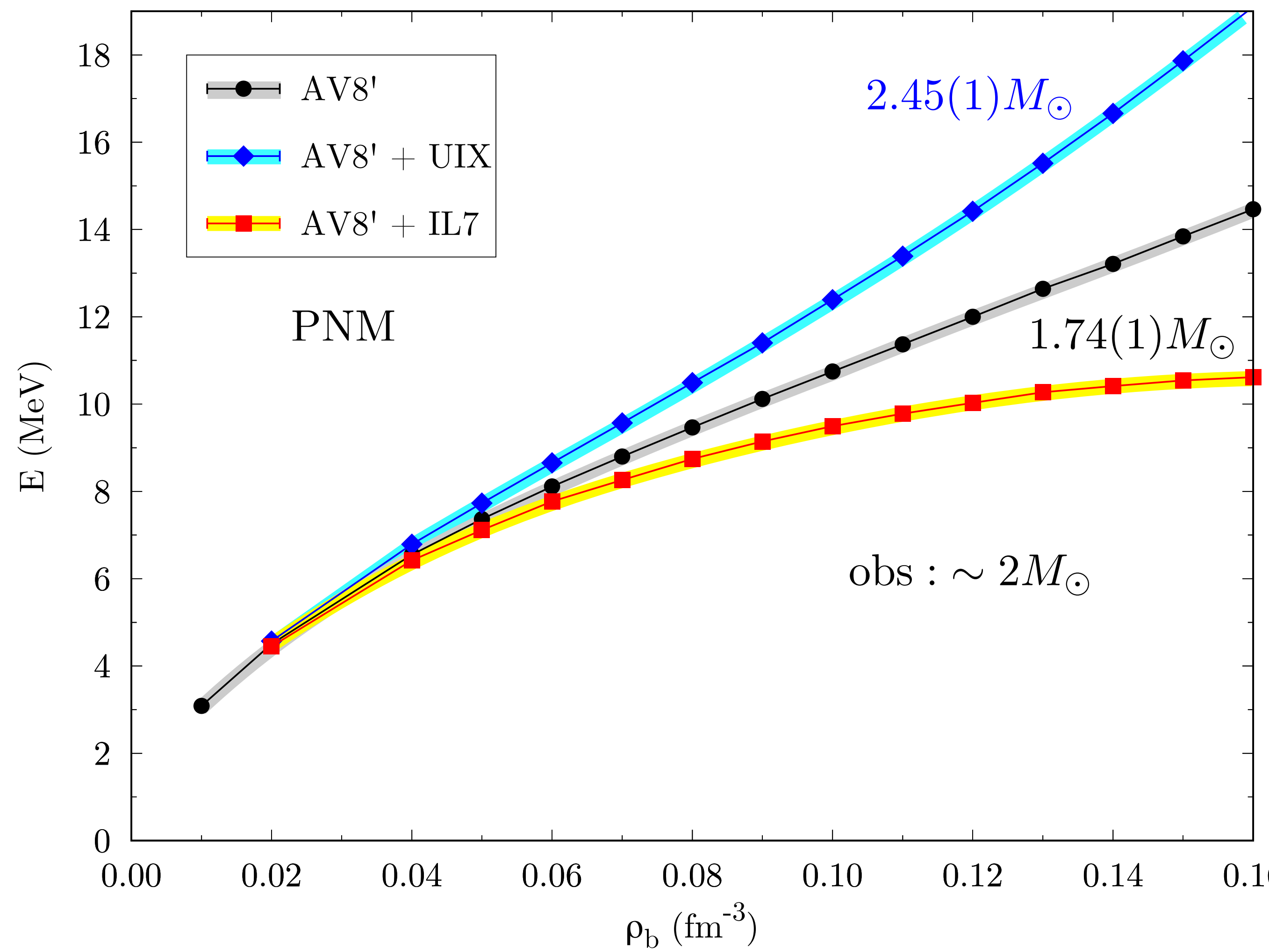
- Argonne interactions fit phase shifts up to high energies. Accurate up to (at least) 2-3 saturation density.
- Suitable for QMC calculations. Very good description of several observables in light nuclei (GFMC ground-state: uncertainties within 1-2%).

Cons:

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

Nuclear Hamiltonians: phenomenological potentials





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

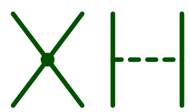
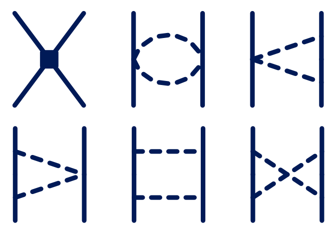
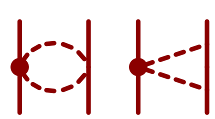
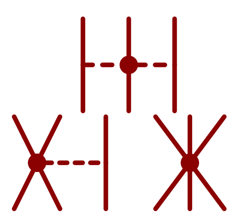
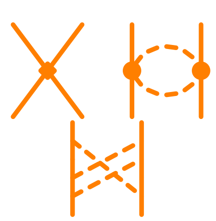
light nuclei
terrestrial experiments

how to
reconcile?

infinite matter
astrophysical observations (M, R)

- ✓ medium-mass region, neutron-rich system → AFDMC
- ✓ other framework → local chiral forces

Nuclear Hamiltonians: chiral EFT potentials

		NN	*NNN*
LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^0$		—
NLO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^2$		—
$\mathrm{N^2LO}$	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^3$		
$\mathrm{N^3LO}$	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^4$	 $+\cdots$	 $+\cdots$

- X-EFT is an expansion in powers of Q/Λ_b

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

Nuclear Hamiltonians: chiral EFT potentials

Pros:

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

Cons:

- Chiral interactions describe low-energy (momentum) physics. How do they work at large momenta?
- ~~In the standard formulation they are non-local and they are written in momentum-space. Not suitable for AFDMC calculations.~~

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)

Nuclear Hamiltonians: local chiral EFT potentials

✓ 2-body NN @ N^2LO

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

- contact terms: 2 LECs @ LO ⟶ no momentum dependence

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

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

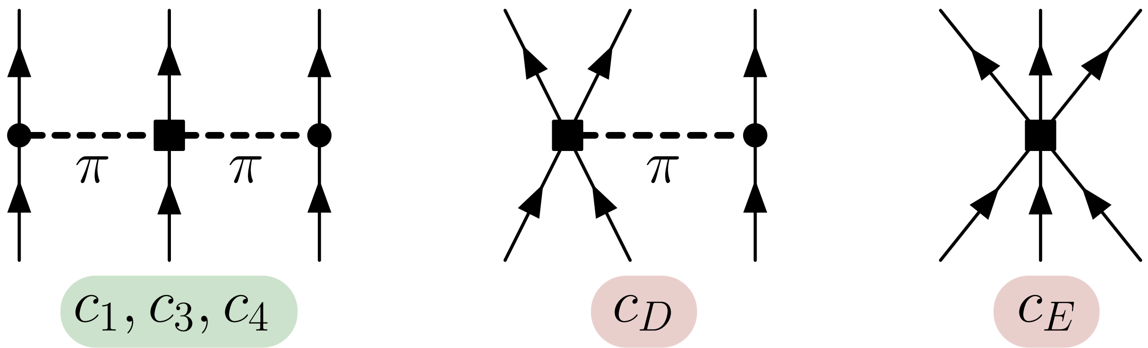
cutoff: $R_0 = 1.0 - 1.2\ \mathrm{fm}$ ⟷ momentum cutoff $\sim 500 - 400\ \mathrm{MeV}$

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

included in both GFMC
and AFDMC propagators

Nuclear Hamiltonians: local chiral EFT potentials

✓ 3-body NNN @ N^{2}LO



same as NN

need to be fit

fit on:

- $^4\mathrm{He}$ binding energy
- low-energy n-α scattering p-wave phase shifts

Note: same regulator functions and cutoff as 2-body NN

Note: finite cutoff

↓

different possible operator structures:

$$V_D \longrightarrow D1,\ D2$$

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

local!! appealing for QMC not only…

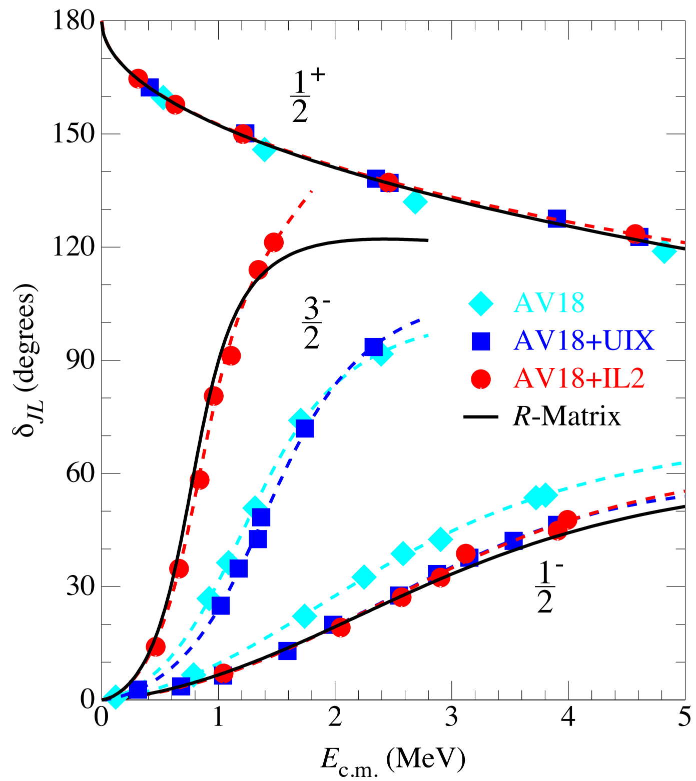
TABLE I. Fit values for the couplings c_D and c_E for different choices of $3N$ forces and cutoffs.

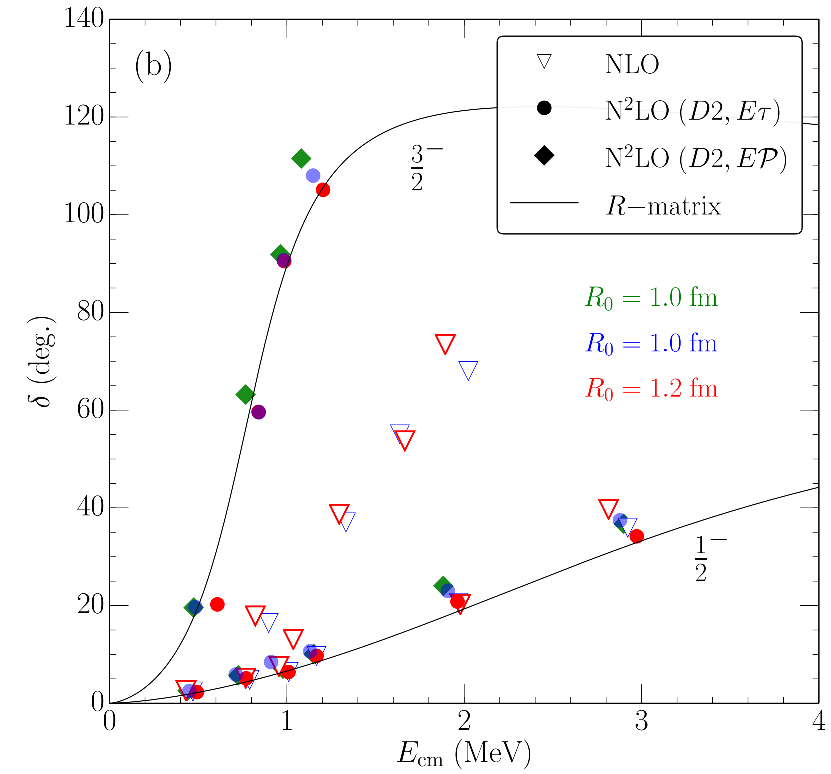
V_{3N}	R_0 (fm)	c_E	c_D
N^{2}LO $(D1, E\tau)$	1.0	−0.63	0.0
	1.2		
N^{2}LO $(D2, E\tau)$	1.0	−0.63	0.0
	1.2	0.09	3.5
N^{2}LO $(D2, E\mathbb{1})$	1.0	0.62	0.5
N^{2}LO $(D2, E\mathcal{P})$	1.0	0.59	0.0

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

Nuclear Hamiltonian: local chiral EFT potentials

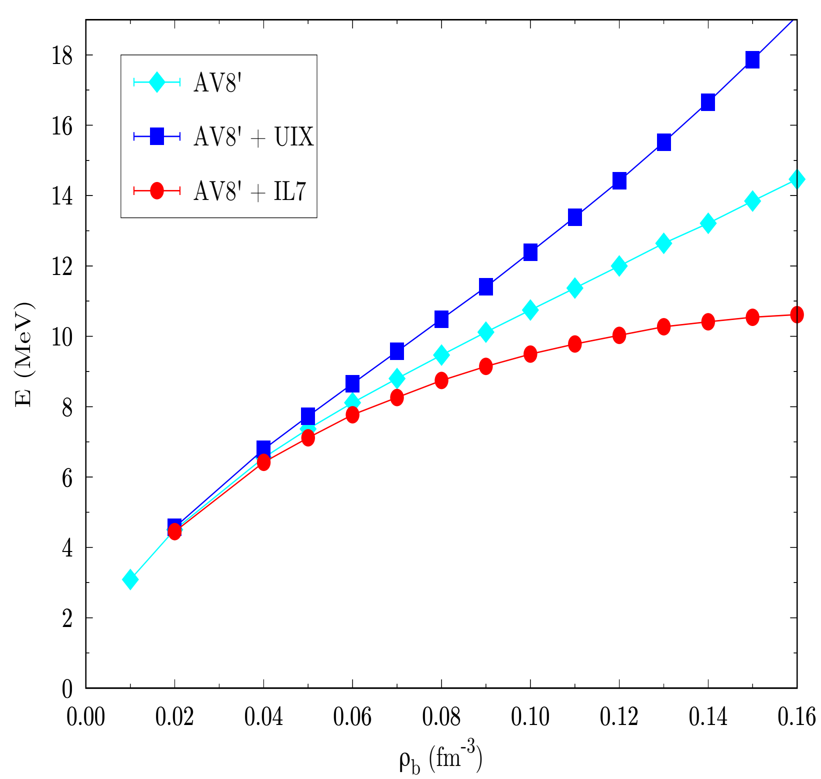
K. M. Nollett et al., Phys. Rev. Lett. 99, 022502 (2007)

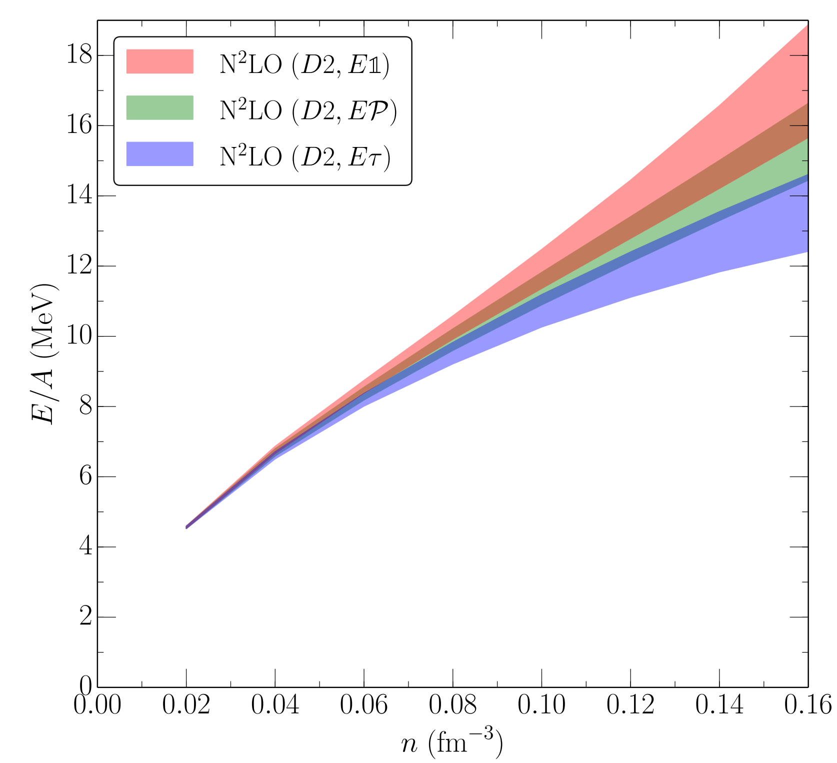




phenomen

chiral





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

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

AFDMC & local chiral EFT potentials

Status:

- 2-body and 3-body local chiral N^2 LO potentials have been implemented in GFMC but so far they have been tested on s-shell nuclei only (A=3,4) and neutron matter
- 2-body potentials have been implemented in AFDMC: need to be tested in nuclei
- 3-body potentials have been implemented in AFDMC: need to be tested

Problem: commutators from TPE in NNN cannot be included in the AFDMC propagator

Idea: use an approximate propagator for NNN

1. enhance the other NNN components in the propagator to compensate for the missing operators
2. minimize the expectation value of the difference between enhanced and real NNN force: $\langle V_{3b}^{diff} \rangle$

Note: similar idea used in GFMC for AV18: propagation done with $\alpha\cdot$ AV8', where α is chosen so as to minimize the difference <AV18 - $\alpha\cdot$AV8'>

AFDMC & local chiral EFT potentials: A = 3

$^3\mathrm{H}\,(\frac{1}{2}^+, \frac{1}{2})$ $E_b = -8.482\,\mathrm{MeV}$ $\sqrt{\langle r^2_{ch}\rangle} = 1.759(36)\,\mathrm{fm}$

Method	cut-off	2b		2b+3b $(D2, E\tau)$	
	R_0 (fm)	E_b (MeV)	$\sqrt{\langle r^2_{ch}\rangle}$ (fm)	E_b (MeV)	$\sqrt{\langle r^2_{ch}\rangle}$ (fm)
GFMC	1.0	−7.55(1)	1.79(2)	−8.34(1)	1.74(3)
	1.2	−7.74(1)	1.76(2)	−8.35(4)	1.74(4)
AFDMC	1.0	−7.54(4)	1.76(2)	−8.35(7)	1.73(2)
	1.2	−7.76(3)	1.75(2)	−8.27(6)	1.73(2)

$^3\mathrm{He}\,(\frac{1}{2}^+, \frac{1}{2})$ $E_b = -7.718\,\mathrm{MeV}$ $\sqrt{\langle r^2_{ch}\rangle} = 1.966(3)\,\mathrm{fm}$

Method	cut-off	2b		2b+3b $(D2, E\tau)$	
	R_0 (fm)	E_b (MeV)	$\sqrt{\langle r^2_{ch}\rangle}$ (fm)	E_b (MeV)	$\sqrt{\langle r^2_{ch}\rangle}$ (fm)
GFMC	1.0	−6.78(1)	2.07(2)	−7.65(2)	1.98(2)
	1.2	−7.01(1)	2.02(1)	−7.63(4)	1.98(1)
AFDMC	1.0	−6.89(5)	2.02(2)	−7.55(8)	1.97(2)
	1.2	−7.12(3)	1.99(1)	−7.60(6)	1.90(2)

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

AFDMC & local chiral EFT potentials: A = 4

$^4\mathrm{He}\,(0^+,0)$ $E_b = -28.296\,\mathrm{MeV}$ $\sqrt{\langle r^2_{ch}\rangle} = 1.676(3)\,\mathrm{fm}$

Method	cut-off	2b		2b+3b $(D2, E\tau)$	
	R_0 (fm)	E_b (MeV)	$\sqrt{\langle r^2_{ch}\rangle}$ (fm)	E_b (MeV)	$\sqrt{\langle r^2_{ch}\rangle}$ (fm)
GFMC	1.0	−23.72(1)	1.74(1)	−28.30(1)	1.66(2)
	1.2	−24.86(1)	1.69(1)	−28.30(1)	1.66(1)
AFDMC	1.0	−23.88(6)	1.73(1)	−27.97(12)	1.69(1)
	1.2	−25.24(6)	1.70(1)	−28.33(10)	1.67(1)

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

good agreement AFDMC-GFMC both at
2-body and 3-body level

Note:
- same coefficients in the NNN propagator for A = 3, 4
- $\langle V_{3b}^{diff}\rangle \le 1\%$ compared to the total binding energy
- variations of the coefficients do no affect the final result

AFDMC $\longrightarrow$ open-shell systems & larger systems

AFDMC & local chiral EFT potentials: A = 6

$^6\text{He}\,(0^+,1)$ $\quad E_b = -29.271\,\text{MeV}$ $\quad \sqrt{\langle r^2_{ch}\rangle} = 2.066(11)\,\text{fm}$

Method	cut-off	2b		2b+3b $(D2, E\tau)$	
	R_0 (fm)	E_b (MeV)	$\sqrt{\langle r^2_{ch}\rangle}$ (fm)	E_b (MeV)	$\sqrt{\langle r^2_{ch}\rangle}$ (fm)
AFDMC	1.0	−22.1(5)	2.11(2)	−28.0(5)	2.06(2)
	1.2	−24.2(2)	2.07(2)	−29.4(8)	1.98(2)

$^6\text{Li}\,(1^+,0)$ $\quad E_b = -31.994\,\text{MeV}$ $\quad \sqrt{\langle r^2_{ch}\rangle} = 2.589(34)\,\text{fm}$

Method	cut-off	2b		2b+3b $(D2, E\tau)$	
	R_0 (fm)	E_b (MeV)	$\sqrt{\langle r^2_{ch}\rangle}$ (fm)	E_b (MeV)	$\sqrt{\langle r^2_{ch}\rangle}$ (fm)
AFDMC	1.0	−24.7(5)	2.62(3)	−29.6(8)	2.43(3)
	1.2	−26.9(5)	2.44(5)	−31.0(8)	2.26(3)

Note:
- same coefficients in the NNN propagator for A = 4: $\langle V_{3b}^{diff}\rangle < 3\%$
- w.f. built with s-p-d single particle states

AFDMC & local chiral EFT potentials: A = 16 - 40

$^{16}\mathrm{O}\,(0^+,0)$ $\quad E_b = -127.619\,\mathrm{MeV}$ $\quad \sqrt{\langle r^2_{ch}\rangle} = 2.699(5)\,\mathrm{fm}$

Method	cut-off	2b		2b+3b $(D2, E\tau)$	
	R_0 (fm)	E_b (MeV)	$\sqrt{\langle r^2_{ch}\rangle}$ (fm)	E_b (MeV)	$\sqrt{\langle r^2_{ch}\rangle}$ (fm)
AFDMC	1.0	$-79(3)$	2.76(3)	$-97(6)^*$	2.78(5)
	1.2	$-105(5)$	2.48(2)	$-150(5)^*$	2.18(5)

$^{40}\mathrm{Ca}\,(0^+,0)$ $\quad E_b = -342.052\,\mathrm{MeV}$ $\quad \sqrt{\langle r^2_{ch}\rangle} = 3.478(1)\,\mathrm{fm}$

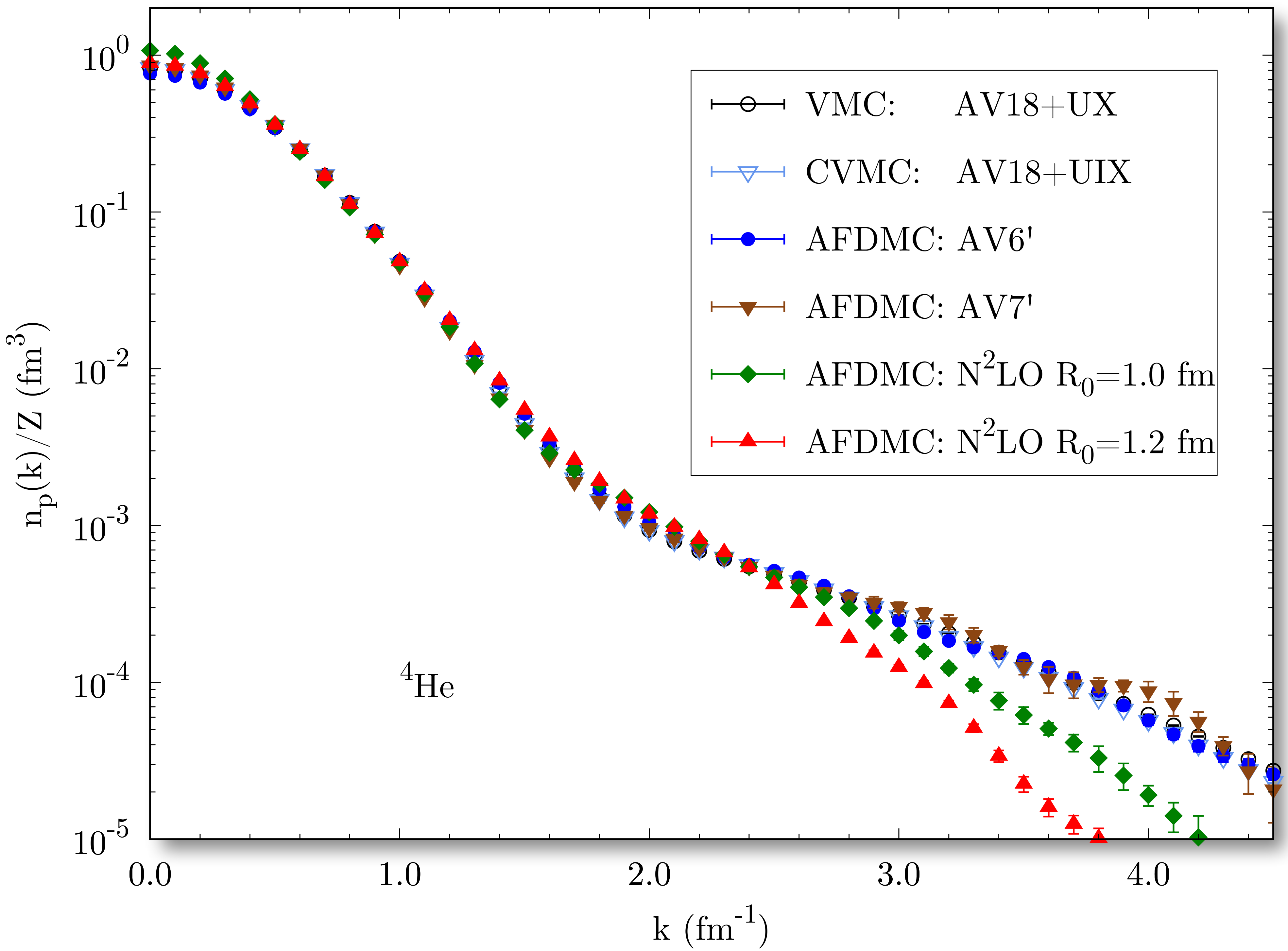
Method	cut-off	2b		2b+3b $(D2, E\tau)$	
	R_0 (fm)	E_b (MeV)	$\sqrt{\langle r^2_{ch}\rangle}$ (fm)	E_b (MeV)	$\sqrt{\langle r^2_{ch}\rangle}$ (fm)
AFDMC	1.0	$-120(10)^*$	-	-	-
	1.2	$-230(10)^*$	-	-	-

Note:
- need to change the coefficients in the propagation
- still possible to keep $\langle V_{3b}^{diff}\rangle$ small

Question: how is this interaction working?

AFDMC & local chiral EFT potentials: n(k)

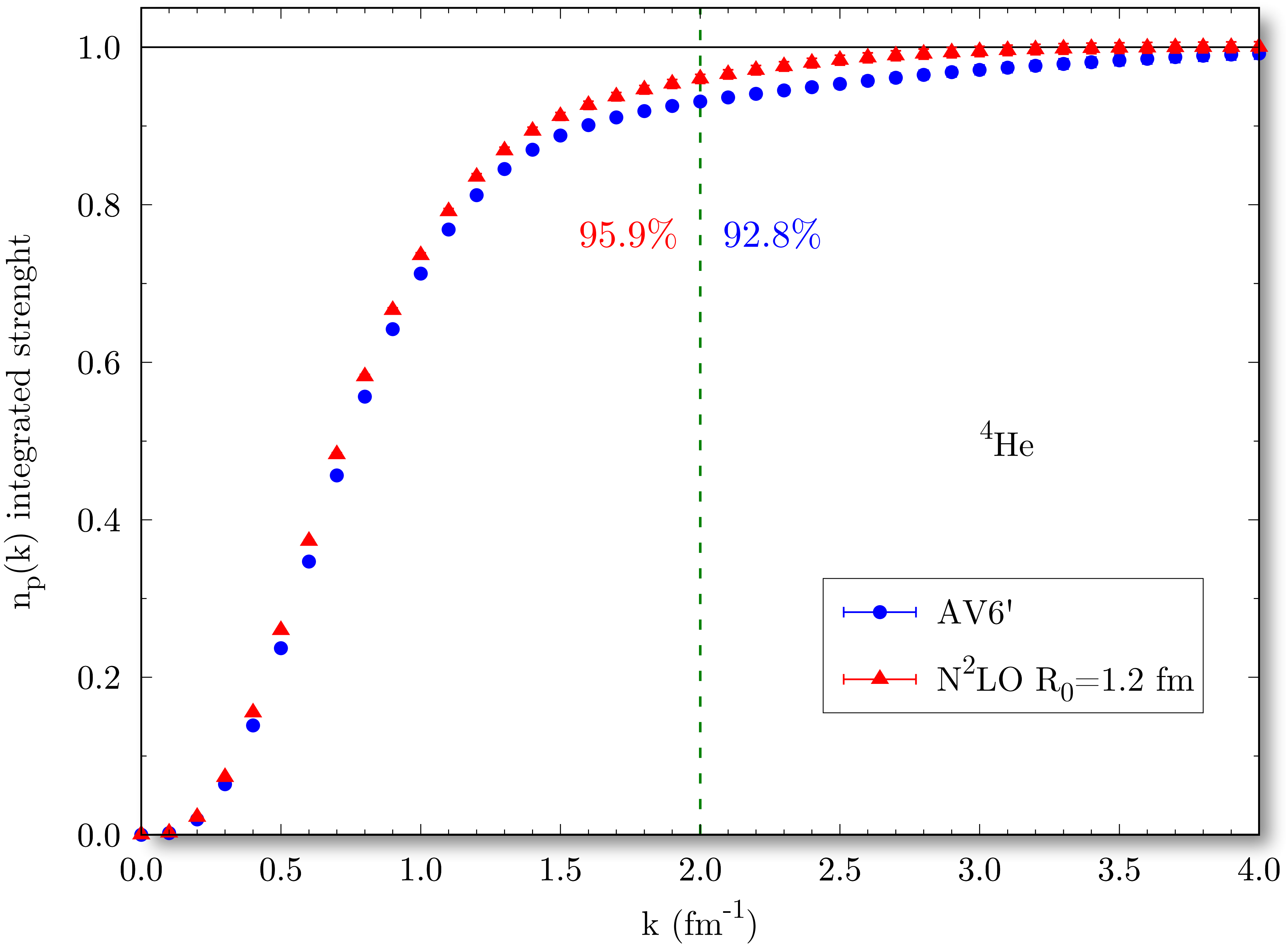
single-nucleon momentum distribution



CVMC: D.L., A. Lovato, S. C. Pieper, R. B. Wiringa, in preparation; AFDMC: S. Gandolfi, J. Carlson, D.L., X. Wang, in preparation

AFDMC & local chiral EFT potentials: n(k)

single-nucleon momentum distribution



AFDMC & local chiral EFT potentials: n(k)

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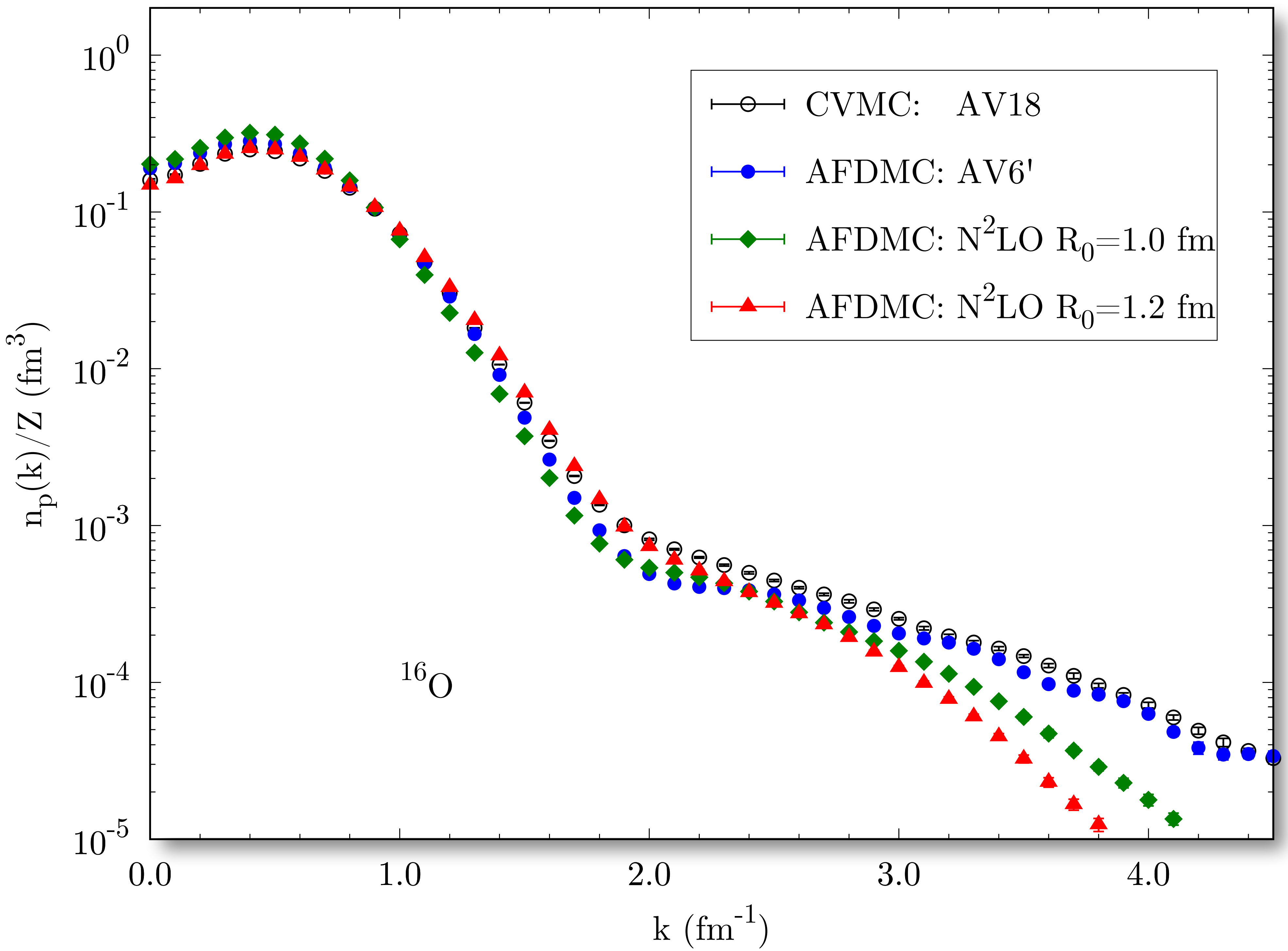

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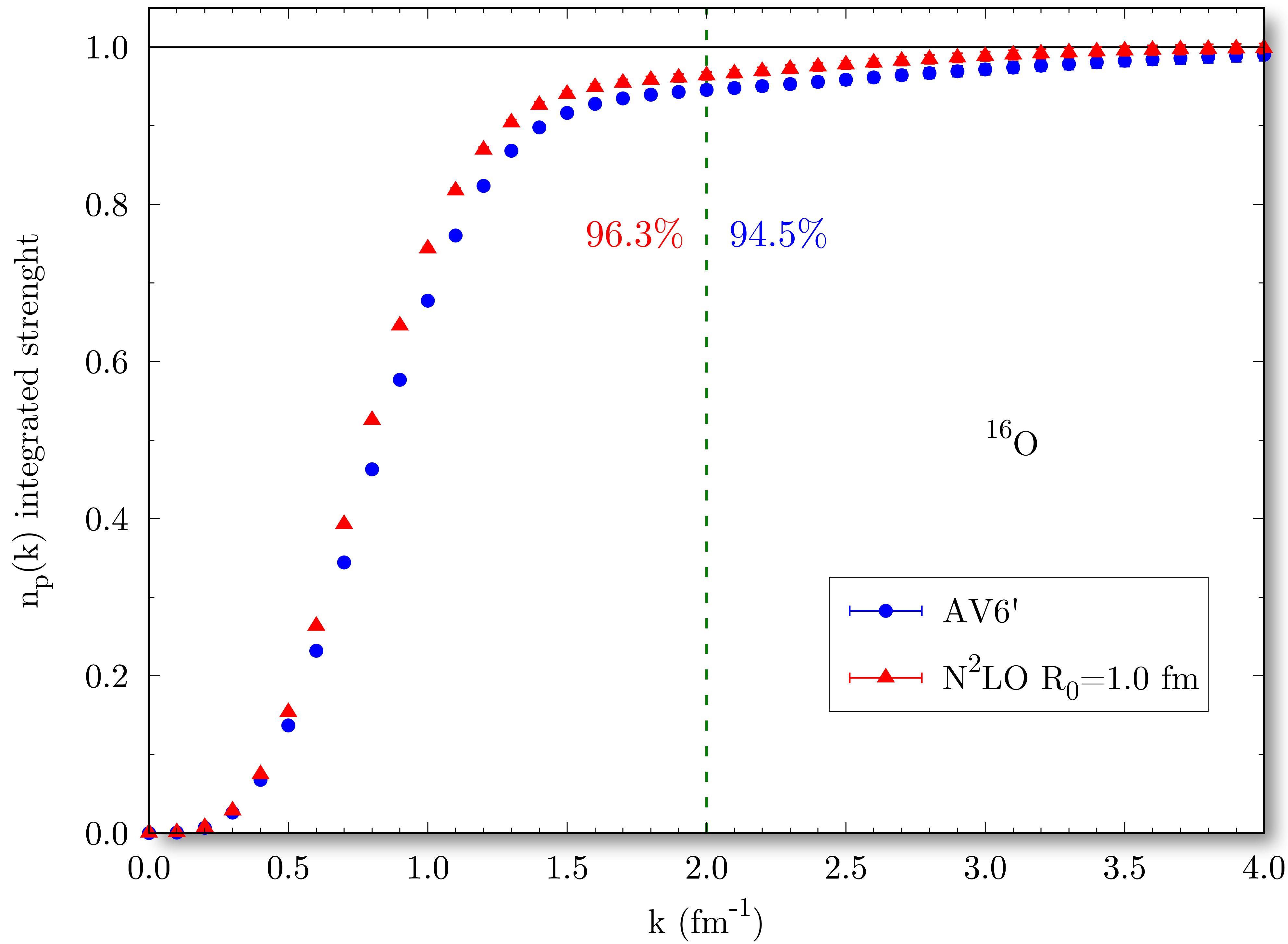
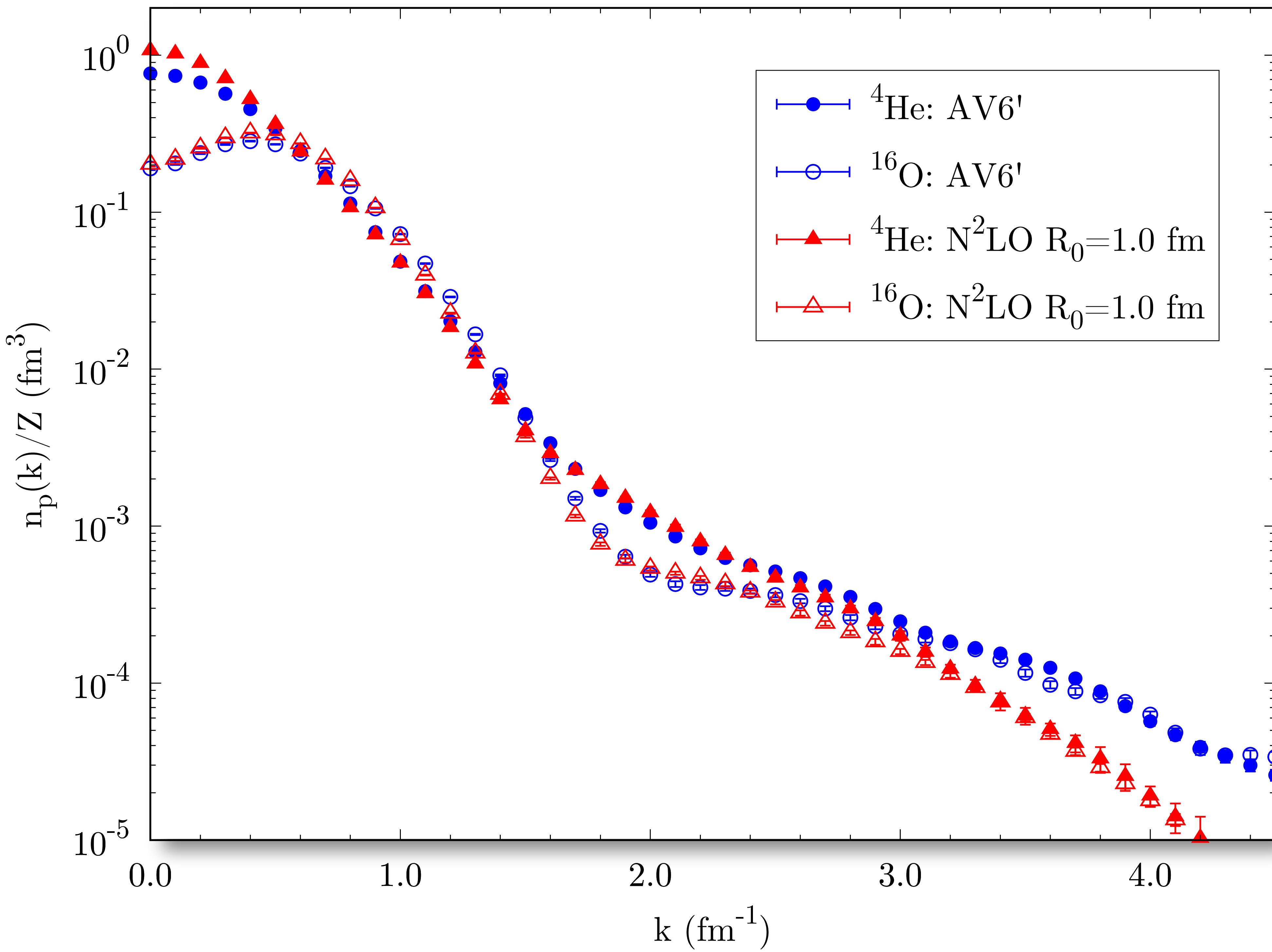
AFDMC & local chiral EFT potentials: n(k)

single-nucleon momentum distribution



AFDMC & local chiral EFT potentials: n(k)

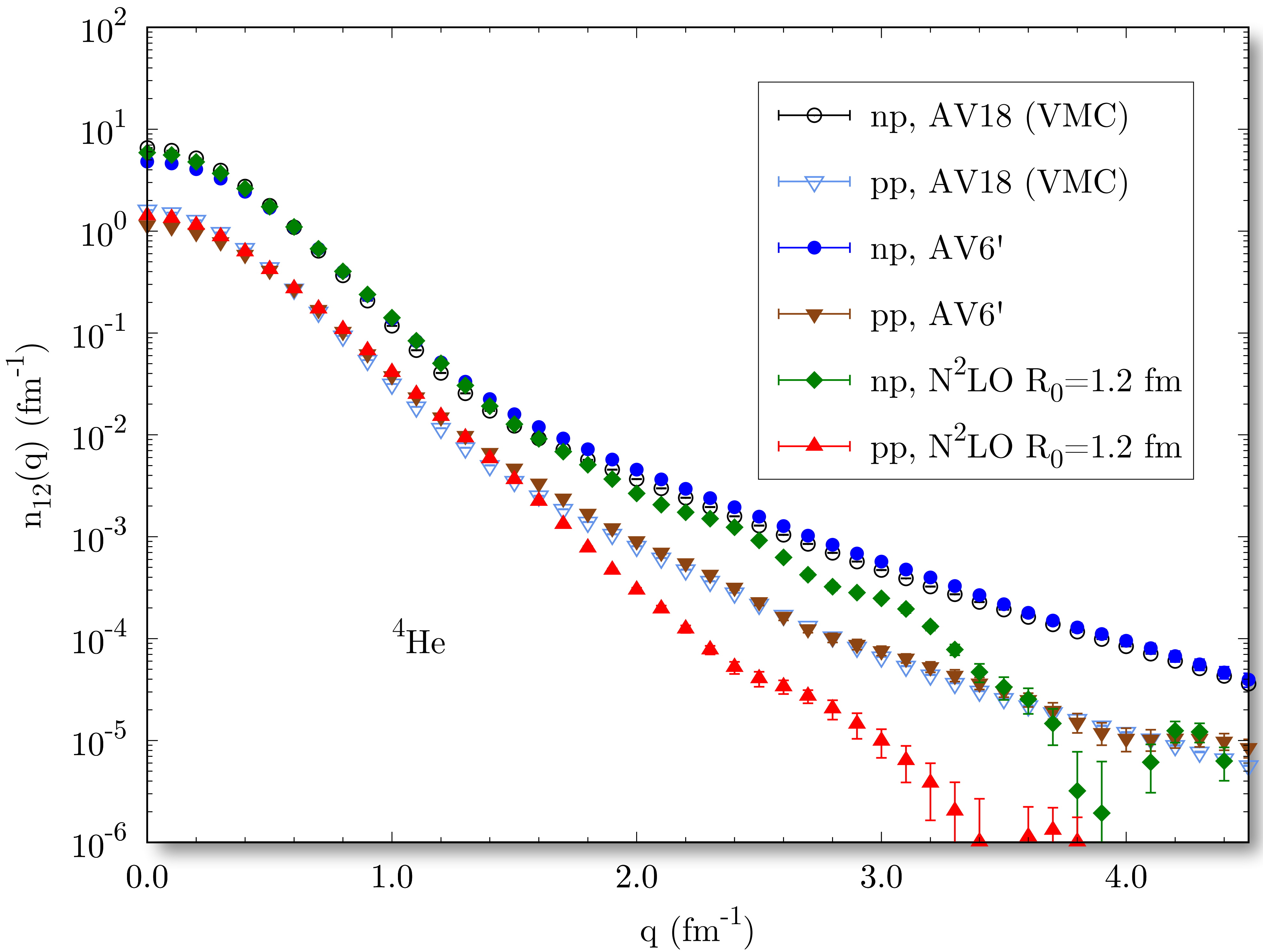
single-nucleon momentum distribution



S. Gandolfi, J. Carlson, D.L., X. Wang, in preparation

AFDMC & local chiral EFT potentials: $n_{12}(q)$

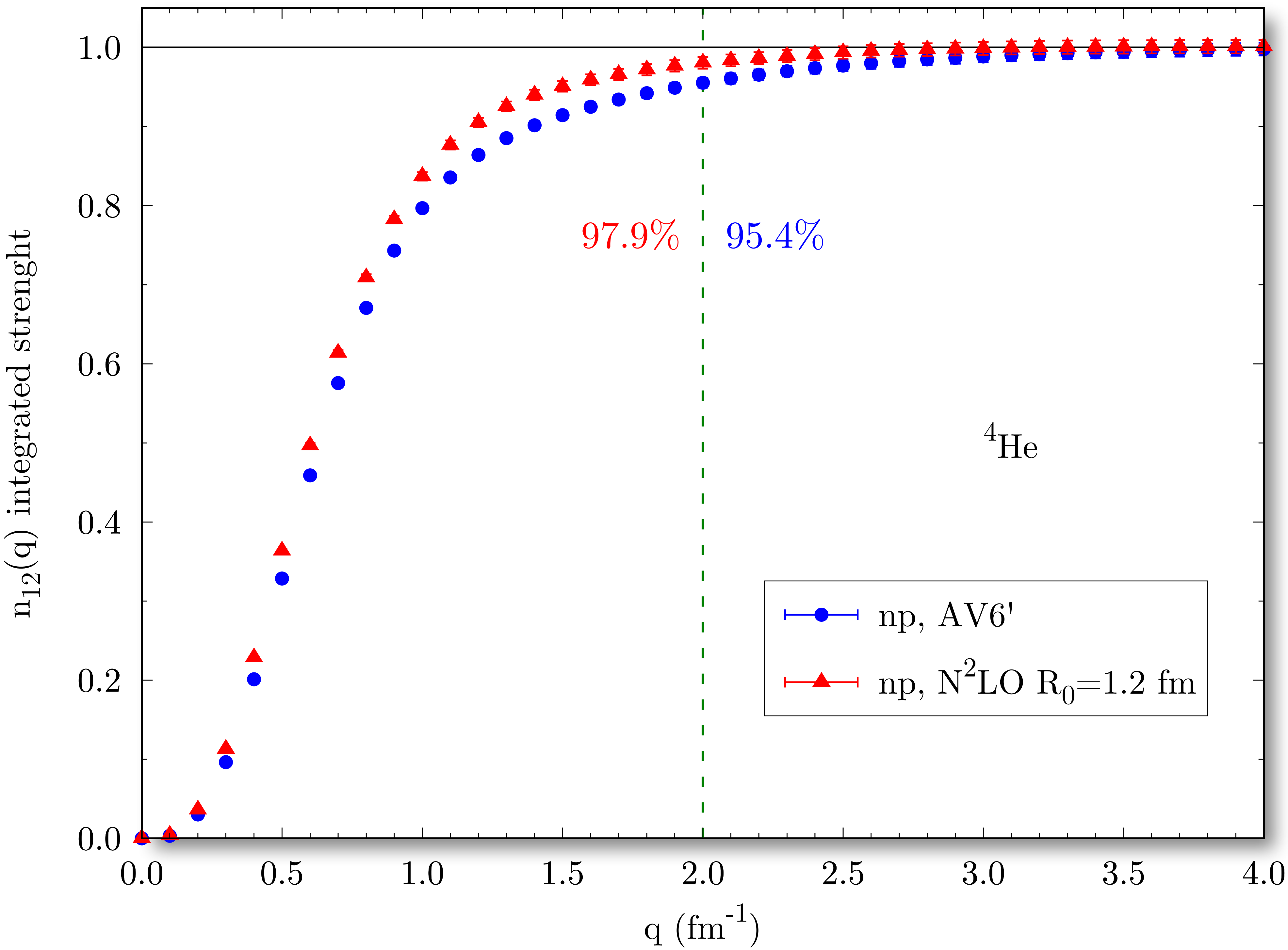
two-nucleon momentum distribution (integrated Q)



VMC: R. B. Wiringa et al., Phys. Rev. C 89, 024305 (2014); AFDMC: S. Gandolfi, J. Carlson, D.L., X. Wang, in preparation

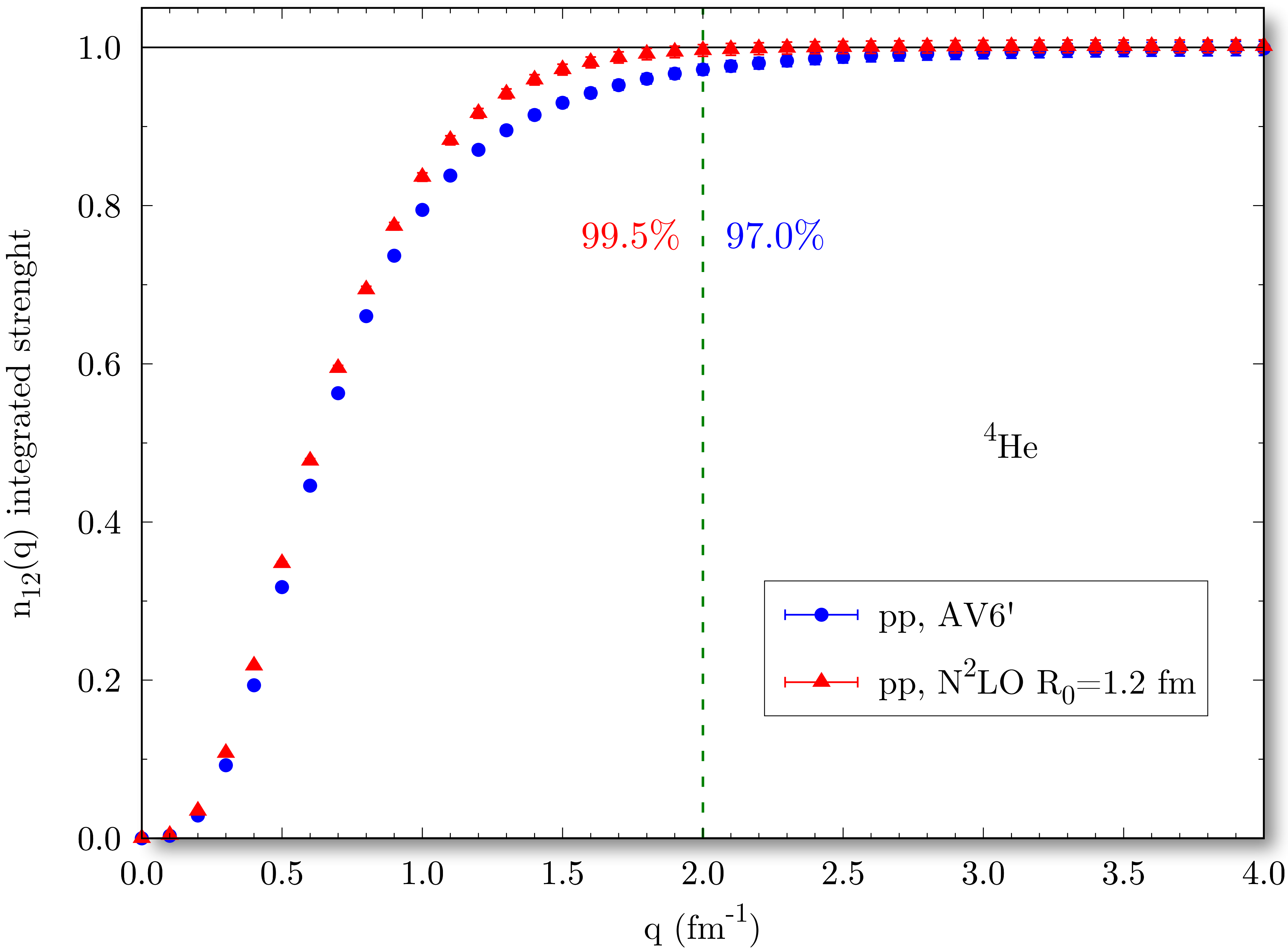
AFDMC & local chiral EFT potentials: $n_{12}(q)$

two-nucleon momentum distribution (integrated Q)



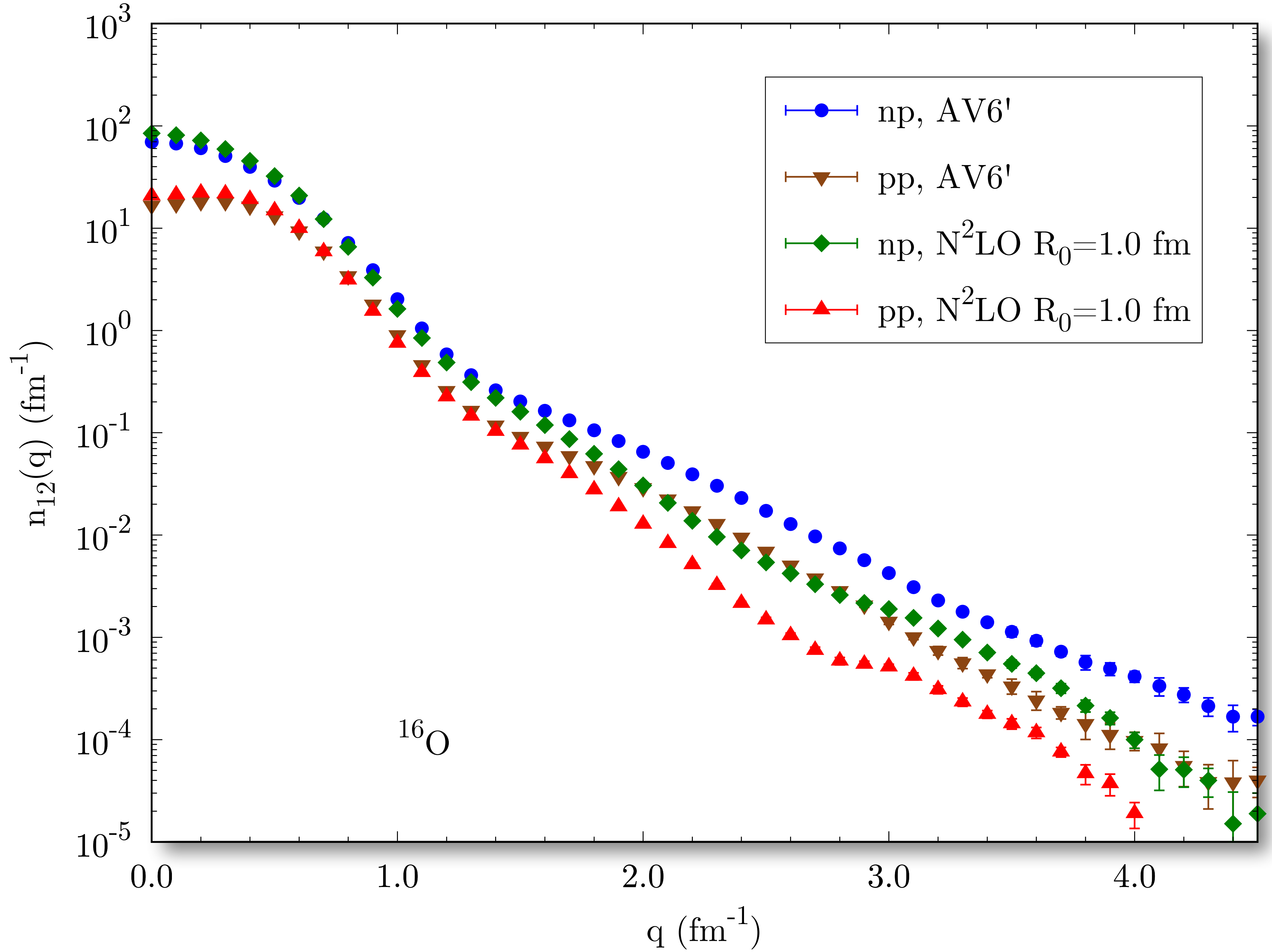
AFDMC & local chiral EFT potentials: $n_{12}(q)$

two-nucleon momentum distribution (integrated Q)



AFDMC & local chiral EFT potentials: $n_{12}(q)$

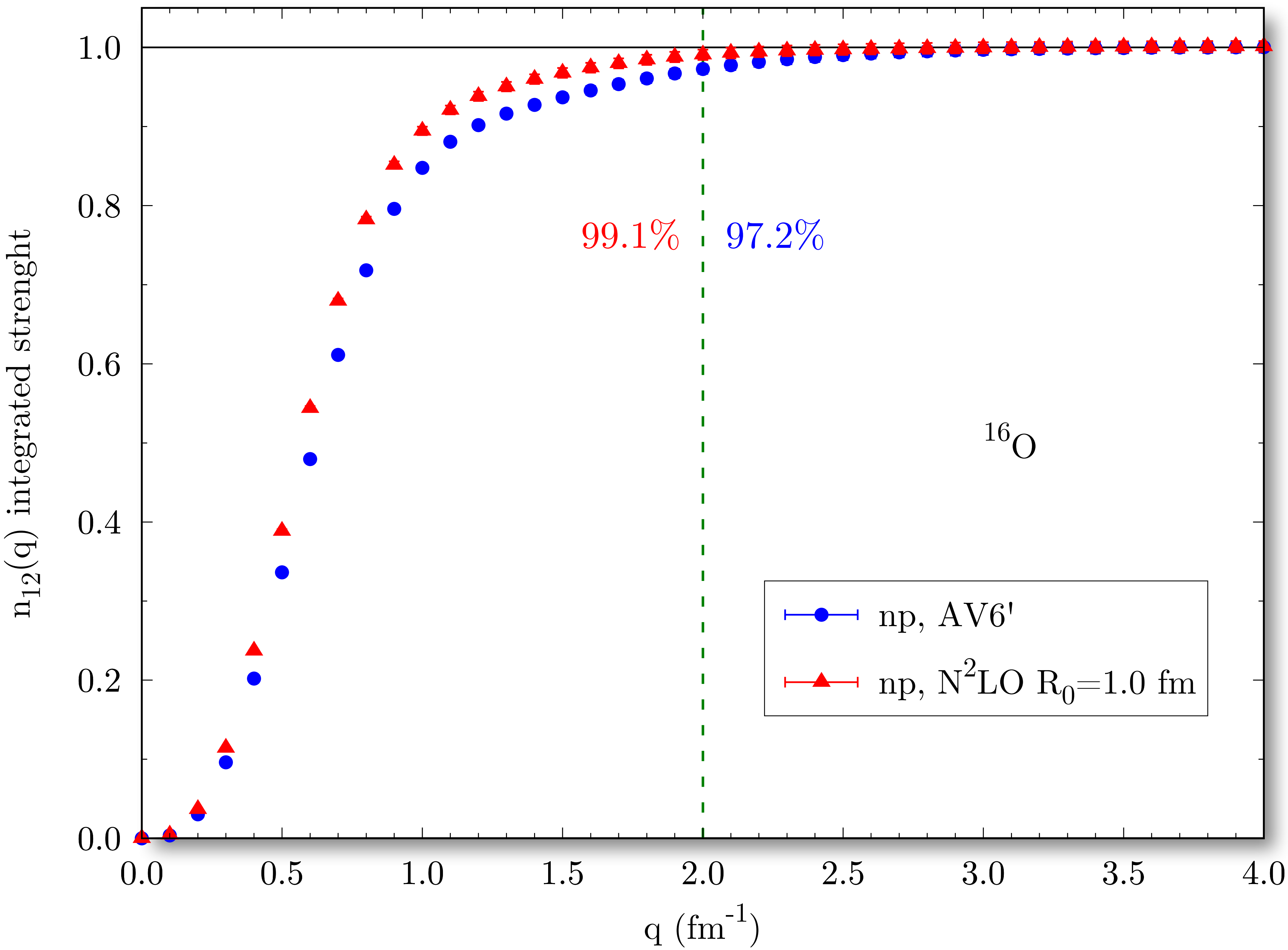
two-nucleon momentum distribution (integrated Q)



S. Gandolfi, J. Carlson, D.L., X. Wang, in preparation

AFDMC & local chiral EFT potentials: $n_{12}(q)$

two-nucleon momentum distribution (integrated Q)



AFDMC & local chiral EFT potentials: $n_{12}(q)$

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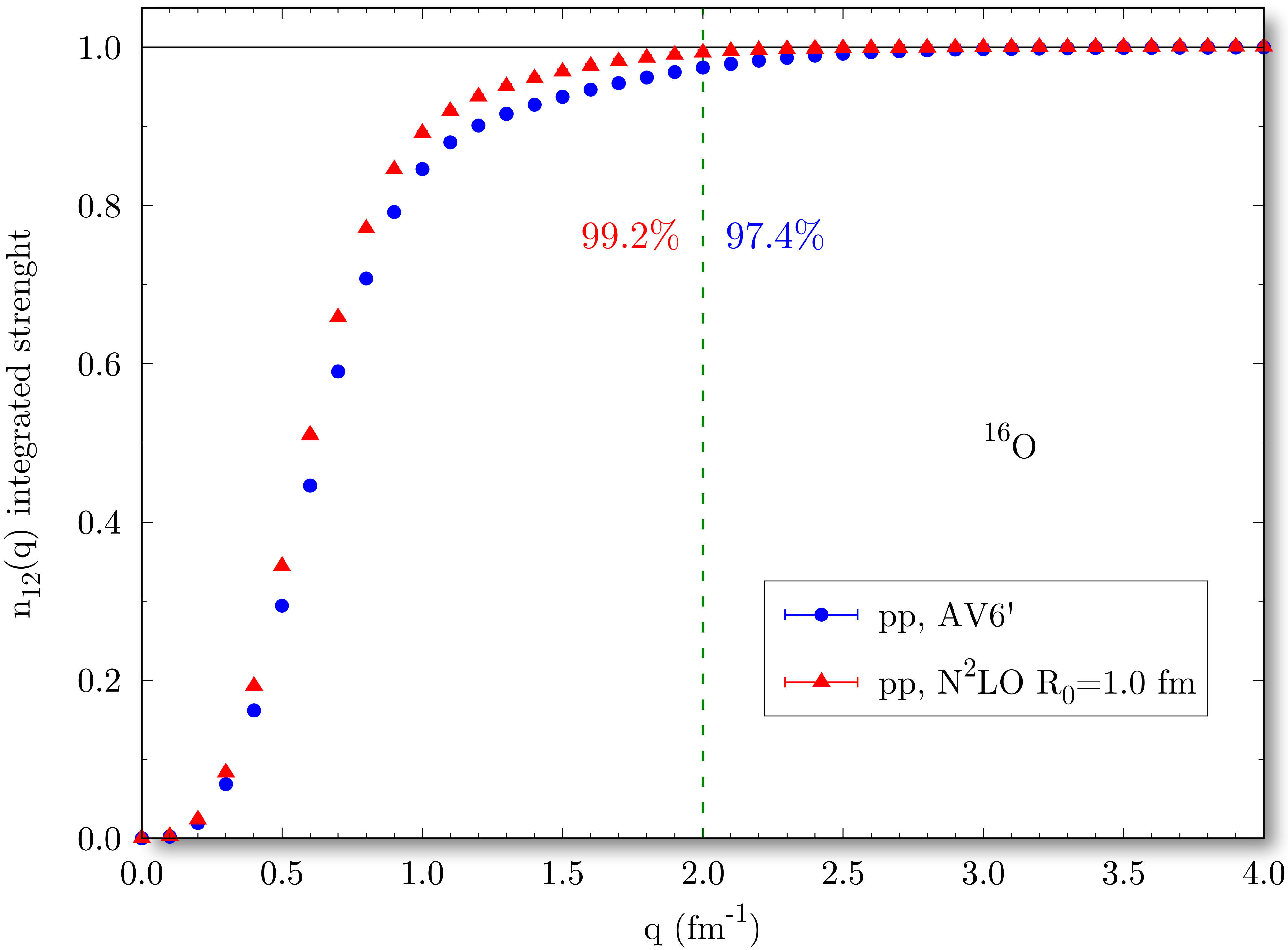
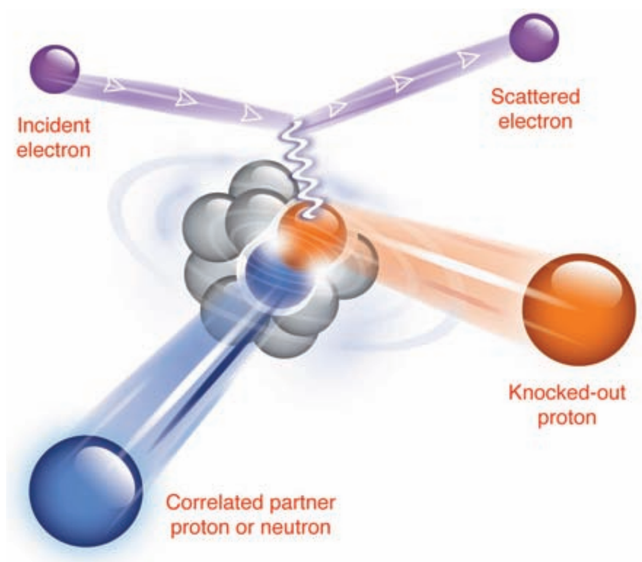


AFDMC & local chiral EFT potentials: $n_{12}(q)$

two-nucleon momentum distribution (q & Q): **on the way!!**



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

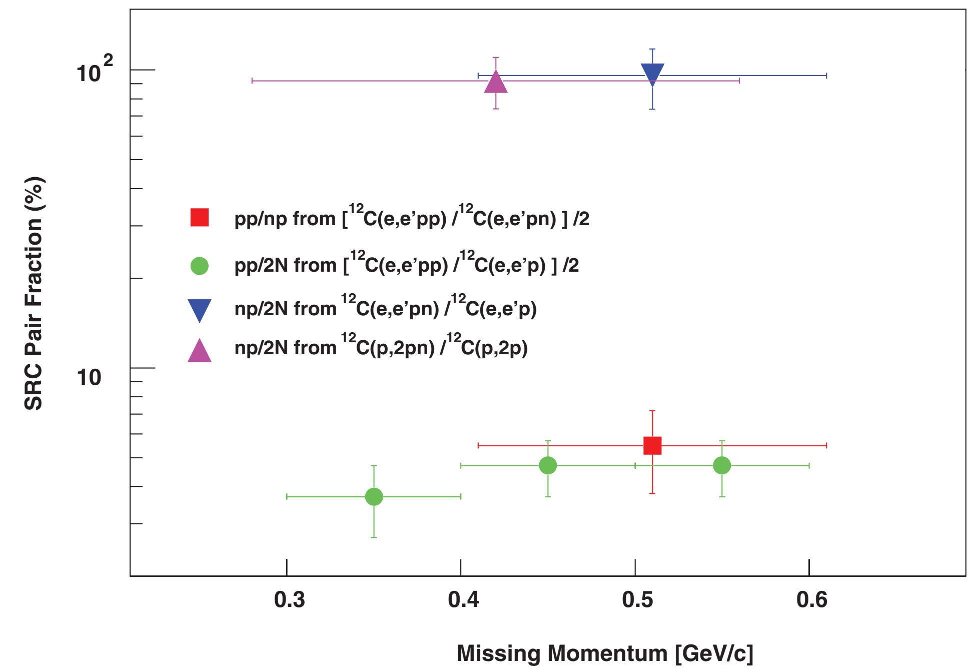


Fig. 2. The fractions of correlated pair combinations in carbon as obtained from the (e,e'pp) and (e,e'pn) reactions, as well as from previous (p,2pn) data. The results and references are listed in table S1.

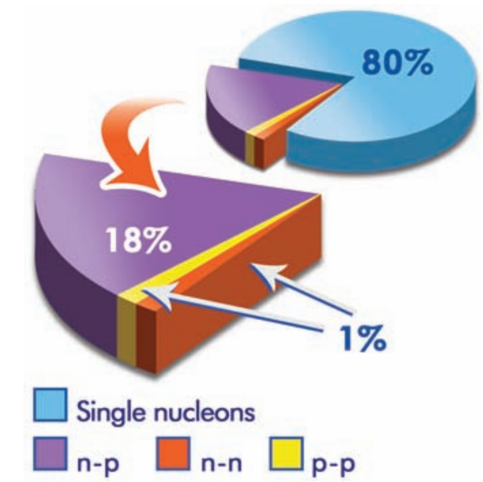
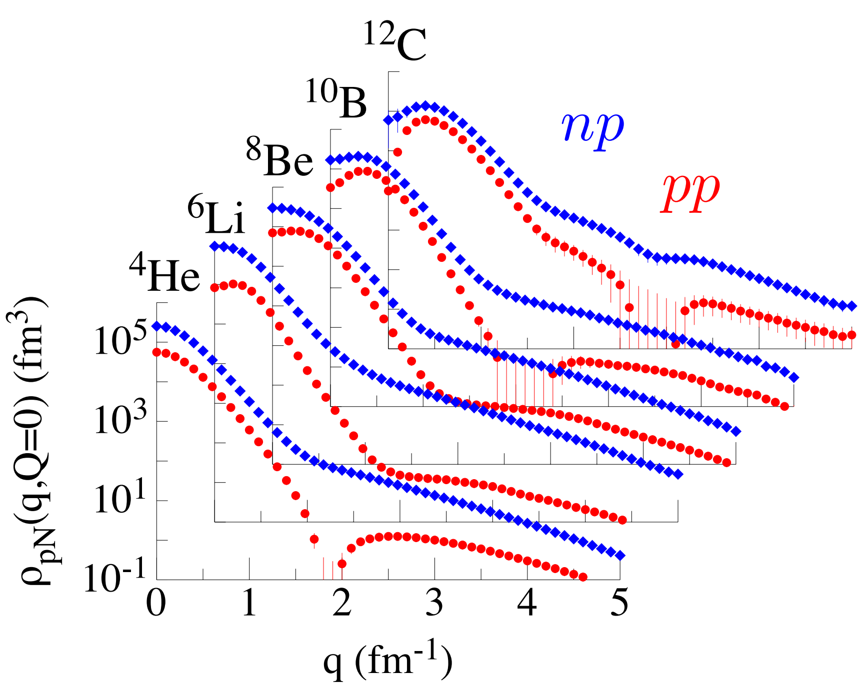


Fig. 3. The average fraction of nucleons in the various initial-state configurations of ^{12}C.

short-range correlated pairs

↓

induced by the nuclear force (tensor force)



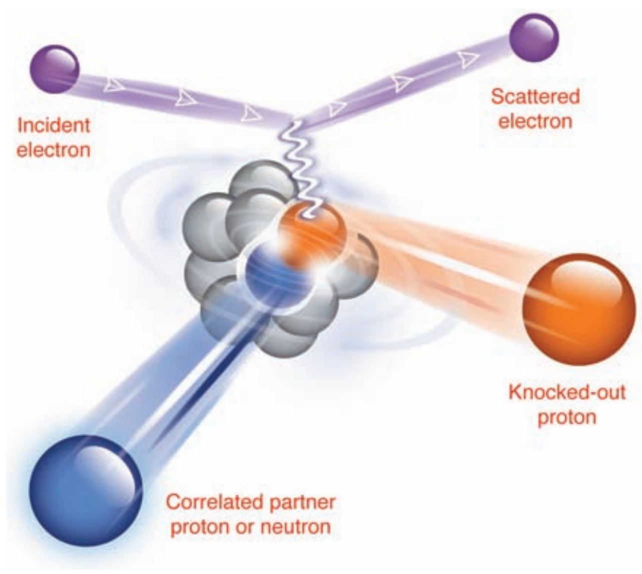
R. B. Wiringa et al., Phys. Rev. C 89, 024305 (2014)

behavior expected to be universal across a wide range of nuclei

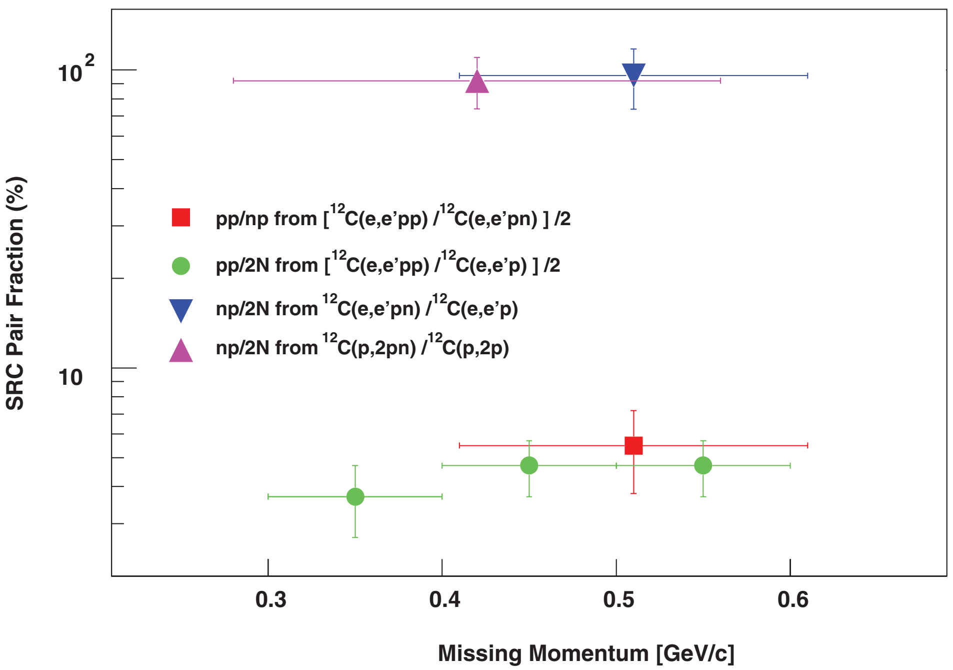
true??
model dependent??

AFDMC & local chiral EFT potentials: $n_{12}(q)$

two-nucleon momentum distribution (q & Q): on the way!!



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



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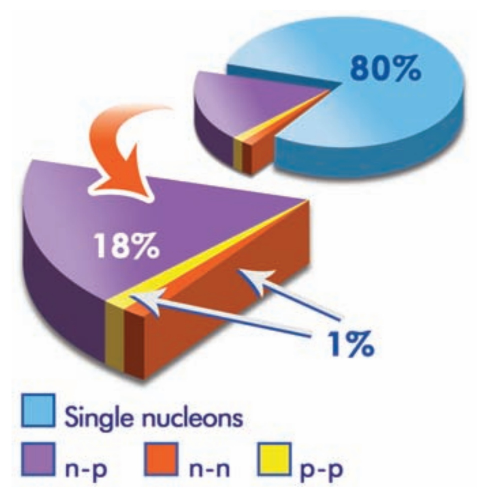

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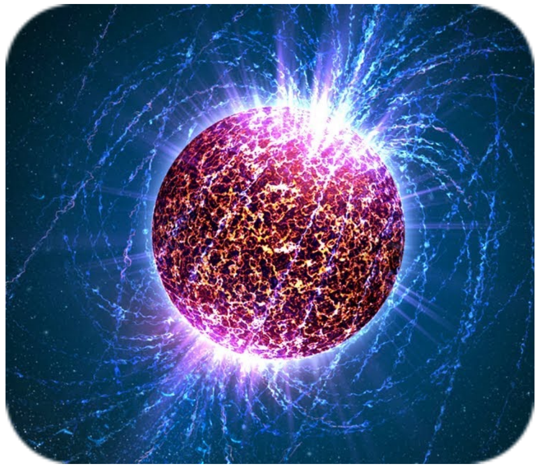


neutron stars:
5-10% protons

realistic calculations of NS need to take into account these correlation effect

↕

employed interaction (and method)

Future directions

progresses in AFDMC calculations → moving towards an ab-initio description of the medium region of the nuclear chart

✓ neutron-rich nuclei

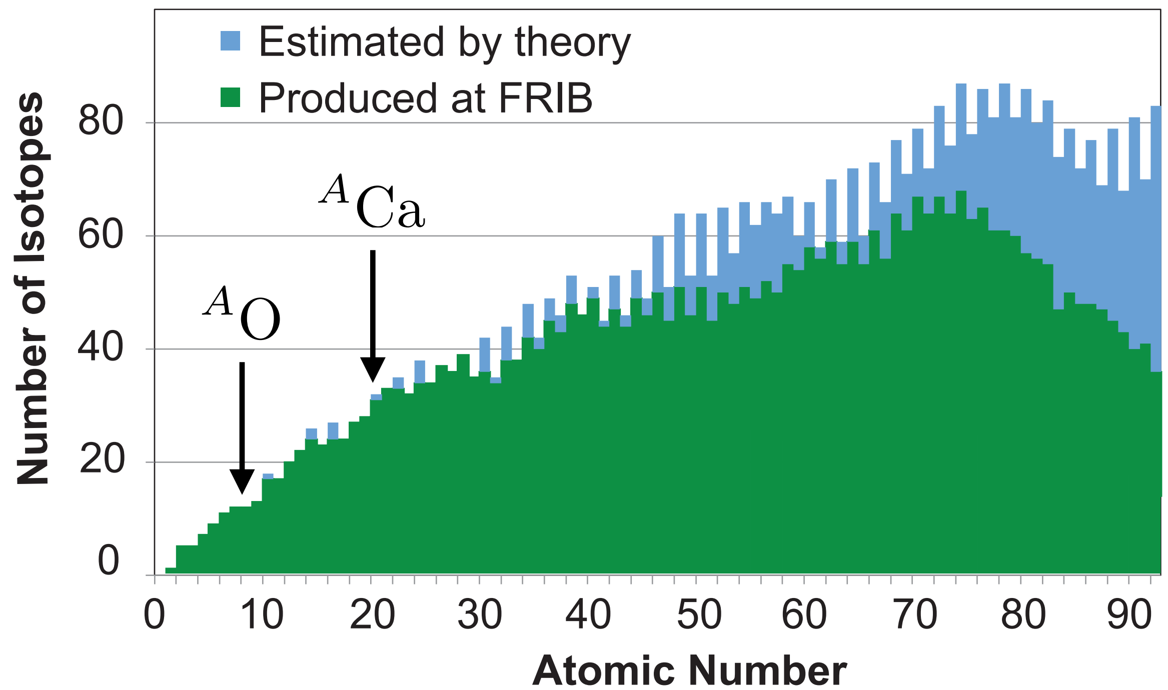
- better understanding of the 3n force:

  fundamental for NS description

- moving towards the neutron drip line:

  appearance of new magic number & last stable isotopes

  nuclear correlations



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

- neutron skin → CREX @ JLab $(^{48}\mathrm{Ca})$

  constraints for the symmetry energy (and its slope)

NS observables:
the mass-radius relationship
(cooling rates, the thickness of the crust)

↔

constraints on NNN force

Conclusions

- ✓ Substantial progresses in AFDMC calculations
  - inclusion of 2b & 3b local N^2LO chiral forces
  - good agreement with GFMC for A = 3, 4
  - first QMC calculations for A = 6, 16, 40 (binding energies & radii)
  - single- and two-nucleon momentum distributions for different forces

↓

- ✓ Develop the technology to study the medium-mass region of the nuclear chart in a non perturbative fashion
- ✓ Access the physics of neutron-rich systems: better understanding of nuclear forces & the connection to the physics of neutron stars

Thank you!!