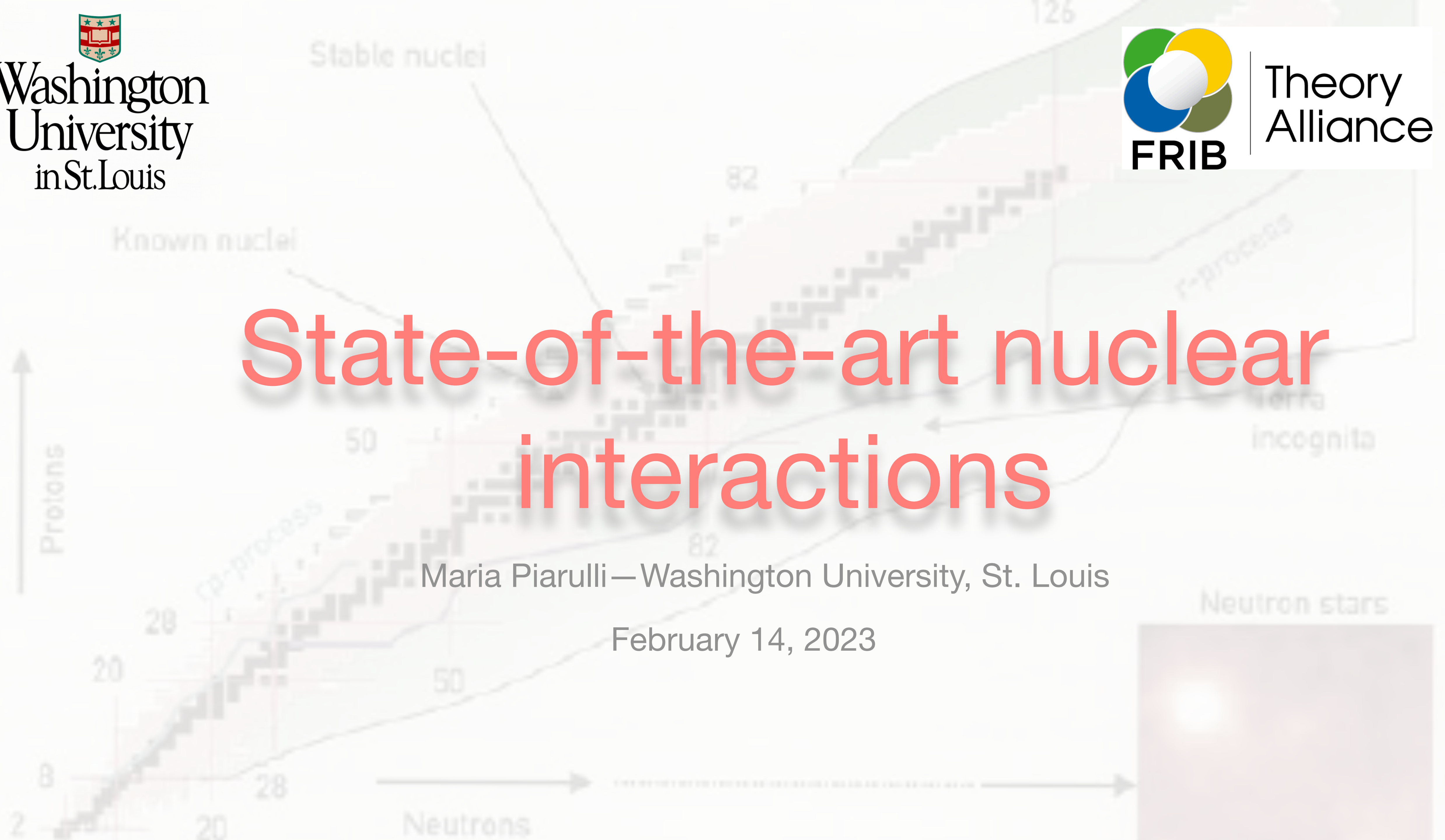


# State-of-the-art nuclear interactions

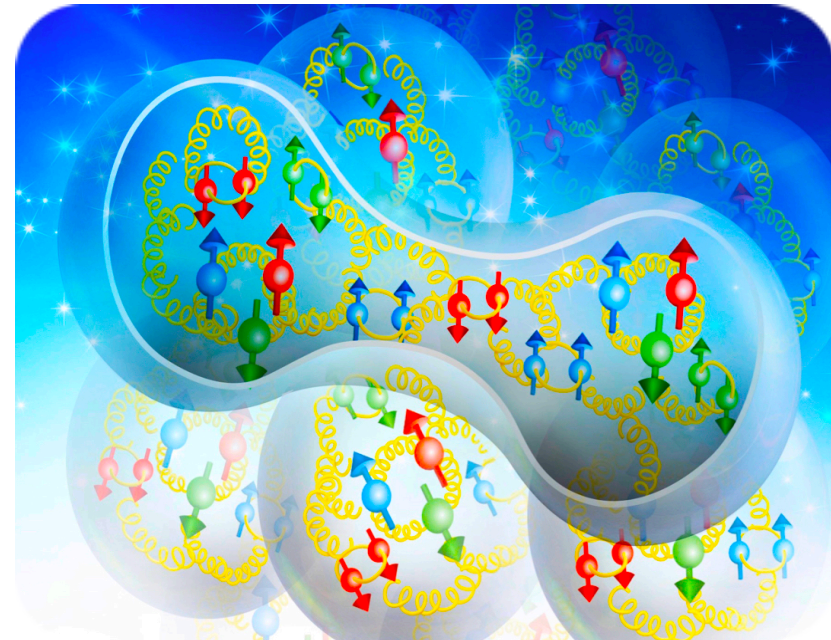
Maria Piarulli — Washington University, St. Louis

February 14, 2023

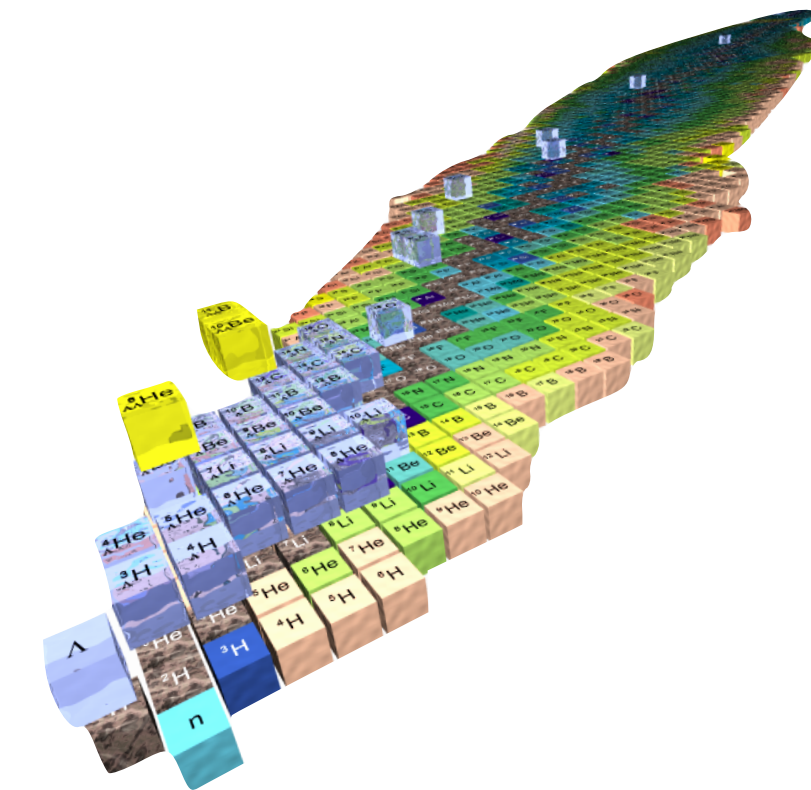
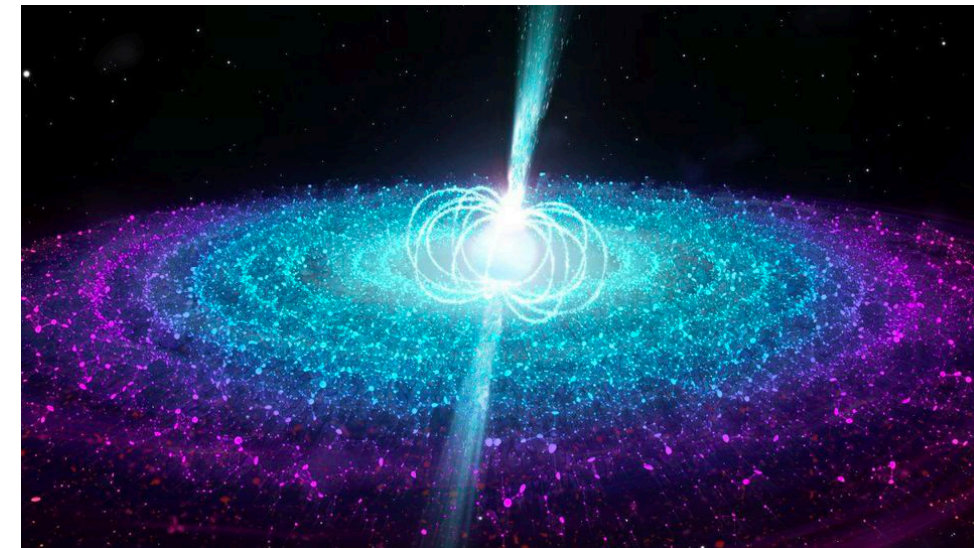


# Introduction

**Question:** where does the nuclear force which binds nucleons together gets its main characteristics, and how it is rooted in the fundamental theory of strong interactions?

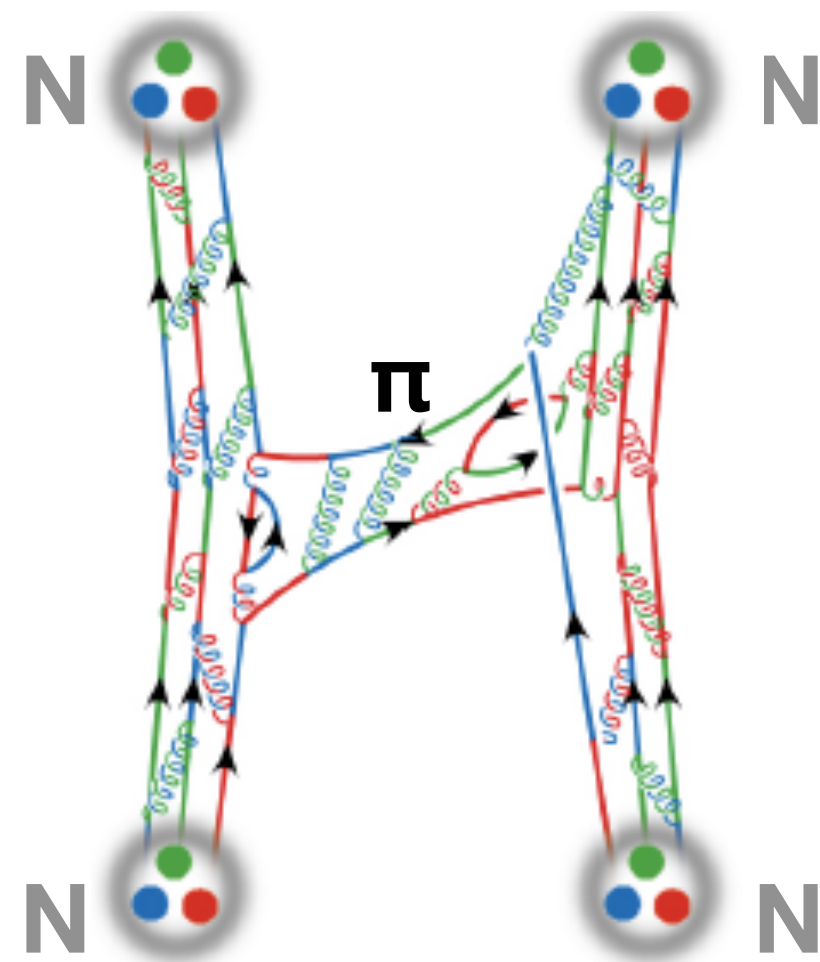


Quantum Chromodynamics



Atomic nuclei and nucleonic matter

This is not a trivial problem due to the nonperturbative nature of QCD at low energy

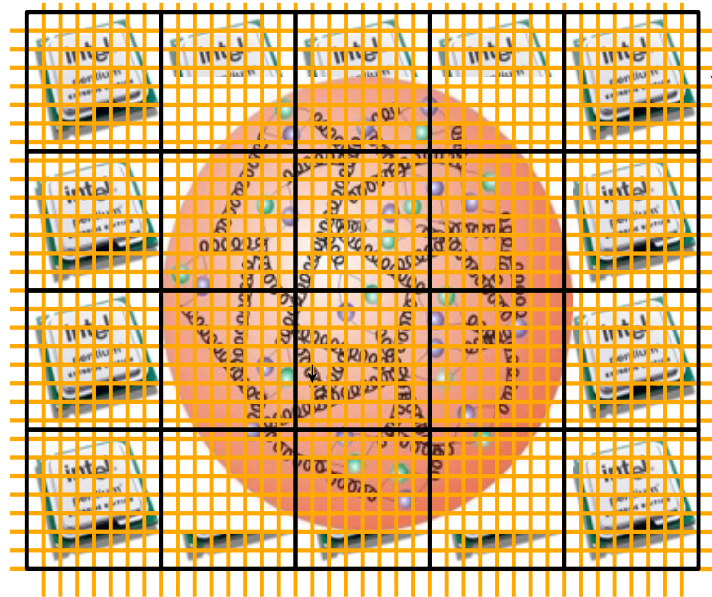


- \* Cartoon of the exchange of a pion (OPE) between two nucleons in the quark picture
- \* OPE: responsible of the long range part of nuclear forces ( $r \gtrsim 2$  fm)

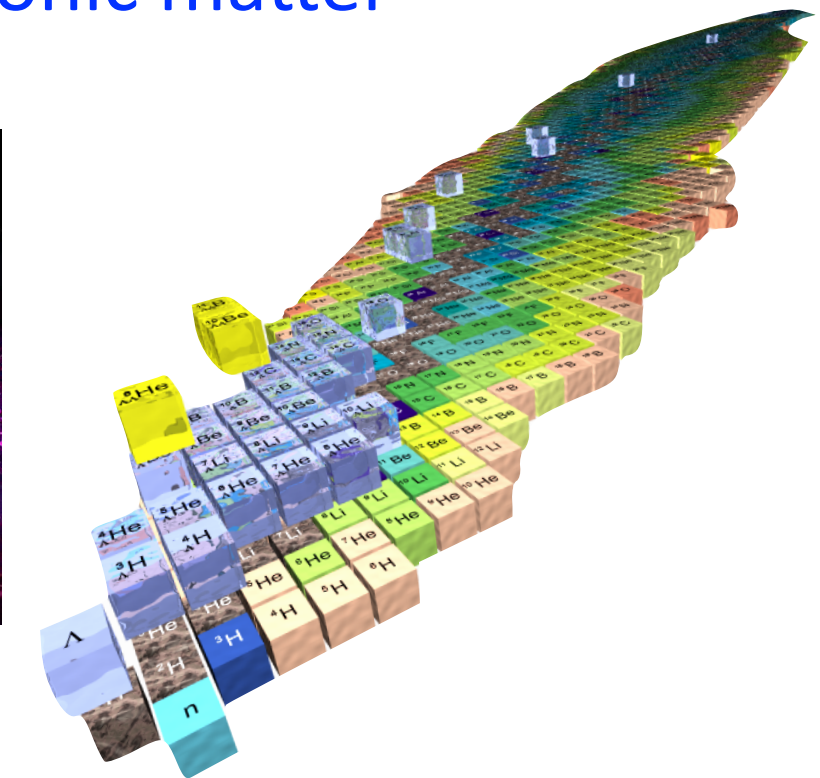
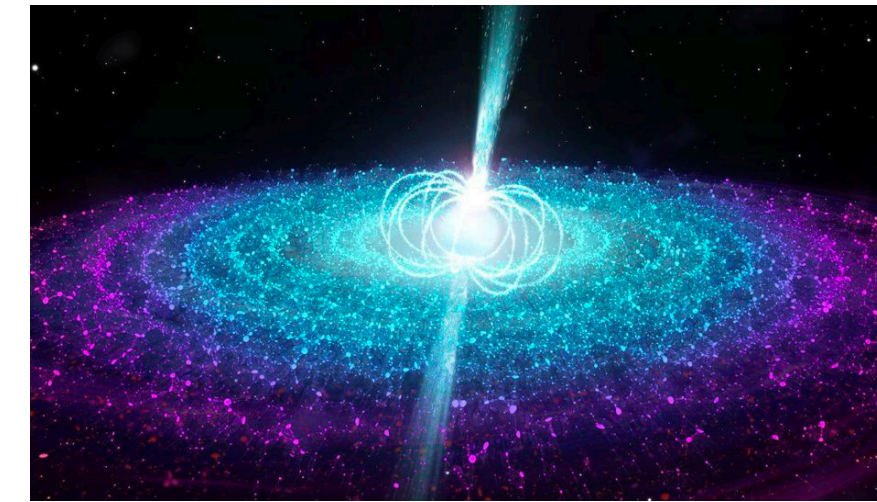
At low-energy nucleons are the relative degrees of freedom leading to the idea of effective nuclear potential

# Nevertheless Lattice QCD

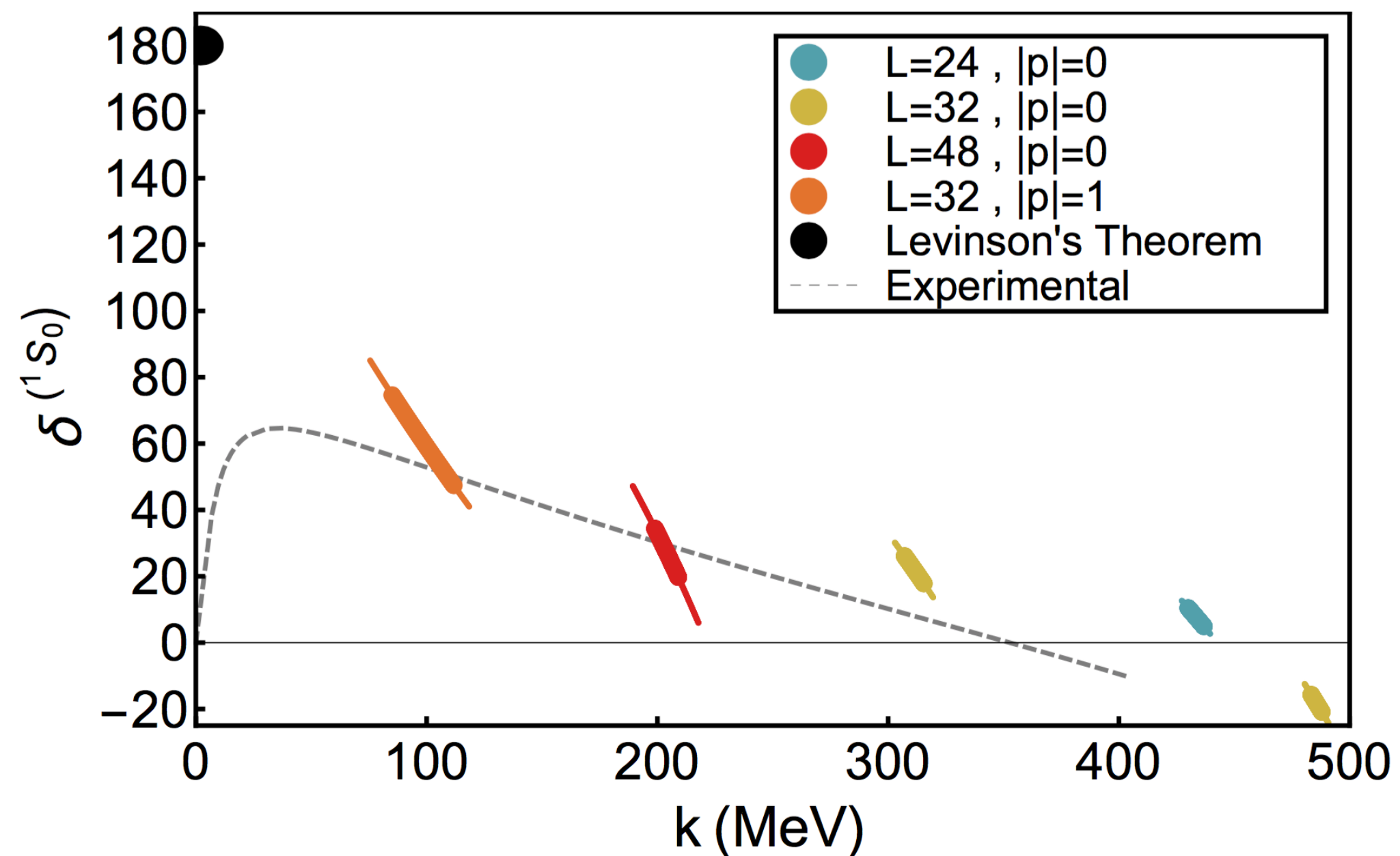
Lattice Quantum Chromodynamics



Atomic nuclei and nucleonic matter

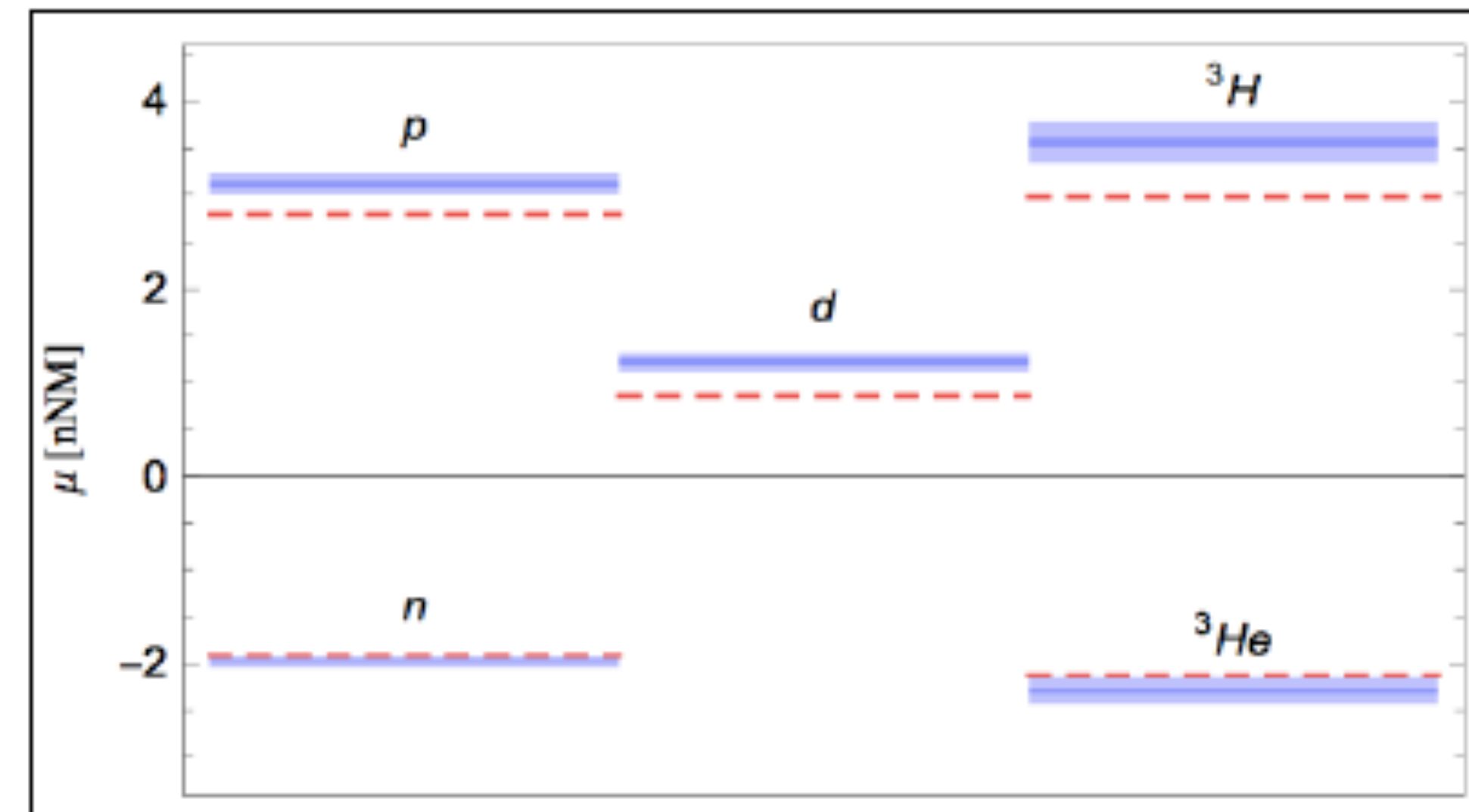


Scattering in the  $^1S_0$  channel  $m_\pi \sim 450$  MeV



Orginos et Phys. Rev. D **92**, 114512 (2015); NPLQCD

LQCD predictions for magnetic moments  $A < 4$ ,  $m_\pi \sim 800$  MeV



Beane et al., PRL113, 252001 (2014); NPLQCD

*Despite the many advances, LQCD calculations are still limited to small nucleon numbers and/or large pion masses.*

# The microscopic model of nuclear theory

*Goal: develop a predictive understanding of nuclei in terms of the interactions between individual nucleons and external probes*

**Nucleon-nucleon (NN) and 3N scattering data:** “thousands” of experimental data available

**Spectra, properties, and transition of nuclei:** BE, radii, magnetic moments, beta decays rates, weak/radiative captures, electroweak form factors, etc,...

**Nucleonic matter equation of state:** for ex. EOS neutron matter

**Disentangle new physics from nuclear effects:** for ex.  $0\nu\beta\beta$ , BSM with  $\beta$ -decay, EDMs,  $\nu - A$  xsec, etc,...

# The microscopic model of nuclear theory

- *What we need?*

Two and many-body interactions:

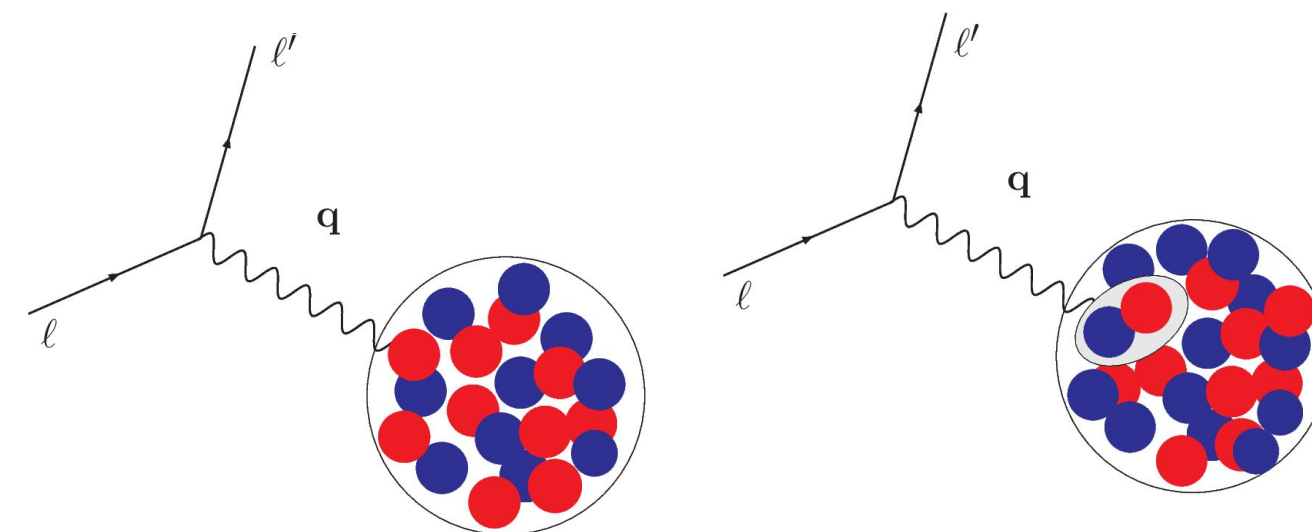
$$H = \sum_{i=1}^A \frac{\mathbf{p}_i^2}{2m_i} + \sum_{i<j=1}^A v_{ij} + \sum_{i<j<k=1}^A V_{ijk} + \dots$$

one-body
two-body (NN)
three-body (3N)

Electroweak current operators:

$$j^{\text{EW}} = \sum_{i=1}^A j_i + \sum_{i<j=1}^A j_{ij} + \sum_{i<j<k=1}^A j_{ijk} + \dots$$

one-body
two-body
three-body



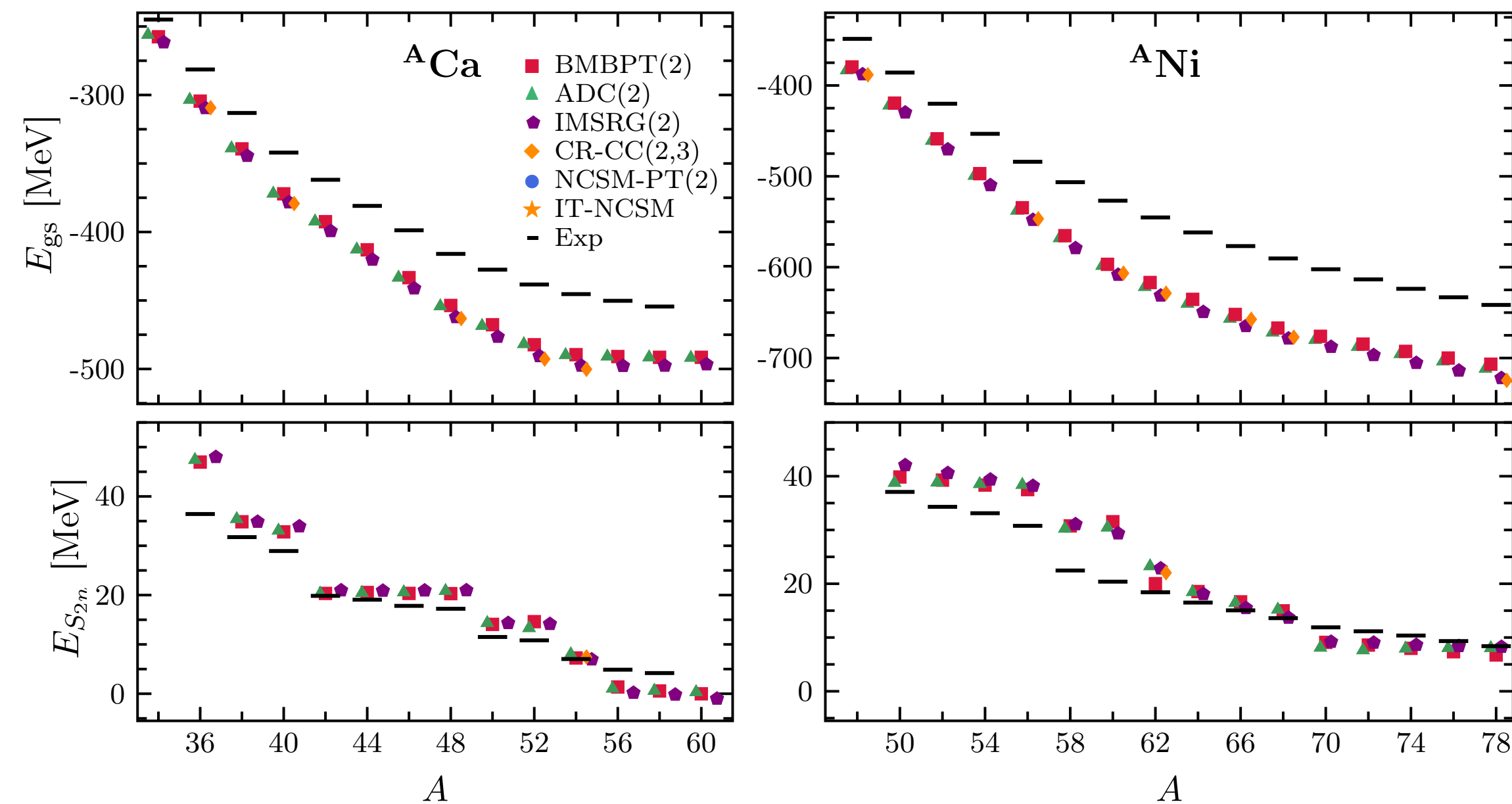
# The microscopic model of nuclear theory

- *What we need?*

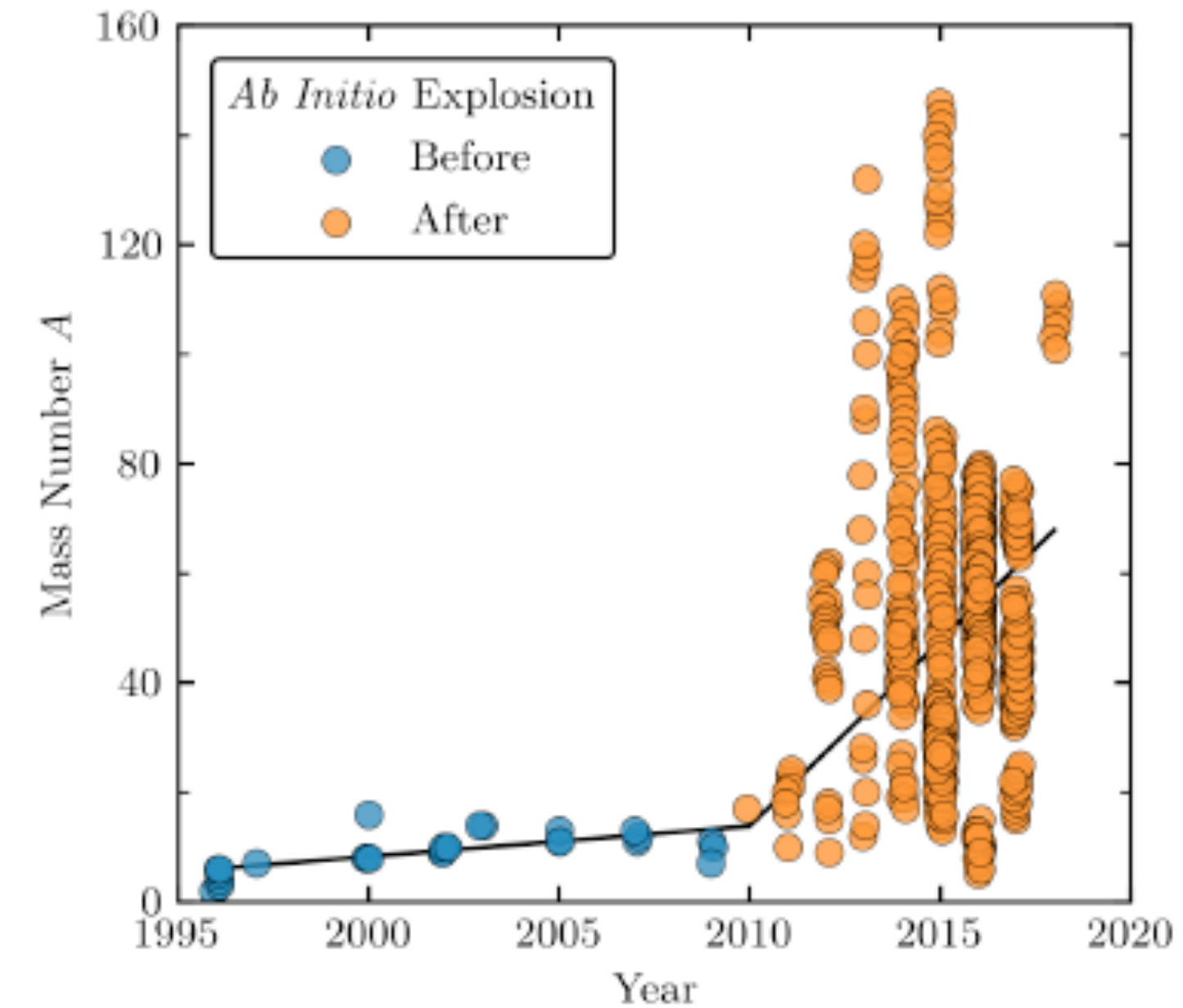
## Ab-initio methods: solve the nuclear many-body problem

- Improved and novel many-body frameworks
- Nuclear interactions and currents based on EFTs
- Increased computational resources
- Theoretical uncertainty quantification

Tichai *et al.* PLB 786, 195 (2018)



Credit to Heiko Hergert (MSU/FRIB) for collecting the data



- Increased many-body capability, algorithms under control
- Remarkable agreement between different ab initio many-body methods for the structure of nuclei (not the same for infinite matter, continuum coupling,..)

# The nuclear many-body problem

Many-body Schrödinger equation:

$$\begin{aligned} H \Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A; s_1, s_2, \dots, s_A; t_1, t_2, \dots, t_A) \\ = E \Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A; s_1, s_2, \dots, s_A; t_1, t_2, \dots, t_A) \end{aligned}$$



Erwin Schrödinger



where  $\mathbf{r}_i$ ,  $s_i$ , and  $t_i$  are the nucleon coordinates, spins, and isospins, respectively

This corresponds to solve

$2^A \times \binom{A}{Z}$  coupled second-order differential equations in  $3A$  dimensions.

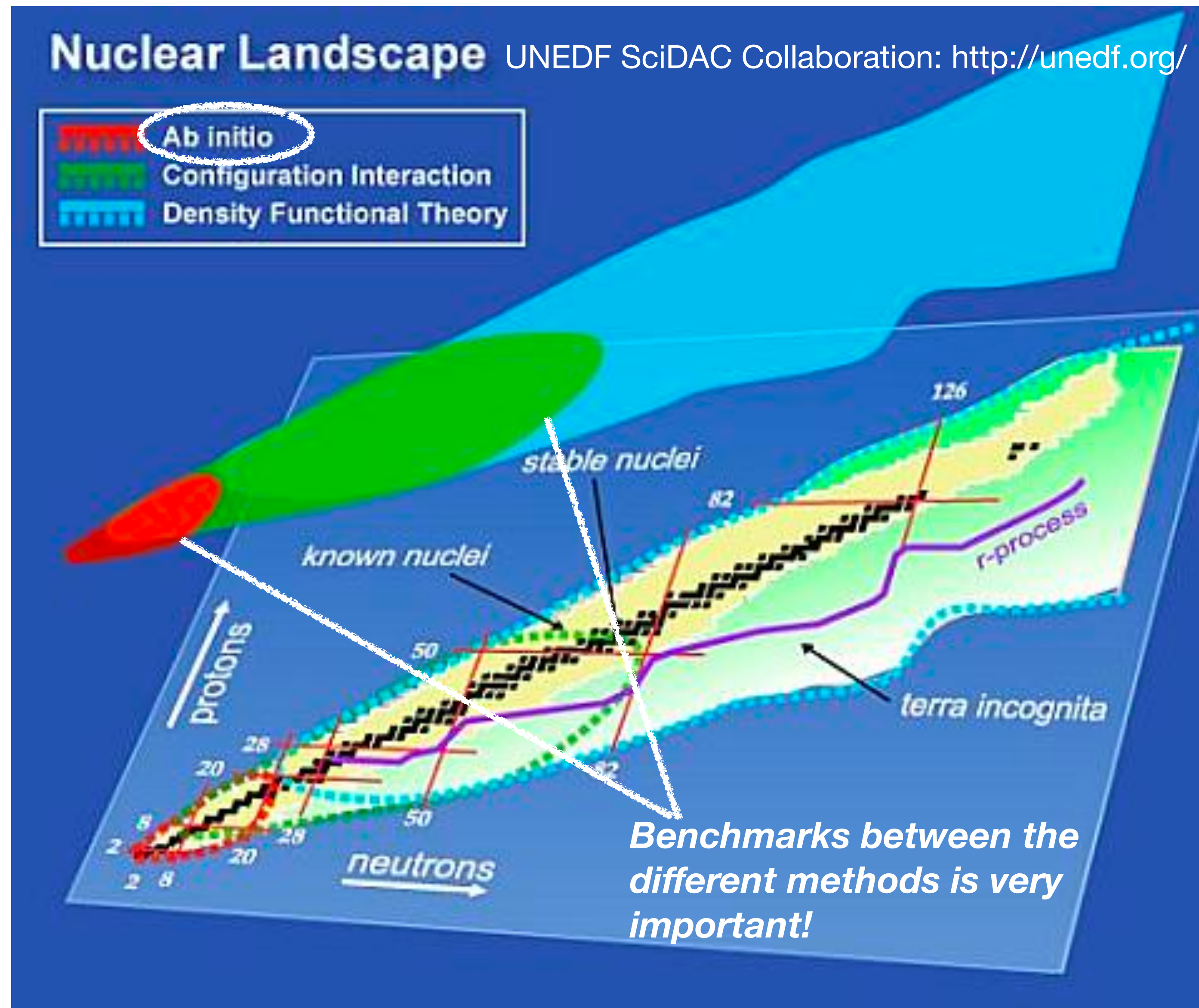
96 for  ${}^4\text{He}$

17,920 for  ${}^8\text{Be}$

3,784,704 for  ${}^{12}\text{C}$

*This is a challenging many-body problem!*

# The nuclear landscape

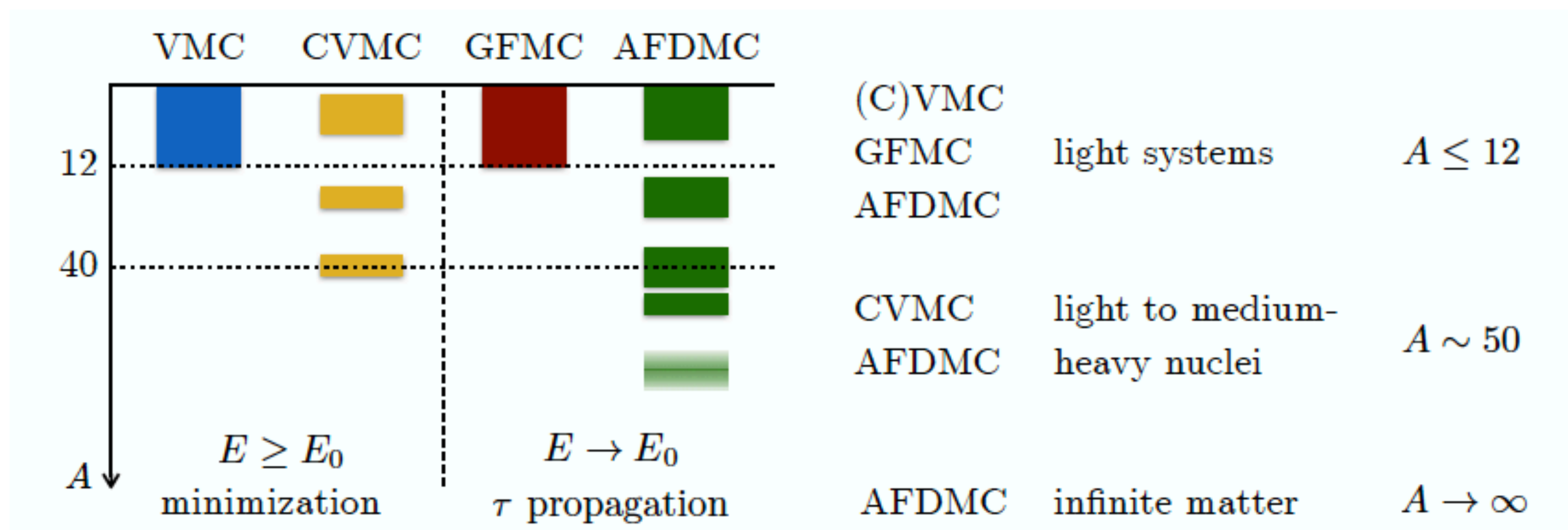


**Definition:** the *ab-initio* methods seek to describe atomic nucleus from the ground up by solving the non-relativistic Schrödinger equation for all constituent nucleons and the forces between them



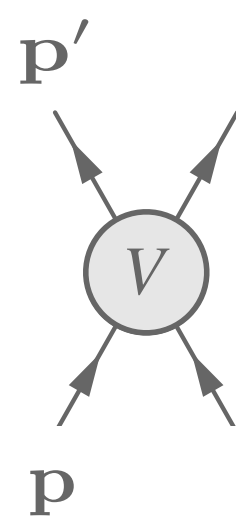
# Nuclear quantum Monte Carlo methods

- Quantum Monte Carlo (QMC) methods: a large family of computational methods whose common aim is the study of complex quantum systems—J. Carlson et al., RMP. 87, 1067 (2015); J.E. Lynn et al., Ann. Rev. Nucl. Part. Sci 279, 69 (2019); S. Gandolfi, MP et. al., Front.in Phys. 8 (2020) 117



Computational resources awarded by the DOE ALCC and INCITE programs

- Work with bare interactions but local r-space representation of the Hamiltonian



$$\mathbf{k} = \mathbf{p}' - \mathbf{p}$$

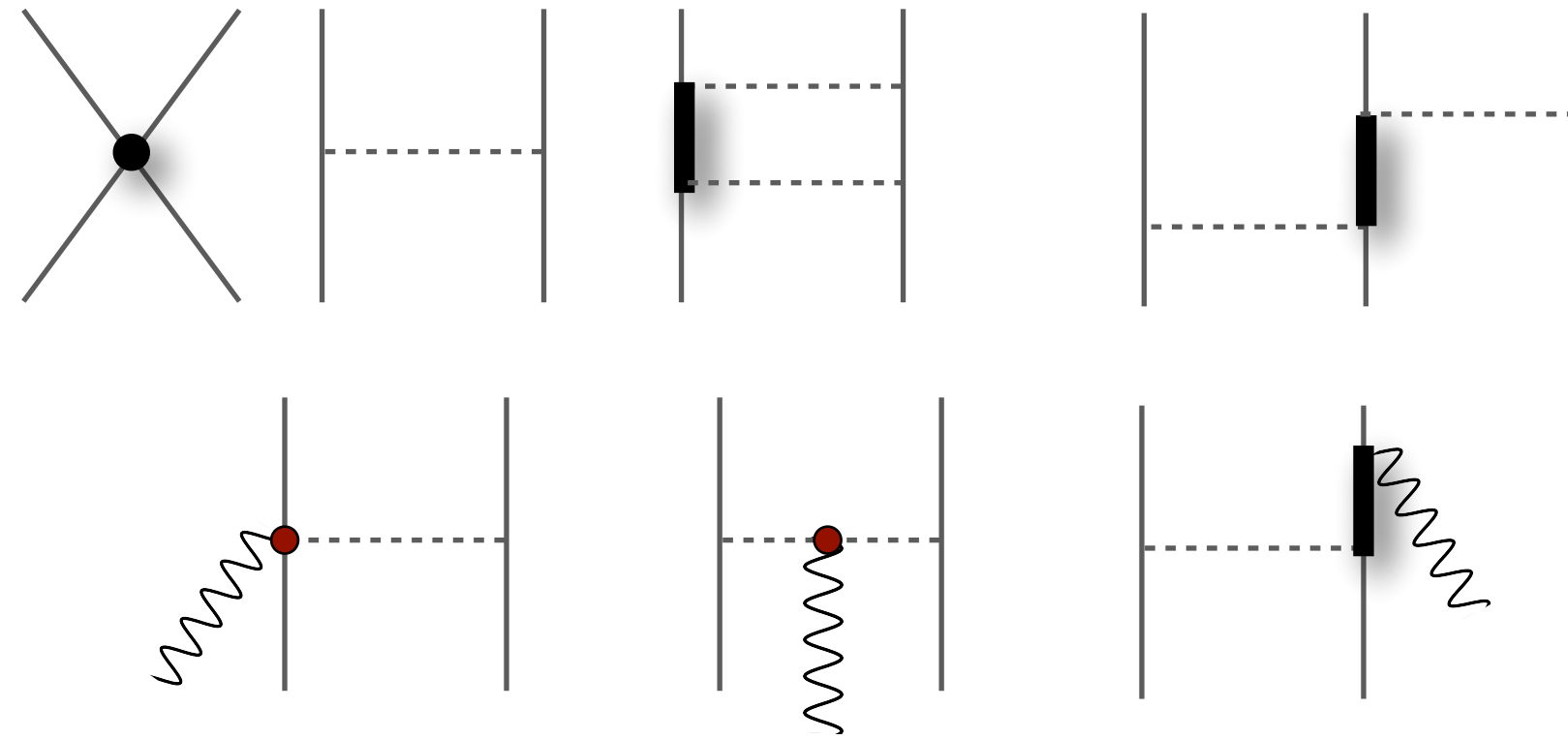
Local

$$\mathbf{K} = (\mathbf{p}' + \mathbf{p})/2$$

Non-Local

- Stochastic method: based on recursive sampling of a probability density, statistical errors quantifiable and systematically improvable

# Hamiltonian and electroweak currents



Historically research on the nuclear force (and corresponding electroweak operators) has proceeded along different ways for example:

## Phenomenological approach:

use the general form of a potential allowed by the symmetries (rotation, translation, isospin, etc); potential terms are needed to describe various phenomena remarked in nuclear interactions

## $\chi$ EFT approach:

pion and nucleon degrees of freedom constructing their interactions consistently with the symmetries and symmetry breaking of the underlying theory, low-energy QCD

# Phenomenological approach

- Use the general form of a potential allowed by the symmetries:

- |                               |  |
|-------------------------------|--|
| - Translation invariance      | - Time reversal invariance                             |
| - Galilean invariance         | - Invariance under the interchange of particle 1 and 2 |
| - Rotation invariance         | - Isospin symmetry                                     |
| - Space reflection invariance | - Hermiticity  |

- Most general two-body potential under those symmetries: ([Okubo and Marshak, Ann. Phys. 4, 166 \(1958\)](#))

$$\begin{aligned}
 V_{NN} = & V_0(r) + V_\sigma \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 + V_\tau \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 + V_{\sigma\tau} \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \text{ central} \\
 & + V_T(r) S_{12} + V_{T\tau}(r) S_{12} \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \text{ tensor} \\
 & + V_{LS}(\mathbf{L} \cdot \mathbf{S}) + V_{LS\tau}(\mathbf{L} \cdot \mathbf{S}) \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \text{ spin-orbit} \\
 & + V_Q Q_{12} + V_{Q\tau} Q_{12} \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \text{ quadratic spin-orbit} \\
 & + V_{PP}(r) (\boldsymbol{\sigma}_1 \cdot \mathbf{p})(\boldsymbol{\sigma}_2 \cdot \mathbf{p}) + V_{PP\tau}(r) (\boldsymbol{\sigma}_1 \cdot \mathbf{p})(\boldsymbol{\sigma}_2 \cdot \mathbf{p}) \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \text{ p-dependent}
 \end{aligned}$$

$$S_{12} = 3 \boldsymbol{\sigma}_2 \cdot \mathbf{r} \boldsymbol{\sigma}_2 \cdot \mathbf{r} - r^2 \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \quad Q_{12} = 1/2 \{ (\boldsymbol{\sigma}_1 \cdot \mathbf{L})(\boldsymbol{\sigma}_2 \cdot \mathbf{L}) + (\boldsymbol{\sigma}_2 \cdot \mathbf{L})(\boldsymbol{\sigma}_1 \cdot \mathbf{L}) \}$$

## Examples:

- Gammel-Thaler potential ( Phys. Rev. **107**, 291, 1339 (1957)), hard-core.
- Hamada-Johnston potential (Nucl. Phys. **34**, 382 (1962)), hard core.
- Reid potential (Ann. Phys. (N.Y.) **50**, 411 (1968)), soft core.
- Argonne **V14** potential (Wiringa *et al.*, Phys. Rev. C **29**, 1207 (1984)), uses 14 operators.
- Argonne **V18** potential (Wiringa *et al.*, Phys. Rev. C **51**, 38 (1995)), uses 18 operators.

# Phenomenological nucleon-nucleon AV18

- It is a r-space potential expressed as a sum of EM and OPE terms and phenomenological intermediate- and short-range parts:

Argonne v18

$$v_{ij} = v_{ij}^{\gamma} + v_{ij}^{\pi} + v_{ij}^I + v_{ij}^S = \sum v_p(r_{ij}) O_{ij}^p$$

$v_{ij}^{\gamma}$ : *pp, pn & nn electromagnetic terms*

$$v_{ij}^{\pi} \sim [Y_{\pi}(r_{ij})\sigma_i \cdot \sigma_j + T_{\pi}(r_{ij})S_{ij}] \otimes \tau_i \cdot \tau_j$$

$$v_{ij}^I = \sum_p I^p T_{\pi}^2(r_{ij}) O_{ij}^p$$

$$v_{ij}^S = \sum_p [P^p + Q^p r + R^p r^2] W(r) O_{ij}^p$$

- Minimum of eight different potential terms needed to fit S- and P- wave data: four for different S, T combinations, plus two tensor and two spin-orbit terms in S = 1 states for different T.

$$O_{ij}^{p=1,8} = [1, \sigma_i \cdot \sigma_j, S_{ij}, \mathbf{L} \cdot \mathbf{S}] \otimes [1, \tau_i \cdot \tau_j]$$

$$S_{ij} = 3 \sigma_i \cdot \mathbf{r} \sigma_j \cdot \mathbf{r} - r^2 \sigma_i \cdot \sigma_j$$

- To fit higher partial waves, momentum-dependent terms are needed, e.g.,

$$O_{ij}^{p=9,14} = [L^2, L^2 \sigma_i \cdot \sigma_j, (\mathbf{L} \cdot \mathbf{S})^2] \otimes [1, \tau_i \cdot \tau_j]$$

- Add small isospin-breaking terms:

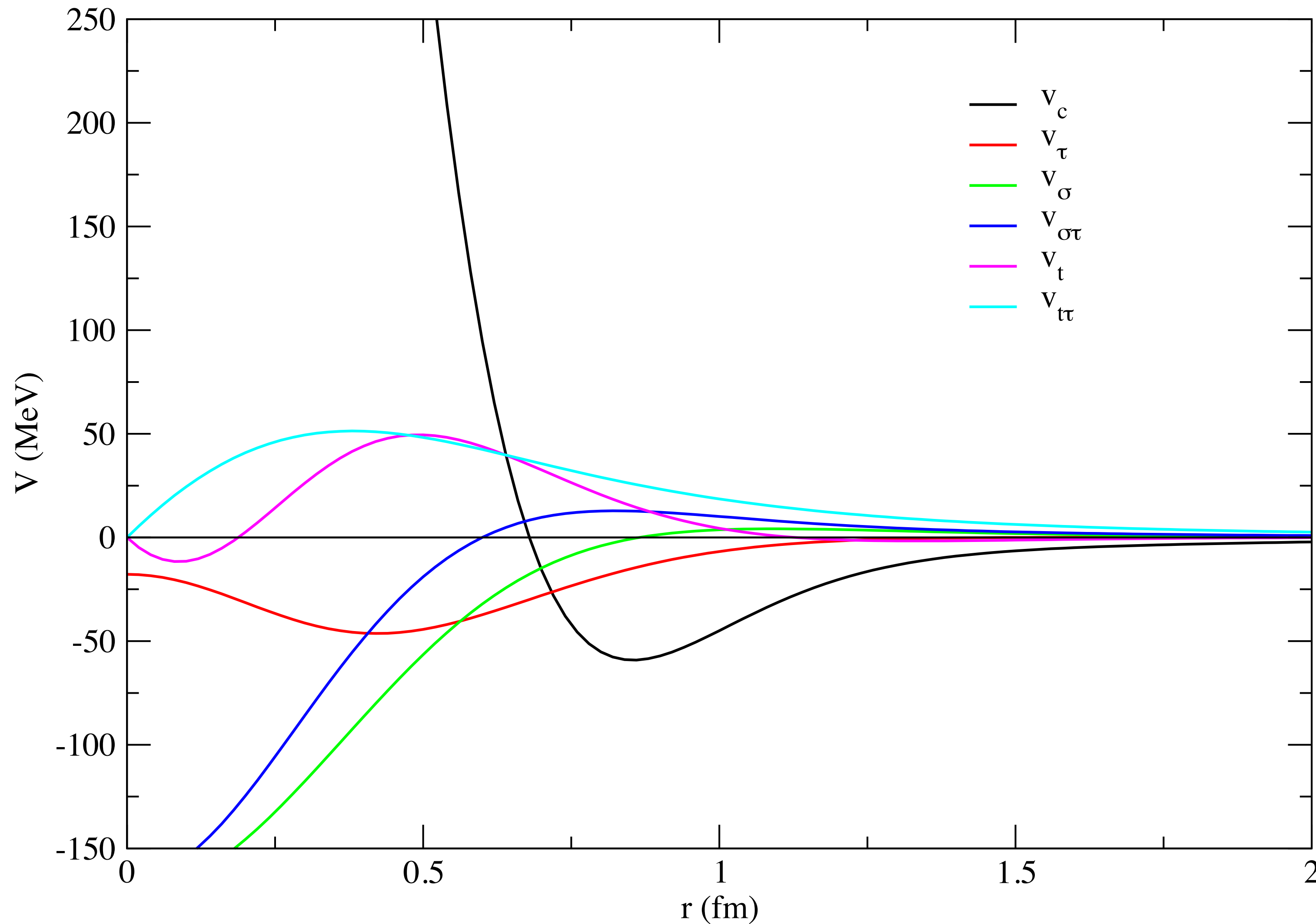
$$O_{ij}^{p=15,22} = [1, \sigma_i \cdot \sigma_j, S_{ij}, \mathbf{L} \cdot \mathbf{S}] \otimes [T_{ij}, \tau_{z_i} + \tau_{z_j}]$$

$$T_{ij} = 3 \tau_{iz} \tau_{jz} - \tau_i \cdot \tau_j$$



Wiringa, Stoks, Schiavilla, PRC  
51, 38 (1995)

# Argonne nucleon-nucleon V18



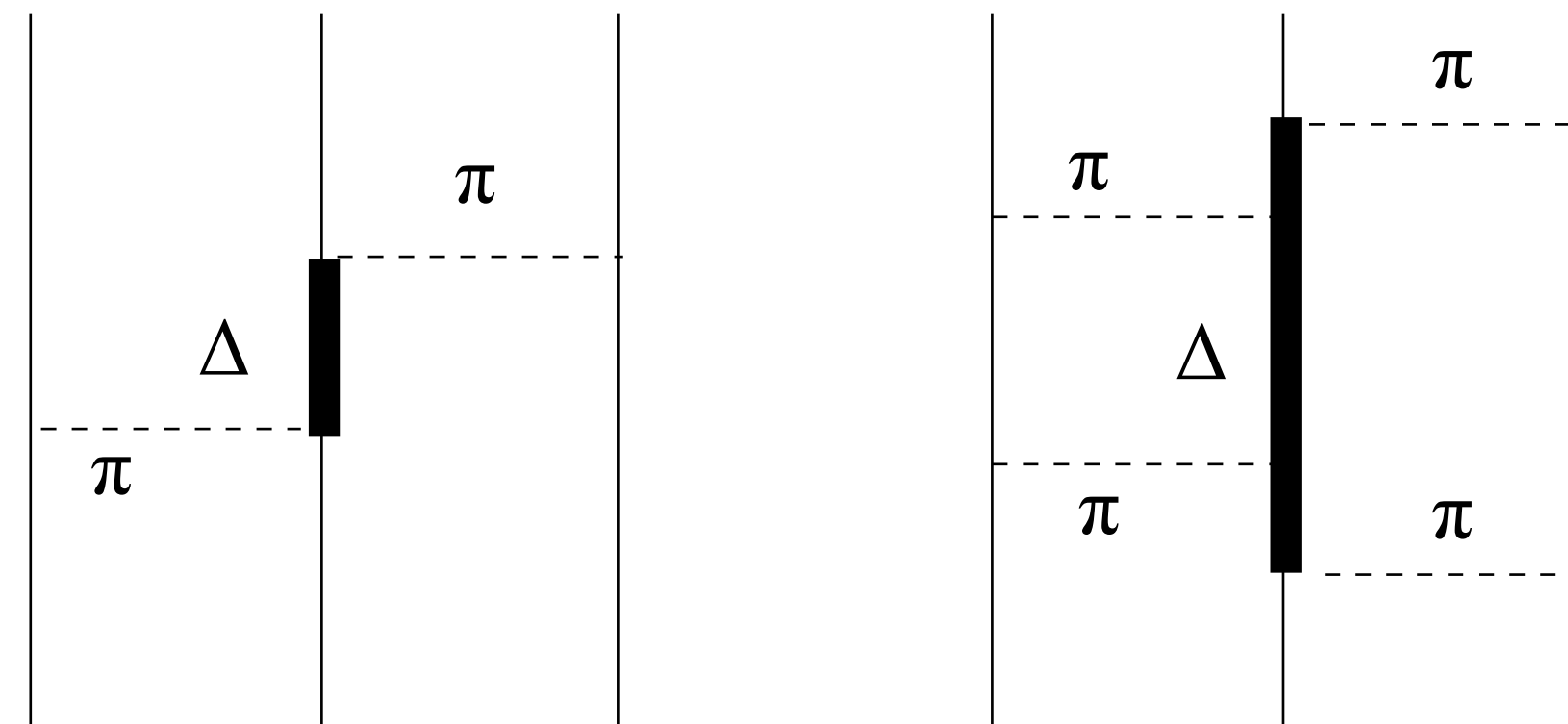
- The AV18 model uses 42  $I^P, P^P, Q^P, R^P$  parameters, one cutoff parameter in  $Y_\pi(r), T_\pi(r)$ .
- These parameters have been fixed by fitting the Nijmegen database of  $\sim 4300$  np and pp scattering data for  $E_{\text{lab}} \leq 350$  MeV with a total  $\chi^2 \cong 1$  plus nn scattering length and deuteron binding energy.

# Phenomenological three-nucleon potentials: Urbana-Illinois

- **3N Urbana-Illinois (UIX-IL7)**: an Hamiltonian which only includes AV18 does not provide enough binding in the light nuclei. In light nuclei we find [thanks to large cancellations between  $\langle T \rangle$  and  $\langle v_{ij} \rangle$ ]:  $\langle V_{ijk} \rangle \sim (0.02 - 0.07) \langle v_{ij} \rangle \sim (0.2 - 0.5) \langle H \rangle$

**Urbana:** J. Carlson et al. NP A401, 59 (1983)

contains the attractive Fujita and Miyazawa two-pion exchange interaction and a phenomenological repulsive term

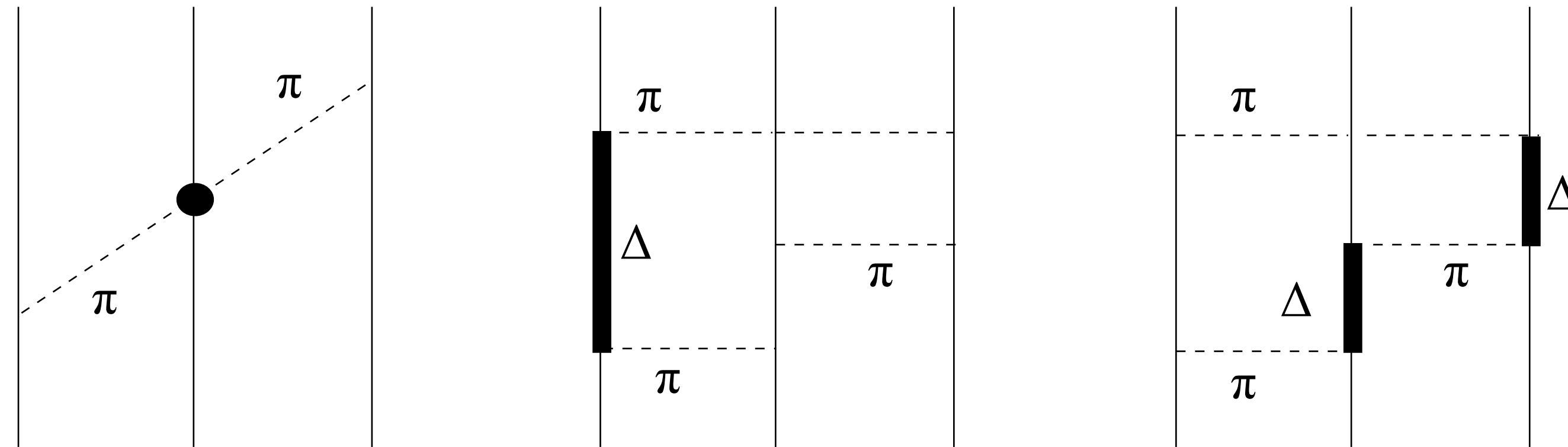


2 independent parameters controlled by  ${}^3\text{H}$  binding energy & saturation density of symmetric nuclear matter. Good description for s-shell nuclei ( $A=3,4$ ) and neutron stars; *inadequate description of the absolute p-shell and spin-orbit splitting of heavier nuclei*

Illinois: S. Pieper et al. PRC 64, 014001 (2001)

also includes terms originating from three-pion rings containing one or two  $\Delta$ s and the two-pion S-wave contribution. This interaction is attractive in  $nnn$  triplets with  $T = 3/2$  and provides extra attraction observed in neutron rich nuclei.

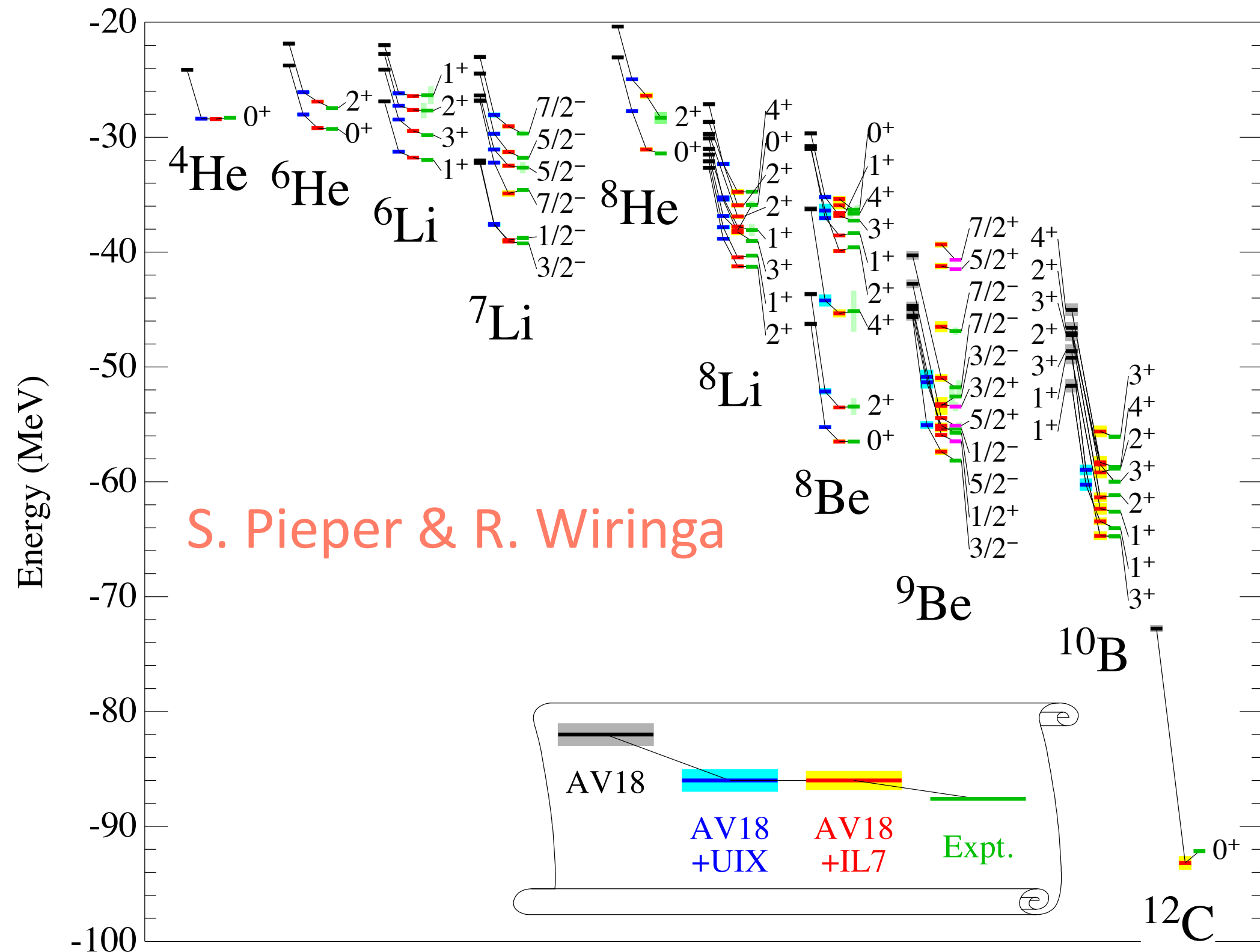
Urbana +



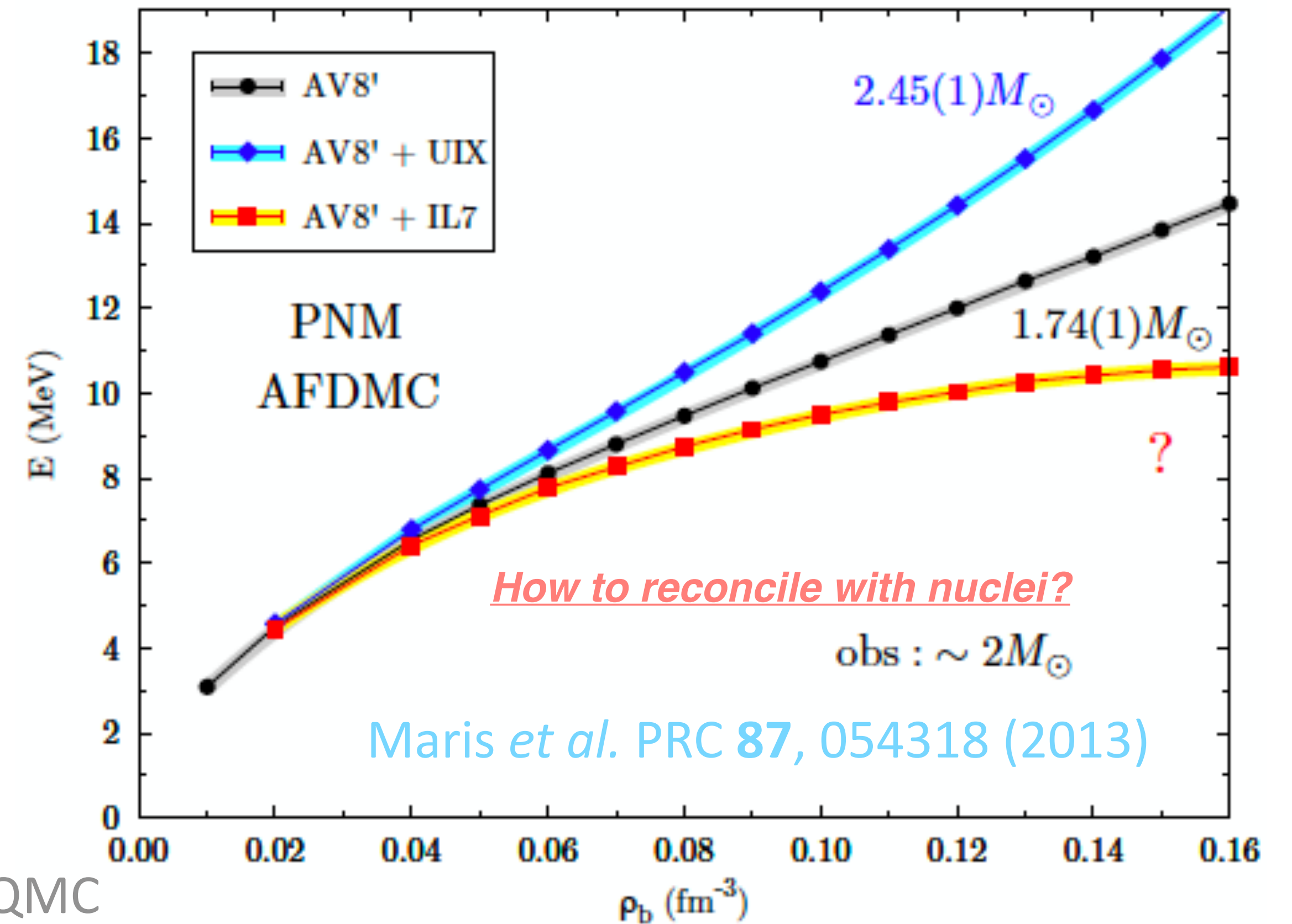
5 independent parameters controlled by ground-state energies of  $A \leq 10$ . Good description for light nuclei up to  $A=12$ ; *inadequate description of the neutron star matter equation of state.*

# Phenomenological potentials & QMC

GFMC calculations of the spectra of light-nuclei using **AV18** without and with **UIX** or **IL7**



The EoS of pure neutron matter (PNM): useful tool to understand properties of neutrons stars



- Suitable for computational methods like QMC

## Pros:

- Very good description of several nuclear observables: ex. GFMC binding energies up to  $A=12$  with AV18+IL7 (GFMC energies: uncertainties within 1-2%)

## Cons:

- Phenomenological interactions are phenomenological, not clear how to improve their quality
- They do not provide rigorous schemes to consistently derive NN and 3N forces and compatible electroweak currents



# Chiral effective field theory: the framework in a nutshell

S. Weinberg, Phys. Lett. **B251**, 288 (1990); Nucl. Phys. **B363**, 3 (1991); Phys. Lett **B295**, 114 (1992)

QCD

Symmetries in particular the approximate chiral symmetry between hadronic d.o.f ( $\pi$ ,  $N$ ,  $\Delta$ )

Approximate chiral symmetry requires the pion to couple to other pions and to baryons by powers of its momentum

Effective chiral Lagrangian  $\mathcal{L}_{eff}(\pi, N, \Delta)$

Calculate amplitudes+prescription to obtain potentials + regularization (of high momentum components)



Nuclear forces and currents

$$\mathcal{L}_{eff} = \mathcal{L}^{(0)} + \mathcal{L}^{(1)} + \mathcal{L}^{(2)} + \dots$$

Given a power counting scheme

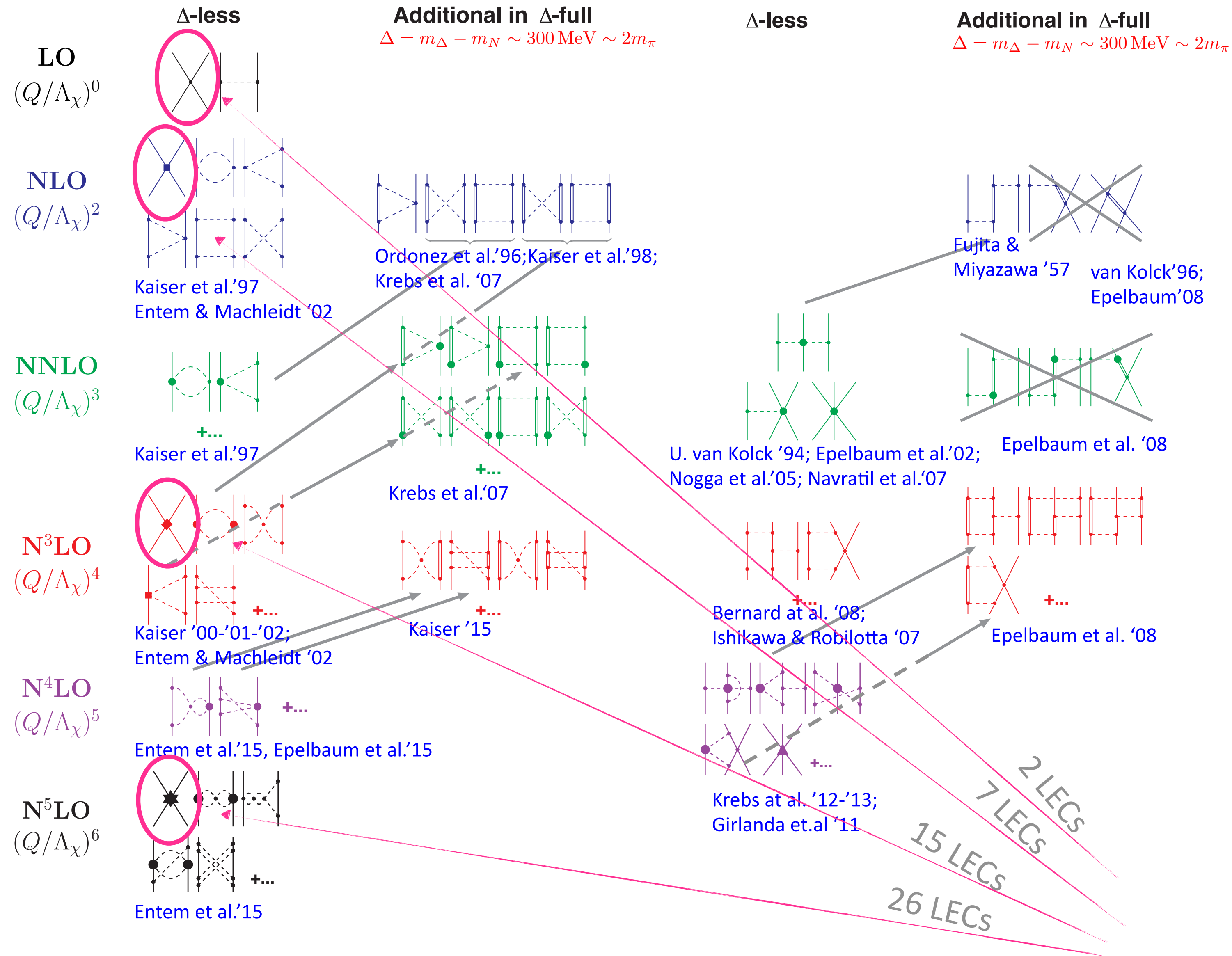
$$\mathcal{L}^{(n)} \sim \left( \frac{Q}{\Lambda_\chi} \right)^n \begin{array}{l} \sim 100 \text{ MeV soft scale} \\ \sim 1 \text{ GeV hard scale} \end{array}$$

Few- and many-body methods: QMC, NCSM, CC, etc



Nuclear structure and dynamics

# State-of-the art Chiral EFT interactions



## Advantages:

- Consistent description of two- and many-body interactions and currents
- Different processes described on the same footing: piN, NN, electroweak
- UQ due to the truncation in the chiral expansion
- Scheme can be systematically improved

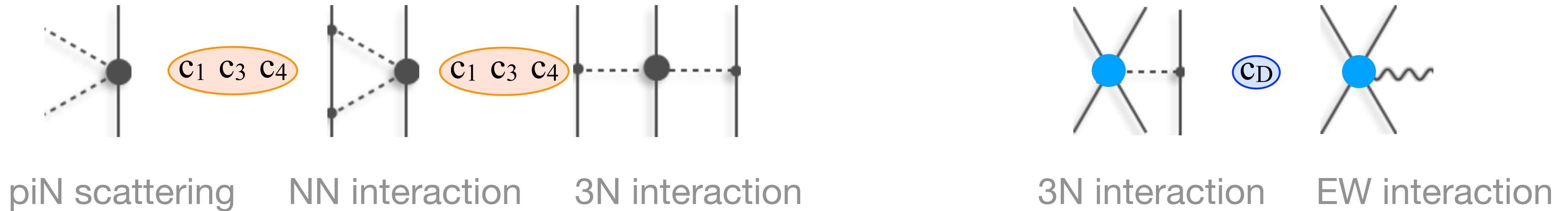
## Disadvantages:

- Increase in number of diagrams at higher orders; When do we stop in the chiral expansion? Convergence, power counting, etc....
- Consistency between strong- and electroweak sector very hard to achieve
- More LECs appearing at higher orders; challenging optimization problem

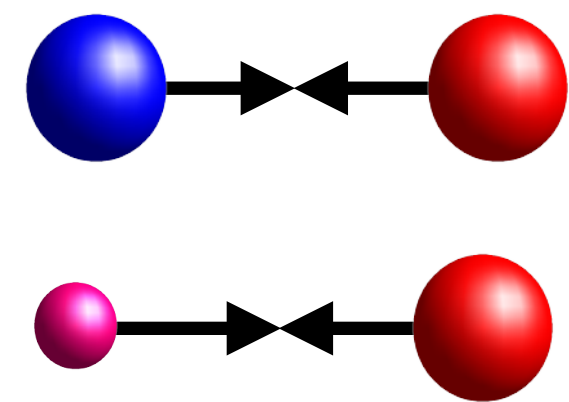
# How to fix the LECs?

First Challenge: *What experimental data should we use to find the LECs?*

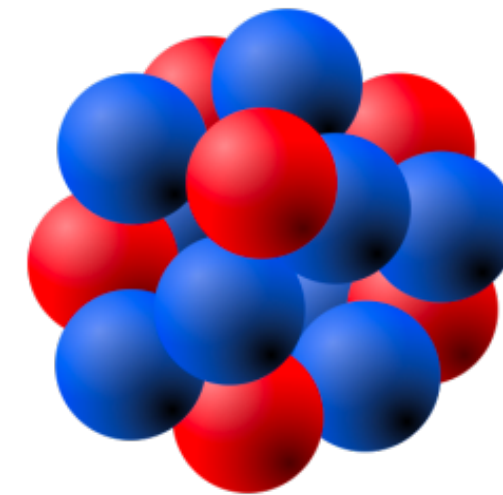
some LECs in chiral EFT appear in different low energy processes



Remaining LECs constrained to:



Scattering observables: piN, NN, NNN..



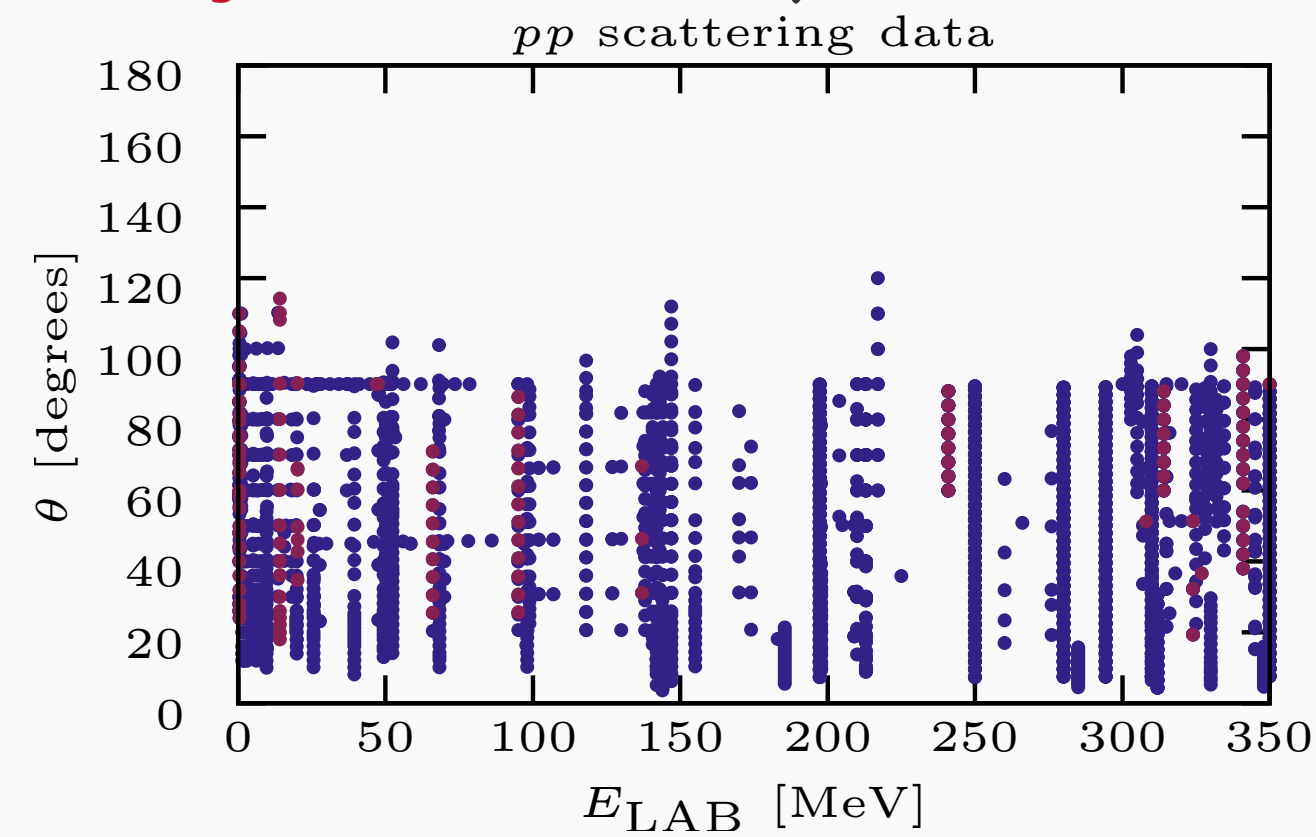
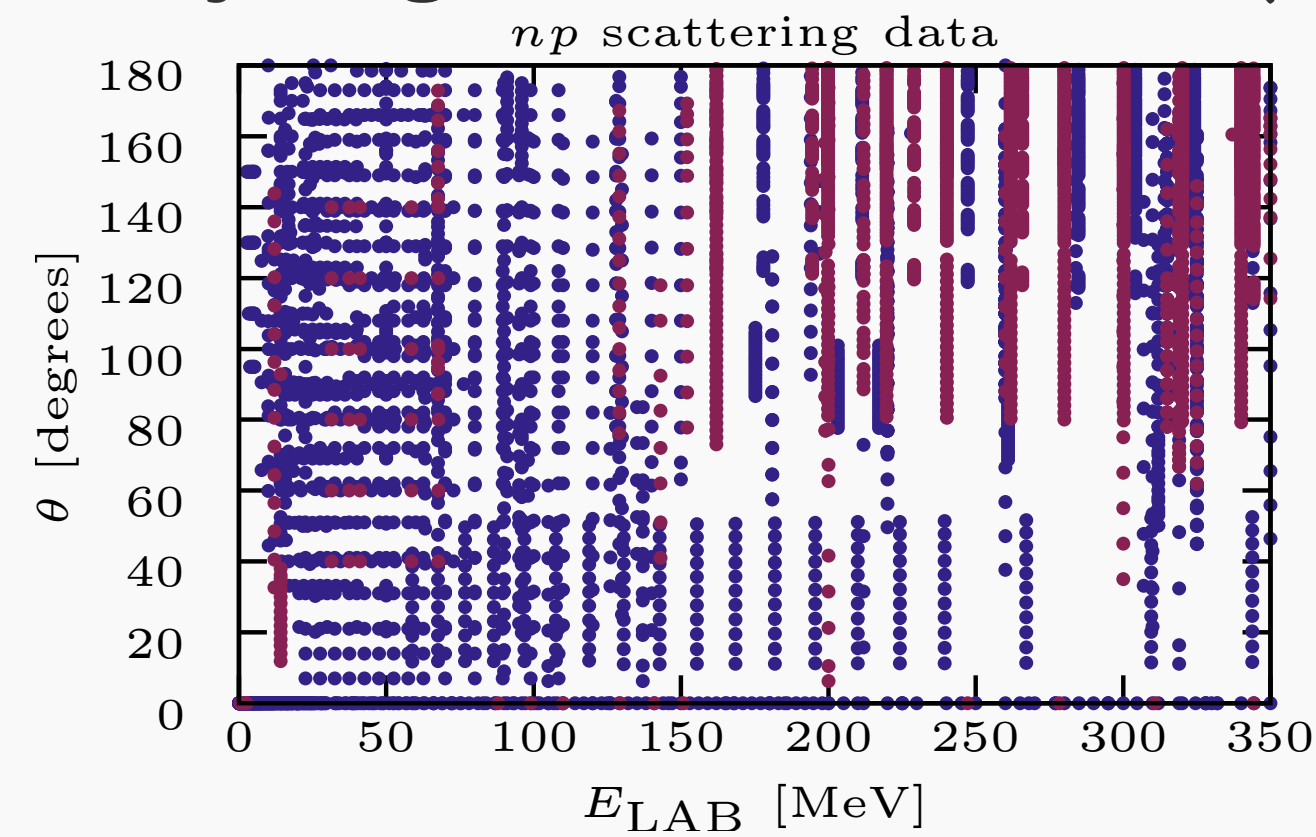
Static and dynamic properties of few- and many-body systems

# Fits of NN Interactions: nucleon-nucleon scattering data

The Granada NN database is the most up to date database. The analysis includes data within the years 1950 to 2013. <http://www.ugr.es/~amaro/nndatabase/>

More than 7800 elastic scattering data up to  $E_{\text{LAB}}=350$  MeV

Usual Nijmegen  $3\sigma$  criterion (1677 rejected data)

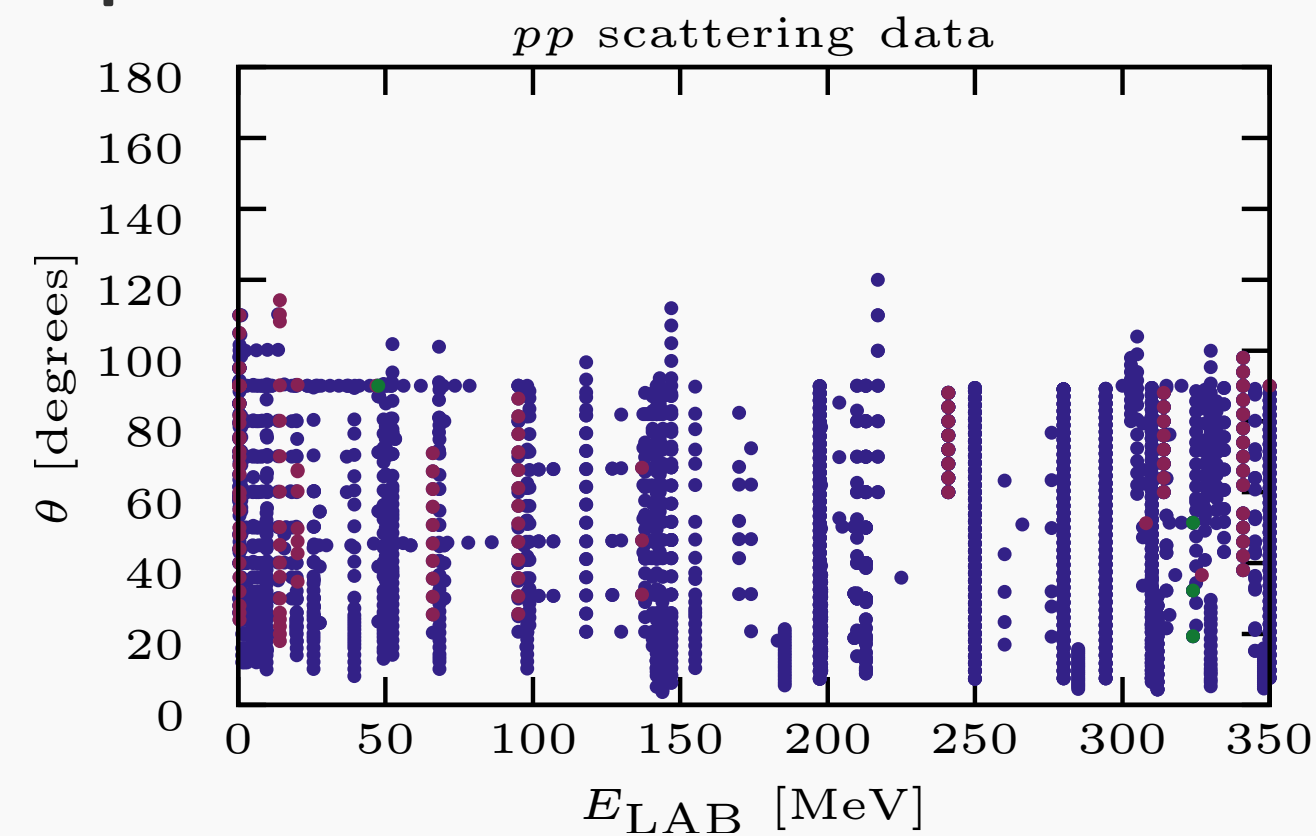
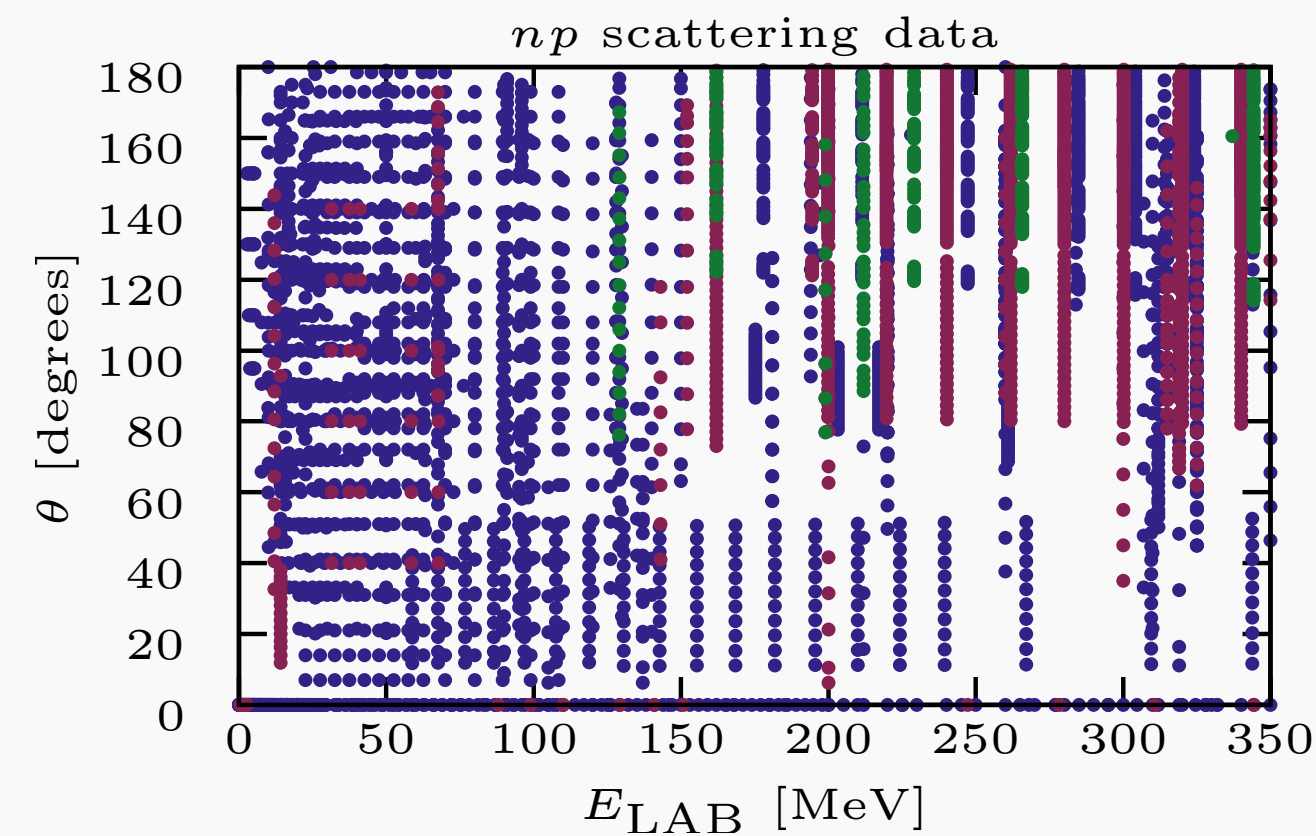


Maximization of the experimental consensus:

Fit to all data  
Apply  $3\sigma$  criterion  
Refit parameters

Re-apply  $3\sigma$  criterion to all data  
Repeat until no more data is excluded or recovered

300 recovered data with Granada procedure



Perez, Amaro, Arriola PRC88 (2013) 064002

# Chiral NN potentials: some recent developments

- Optimized N2LO NN potential ( $\pi$ N LECs are tuned to NN peripheral scattering): [Ekström et al. \(PRL \*\*110\*\*, 192502 2013; JPG \*\*42\*\*, 034003 2015\)](#)
- N2LO potential: a simultaneous fit of NN and 3N forces to low NN data ( $E_{\text{lab}}=35$  MeV), deuteron BE, BE and CR of hydrogen, helium, carbon and oxygen isotopes; [Carlsson et al. \(PRC \*\*91\*\*, 051301\(R\) 2015\)](#)
- New generation of chiral NN potentials up to N4LO: improved choice of the regulator, no SFR; [Epelbaum et al. \(PRL. \*\*112\*\*, 102501, 2014; EPJ A \*\*51\*\*, 53 2015; PRL. \*\*115\*\*, 122301, 2015\)](#)
- Chiral  $2\pi$  and  $3\pi$  exchange up to N4LO and up to N5LO in NN peripheral scattering; [Entem et al. \(PRC \*\*91\*\*, 014002 2015; PRC \*\*92\*\*, 064001 2015\)](#)
- High-quality two-nucleon potentials up to fifth order of the chiral expansion ([PRC \*\*96\*\*, 024004 2017; Front.in Phys. \*\*8\*\* 57 2020](#))
- High-Precision Nucleon-Nucleon Potentials from Chiral EFT; [Reinert, Krebs, Epelbaum \(Springer Proc. Phys. \*\*238\*\* 497-501 \(2020\)](#))
- ....

NOTE: – Many of the available versions of chiral potentials are formulated in p-space and are strongly nonlocal:

Nonlocalities due to contact interactions  
Nonlocalities due to regulator functions   $\mathbf{p} \rightarrow -i\nabla$

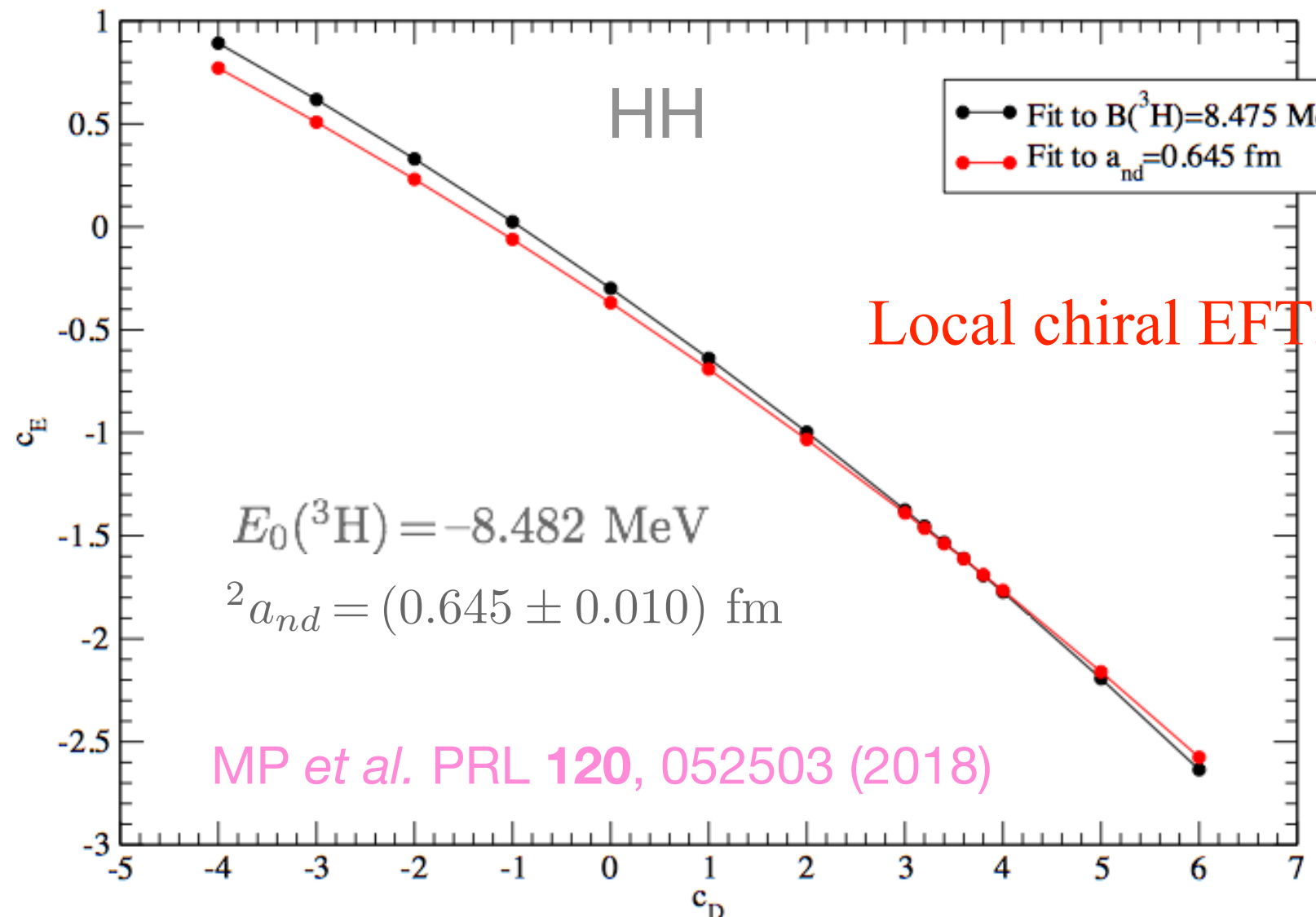
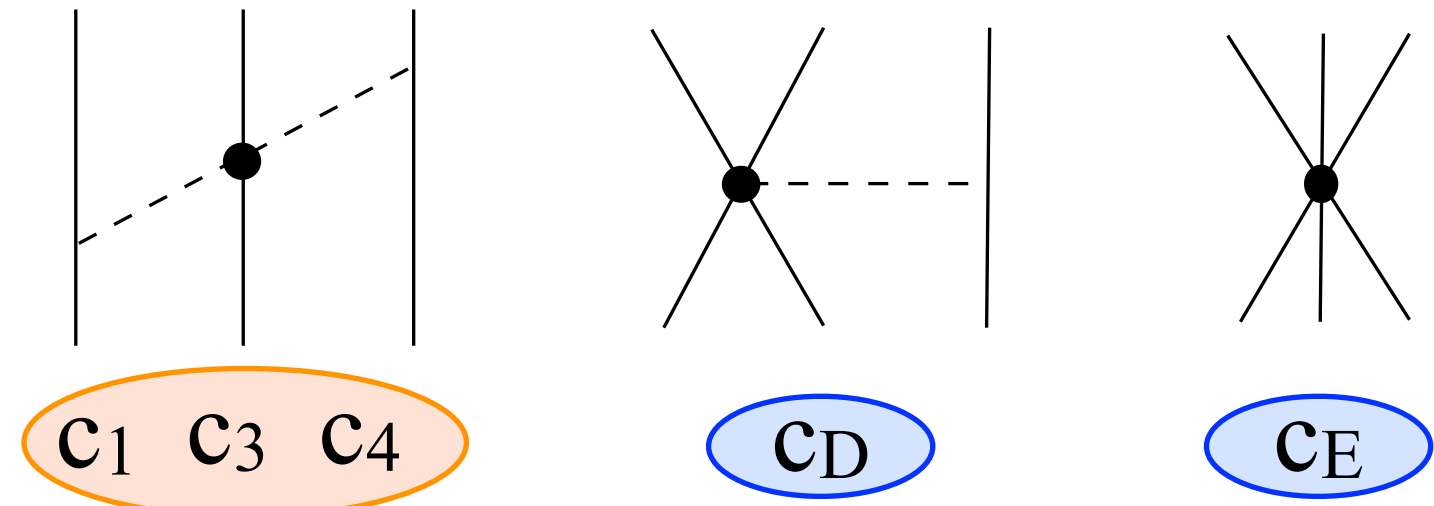
– Nonlocal interactions hard to handle in for example Quantum Monte Carlo (QMC) methods

- Local NN potentials up to N2LO: Gezerlis et al. ([PRL \*\*111\*\*, 032501 2013, PRC \*\*90\*\*, 054323 2014](#)); Lynn et al. ([PRL \*\*113\*\* 192501, 2014](#))
- Minimally nonlocal NN potentials up to N3LO (including N2LO  $\Delta$  contributions); [Piarulli et al. \(PRC \*\*91\*\*, 024003 2015\)](#)
- Local chiral potential with  $\Delta$ -intermediate states up to N3LO; [Piarulli et al. \(PRC \*\*94\*\*, 054007 2016\)](#)
- Local position-space two-nucleon potentials from leading to fourth order of chiral effective field theory; [S.K. Saha \(arxiv \*\*2209.13170\*\*\)](#)

# Fits of 3N Interactions: three-body scattering cross sections

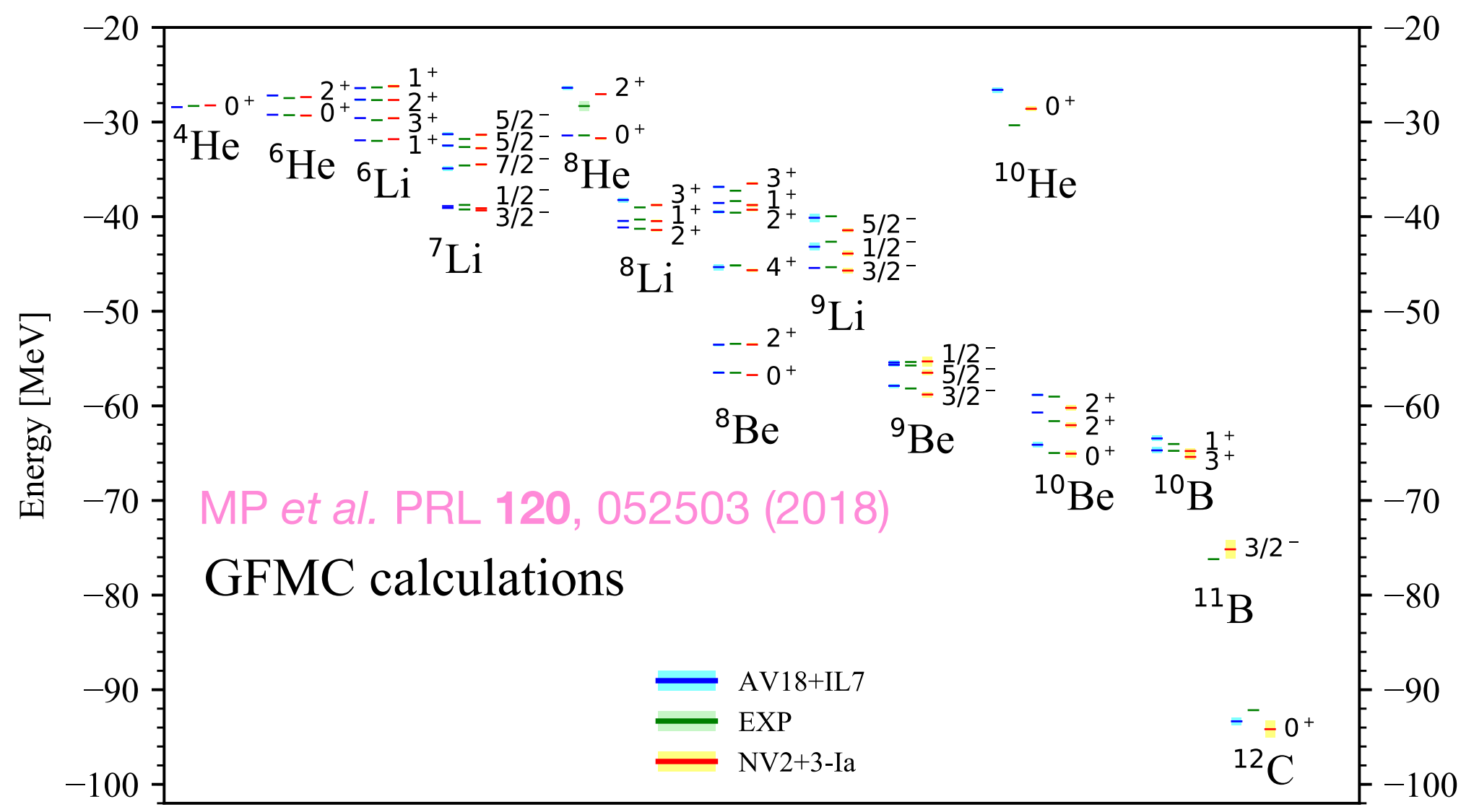
- Inclusion of 3N forces at N2LO:

Constrained from  $\pi N$  scattering or  $NN$ : ex.  
 Hoferichter et al., Phys.Rept. 625 (2016) 1

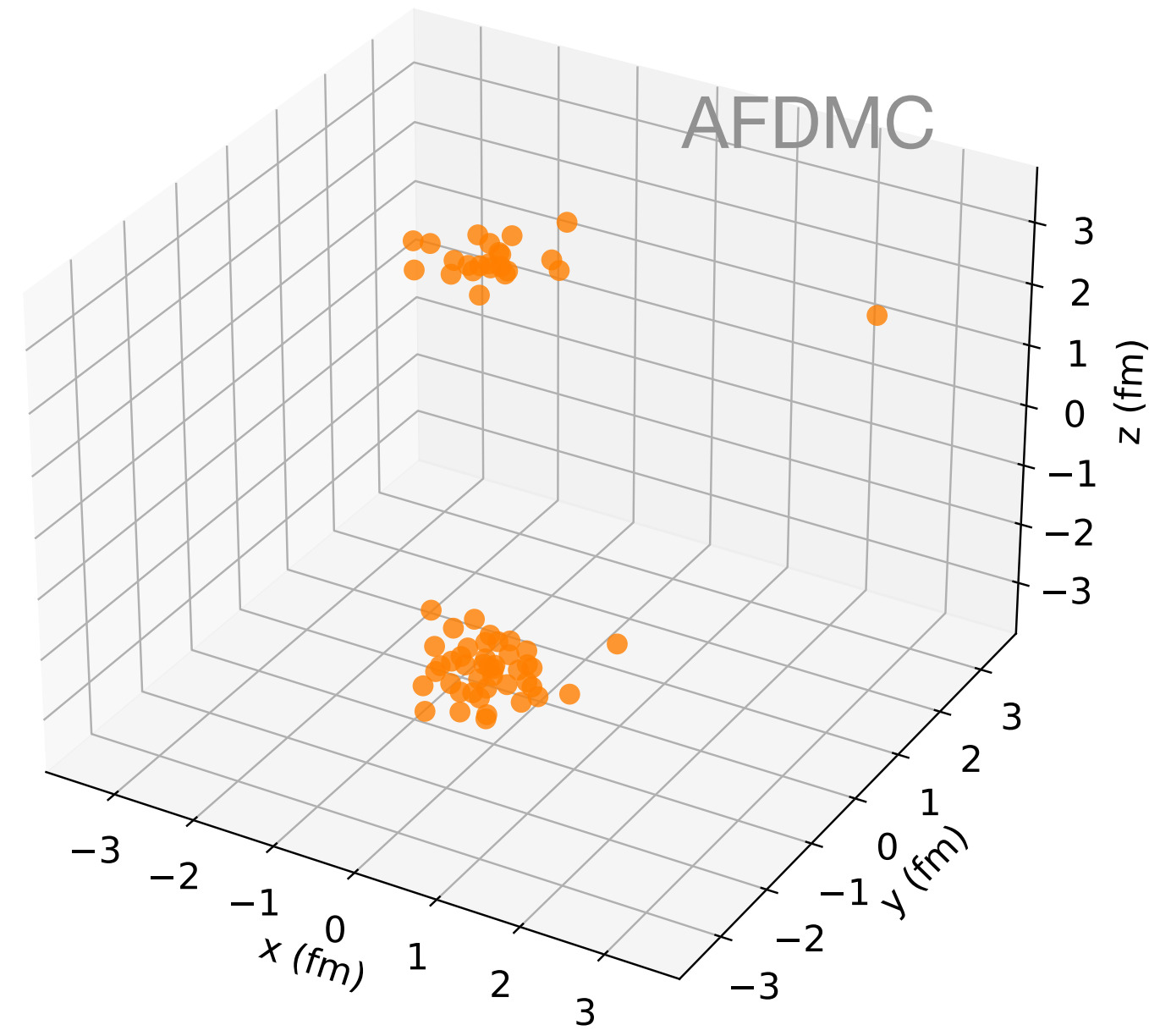


Model	$c_D$	$c_E$
Ia	3.666	-1.638
Ib	-2.061	-0.982
IIa	1.278	-1.029
IIb	-4.480	-0.412

Spectra of light nuclei and charge radii in good agreement with data but....



- ..... relatively large and negative values of  $c_E$ : “collapse” of PNM, whose energy per particles became large ( $\sim$  several GeV per particle).
- The collapse is associated with the formation of “droplets” of closely packed neutrons, ultimately caused by the attractive nature of the  $c_E$  term in the 3N force.



a single scattering observable not too constraining (correlated with energy of  $^3\text{H}$ )

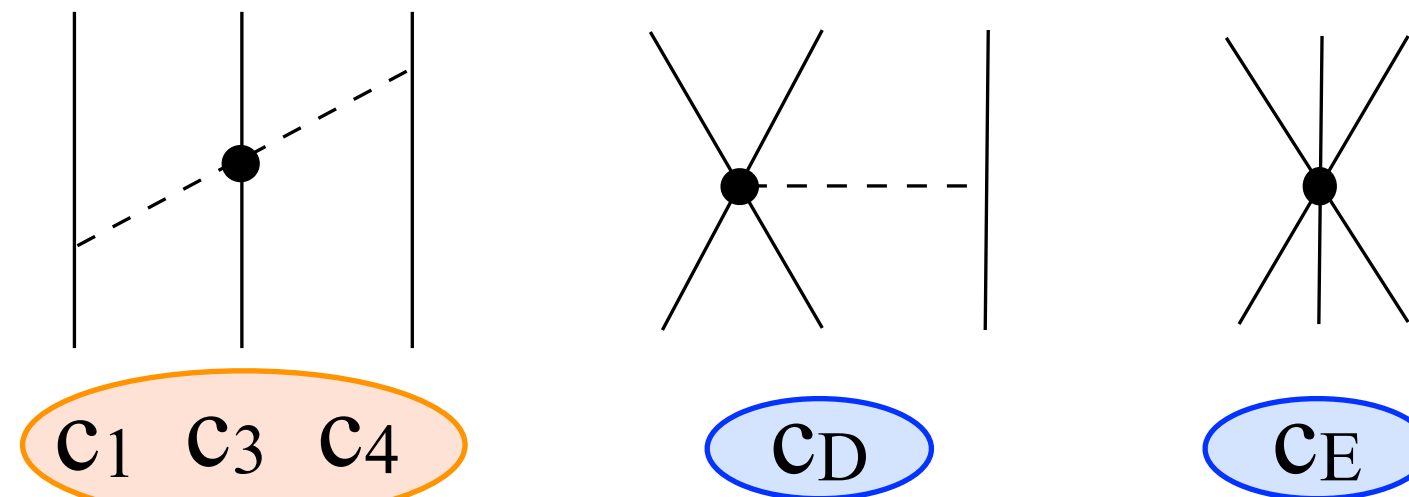
Lovato, MP et al. PRC105 (2022) 055808

# Fits of 3N Interactions: triton beta decay half life

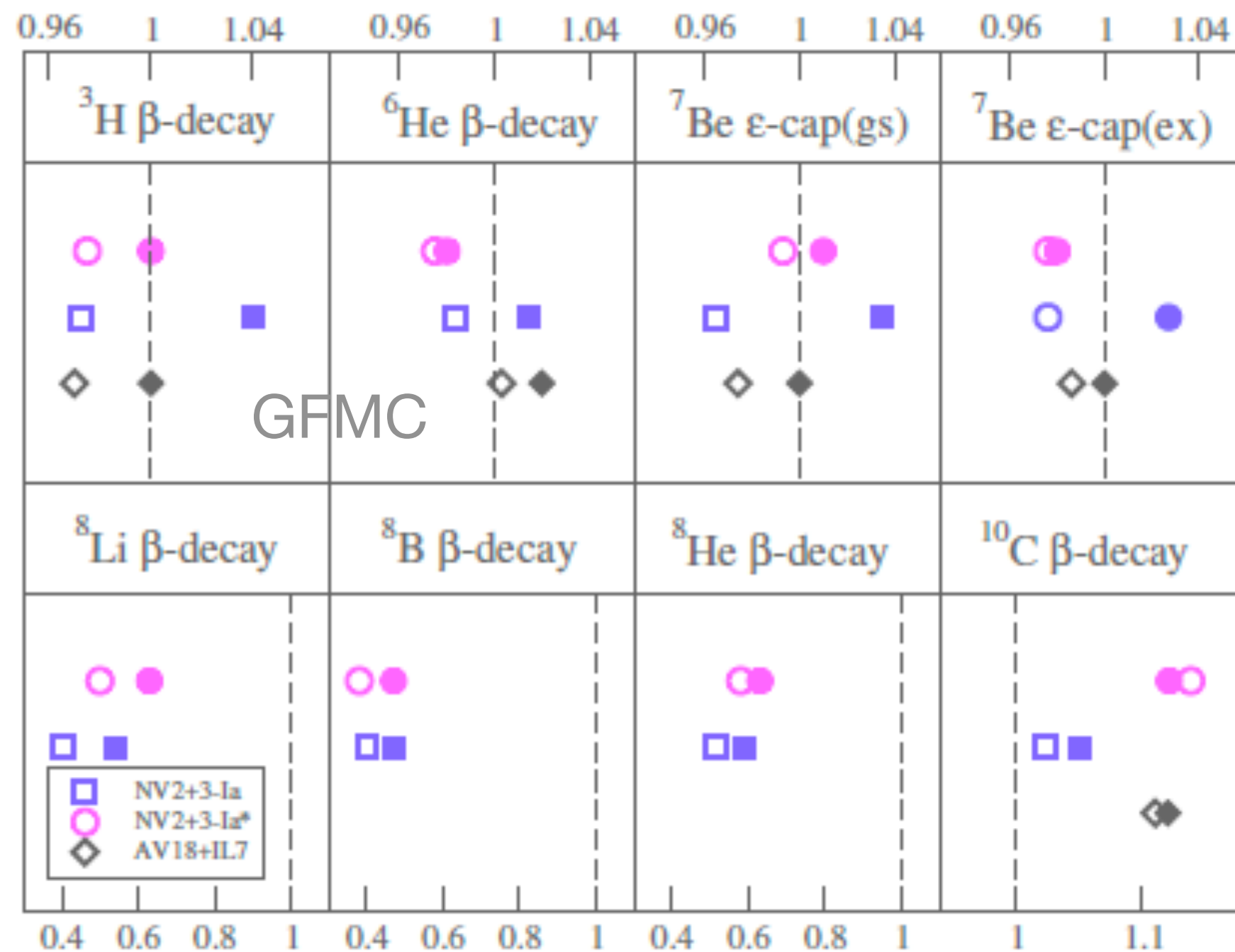
Baroni, MP et al. PRC 98 (2018) 4, 044003

- Inclusion of 3N forces at N2LO:

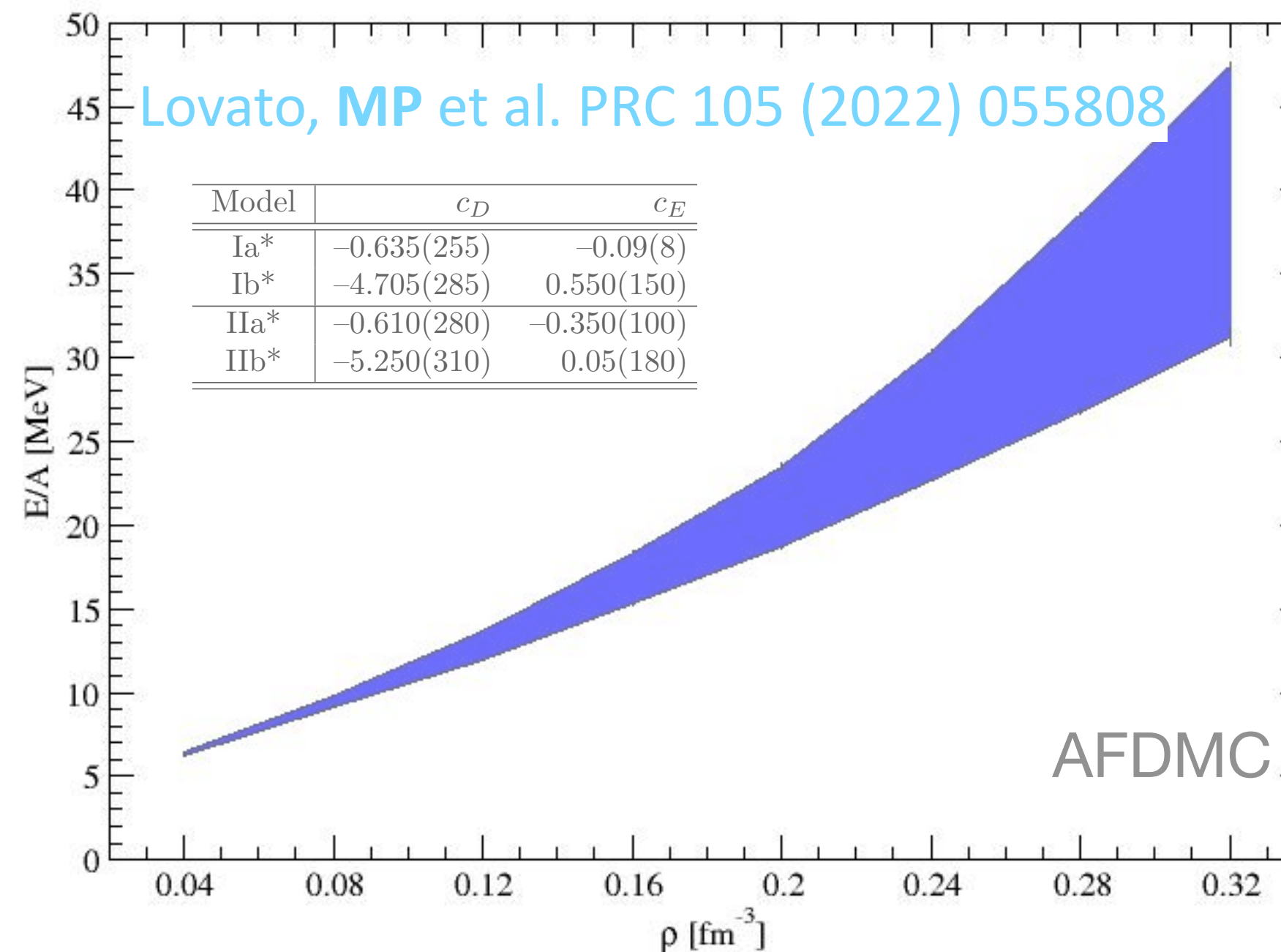
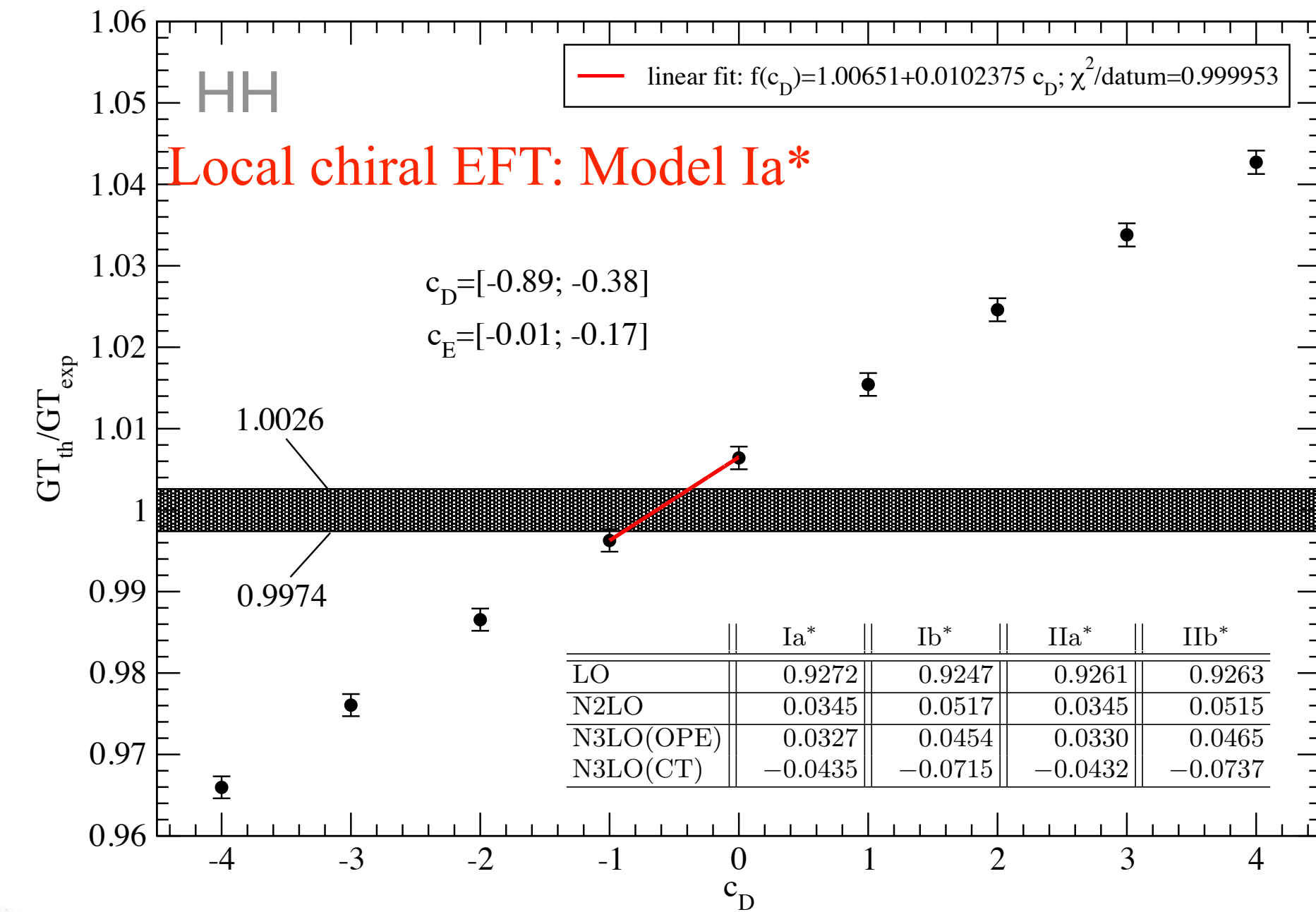
Constrained from  $\pi N$  scattering or  $NN$ : ex  
Hoferichter et al., Phys.Rept. 625 (2016) 1



$$z_0 = \frac{g_A}{2} \frac{m_\pi^2}{f_\pi^2} \frac{1}{(m_\pi R_S)^3} \left[ -\frac{m_\pi}{4 g_A \Lambda_\chi} c_D + \frac{m_\pi}{3} (c_3 + 2 c_4) + \frac{m_\pi}{6 m} \right]$$



King, MP et al. PRC 102, 025501 (2020)

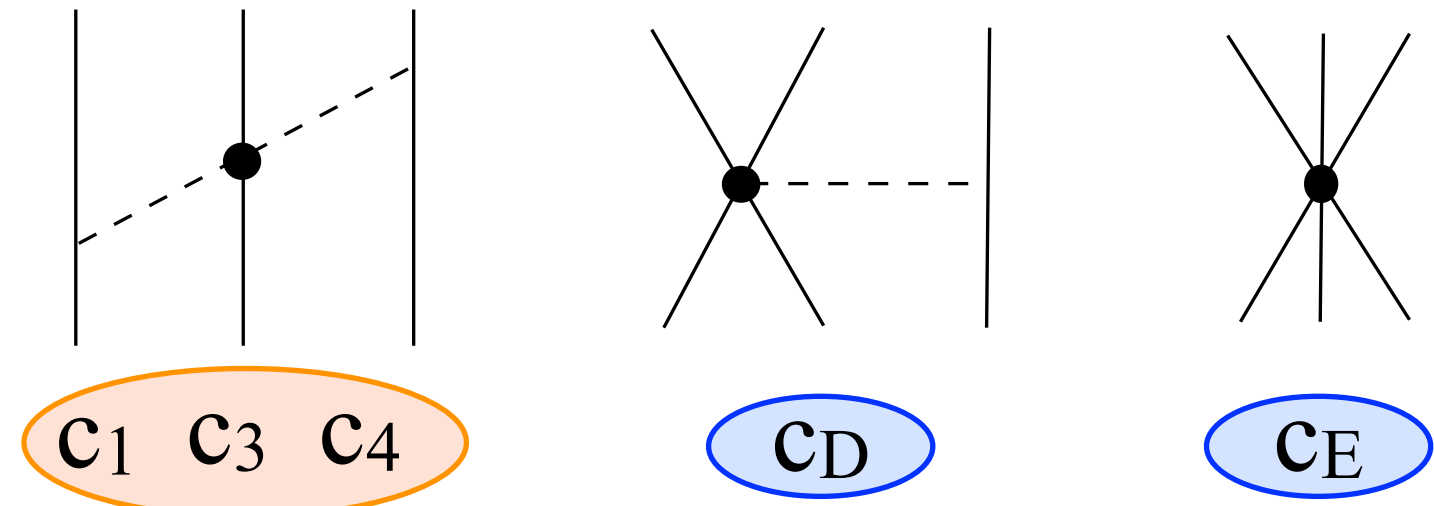


- Model dependence of the EOS at three-body level  $\rho = 2\rho_0$  ( $\sim 16$  MeV)
- The exp error on the  $^3\text{H}$  beta decays in the NV2+3s\* (numbers in parenthesis) is not propagated yet

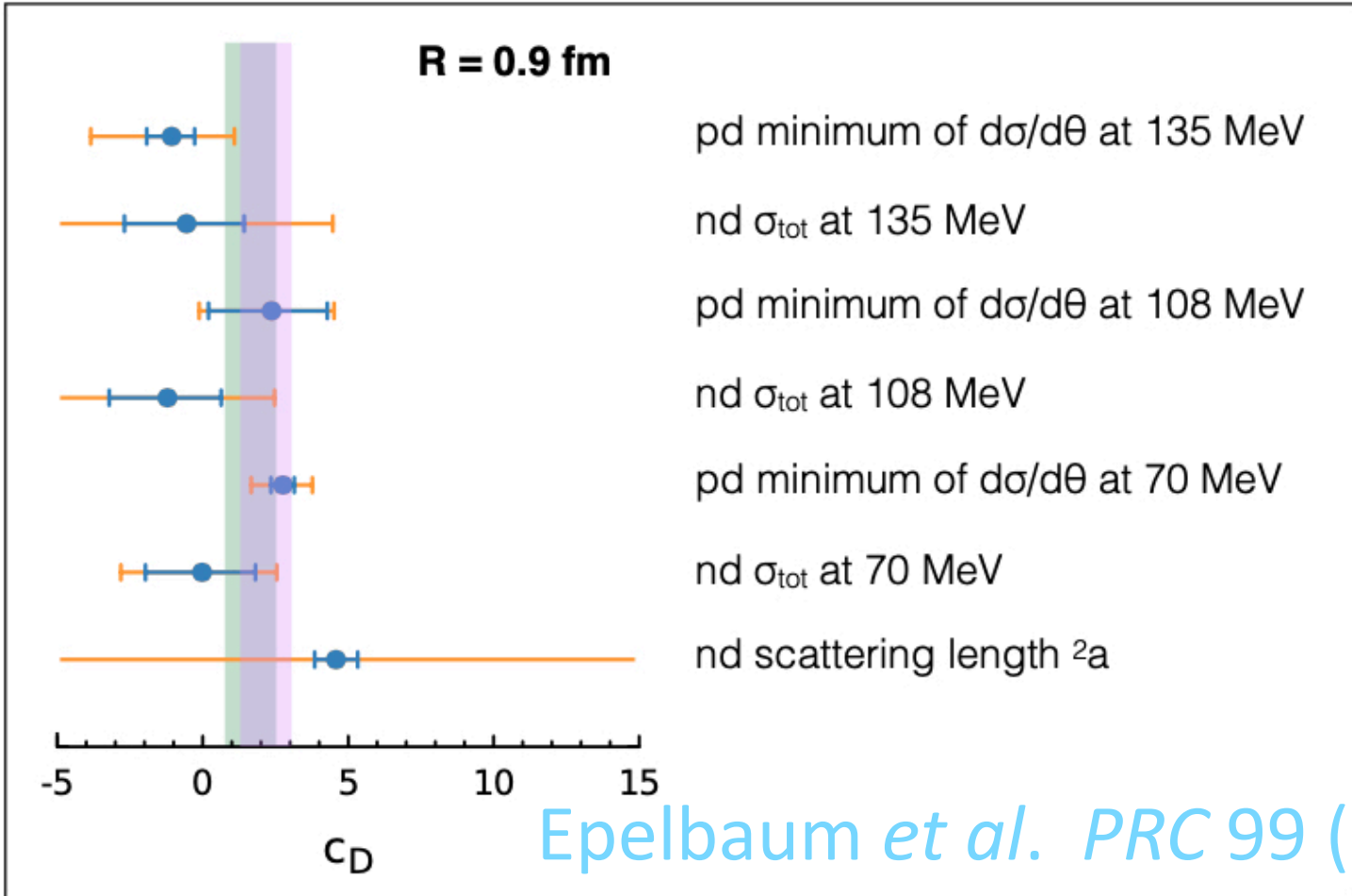
# Fits of 3N Interactions: three-body scattering cross sections

- Inclusion of 3N forces at N2LO:

Constrained from  $\pi N$  scattering or  $NN$ : ex  
Hoferichter et al.,  
Phys.Rept. 625 (2016) 1



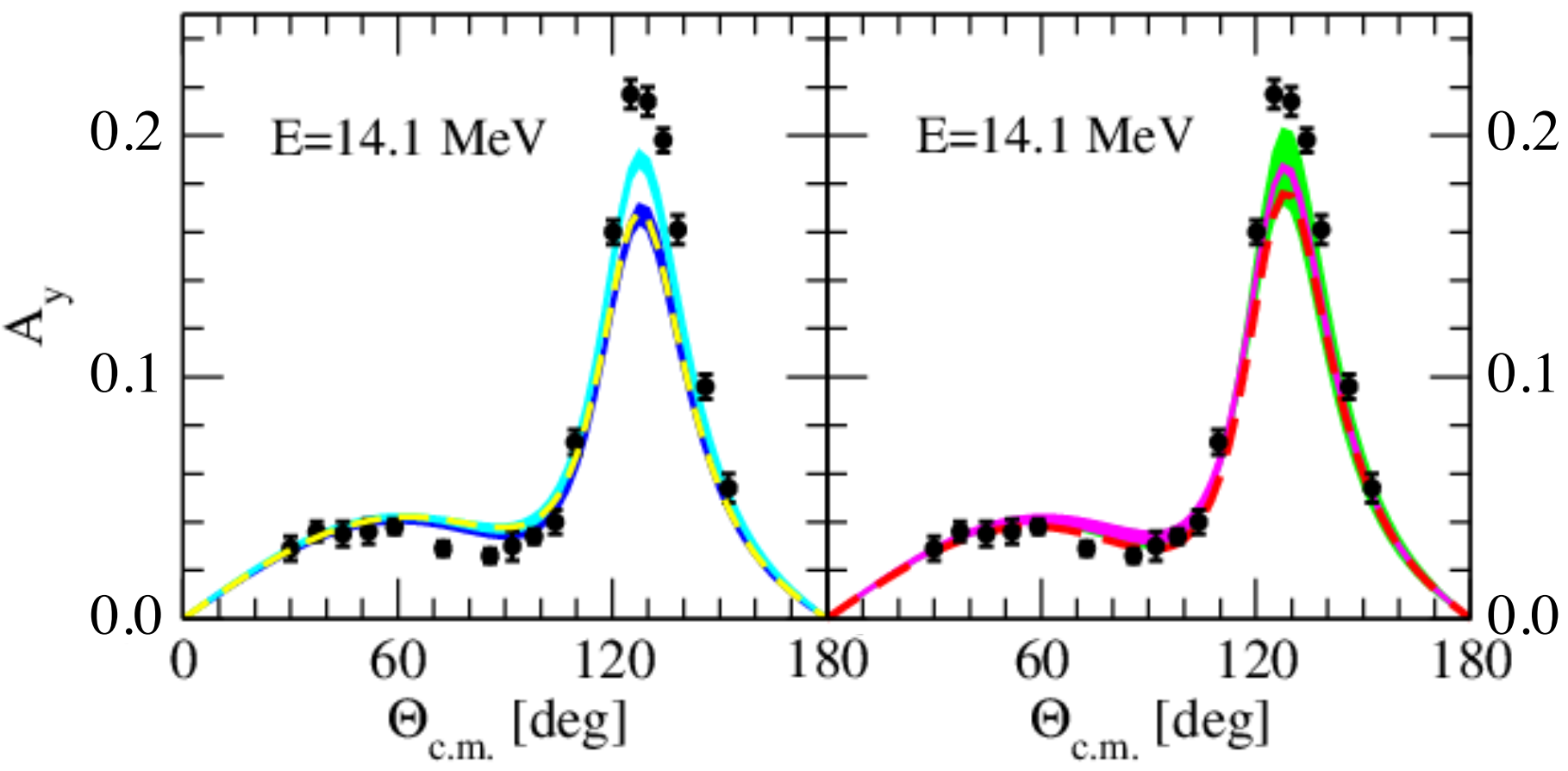
a more global fit using several observables more robust!!



Epelbaum et al. PRC 99 (2019) 2, 024313

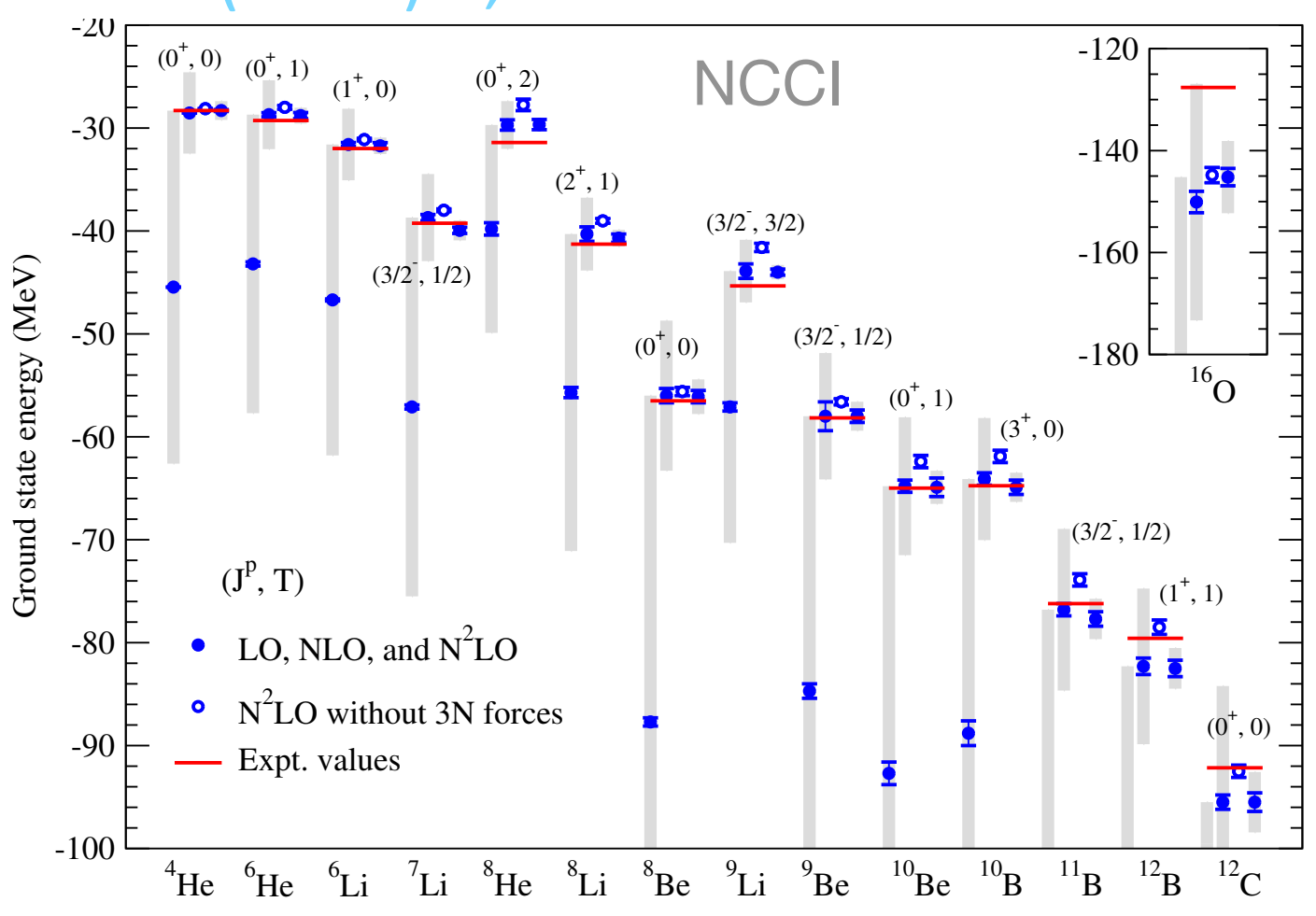
The neutron analyzing power  $A_y$  in nd elastic scattering at  $E_n = 14.1$  MeV

Epelbaum et al. PRC 99 (2019) 2, 024313

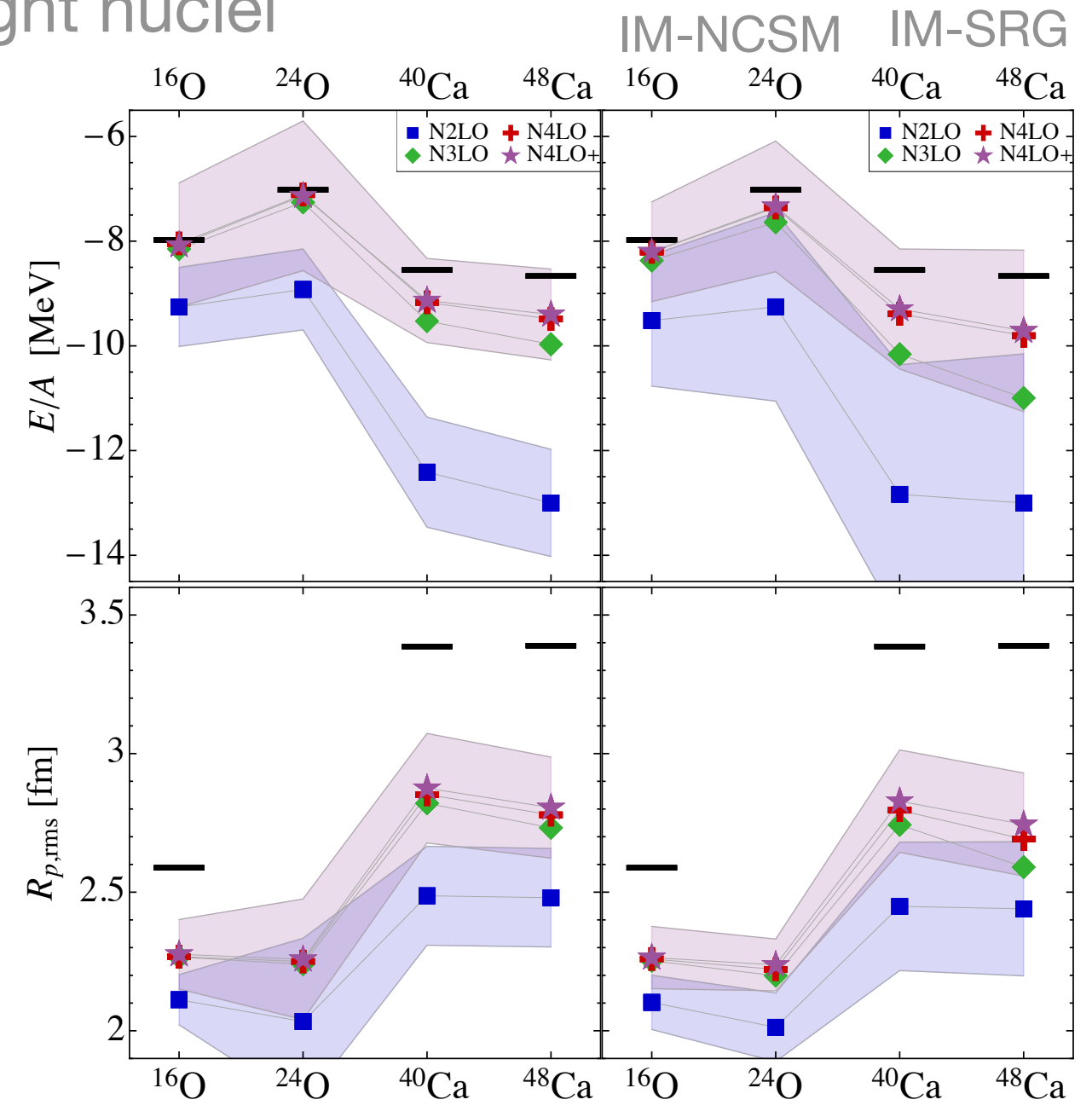


- AV18, CD Bonn, Nijm1, Nijm2
- AV18, CD Bonn, Nijm1, Nijm2 +TM99
- AV18+UIX
- NN N2LO
- NN+NNN @ N2LO
- NN+NNN @ N2LO +UQ

Ground-state energies in light nuclei



Indication that subleading 3N contact interactions are relevant to solve the discrepancies!

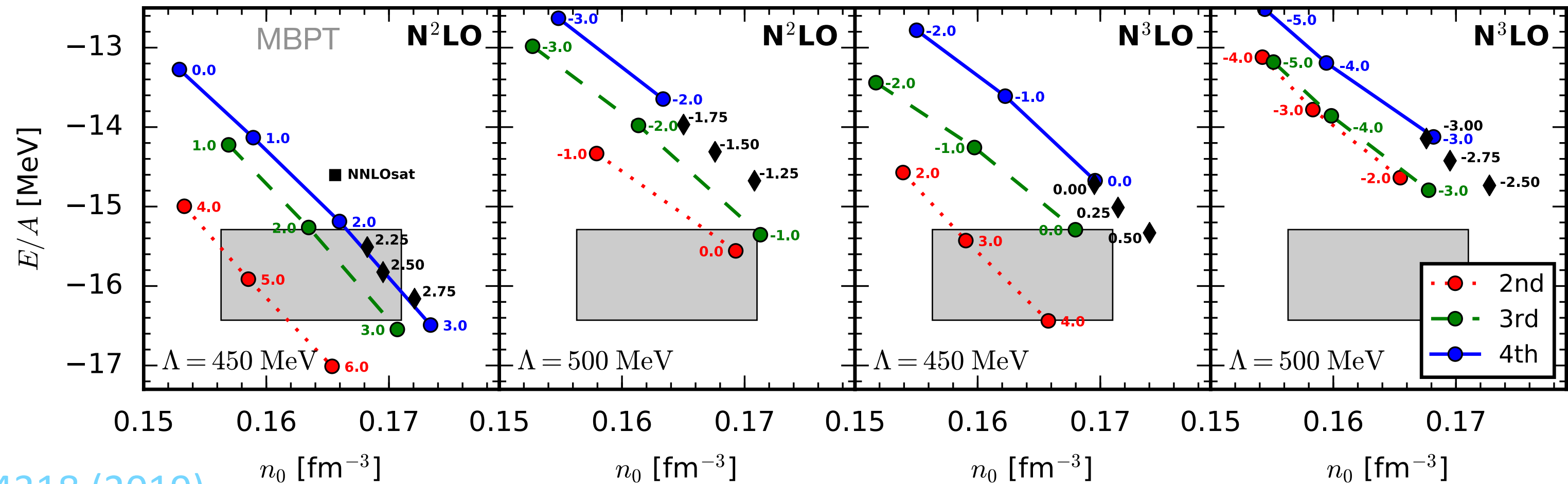
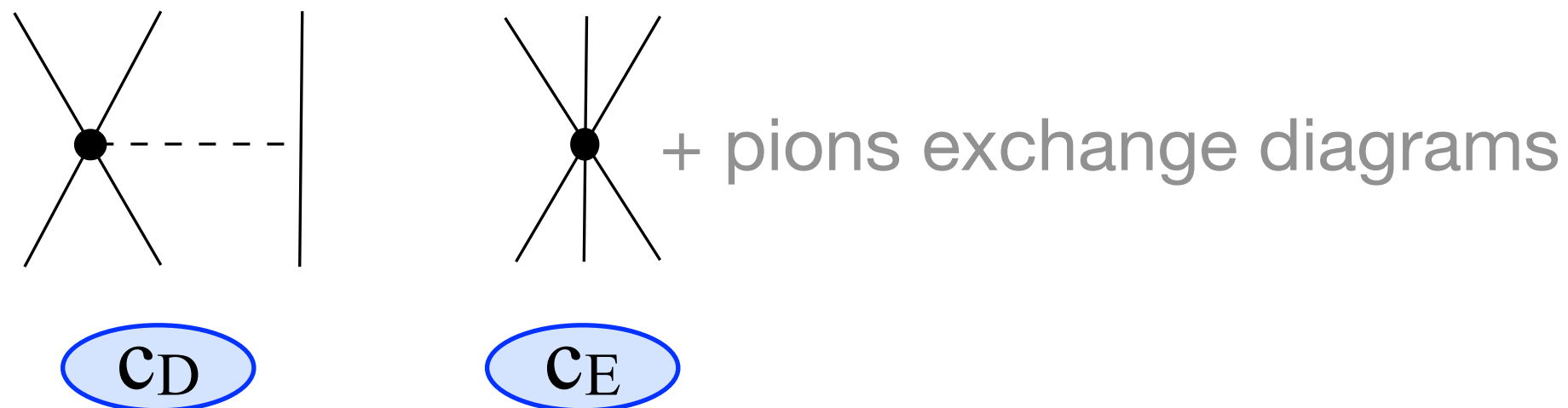


Maris et al. PRC 106 (2022) 6, 064002



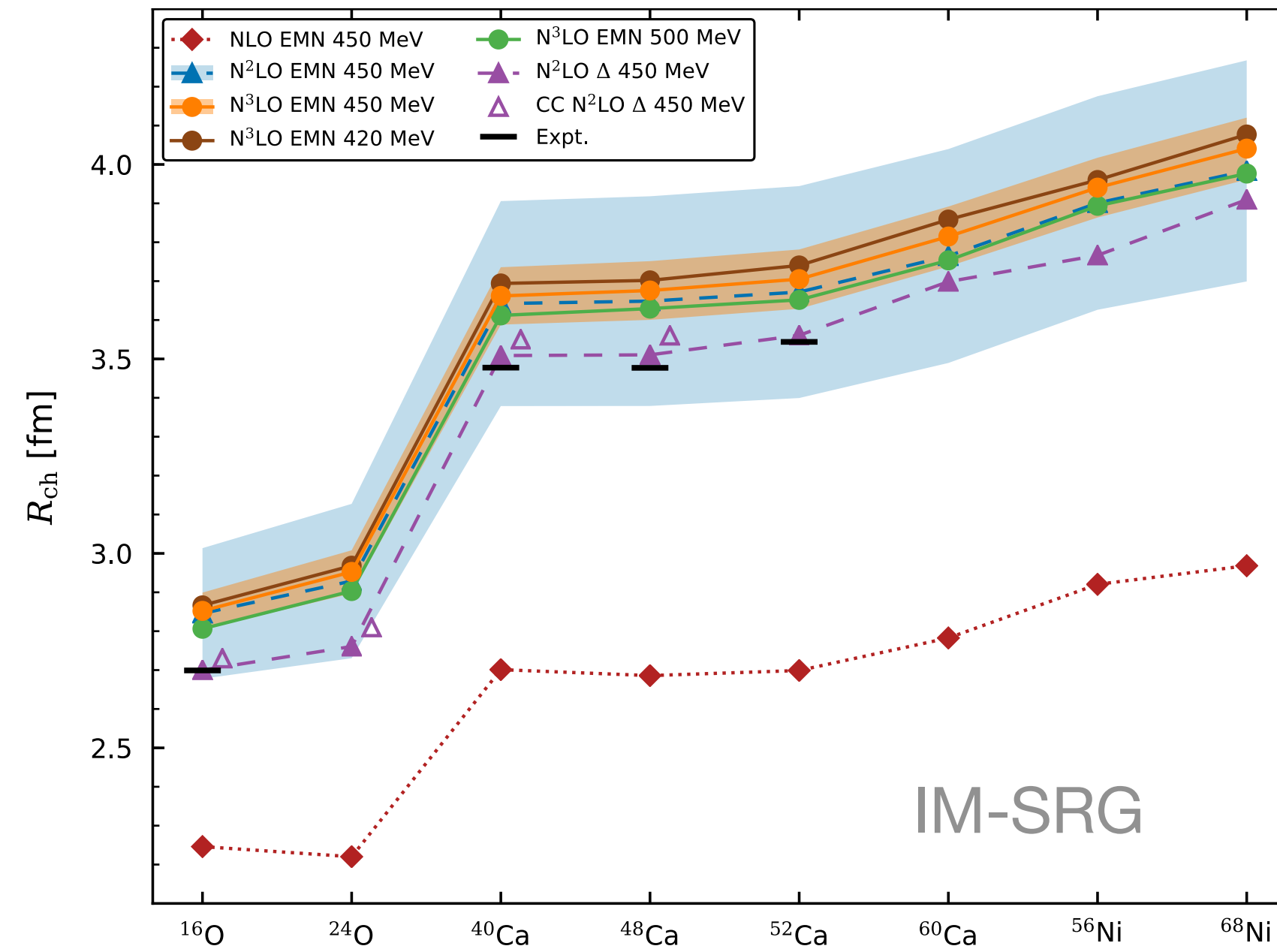
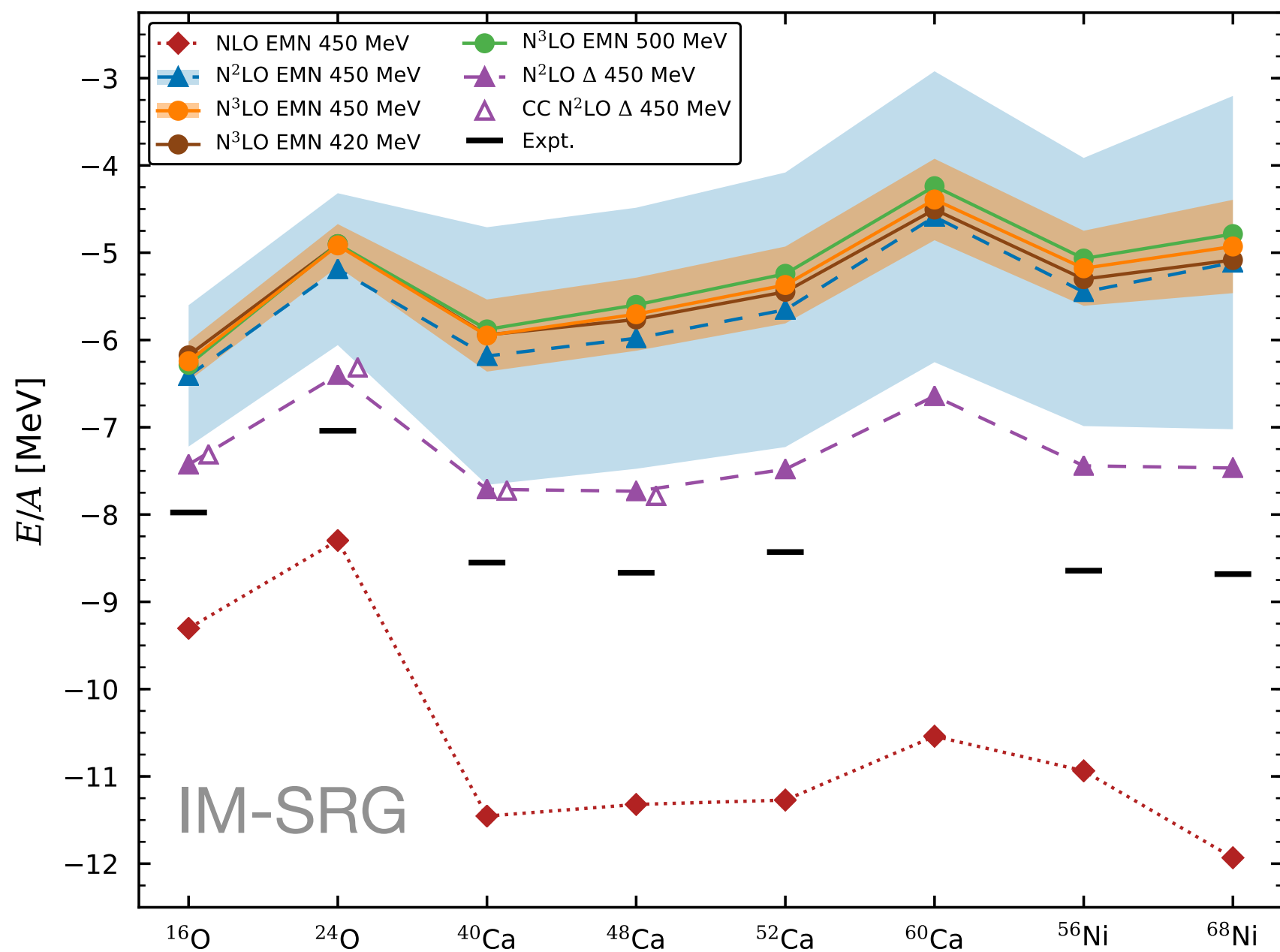
# Fits of 3N Interactions: nuclear matter saturation point

- Inclusion of 3N forces at N2LO and N3LO:



Hoppe et al. PRC 100, 024318 (2019)

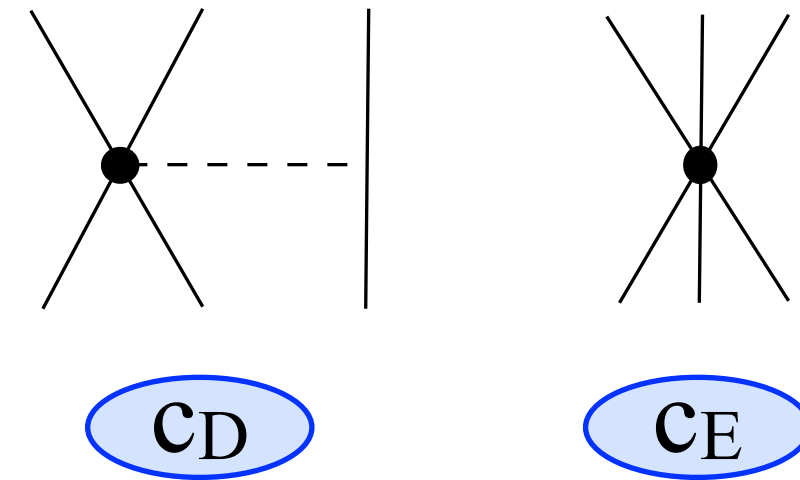
Drischler et al., PRL 122 (2019) 042501



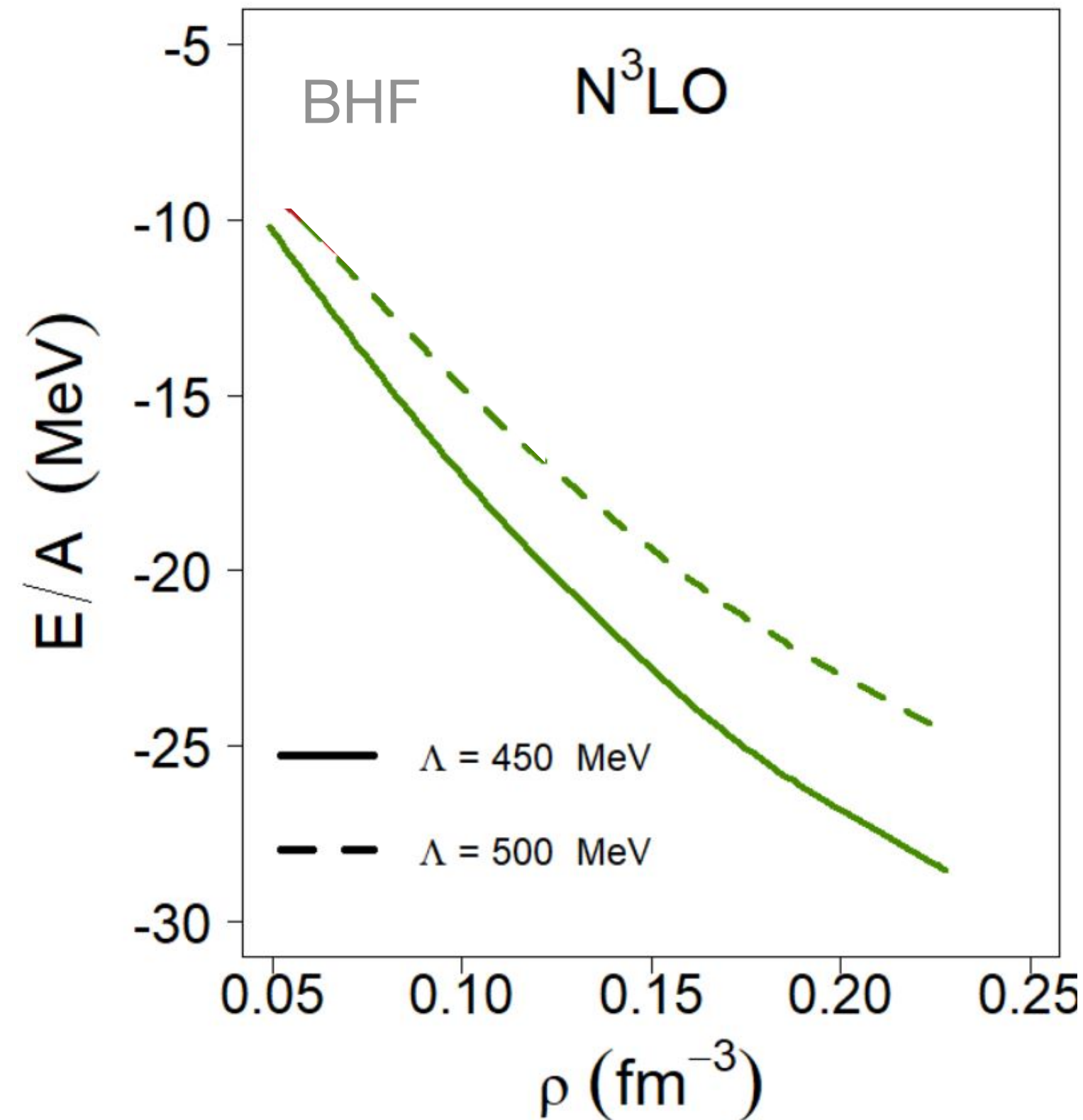
- Use nuclear matter saturation energy and density to adjust LECs
- Reasonable reproduction of both quantities possible
- Results for medium-mass nuclei still not satisfactory

# Fits of 3N Interactions: g.s. energies of nuclei

- Inclusion of 3N forces at N2LO and N3LO:

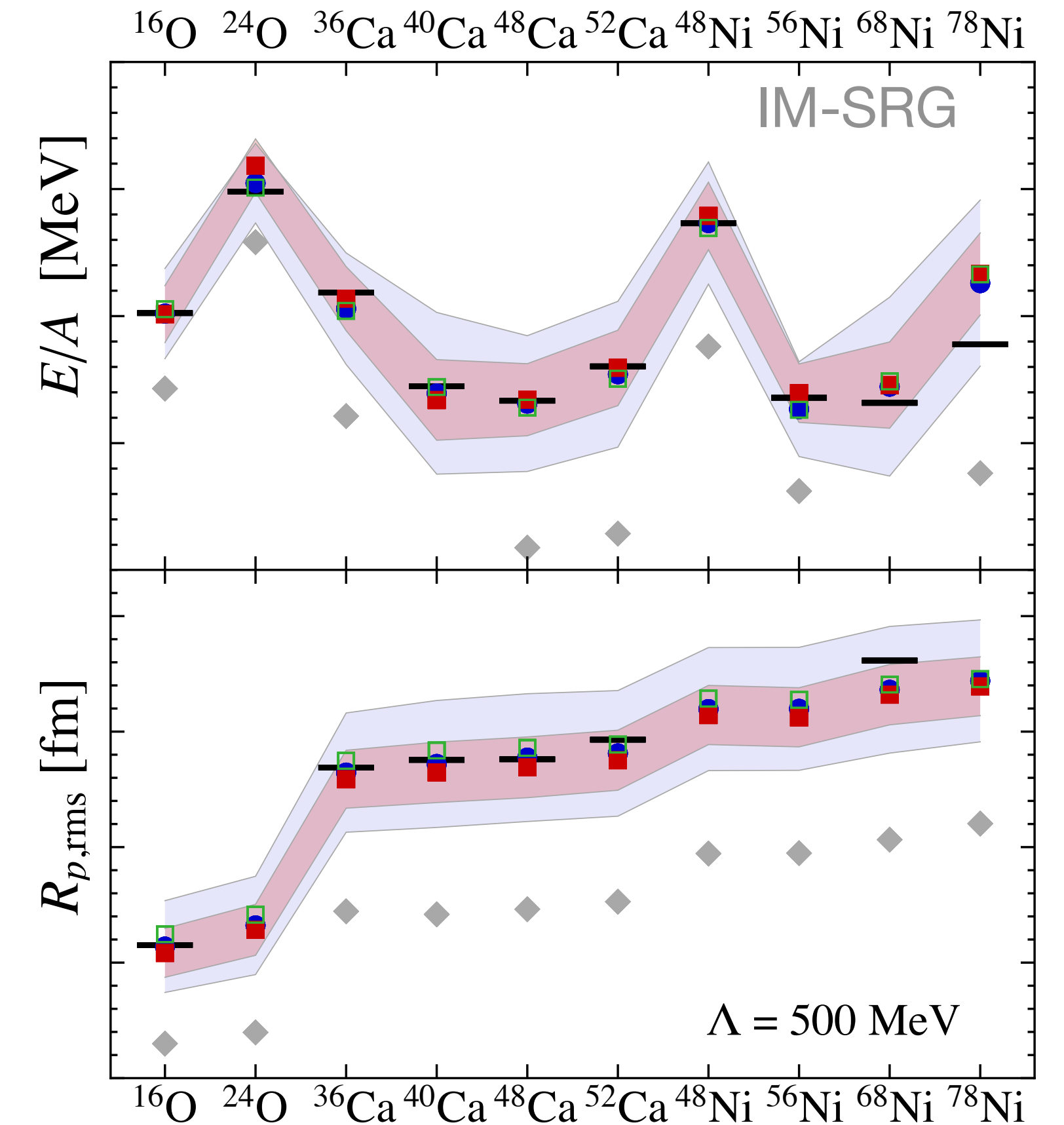


3N fitted to 3H and  $^{16}\text{O}$  g.s. energies



Constraints from the few-nucleon system and a relatively light nucleus such as  $^{16}\text{O}$  produce chiral interactions which are excessively attractive when applied in nuclear matter showing no sign of saturation.

Sammarruca et al., PRC 102, 034313 (2020)



Huther et al., PLB 808, 135651 (2020)

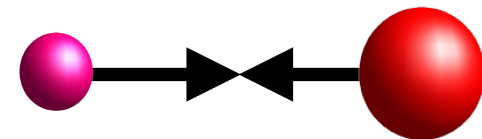
A good reproduction of both experimental energies and radii from p-shell nuclei up to the nickel isotopes within theoretical uncertainties

# How to fix the LECs?

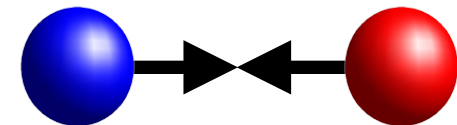
Second Challenge: *What is the best fitting procedure?*

“Traditional” approach: separate fits

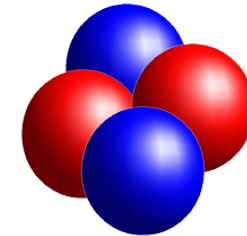
piN



NN



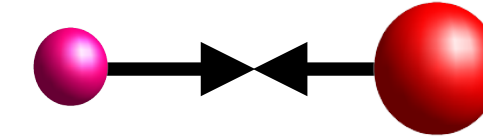
Light nuclei,  $A=2,3,4$



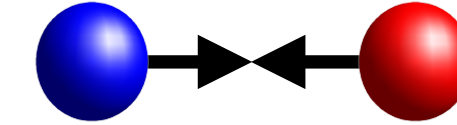
- D. R. Entem et al., Phys. Rev. C 96, 024004 2017
- A. Gezerlis et al., Phys.Rev. C 90, 054323 2014
- M. Piarulli et al., Phys. Rev. C, 024003 2015
- E. Epelbaum et al., Eur. Phys. J. A 51, 53 2015
- P. Reinert et al., Eur.Phys.J. A54 no.5, 86 2018
- Ekström et al. Phys. Rev. Lett. 110, 192502 2013 (NNLOopt)
- Ekström et al. Phys. Rev. C **97**, 024332 2018
- B. Carlsson et al., Phys. Rev. X, 011019 2015 (NNLOsep)
- .....

A “more modern” approach: simultaneous fits

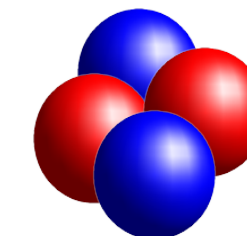
piN



NN

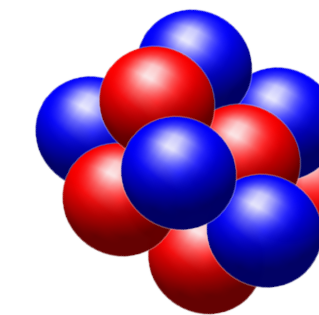


Light nuclei,  $A=2,3,4$



Or

Heavier nuclei:  $A>12$



- B. Carlsson et al., Phys. Rev. X, 011019, 2015 (NNLOsim)

- Indications that simultaneous fits lead to more systematic EFT convergence
- Results for heavier systems not consistent with experimental results

- A. Ekström et al., J. Phys. G 42, 034003 2015 (NNLOsat)

- Good results for  $^{40}\text{Ca}$  even though the fit included information up to oxygen.
- But NN scattering data included only up to 35 MeV  $E_{\text{LAB}}$

Computationally a very challenging problem!

# Optimization procedure for the LECs

Third Challenge: Minimize a objective function to find  $\mathbf{a}^*$  (LECs) in the parameter space

Least-square objective function for a set of observables

$$\mathbf{a}^* = \min_{\mathbf{a}} \chi^2(\mathbf{a}) \quad \text{with} \quad \chi^2(\mathbf{a}) = \sum_{i=1}^{N_{\text{data}}} \left( \frac{o_i - t_i(\mathbf{a})}{\delta o_i} \right)^2$$

$o_i$  : measured values

$t_i$  : calculated values

$\delta o_i$ : uncertainty observables

“Conventional” least-square minimization:

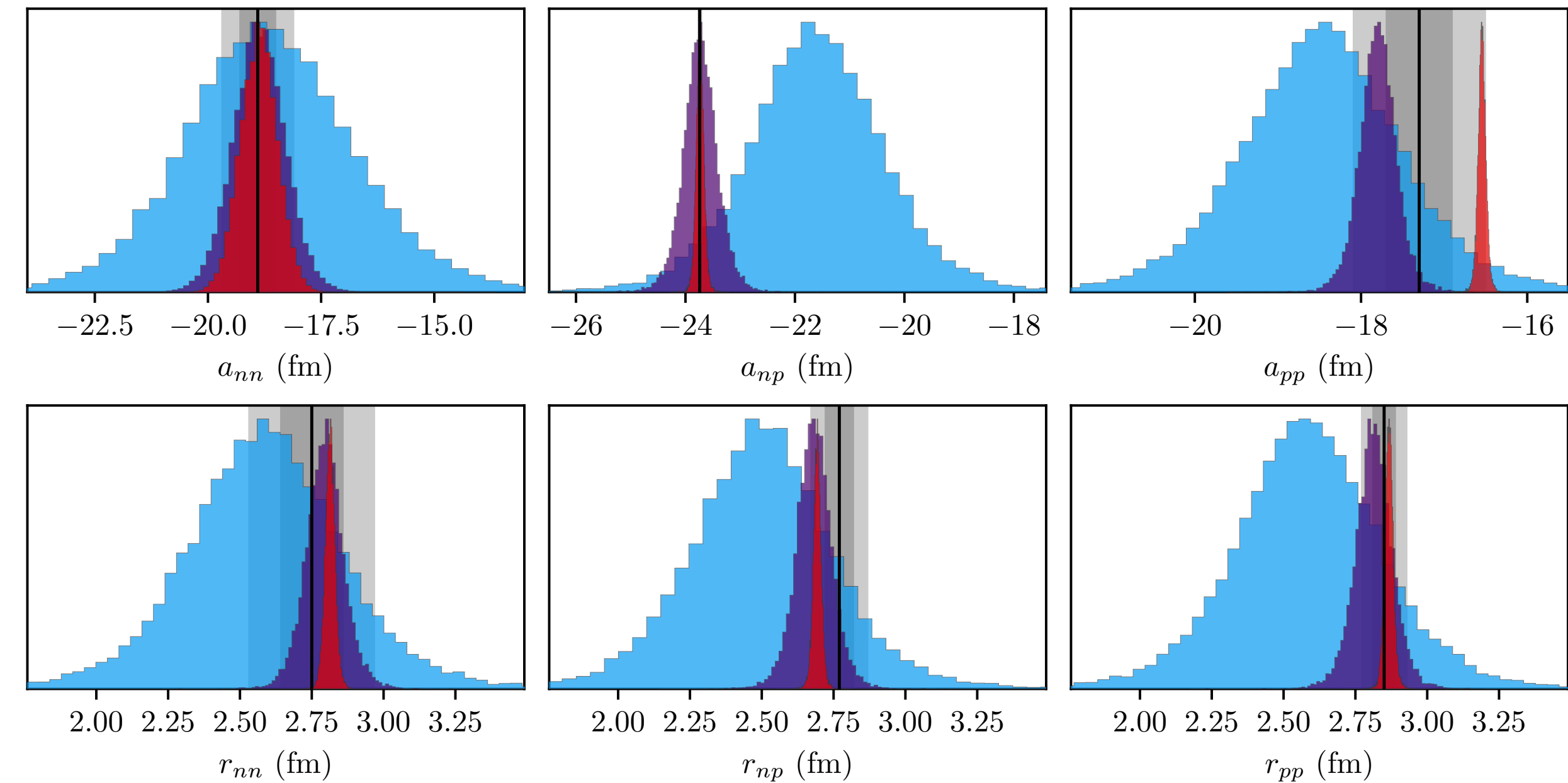
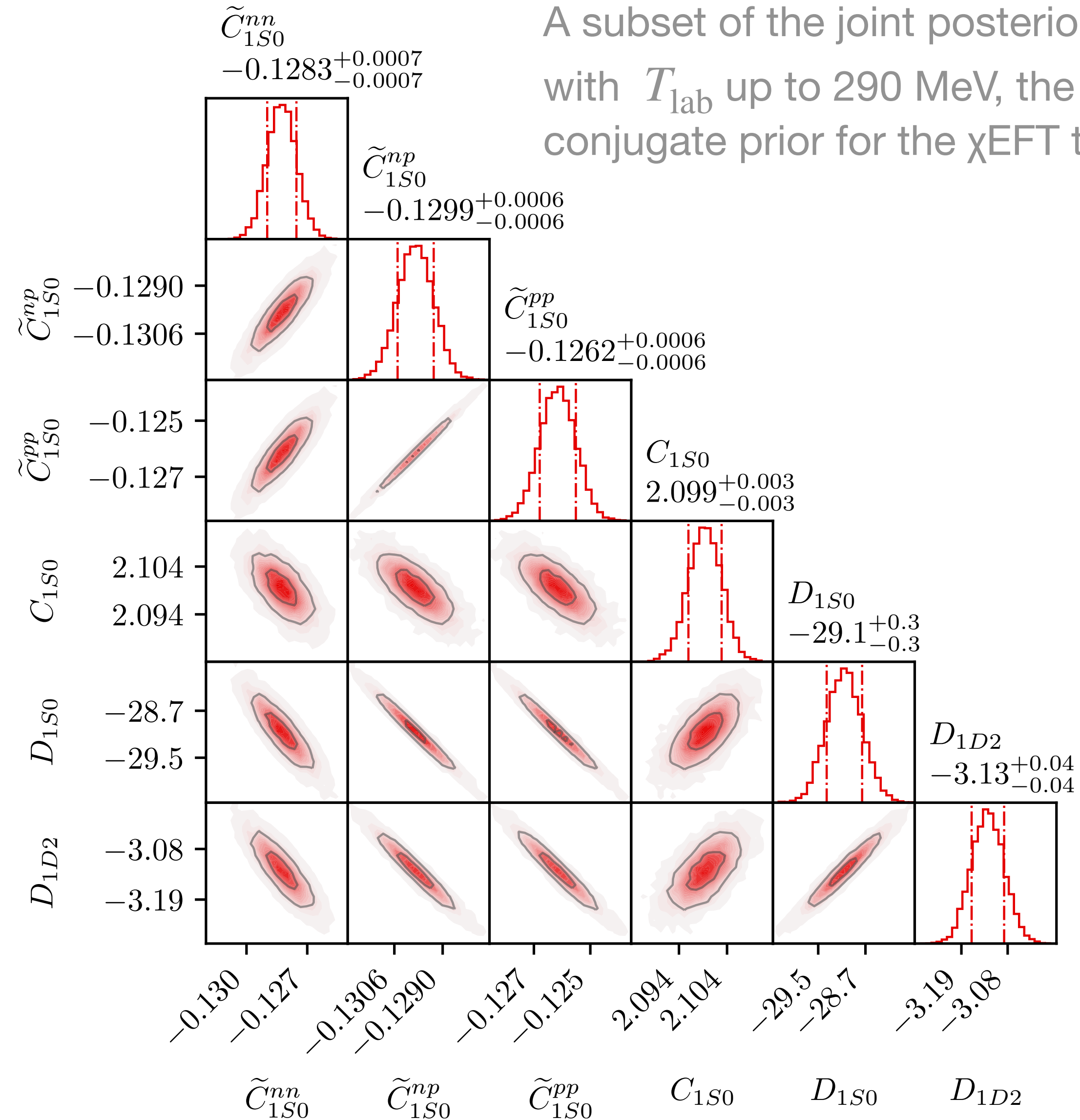
- Take  $\delta o_i$  to be the experimental error (or same modification to take into account theoretical errors)
- Many optimization techniques suitable for this problem such as POUNDers, Newtons Methods,....
- UQ addressed as: Covariance methods, Bootstrapping, standard protocols for chiral truncation errors, cutoff dependence
- over/under-fitting parameter ,..

Bayesian parameter estimation:

$$\underbrace{\text{pr}(\mathbf{a}|\text{Data}, I)}_{\text{posterior}} \propto \underbrace{\text{pr}(\text{Data}|\mathbf{a}, I)}_{\text{likelihood}} \times \underbrace{\text{pr}(\mathbf{a}|I)}_{\text{prior}} \\ \propto e^{-\chi^2(\mathbf{a})/2}$$

- Bayesian statistics is a powerful framework for (chiral) EFT uncertainty quantification (UQ). *Everything is a pdf*
- Assumptions are made explicit (e.g. naturalness of LECs, truncation errors)
- Bayesian: *sample* for parameter estimation and the propagation of uncertainties; use *emulators* (like EC)!
- Using priors and truncation errors minimizes overfitting and dependence on how much data is used; posteriors can be used for diagnostics.
- Clear prescriptions for combining errors

# Bayesian estimation of LECs up to N3LO for the NN $\chi$ EFT



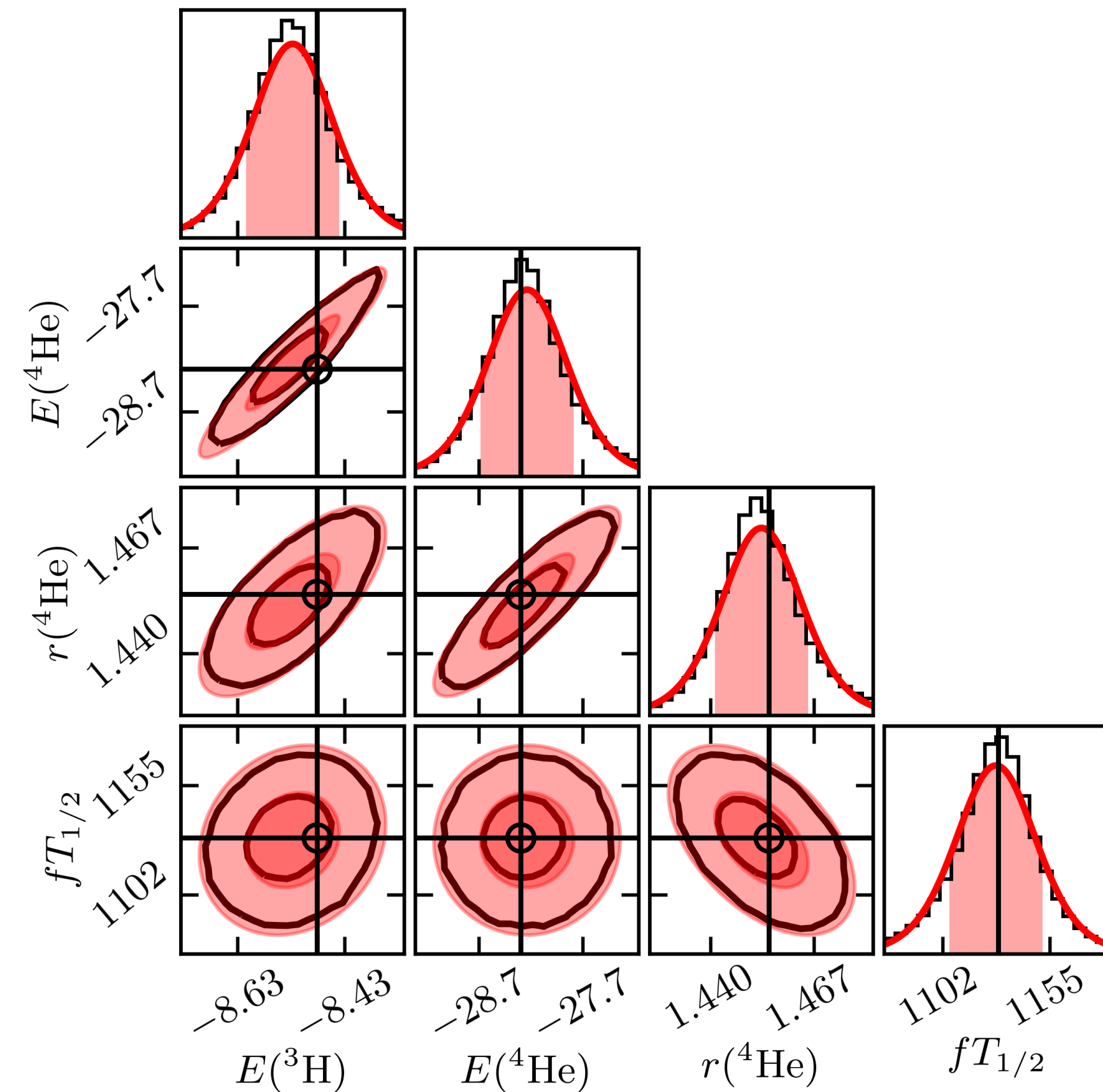
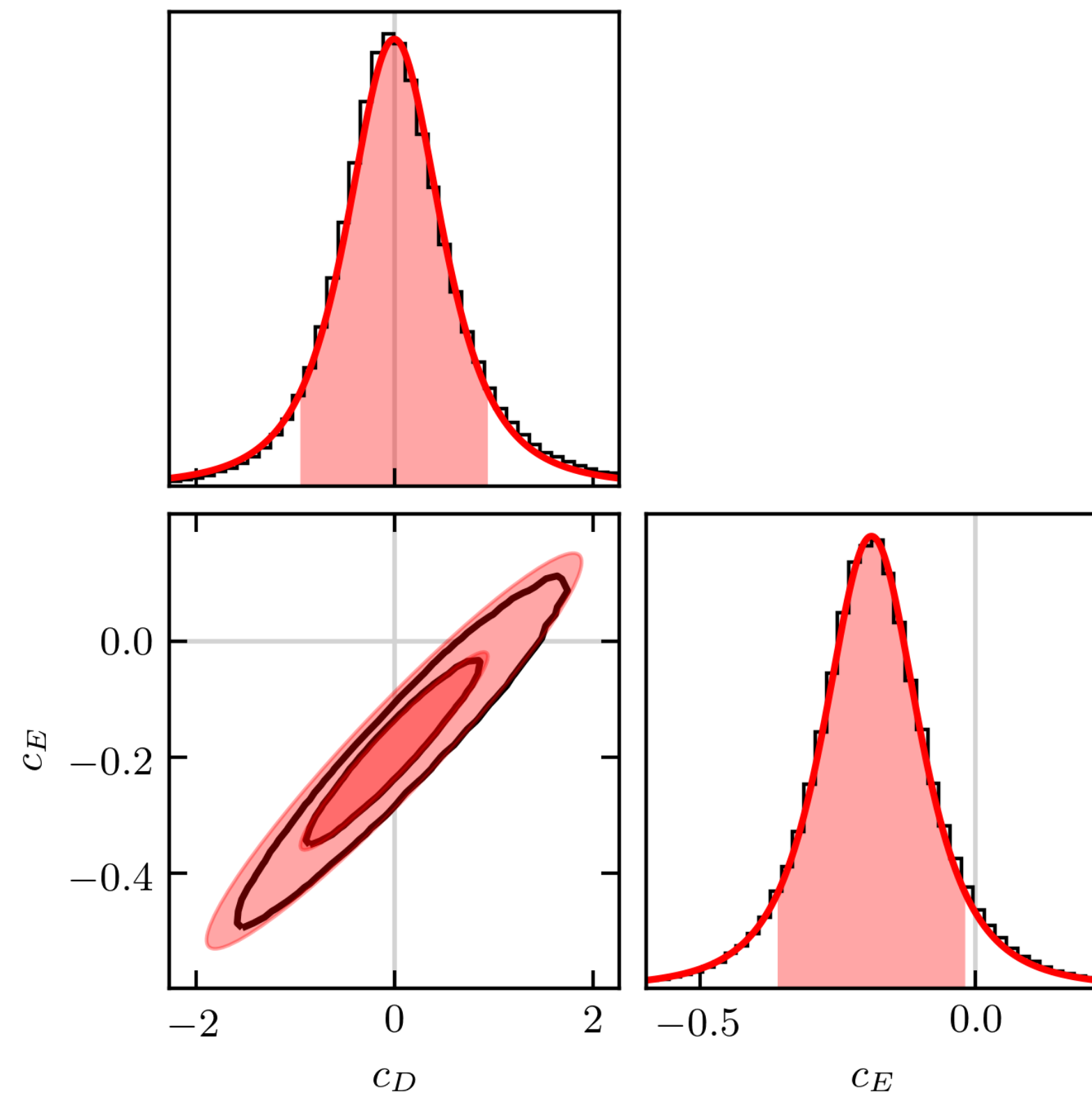
PPDs of scattering lengths and effective ranges at NLO (blue), NNLO (purple), and N3LO (red). Empirical results are shown as black lines, with corresponding  $1\sigma$  ( $2\sigma$ ) uncertainties as a dark (light) gray area

# Bayesian estimation of LECs up to N2LO for the 3N $\chi$ EFT

Statistically rigorous analysis that incorporates experimental error, computational method uncertainty, and the uncertainty due to truncation of the  $\chi$ EFT expansion at N2LO

Wesolowski et al. Phys.Rev.C 104 (2021) 6, 064001

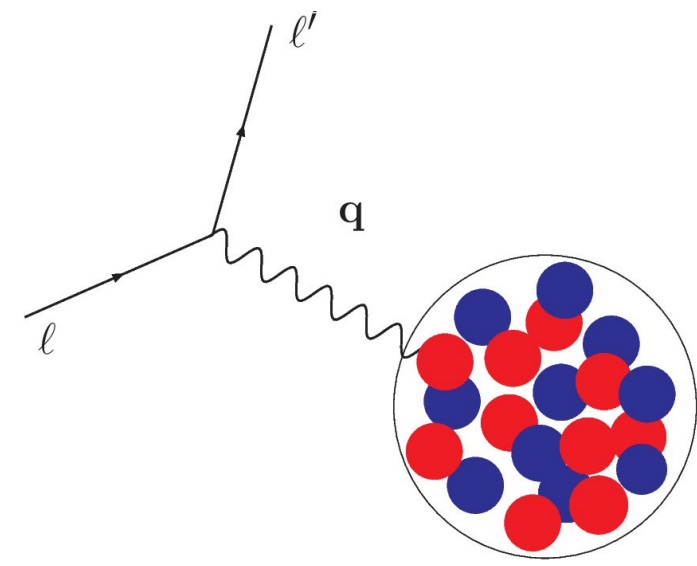
The posterior of  $c_D$  and  $c_E$  fitting to  ${}^3\text{H}$  binding energy, the  ${}^3\text{H}$  e binding energy and radius, and the  ${}^3\text{H}$   $\beta$ -decay rate



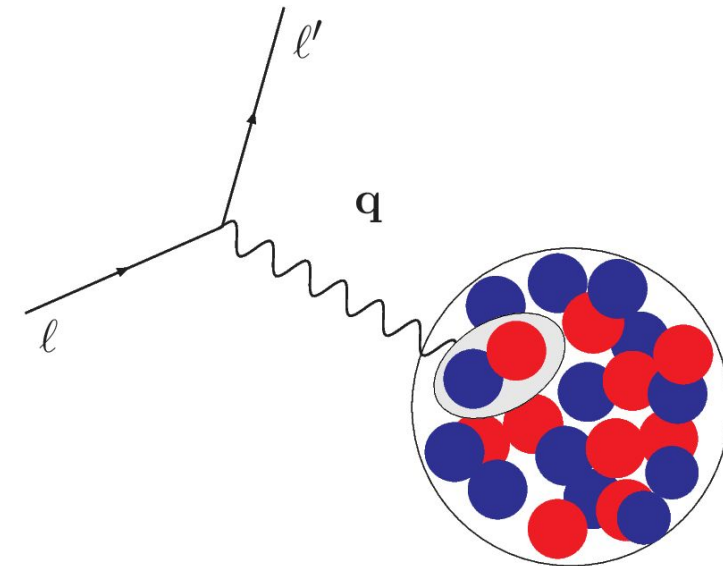
The posterior predictive distribution for the target few-nucleon observables, evaluated from the full posterior

# Many-body Nuclear Electroweak Currents

- Electroweak structure and reactions:



one-body



two-body

- Accurate understanding of the electroweak interactions of external probes with **nucleons**, **correlated nucleon-pairs**,...
- Two-body currents are a manifestation of two-body correlations
- Electromagnetic two-body currents are required to satisfy current conservation

$$\mathbf{q} \cdot \mathbf{j} = [H, \rho] = [t_i + v_{ij} + V_{ijk}, \rho]$$

- Meson exchange currents: [R. Schiavilla et al., PRC 45, 2628 \(1992\)](#), [Marcucci et al. PRC 72, 014001 \(2005\)](#), [L. Marcucci et al., PRC 78, 065501 \(2008\)](#)
- Chiral EFT currents: [Park et al. NPA 596, 515 \(1996\)](#); [Pastore et al. PRC 78, 064002 \(2008\)](#), [PRC 80, 034004 \(2009\)](#); [Piarulli et al. PRC 87, 014006 \(2013\)](#), [Baroni et al. PRC 93, 015501 \(2016\)](#); [Phillips et al. PRC 72, 014006 \(2005\)](#), [Kölling et al. PRC 80, 045502 \(2009\)](#), [PRC 84, 054008](#), [PRC 86, 047001 \(2012\)](#); [Krebs et al., Ann. Phys. 378, 317 \(2017\)](#)

- Electroweak form factors
- Magnetic moments and radii
- Electroweak Response functions
- Radiative/weak captures
- G.T. matrix elements involved in beta decays
- .....

Nuclear charge operator

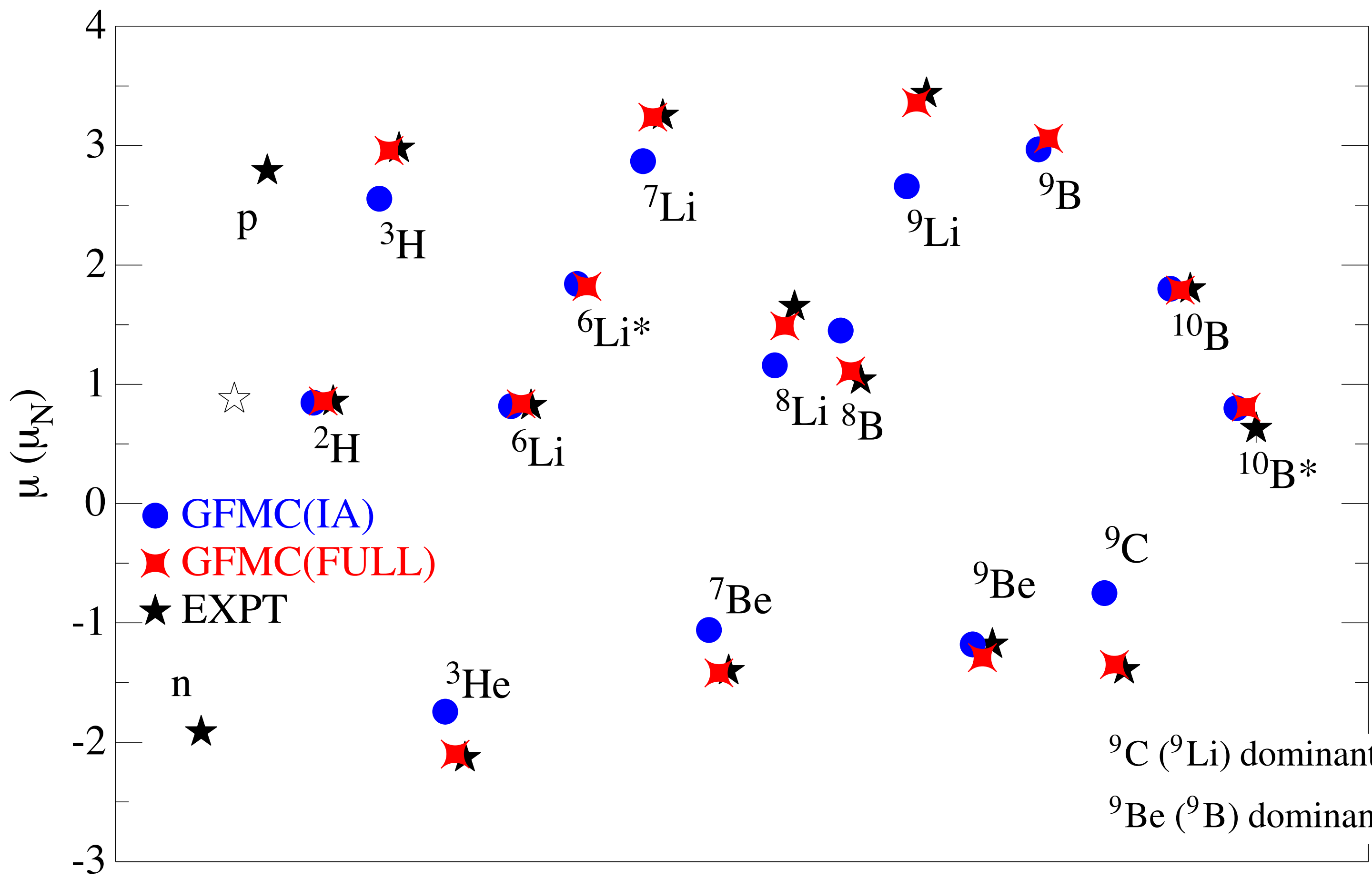
$$\rho = \sum_{i=1}^A \rho_i + \sum_{i<j} \rho_{ij} + \dots$$

Nuclear vector operator

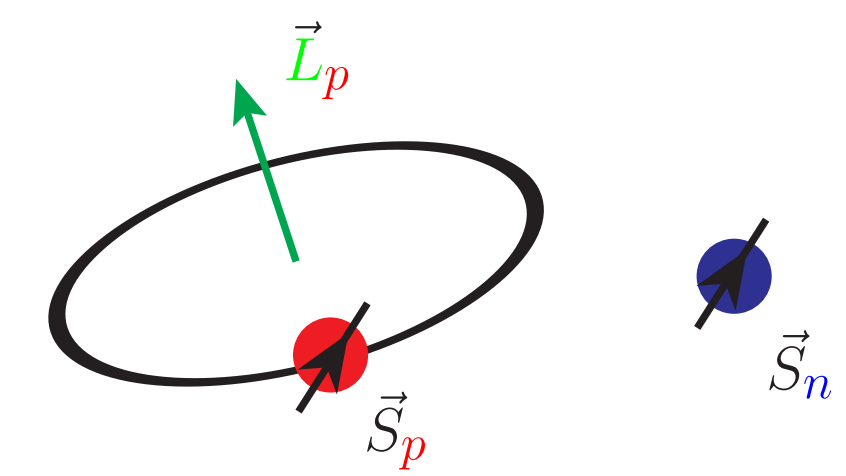
$$\mathbf{j} = \sum_{i=1}^A \mathbf{j}_i + \sum_{i<j} \mathbf{j}_{ij} + \dots$$

# Magnetic moment and EM decay

- GFMC calculations using AV18/IL7 (rather than chiral) and EM  $\chi$ EFT currents— hybrid calculation



$$\mu(\text{IA}) = \mu_N \sum_i [(L_i + g_p S_i)(1 + \tau_{i,z})/2 + g_n S_i(1 - \tau_{i,z})/2]$$



$$\langle J_f^\pi, M_f | \mu^{\text{MEC}} | J_i^\pi, M_i \rangle = -i \lim_{q \rightarrow 0} \frac{2 m_N}{q} \langle J_f^\pi, M_f | j_y^{\text{MEC}}(q \hat{x}) | J_i^\pi, M_i \rangle$$

${}^9\text{C}$  ( ${}^9\text{Li}$ ) dominant spatial symmetry [s.s.] = [432] = [ $\alpha$ ,  ${}^3\text{He}({}^3\text{H}), pp(nn)$ ]  $\rightarrow$  Large MEC  
 ${}^9\text{Be}$  ( ${}^9\text{B}$ ) dominant spatial symmetry [s.s.] = [441] = [ $\alpha$ ,  $\alpha, n(p)$ ]

Pastore *et al.* PRC 87, 035503 (2013)

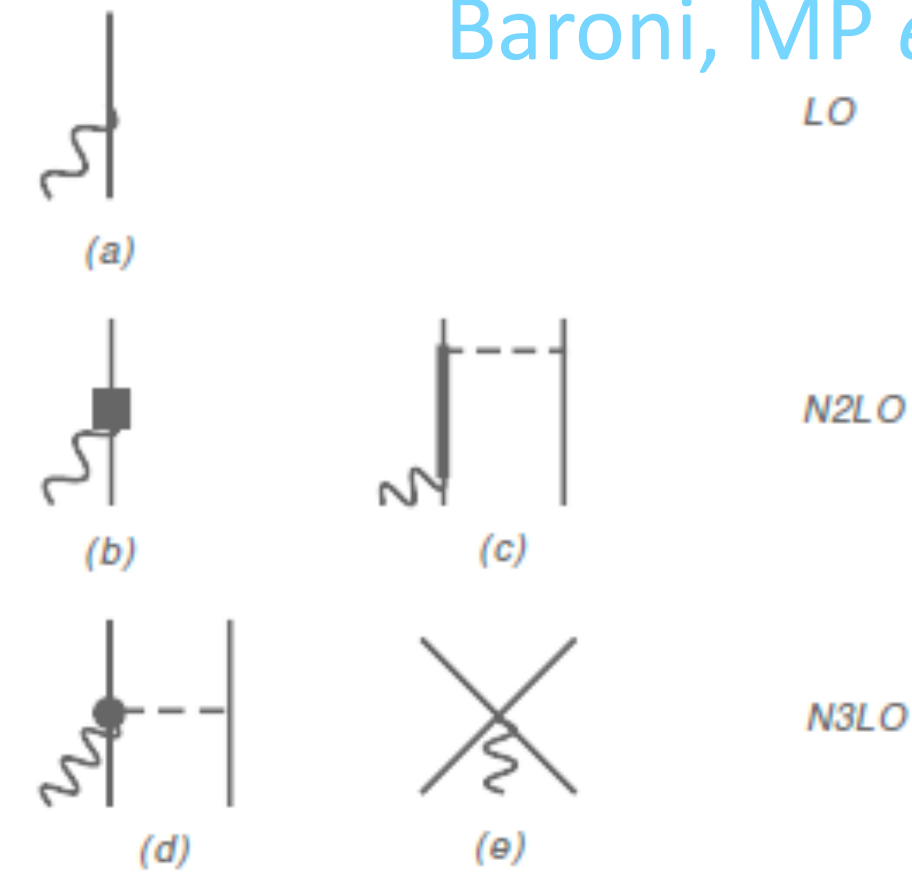
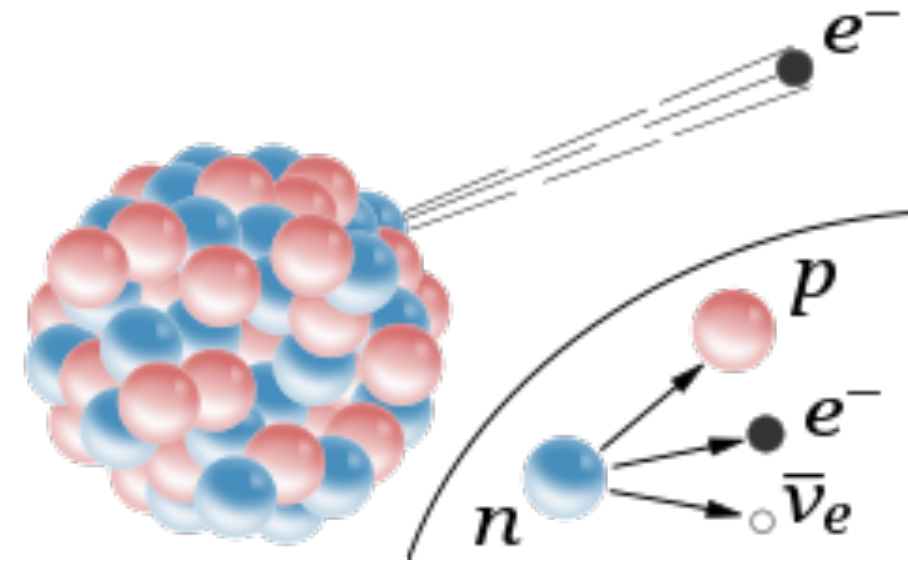
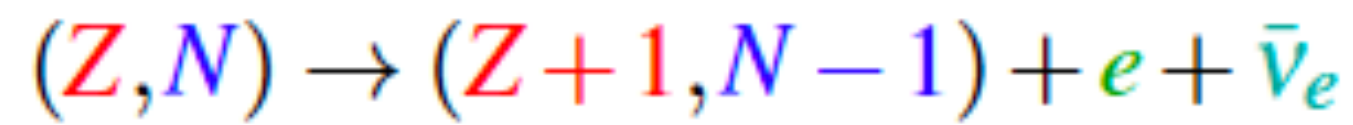
*Electromagnetic data are explained when two-body correlations and currents are accounted for!*



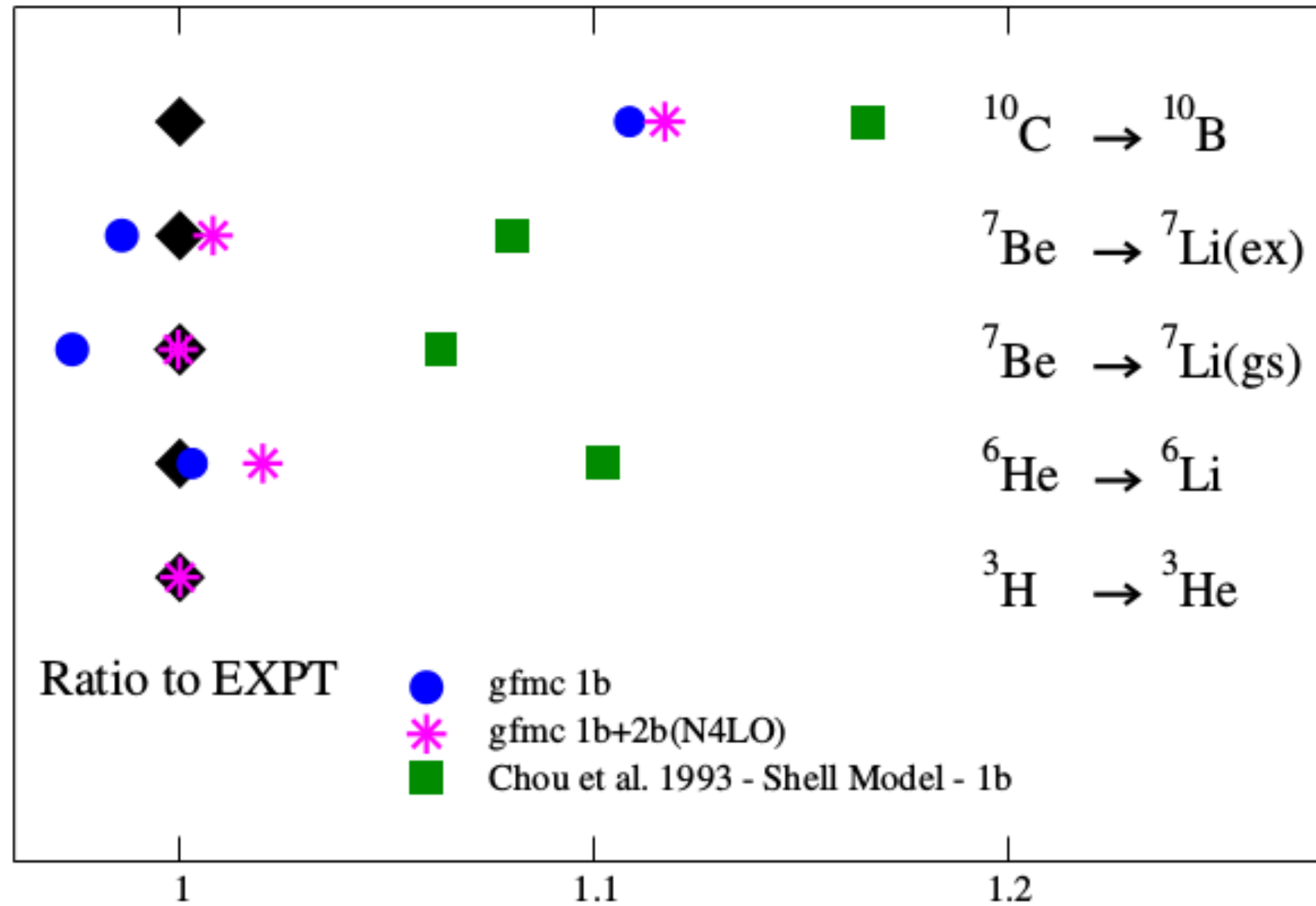
# Single-Beta decay matrix elements

Baroni, MP *et al.* PRC 93, 015501 (2016)

- Beta decay occurs when, in a nucleus with too many protons or too many neutrons, one of the protons or neutrons is transformed into the other.



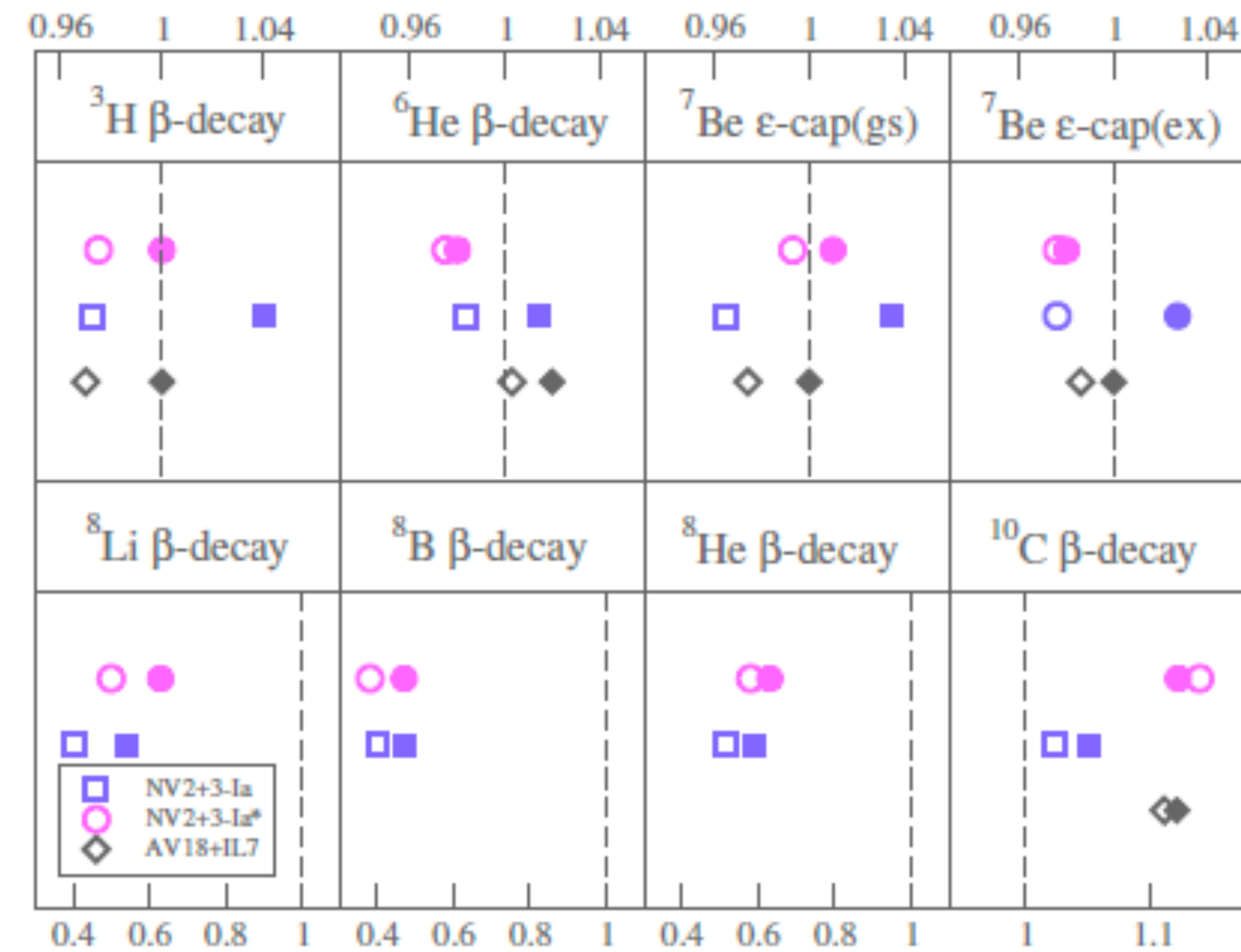
King, MP *et al.* PRC 102, 025501 (2020)



gfmc (1b) and gfmc (1b+2b); shell model (1b)

GFMC calculations using AV18/IL7 (rather than chiral) and axial  $\chi$ EFT currents— hybrid calculation

Pastore *et al.* PRC 97 022501 (2018)



GFMC calculations using chiral and axial  $\chi$ EFT currents— consistent calculation

# Partial Muon Capture in Light Nuclei

Weak-interaction Hamiltonian

$$H_W = \frac{G_V}{\sqrt{2}} \int d\mathbf{x} e^{-i\mathbf{k}_\nu \cdot \mathbf{x}} \tilde{l}_\sigma(\mathbf{x}) j^\sigma(\mathbf{x})$$

- Momentum transfer  $q \sim 100 \text{ MeV}$
- Validation of vector and axial charges and currents
- For light nuclei, you can approximate the muon as at rest in a Hydrogen-like 1s orbital

$$\begin{aligned} \Gamma = & \frac{G_V^2}{2\pi} \frac{|\psi_{1s}^{\text{av}}|^2}{(2J_i + 1) \text{recoil}} \frac{E_\nu^{*2}}{\sum_{M_f, M_i}} \left[ |\langle J_f, M_f | \rho(E_\nu^* \hat{\mathbf{z}}) | J_i, M_i \rangle|^2 + |\langle J_f, M_f | \mathbf{j}_z(E_\nu^* \hat{\mathbf{z}}) | J_i, M_i \rangle|^2 \right. \\ & + 2 \text{Re} \left[ \langle J_f, M_f | \rho(E_\nu^* \hat{\mathbf{z}}) | J_i, M_i \rangle \langle J_f, M_f | \mathbf{j}_z(E_\nu^* \hat{\mathbf{z}}) | J_i, M_i \rangle^* \right] + |\langle J_f, M_f | \mathbf{j}_x(E_\nu^* \hat{\mathbf{z}}) | J_i, M_i \rangle|^2 \\ & \left. + |\langle J_f, M_f | \mathbf{j}_y(E_\nu^* \hat{\mathbf{z}}) | J_i, M_i \rangle|^2 - 2 \text{Im} \left[ \langle J_f, M_f | \mathbf{j}_x(E_\nu^* \hat{\mathbf{z}}) | J_i, M_i \rangle \langle J_f, M_f | \mathbf{j}_y(E_\nu^* \hat{\mathbf{z}}) | J_i, M_i \rangle^* \right] \right] \end{aligned}$$

# Partial Muon Capture Rates with QMC: ${}^3\text{He}(\mu^-, \nu_\mu){}^3\text{H}$

Momentum transfer  $q \sim 100$  MeV

- QMC rate for  ${}^3\text{He}(1/2^+; 1/2) \rightarrow {}^3\text{H}(1/2^+; 1/2)$

- ▶  $\Gamma_{\text{VMC}} = 1512 \text{ s}^{-1} \pm 32 \text{ s}^{-1}$
- ▶  $\Gamma_{\text{GFMC}} = 1476 \text{ s}^{-1} \pm 43 \text{ s}^{-1}$
- ▶  $\Gamma_{\text{expt}} = 1496.0 \text{ s}^{-1} \pm 4.0 \text{ s}^{-1}$

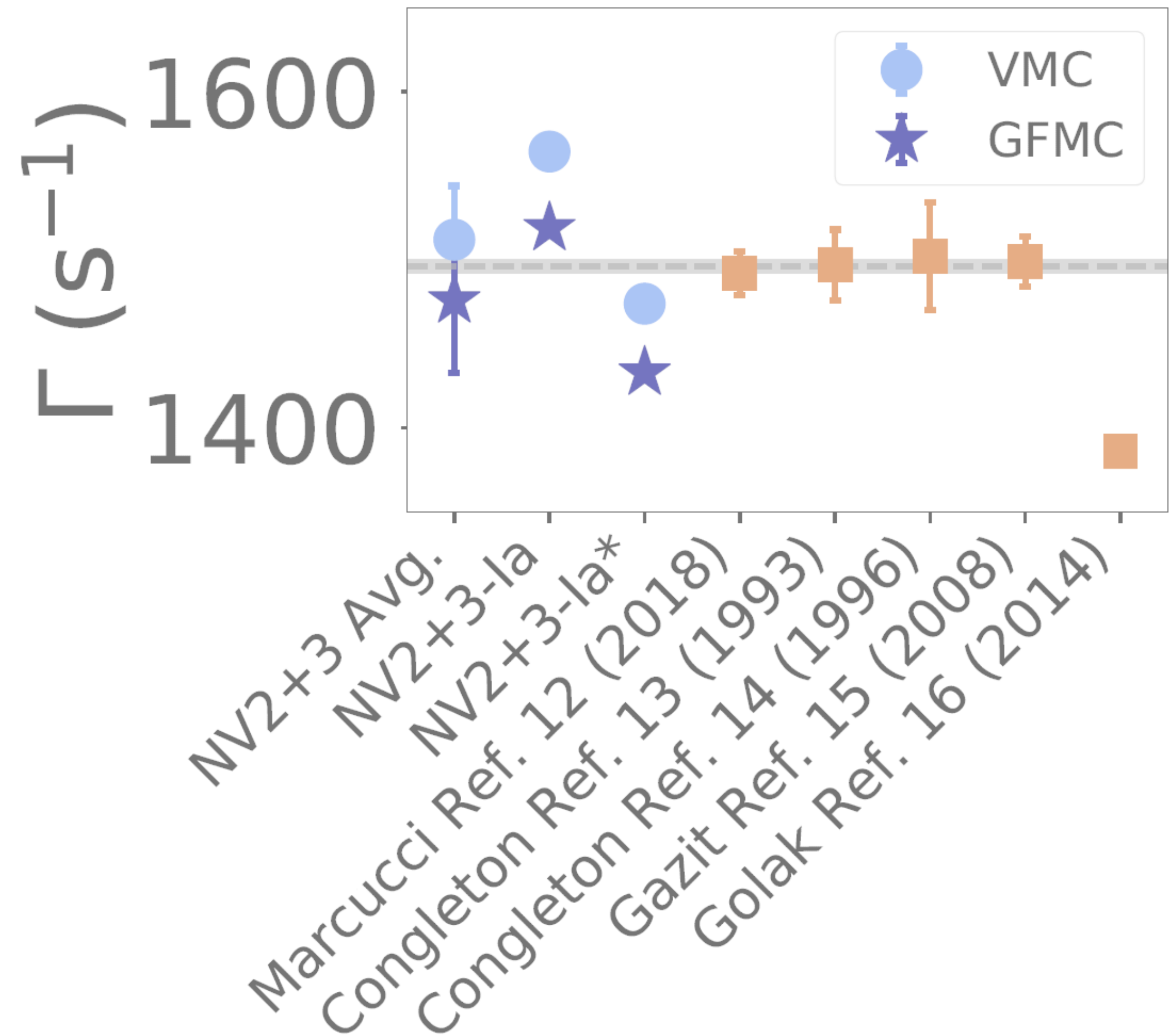
[Ackerbauer et al. Phys. Lett. B417 (1998)]

- The inclusion of 2b electroweak currents increase the rate by about 9% to 16%.

- uncertainty estimates:

- Cutoff:  $8 \text{ s}^{-1}$  (0.5%)
- Energy range of fit:  $11 \text{ s}^{-1}$  (0.7%)
- Three-body fit:  $27 \text{ s}^{-1}$  (1.8%)
- Systematic:  $9 \text{ s}^{-1}$  (0.6%)

King, MP et al. PRC 105 (2022) 4, L042501



# Partial Muon Capture Rates with QMC: ${}^6\text{Li}(\mu^-, \nu_\mu){}^6\text{He}$

Momentum transfer  $q \sim 100$  MeV

- QMC rate for  ${}^6\text{Li}(1^+;0) \rightarrow {}^6\text{He}(0^+;1)$

- $\Gamma_{\text{VMC}} = 1243 \text{ s}^{-1} \pm 59 \text{ s}^{-1}$
- $\Gamma_{\text{GFMC}} = 1056 \text{ s}^{-1} \pm 180 \text{ s}^{-1}$
- $\Gamma_{\text{expt}} = 1600 \text{ s}^{-1} +300/-129 \text{ s}^{-1}$

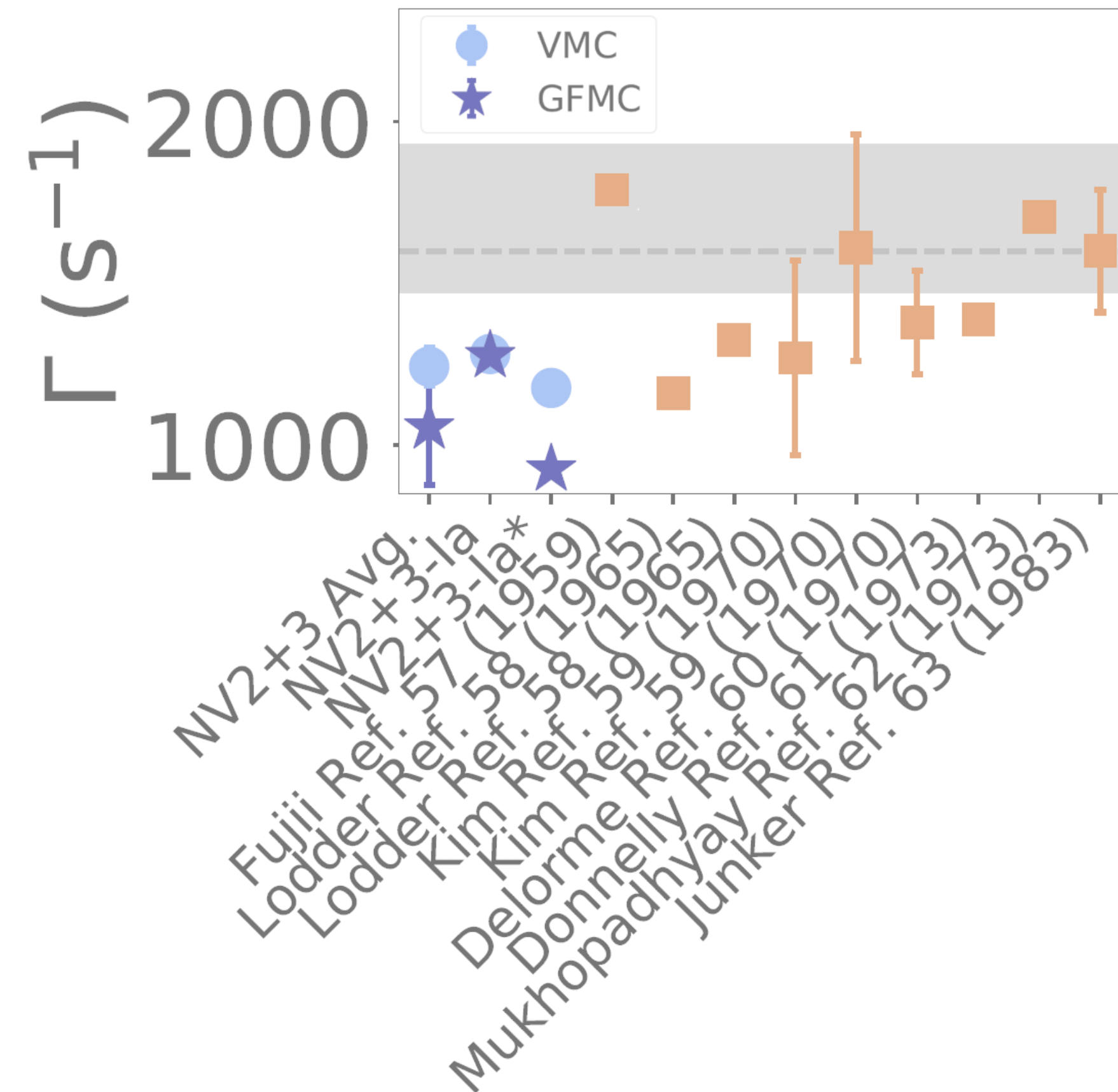
Deutsch et al. Phys. Lett. B26 (1968)

- The inclusion of 2b electroweak currents increase the rate by about 3% to 7%.

- uncertainty estimates:

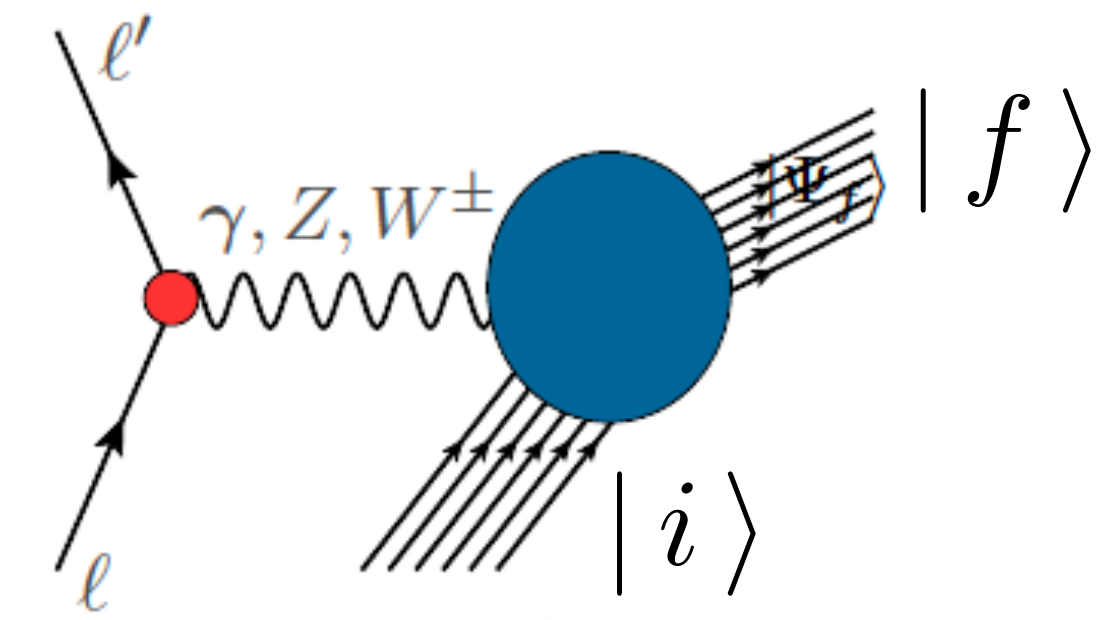
- Cutoff:  $36 \text{ s}^{-1}$  (2.9%)
- Energy range of fit:  $36 \text{ s}^{-1}$  (2.9%)
- Three-body fit:  $30 \text{ s}^{-1}$  (2.4%)
- Systematic:  $8 \text{ s}^{-1}$  (0.6%)

King, MP et al. PRC 105 (2022) 4, L042501



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# Lepton-Nucleus Scattering: Inclusive Processes



- Inclusive lepton scattering off a the nucleus: five response functions

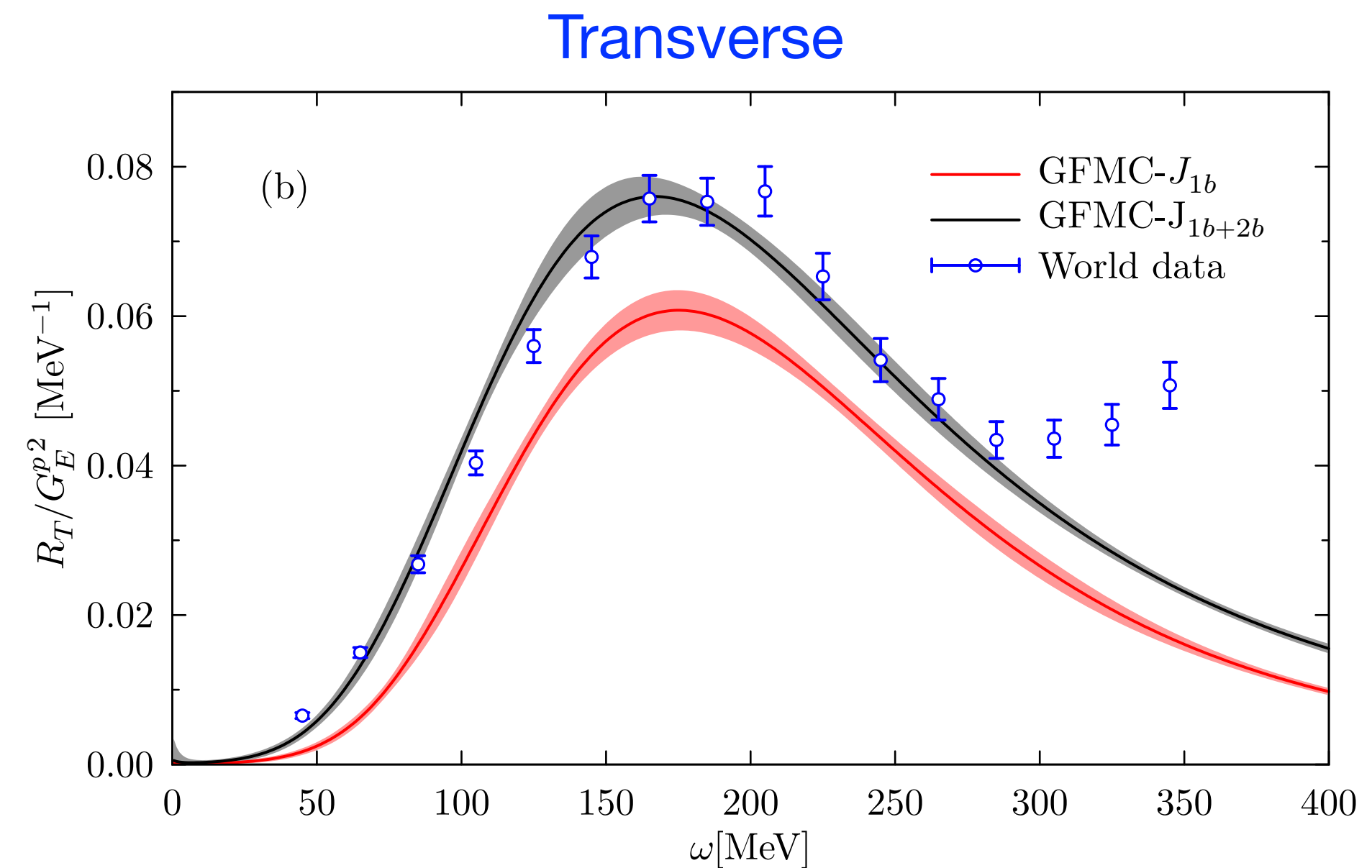
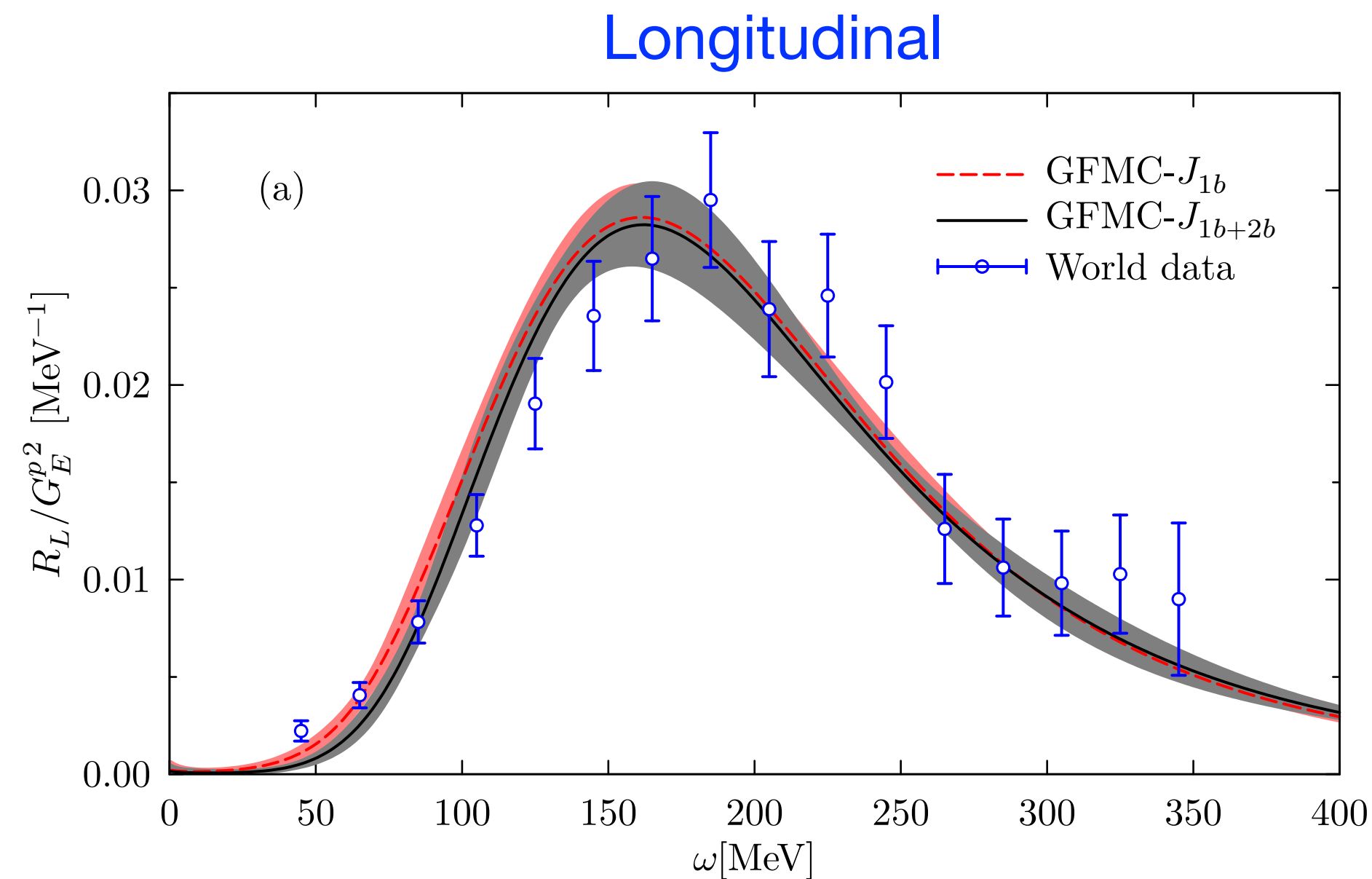
$$\frac{d\sigma}{d\epsilon'_l d\Omega_l} \propto \left[ v_{00} R_{00} + v_{zz} R_{zz} - v_{0z} R_{0z} + v_{xx} R_{xx} \mp v_{xy} R_{xy} \right]$$

- For the EM case only two response functions survive: longitudinal  $R_{00}$  and transverse  $R_{xx}$  which are obtained from the charge and transverse current operators  $R_\alpha(q, \omega) = \sum_f \delta(\omega + E_0 - E_f) |\langle f | O_\alpha(\mathbf{q}) | 0 \rangle|^2$   $O_L = \rho$   
 $O_T = \mathbf{j}$

Euclidean response: GFMC calculations

$$\int_0^\infty d\omega e^{-\tau\omega} R_{\alpha\beta}(q, \omega) = \langle i | j_\alpha^\dagger(\mathbf{q}) e^{-\tau(H-E_i)} j_\beta(\mathbf{q}) | i \rangle$$

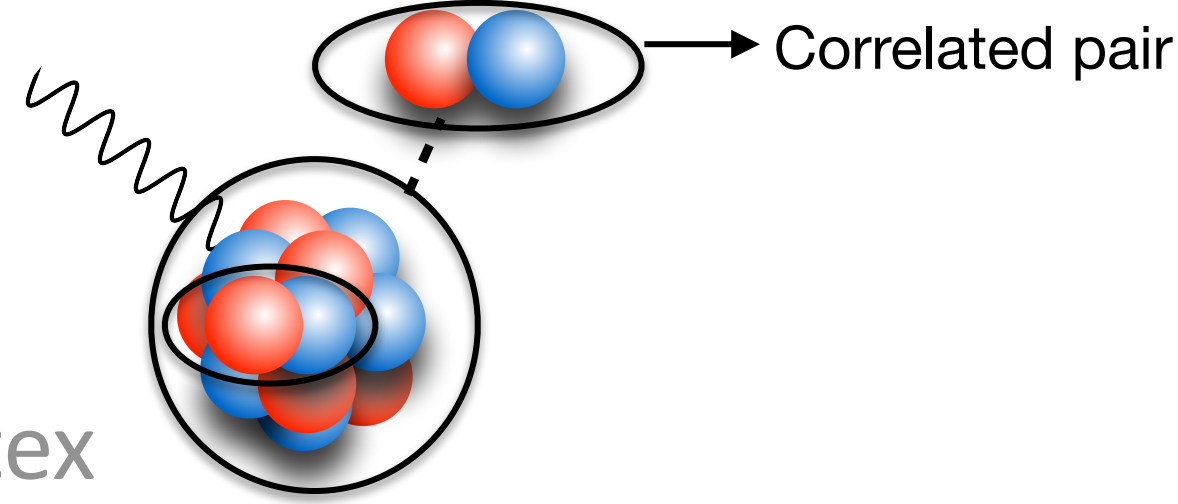
Inversion back to obtain the response by maximum entropy methods



# Lepton-Nucleus Scattering: Exclusive Processes

## Short-Time-Approximation:

- Based on factorization
- Response functions are given by the scattering from pairs of fully interacting nucleons that propagate into a correlated pair of nucleons
- Allows to retain both two-body correlations and currents at the vertex
- Describe electroweak scattering for  $A > 12$  without losing two-body physics
- Incorporate relativistic effects
- Provides “more” exclusive information in terms of nucleon-pair kinematics via the Response Densities



Response **Functions:** integral over real time

$$R_{\alpha\beta}(\omega, \mathbf{q}) = \int \frac{dt}{2\pi} e^{i(\omega + E_0)t} \langle 0 | J_{\alpha}^{\dagger}(\mathbf{q}) e^{-iHt} J_{\beta}(\mathbf{q}) | 0 \rangle$$

The two main assumption underlying the STA are:

1. Only the one- and two-body terms are kept in the current-current correlator

$$j^{\dagger}(i) e^{-iHt} j(i) + j^{\dagger}(i) e^{-iHt} j(j) + j^{\dagger}(i) e^{-iHt} j(ij) + j^{\dagger}(ij) e^{-iHt} j(ij)$$

2. In the particle propagator the Hamiltonian is rewritten as

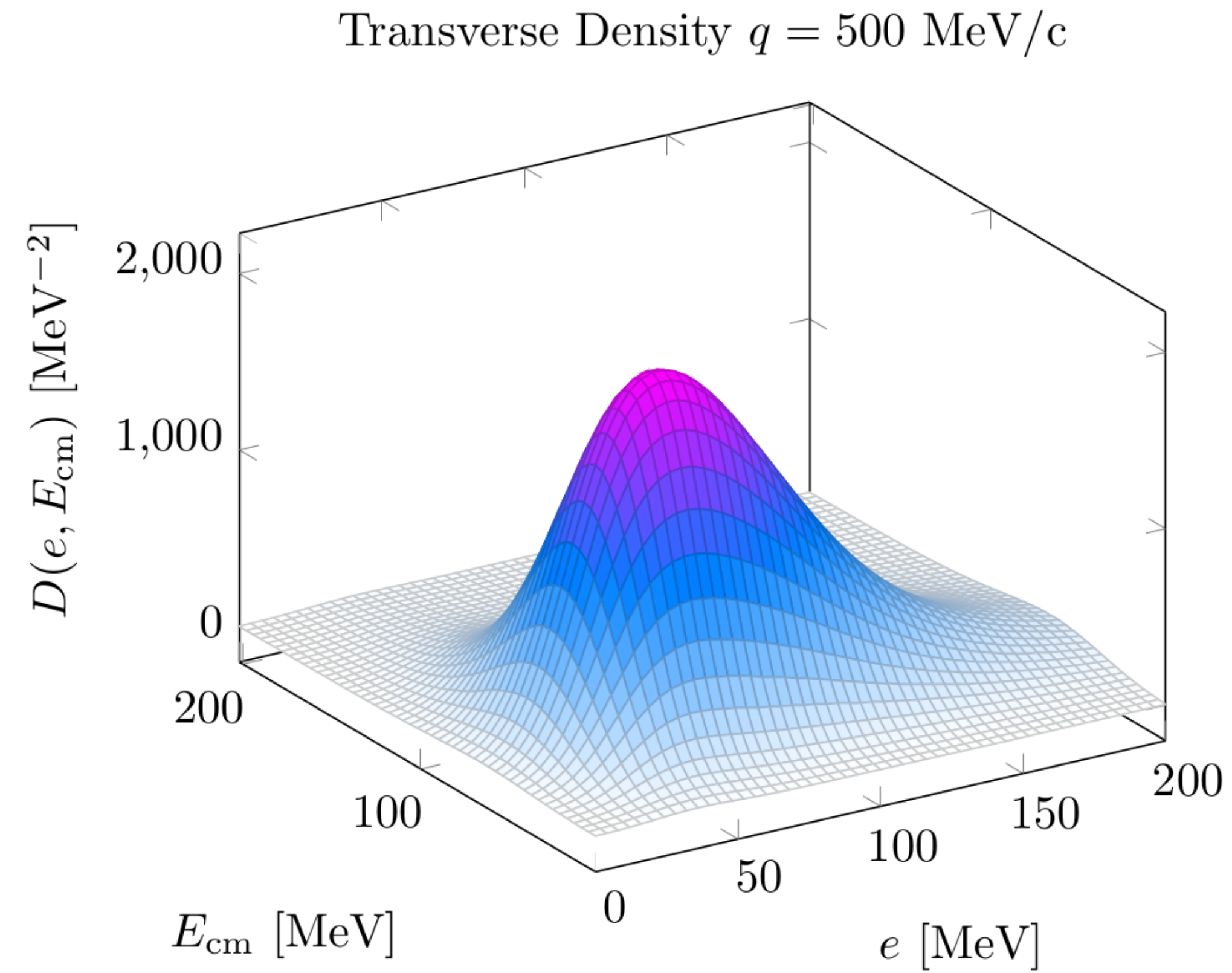
$$H = \sum_i \frac{p_i^2}{2m} + \sum_{ij} v_{ij}$$

Response **Densities:**

$$R(q, \omega) = \int_0^{\infty} de dE_{\text{cm}} \delta(\omega + E_0 - e - E_{\text{cm}}) D(e, E_{\text{cm}})$$

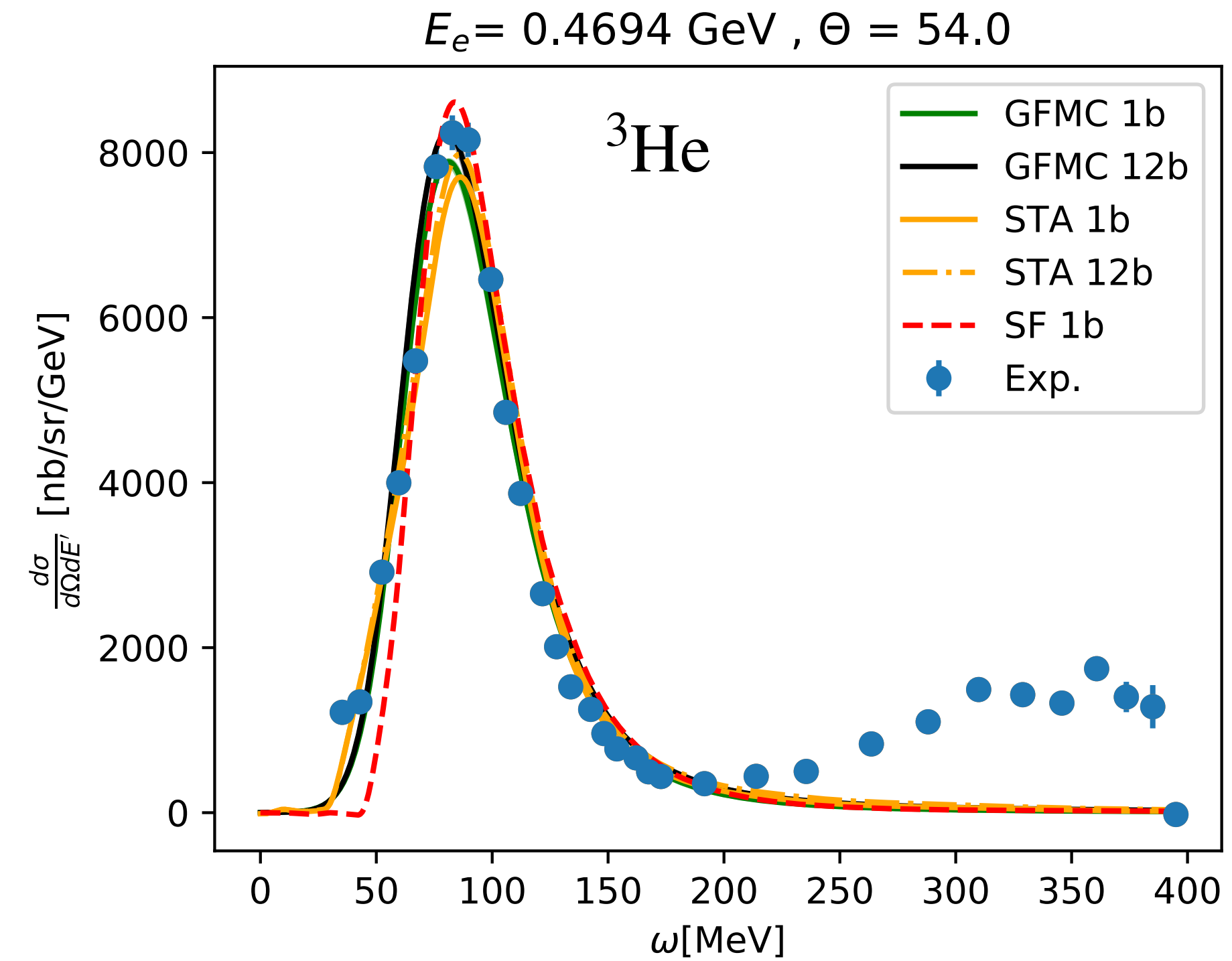
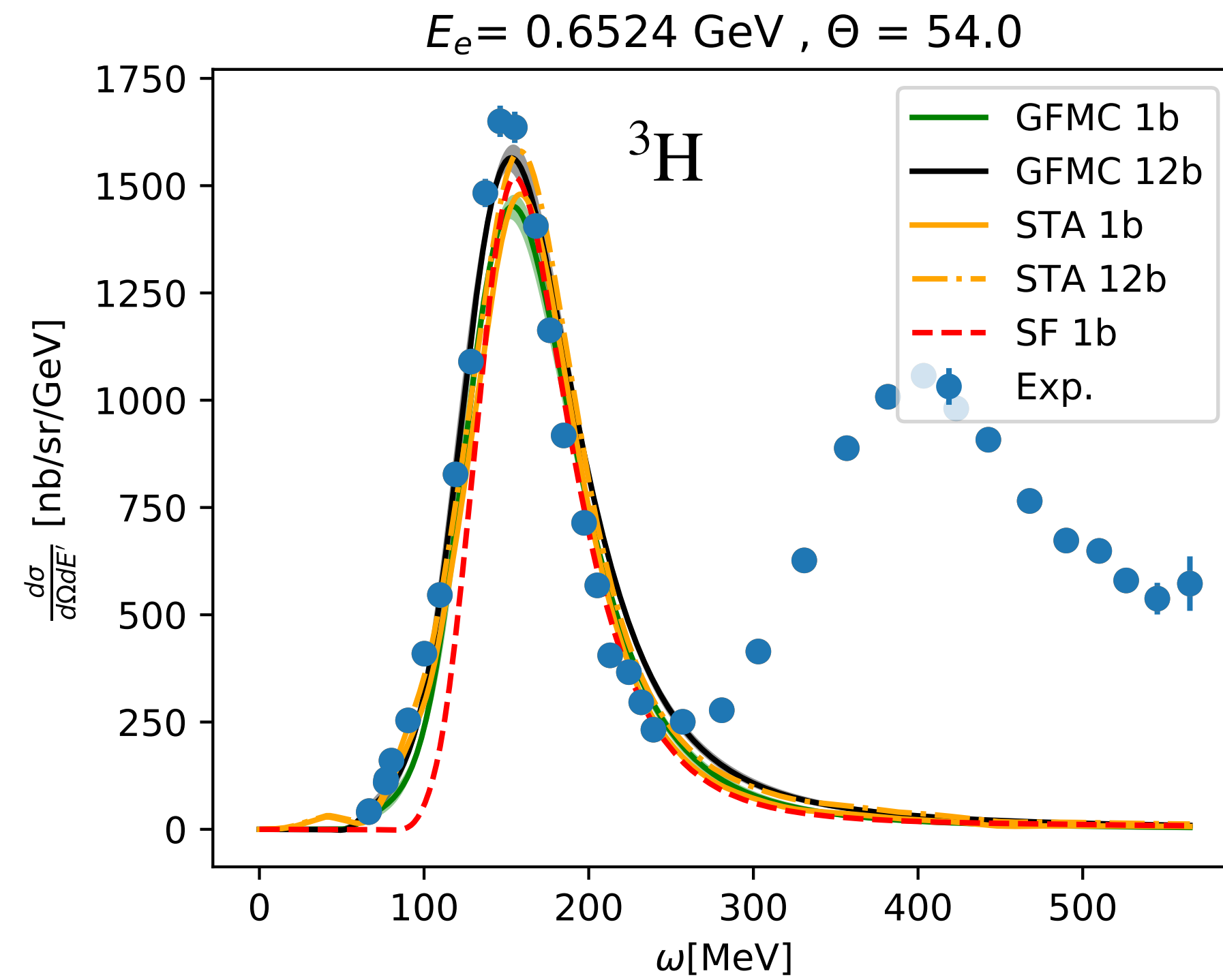
$E_{\text{cm}}$  and  $e$  are the CM and relative energy of the struck nucleon pair

# Transverse Response Density: $e$ - ${}^4\text{He}$ scattering



Pastore *et al.* PRC101(2020)044612

# Cross sections $^3\text{H}$ and $^3\text{He}$ : benchmark between GFMC and STA

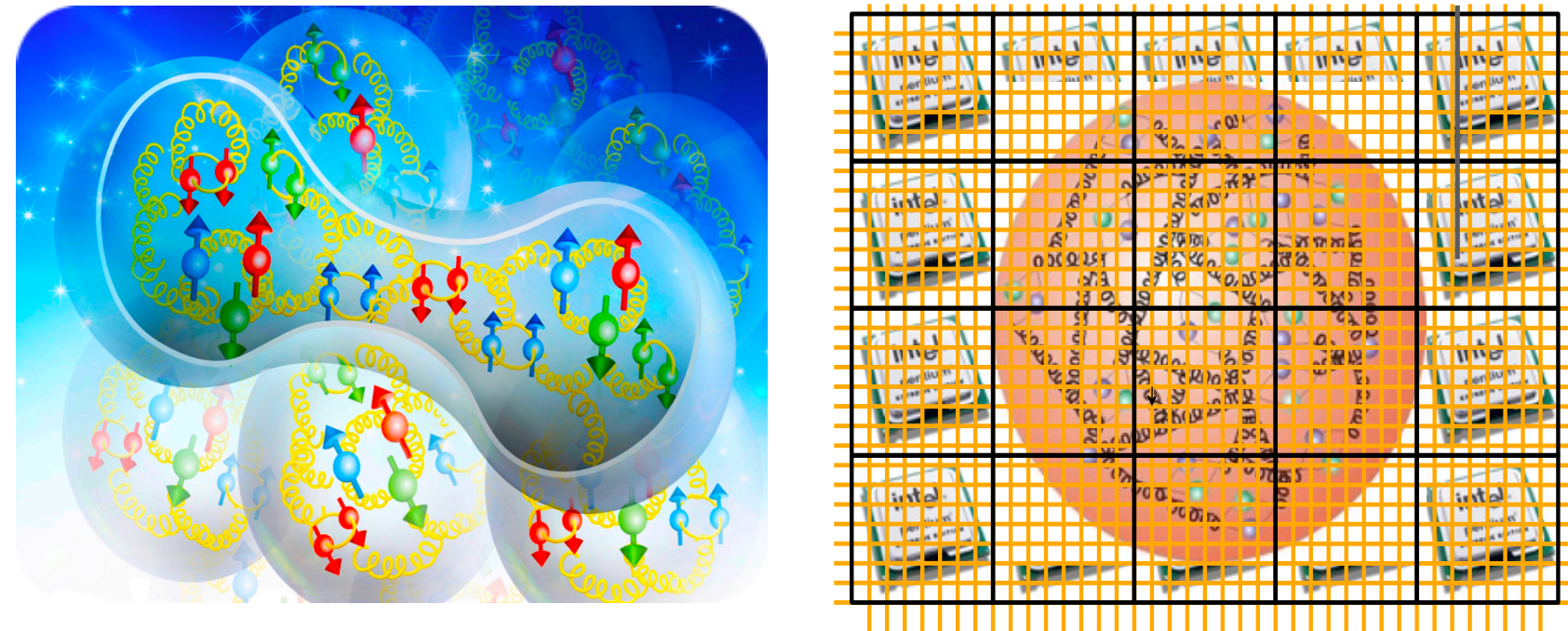


Andreoli et al. Phys. Rev. C 105, 014002

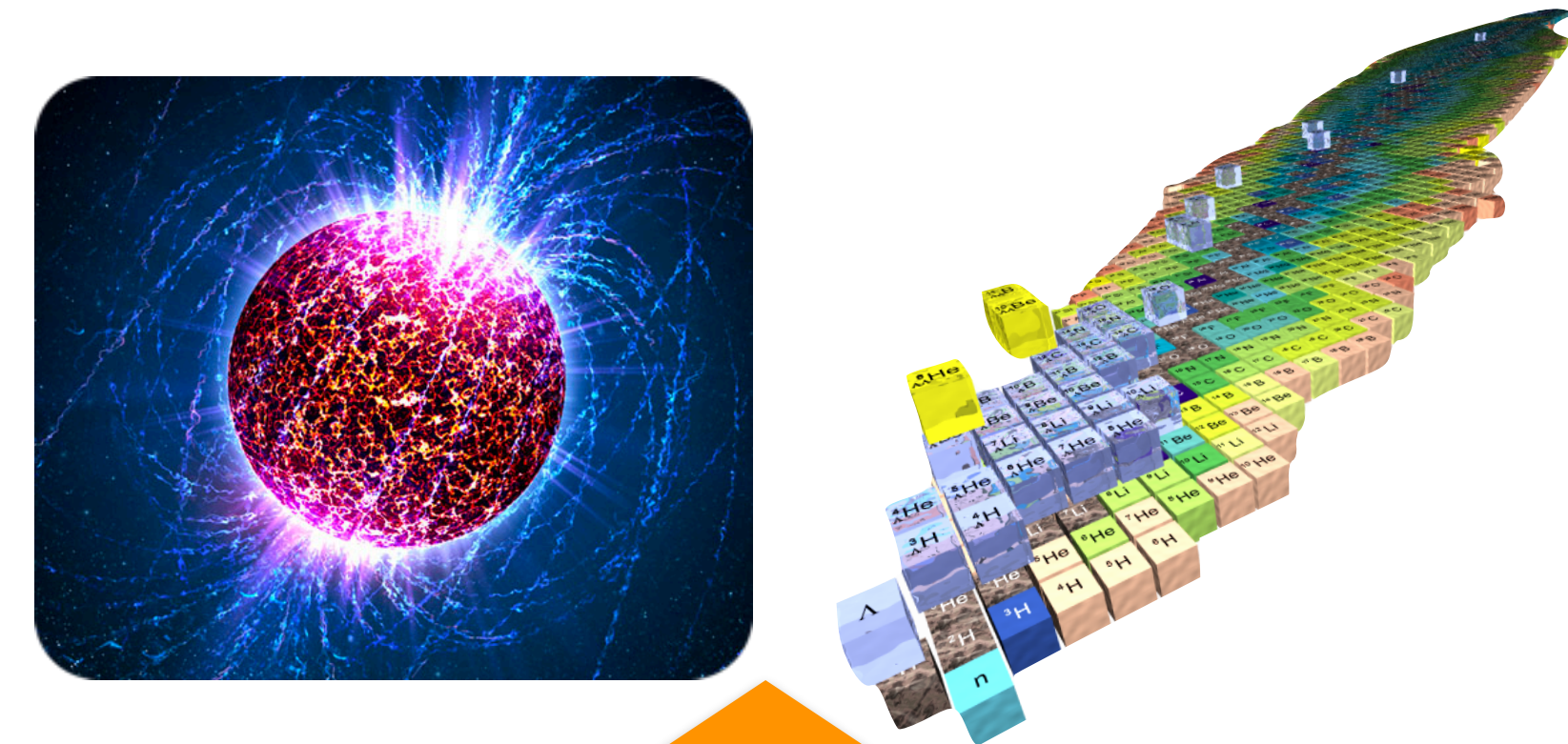


# Summary: Workflow for the microscopic model nuclear theory

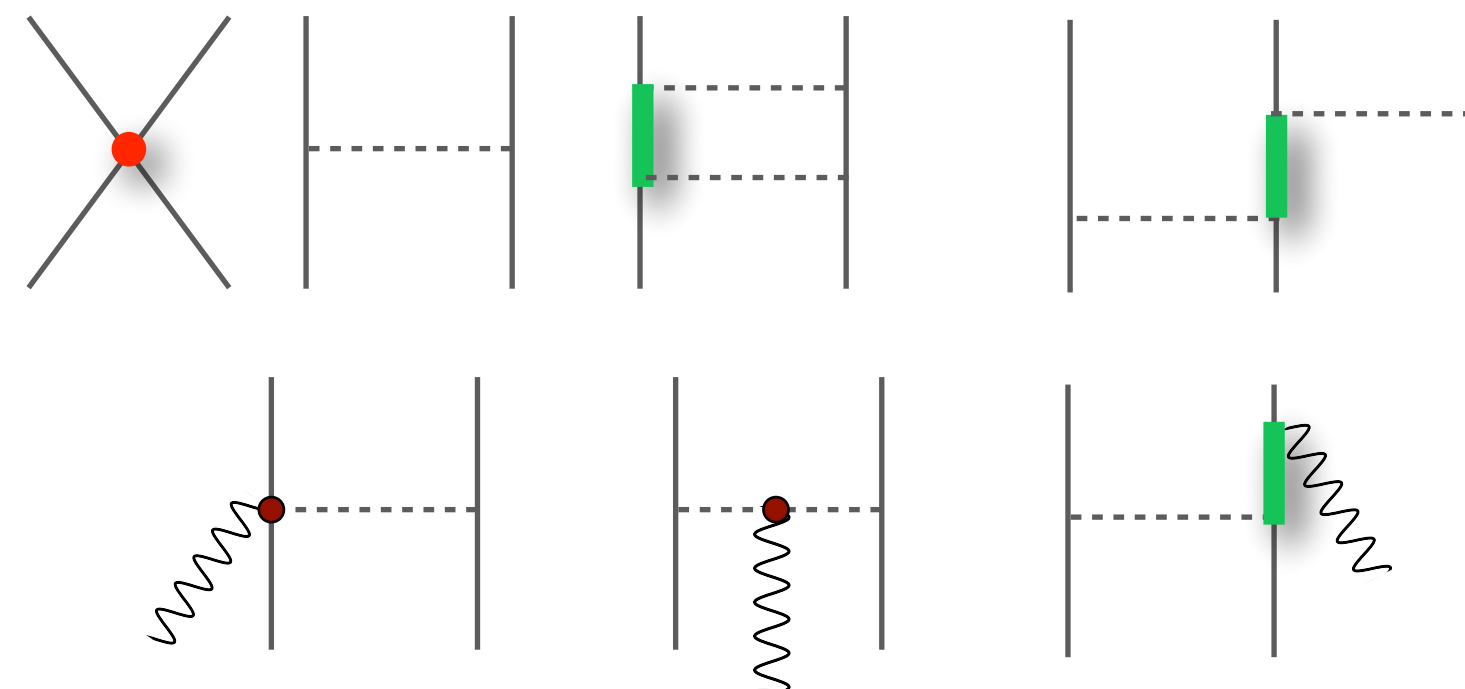
## Quantum Chromodynamics



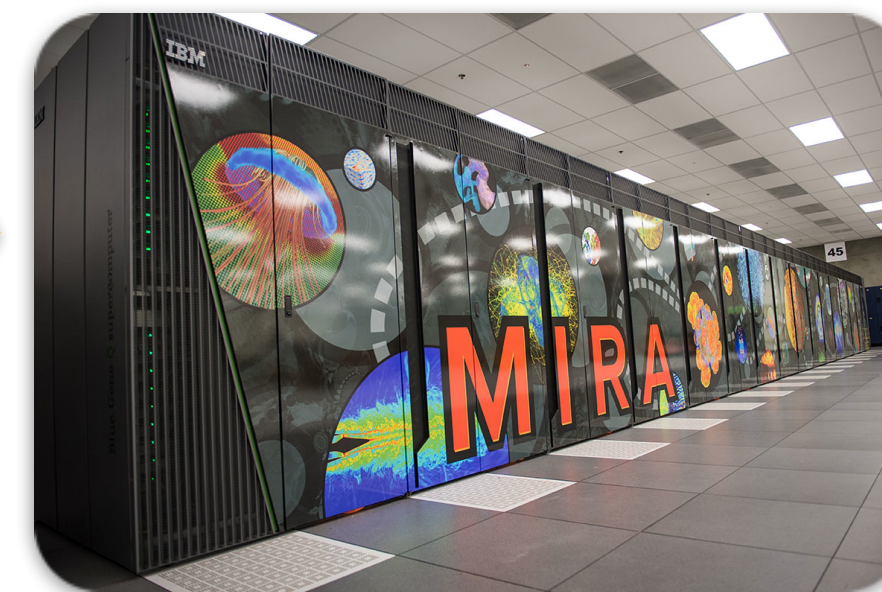
## Atomic nuclei and nucleonic matter



## Hamiltonian and electroweak currents



## Accurate nuclear many-body methods



$$H|\Psi_n\rangle = E_n|\Psi_n\rangle$$

$$J_{mn} = \langle\Psi_m|J|\Psi_n\rangle$$

# Summary:

- *(Progress)*: Tremendous progress in ab-initio theory: algorithms and interactions
  - increased algorithm efficiency,
  - new algorithms (hybrid),
  - successful algorithm benchmarks,
  - advent of EFTs and UQ
- *(Progress)*: Microscopic description of nuclei represent a powerful tool to elucidate the role of two-body effects in nuclear interactions and currents:
  - two-body corrections can be sizable and improve the agreement of theory with experiment
- *(Progress)*: Possibility to perform consistent calculations for nuclei and infinite matter, connecting nuclei observables to astrophysical quantities and observations
- *(Needs)*: New protocols to build realistic nuclear interactions:
  - which observables to use? In which mass range? Uncertainty quantification?
  - improvements in the formulation of the 3NFs
- *(Needs)*: A deeper and more quantitative understanding of the connection between properties of matter and finite nuclei is needed

# Quantum Monte Carlo Group for Nuclear Physics

<https://physics.wustl.edu/quantum-monte-carlo-group>



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*Thank you for your attention!*

