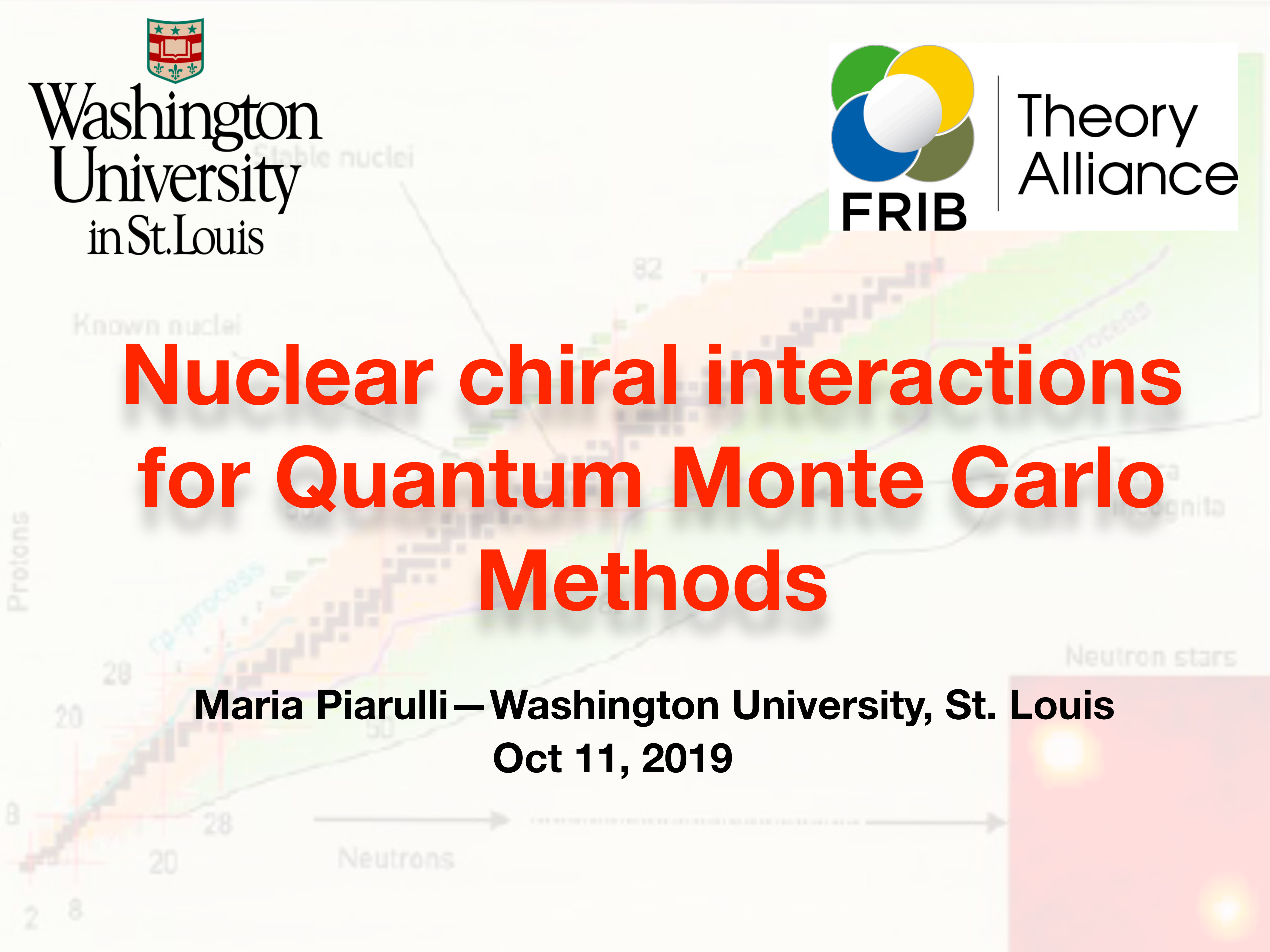
Washington University in St. Louis

FRIB Theory Alliance



Nuclear chiral interactions for Quantum Monte Carlo Methods

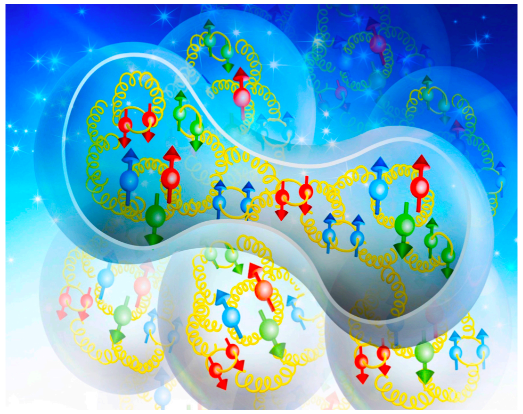
Maria Piarulli—Washington University, St. Louis

Oct 11, 2019

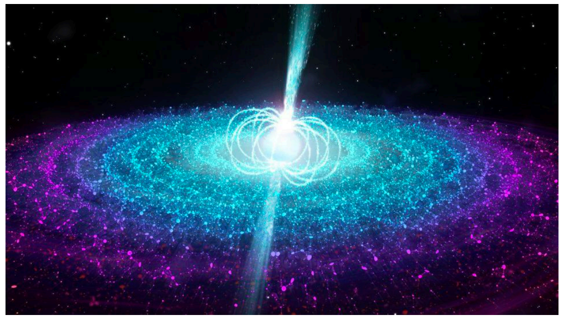
Nuclear Physics

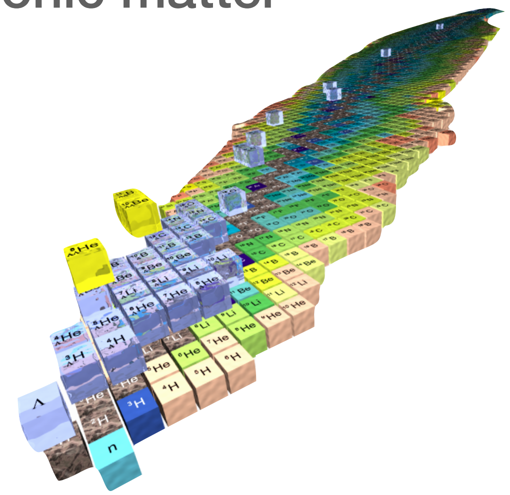
Question: where does the nuclear force which binds nucleons together gets its main characteristics, and how it is rooted in the fundamental theory of strong interactions?

Quantum Chromodynamcs

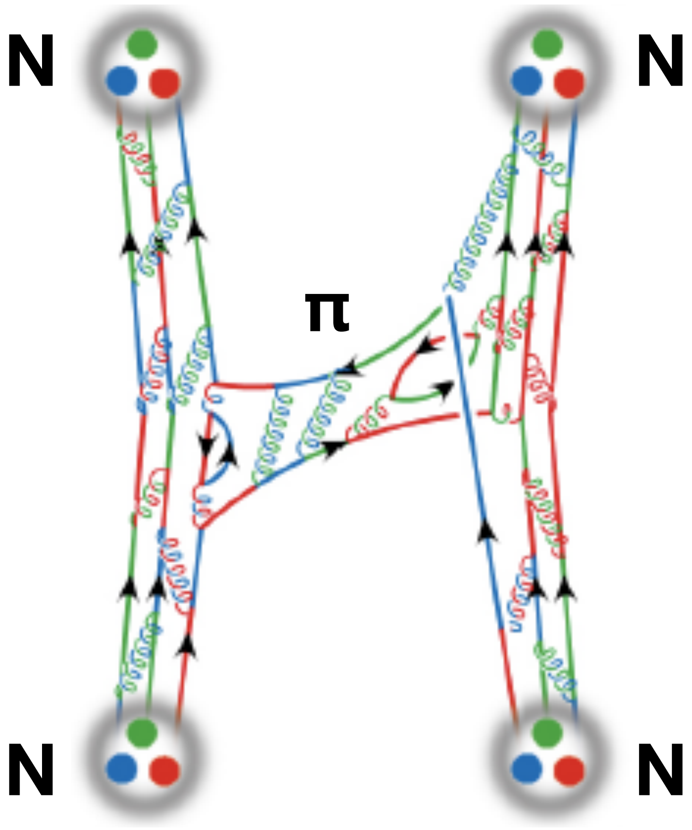


Atomic nuclei and nucleonic matter





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



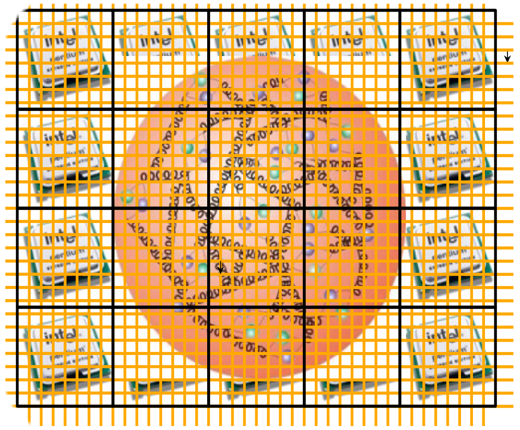
Cartoon of the exchange of a pion (OPE) between two nucleons in the quark picture

OPE: describes the long range part of nuclear forces ($r \gtrsim 2$ fm) to describe the net attraction to form bound nuclei

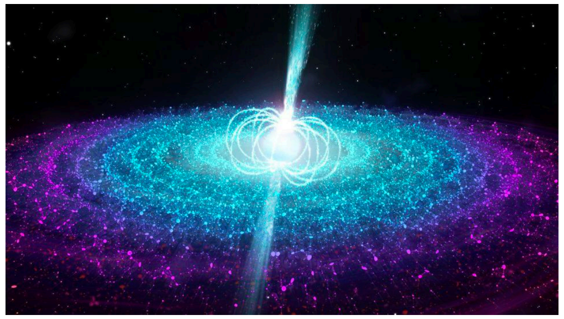
Meson exchange theory: introduced by Yukawa in 1935; in 1947 discovery of a massive particle called pion

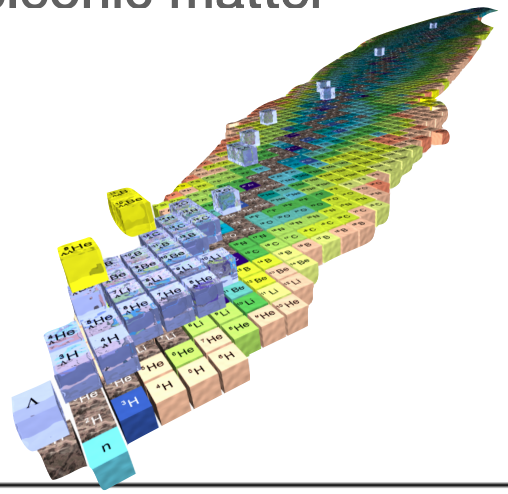
Nevertheless Lattice QCD

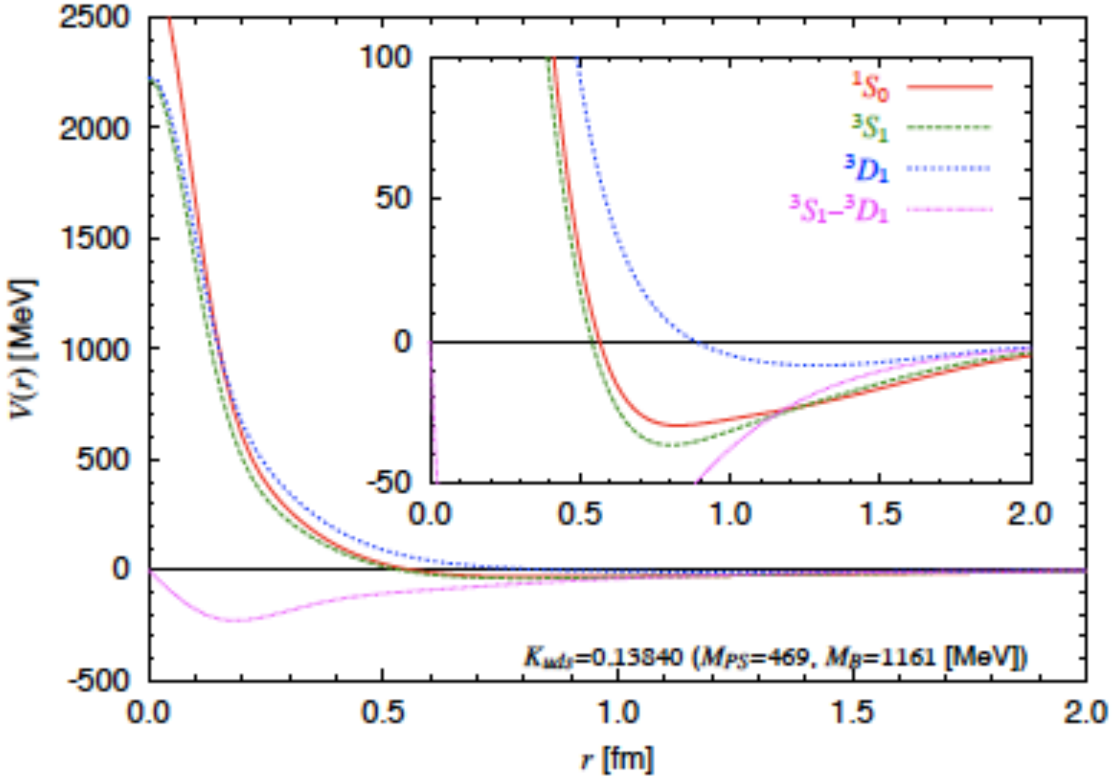
Lattice Quantum Chromodynamcs



Atomic nuclei and nucleonic matter

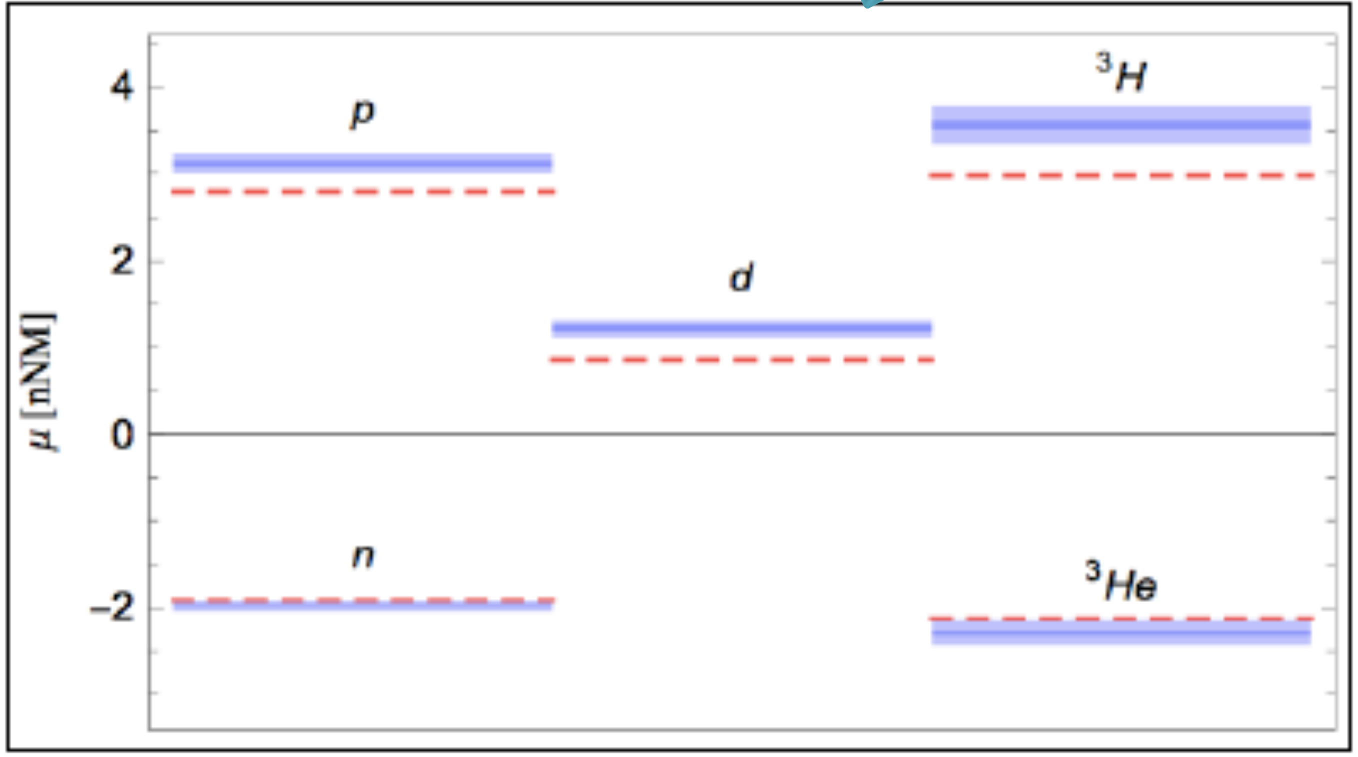






Nuclear Force from LQCD

Inoue et al. PRL 111, 112503 (2013); HALQCD/HPCI



LQCD predictions for magnetic moments A < 4

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

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

The *basic model* of nuclear theory

The *basic model* of nuclear theory: achieving a comprehensive description of the wealth of data and peculiarities exhibited by nuclear systems

Nucleon-nucleon (NN) and 3N scattering data;
Spectra, properties, and transition of nuclei;
Nucleonic matter equation of state;

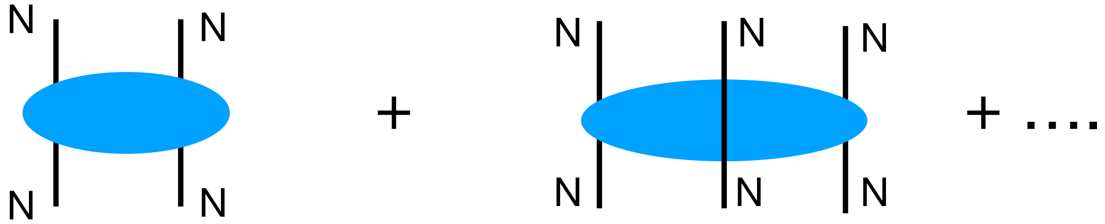
……

Inputs for the *basic model*:

Many-body interactions between the constituents

$$H = \sum_{i=1}^{A} \frac{\mathbf{p}_i^2}{2m_i} + \sum_{i<j=1}^{A} \overbrace{v_{ij}}^{\text{th+exp}} + \sum_{i<j<k=1}^{A} \overbrace{V_{ijk}}^{\text{th+exp}} + \ldots..$$

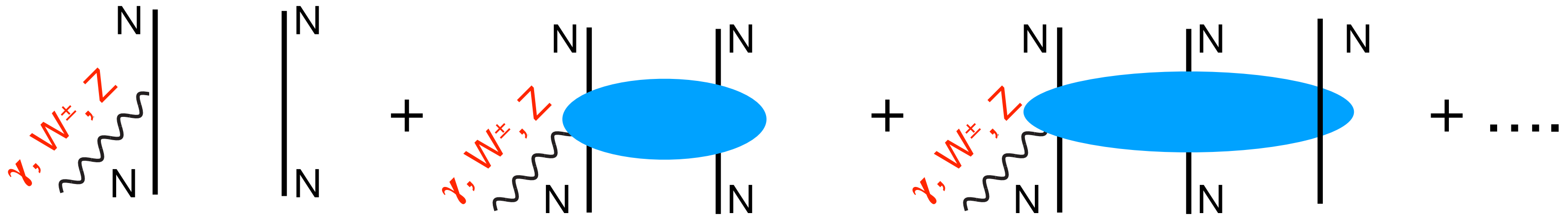
One-body   Two-body (NN)   Three-body (3N)



Electroweak current operators:

$$j^{\text{EW}} = \sum_{i=1}^{A} j_i + \sum_{i<j=1}^{A} \overbrace{j_{ij}}^{\text{th+exp}} + \sum_{i<j<k=1}^{A} \overbrace{j_{ijk}}^{\text{th+exp}} + \ldots.$$

One-body   Two-body   Many-body

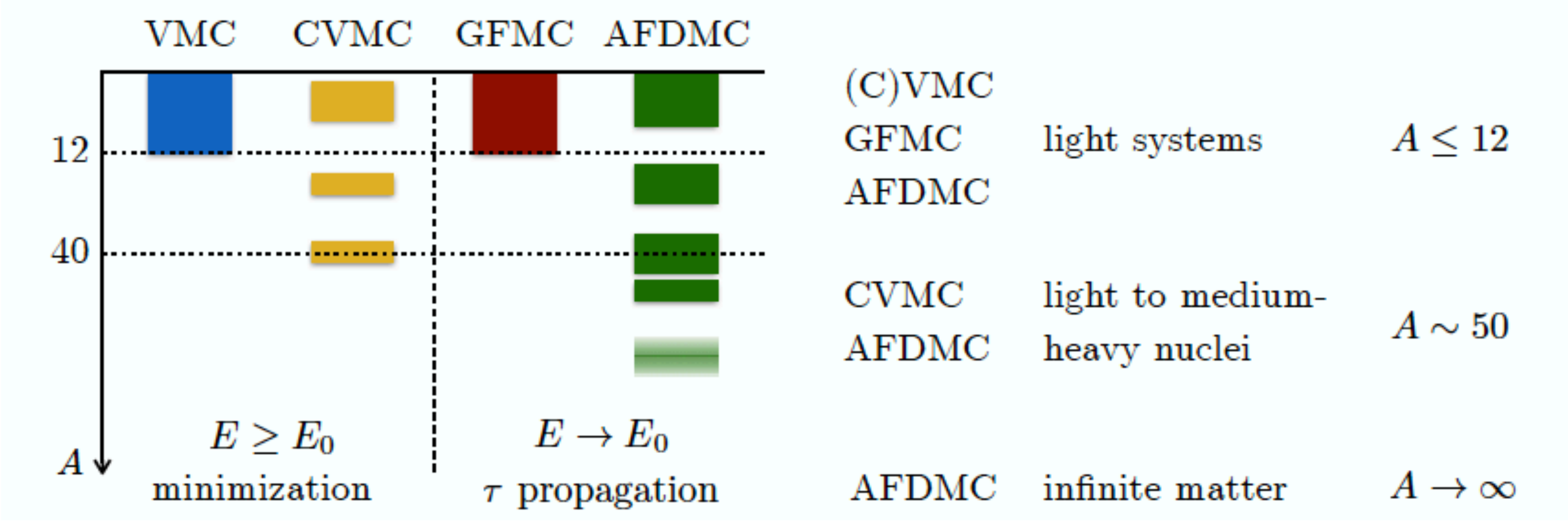


Quantum Monte Carlo methods

Goal: $H\,\Psi(\mathbf{R}; s_1, .., s_A; t_1, .., t_A) = E\,\Psi(\mathbf{R}; s_1, .., s_A; t_1, .., t_A)$

3A coordinates in r-space Nucleon spin Nucleon isospin (p or n)

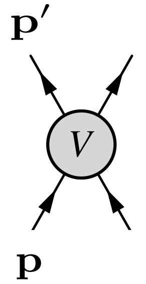
QMC methods: large family of computational methods used to study complex quantum systems



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

Figure by Diego Lonardoni, LANL

- 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

QMC: Variational Monte Carlo (VMC)

R.B. Wiringa, PRC **43**, 1585 (1991)

Minimize the expectation value of H:

$$\boxed{E_T = \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} \geq E_0}$$

Trial wave function (involves variational parameters):

$$\boxed{|\Psi_T\rangle = \left[1 + \sum_{i<j<k} U_{ijk}\right] \left[S \prod_{i<j} (1 + U_{ij})\right] |\Psi_J\rangle}$$

$|\Psi_J\rangle = \left[\prod_{i<j} f_c(r_{ij})\right] |\Phi(JMTT_z)\rangle$ (s-shell nuclei): Jastrow wave function, fully antisymmetric

$S \prod_{i<j}$: represents a symmetrized product

$U_{ij} = \sum_{p=2,6} u_p(r_{ij})\, O_{ij}^p$: pair correlation operators

$U_{ijk} = \sum_x \epsilon_x V_{ijk}^x$: three-body correlation operators

$|\Psi_T\rangle$ are spin-isospin vectors in 3A dimension with $2^A \begin{pmatrix} A \\ Z \end{pmatrix}$

The search in the parameter space is made using COBYLA (Constrained Optimization BY Linear Approximations) algorithm available in NLopt library

QMC: Diffusion Monte Carlo (DMC)

The diffusion Monte Carlo (DMC) method (ex. GFMC or AFDMC) overcomes the limitations of VMC by using a projection technique to determine the true ground-state

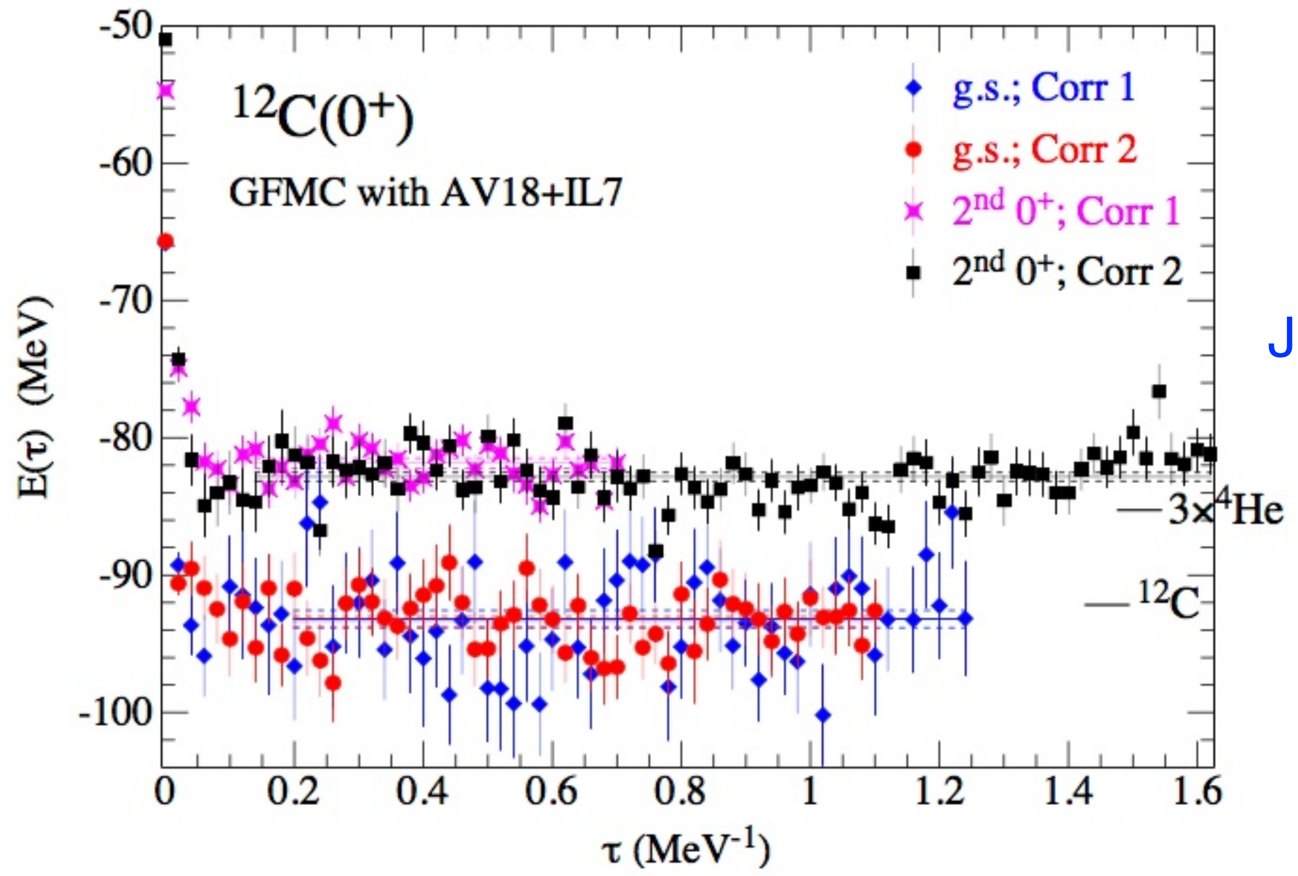
The method relies on the observation that Ψ_T can be expanded in the complete set of eigenstates of the Hamiltonian according to

$$|\Psi_T\rangle = \sum_n c_n |\Psi_n\rangle \qquad H|\Psi_n\rangle = E_n|\Psi_n\rangle$$

$$\boxed{\lim_{\tau\to\infty} |\Psi(\tau)\rangle = \lim_{\tau\to\infty} e^{-(H-E_0)\,\tau}\,|\Psi_T\rangle = c_0|\Psi_0\rangle} \qquad |\Psi(\tau=0)\rangle = |\Psi_T\rangle$$

where τ is the imaginary time

The evaluation of $\Psi(\tau)$ is done stochastically in small time steps $\Delta\tau$ ($\tau = n\,\Delta\tau$) using a Green's function formulation



J. Carlson et al., RMP. **87**, 1067 (2015)

Nuclear Hamiltonian: phenomenological formulation of the *basic model*

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

NN: Argonne V18 $v_{18}(r_{12}) = v^{\gamma}_{12} + v^{\pi}_{12} + v^{I}_{12} + v^{S}_{12} = \sum_{p=1}^{18} v^{p}(r_{12}) O^{p}_{12}$

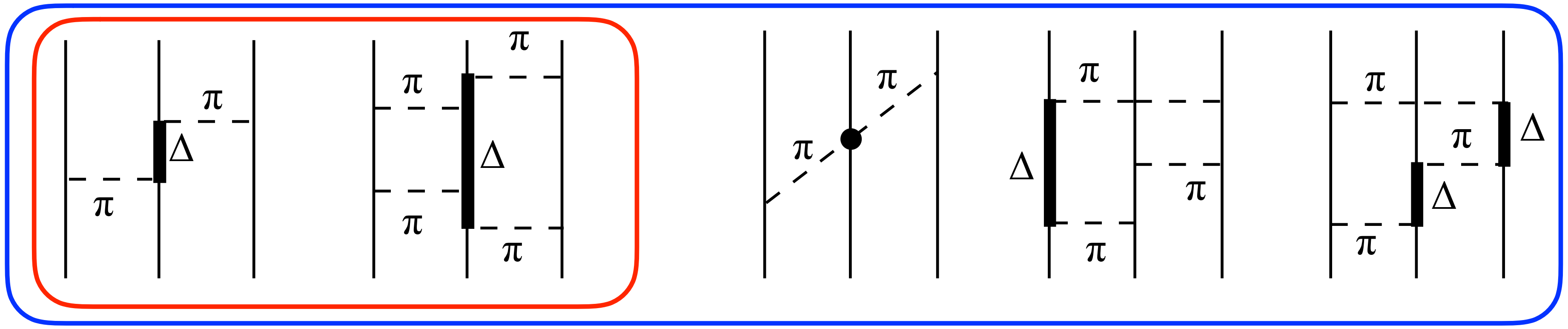
- v^{γ}_{12}: pp, np, nn electromagnetic terms
- v^{π}_{12}: one pion exchange (OPE)
- 18 spin, tensor, spin-orbit, isospin, etc., operators
- 42 independent parameters controlled by ~4300 np and pp scattering data below 350 MeV lab energy

An Hamiltonian including only AV18 does not provide enough binding in the light-nuclei

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

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

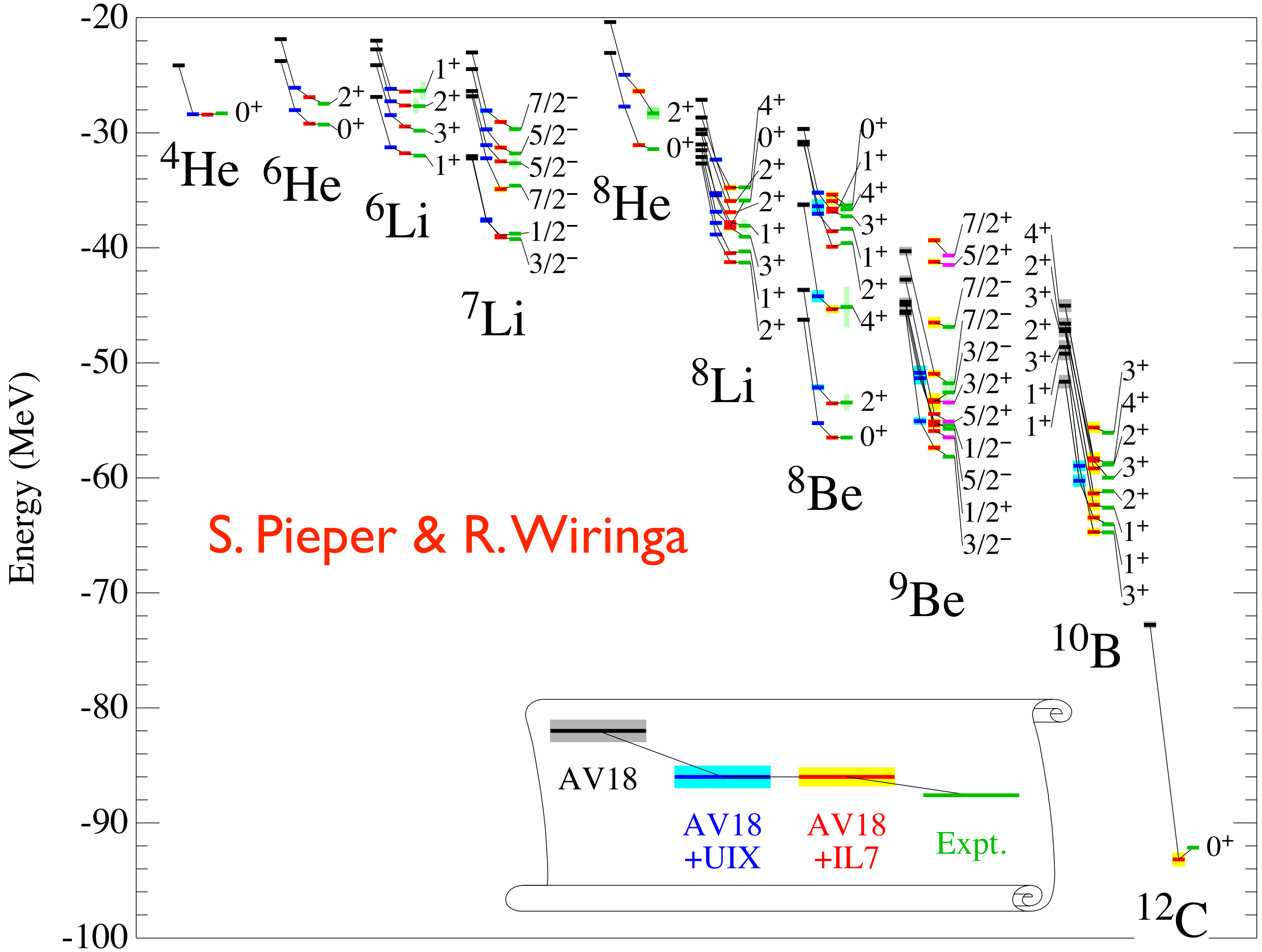
3N Urbana/Illinois



- 2 independent parameters controlled by 3H binding energy & saturation density of symmetric nuclear matter: some problems to describe p-shell nuclei
- 5 independent parameters controlled by ground-state energies of A ≤ 10

Phenomenological potentials & QMC

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

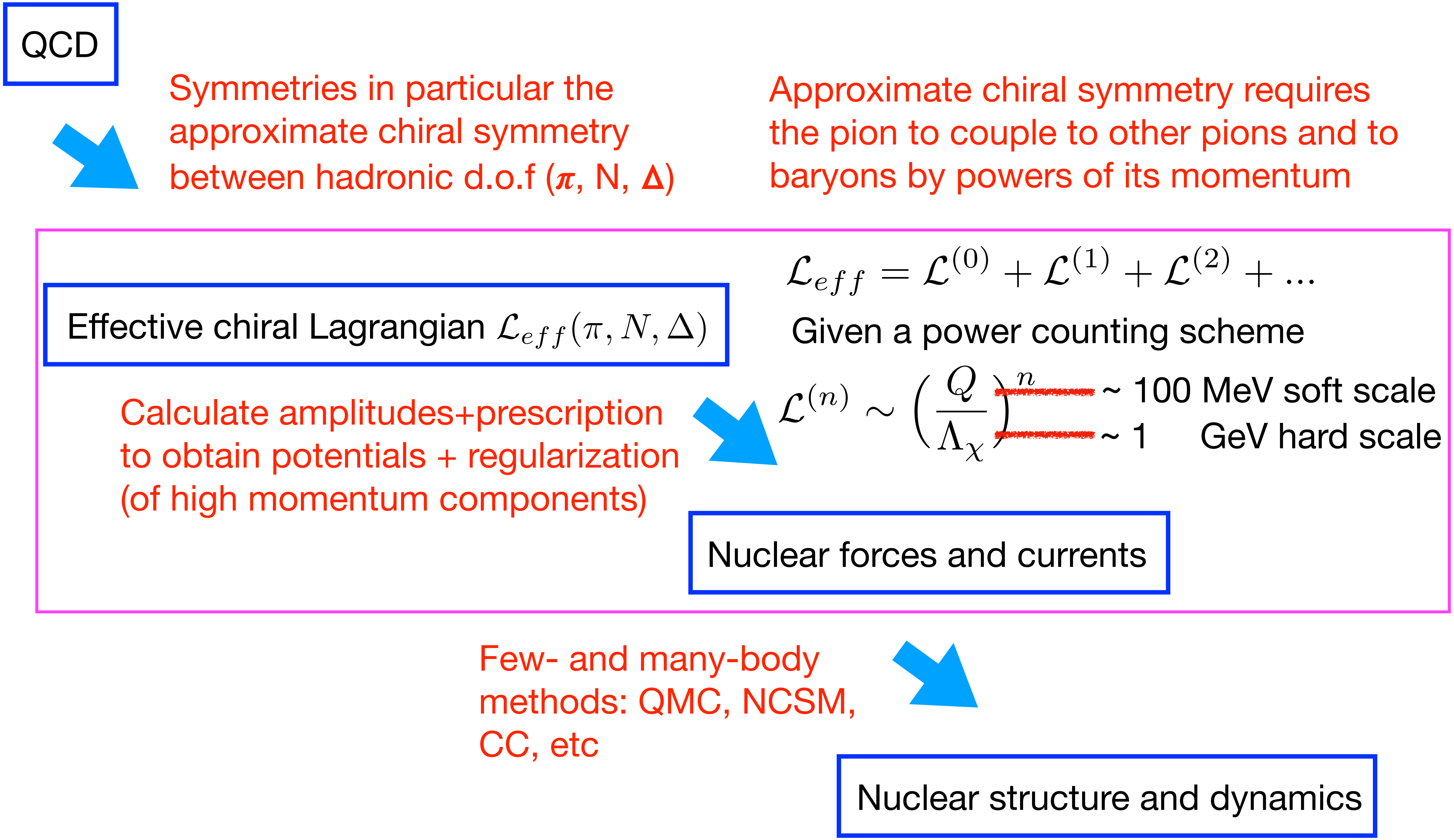


Pros:
- Suitable for QMC
- Very good description of several nuclear observables: ex. GFMC binding energies up to A=12 with AV18+IL7 (GFMC energies: uncertainties within 1-2%)

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 EFT: from QCD to nuclear systems

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 (**π**, N, **Δ**)

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

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

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

Given a power counting scheme

$$\mathcal{L}^{(n)} \sim \left(\frac{Q}{\Lambda_\chi}\right)^n$$

~ 100 MeV soft scale

~ 1 GeV hard scale

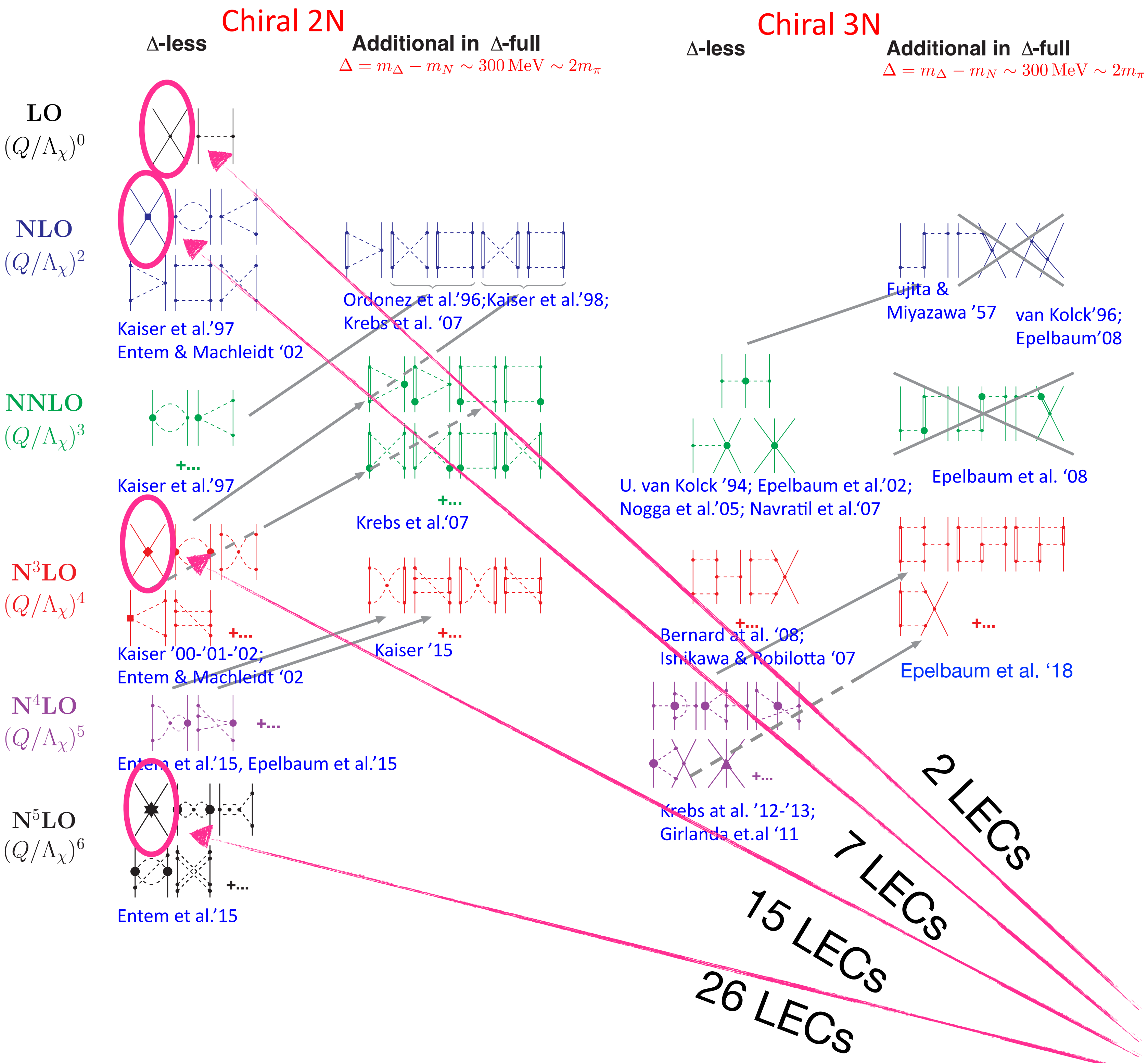
Calculate amplitudes+prescription to obtain potentials + regularization (of high momentum components)

Nuclear forces and currents

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

Nuclear structure and dynamics

Nuclear Hamiltonian: Chiral EFT formulation of the *basic model*



Advantages:

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

Disadvantages:

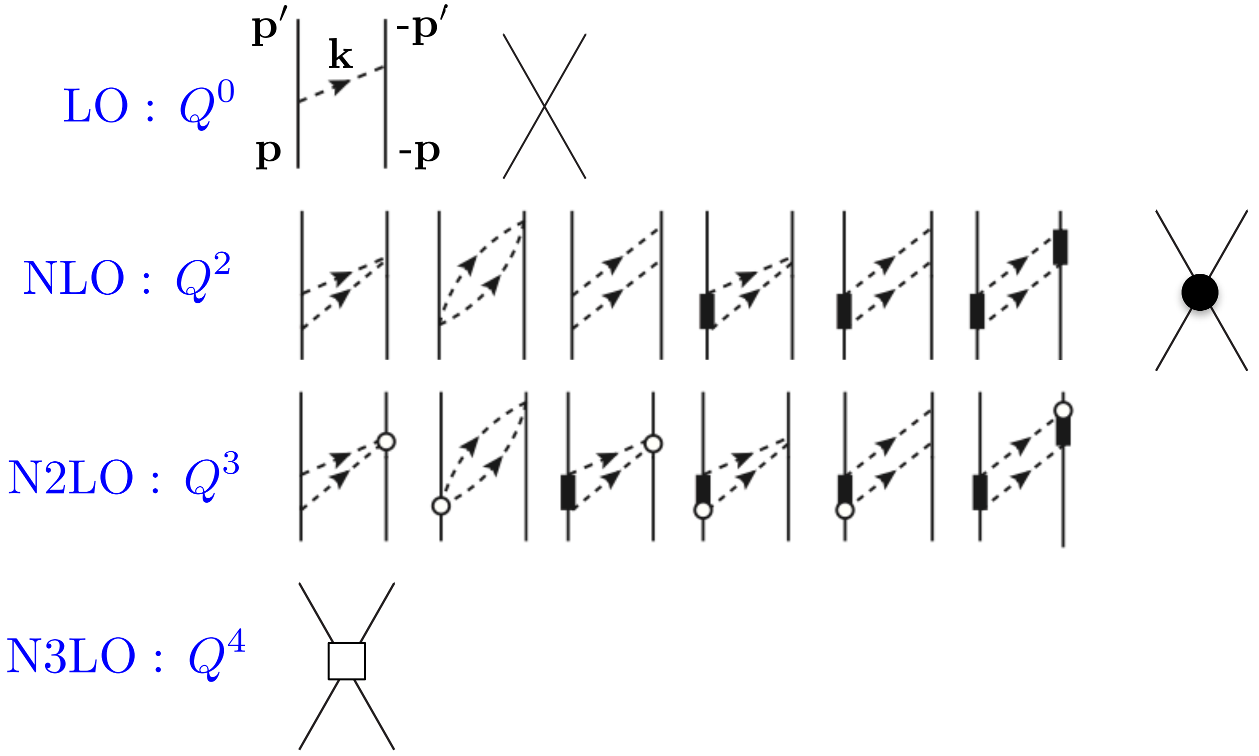
- Increase in number of diagrams as we move to higher orders; When do we stop in the chiral expansion? Convergence, power counting, etc….
- Consistency between strong sector and electroweak sector is very hard to achieve
- More LECs appearing when we go up to higher orders; how do we fix them?

Many of the available versions of chiral potentials are formulated in momentum-space

Gezerlis et al. PRL 111, 032501 2013; PRC 90, 054323 2014;
Lynn et al. PRL 113, 192501 2014
Piarulli et al. PRC 91, 024003 2015; PRC 94, 054007 2016

“Fist generation” local chiral NN potential with Δ’s

Piarulli et al. PRC **91**, 024003 2015; PRC **94**, 054007 2016



v_{12}^{L} : chiral OPE and TPE component with Δ’s

- dependence only on the momentum transfer **k=p′-p**

  $c_1,\ c_2,\ c_3,\ c_4\ (\mathcal{L}^{(2)}_{\pi N}) \quad b_3 + b_8\ (\mathcal{L}^{(2)}_{\pi N\Delta})$

  (Krebs at al. EPJ **A32,** 127 2007), piN scattering, more updated analysis Roy-Steiner)

v_{12}^{S} : contacts up to N3LO (Q^4) 26 LECs

- the functional form taken as $C_{R_S}(r) \propto e^{-(r/R_S)^2}$

  $R_S = 0.8\ (0.7)$ fm

Model for local chiral interaction:

- 26 LECs obtained fitting the pp and np Granada database: two ranges of E_{lab} = 125 MeV and 200 MeV, the deuteron BE and the nn scattering length
- To minimizing the χ^2 we have used the Practical Optimization Using No Derivatives (for Squares), POUNDers

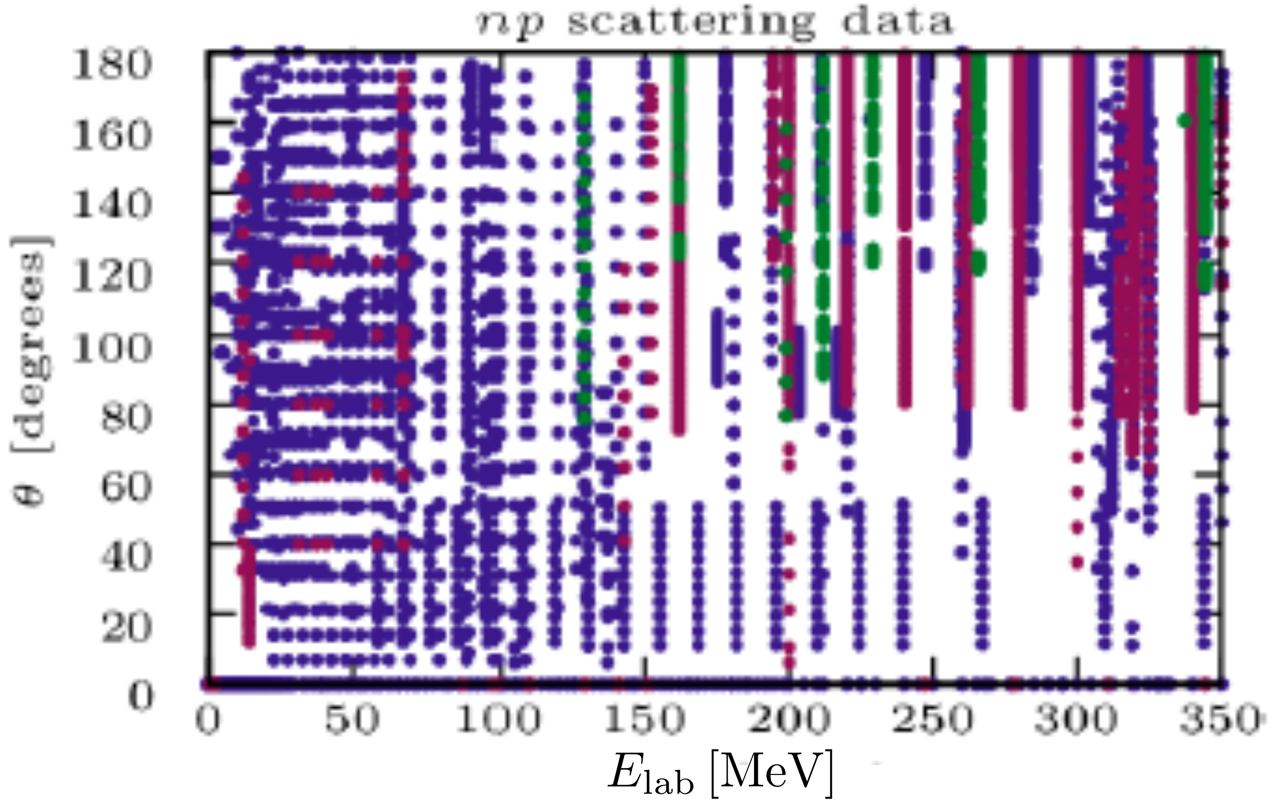
Assumptions:

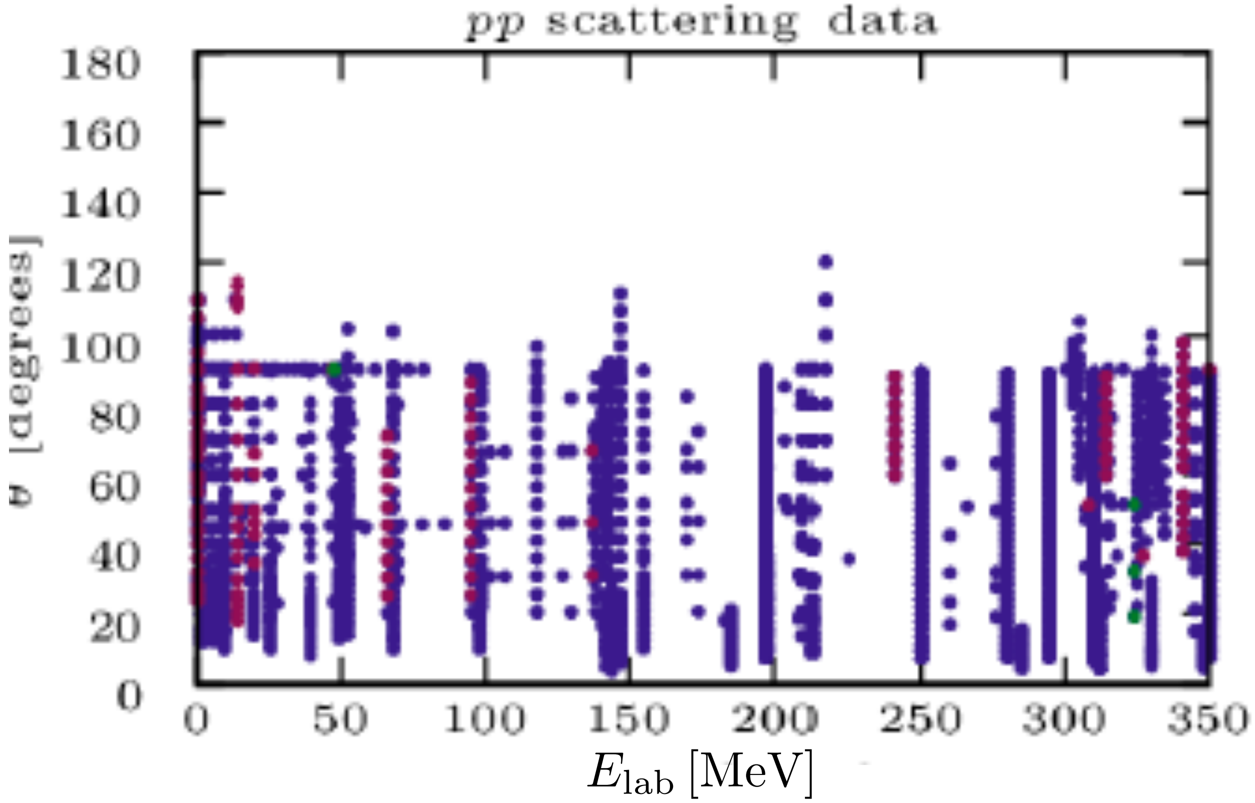
- Neglecting long range component at N3LO; could be justified by the fact we are including Δ-isobar
- Neglecting four nonlocal terms in the contacts at N3LO during the fit procedure; we limited the fitting up to lab energy 200 MeV

Nucleon-Nucleon database

Granada database: consistent database ~8000 data up to pion production threshold

Perez at al. Phys. Rev. C 88, 064002 (2013)





model	order	E_{Lab} (MeV)	N_{pp+np}	χ^2/datum
Ia	N3LO	0–125	2668	1.05
Ib	N3LO	0–125	2665	1.07
IIa	N3LO	0–200	3698	1.37
IIb	N3LO	0–200	3695	1.37

Models a (b) cutoff~500 MeV (600 MeV) in momentum-space

Binding energies with only NN

		^{3}H		^{4}He	
Model	order	E_0	$\sqrt{\langle r_p^2 \rangle}$	E_0	$\sqrt{\langle r_p^2 \rangle}$
b	LO	–13.407(9)	1.23	–55.53(1)	0.90
b	NLO	–7.379(4)	1.69	–23.04(2)	1.55
b	N2LO	–7.574(9)	1.65	–23.95(3)	1.52
b	N3LO	–7.627(17)	1.65	–23.88(5)	1.53

Piarulli et al. PRC **94**, 054007 2016

At LO nuclei are significantly overbound: 5 MeV (for ^{3}H) and 27 MeV (for ^{4}He) more bound of their corresponding exp values (-8.482 MeV and -28.30 MeV)

The NLO contribution is an important correction to the LO results: respectively, $\sim$1 MeV and $\sim$5 MeV underbound compared to their exp values

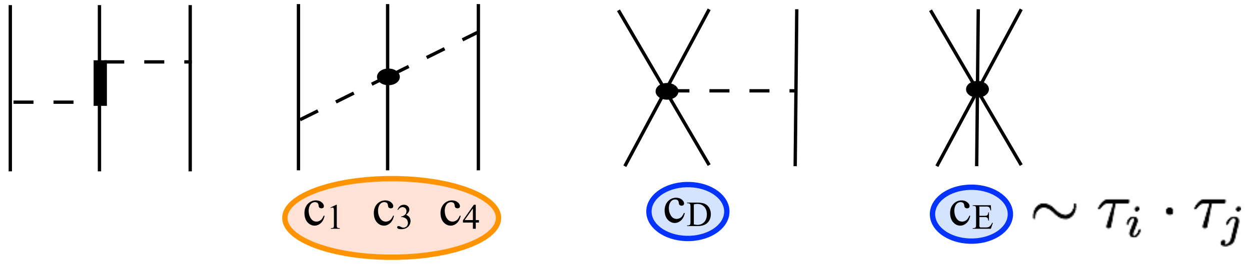
At N2LO and N3LO the nuclei are still underbound (closer to exp)

$|\text{LO-NLO}| > |\text{NLO-N2LO}| > |\text{N2LO-N3LO}|$

3N interactions are needed!!

Local chiral 3N potential with Δ's

Inclusion of 3N forces at N2LO:



1) Fit to:

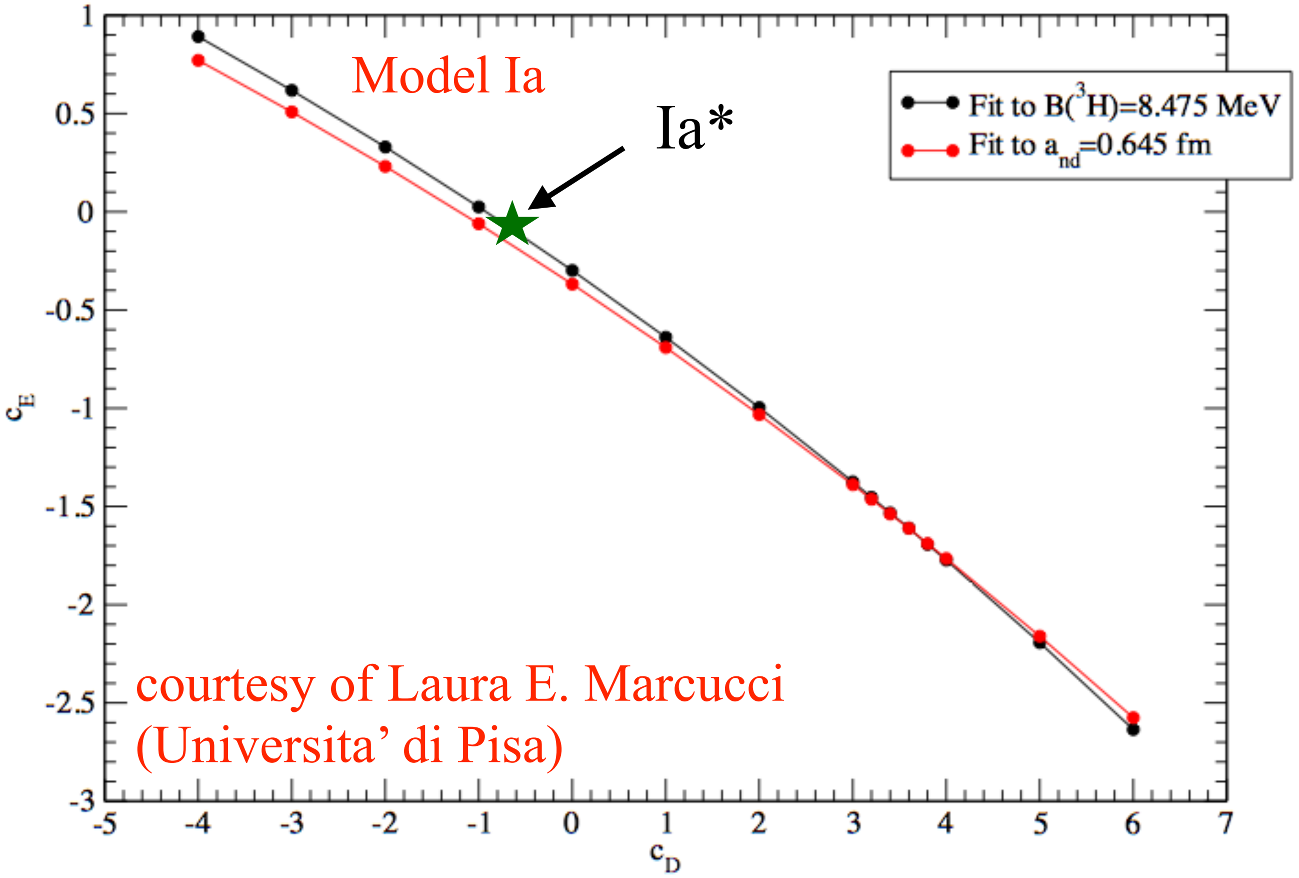
- $E_0(^3\mathrm{H}) = -8.482$ MeV
- $^2a_{nd} = (0.645 \pm 0.010)$ fm

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

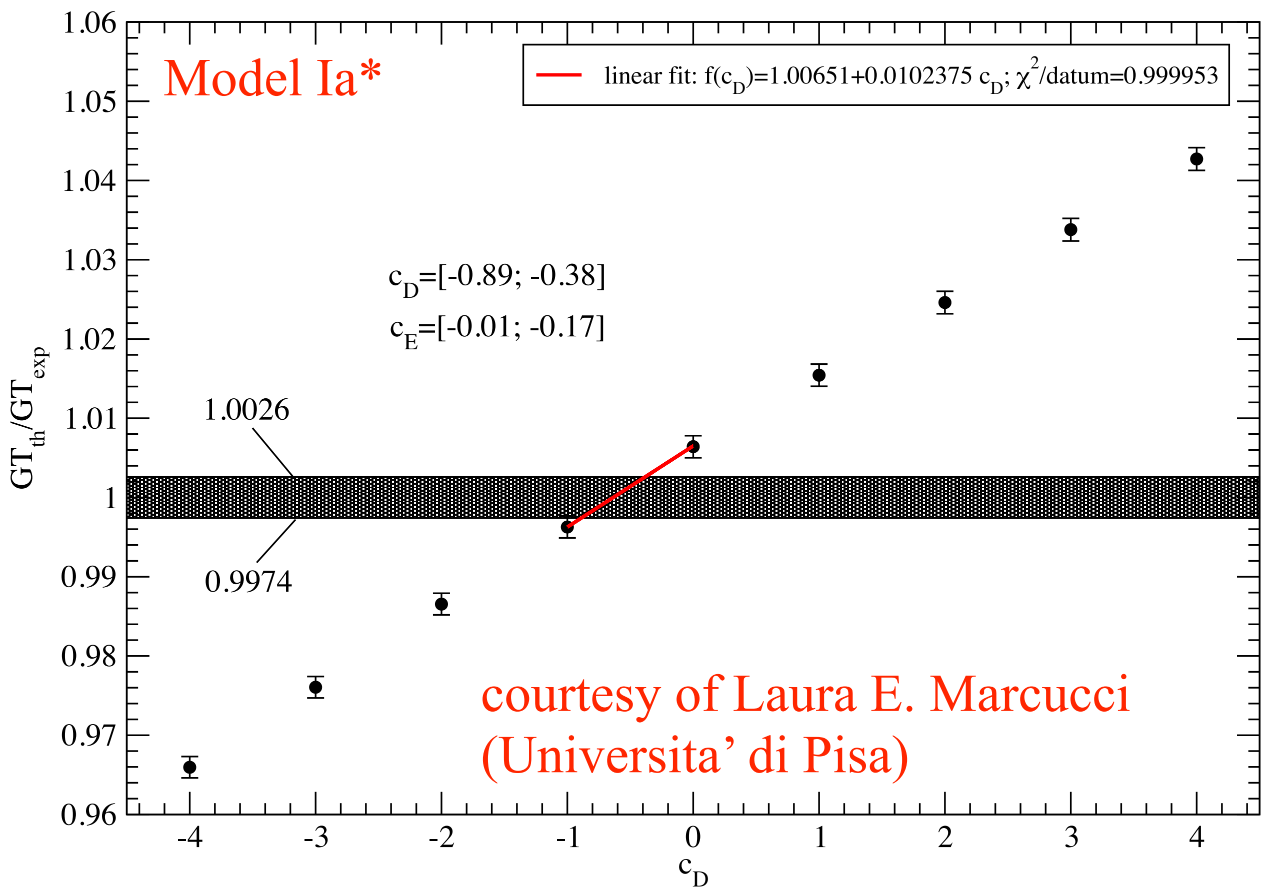
2) Fit to:

- $E_0(^3\mathrm{H}) = -8.482$ MeV
- GT m.e. in ^{3}H β-decay

Model	c_D	c_E
Ia*	–0.635(255)	–0.09(8)
Ib*	–4.705(285)	0.550(150)
IIa*	–0.610(280)	–0.350(100)
IIb*	–5.250(310)	0.05(180)

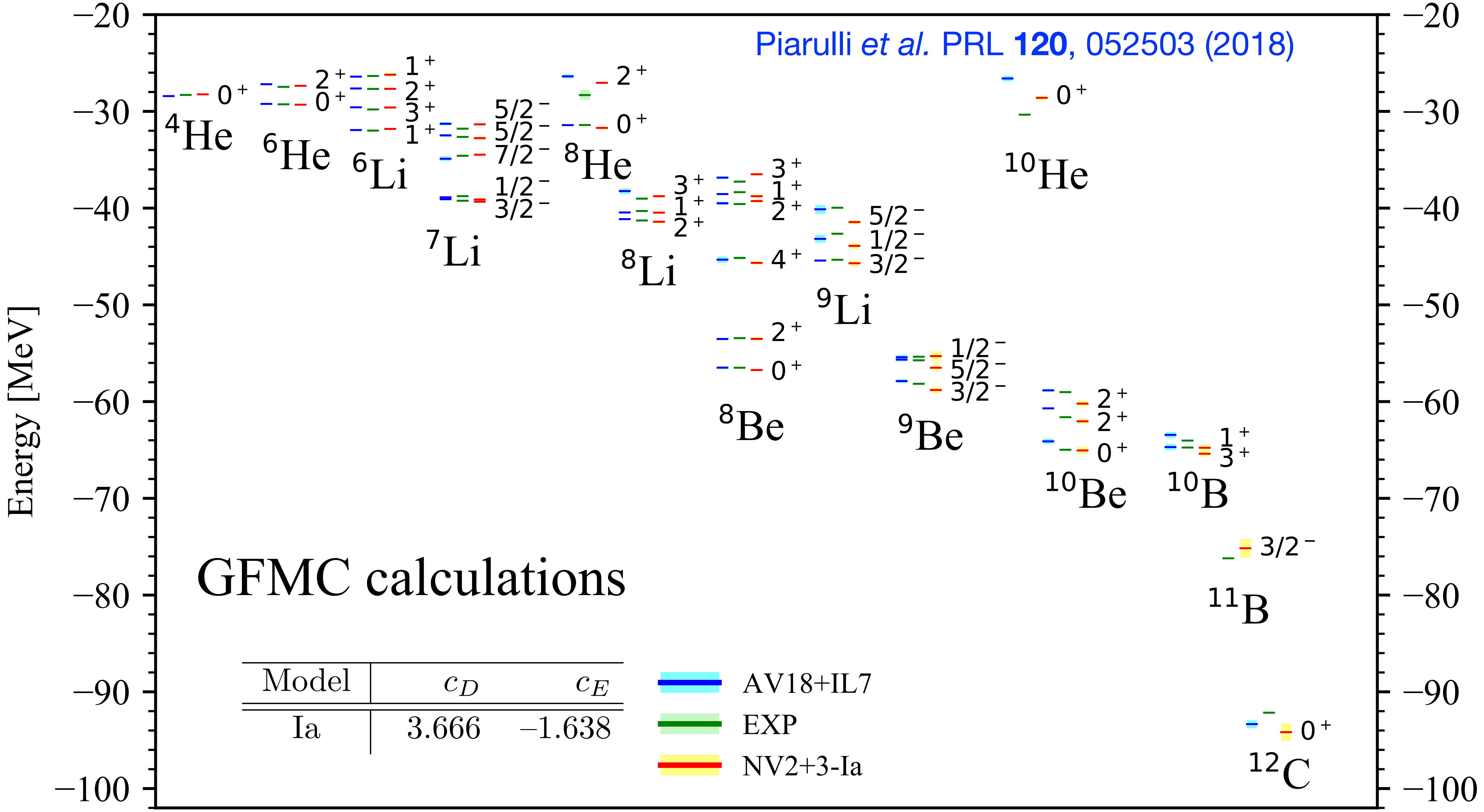


courtesy of Laura E. Marcucci
(Universita' di Pisa)



courtesy of Laura E. Marcucci
(Universita' di Pisa)

Spectra of Light Nuclei: Phenomenology vs χEFT



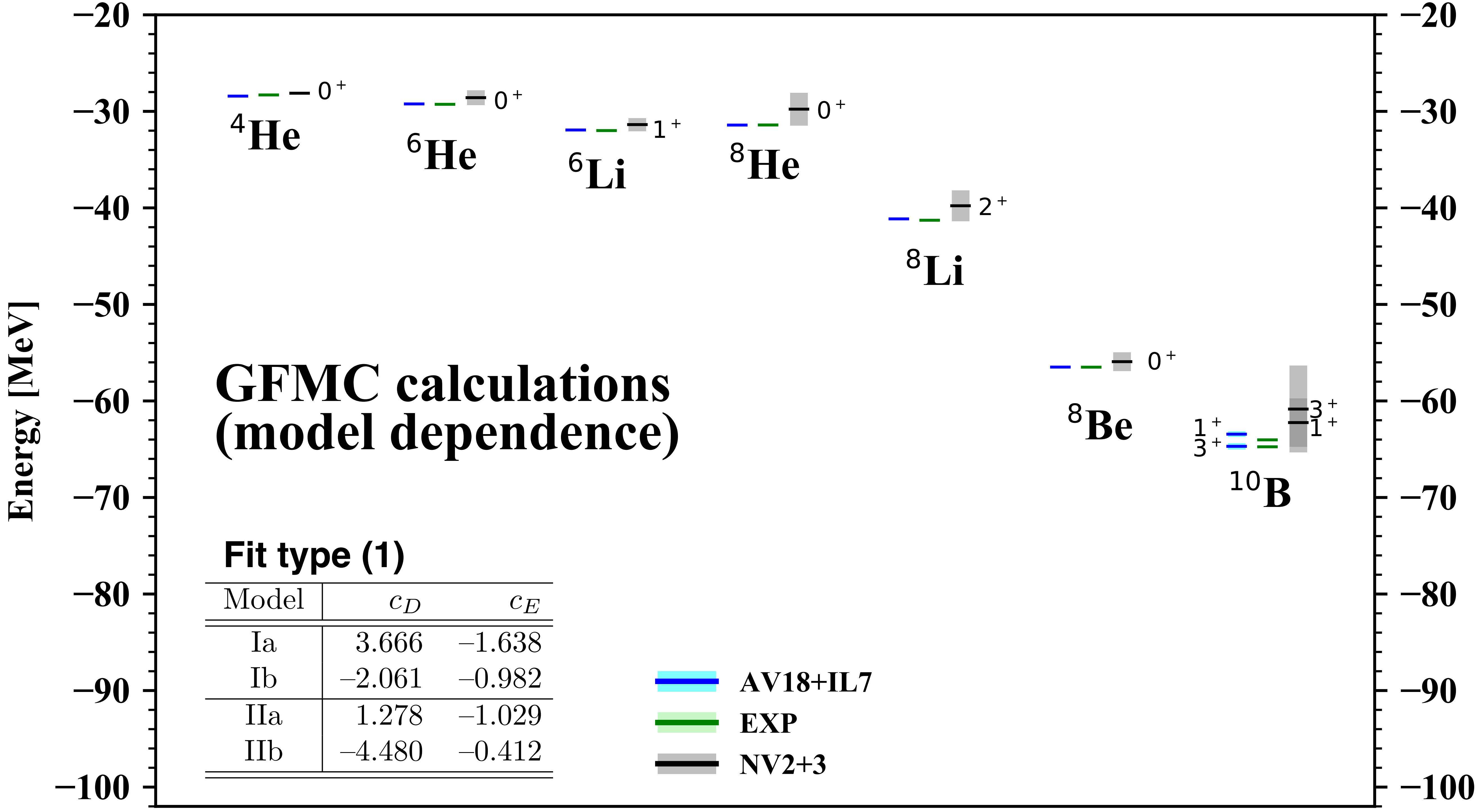
$c_E < (>)0$: repulsion (attraction) in light-nuclei (the opposite effect in PNM)

$c_D < (>)0$: repulsion (attraction) in light-nuclei (same effect in PNM but very small)

Model-dependence for NV2+3 up to 5-6% of the total binding energy: mostly due to the fact that all the four models do not reproduce the spitting in 10B

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

Energies of Light Nuclei: Model-dependence

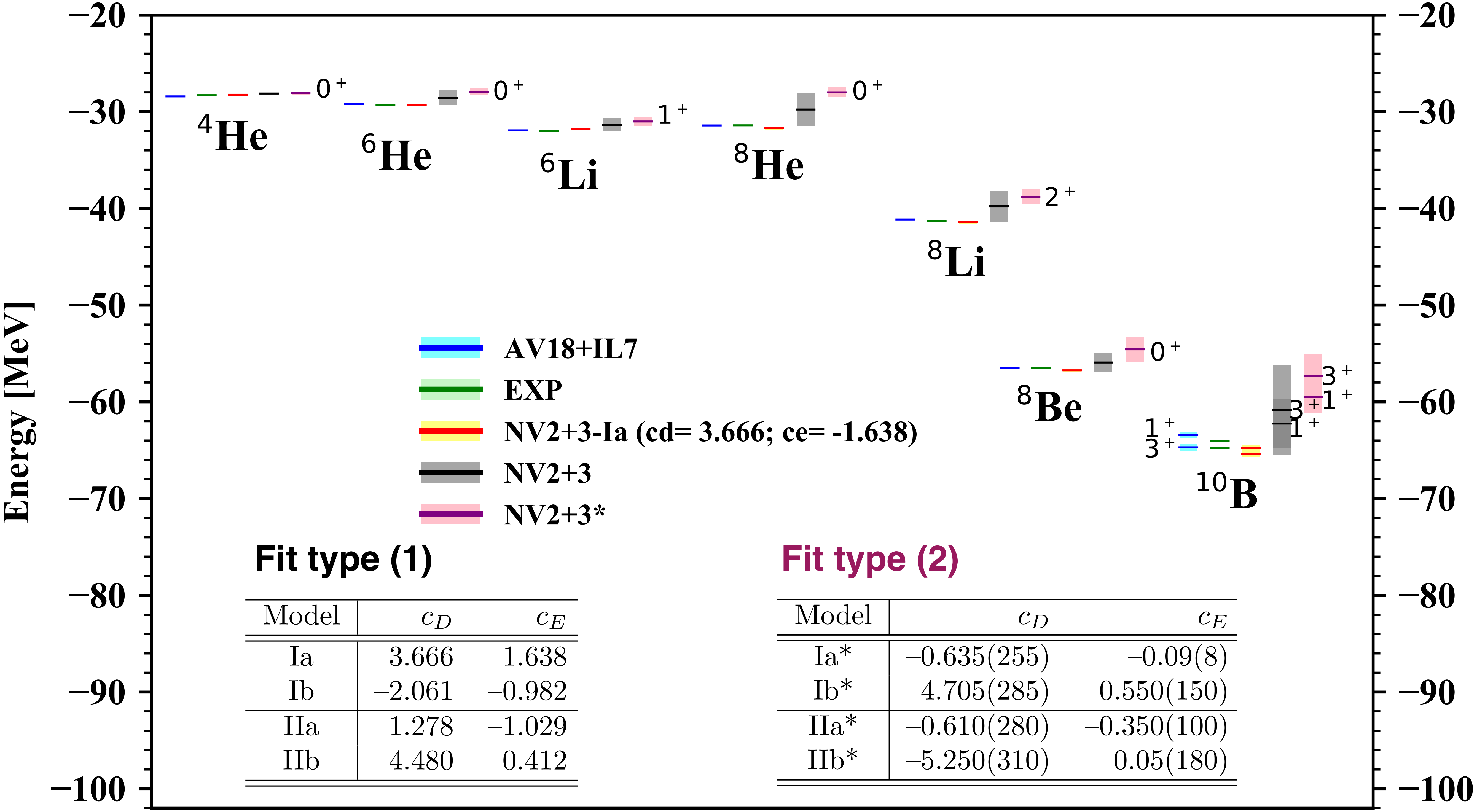


Fit type (1)

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

Model-dependence for NV2+3 up to 5-6% of the total binding energy mostly due to the splitting in 10B: this is an issue related to the NNN interaction

Energies of Light Nuclei: Model-dependence



Fit type (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

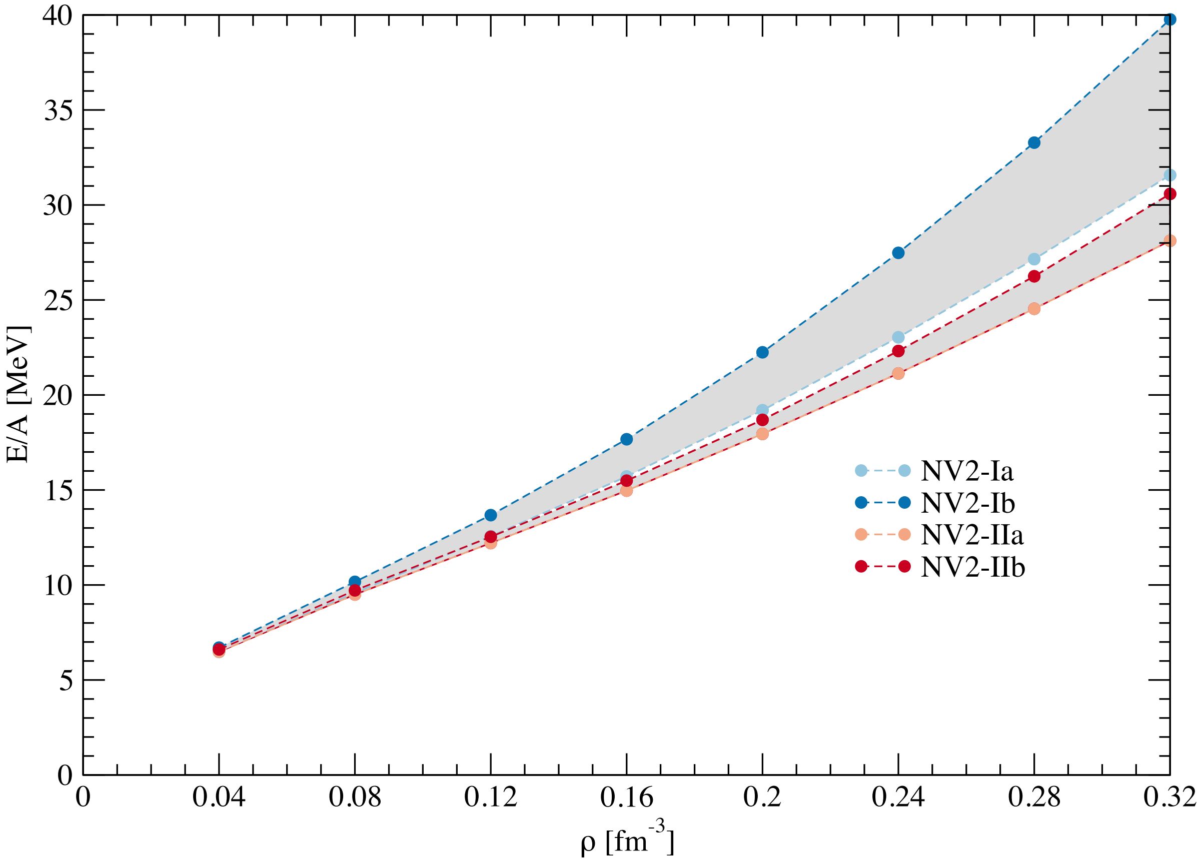
Fit type (2)

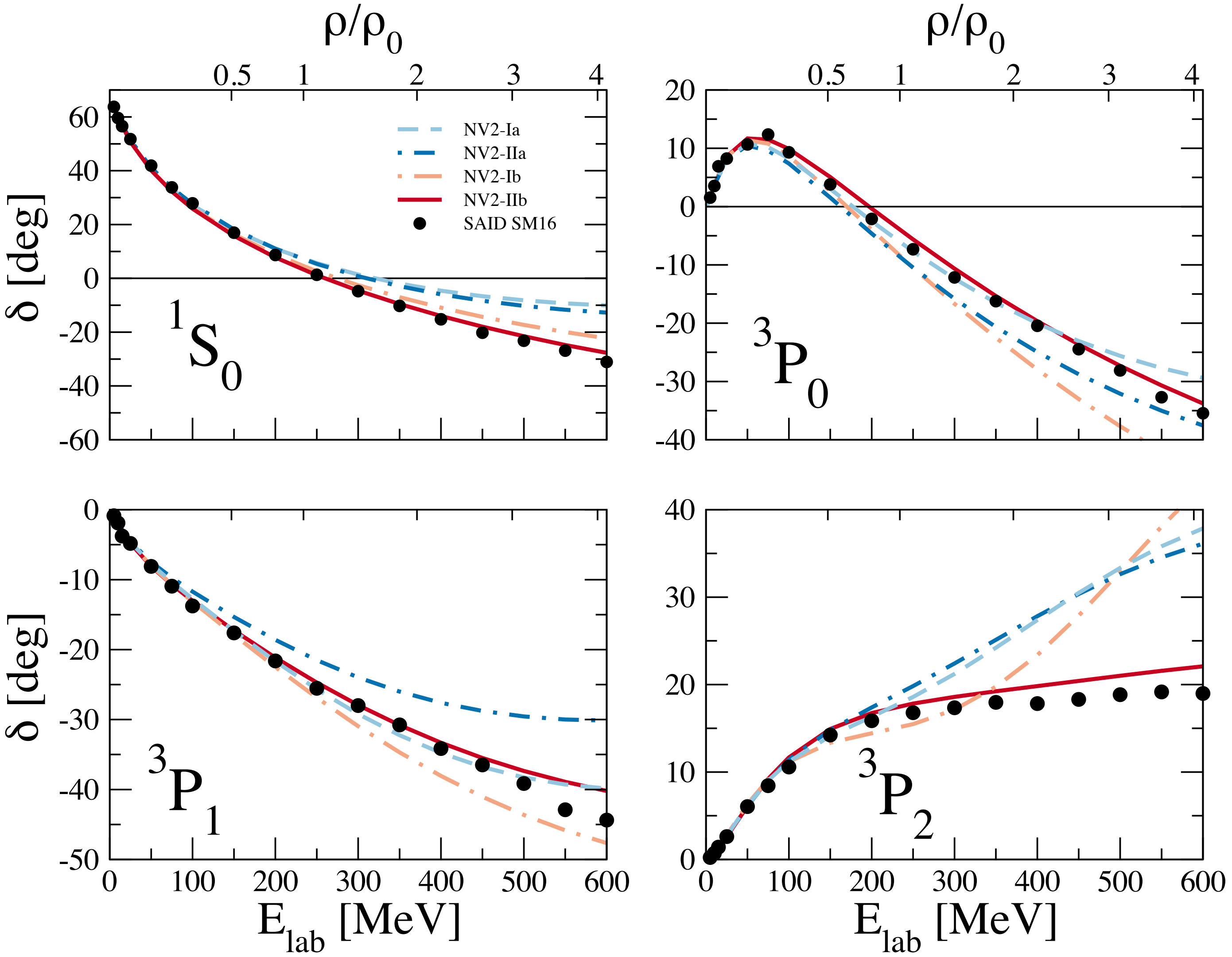
Model	c_D	c_E
Ia*	–0.635(255)	–0.09(8)
Ib*	–4.705(285)	0.550(150)
IIa*	–0.610(280)	–0.350(100)
IIb*	–5.250(310)	0.05(180)

Model-dependence for NV2+3 up to 5-6% of the total binding energy

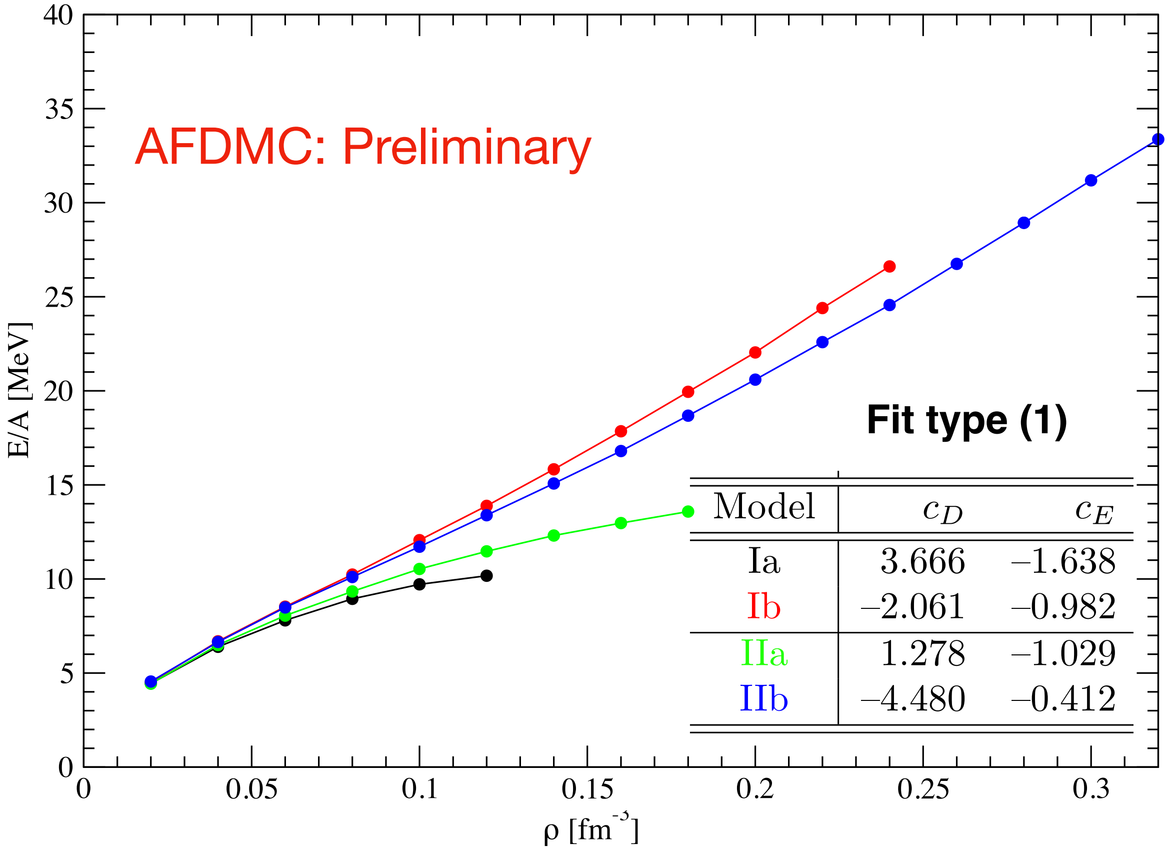
Model-dependence for NV2+3* up to 2-3% of the total binding energy

Issues with 3N: EOS of Pure Neutron Matter in χEFT





M. Piarulli, I. Bombaci, D. Logoteta, A. Lovato, R. B. Wiringa
arXiv:1908.04426



Fit type (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

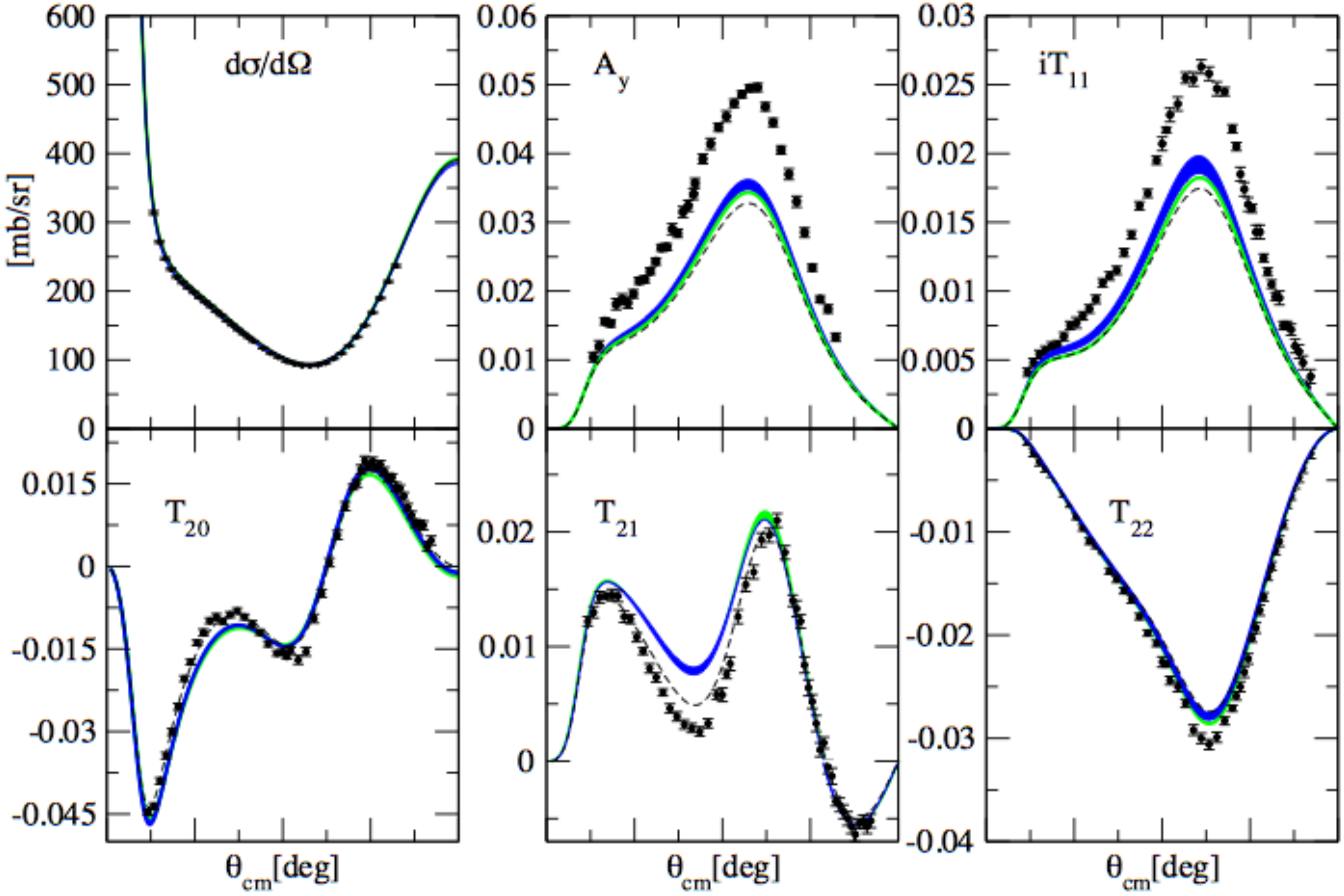
Cutoff sensitivity: modest in NV2 models; very large in NV2+3 models

Fit type (2)

Model	c_D	c_E
Ia*	−0.635(255)	−0.09(8)
Ib*	−4.705(285)	0.550(150)
IIa*	−0.610(280)	−0.350(100)
IIb*	−5.250(310)	0.05(180)

Polarization observables in pd elastic scattering at 3 MeV: HH calculations with the NV2+3 models Ia-Ib (IIa-IIb), are shown by the green (blue) band. The black dashed line are results obtained with only the two-body interaction NV2-Ia

Girlanda, Kievsky, Marcucci, Viviani



More sophisticated 3N force??? Different way to fix the 3N??? subleading contact terms in 3N interaction???

Beyond Energy Calculations

Electroweak structure and reactions:

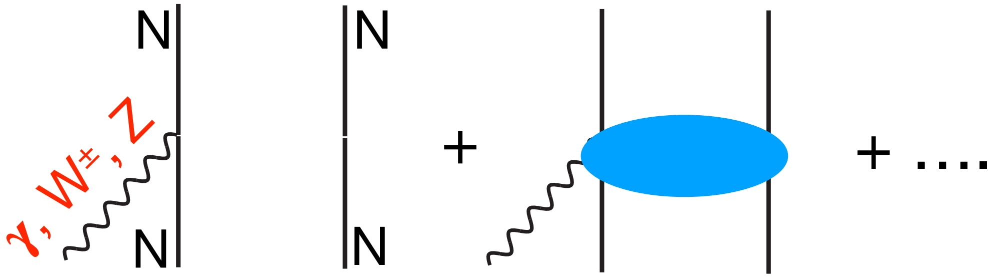
- Electroweak form factors
- Magnetic moments and radii
- Electroweak Response functions
- Radiative/weak captures
- G.T. matrix elements involved in beta decays

……..

Inputs besides nuclear interactions:

Electroweak current operators:

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



Current operators constructed in correspondence to the phenomenological interactions based on meson-exchange approach Marcucci *et al.* PRC **72**, 014001 (2005)

Current operators derived in χEFT: 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); Kölling *et al.* PRC **86**, 047001 (2012), Krebs et al., Ann. Phys. **378**, 317 (2017)

Nuclear axial currents and beta-decays in light-nuclei

$(Z,N) \rightarrow (Z+1,N-1)+e+\bar{\nu}_e$

Matrix Element $< \Psi_f|\mathrm{GT}|\Psi_i > \sim g_A$ and decay rate $\sim g_A^2$

Understanding “quenching” of $\sim g_A$

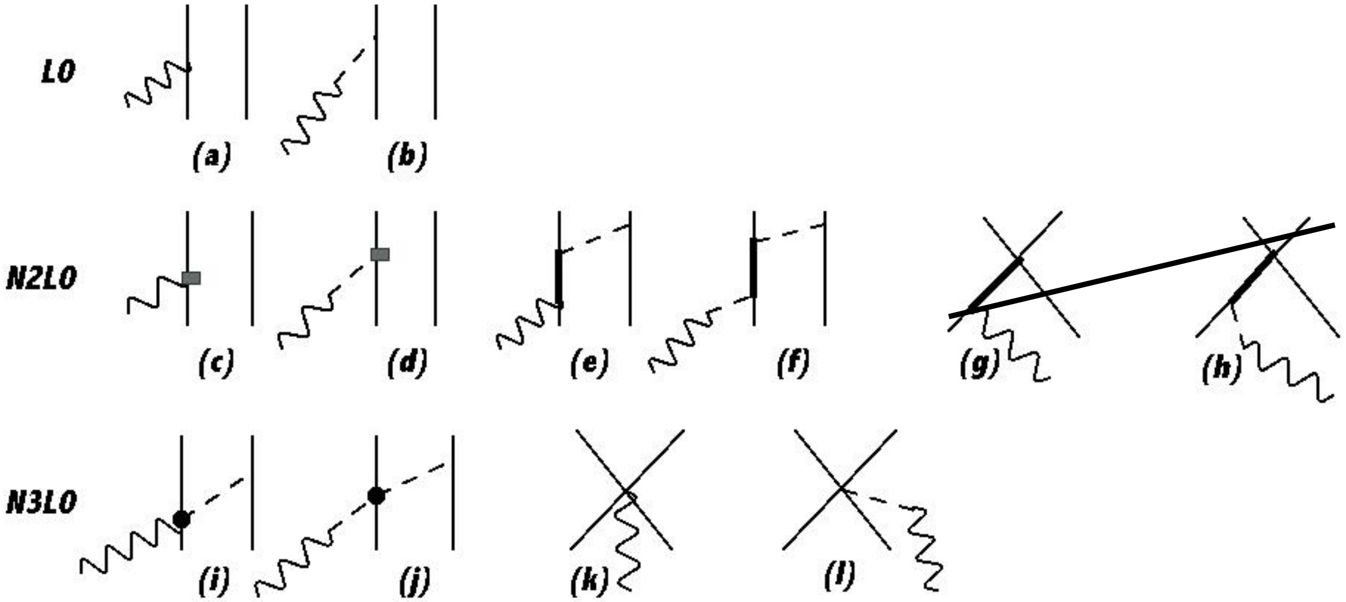
Relevant for neutrinoless double beta decay since rate $\sim g_A^4$

Nuclear astrophysics (Sun chain reaction)

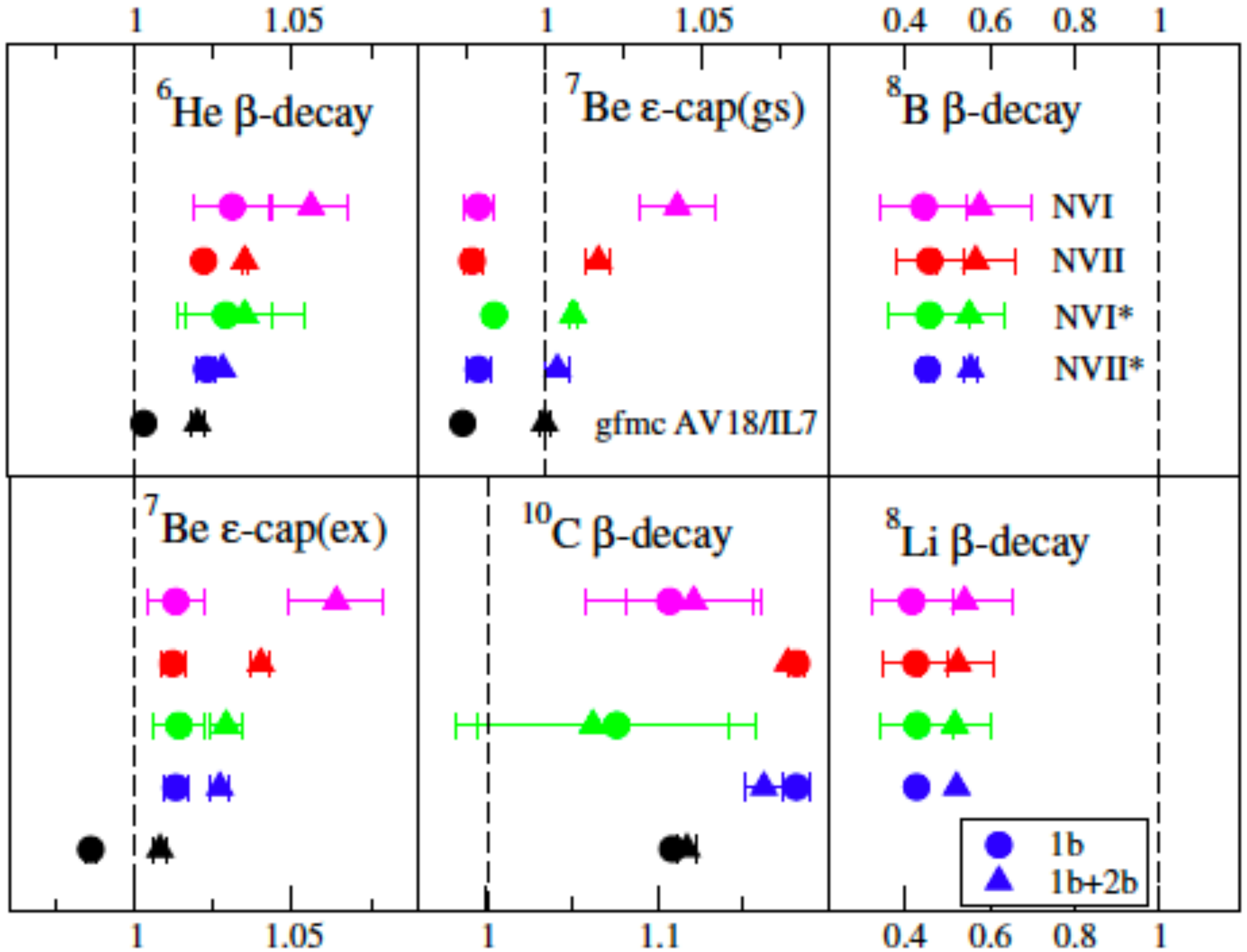
Schiavilla et al. PRC 99, 034005 (2019)

Baroni et al. PRC 93, 015501 (2016)

Pastore et al. PRC 78, 064002 (2008)



A single unknown LEC in the axial contact current fixed in 3H beta-decay



NVI - database fitted up to 125 MeV - c_D, c_E fitted to B.E. and *nd*-scattering length (VMC calculations)
NVII - database fitted up to 200 MeV - c_D, c_E fitted to B.E. and *nd*-scattering length (VMC calculations)
NVI* - database fitted up to 125 MeV - c_D, c_E fitted to B.E. and GT triton (VMC calculations)
NVII* - database fitted up to 200 MeV - c_D, c_E fitted to B.E. and GT triton (VMC calculations)

Pastore, Piarulli, Schiavilla, Wiringa, Baroni, Carlson, Gandolfi, in preparation

PRELIMINARY

AV18+IL7 - database fitted up to 350 MeV - c_D fitted to GT triton (GFMC calculations) Pastore et al. PRC **97** 022501 (2018)

Conclusions

We are testing our models of NN+3N interactions with Δ-isobar based on chiral EFT framework in both light-nuclei and infinite nuclear matter

We mainly focused our attention on studying properties of nuclei up to A=12 and EoS of infinite neutron matter

For the time being, we are interested in studying the model-dependence of the nuclear observables by exploring different cutoffs and range of energies used to fit the NN interactions as well as analyzing different strategies fo fit the TNI

It looks like that the formulation of the TNI with only c_D and c_E terms is too simplistic if we want to have a good descriptions of spectra, properties of light-nuclei, infinite nuclear matter, three-body observables with a certain degree of accuracy

We are investigating the effect of subleading 3N contact interactions in light-nuclei (we will do so also for infinite nuclear matter)

THANK YOU

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Argonne NATIONAL LABORATORY

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NUCLEI
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This is how I like to remember my days here at ANL: