No Core Shell Model (NCSM) With Consistent Electroweak Interactions and Other Recent Developments

James P. Vary, Iowa State University

TRIUMF Workshop, Feb 26 - Mar 1, 2019

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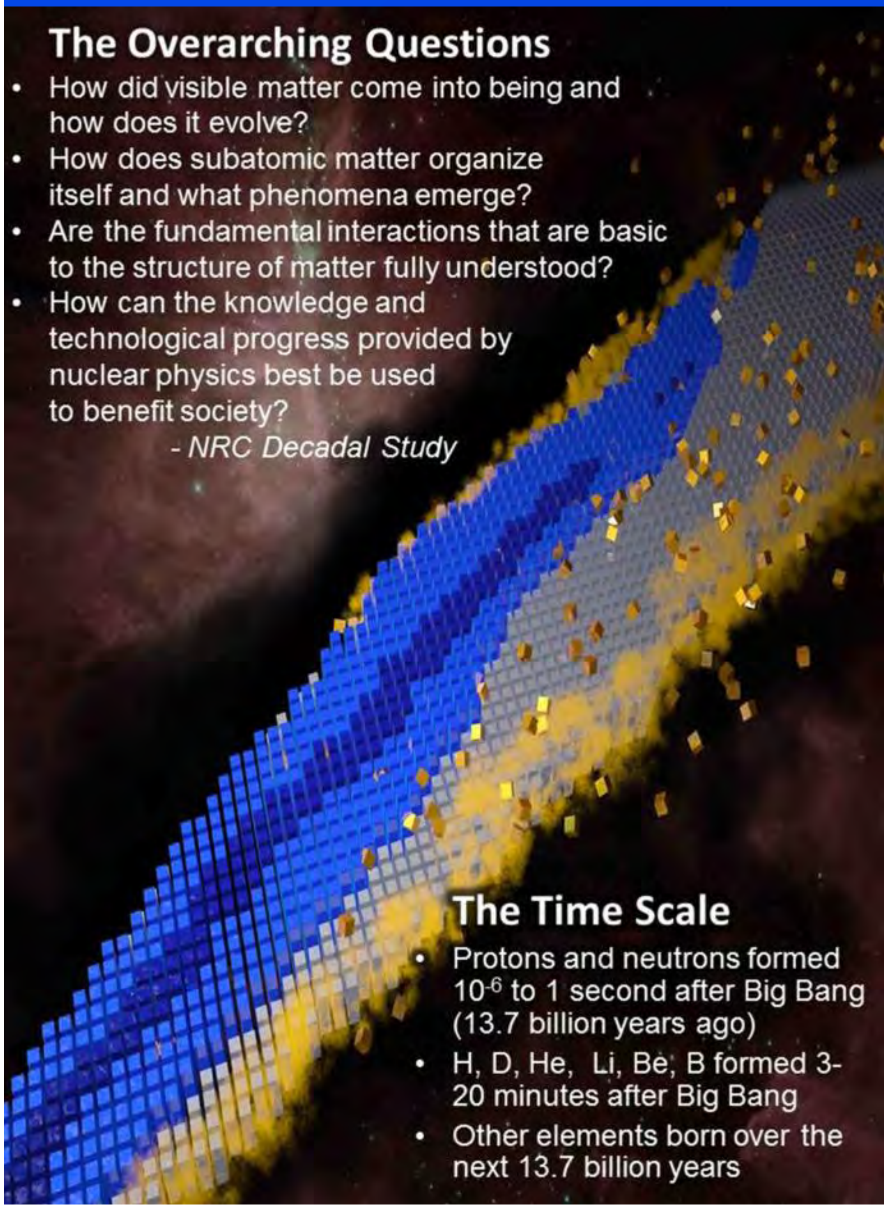
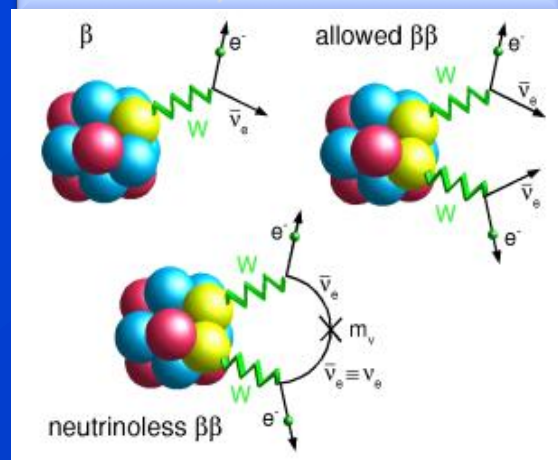
SciDAC Scientific Discovery through Advanced Computing



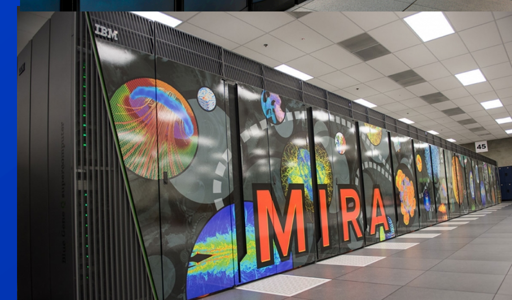
Topical Collaboration on Neutrinos and Fundamental Symmetries



LENPIC

NUCLEI Nuclear Computational Low-Energy Initiative

U.S. DEPARTMENT OF ENERGY INCITE LEADERSHIP COMPUTING



No-Core Configuration Interaction calculations

Barrett, Navrátil, Vary, *Ab initio no-core shell model*, PPNP69, 131 (2013)

Given a Hamiltonian operator

$$\hat{\mathbf{H}} = \sum_{i<j} \frac{(\vec{p}_i - \vec{p}_j)^2}{2\,m\,A} + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \ldots$$

solve the eigenvalue problem for wavefunction of A nucleons

$$\hat{\mathbf{H}}\,\Psi(r_1,\ldots,r_A) = \lambda\,\Psi(r_1,\ldots,r_A)$$

- Expand eigenstates in basis states $|\Psi\rangle = \sum a_i|\Phi_i\rangle$
- Diagonalize Hamiltonian matrix $H_{ij} = \langle\Phi_j|\hat{\mathbf{H}}|\Phi_i\rangle$
- No Core Full Configuration (NCFC) – All A nucleons treated equally
- Complete basis $\longrightarrow$ exact result
- In practice
  - truncate basis
  - study behavior of observables as function of truncation

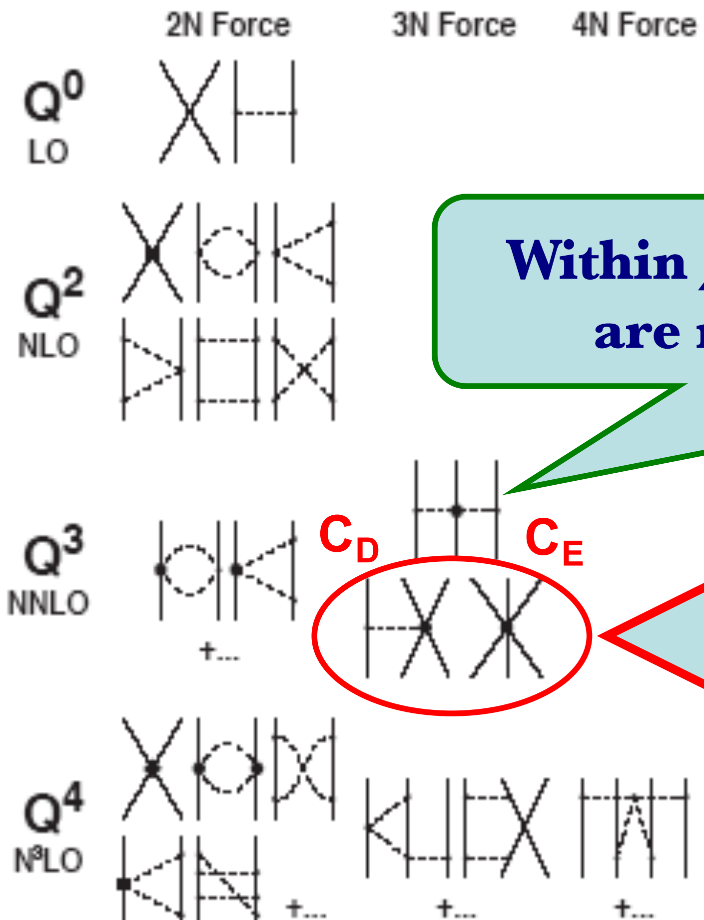
Effective Nucleon Interaction

(Chiral Perturbation Theory)

Chiral perturbation theory (χPT) allows for controlled power series expansion

Expansion parameter : $\left(\frac{Q}{\Lambda_\chi}\right)^{\upsilon}$, $Q-$momentum transfer,

$\Lambda_\chi \approx 1\ GeV$, χ - symmetry breaking scale



Within χPT 2π-NNN Low Energy Constants (LEC) are related to the NN-interaction LECs $\{c_i\}$.

Terms suggested within the
Chiral Perturbation Theory

Regularization is essential, which is also implicit within the Harmonic Oscillator (HO) wave function basis

R. Machleidt and D.R. Entem, Phys. Rep. 503, 1 (2011);
E. Epelbaum, H. Krebs, U.-G Meissner, Eur. Phys. J. A51, 53 (2015); Phys. Rev. Lett. 115, 122301 (2015)

Calculation of three-body forces at N^{3}LO

Low
Energy
Nuclear
Physics
International
Collaboration

LENPIC

J. Golak, R. Skibinski, K. Tolponicki, H. Witala

RUB — E. Epelbaum, H. Krebs

JÜLICH — A. Nogga

The Ohio State University — R. Furnstahl

Technische Universität Darmstadt — S. Binder, A. Calci, K. Hebeler, J. Langhammer, R. Roth

Iowa State — P. Maris, J. Vary

Kyutech — H. Kamada

U.-G Meissner

Goal

Calculate matrix elements of 3NF in a partial-wave decomposed form which is suitable for different few- and many-body frameworks

Challenge

Due to the large number of matrix elements, the calculation is extremely expensive.

Strategy

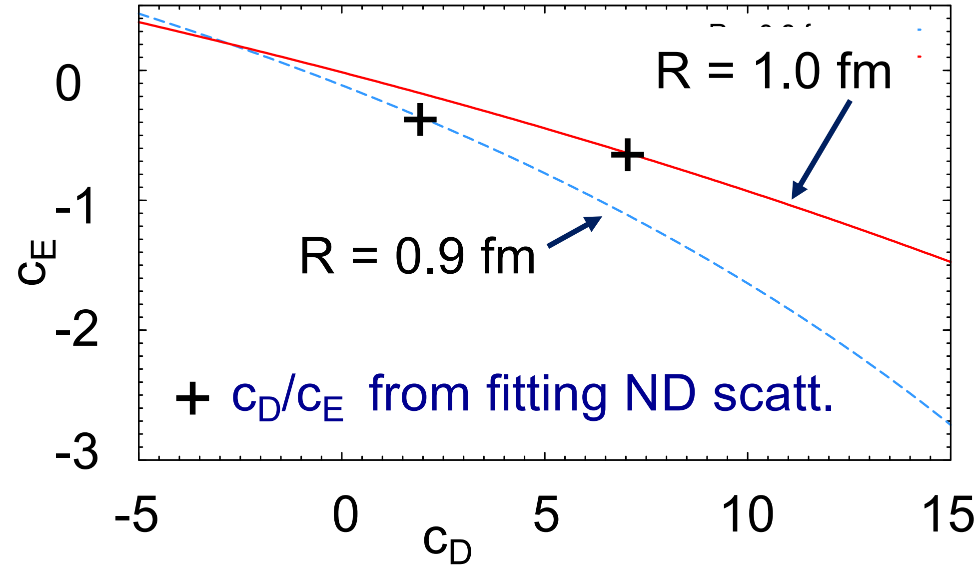
Develop an efficient code which allows to treat arbitrary local 3N interactions. (Krebs and Hebeler)

Additional Goal: Develop consistent chiral EFT theory for electroweak operators

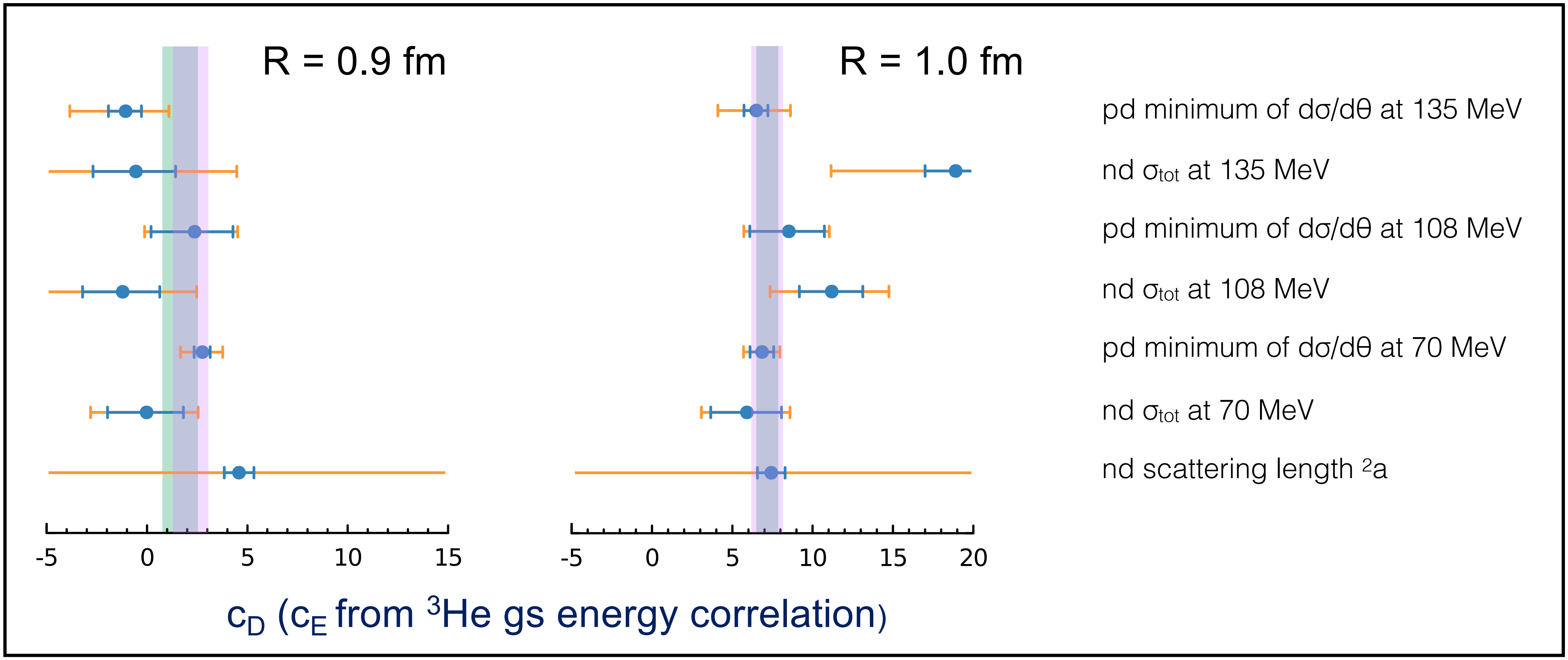
Coordinate space regulator:

$$f\left(\frac{r}{R}\right)=\left(1-\exp\left(-\frac{r^2}{R^2}\right)\right)^6$$

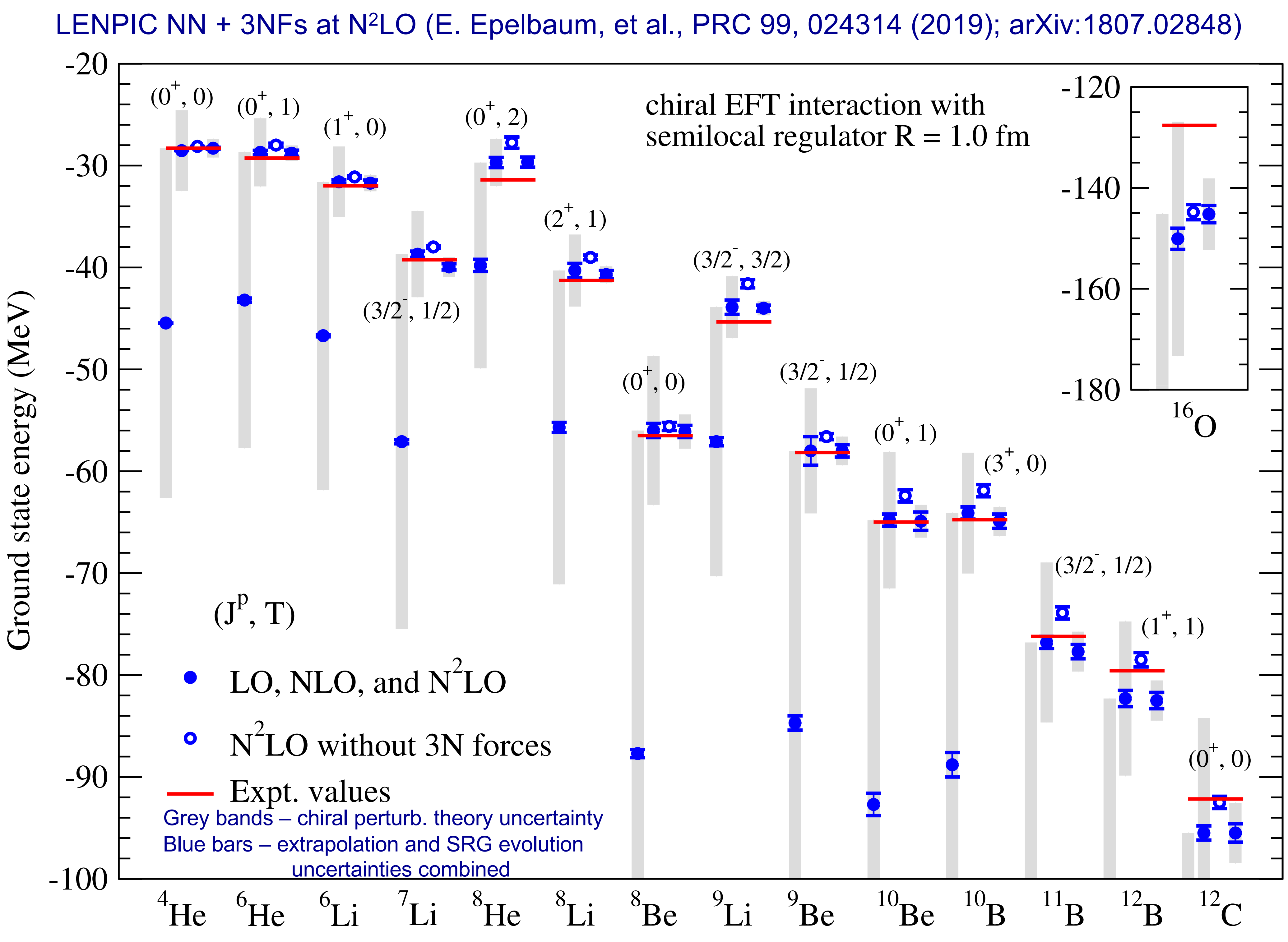
c_D/c_E correlation from fitting ^{3}He gs Energy



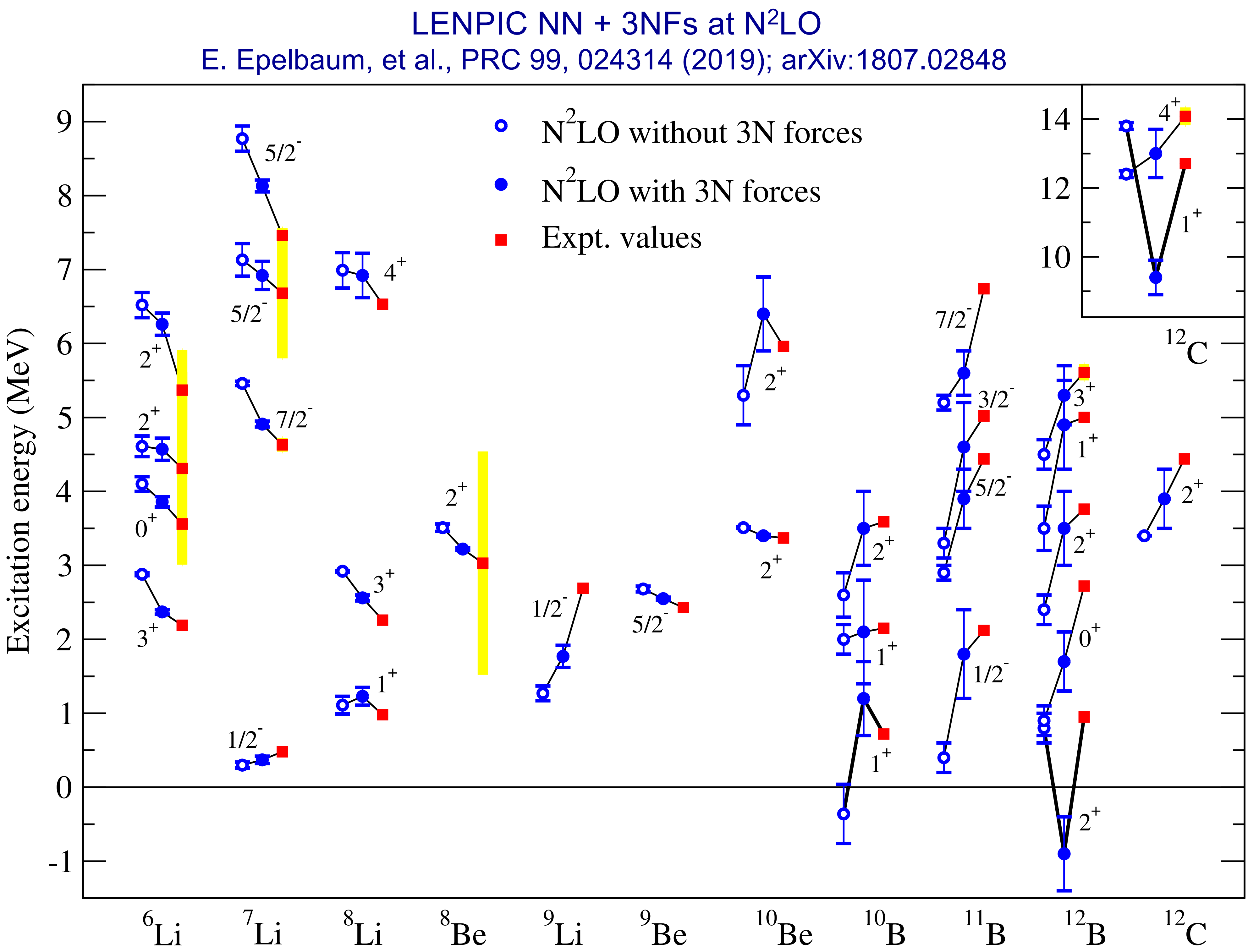
c_D (c_E) selected via ND scattering analyses:



LENPIC NN + 3NFs at N^{2}LO (E. Epelbaum, et al., PRC 99, 024314 (2019); arXiv:1807.02848)

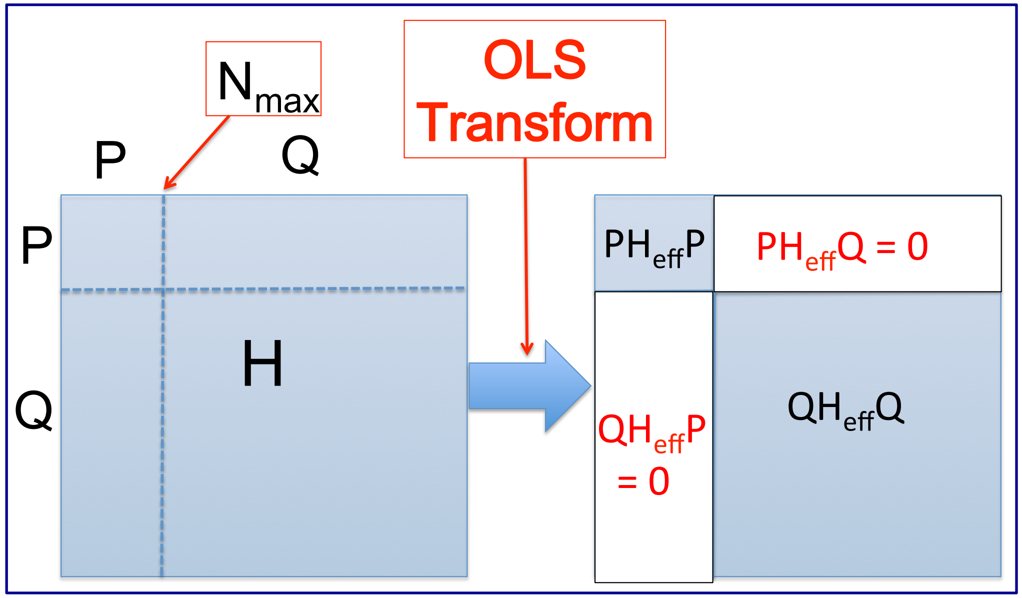


LENPIC NN + 3NFs at N²LO (E. Epelbaum, et al., PRC 99, 024314 (2019); arXiv:1807.02848)
chiral EFT interaction with
semilocal regulator R = 1.0 fm
Ground state energy (MeV)
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
16O
(0+, 0)
(0+, 1)
(1+, 0)
(3/2-, 1/2)
(0+, 2)
(2+, 1)
(0+, 0)
(3/2-, 3/2)
(3/2-, 1/2)
(0+, 1)
(3+, 0)
(3/2-, 1/2)
(1+, 1)
(0+, 0)
(Jp, T)
LO, NLO, and N2LO
N2LO without 3N forces
Expt. values
Grey bands – chiral perturb. theory uncertainty
Blue bars – extrapolation and SRG evolution
uncertainties combined
4He
6He
6Li
7Li
8He
8Li
8Be
9Li
9Be
10Be
10B
11B
12B
12C


LENPIC NN + 3NFs at N2LO
E. Epelbaum, et al., PRC 99, 024314 (2019); arXiv:1807.02848
Excitation energy (MeV)
N2LO without 3N forces
N2LO with 3N forces
Expt. values
6Li
7Li
8Li
8Be
9Li
9Be
10Be
10B
11B
12B
12C
3+
0+
2+
2+
5/2-
5/2-
7/2-
1/2-
4+
3+
1+
2+
1/2-
5/2-
2+
2+
7/2-
3/2-
5/2-
1/2-
1+
2+
1+
3+
1+
2+
0+
2+
2+
4+
1+

OLS Transform:

Unitary transformation that block-diagonalizes the Hamiltonian – i.e. it integrates out Q-space degrees of freedom.



$$UHU^{\dagger} = U[T+V]U^{\dagger} = H_d, \text{ the diagonalized } H$$

$$H_{\text{eff}} \equiv U_{OLS} H U_{OLS}^{\dagger} = PH_{\text{eff}}P = P[T+V_{\text{eff}}]P$$

$$W^P \equiv PUP$$

$$\tilde{U}^P \equiv P\tilde{U}^P P \equiv \frac{W^P}{\sqrt{W^{P\dagger}W^P}}$$

$$H_{\text{eff}} = \tilde{U}^{P\dagger} H_d \tilde{U}^P = \tilde{U}^{P\dagger} UHU^{\dagger} \tilde{U}^P = P[T+V_{\text{eff}}]P$$

We conclude that:

$$U_{OLS} = \tilde{U}^{P\dagger} U$$

Similarly, we have effective operators for observables:

$$O_{\text{eff}} \equiv \tilde{U}^{P\dagger} UOU^{\dagger} \tilde{U}^P = P[O_{\text{eff}}]P$$

← Consistent observables

See: J.P. Vary, et al., PRC98, 065502 (2018) arXiv:1809.00276 for applications

Consider two nucleons as a model problem with V = LENPIC chiral NN solved in the harmonic oscillator basis with ħΩ = 5, 10 and 20 MeV. Also, consider the role of an added harmonic oscillator quasipotential

Hamiltonian #1 $H = T + V$

Hamiltonian #2 $H = T + U_{\mathrm{osc}}(\hbar\Omega_{\mathrm{basis}}) + V$

Other observables:

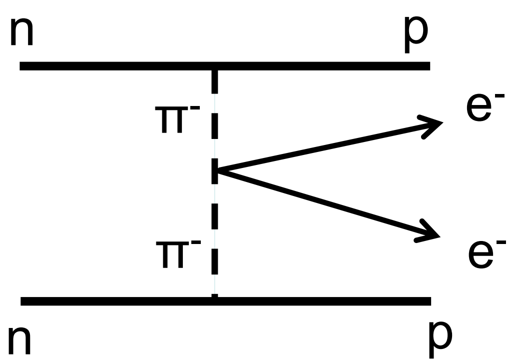
Root mean square radius	R
Magnetic dipole operator	M1
Electric dipole operator	E1
Electric quadrupole moment	Q
Electric quadrupole transition	E2
Gamow-Teller	GT
Neutrinoless double-beta decay	M(0ν2β)

Dimension of the "full space" is 400 for all results depicted here

J.P. Vary, et al., PRC98, 065502 (2018);arXiv:1809.00276

We initially considered a 2-body contribution within EFT to 0νββ-decay at N^2LO

G. Prézeau, M. Ramsey-Musolf and P. Vogel, Phys. Rev. D 68, 034016 (2003)



$$M^0 = \langle \Psi_{A,Z+2} | \sum_{ii} \frac{R}{r_{ij}} \left[F_1(x_{ij}) \vec{\sigma}_i \vec{\sigma}_j + F_2(x_{ij}) T_{ij} \right] \tau_i^+ \tau_j^+ | \Psi_{A,Z} \rangle$$

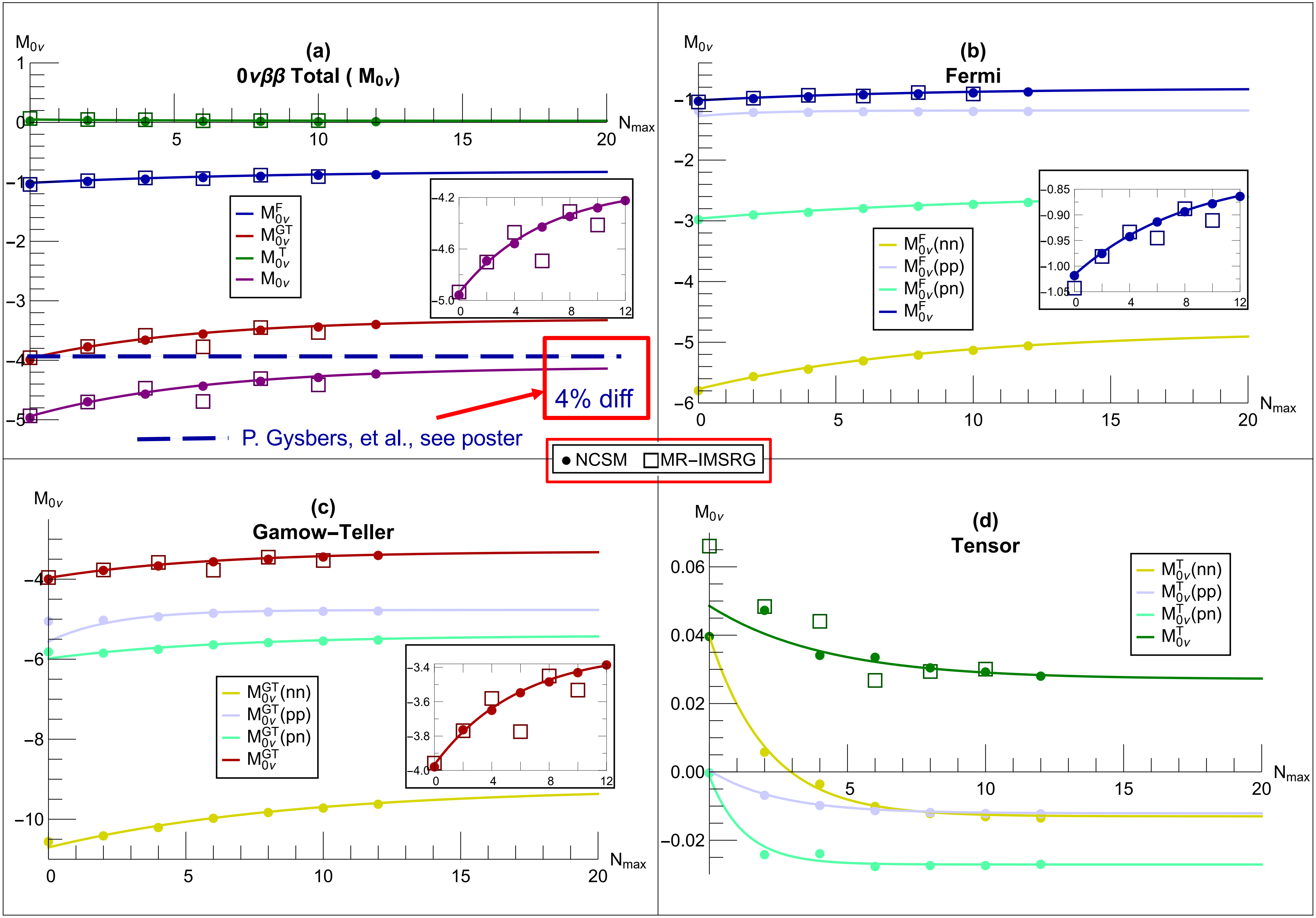
$$F_1(x) = (x-2)e^{-x} \quad , F_2(x) = (x+1)e^{-x} \, , \; x = m_\pi |\vec{r}|$$

$$T_{ij} = 3\vec{\sigma}_i . \hat{r}_{ij} \vec{\sigma}_j . \hat{r}_{ij} - \vec{\sigma}_i \vec{\sigma}_j$$

This operator is used in: J.P. Vary, et al., PRC98, 065502 (2018);
Jon Engel's operator used in: ISU-UNC-MSU Collaboration benchmarking NCSM and MR-IMSRG (paper in preparation)

Iowa State work-in-progress – take 0νββ-decay operators, term-by-term, available from V. Cirigliano, W. Dekens, J. de Vries, M.L. Graesser and E. Mereghetti, arXiv:1806.02780; calculate them in the harmonic oscillator basis and use LENPIC LECs for NCSM apps with LENPIC interactions.

ISU – UNC – MSU collaboration to benchmark 0νββ-decay matrix elements for $^{6}He \rightarrow {}^{6}Be$

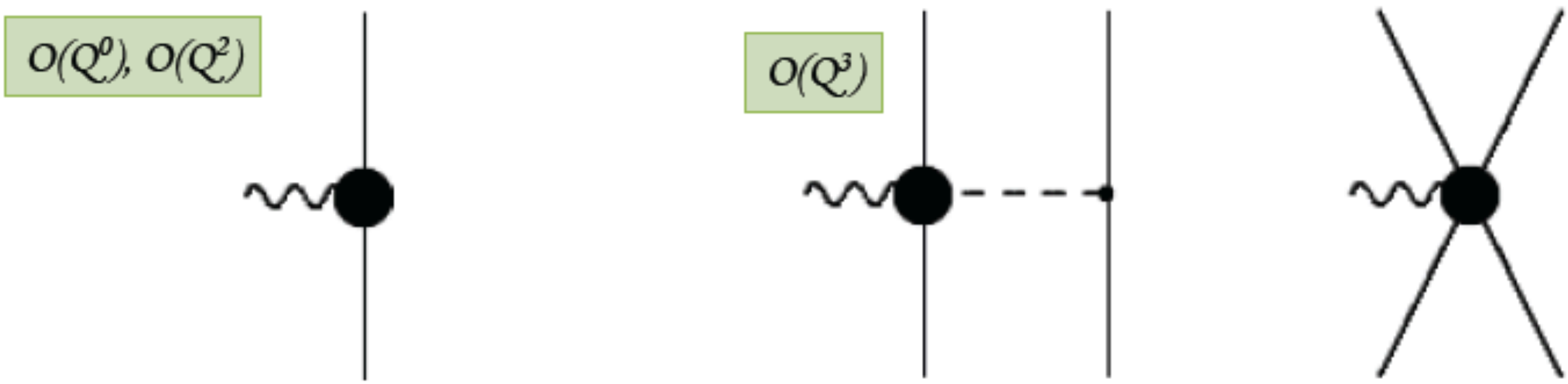


Coupling to External Probes in Chiral EFT

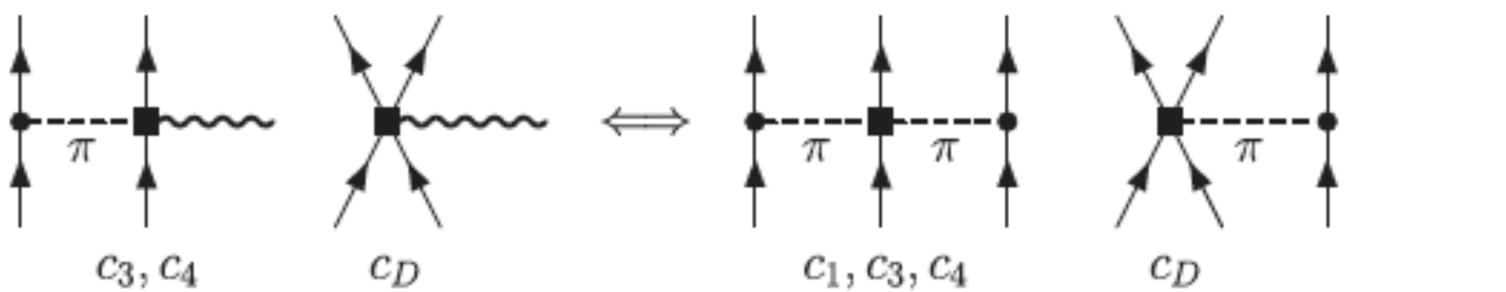
LENPIC collaboration (in process) – adopts momentum space regulators

- Nuclear Axial Current Operators e.g. Krebs, et al., Ann. Phys. 378, 317 (2017)

Single nucleon current | 1 pion exchange | Contact term



Two-Body Currents (N^2LO)



Note: we are working to retain dependence on external momentum transfer

Charge radius

- The charge radius squared is defined as the second moment of the charge form factor,

$$\langle r^2 \rangle = -\frac{dG_C(k^2)}{dk^2}\bigg|_{k^2=0}. \tag{4}$$

- The charge form factor is obtained from the scalar component of the charge operator.
- At leading order (Q^{-3}) the charge operator consists of point-like nucleons,

$$\hat{\rho}_{LO} = |e| \sum_i \frac{1+\tau_i^z}{2} \delta(\vec{p}_i' - \vec{p}_i - \vec{k}). \tag{5}$$

- There is no contribution to the charge operator at next-to-leading order.
- At N2LO (Q^{-1}), there are relativistic corrections arising from the finite size of the nucleons, [Phillips, 2003]

$$\hat{\rho}_{N2LO} = -\frac{|e|}{6} \langle r_{Es}^2 \rangle \sum_i \frac{1+\tau_i^z}{2} \delta(\vec{p}_i' - \vec{p}_i - \vec{k}). \tag{6}$$

Charge radius

- The first two body correction appears at N3LO (Q^0),

[Kölling *et.al.*, 2011]

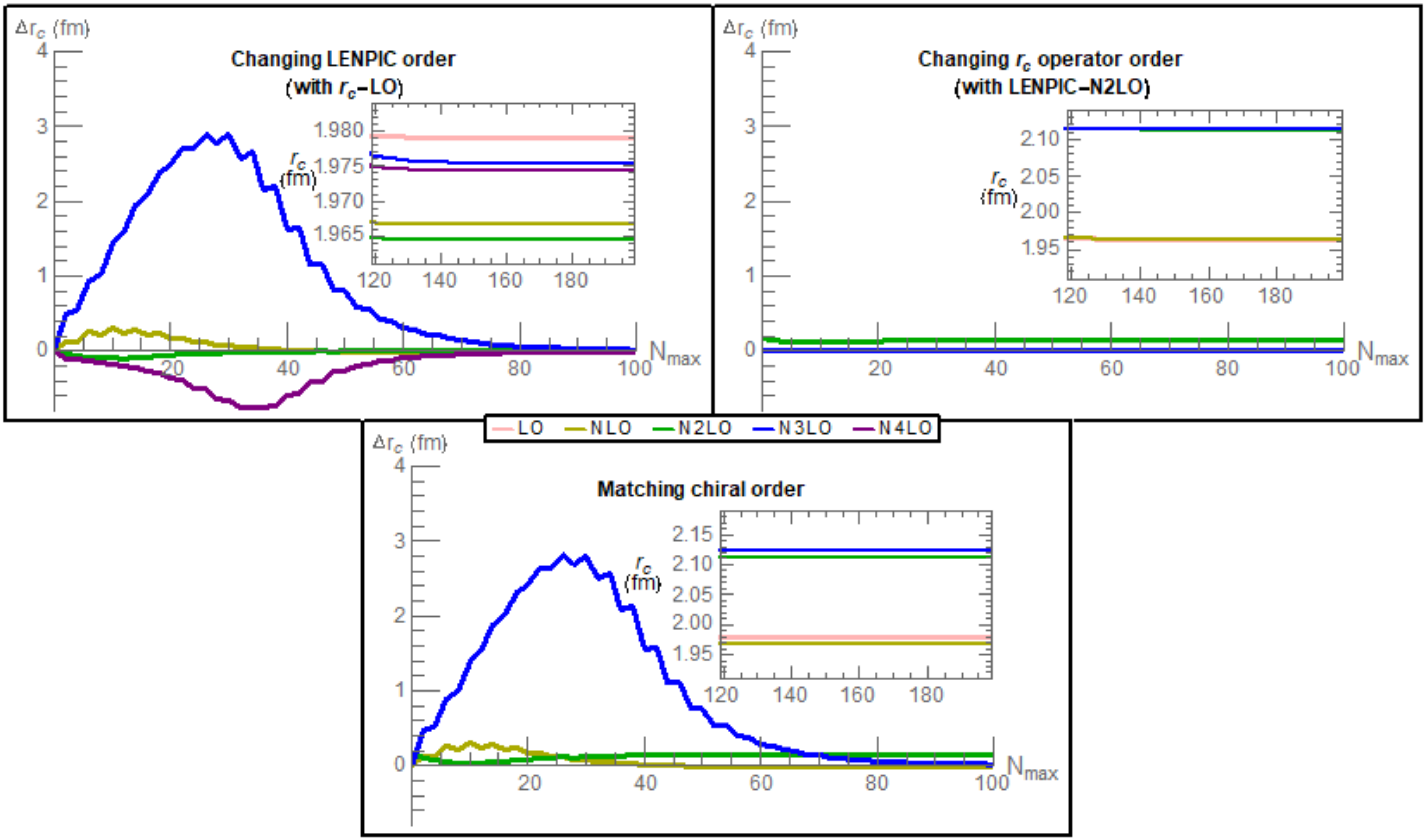
$$\hat{\rho}_{N3LO} = \frac{|e| g_A^2}{16 F_\pi^2 m_N} \left(1 - 2\bar{\beta}_9\right) \sum_{i<j} \left\{ (\tau_i^z + \vec{\tau}_i \cdot \vec{\tau}_j) \frac{\vec{\sigma}_i \cdot \vec{q}_i \vec{\sigma}_j \cdot \vec{k}}{q_i^2 + m_\pi^2} + i \leftrightarrow j \right\} \delta(\vec{p}_i' + \vec{p}_j' - \vec{p}_i - \vec{p}_j - \vec{k}). \quad (7)$$

- $\bar{\beta}_9$ is a parameter of the unitary transformation used to renormalize the one-pion exchange potential, and the charge operator. We have used $\bar{\beta}_9 = 0$.
- There are two more terms that contribute to the charge operator at N3LO, however they do not contribute to the charge radius.

Deuteron rms charge radius (r_c)

$\Delta r_c^{\lambda} = r_c^{\lambda} - r_c^{\lambda-1}$

LENPIC, R=1.0 fm, $\hbar\omega$=10 MeV



Gamow-Teller transition

- We consider the operators at zero momentum transfer.
- The leading order contribution (Q^{-3} in power counting) obtained from chiral EFT coincides with the impulse approximation operator,

$$\hat{O}^{\pm}_{GT,LO} = -g_A \sum_i \tau_i^{\pm} \hat{\sigma}_i \delta(\vec{p}_i' - \vec{p}_i). \tag{1}$$

- The first two body correction from chiral EFT appears at N2LO (Q^0 in power counting), [Krebs, *et.al.*, 2017]

$$\hat{O}^{\pm}_{GT,N2LO} = -\frac{1}{2(2\pi)^3} D \sum_{i<j} \left(\tau_i^{\pm} \hat{\sigma}_i + i \leftrightarrow j\right) \delta(\vec{p}_i' + \vec{p}_j' - \vec{p}_i - \vec{p}_j). \tag{2}$$

- The low energy constant D comes from the one pion exchange loop diagram, and is usually expressed in terms of a more well-known low energy constant, c_D,

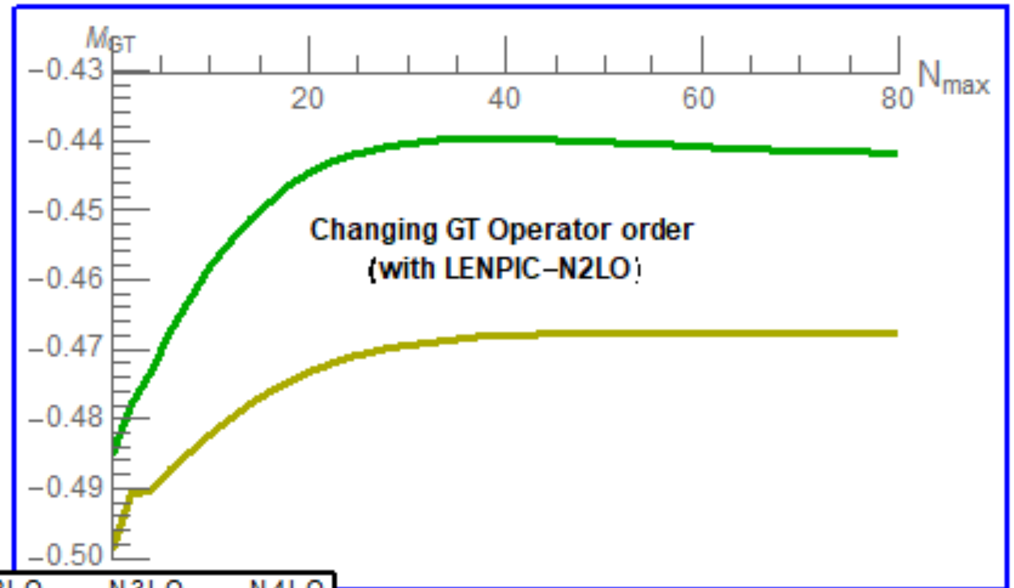
$$D = \frac{c_D}{F_\pi^2 \Lambda_\chi}. \tag{3}$$

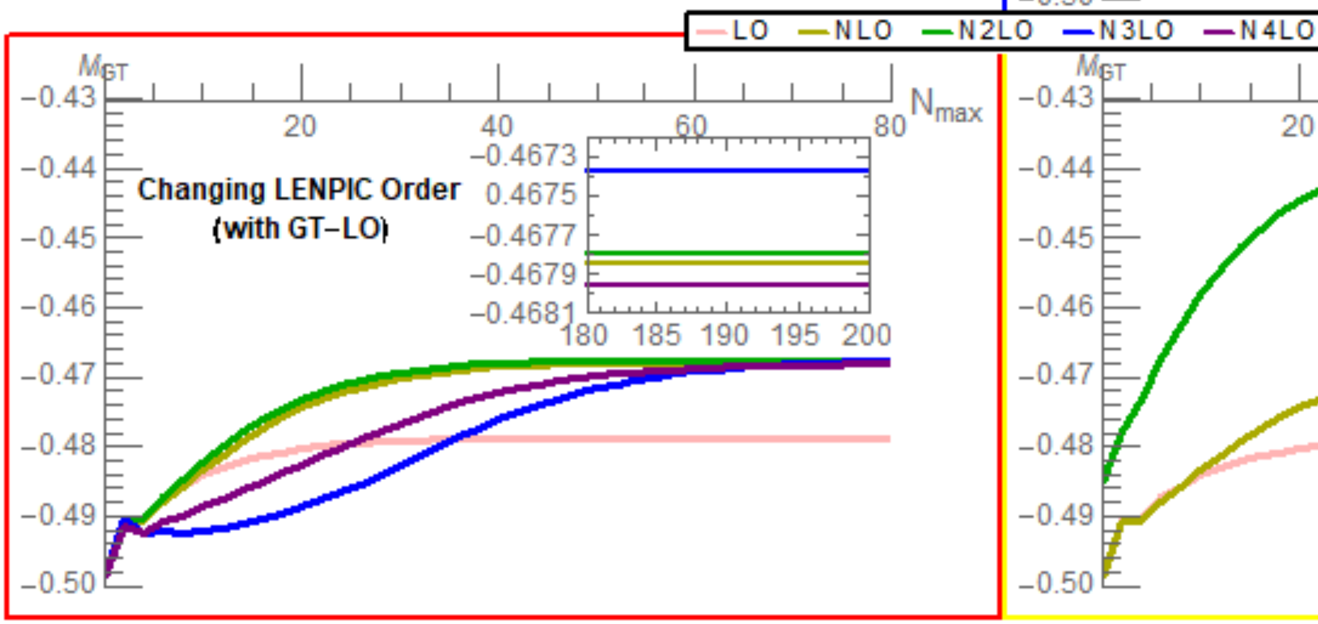
- We have used $c_D = -1$ [Navratil *et.al.*, 2007 and the chiral symmetry breaking scale $\Lambda_\chi = 700$ MeV.

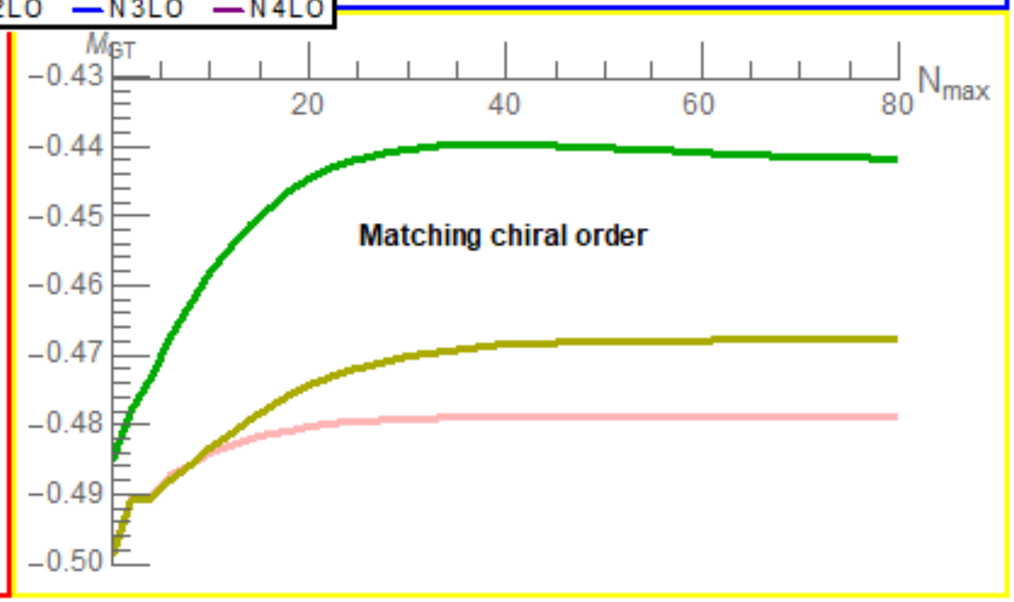
$s_0(nn) \to {}^3s_1 - {}^3d_1(np)$ GT Matrix Element (M_{GT})

LENPIC + V_{HO}, R=1.0 fm, $\hbar\omega$=10 MeV

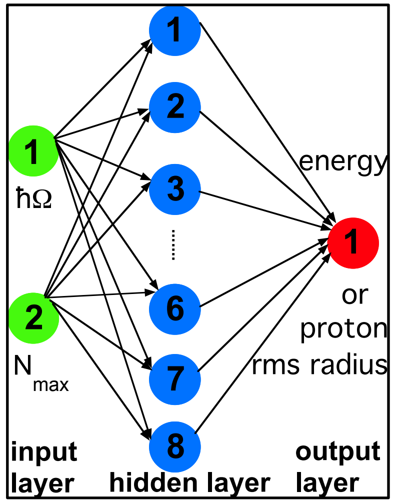
$M_{GT}(N_{max} \to 200)$		Operator Order				
		LO	NLO	N2LO	N3LO	N4LO
Interaction Order	LO	-0.478738	-0.478738	-0.424923	...	...
	NLO	-0.467850	-0.467850	-0.437194	...	...
	N2LO	-0.467793	-0.467793	-0.441937	...	...
	N3LO	-0.467378	-0.467378	-0.466229	...	...
	N4LO	-0.467964	-0.467964	-0.467793	...	...

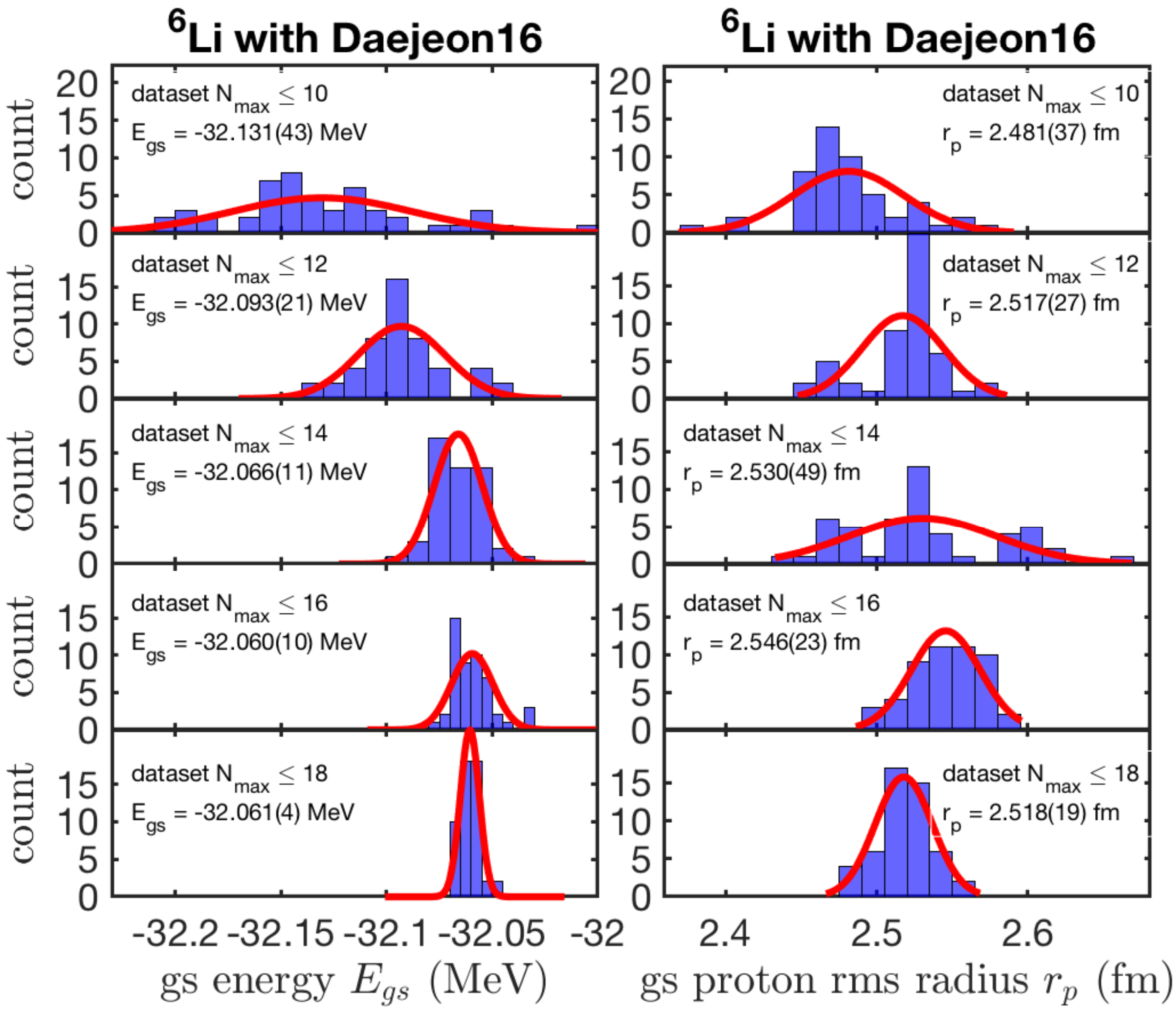


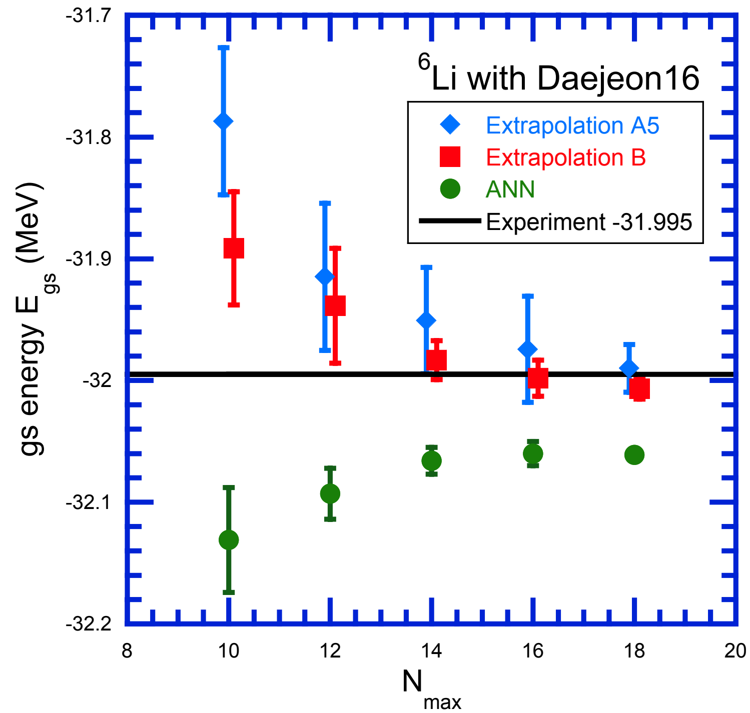


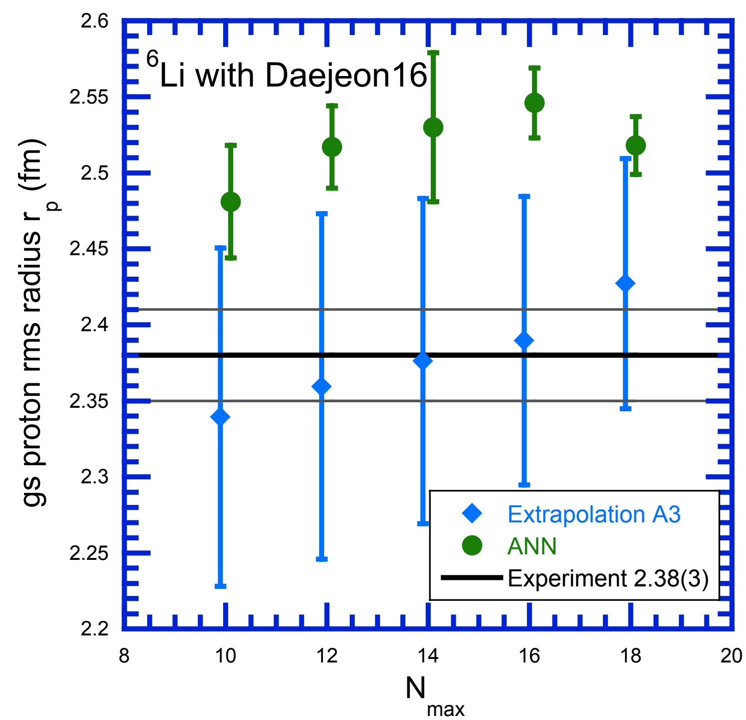


Deep Learning:
Extrapolation Tool for
Ab Initio Nuclear Theory,
G.A. Negoita, et al.,
arXiv:1810.04009

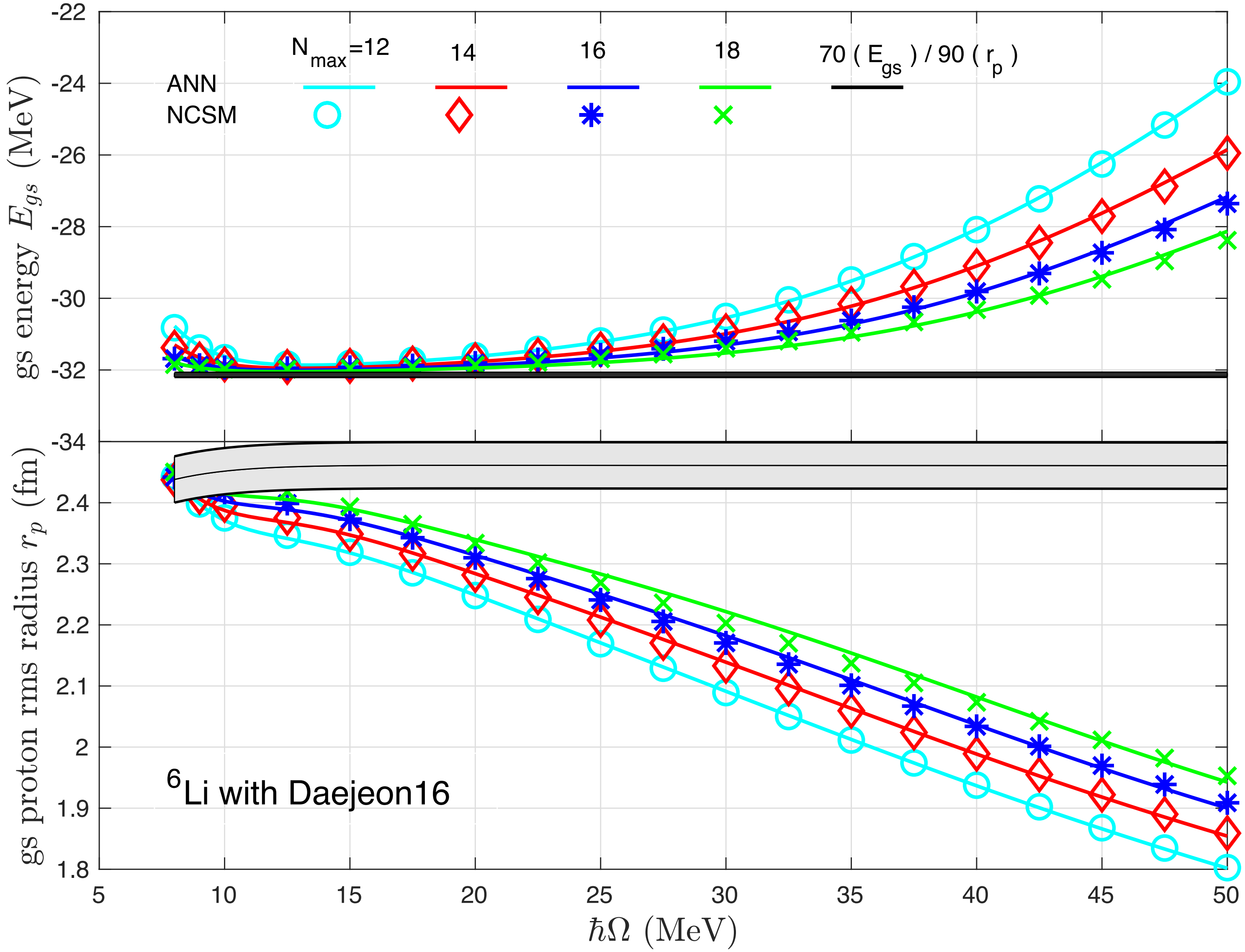








ANN results when training data limited to Nmax ≤ 10



G.A. Negoita, et al., “Deep Learning: Extrapolation Tool for Computational Nuclear Physics,” submitted to PRC; arXiv: 1811.01782

Progress:

LENPIC NN+NNN (at N2LO) paper: **PRC accepted**; arXiv:1807.02848

Completed studies of model 2-body systems: **PRC98, 065502 (2018);**
arXiv: 1809:00276

Implement electroweak operators in finite nuclei:

Benchmark A=6 calculations of 0v2β-decay with UNC & MSU groups (**paper in preparation**)

Postprocessor code for scalar and non-scalar observables (**in testing stage**)
Iowa State – Notre Dame collaboration

Develop extrapolations and uncertainties with Artificial Neural Networks:
A. Negoita, et al., submitted to PRC; arXiv:1810.04009

Outlook:

Expand treatment to full range of EW operators within Chiral EFT
at NLO, N2LO & N3LO (studies underway)

Extend effective EW operator approach to medium weight nuclei with "Double OLS" approach (sd shell investigations underway: N. Smirnova, et al)

Iowa State University
Members of NUCLEI and Topical Collaboration Teams

Faculty

J.P. Vary and P. Maris

Grad Students

Robert Basili
Weijie Du
Mengyao Huang
Matthew Lockner
Alina Negoita
Soham Pal
Shiplu Sarker

New faculty position at Iowa State in Nuclear Theory
Supported, in part, by the Fundamental Interactions
Topical Collaboration

Interviews in process

Breaking News

Time-Dependent Basis Function approach to Coulomb Excitation

Deuteron (JISP16) on ^{208}Pb target

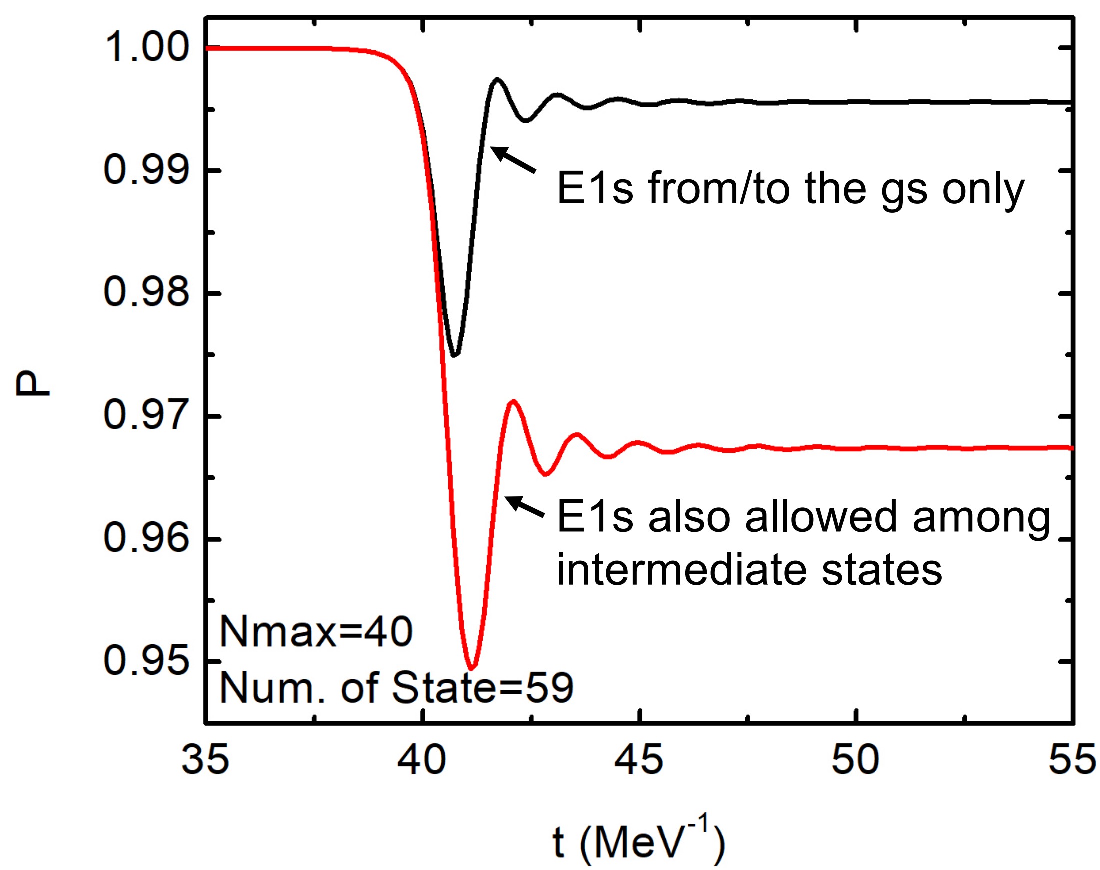
E_d (lab) = 12 MeV, Lab scattering angle of n-p CM = 70^o

Peng Yin, et al., in preparation

P = probability the deuteron remains in the elastic channel as function of t.

Non-perturbative treatment of electric dipole transitions to continuum states.

1-P = breakup probability



W. Du, et al., PRC 97, 064620 (2018); arXiv 1804.01156