No-Core Shell Model
with Chiral Effective Field Theory Interactions

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Nuclear Computational Low-Energy Initiative

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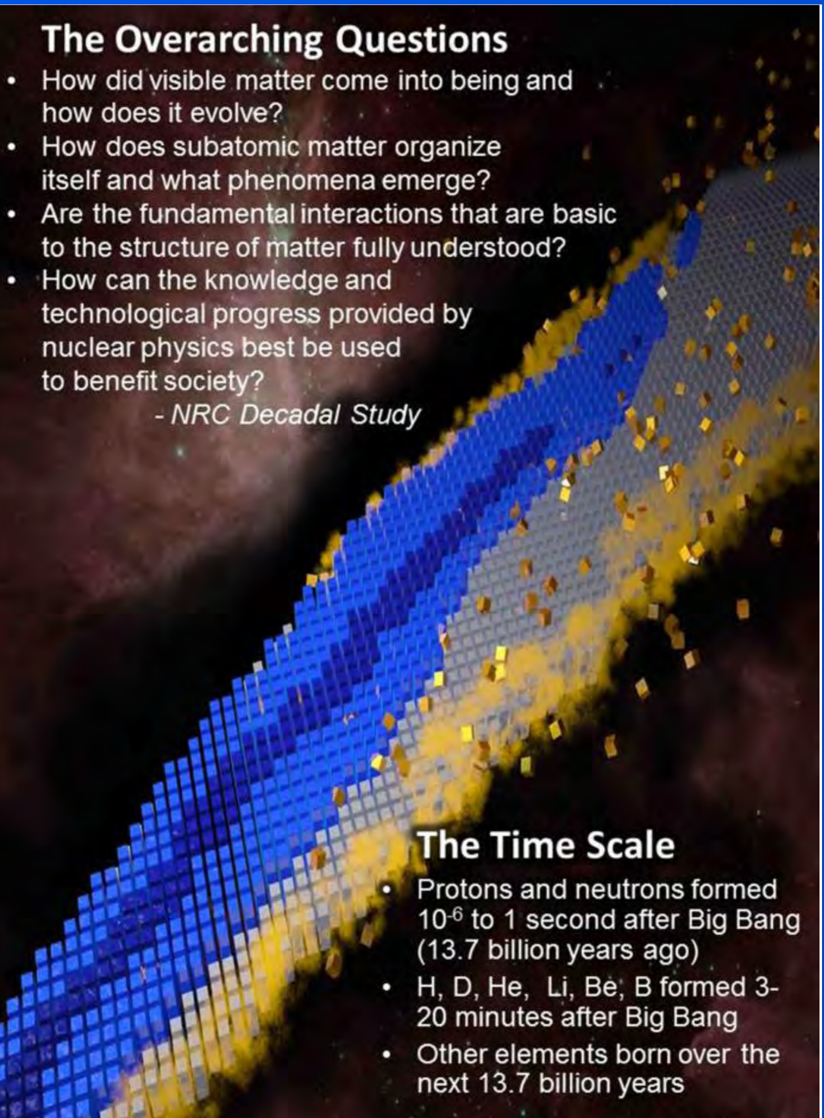
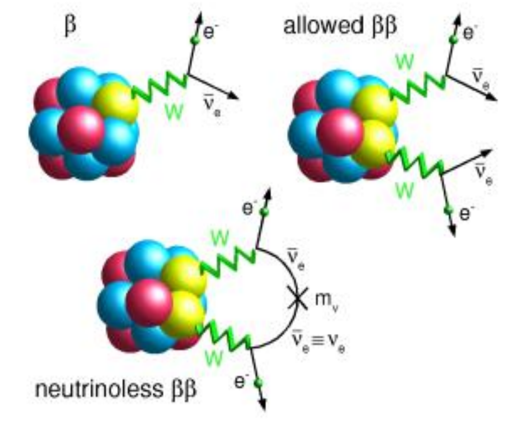


Topical Collaboration on Neutrinos and Fundamental Symmetries



LENPIC

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

Basis expansion $\Psi(r_1,\ldots,r_A) = \sum a_i \Phi_i(r_1,\ldots,r_A)$

- Many-Body basis states $\Phi_i(r_1,\ldots,r_A)$ Slater Determinants
- Single-Particle basis states $\phi_\alpha(r_k)$ with $\alpha = (n, l, s, j, m_j)$
- Radial wavefunctions: Harmonic Oscillator (HO), natural orbitals, Woods-Saxon, Coulomb-Sturmian, Complex Scaled HO, Berggren,. . .
- M-scheme: Many-Body basis states eigenstates of $\hat{\mathbf{J}}_\mathbf{z}$

$$\hat{\mathbf{J}}_\mathbf{z}|\Phi_i\rangle = M|\Phi_i\rangle = \sum_{k=1}^{A} m_{ik}|\Phi_i\rangle$$

- $N_{\rm max}$ truncation: Many-Body basis states satisfy

$$\sum_{\alpha \text{ occ.}}^{A} (2n+l)_\alpha \leq N_0 + N_{\rm max}$$

$N_{\rm max}$ runs from zero to computational limit. ($N_{\rm max}$, $\hbar\Omega$) fix HO basis

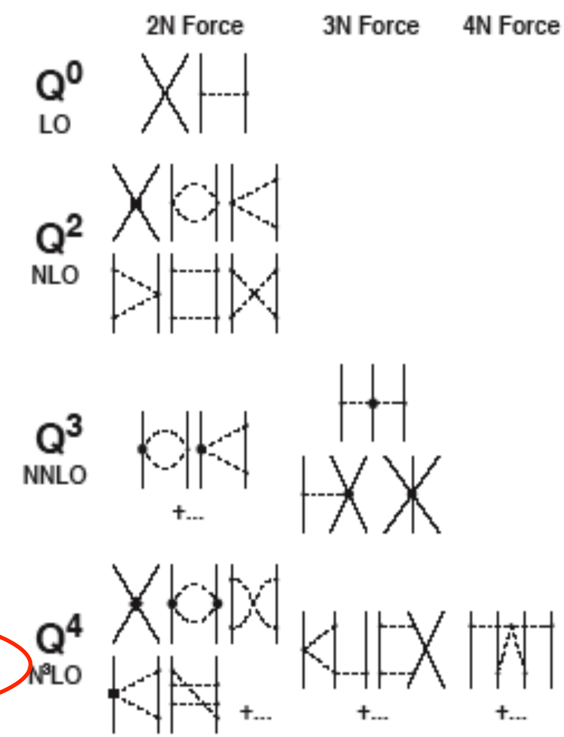
- Alternatives:
  - Full Configuration Interaction (single-particle basis truncation)
  - Importance Truncation — Roth, PRC79, 064324 (2009)
  - No-Core Monte-Carlo Shell Model — Abe *et al*, PRC86, 054301 (2012)
  - SU(3) Truncation — Dytrych *et al*, PRL111, 252501 (2013)

Nuclear interaction

Major development during the past ~10 years:
High-precision ab initio calculations now used to "discover" the correct strong NN+NNN interaction

Nuclear potential not well-known,
though in principle calculable from QCD

$$\hat{\mathbf{H}} = \hat{\mathbf{T}}_{\text{rel}} + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \ldots$$



In practice, alphabet of realistic potentials

- Argonne potentials: AV8′, AV18
  - plus Urbana 3NF (UIX)
  - plus Illinois 3NF (IL7)
- Bonn potentials
- Chiral NN interactions - e.g. LENPIC
  - plus chiral 3NF, ideally to the same order
- JISP16

Kim, Abe, Caprio, Mazur, Shirokov talks

- Daejeon16
- . . .

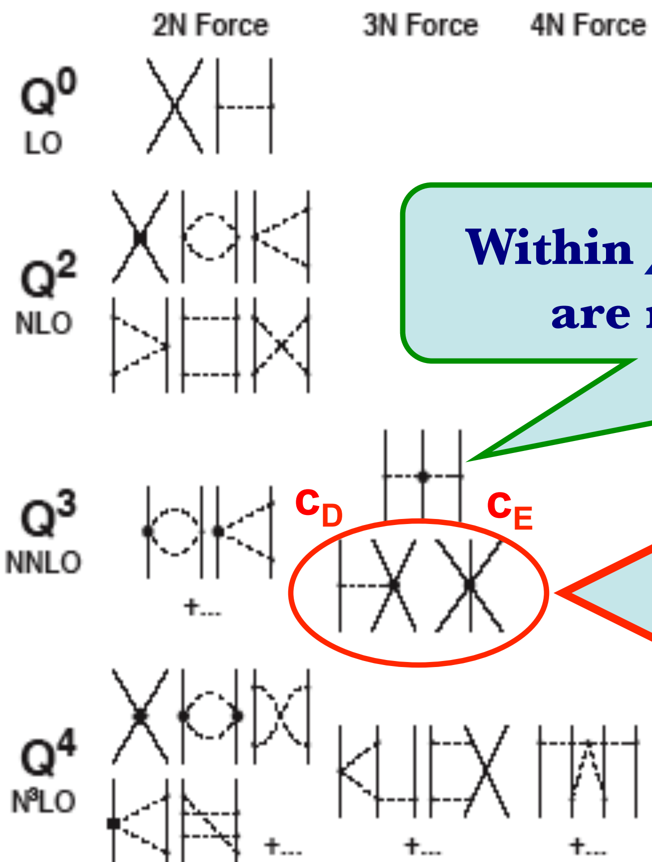
Extrapolations with Artificial Neural Networks: Brief comment at the end

Effective Nucleon Interaction
(Chiral Perturbation Theory)

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

Expansion parameter : $\left(\frac{Q}{\Lambda_\chi}\right)^{\nu}$, 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 (see below)

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 Forschungszentrum — 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

Goal

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

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Challenge

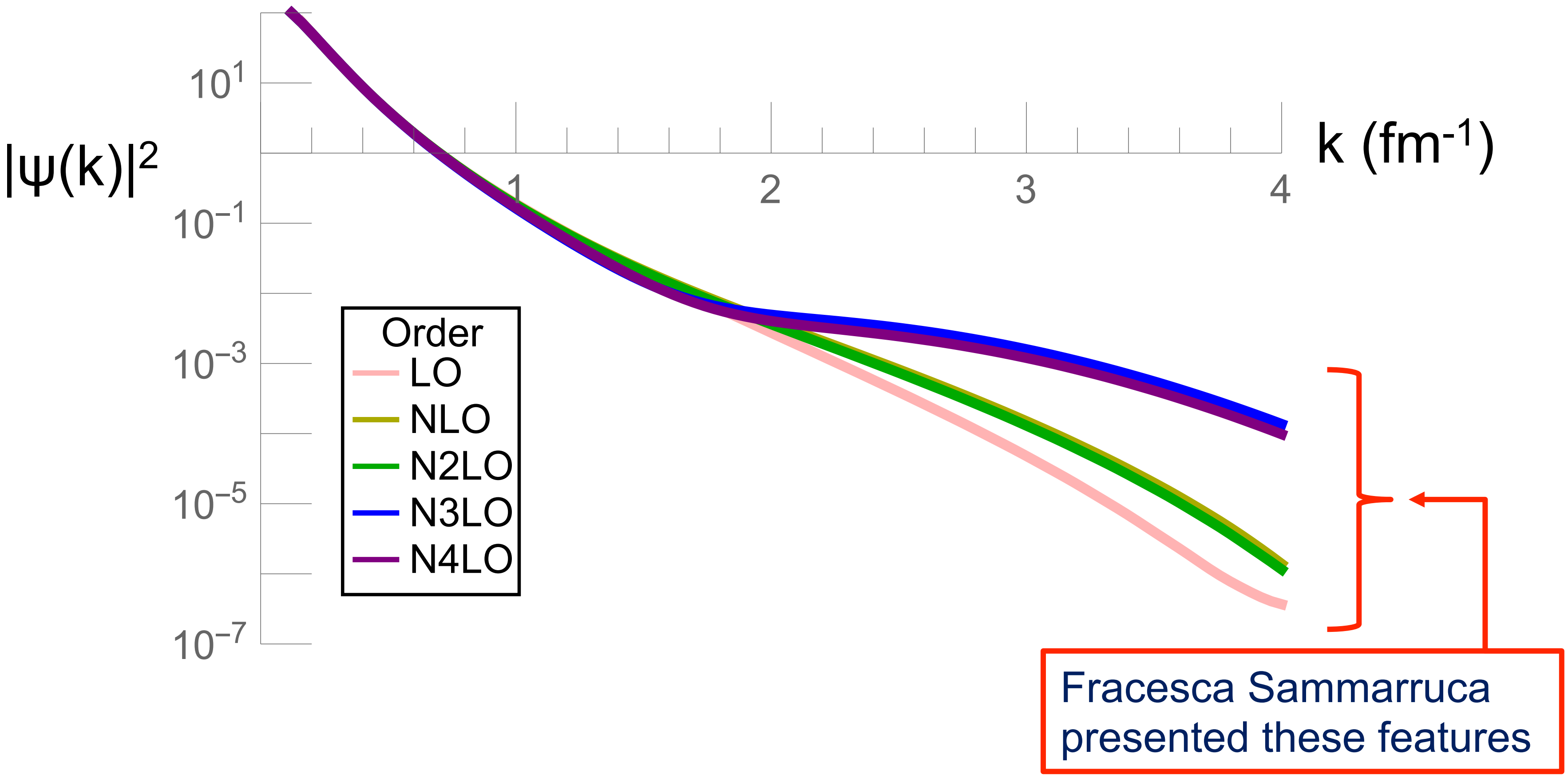
Due to the large number of matrix elements, the calculation is extremely expensive.

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

Progressing to higher chiral order builds higher momentum components into the deuteron ground state wave function: bellwether for convergence in NCSM applications

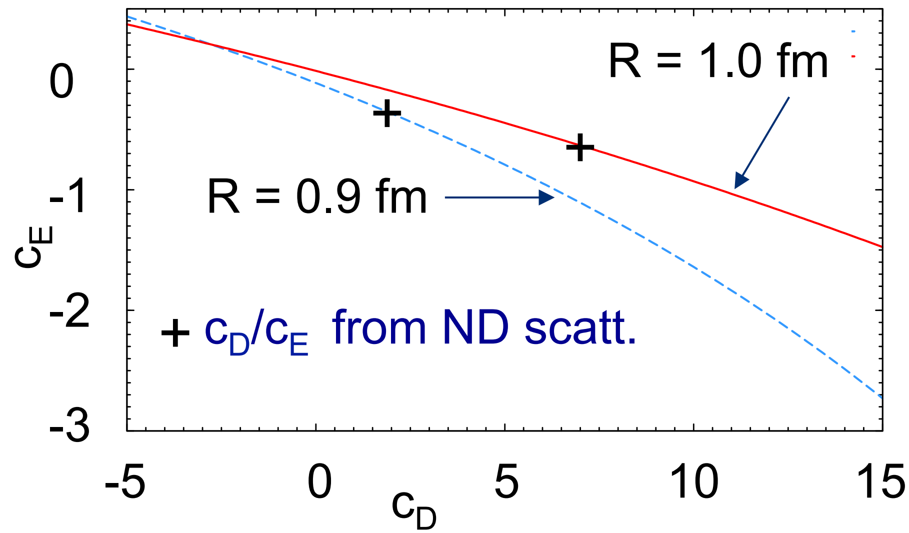


R. Basili, W. Du, et al., in preparation

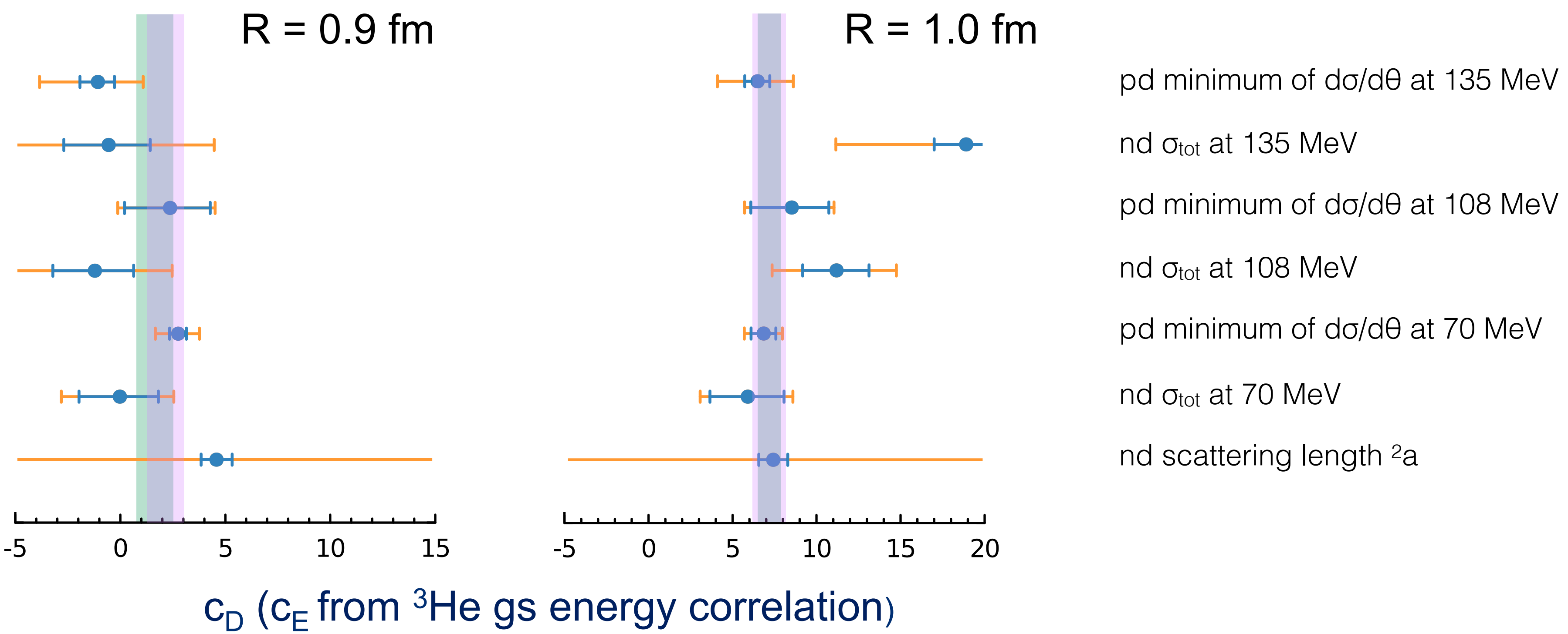
Coordinate space regulator:

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

c_D/c_E correlation from fits to ^3He gs Energy

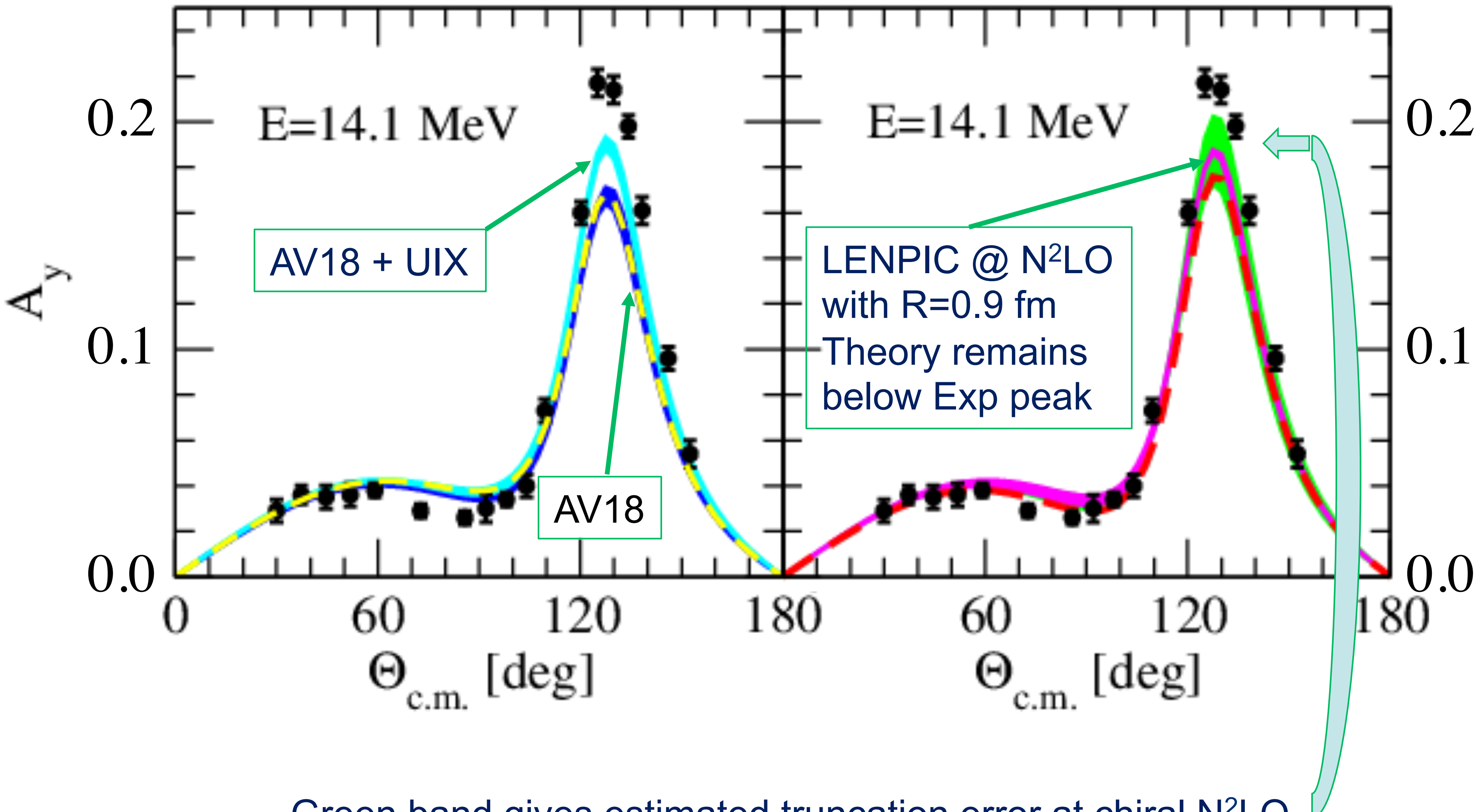


c_D (c_E) selected via ND scattering analyses:



LENPIC: E. Epelbaum, et al., arXiv: 1807.02848

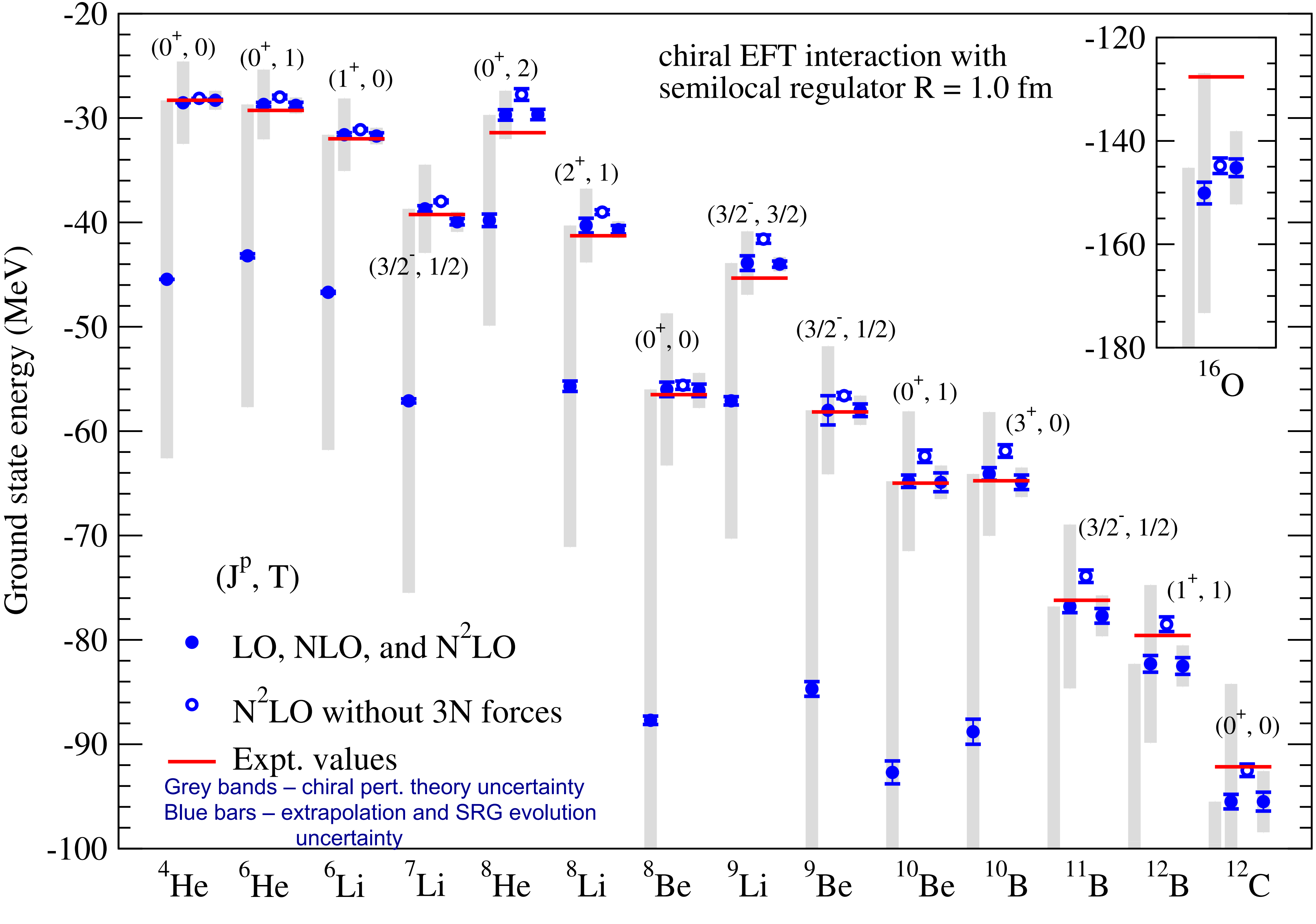
Status of the A_y puzzle (talk by Roman Skibinski)

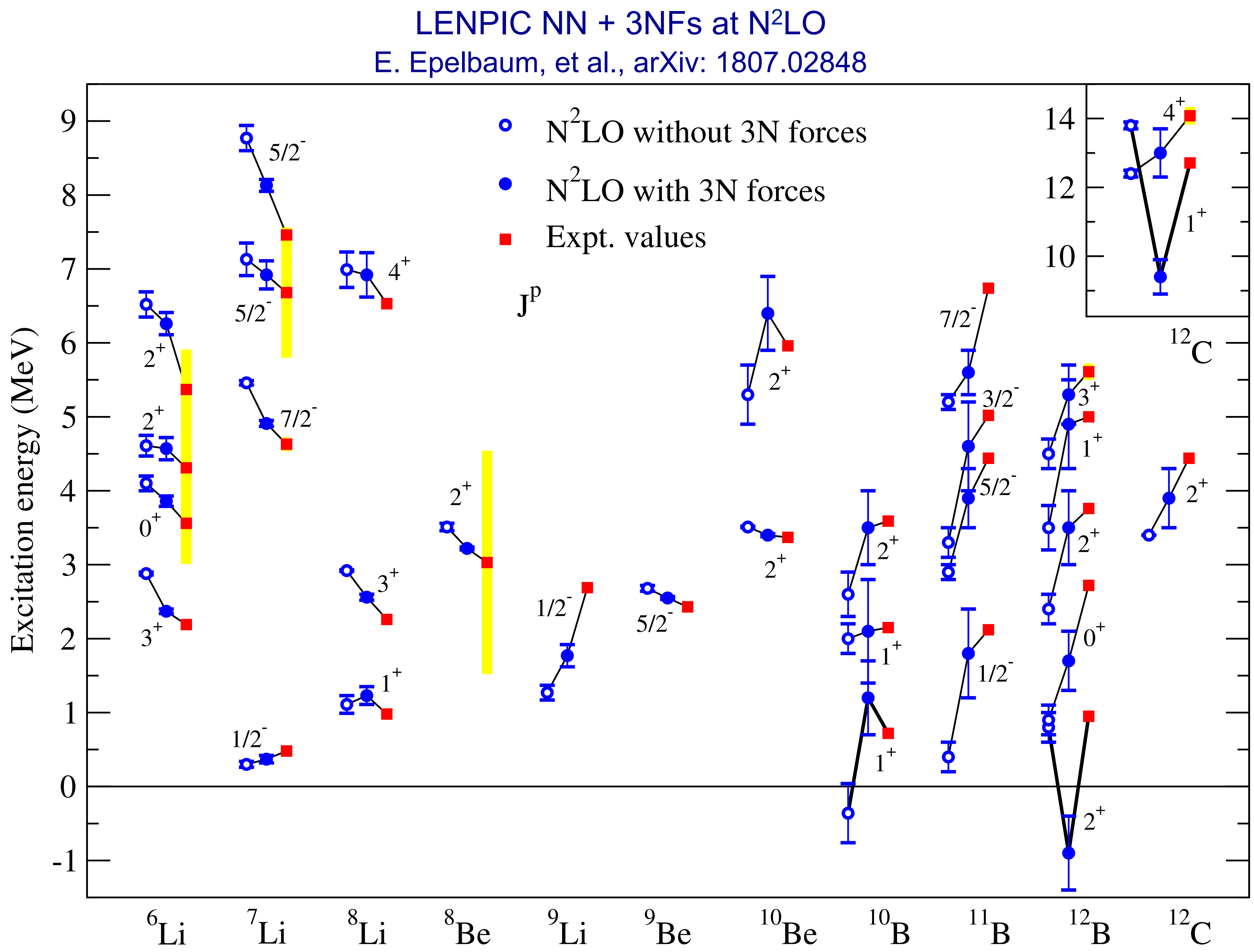


Green band gives estimated truncation error at chiral N^2LO

LENPIC: E. Epelbaum, et al., arXiv: 1807.02848

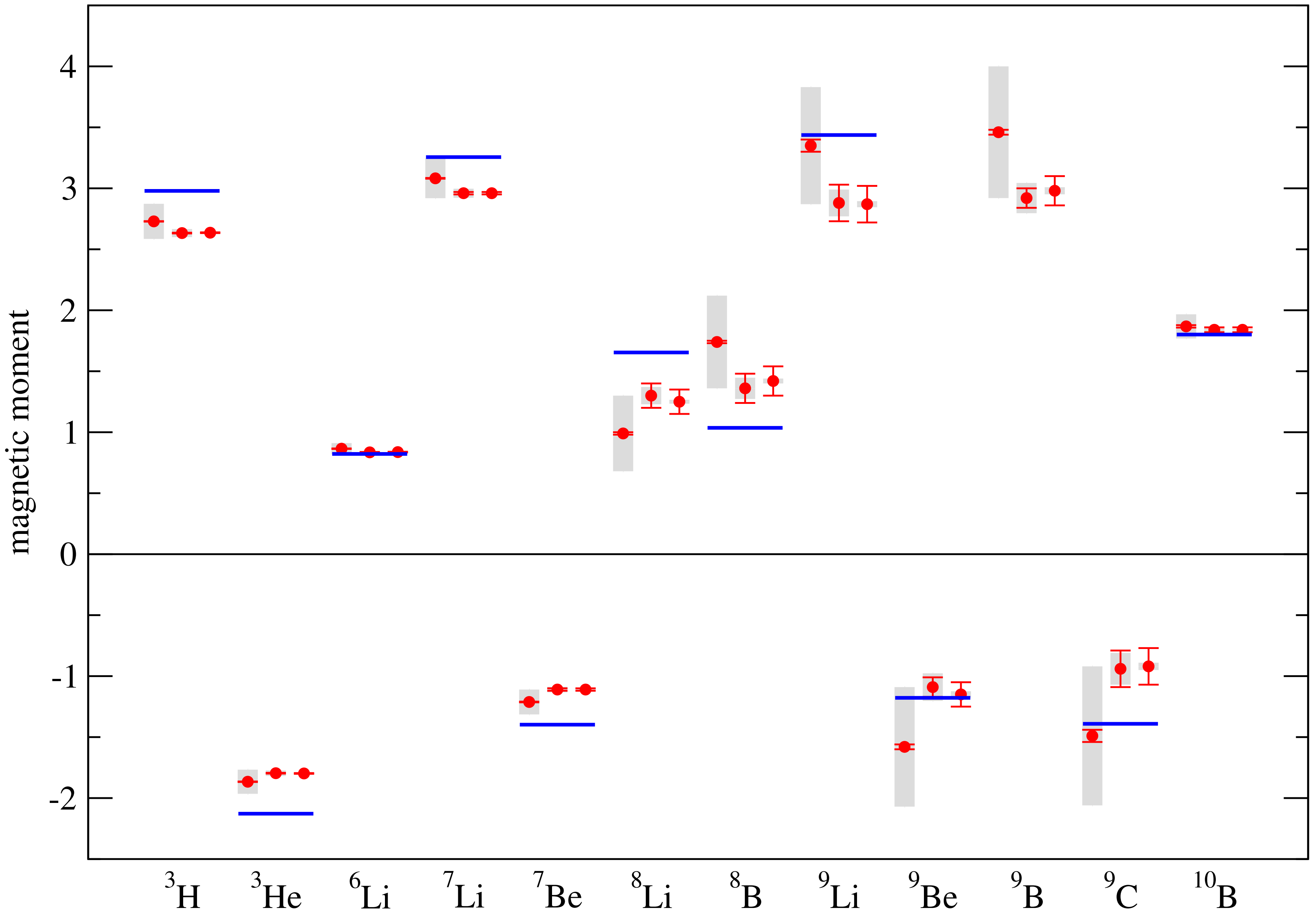
LENPIC NN + 3NFs at N²LO (E. Epelbaum, et al., arXiv: 1807.02848)





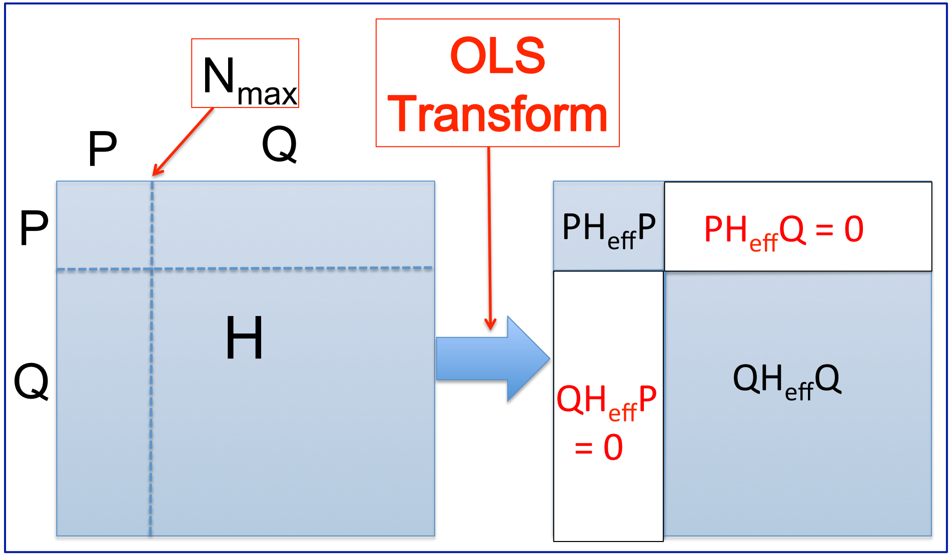
LENPIC NN + 3NFs at N2LO
E. Epelbaum, et al., arXiv: 1807.02848
N2LO without 3N forces
N2LO with 3N forces
Expt. values
Jp
Excitation energy (MeV)
6Li
7Li
8Li
8Be
9Li
9Be
10Be
10B
11B
12B
12C

Preliminary results – yet to include 3NF and corrections to M1 moment operator



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., arXiv: 1809.00276 for applications

Consider two nucleons as a model problem with V = LENPIC chiral NN solved in the harmonic oscillator basis with $\hbar\Omega$ = 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(0v2β)

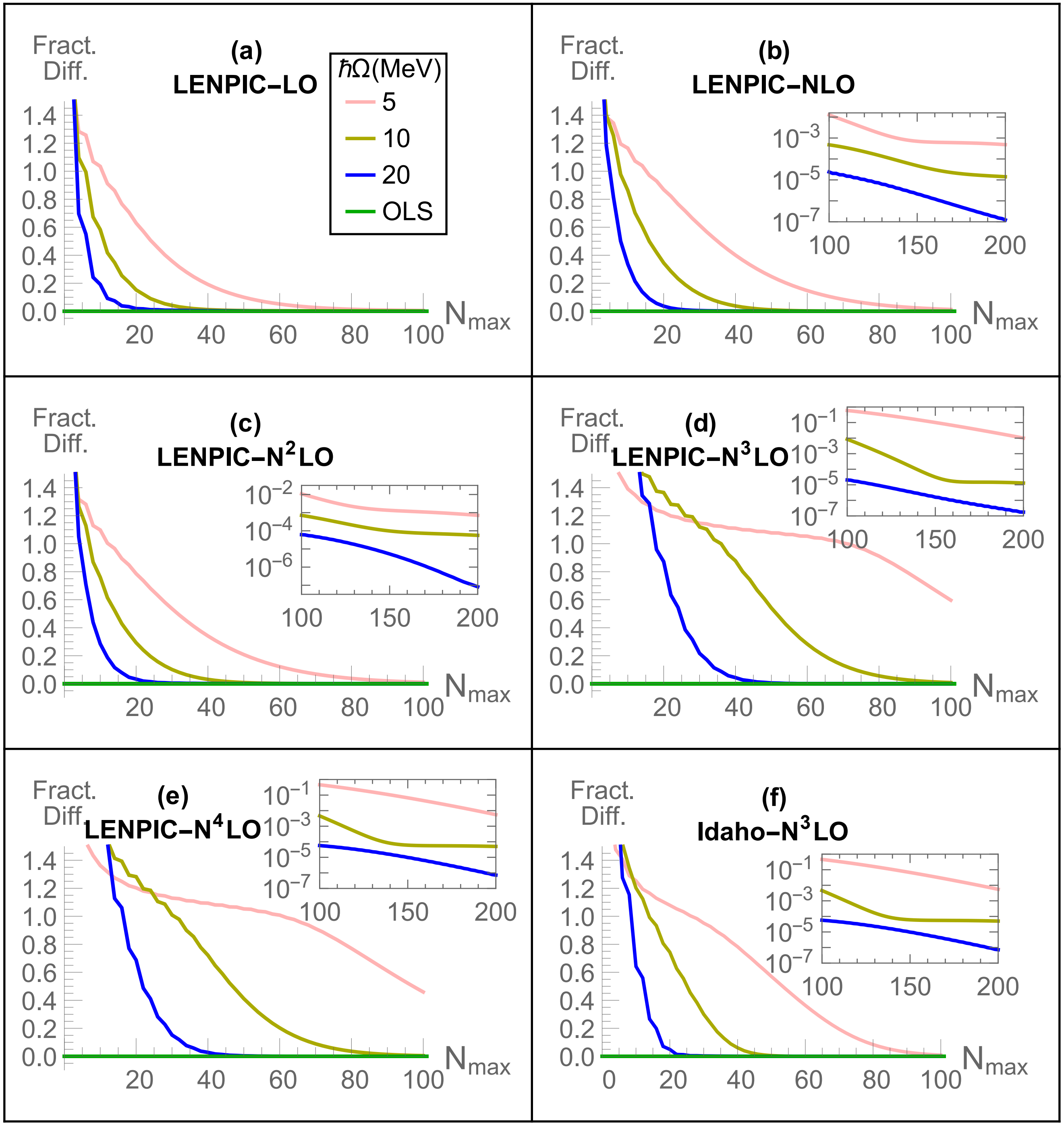
Dimension of the “full space” is 400 for all results depicted here

J.P. Vary, et al., arXiv: 1809.00276

Deuteron gs energy: truncation vs OLS

Fract. Diff. = $(E_{model} - E_{exact})/|E_{exact}|$

Insets: Semilog plots of high N_{max} region



OLS gives exact results for all cases (green lines at Fract. Diff. = 0)

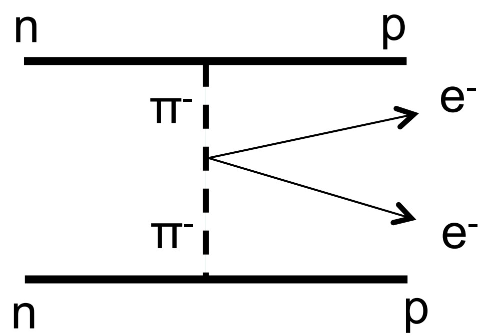
Convergence patterns sensitive to chiral order

Even unbound cases (Fract. Diff. > 1.0) are accurately treated with OLS

J.P. Vary, et al., arXiv: 1809.00276

Consider a 2-body contribution within EFT to 0vββ-decay at N^{2}LO

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



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

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

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

Challenge to apply coordinate space regulator and preserve gauge symmetry

~~Regulator applied to 0vββ-decay operator for consistency with LENPIC interaction~~

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

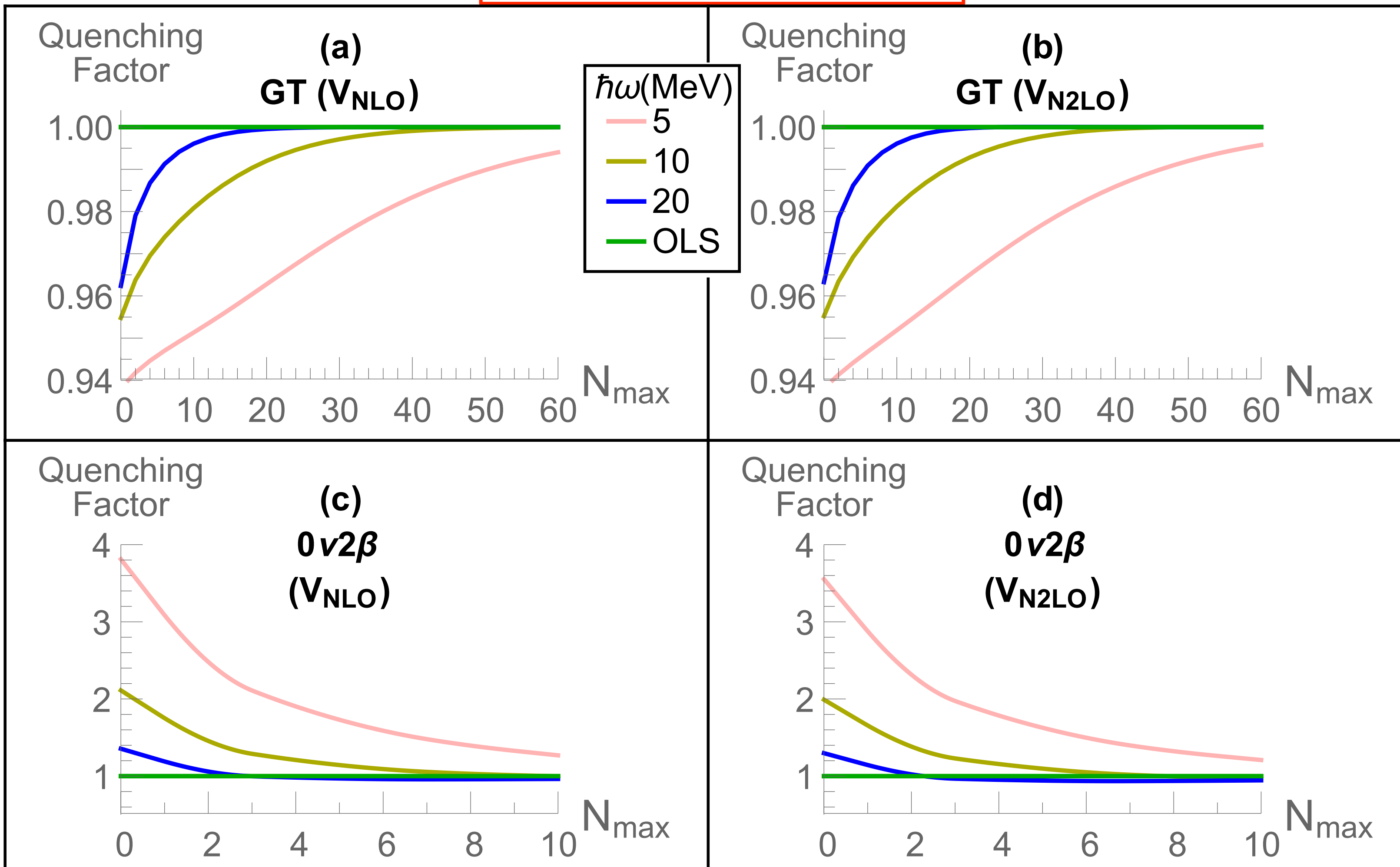
$R = 1.0$ fm for these results

Sensitivity to R and additional operators under development – stay tuned

Two nucleons in a Harmonic Oscillator trap with trap ħΩ = basis ħΩ
LENPIC Chiral NN interaction at N^2LO with R = 1.0 fm
Comparison of GT and 0v2β-decay matrix elements from truncation with Exact/OLS

Quenching Factor = Exact/Model
Note: 0v2β regions at low N_{max} show enhancement

$^1S_0(nn\ \text{gs}) \rightarrow {}^3S_1 - {}^3D_1(np\ \text{gs})$

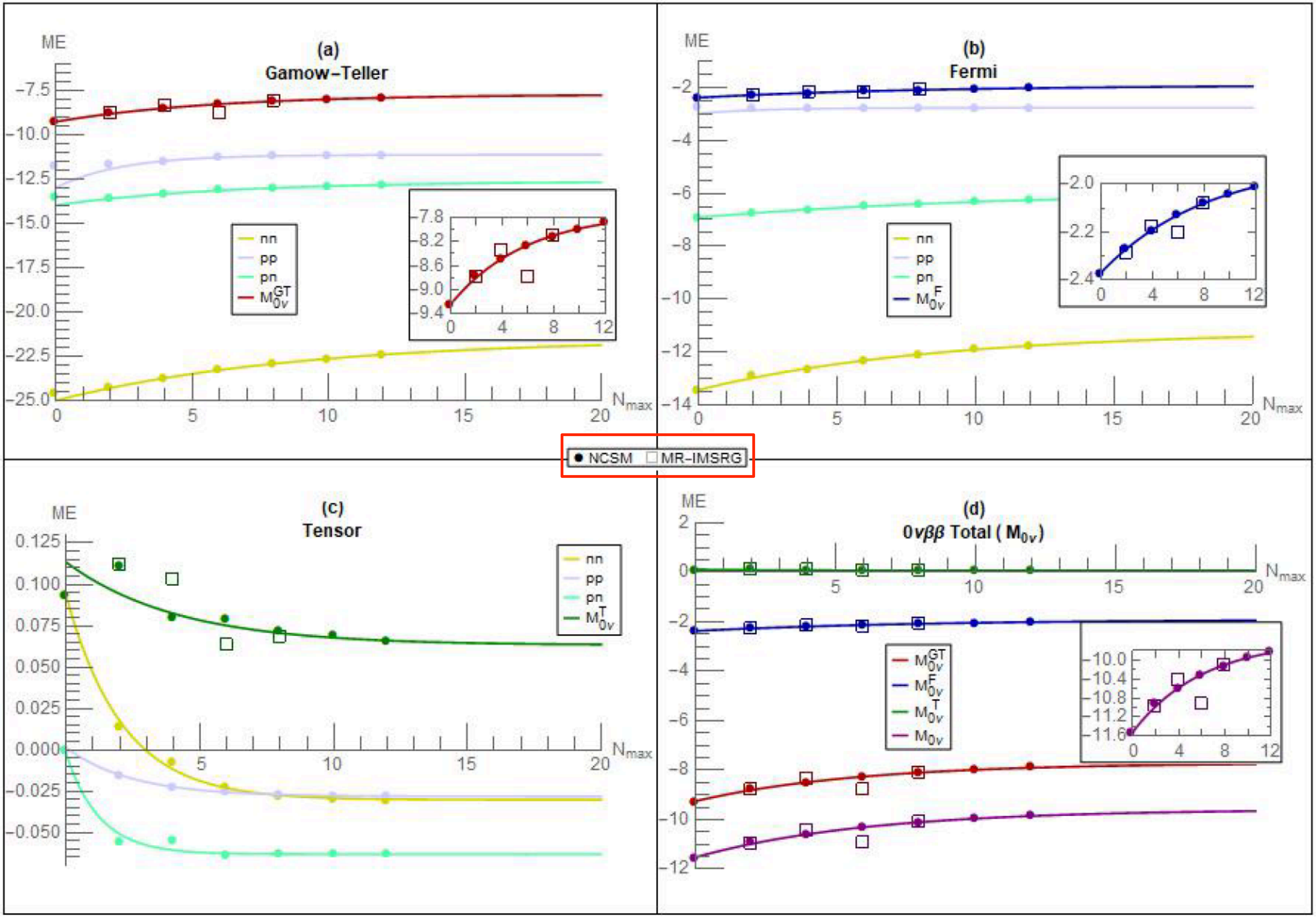


$^1S_0(nn\ \text{gs}) \rightarrow {}^1S_0(pp\ \text{gs})$

J.P. Vary, et al., arXiv: 1809.00276

ISU – UNC collaboration to benchmark 0n2b-decay matrix elements for ^{6}He -> ^{6}Be

EM500 N3LO NN interaction; 0ν2β-decay ops from J. Engel and J. Menendez, Rept. Prog. Phys. 80, 046301 (2017)



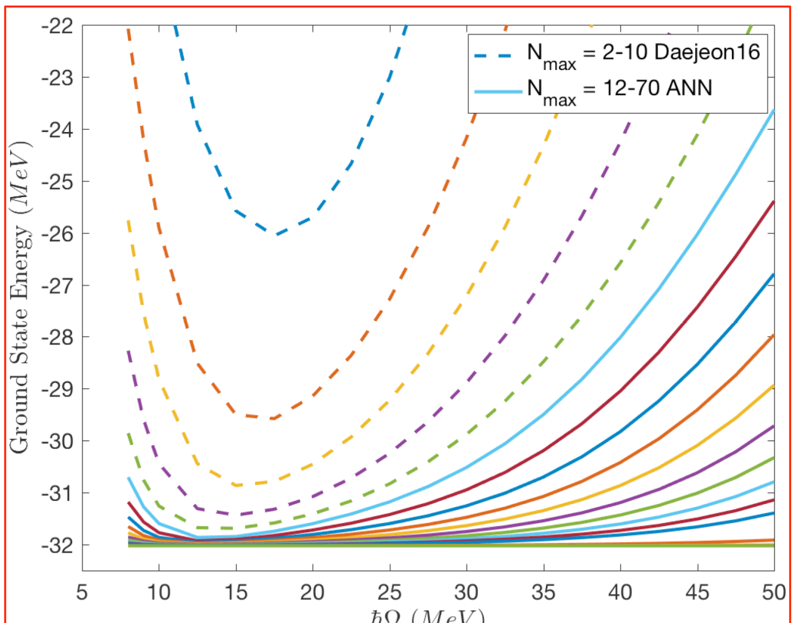
Deep Learning for Nuclear Binding Energy and Radius

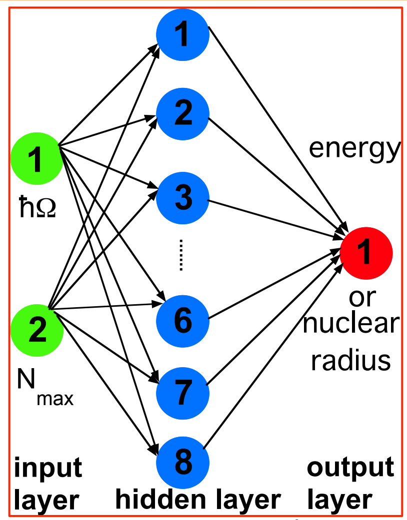
Scientific Achievement

- Development of an artificial neural network (ANN) for extending the application range of the *ab initio* No-Core Shell Model (NCSM)
- Demonstrated predictive power of ANNs for converged solutions of weakly converging simulations of the nuclear radius
- Provided a new paradigm for matching Deep Learning with results from high performance computing simulations

Significance and Impact

- Guides experimental programs at DOE's rare isotope facilities
- Extends the predictive power of *ab initio* nuclear theory beyond the reach of current high performance computing simulations
- Establishes foundation for deep learning tools in nuclear theory useful for a wide range of applications





Architecture of neural network (**above**) used successfully to extrapolate the ^{6}**Li** ground state energy from modest basis spaces (dashed line sequence) to extreme basis spaces (solid line sequence) achieving independence of basis parameters (flat line in **left figure**).

Research Details

- Predict properties of nuclei based on *ab initio* structure calculations in achievable basis spaces
- Develop artificial neural networks that extend the reach of high performance computing simulations of nuclei
- Produce accurate predictions of nuclear properties with quantified uncertainties using fundamental inter-nucleon interactions

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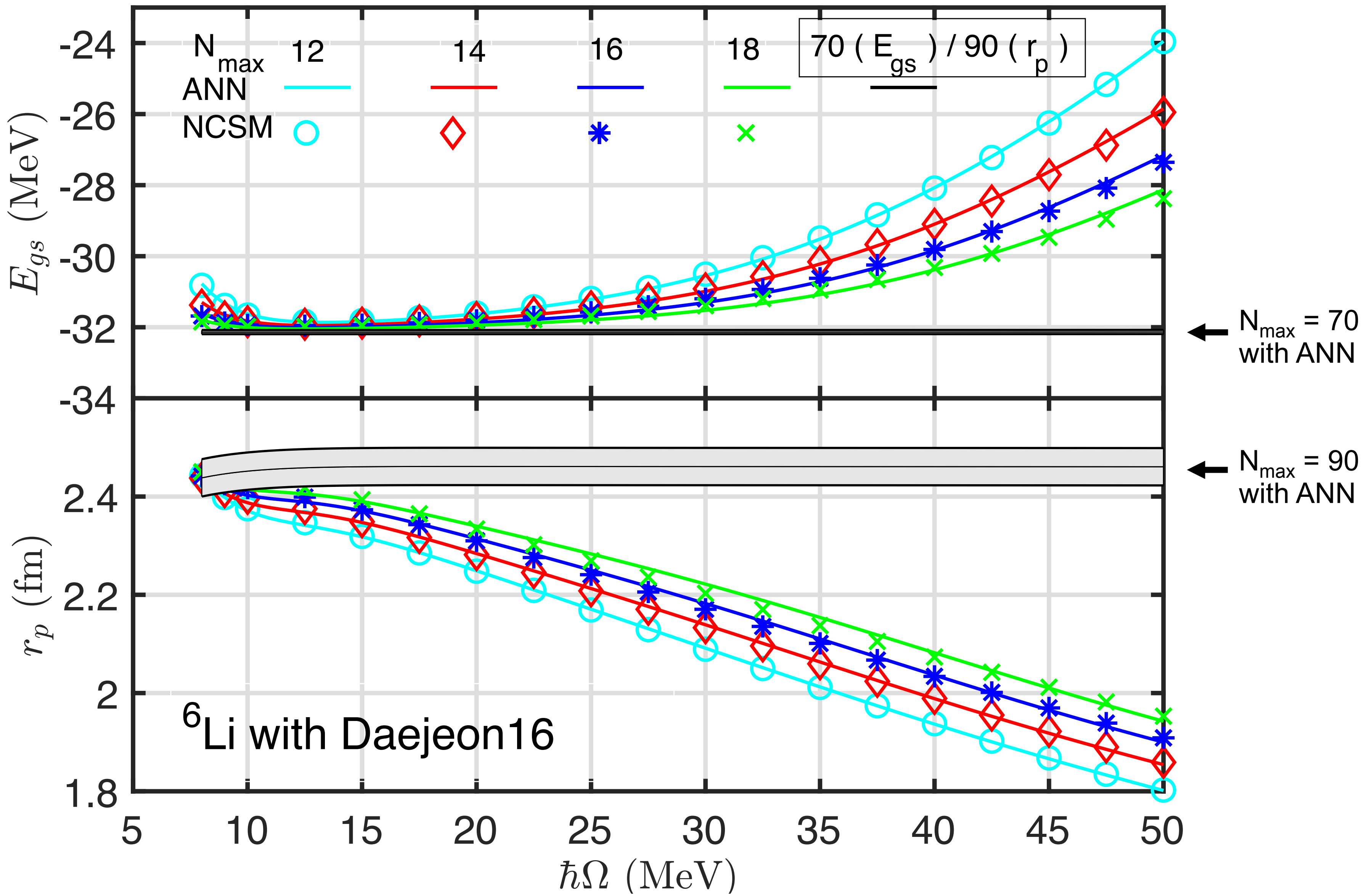
Reference: G. A. Negoita, et al., in COMPUTATION TOOLS 2018, Barcelona, Spain, February 18–22, 2018; http://www.thinkmind.org/index.php?view=article&articleid=computation_tools_2018_1_40_80017

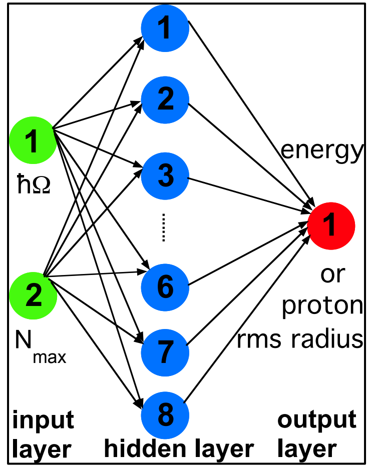
Contacts: jvary@iastate.edu; egng@lbnl.gov

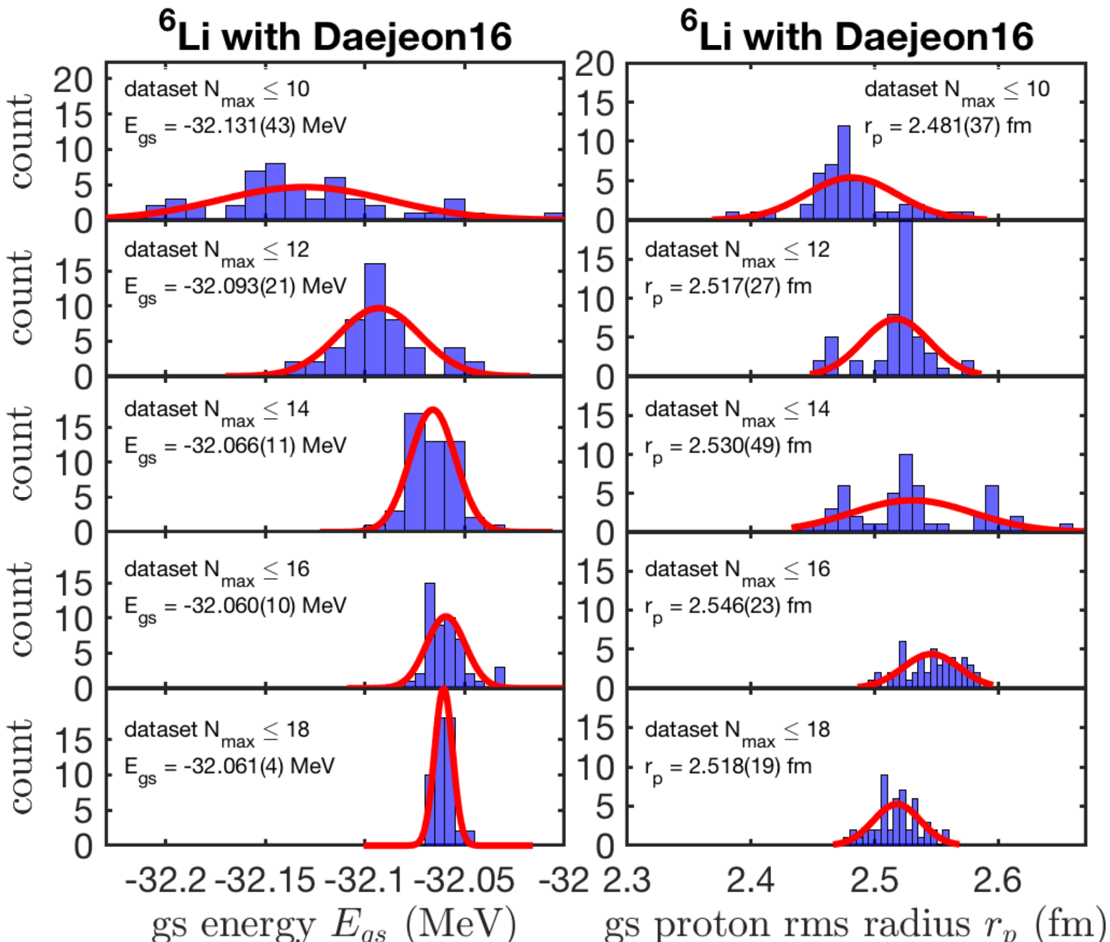
Train/test ANN with NCSM data (Daejeon16) up through N_{max} = 10
then **predict** data for N_{max} > 10

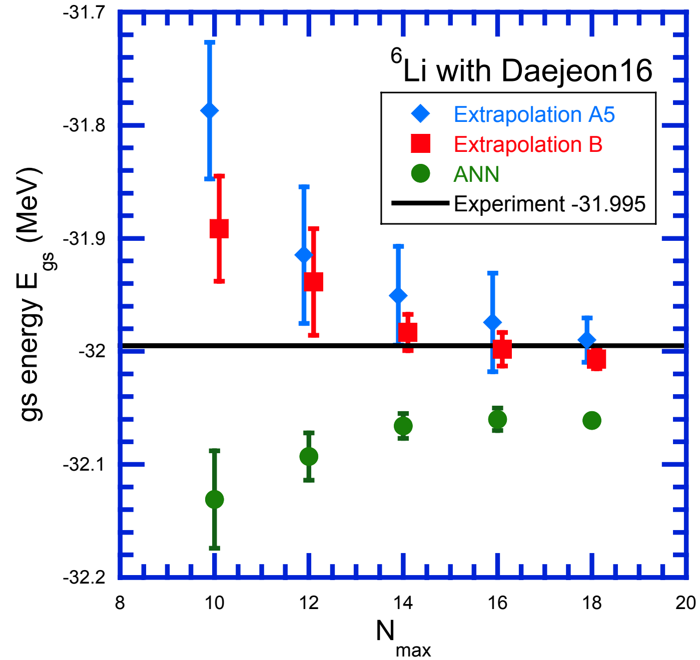


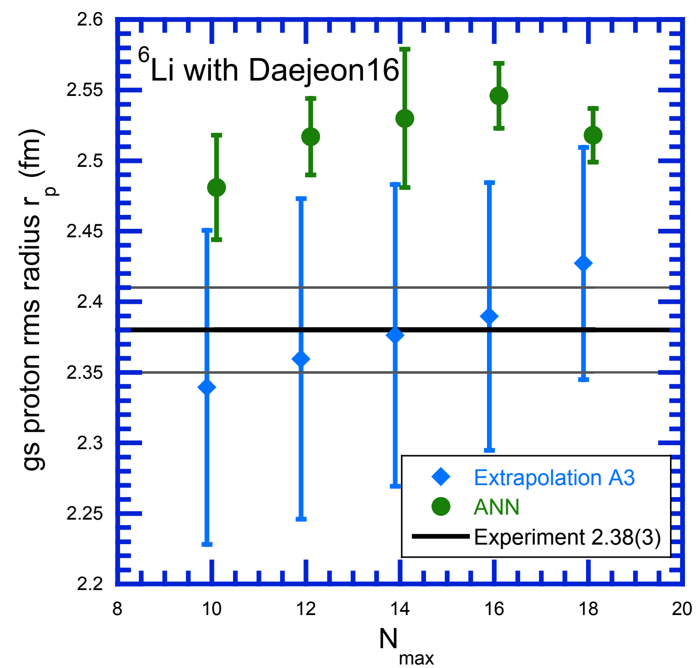
G.A. Negoita, et al., arXiv:1810.04009

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







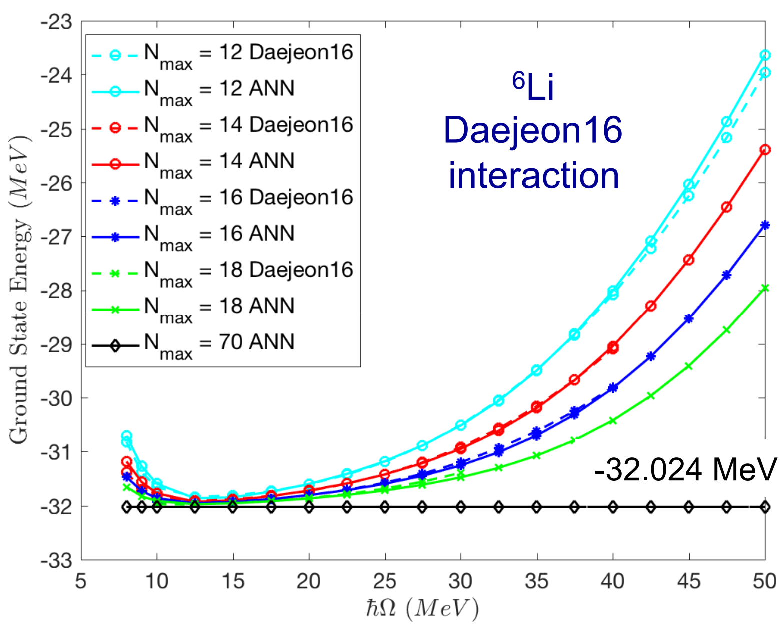


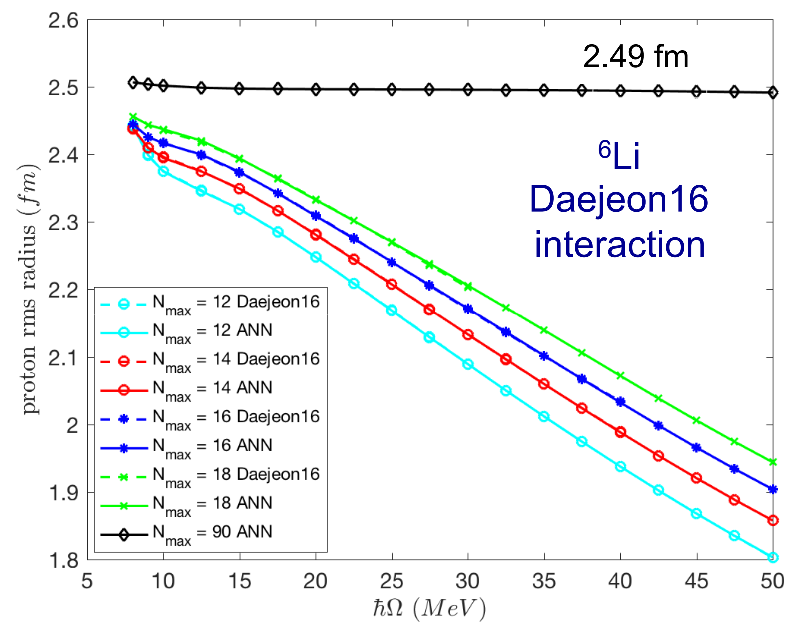
Extrapolating to complete basis

- Perform a series of calculations with increasing N_{max} truncation
- Empirical extrapolation binding energy

$$E^{N}_{\mathrm{binding}} = E^{\infty}_{\mathrm{binding}} + a\exp(-bN_{\mathrm{max}})$$

- Artificial Neural Networks trained with Nmax ≤ 10 NCSM results





Negoita, et al., Computation Tools 2018, Barcelona, Feb. 19, 2018: Best Paper award & Published online:
http://www.thinkmind.org/index.php?view=article&articleid=computation_tools_2018_1_40_80017
arXiv: 1803.03215

Summary

LENPIC NN+NNN (at N2LO) paper: arXiv: 1807.02848

OLS for model 2-body systems: arXiv: 1809:00276

Improved electroweak operators in finite nuclei:

Benchmark A=6 calculations of 0v2β-decay with UNC group (paper in preparation)

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

Extrapolations + uncertainties with Artificial Neural Networks: arXiv:1810:04009

Outlook

Expand treatment to full range of EW operators within Chiral EFT at NLO & N2LO (well underway); employ alternative bases

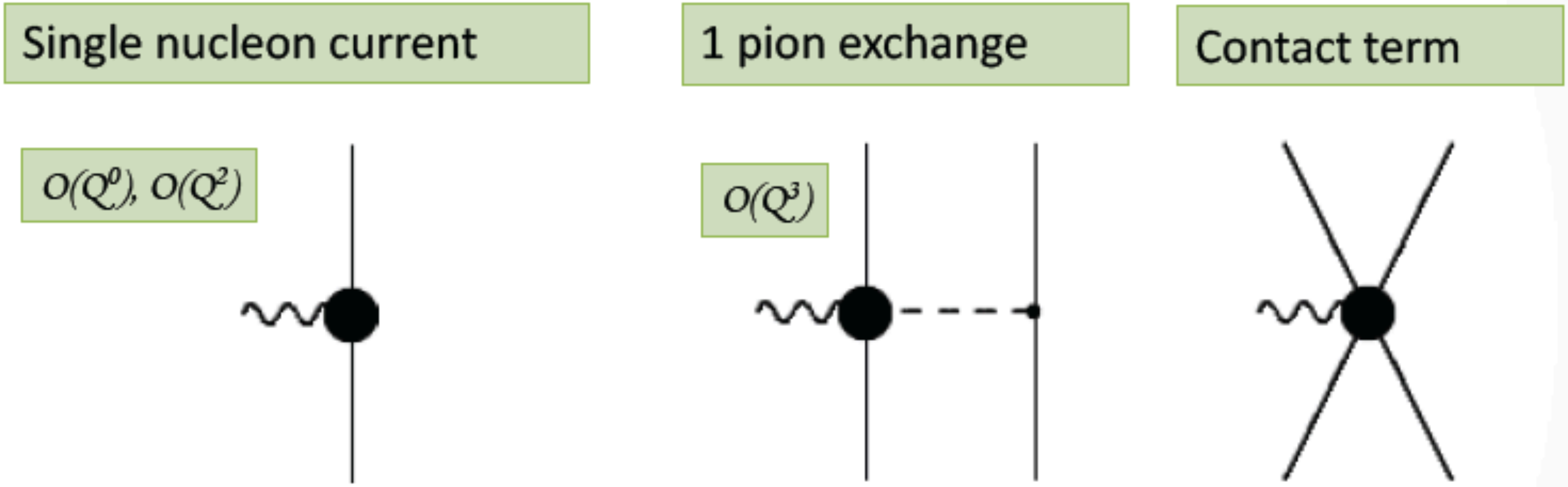
Extend effective interactions and EW operators to medium weight nuclei with "Double OLS" approach – talk by Bruce Barrett

Also underway: more neural network developments, . . .

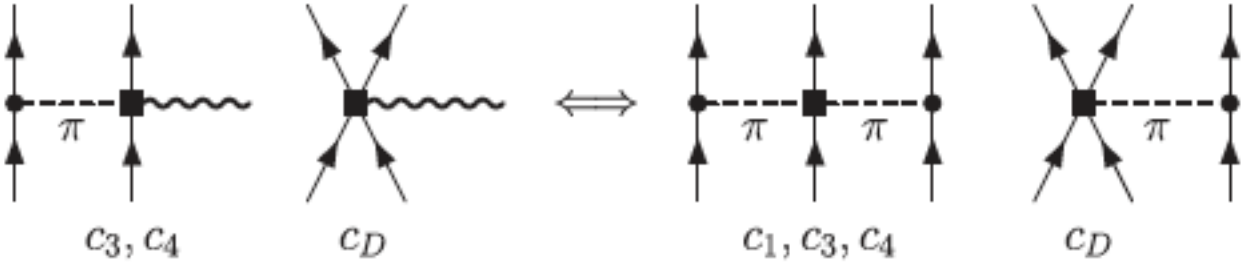
Coupling to External Probes in Chiral EFT

LENPIC collaboration (in process) – adopts momentum space regulators

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



Two-Body Currents (N^2LO)



Note: we retain dependence on external momentum transfer

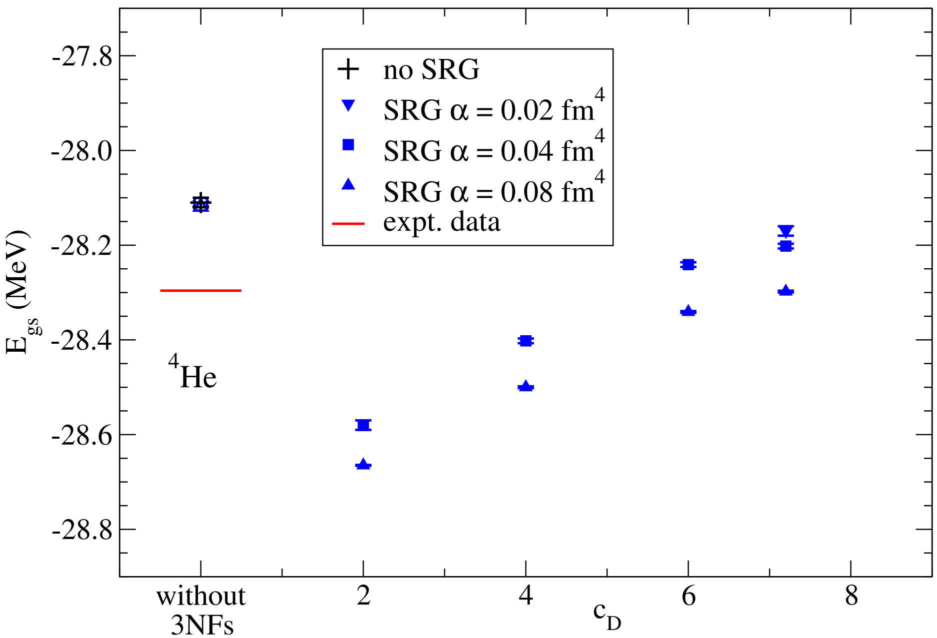
Additional collaborators at Iowa State University
Members of NUCLEI and Topical Collaboration Teams

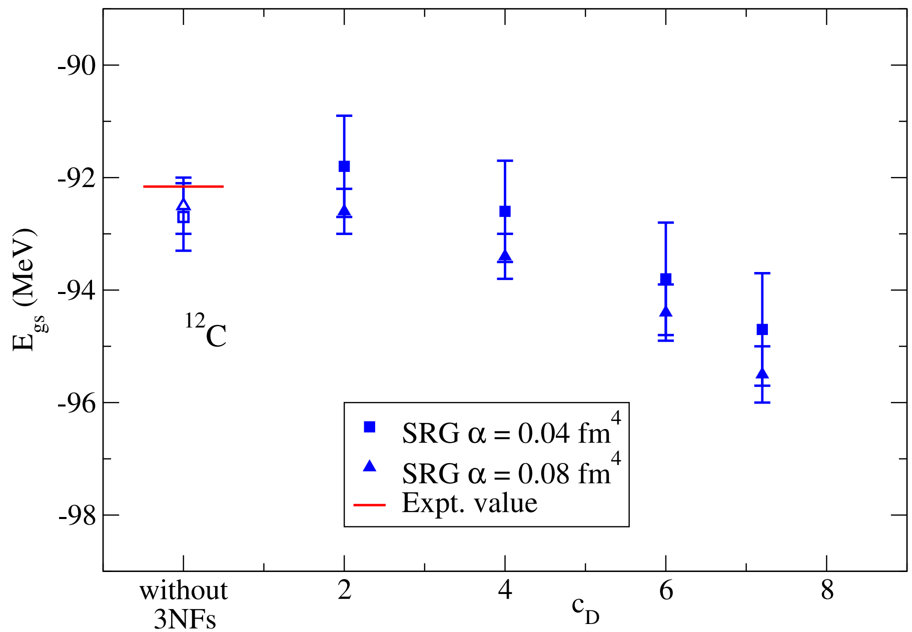
Robert Basili (grad student)
Weijie Du (grad student)
Matthew Lockner (grad student)
Pieter Maris
Alina Negoita (grad student)
Soham Pal (grad student)
Shiplu Sarker (grad student)

New faculty position at Iowa State in Nuclear Theory
Supported, in part, by the Fundamental Interactions
Topical Collaboration – part of a cluster hire:
www.physastro.iastate.edu/employment

Backup Slides

Dependence of gs energy on SRG evolution is small within the range we employ. We include sensitivity to SRG evolution parameter and extrapolation uncertainties in our estimate of numerical uncertainty of the gs energy.





E. Epelbaum, et al., arXiv: 1807.02848