No Core Shell Model (NCSM) With Electroweak Interactions

James P. Vary, Iowa State University

DOE Topical Collaboration Semi-Annual Meeting
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U.S. DEPARTMENT OF ENERGY | Office of Science

SciDAC Scientific Discovery through Advanced Computing

NUCLEI Nuclear Computational Low-Energy Initiative

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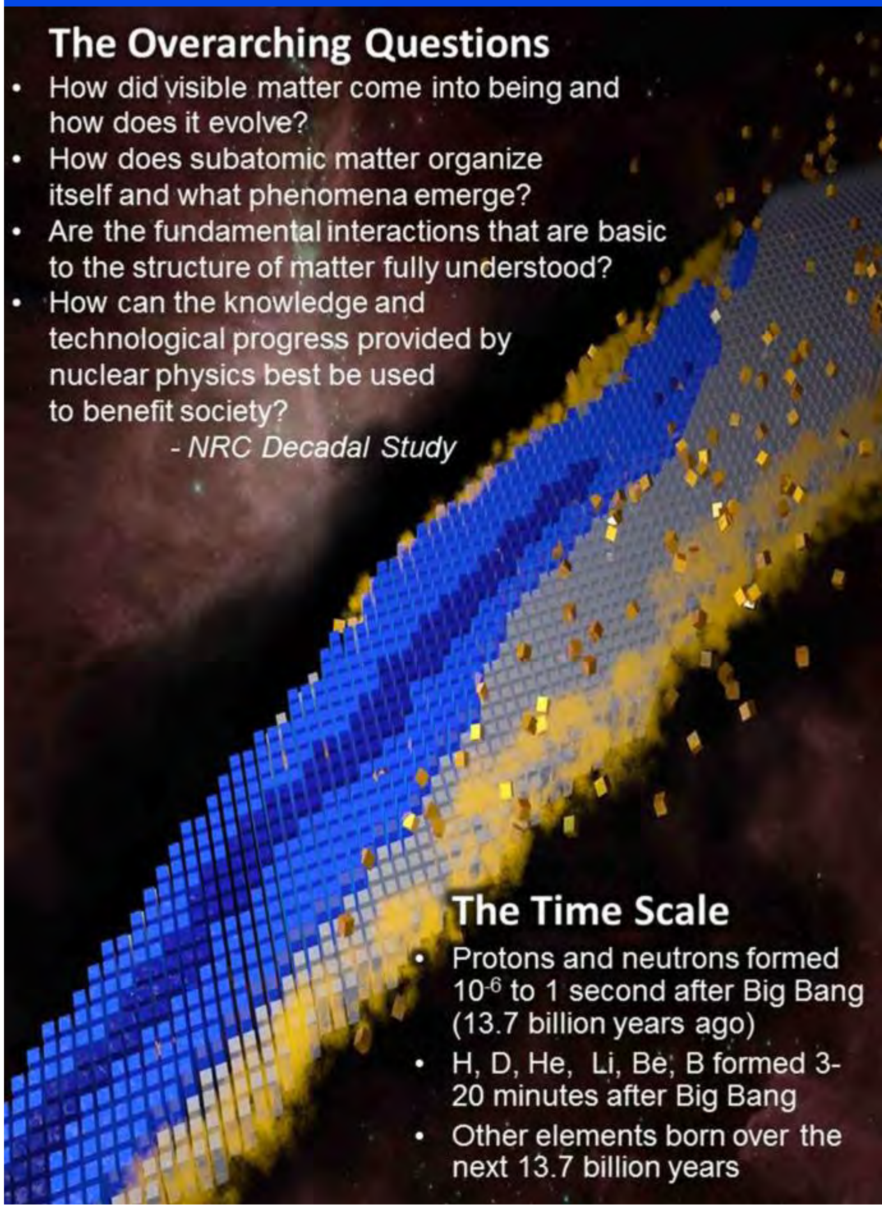
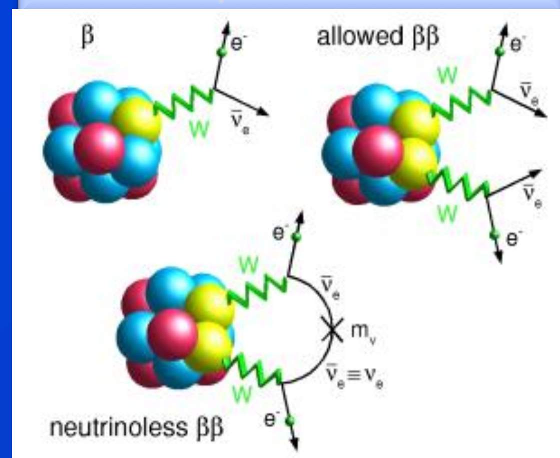


Topical Collaboration on Neutrinos and Fundamental Symmetries



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

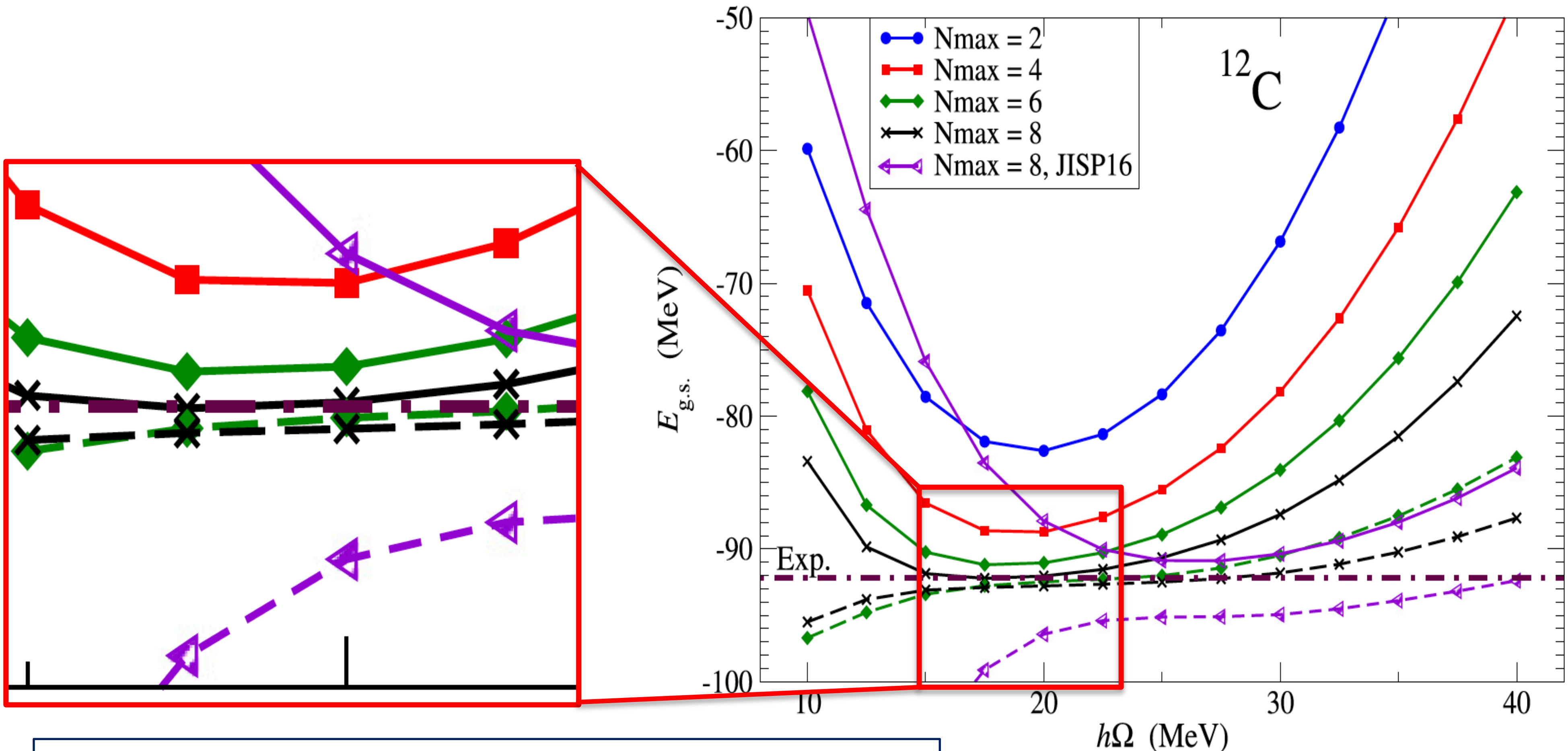
$$\hat{\mathbf{H}}\, \Psi(r_1, \ldots, r_A) = \lambda\, \Psi(r_1, \ldots, r_A)$$

- 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

Daejeon16 NN interaction

Based on SRG evolution of Entem-Machleidt “500” chiral N3LO to $\lambda = 1.5\ \mathrm{fm}^{-1}$ followed by Phase-Equivalent Transformations (PETs) to fit selected properties of light nuclei.

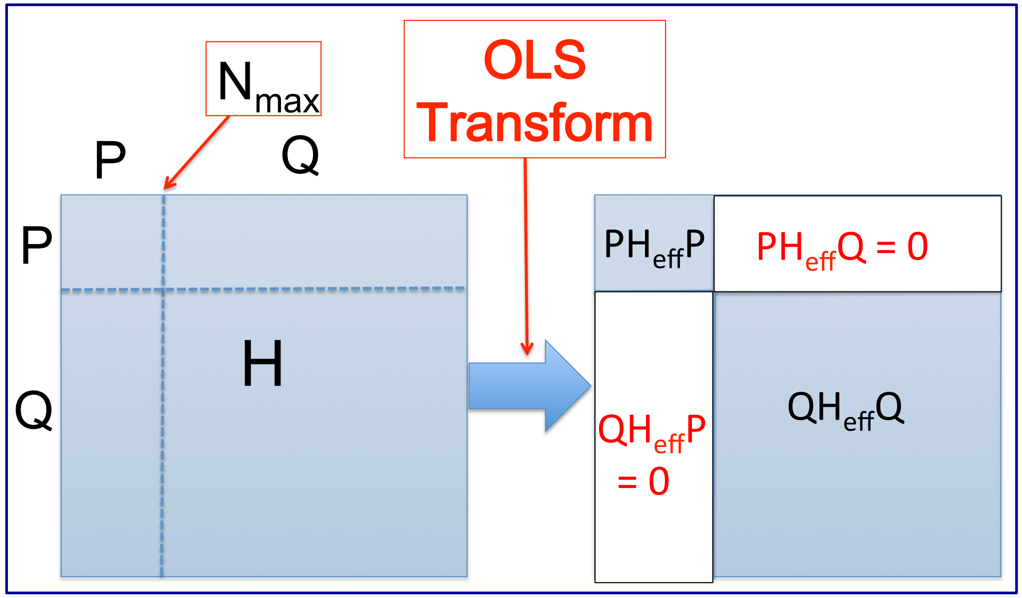
A.M. Shirokov, I.J. Shin, Y. Kim, M. Sosonkina, P. Maris and J.P. Vary, “N3LO NN interaction adjusted to light nuclei in ab exitu approach,” Phys. Letts. B 761, 87 (2016); arXiv: 1605.00413



GS radius also agrees with experiment to within 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:

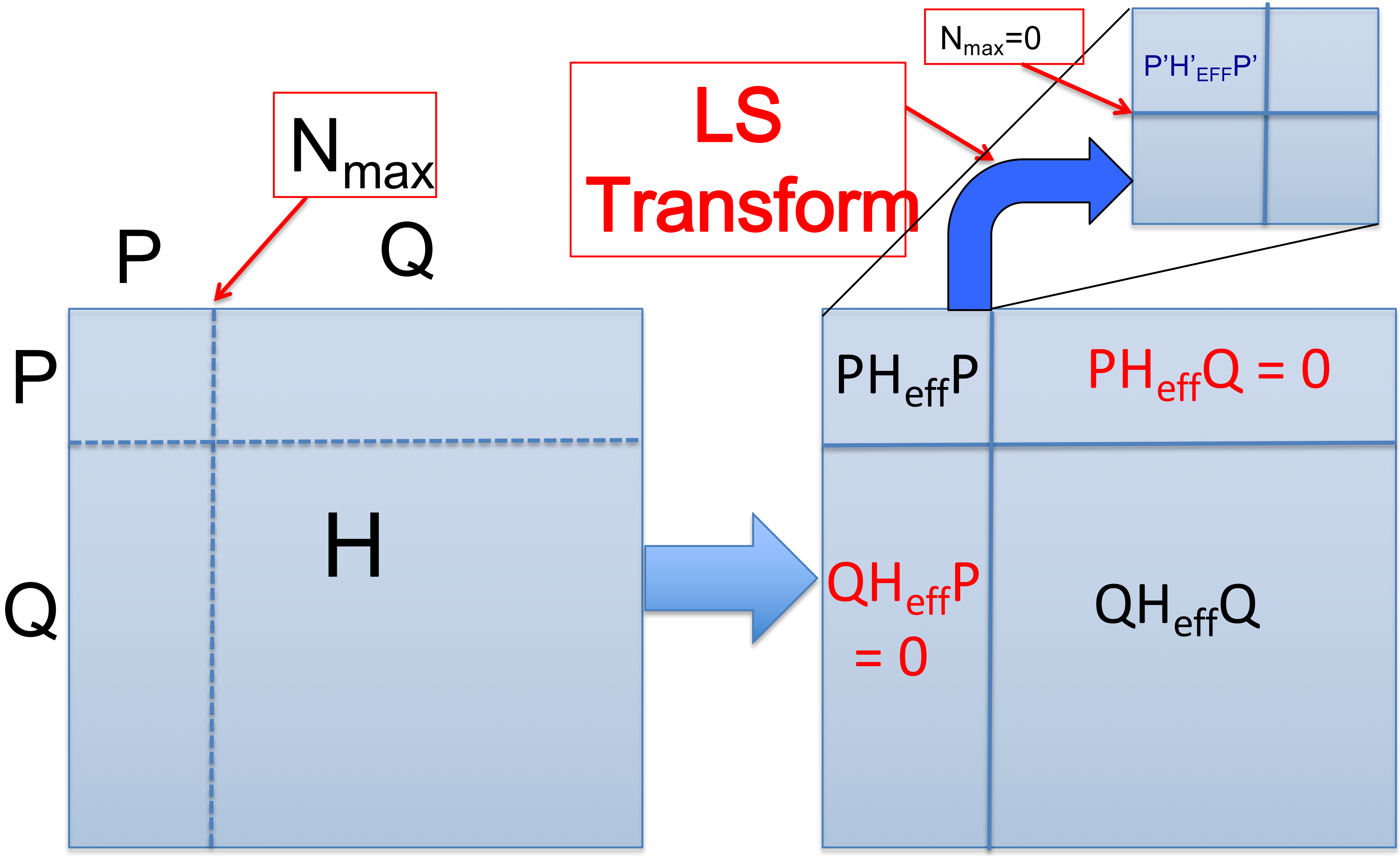
$$U_{OLS} = \tilde{U}^{P\dagger} U$$

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

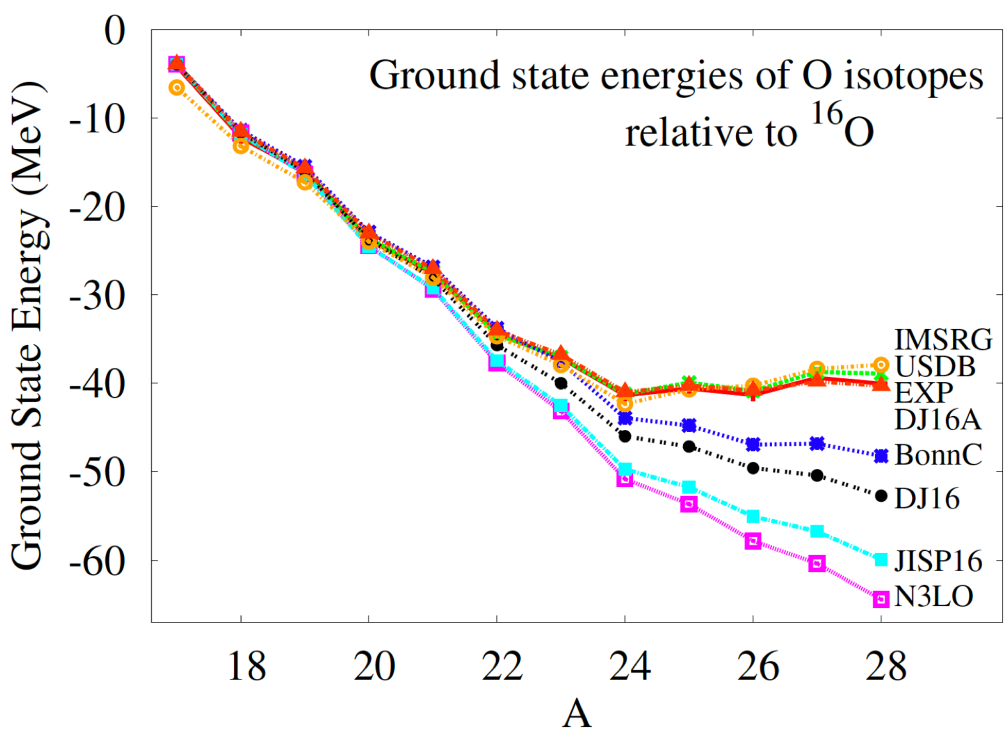
J.P. Vary, et al., PRC98, 065502 (2018); E, μ, Q, GT, $0\nu\beta\beta$, in 2-nucleon systems

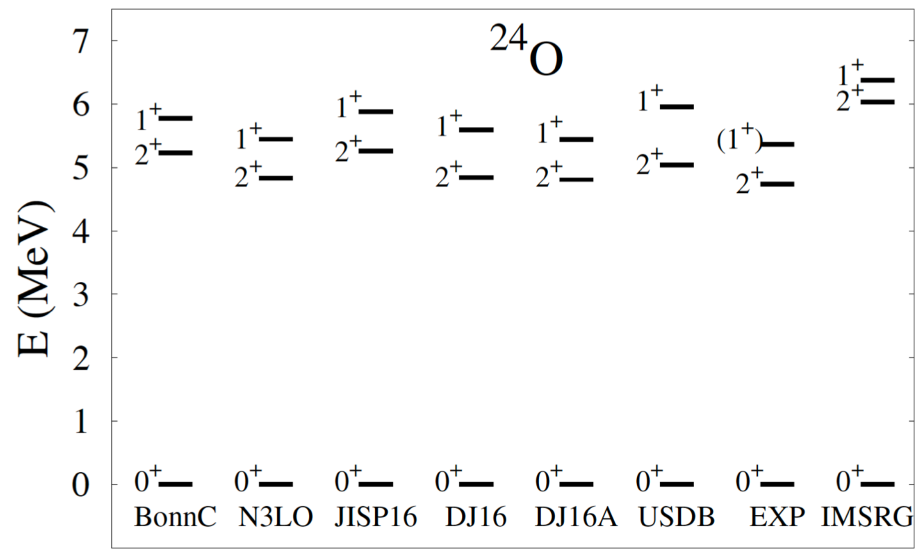


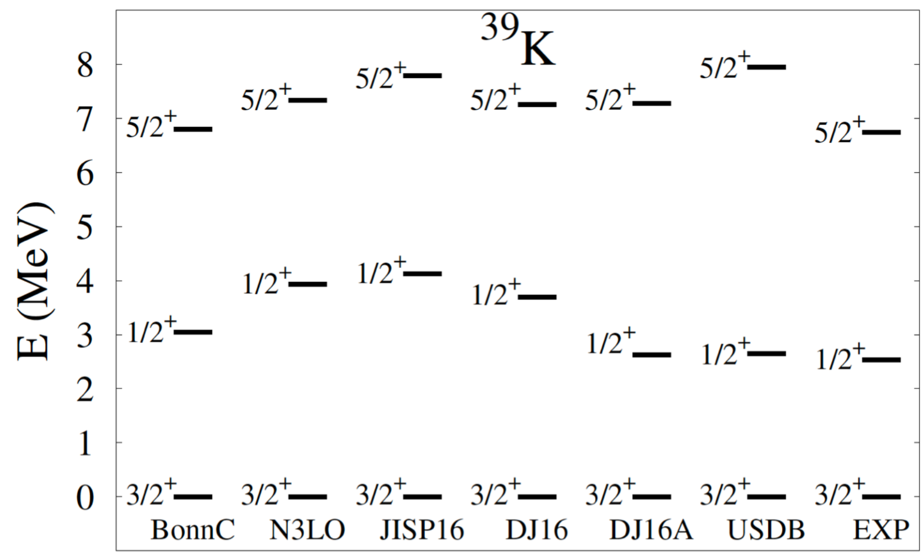
The "double Okubo-Lee-Suzuki transform" = valence H_{eff} and O_{eff}

A.F. Lisetskiy, B. R. Barrett, M. K. G. Kruse, P. Navratil, I. Stetcu, J. P. Vary, Phys. Rev. C. 78, 044302 (2008)
E. Dikmen, A.F. Lisetskiy, B.R. Barrett, P. Maris, A. M. Shirokov, J.P. Vary, Phys. Rev. C. 91, 064301 (2015)
N.A. Smirnova, B.R. Barrett, Y. Kim, I.J. Shin, A.M. Shirokov, E. Dikmen, P. Maris and J.P. Vary, arXiv:1909.00628

Derive V_{eff} TBMEs for valence systems using the NCSM
"Double Okubo-Lee-Suzuki" approach
All calcs (exc IMSRG) use spe's from USDB & TBME's with $A^{-1/3}$ scaling
DJ16A has modest monopole adjustment
N.A. Smirnova, et al., arXiv: 1909.00628







What's next: Nmax = 6;
Chiral NN + 3N; Veff for pf-shell

Benchmark neutrinoless double-beta decay matrix elements in a light nucleus

R.A. Basili,[1] J.M. Yao,[2,3] J. Engel,[2] H. Hergert,[3] M. Lockner,[1] P. Maris,[1] and J.P. Vary[1]

ISU – UNC – MSU collaboration

Benchmark: MR-IMSRG with NCSM

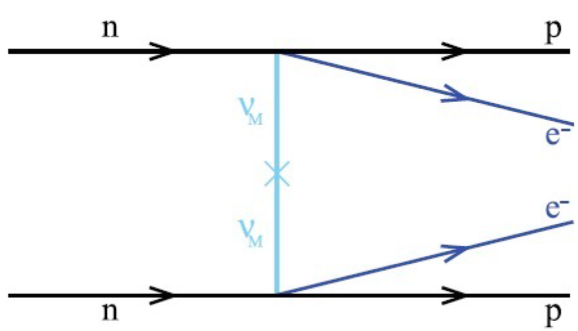
System: ^{6}He ⇨ ^{6}Be assuming isospin symmetry

Correlation: emax = N_{max} + 1

Interaction: EM500 (SRG at 2.0fm-1)

Basis: Harmonic Oscillator with $\hbar\Omega$ = 20 MeV

$$M_{0\nu} = M^{F}_{0\nu} + M^{GT}_{0\nu} + M^{T}_{0\nu}$$



$$O^{F}_{0\nu}(r) = \frac{4R}{\pi g_A^2}\int_0^\infty |\mathbf{q}|d|\mathbf{q}|\frac{j_0(|\mathbf{q}|r)h_F(|\mathbf{q}|)}{|\mathbf{q}|+\bar{E}-(E_i+E_f)/2}\tau_1^+\tau_2^+ ;$$

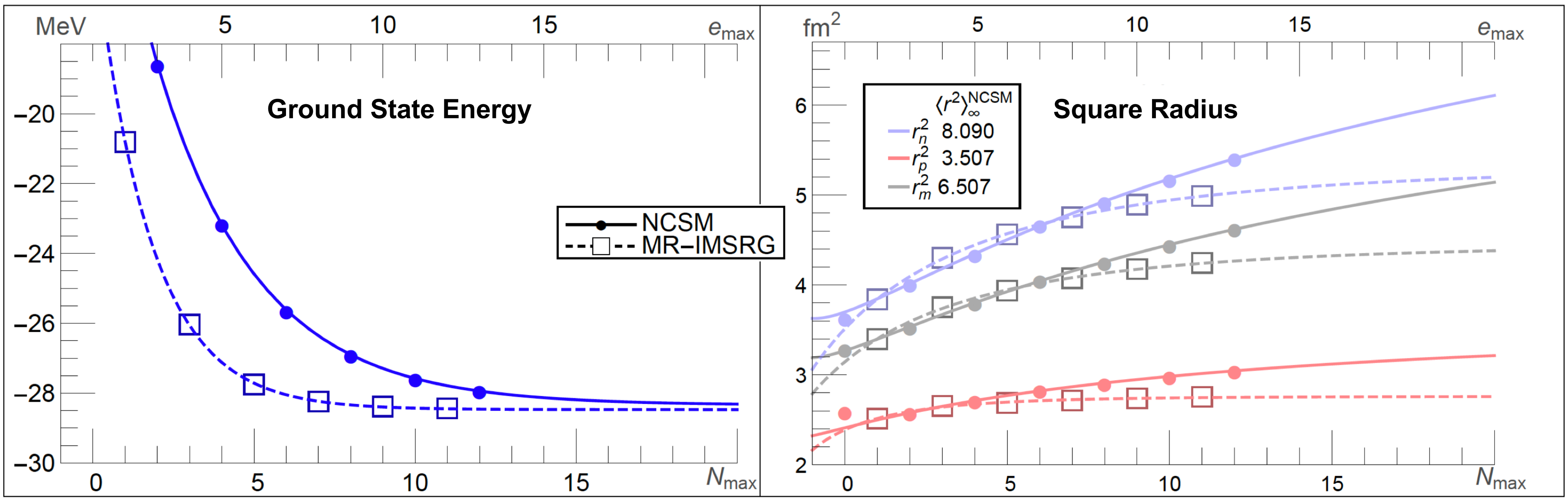
$$O^{GT}_{0\nu}(r) = \frac{4R}{\pi g_A^2}\int_0^\infty |\mathbf{q}|d|\mathbf{q}|\frac{j_0(|\mathbf{q}|r)h_{GT}(|\mathbf{q}|)\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2}{|\mathbf{q}|+\bar{E}-(E_i+E_f)/2}\tau_1^+\tau_2^+$$

$$O^{T}_{0\nu}(r) = \frac{4R}{\pi g_A^2}\int_0^\infty |\mathbf{q}|d|\mathbf{q}|\frac{j_2(|\mathbf{q}|r)h_T(|\mathbf{q}|)\boldsymbol{S}_{12}}{|\mathbf{q}|+\bar{E}-(E_i+E_f)/2}\tau_1^+\tau_2^+ ;$$

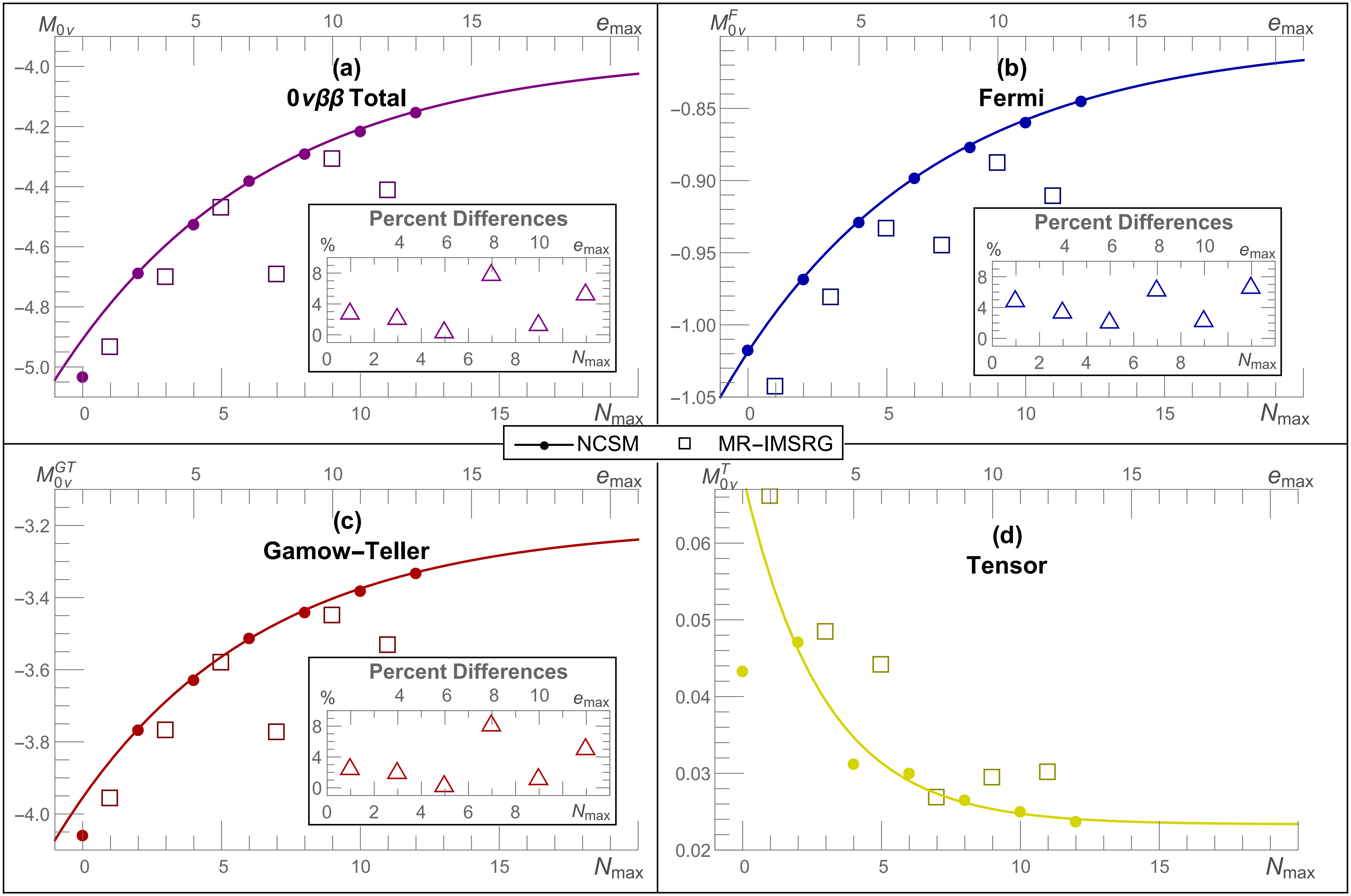
J. Engel and J. Menendez, Rept. Prog. Phys. 80, 046301 (2017)

ISU – UNC – MSU collaboration; R. Basili, et al., in preparation
Benchmark 0νββ-decay matrix elements for $^{6}He \rightarrow {}^{6}Be$

Ground State Energy and Square Radii



ISU – UNC – MSU collaboration; R. Basili, et al., in preparation
Benchmark 0νββ-decay matrix elements for ^{6}He -> ^{6}Be



ISU – UNC – MSU collaboration; R. Basili, et al., in preparation
Benchmark 0νββ-decay matrix elements for ^{6}He -> ^{6}Be

Our result for total |NME| at N_{max} = 12:

4.1485

Compare with the result from Peter Gysbers (this meeting) who uses the same NN interaction and $0\nu\beta\beta$ -decay operator, but also includes 3NF and isospin breaking effects:

3.9543

The difference is 5%

Consistent strong and electroweak interactions from Chiral EFT

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

Current Focus

Introduce momentum space regulators to facilitate gauge invariance

Extensive studies of the NN systems: moments, form factors and transitions

Light nuclei: magnetic moments, GT quenching, M1 transitions

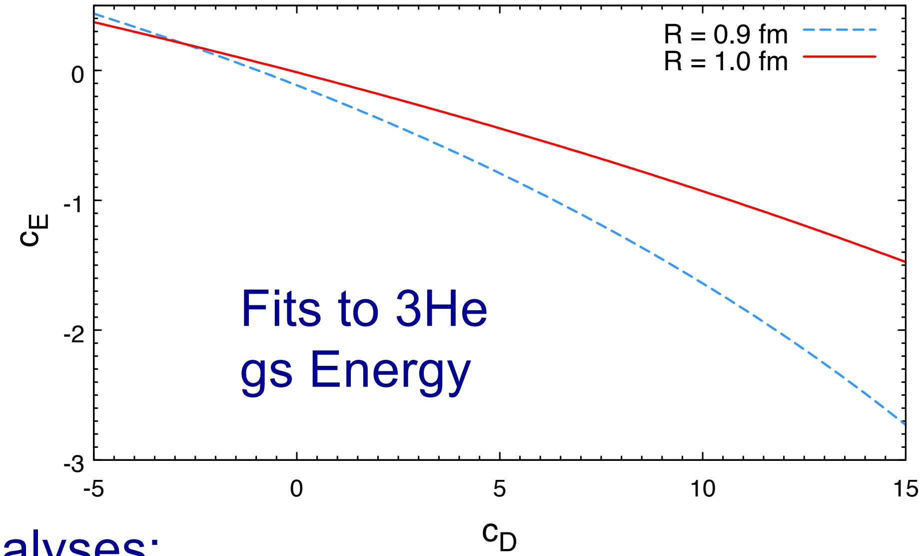
Medium weight nuclei with coupled cluster

Longer term – sd-shell and pf-shell (V_{eff})

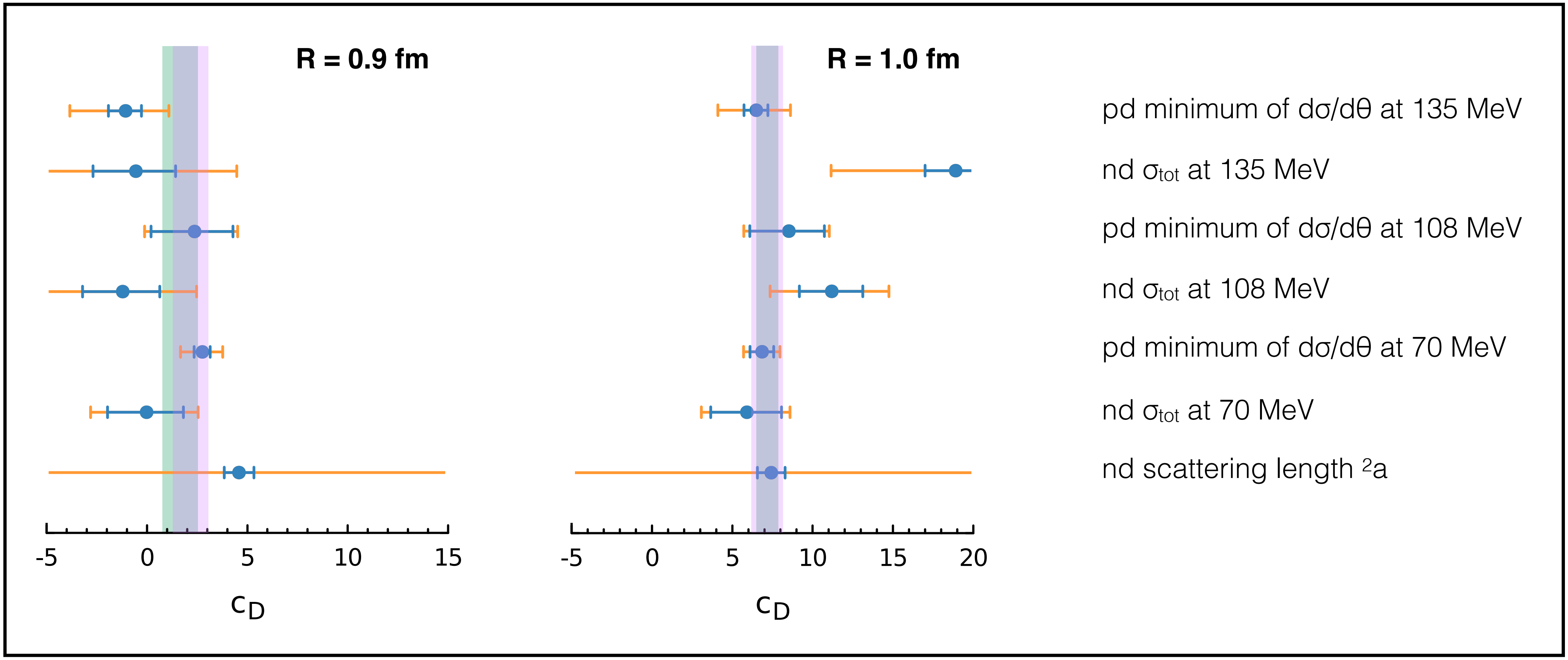
Develop operators consistent through N3LO

Coordinate space regulator:

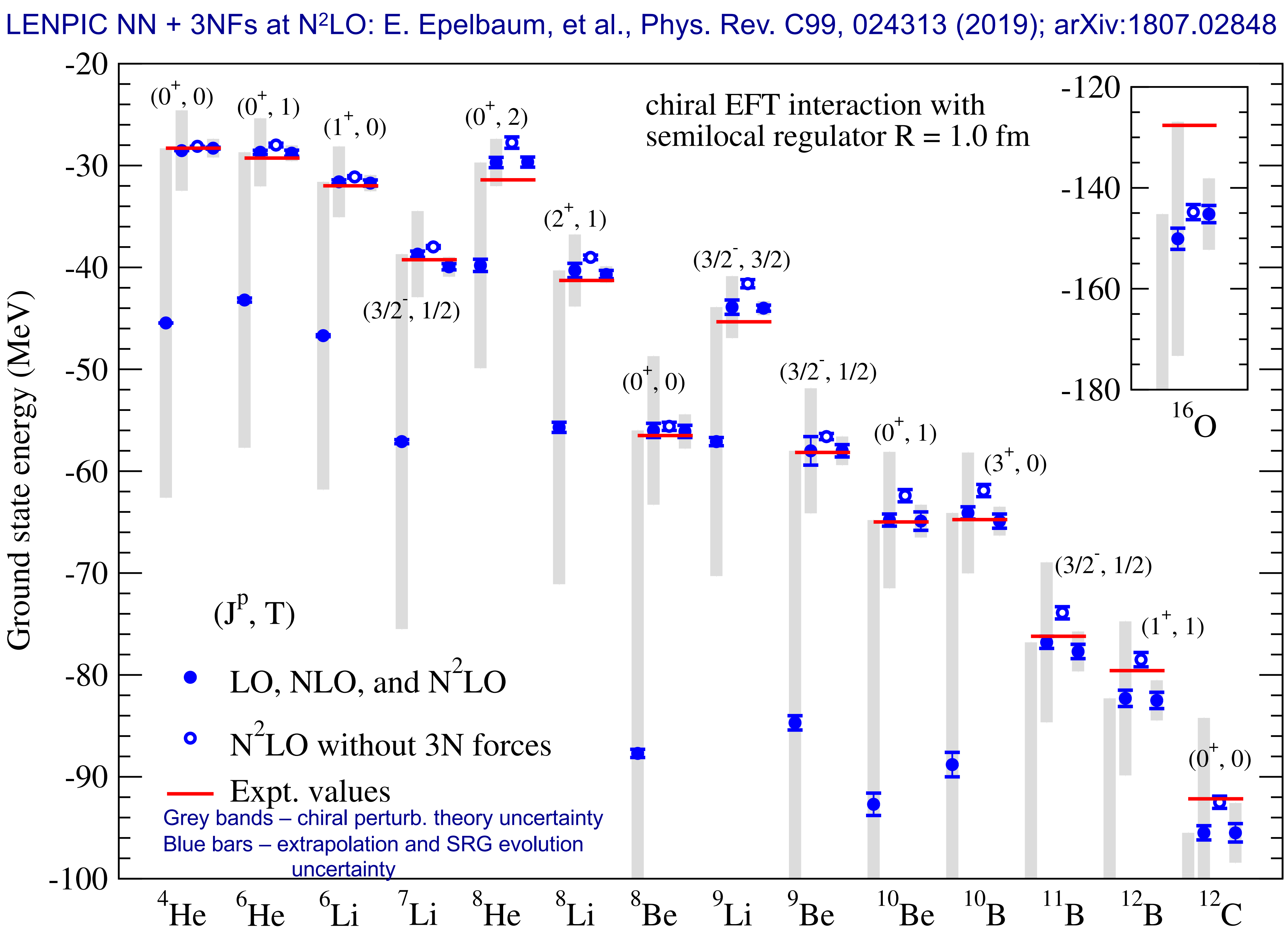
$$f\left(\frac{r}{R}\right)=\left(1-\exp\left(-\frac{r^2}{R^2}\right)\right)^6$$



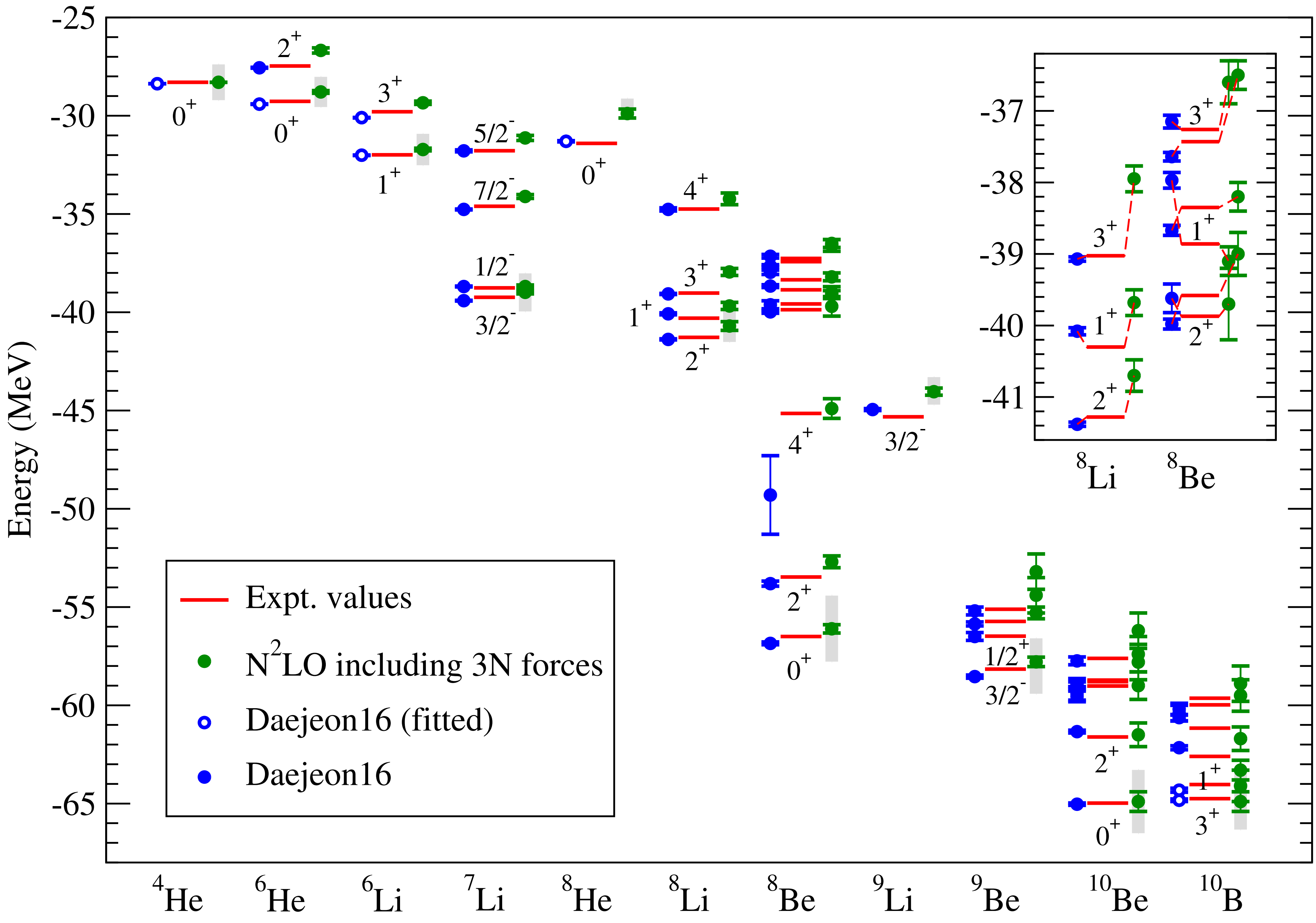
Optimal cD (cE) selected via ND scattering analyses:



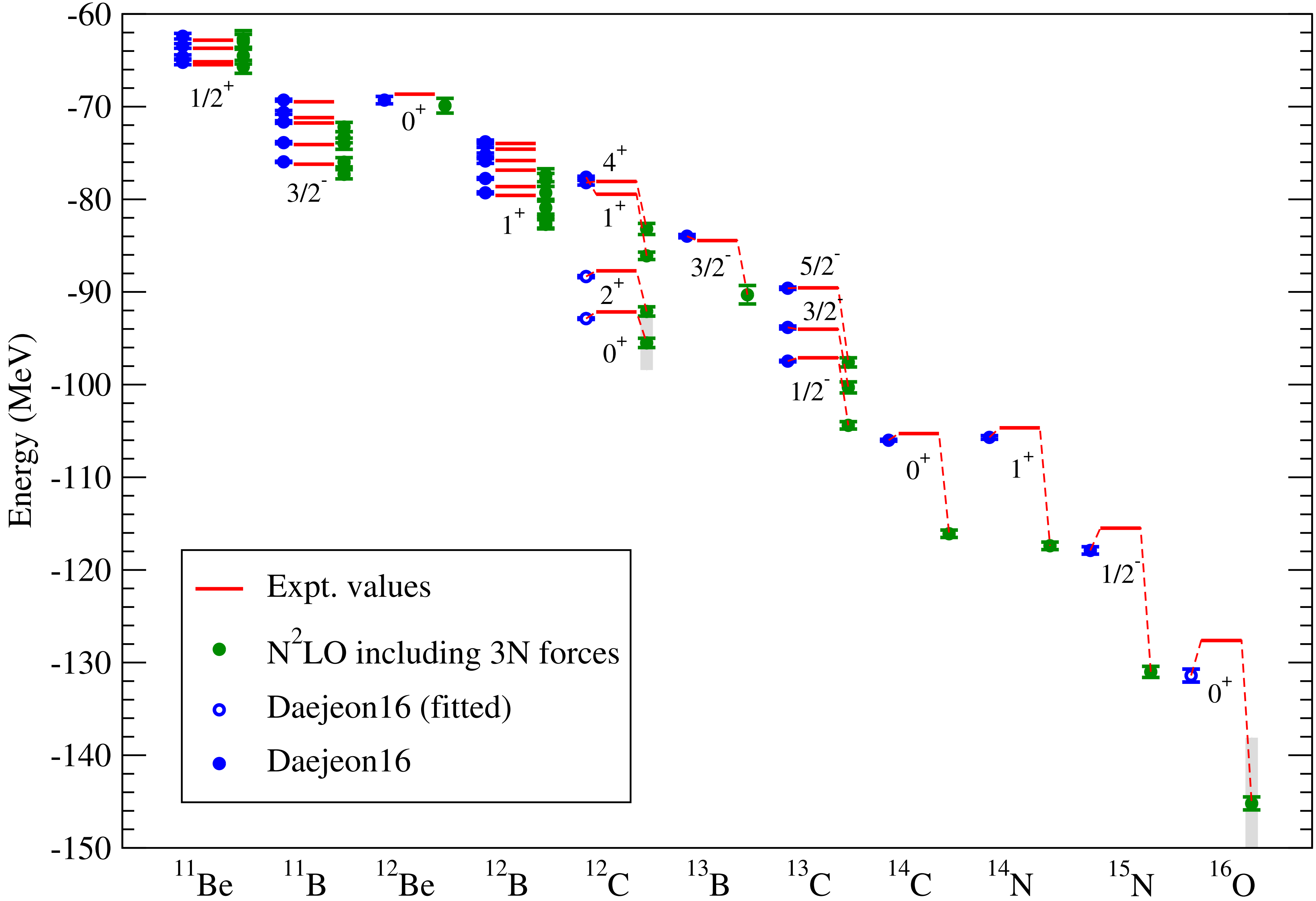
LENPIC: E. Epelbaum, et al., Phys. Rev. C99, 024313 (2019); arXiv: 1807.02848



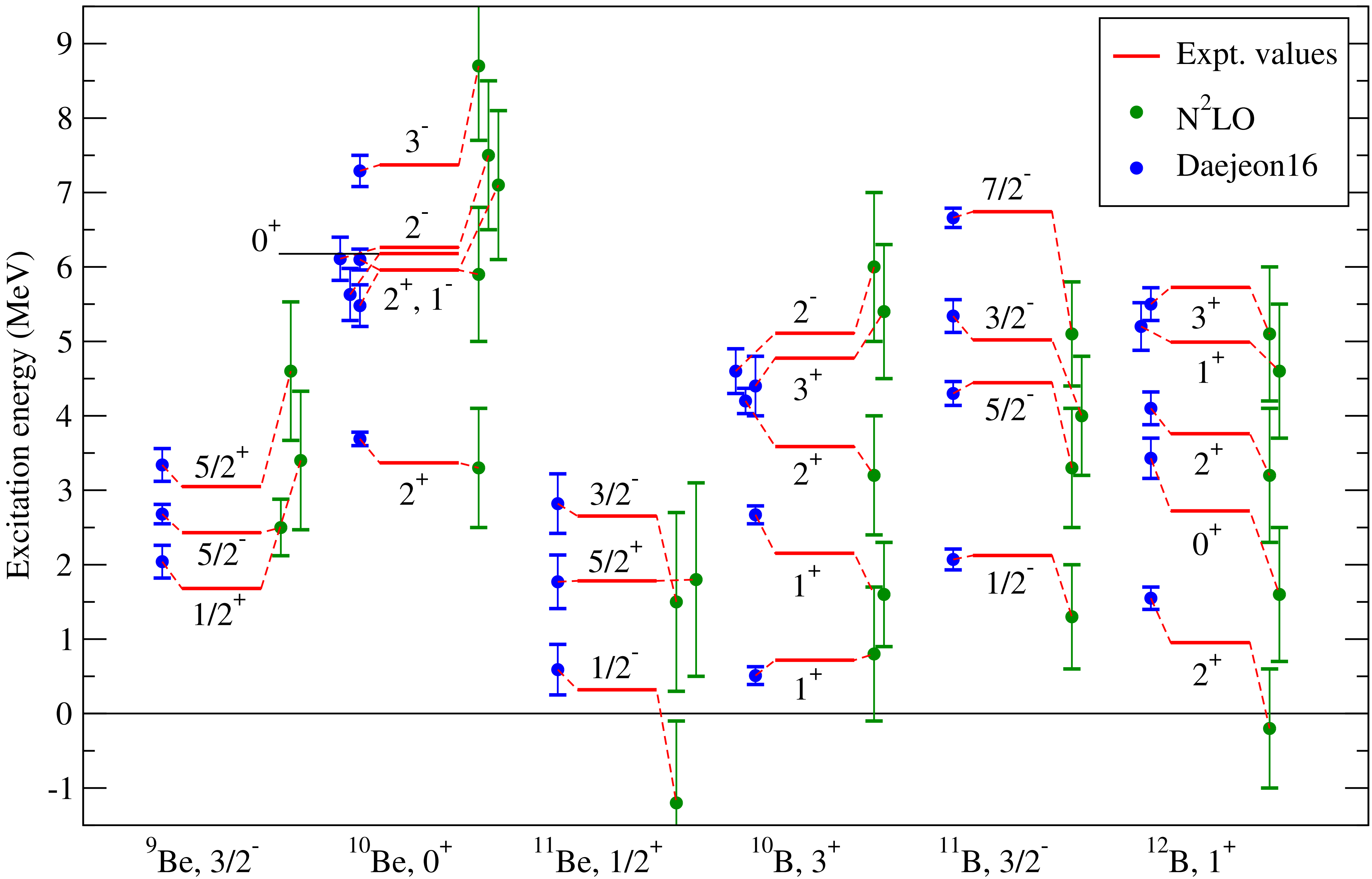
LENPIC NN + 3NFs at N2LO: E. Epelbaum, et al., Phys. Rev. C99, 024313 (2019); arXiv:1807.02848
chiral EFT interaction with
semilocal regulator R = 1.0 fm
Ground state energy (MeV)
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
(0+, 0)
(0+, 1)
(1+, 0)
(3/2-, 1/2)
(0+, 2)
(2+, 1)
(0+, 0)
(3/2-, 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
uncertainty
4He
6He
6Li
7Li
8He
8Li
8Be
9Li
9Be
10Be
10B
11B
12B
12C
16O



P. Maris, I.J. Shin and J.P. Vary, NTSE2018 Proceedings, arXiv: 1908.00155



P. Maris, I.J. Shin and J.P. Vary, NTSE2018 Proceedings, arXiv: 1908.00155



P. Maris, I.J. Shin and J.P. Vary, NTSE2018 Proceedings, arXiv: 1908.00155

Chiral EFT order

- Perturbative expansion of potentials and currents in $Q \in \{\frac{m_\pi}{\lambda_\chi}, \frac{p}{\lambda_\chi}\}$.
- Order of the operator is determined by the "power" of Q (Power Counting).
- LENPIC power counting:
    - Q^{-3}: Leading Order (LO)
    - Q^{-1}: Next to leading order (NLO)
    - Q^{0} : N2LO
    - Q^{+1}: N3LO

Coupling to External Probes in Chiral EFT

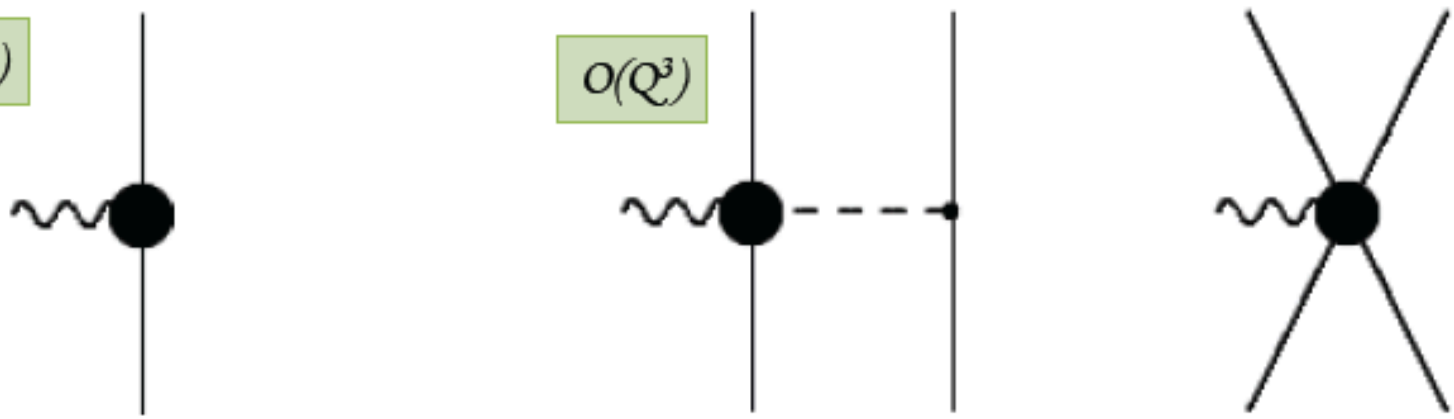
LENPIC collaboration (in process) – adopts momentum space regulators

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

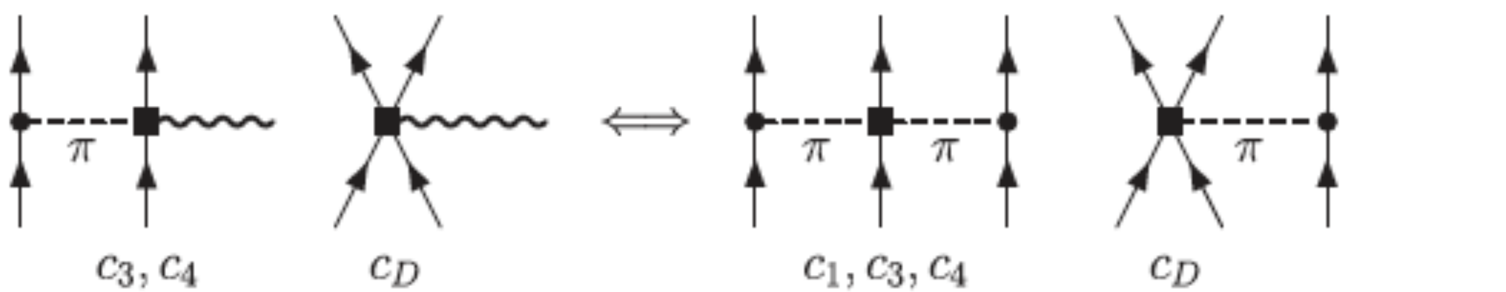
Single nucleon current | 1 pion exchange | Contact term

$O(Q^0)$, $O(Q^2)$

$O(Q^3)$



Two-Body Currents (N^2LO)



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

Regularization

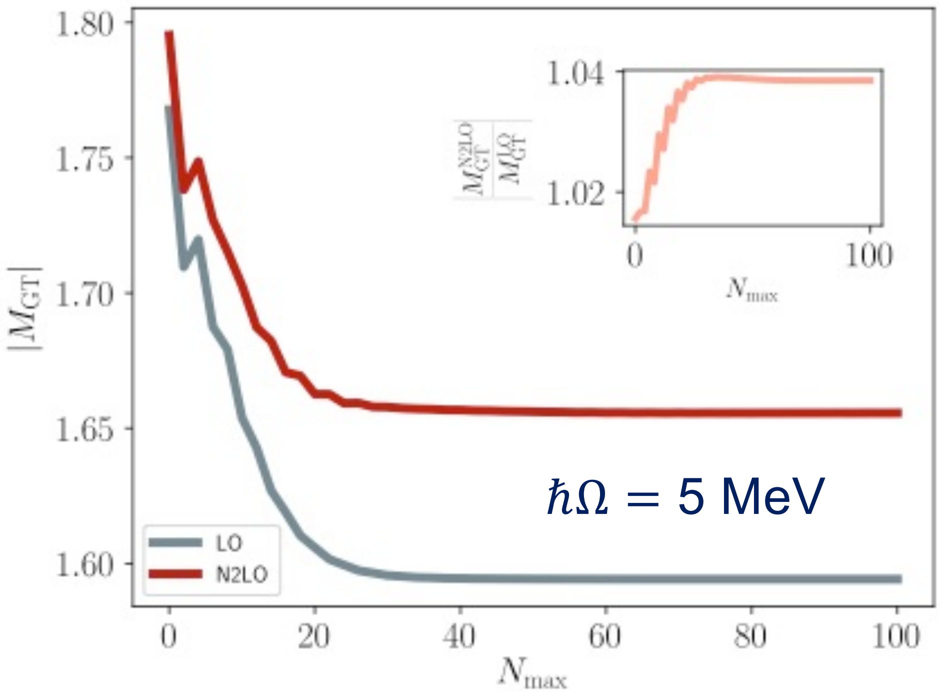
- Pion exchange terms are regularized by LENPIC semi-local coordinate space regulator: $(1 - e^{r^2/R^2})^6$.
- Contact terms are regularized by non-local Gaussian regulator in momentum space with cut-off $\lambda = 2/R$.

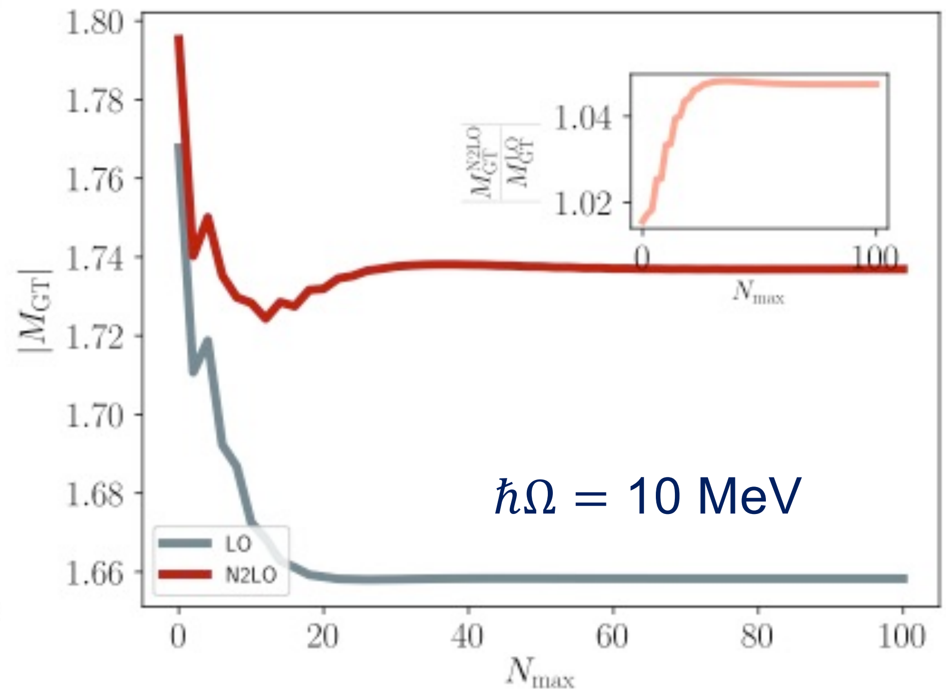
Axial currents and GT operator

- $\mathcal{M}_{GT} = \int \mathrm{d}^3x \, \tilde{\vec{A}}^a(\vec{x}) = \vec{A}^a(\vec{k})\Big|_{k=0}$, $\vec{A}(\vec{k})$ is the weak axial current.
- Relevant (at $k=0$) weak axial currents from *Krebs, Epelbaum, Meissner (2016)*
  - LO: $-\frac{g_A}{2}\tau_1^a\vec{\sigma}_1$ (same as IA)
  - N2LO:
    - pion-exchange term (depends on the LECs c_3 and c_4)
    - contact term (depends on the LEC D)

N2LO currents

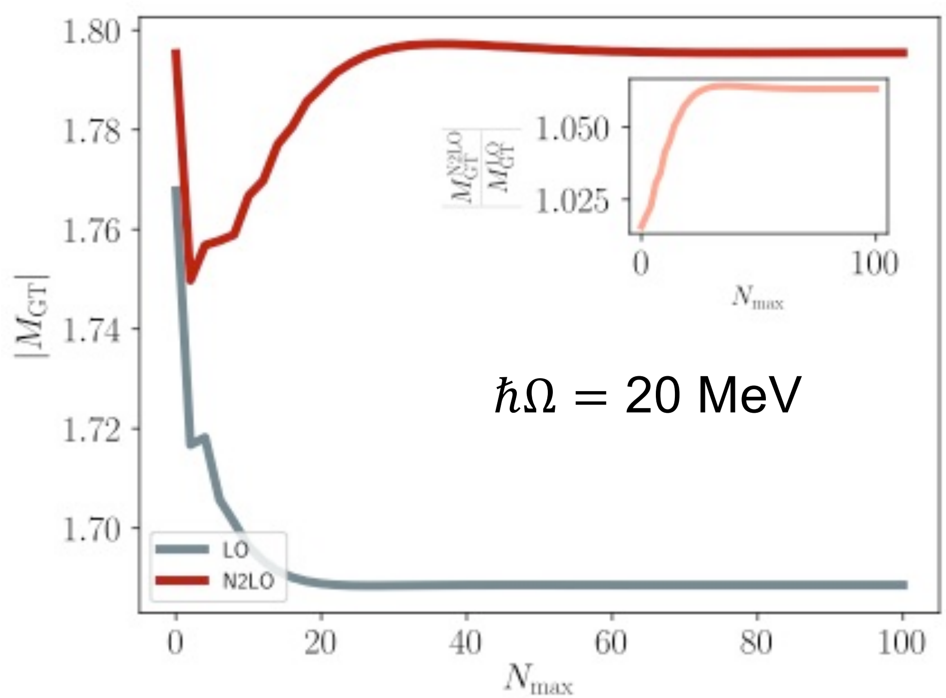
- c_3 current: $\dfrac{g_A}{2F_\pi^2} 2c_3 \tau_1^a \dfrac{\vec{\sigma}_1 \cdot \vec{q}_1}{q_1^2 + m_\pi^2} \vec{q}_1 + (1 \leftrightarrow 2)$
- c_4 current: $\dfrac{g_A}{2F_\pi^2} c_4 [\vec{\tau}_1 \times \vec{\tau}_2]^a \dfrac{(\vec{\sigma}_1 \cdot \vec{q}_1)(\vec{q}_1 \times \vec{\sigma}_2)}{q_1^2 + m_\pi^2} + (1 \leftrightarrow 2)$
- D current: $-\dfrac{1}{4} D \tau_1^a \vec{\sigma}_1 + (1 \leftrightarrow 2)$





$^1S_0$ to deuteron gs transition
in harmonic oscillator trap
LENPIC NN **and** GT operators
LENPIC regulator: R=1.0 fm

Stronger trap => larger enhancement from N2LO relative to LO.



Soham Pal, et al, in preparation

Now consider the M1 operator

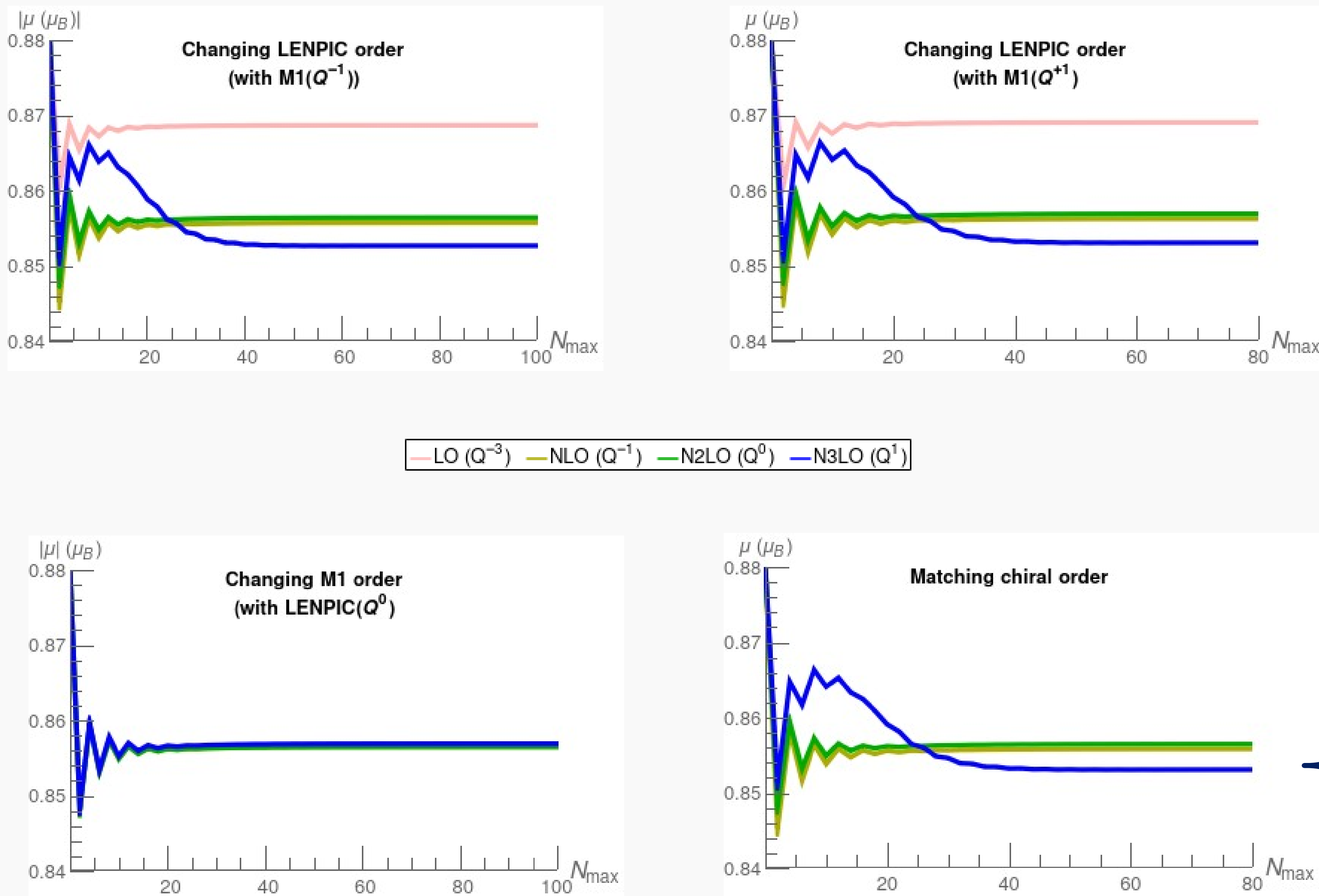
Chiral Power Counting Scheme

- Chiral expansion parameter, $Q \in \{m_\pi/\lambda_b, p/\lambda_b\}$.
- ρ_{1B} operator starts contributing at Q^{-3}. This order is considered as LO for both charge and current operators.
- At LO (Q^{-3}) there is no contribution of $\boldsymbol{J}$ operator
- No correction to the ρ or $\boldsymbol{J}$ appear at Q^{-2}
- First contribution to $\boldsymbol{J_{1B}}$ and first correction to $\boldsymbol{J_{2B}}$ (isovector) both appear at Q^{-1}. This order is considered as NLO.
- No correction to $\boldsymbol{J_{2B}}$ at N2LO (Q^0)
- First isoscalar correction to $\boldsymbol{J_{2B}}$ appears at N3LO (Q^{+1}). We are ~~only~~ interested in N3LO currents for the deuteron.

Low Energy Constants in Chiral EM Current

- One body current appearing at NLO contains two LEC's: iso-scalar and iso-vector anomalous magnetic moment of nucleon. The values of μ_s and μ_v are taken to be 0.88 and 4.706 respectively in unit of nuclear magneton.
- Two body iso-vector current appearing at NLO contains one LEC: $\bar{d}_{18}$ originating from N2LO Chiral Pion-Nucleon Lagrangian. $\bar{d}_{18} =$ -10.14 GeV^{-2}.
- Two body iso-scalar current at N3LO contains one LEC: $\bar{d}_9$ originating from N2LO Chiral Pion-Nucleon Lagrangian.
- Contact term at N3LO contains one LEC: L_2 originating from NLO Chiral Nucleon-Nucleon Lagrangian.
- $L_2 =$ -0.149 fm^4 and $\bar{d}_9 =$ - 0.06 GeV^{-2} are used in this work.

Deuteron gs magnetic moment with LENPIC NN and M1 operators
Regulator R = 1.0 fm



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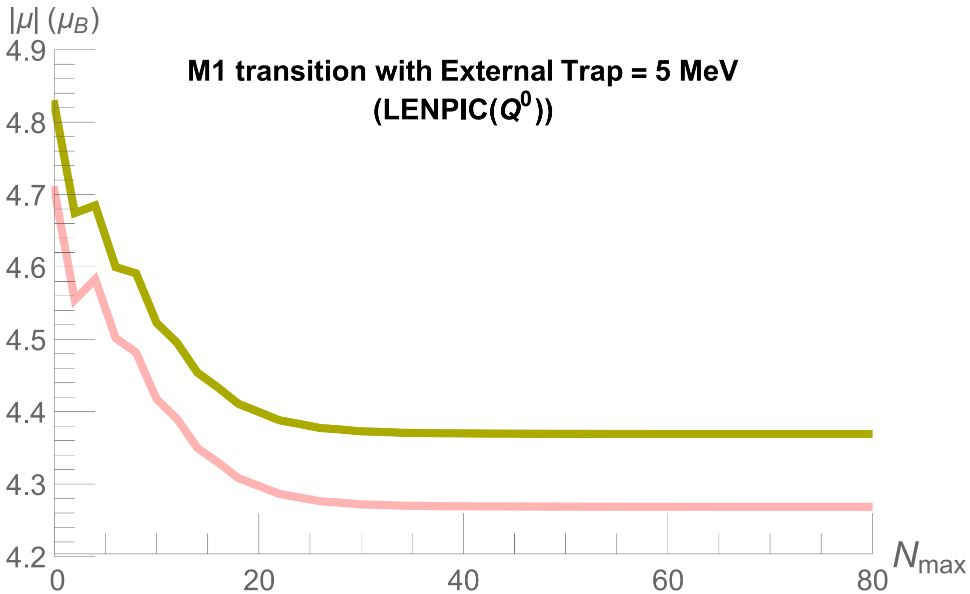
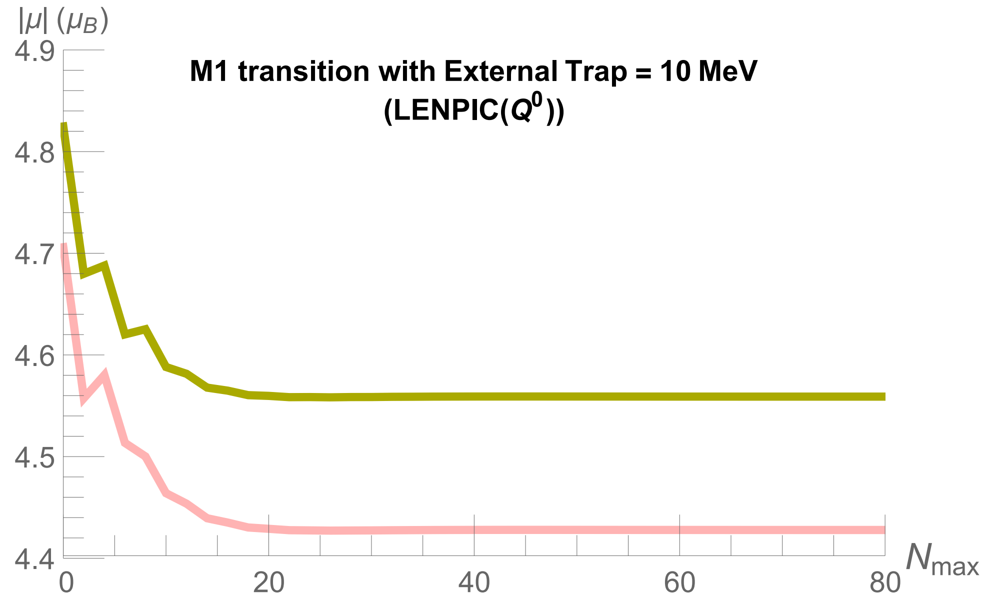
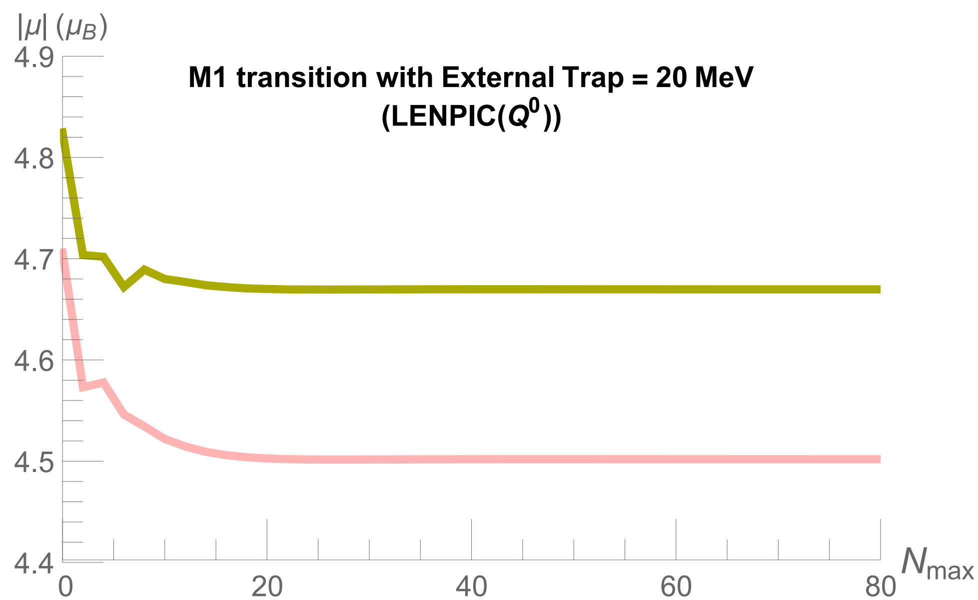




$^1S_0$ to deuteron gs transition
in harmonic oscillator trap
LENPIC NN **and** M1 operators
LENPIC regulator: R=1.0 fm
HO basis = 20 MeV



Stronger trap => larger enhancement from N2LO relative to LO.

Shiplu Sarker, et al., in preparation

Progress:

Completed LENPIC NN+NNN at N2LO paper: **PRC99, 024313 (2019);**
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 – results reported today**)

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

Develop extrapolations with Artificial Neural Networks:
A. Negoita, et al., PRC99, 054308 (2019); arXiv:1810.04009

Outlook:

Expand treatment to full range of EW operators within Chiral EFT
at NLO, N2LO & N3LO (**studies underway – GT & M1 progress reported today**)

Extend effective EW operator approach to medium weight nuclei with "Double OLS" approach (**initial sd-shell V_{eff} investigations completed: N. Smirnova, et al; arXiv:1909.00628**)

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
Soham Pal
Shiplu Sarker

Note: Srimoyee Sen has joined our faculty this week