NCSM and neutrinoless double beta decay

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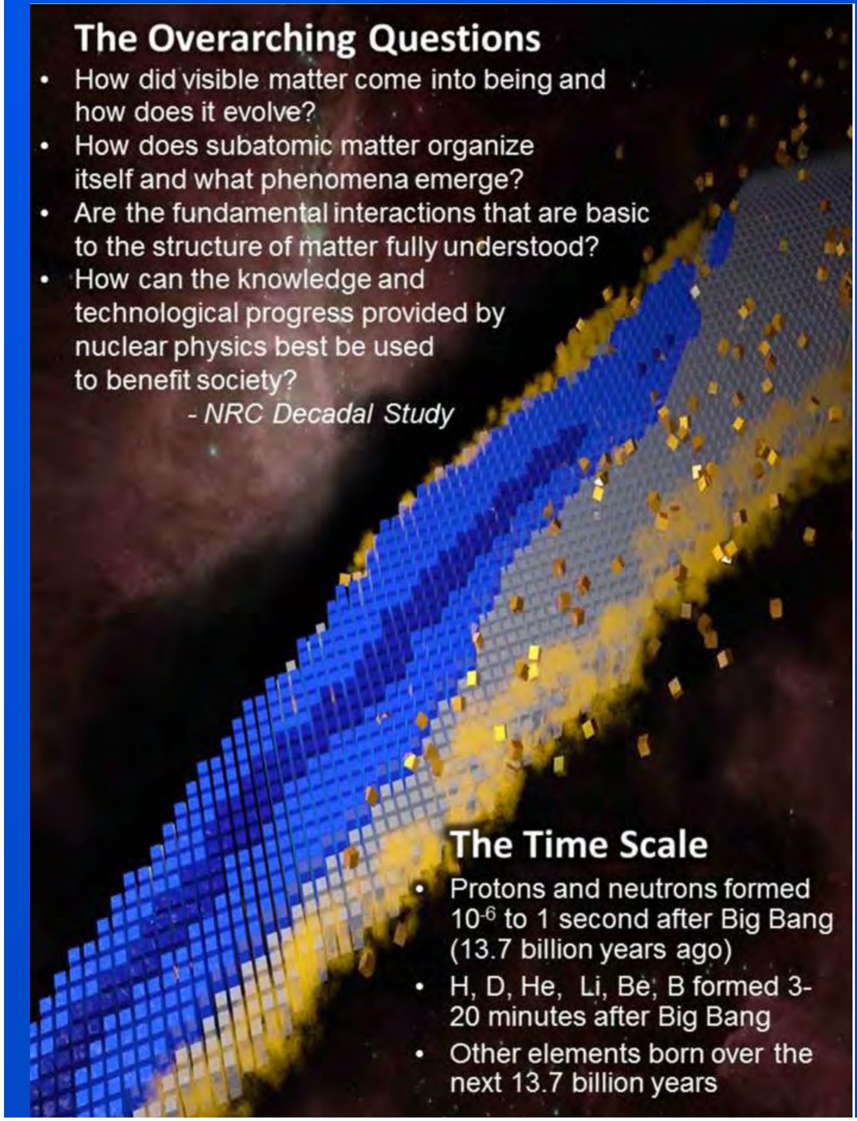


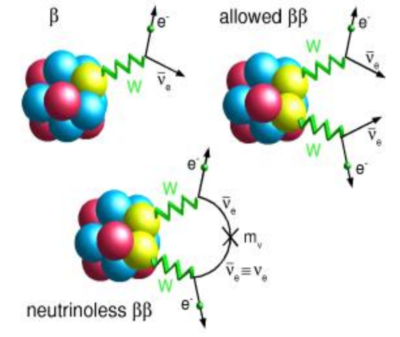
The Overarching Questions

- How did visible matter come into being and how does it evolve?
- How does subatomic matter organize itself and what phenomena emerge?
- Are the fundamental interactions that are basic to the structure of matter fully understood?
- How can the knowledge and technological progress provided by nuclear physics best be used to benefit society?

- NRC Decadal Study

The Time Scale

- Protons and neutrons formed 10^{-6} to 1 second after Big Bang (13.7 billion years ago)
- H, D, He, Li, Be, B formed 3-20 minutes after Big Bang
- Other elements born over the next 13.7 billion years



LENPIC

NUCLEI
Nuclear Computational Low-Energy Initiative

U.S. DEPARTMENT OF ENERGY
INCITE
LEADERSHIP COMPUTING

Sources of observables’ uncertainties with Chiral EFT

Working with Chiral EFT operators – uncertainties due to:

- Fitting of LECs, NN data error propogation (other LENPIC teams)
- Choice of regulator (results here for R = 1.0 fm)
- Truncation at a fixed Chiral order
- Numerical uncertainty at fixed [Nmax, hw] (~1 keV in total gs energy)
- Extrapolation uncertainty (new results for gs energies)
- Other approximations, if adopted, such as normal ordering approximation, importance truncation, . . .

results here

Working with NCSM using OLS – uncertainties due to:

- Truncation vs OLS applied to the operators
- Rank of OLS-derived operator truncation (2-body, 3-body, . . .)

results here

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 CI: all A nucleons are treated the same
- 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), Woods-Saxon, Coulomb-Sturmian, Complex Scaled HO, Berggren,. . .
- M-scheme: Many-Body basis states eigenstates of $\hat{\mathbf{J}}_\mathbf{z}$

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

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

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

N_{max} runs from zero
to computational limit.
(N_{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)

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

Low
Energy
Nuclear
Physics
International
Collaboration

LENPIC

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JÜLICH	A. Nogga
THE OHIO STATE UNIVERSITY	R. Furnstahl
TECHNISCHE UNIVERSITÄT DARMSTADT	S. Binder, A. Calci, K. Hebeler, J. Langhammer, R. Roth
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

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)

E. Epelbaum, H. Krebs, U.G. Meissner, PRL 115, 122301 (2015);
S. Binder, et al., LENPIC, PRC 93, 044002 (2016); and in preparation

Established method for GS energy error estimate adapted to case where results up to N2LO are used:

$$Q \equiv \frac{m_\pi}{\Lambda}$$

$$\delta E^{(0)} = \max(\mathrm{Q}^2\left|E^{(0)}\right|, \left|E^{(2)} - E^{(0)}\right|, \left|E^{(3)} - E^{(0)}\right|, \left|E^{(3)} - E^{(2)}\right|)$$

$$\delta E^{(2)} = \max(\mathrm{Q}^3\left|E^{(0)}\right|, Q\left|E^{(2)} - E^{(0)}\right|, \left|E^{(3)} - E^{(2)}\right|, Q\delta E^{(0)})$$

$$\delta E^{(3)} = \max(\mathrm{Q}^4\left|E^{(0)}\right|, Q^2\left|E^{(2)} - E^{(0)}\right|, Q\left|E^{(3)} - E^{(2)}\right|, Q\delta E^{(2)})$$

Error estimate for finite nuclei results using average relative momentum based on Hartree-Fock results (~NCSM results) at each chiral order:

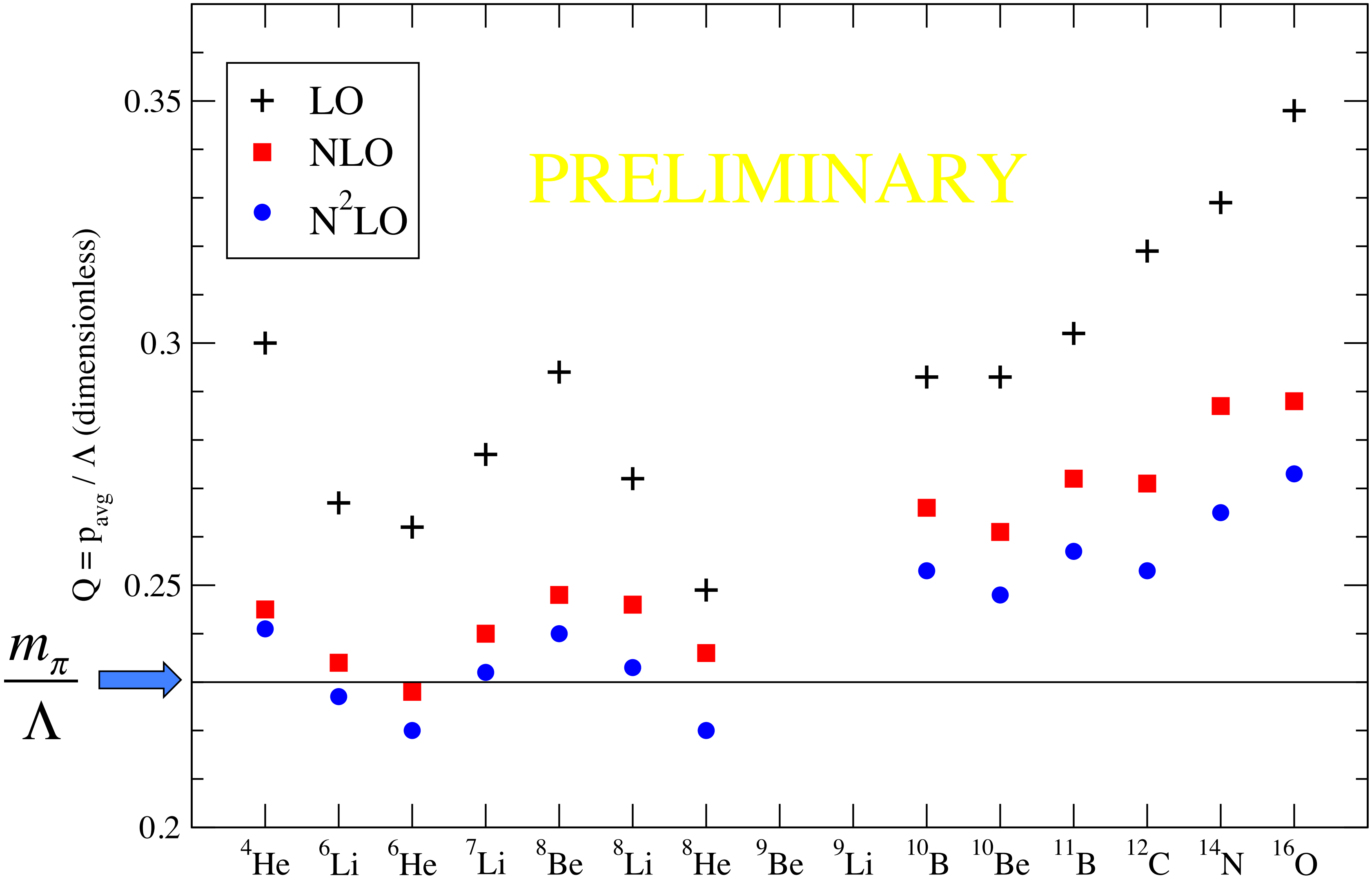
$$\vec{p}^{\,ij} \equiv \frac{\vec{p}_i - \vec{p}_j}{2}$$

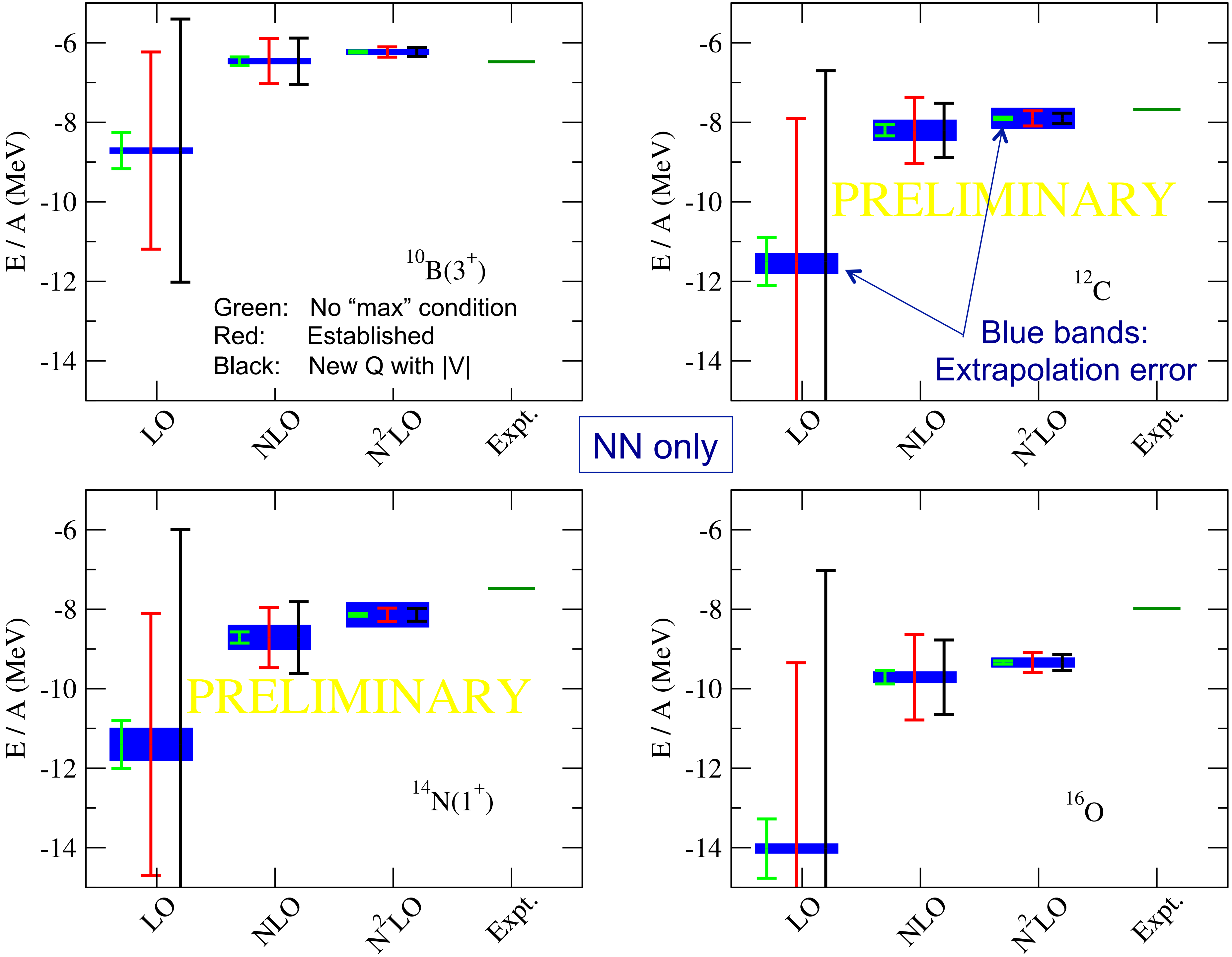
$$T_{\mathrm{rel}} \equiv \frac{2}{A}\sum_{i<j}\frac{\left(\vec{p}^{\,ij}\right)^2}{m} \equiv \frac{2}{A}\,\frac{A(A-1)}{2}\,\frac{\left(p_{\mathrm{avg}}\right)^2}{m}$$

$$p_{\mathrm{avg}} = \sqrt{\frac{m\left(T_{\mathrm{rel}}\right)}{A-1}}; \qquad Q \equiv Max\left(\frac{m_\pi}{\Lambda}, \frac{p_{\mathrm{avg}}}{\Lambda}\right)$$

$$\delta E^{(i)} = Q^{\max(2,\, i+1)}\left|V^{(i)}\right|; \ \text{ where } Q \text{ is evaluated at } i$$

Dimensionless Q based on p_{avg} from NCSM



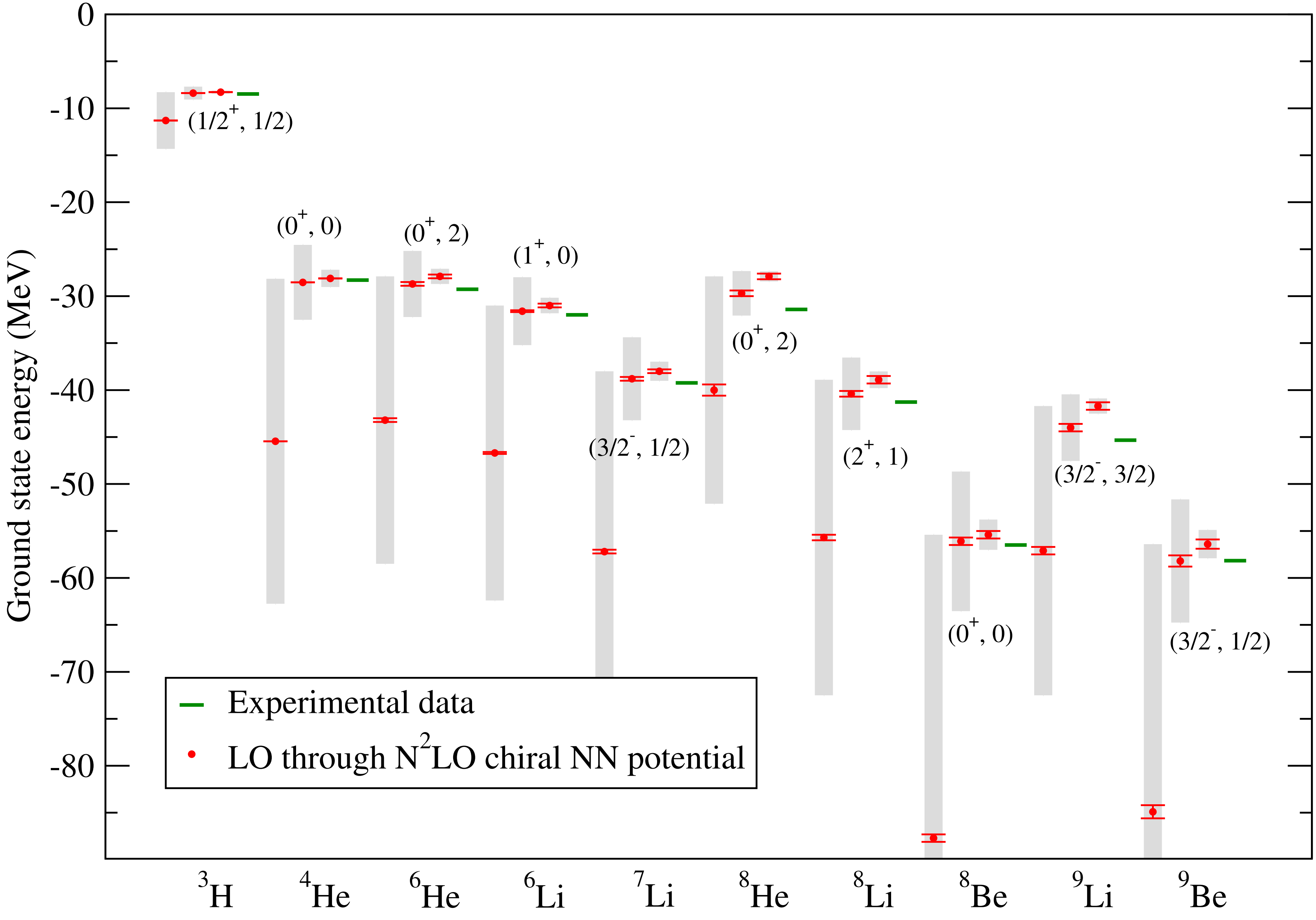


Green: No “max” condition
Red: Established
Black: New Q with |V|

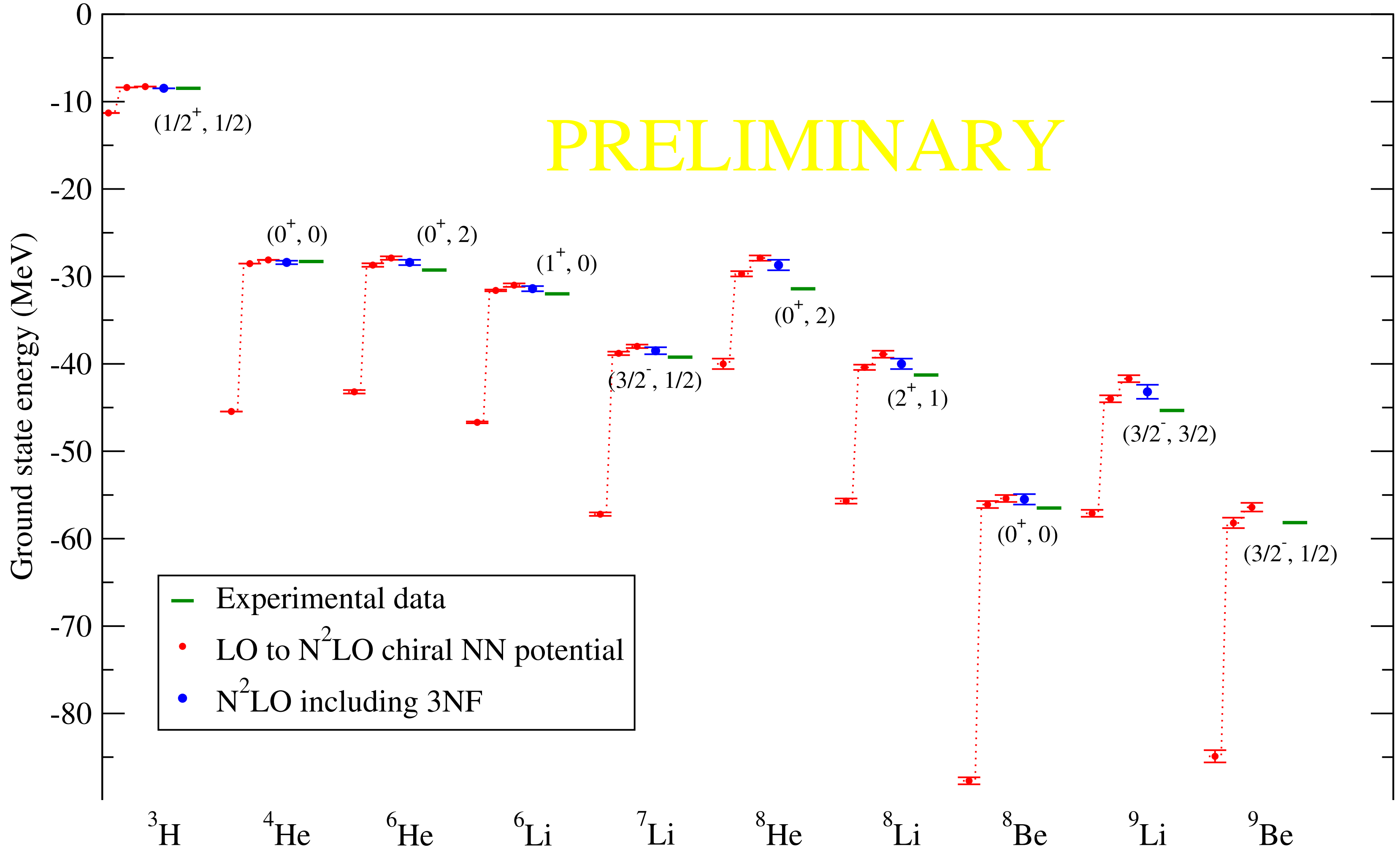
Blue bands:
Extrapolation error

NN only

Preliminary light-nuclei results
S. Binder, et al, LENPIC Collaboration, in preparation



Ground state energies with χEFT up to $A = 9$



Next step: Need to apply these analyses to other observables, e.g. r^2, 0νββ, . . .

Now consider truncation vs Okubo-Lee-Suzuki (OLS) renormalization
for electromagnetic observables using LENPIC interactions in model problems

Consider two nucleons as a model problem with V = LENPIC Chiral EFT Interactions (R = 1.0 fm) 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 $$H = T + V$$

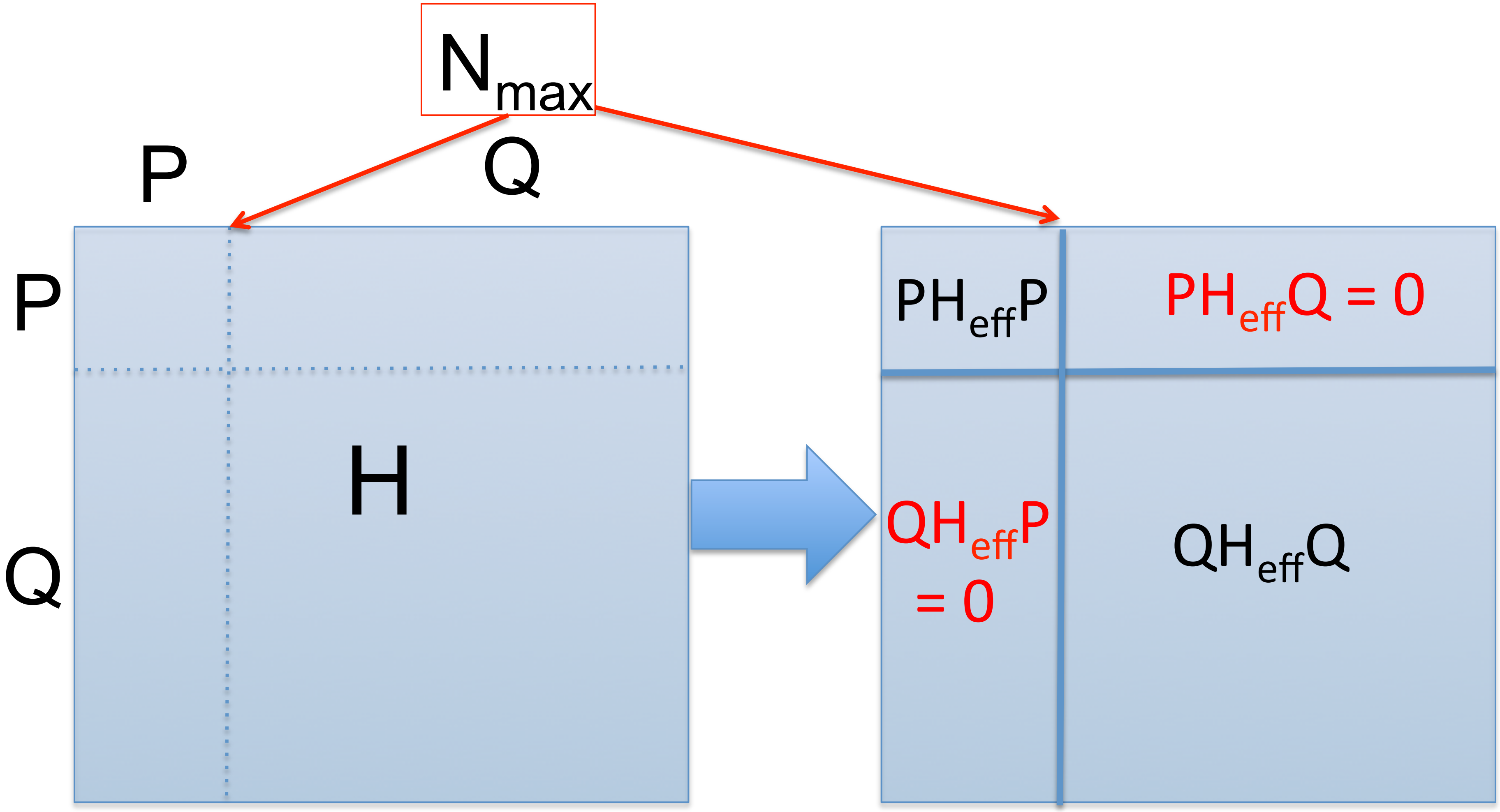
Hamiltonian #2 $$H = T + U_{\mathrm{osc}}(\hbar\Omega_{\mathrm{basis}}) + V$$

Evaluate lowest states' observables:

Ground state energy	E
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(0v)

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

OLS Transform on H



N_{max}

P Q

P

Q

H

$PH_{eff}P$

$PH_{eff}Q = 0$

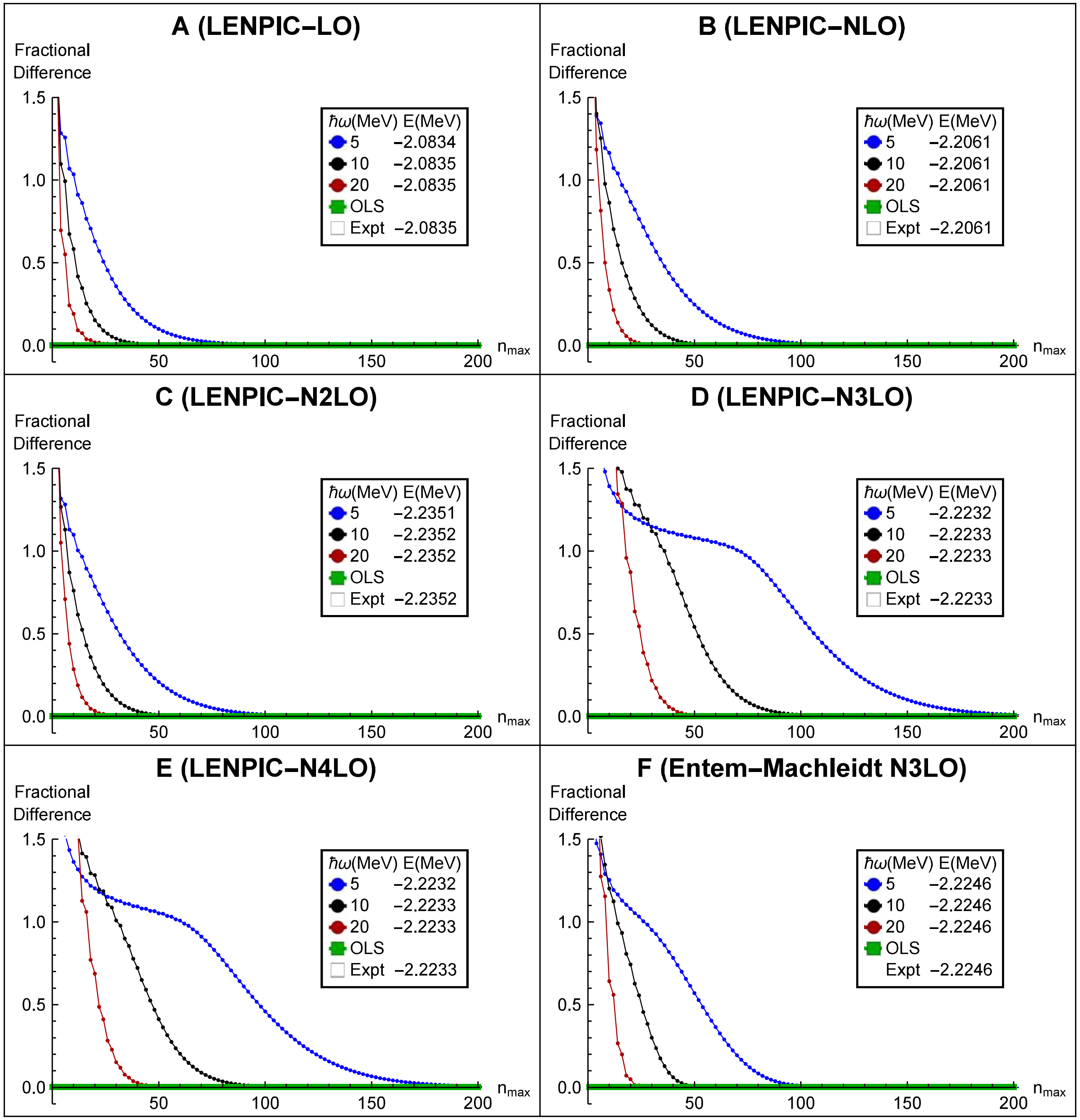
$QH_{eff}P = 0$

$QH_{eff}Q$

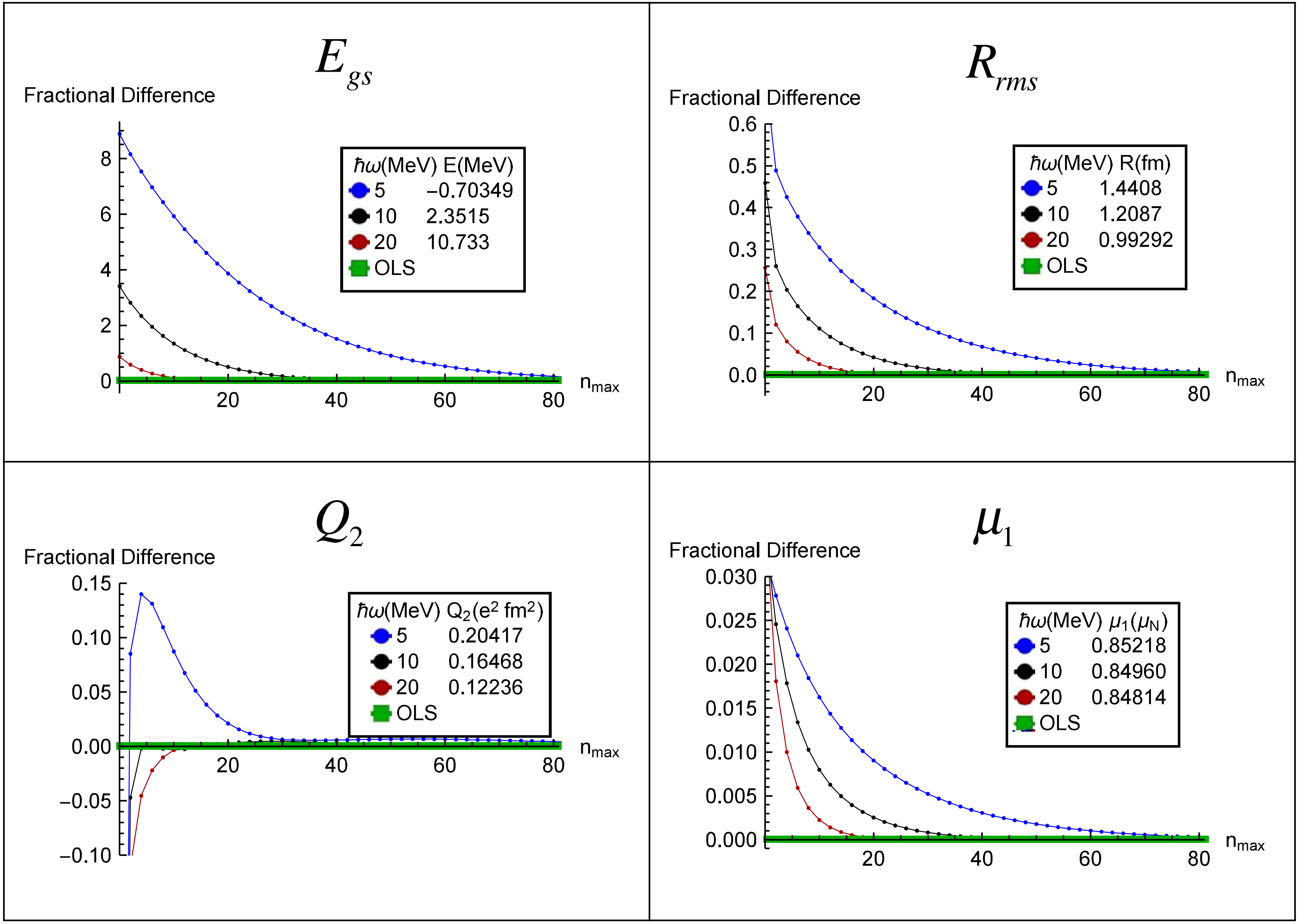
With H defining the OLS transformation,
same picture applies to other Hermitian operators

PRELIMINARY: Deuteron GS energy – Ham #1 – Truncation vs OLS

“Fractional Difference” is $\frac{\text{Model-Exact}}{|\text{Exact}|}$



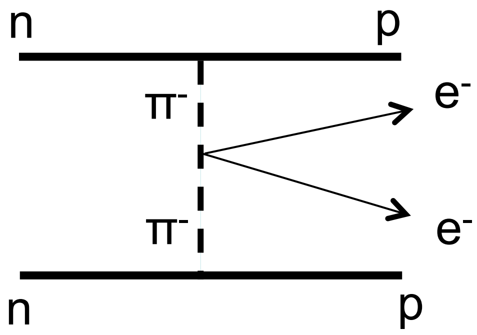
PRELIMINARY: Deuteron properties – Truncation vs OLS
Chiral N2LO for Ham #2 (external trap) & LO for other operators



Preliminary

Consider a 2-body contribution within EFT to 0νββ-decay at NLO

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



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

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

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

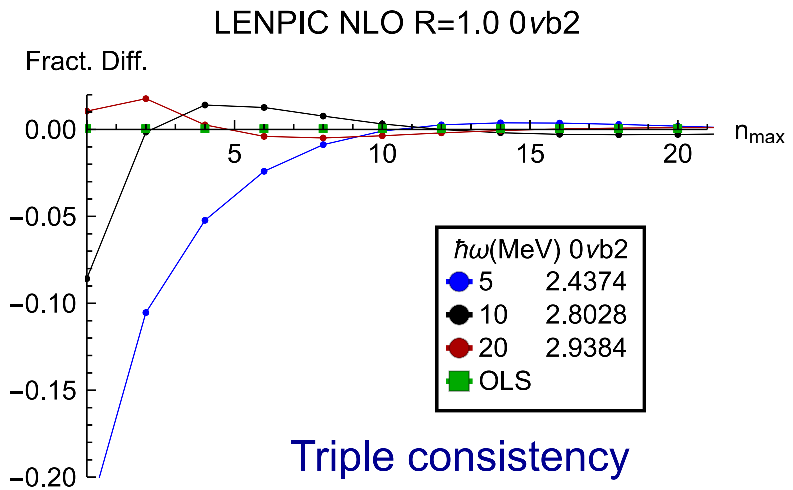
Additional operators being developed – stay tuned

Regulator applied to operators for consistency when using LENPIC interactions

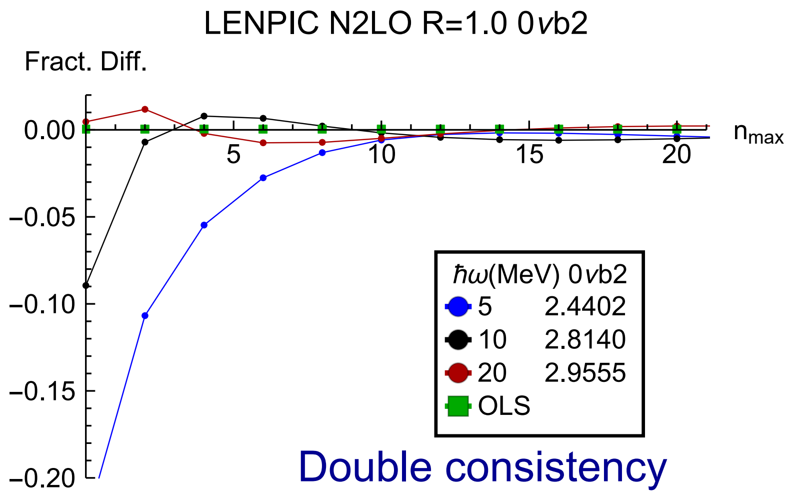
$$f\left(\frac{r}{R}\right) = \left(1 - \exp\left(-\frac{r^2}{R^2}\right)\right)^6$$

$$R = 0.8,\ 0.9,\ 1.0,\ 1.1,\ 1.2\ fm$$

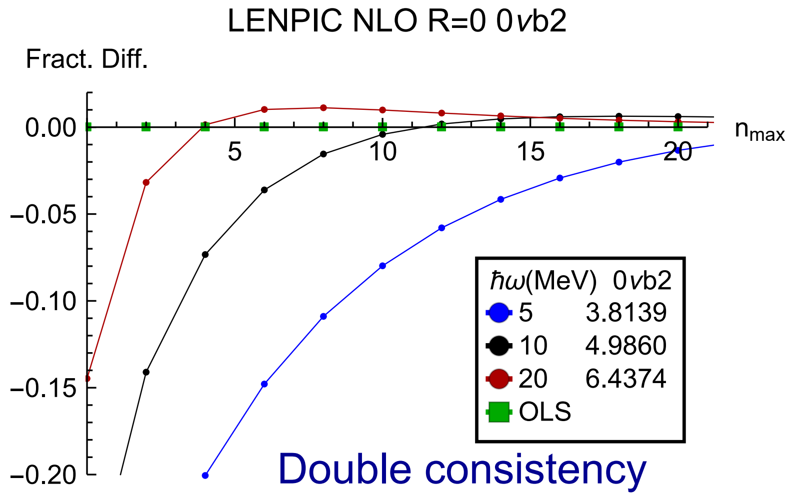
0νββ for 1S0(nn)➔1S0(pp) using Ham #2 (external trap)
Roles of chiral order, consistent regularization and OLS renormalization



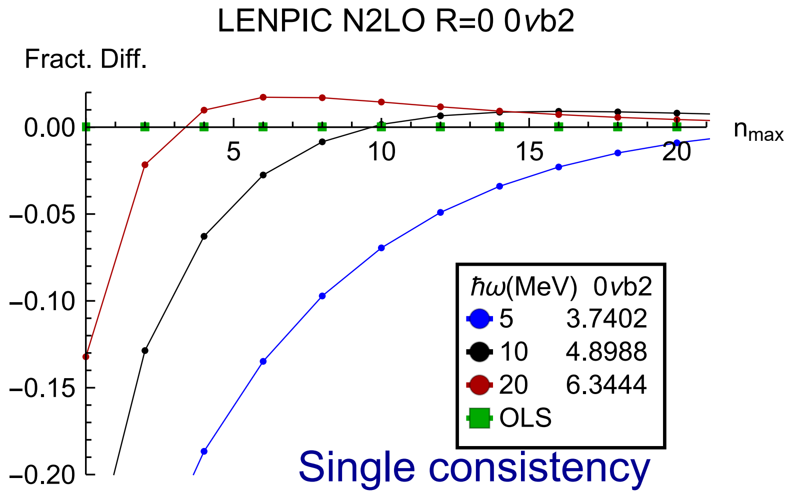
Triple consistency
(chiral order, reg’n, ren’n)



Double consistency
(reg’n, ren’n)



Double consistency
(chiral order, ren’n)



Single consistency
(ren’n)

Plans:

Implement in finite nuclei:

- Input OLS’d operators as TBMEs in single-particle representation

- Perform benchmark A=6 calculations with UNC group (underway)

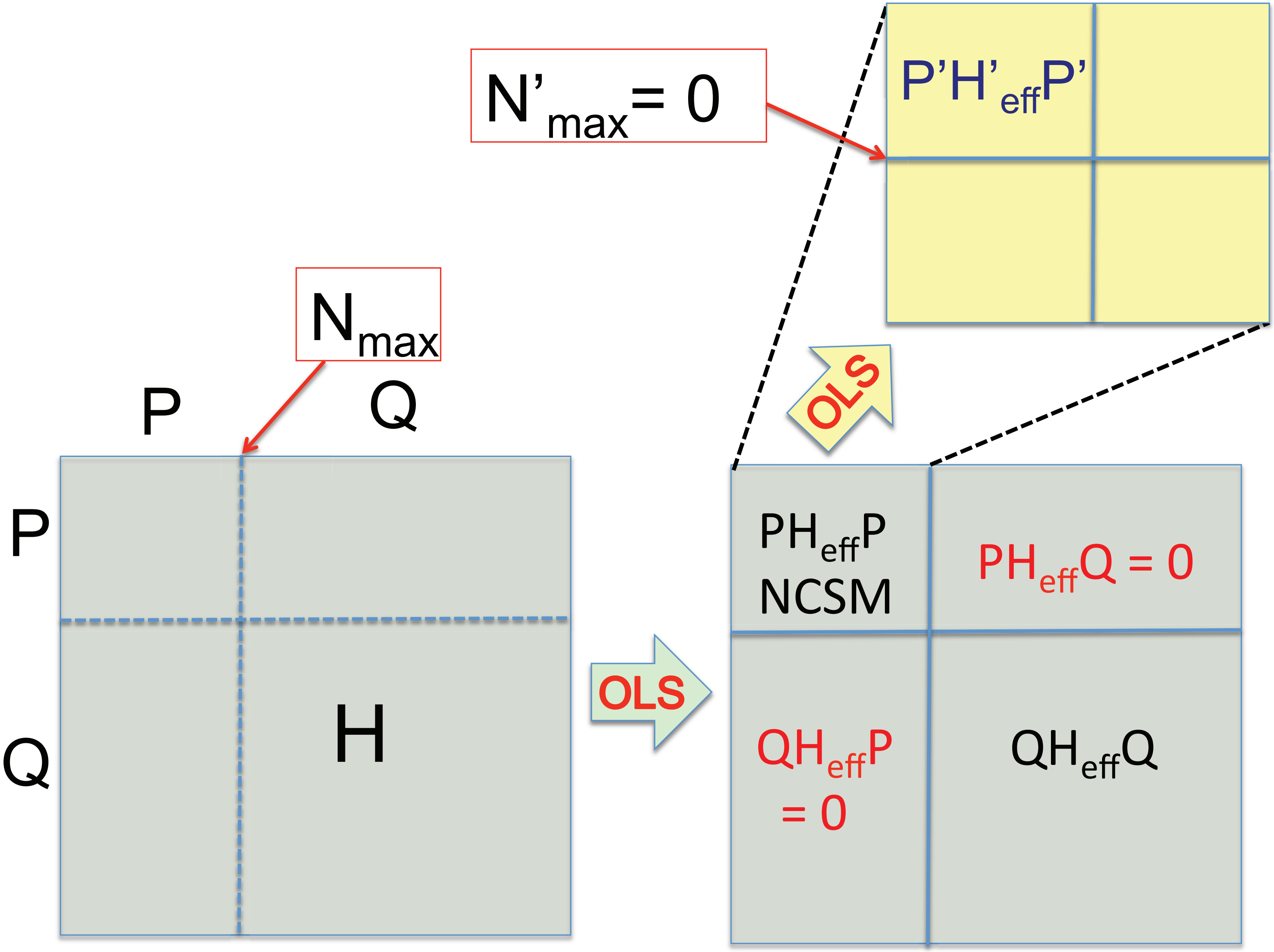
- Evaluate/save density matrices (static and transition) and use them to evaluate OLS’d observables and compare with results from bare observables

Expand treatment to wider range of EW operators within Chiral EFT at NLO & N2LO

Extend to 3-body H with OLS on operators at the 3-body level

Extend to medium weight nuclei with “Double OLS” approach

Double OLS reduction of the basis to a "conventional" shell model valence space



$N'_{max} = 0$

$P'H'_{eff}P'$

N_{max}

OLS

P

Q

P

Q

H

OLS

$PH_{eff}P$

NCSM

$PH_{eff}Q = 0$

$QH_{eff}P$

$= 0$

$QH_{eff}Q$

Dikmen, Lisetskiy, Barrett, Maris, Shirokov, Vary, PRC 91, 064301 (2015); arXiv 1502:00700

Collaborators at Iowa State University
and NUCLEI Team members

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

Note: Proposed faculty hire at Iowa State in NP with support from the Fundamental Interactions Topical Collaboration

Conclusions

Uncertainty vs chiral order is consistent when adopting avg relative momentum from NCSM to set the dimensionless scale Q along with |V| for the energy scale.

OLS succeeds in renormalizing the IR and UV scales in these initial applications to electroweak operators.

Outlook

Novel approach to scattering now established and used to predict the tetraneutron. Opens a path for scattering applications with chiral interactions in light nuclei.

Major additional efforts needed to develop and apply these methods:
effective Hamiltonians, effective electroweak operators, many-body methods, ...