Nuclear Properties with Chiral EFT Interactions
And the Effects of Consistent Electroweak Interactions

James P. Vary, Iowa State University

Multiparticle resonances in hadrons, nuclei and ultracold gases
Hirschegg, January 15-19, 2018

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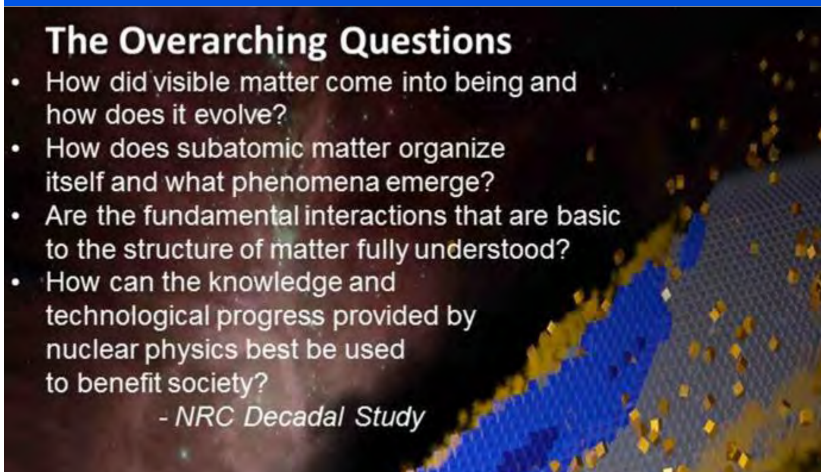
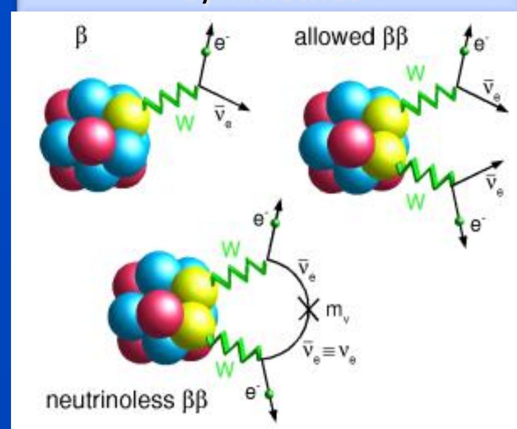


LENPIC

Topical Collaboration on Neutrinos and Fundamental Symmetries



NUCLEI
Nuclear Computational Low-Energy Initiative

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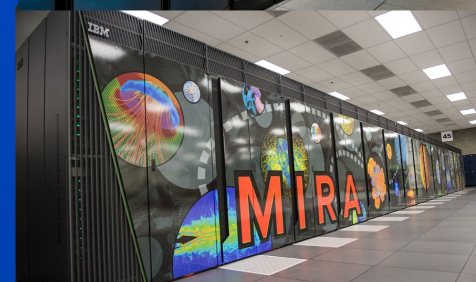
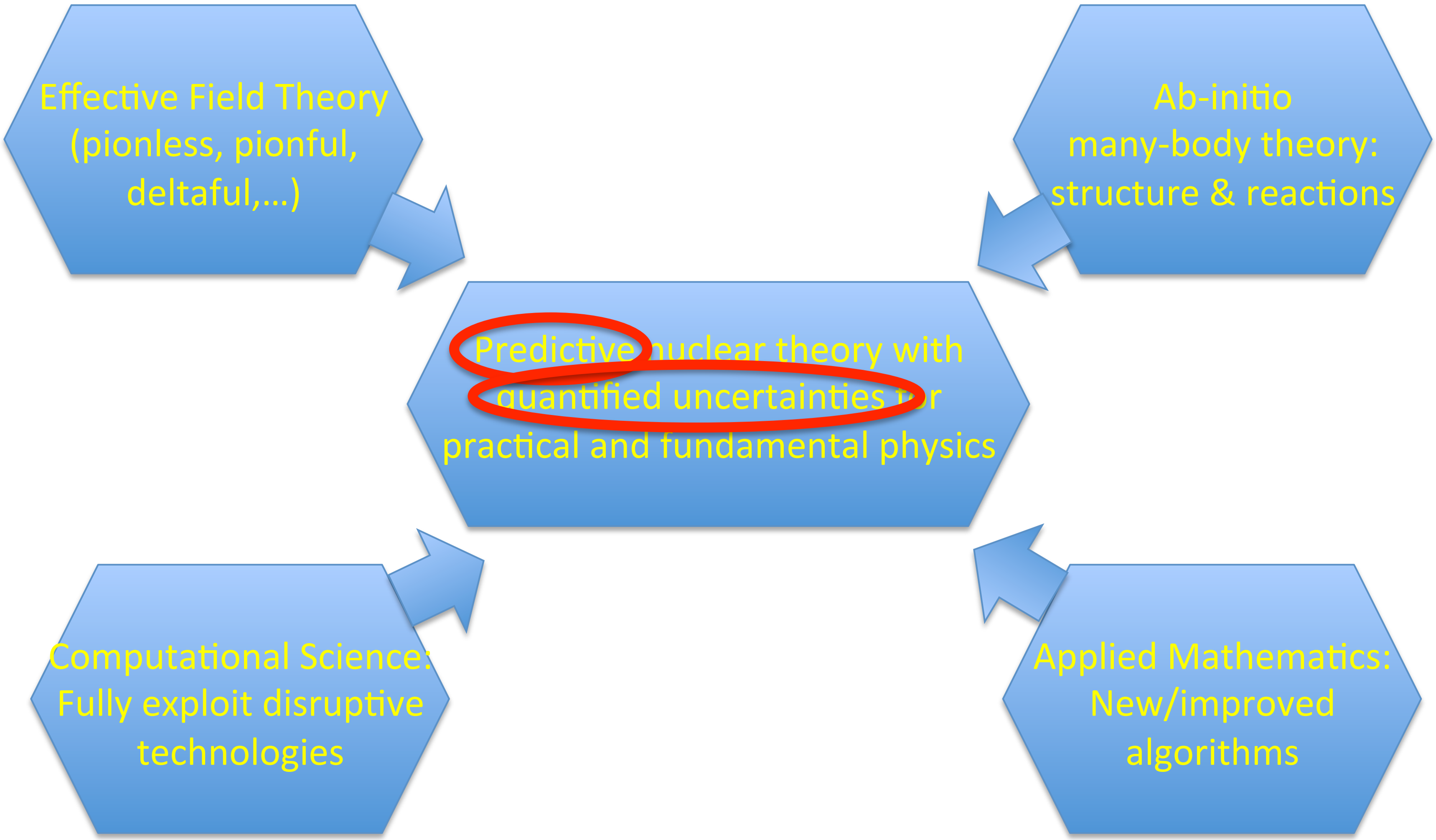



Effective Field Theory (pionless, pionful, deltaful,…)
Ab-initio many-body theory: structure & reactions
Predictive nuclear theory with quantified uncertainties for practical and fundamental physics
Computational Science: Fully exploit disruptive technologies
Applied Mathematics: New/improved algorithms

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

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

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

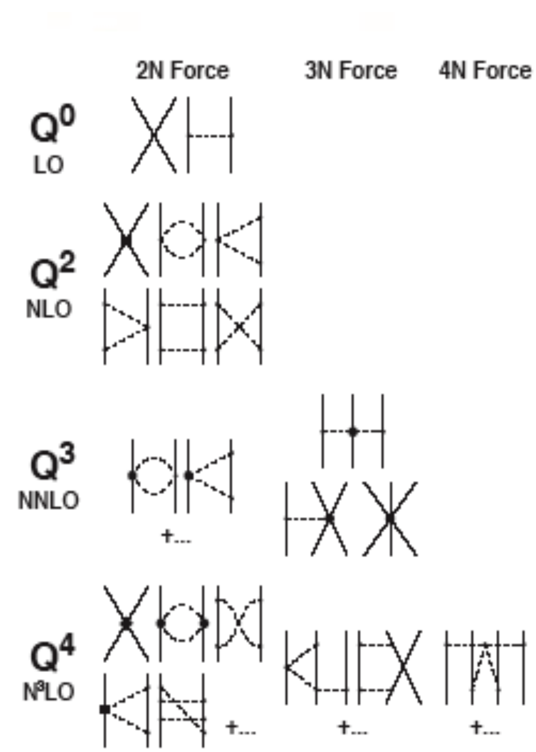
- Alternatives:
  - Full Configuration Interaction (single-particle basis truncation)
  - Importance Truncation — Roth, PRC79, 064324 (2009)
  - No-Core Monte-Carlo Shell Model — Abe *et al*, PRC86, 054301 (2012)
  - SU(3) Truncation — Dytrych *et al*, PRL111, 252501 (2013)

Nuclear interaction

Nuclear potential not well-known,

though in principle calculable from QCD

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



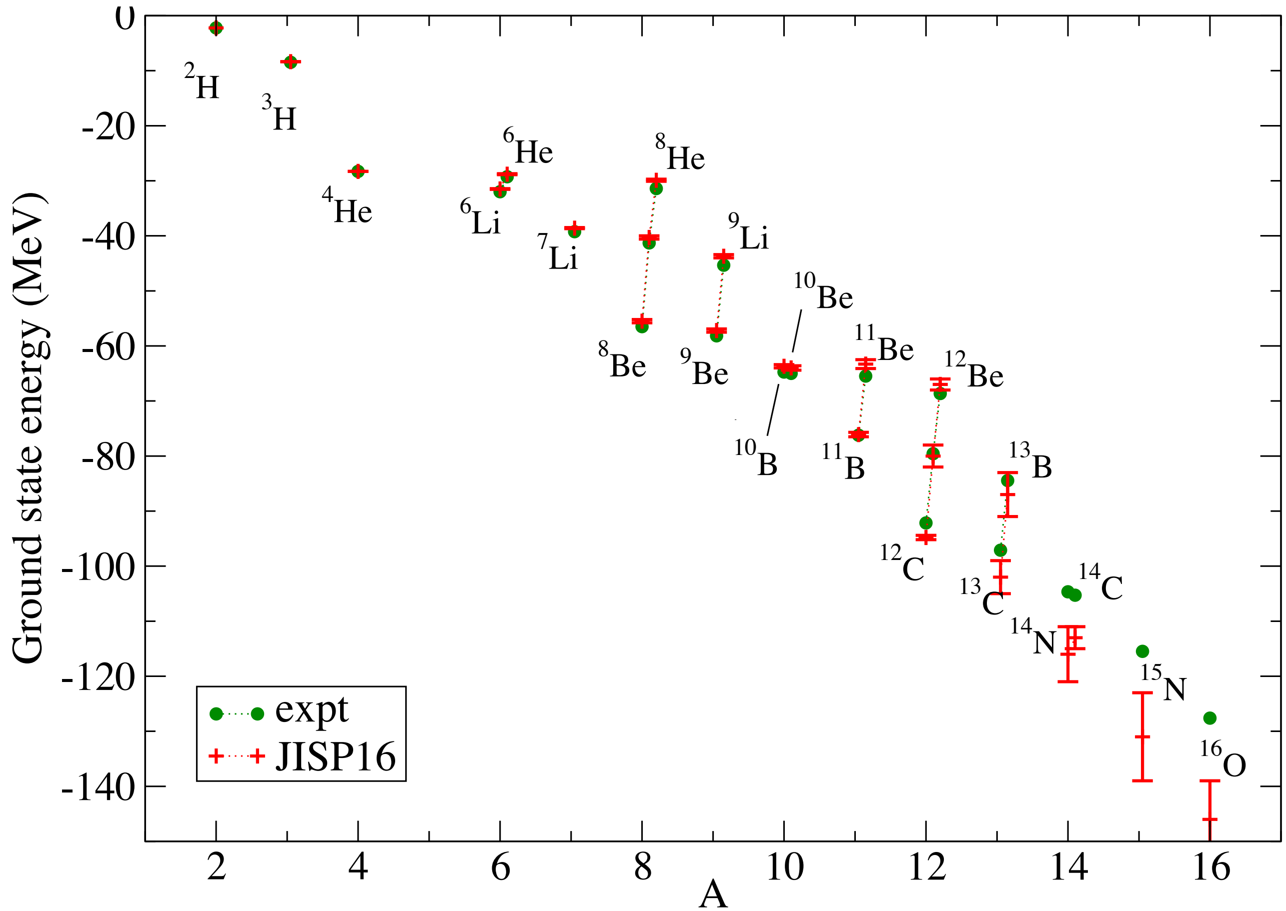
In practice, alphabet of realistic potentials

- Argonne potentials: AV8′, AV18
  - plus Urbana 3NF (UIX)
  - plus Illinois 3NF (IL7)
- Bonn potentials
- Chiral NN interactions
  - plus chiral 3NF, ideally to the same order
- JISP16
- Daejeon16
- . . .

Major development during the past 5-10 years:
High-precision ab initio calculations now used to
"discover" the correct strong NN+NNN interaction

Ground state energy of p-shell nuclei with JISP16

Compare theory and experiment for 24 nuclei Maris, Vary, IJMPE22, 1330016 (2013)



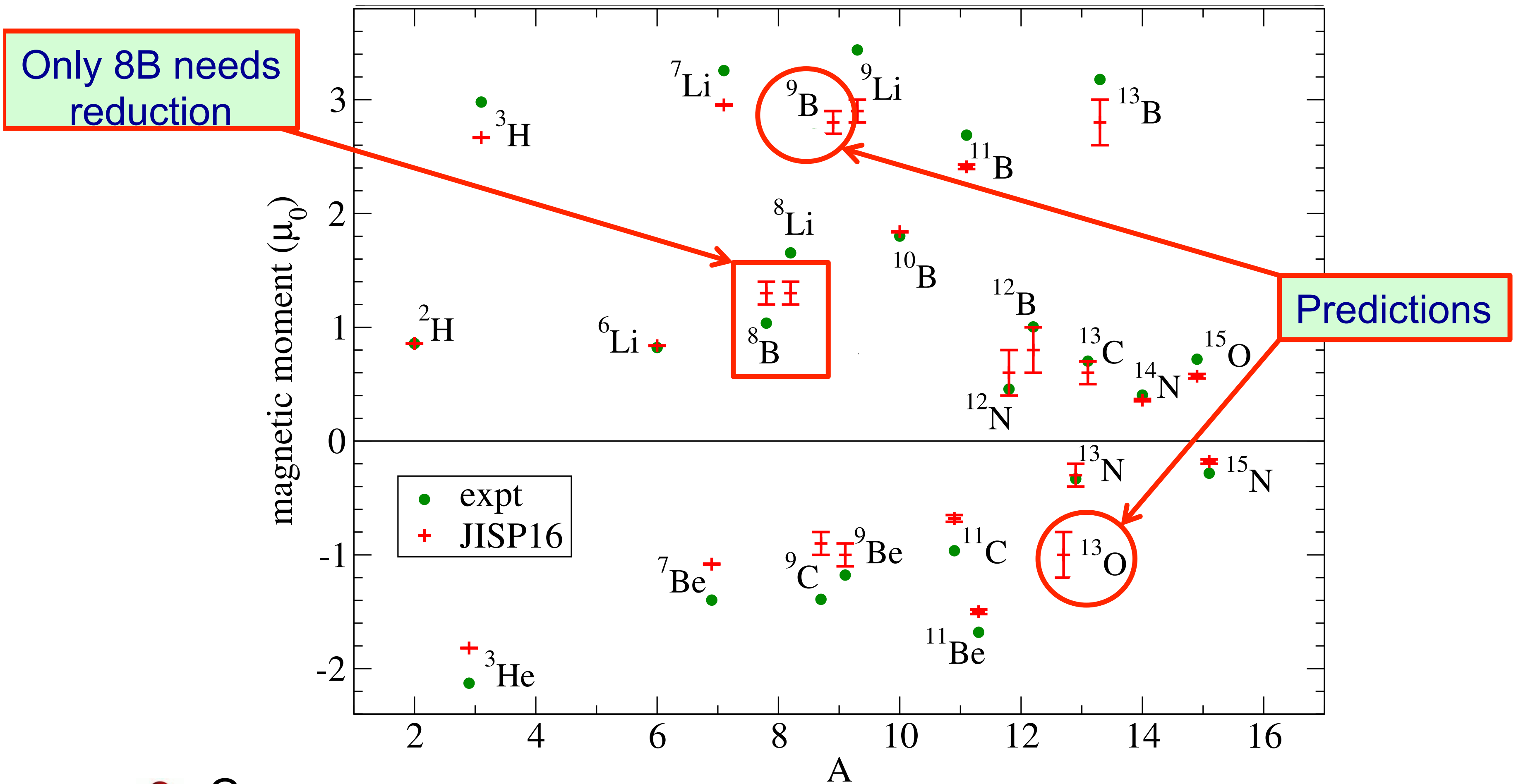
- ^{10}B – most likely JISP16 produces correct 3^+ ground state, but extrapolation of 1^+ states not reliable due to mixing of two 1^+ states
- ^{11}Be – expt. observed parity inversion within error estimates of extrapolation
- ^{12}B and ^{12}N – unclear whether gs is 1^+ or 2^+ (expt. at $E_x = 1$ MeV) with JISP16

Many additional nuclear states: A.M. Shirokov, V.A. Kulikov, P. Maris and J.P. Vary, in Nucleon-Nucleon and Three-Nucleon Interactions, edited by L.D. Blokhintsev and I.I. Strakovsky, (Nova Science, 2014), Chapter 8, p. 231.

Ground state magnetic moments with JISP16

Compare theory and experiment for 23 magnetic moments Maris, Vary, IJMPE22, 1330016 (2013)

$$\mu = \frac{1}{J+1}\Big(\langle \mathbf{J}\cdot\mathbf{L}_p\rangle + 5.586\langle \mathbf{J}\cdot\mathbf{S}_p\rangle - 3.826\langle \mathbf{J}\cdot\mathbf{S}_n\rangle\Big)\,\mu_0$$



- Good agreement with data, given that we do not have any meson-exchange currents

GFMC with AV18 + IL7 interaction
15 magnetic moments compared between theory and experiment
Two-body currents tend to enhance the magnetic moments (exc. ^{8}B)

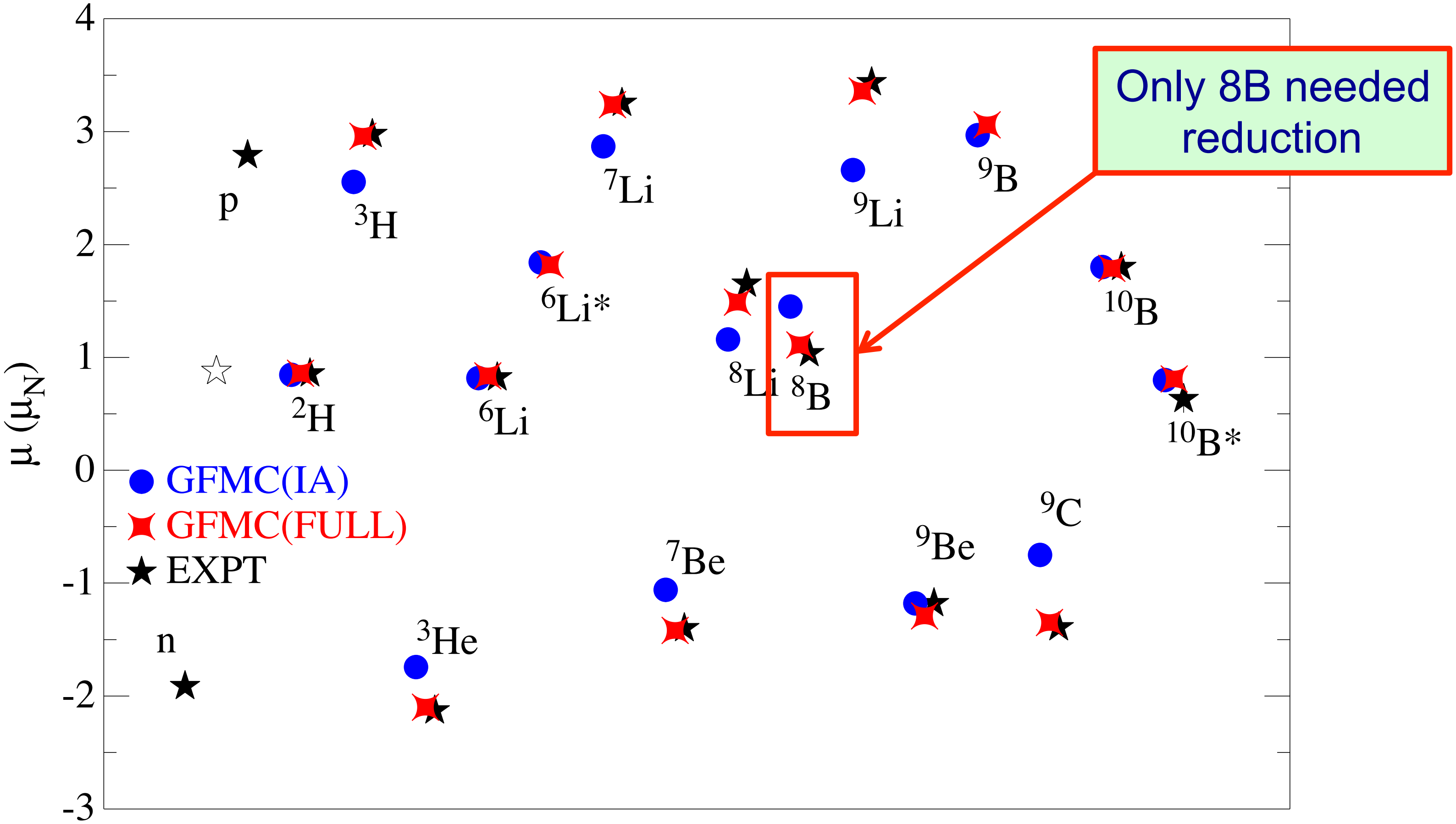
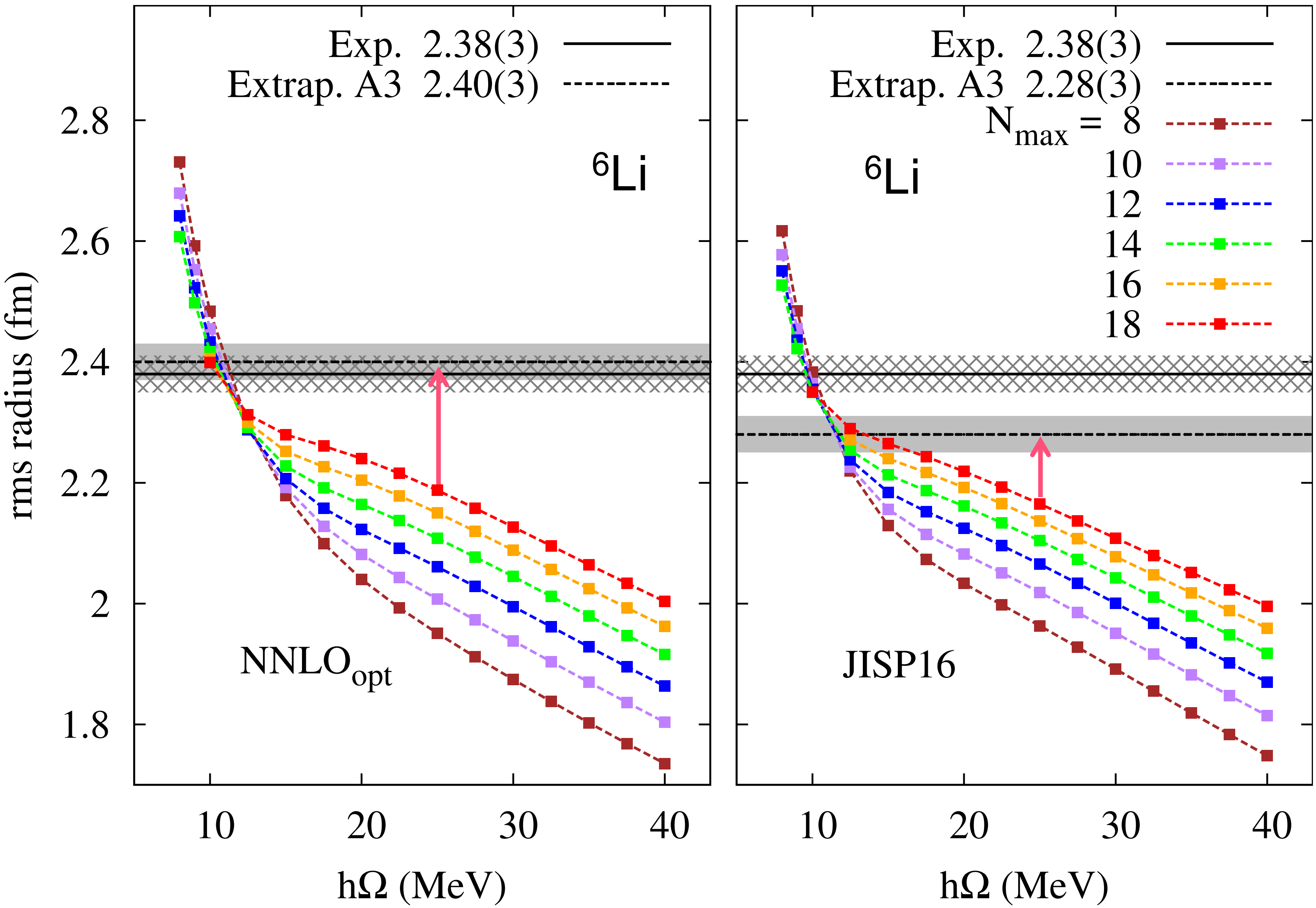
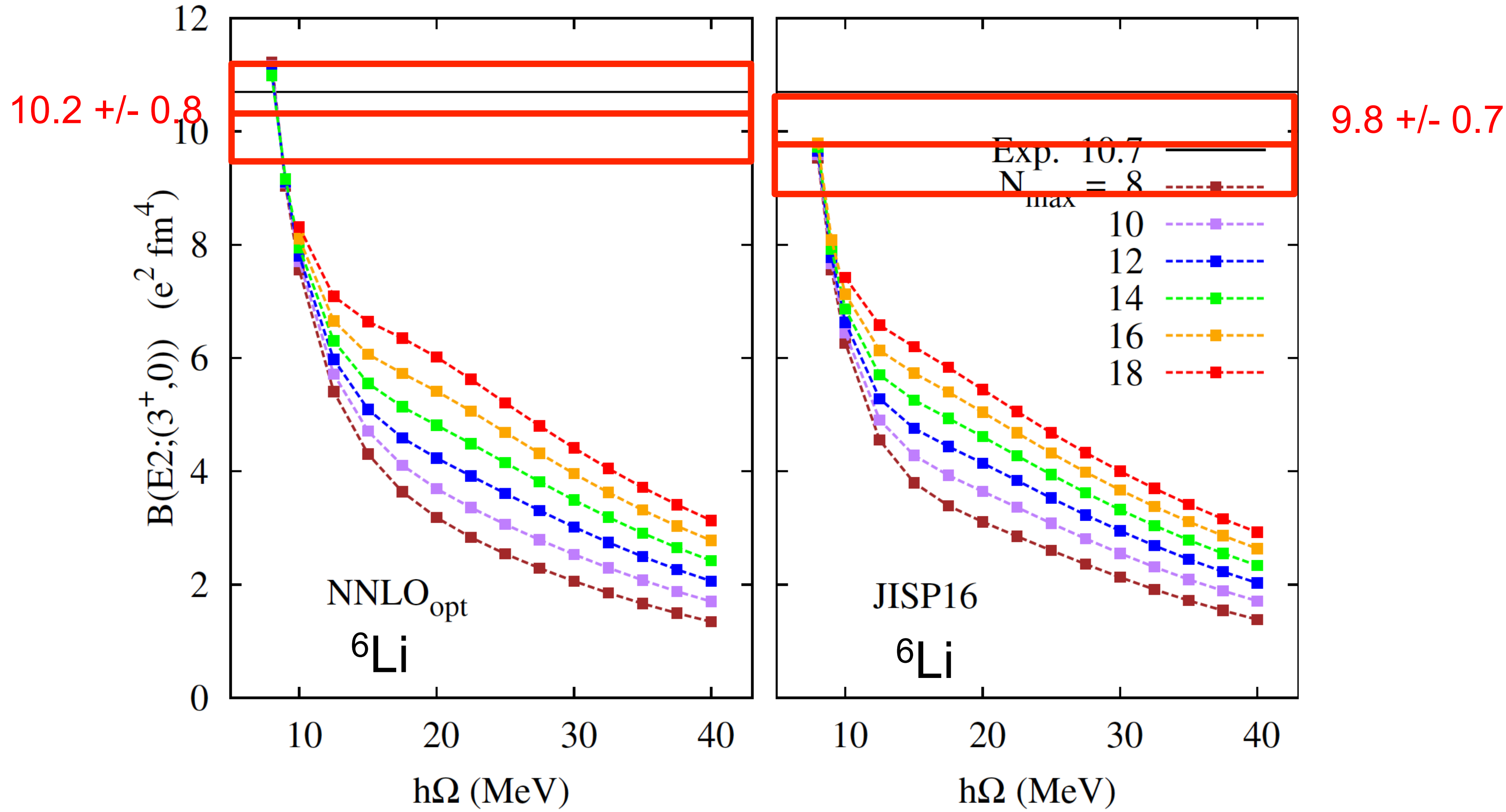


Figure from Rocco Schiavilla



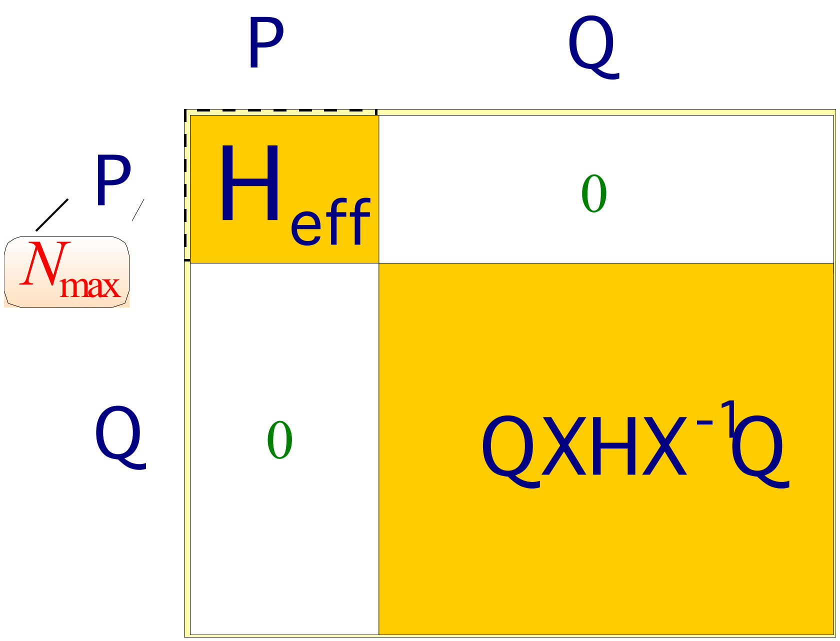
Ik Jae Shin, Youngman Kim, Pieter Maris, James P. Vary, Christian Forssen, Jimmy Rotureau and Nicolas Michel, J. Phys. G., Nuc. Part. Phys. 44, 075103 (2017); arXiv:1605.02819

=> Apply extrapolation method:
D. Odell, T. Papenbrock and L. Platter, Phys. Rev. C93, 044331(2016)



Ik Jae Shin, Youngman Kim, Pieter Maris, James P. Vary, Christian Forssen, Jimmy Rotureau and Nicolas Michel, J. Phys. G., Nuc. Part. Phys. 44, 075103 (2017); arXiv:1605.02819

Effective Hamiltonian in the NCSM
Okubo-Lee-Suzuki (OLS) renormalization scheme



$$H: \quad E_1, E_2, E_3, \ldots E_{d_P}, \ldots E_\infty$$

$$H_{eff}: \quad E_1, E_2, E_3, \ldots E_{d_P}$$

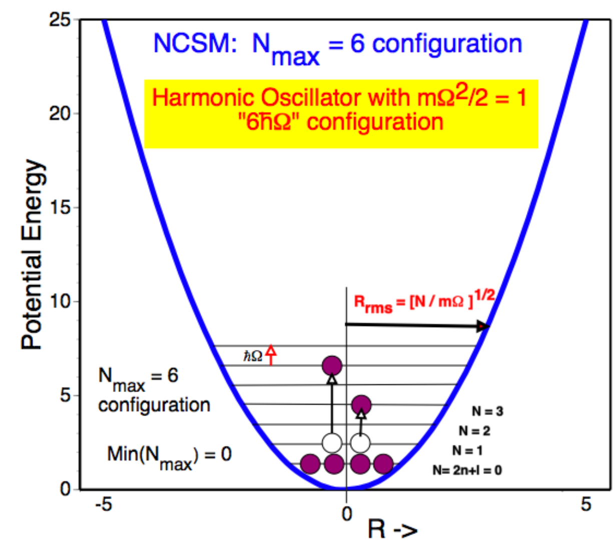
model space dimension

$$QXHX^{-1}P = 0$$

$$H_{eff} = PXHX^{-1}P$$

unitary $X = \exp[-\operatorname{arctan h}(\omega^+ - \omega)]$

- *n*-body cluster approximation, $2 \le n \le A$
- $H^{(n)}_{eff}$ *n*-body operator
- Two ways of convergence:
  - For $P \to 1$ $\quad H^{(n)}_{eff} \to H$
  - For $n \to A$ and fixed P: $H^{(n)}_{eff} \to H_{eff}$



Adapted from Petr Navratil

Outline of the OLS process

$$UHU^{\dagger} = U[T+V]U^{\dagger} = H_d$$

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

$$U^P = PUP$$

$$\tilde{U}^P = P\tilde{U}^P P = \frac{U^P}{\sqrt{U^{P\dagger} U^P}}$$

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

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

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

Calculation of three-body forces at N^3LO

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

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

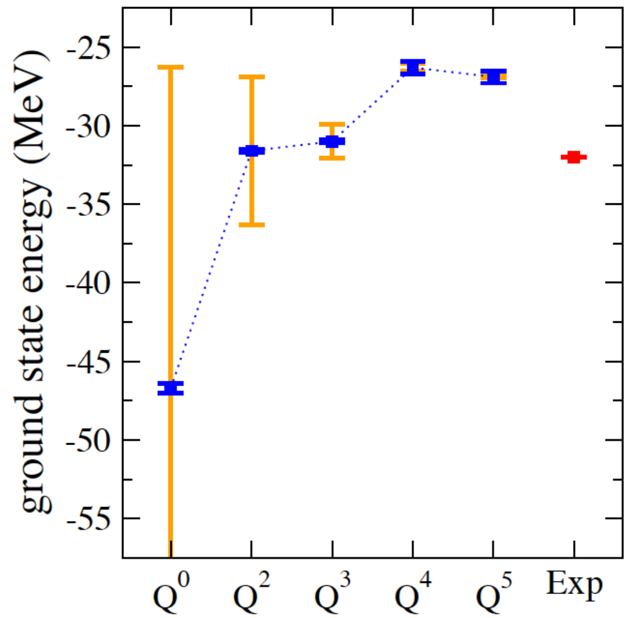
Due to the large number of matrix elements, the calculation is extremely expensive.

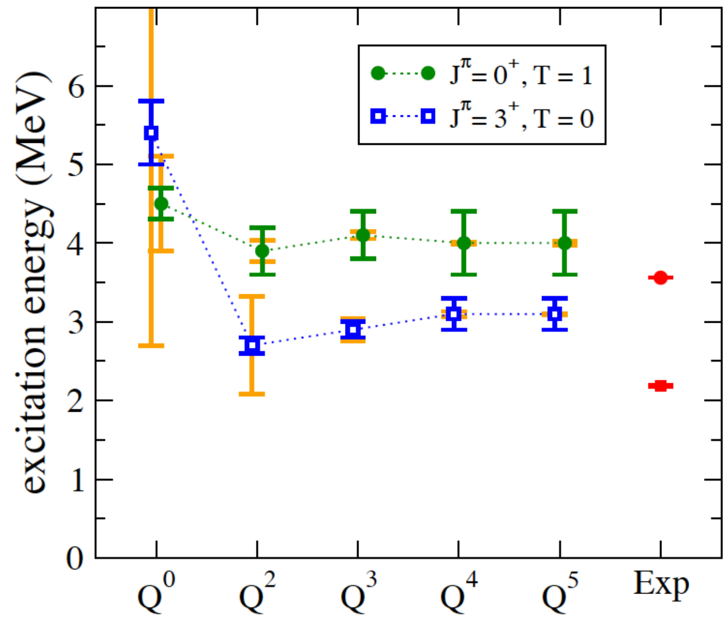
Strategy

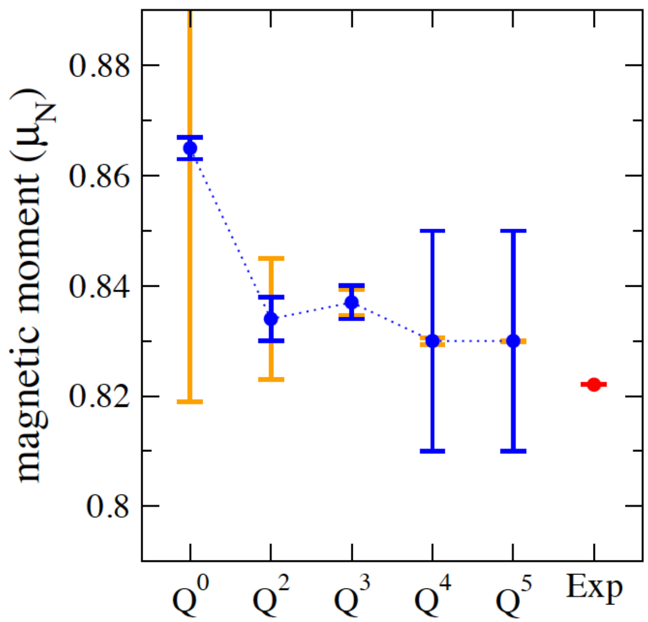
Develop an efficient code which allows to treat arbitrary local 3N interactions.
(Krebs and Hebeler)

Initial LENPIC Collaboration results: Chiral NN results for ^{6}Li by Chiral order

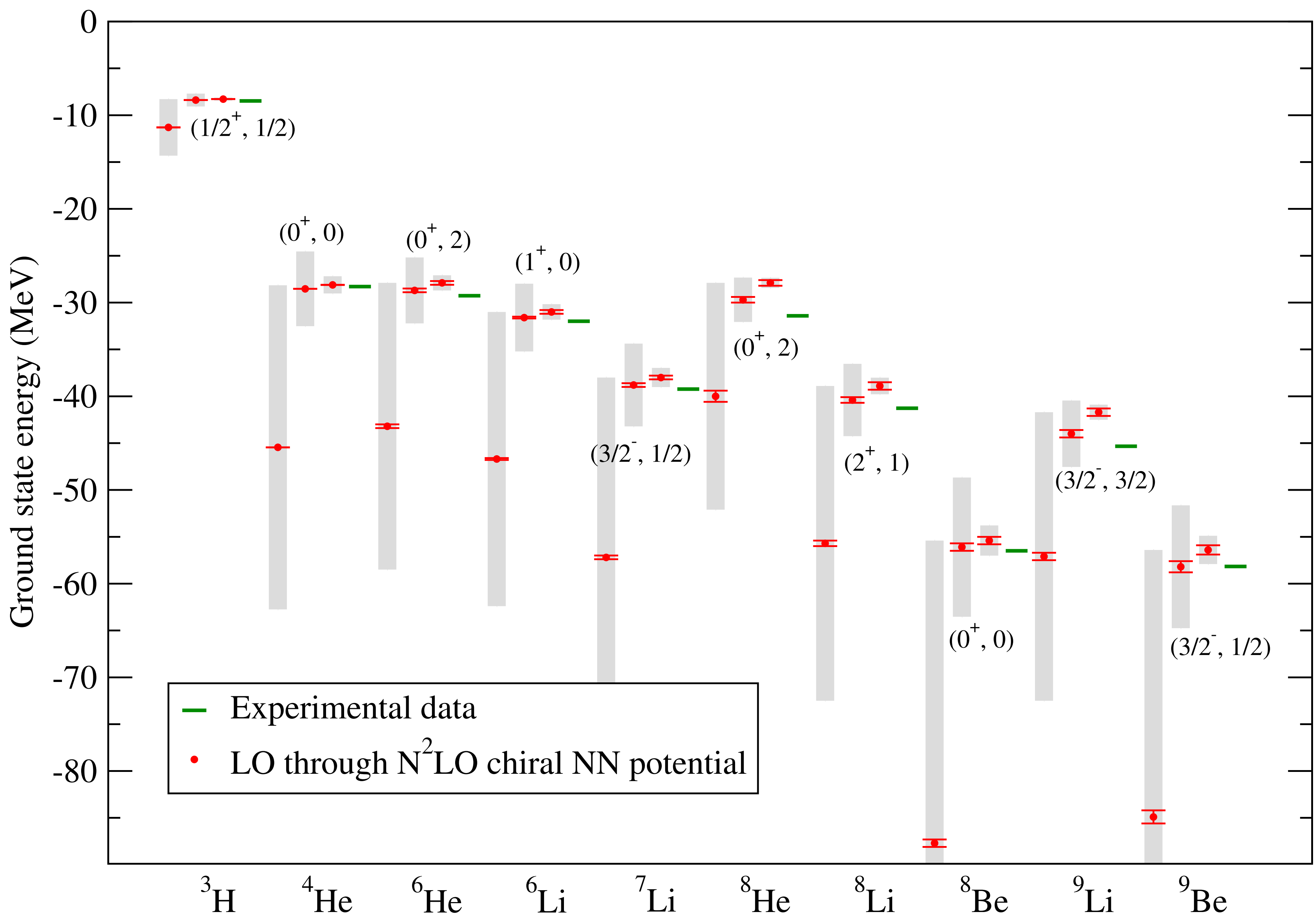
Orange: Chiral order uncertainties; Blue/Green: Many-body method uncertainties
S. Binder, et al, Phys. Rev. C **93,** 044002 (2016); arXiv:1505.07218





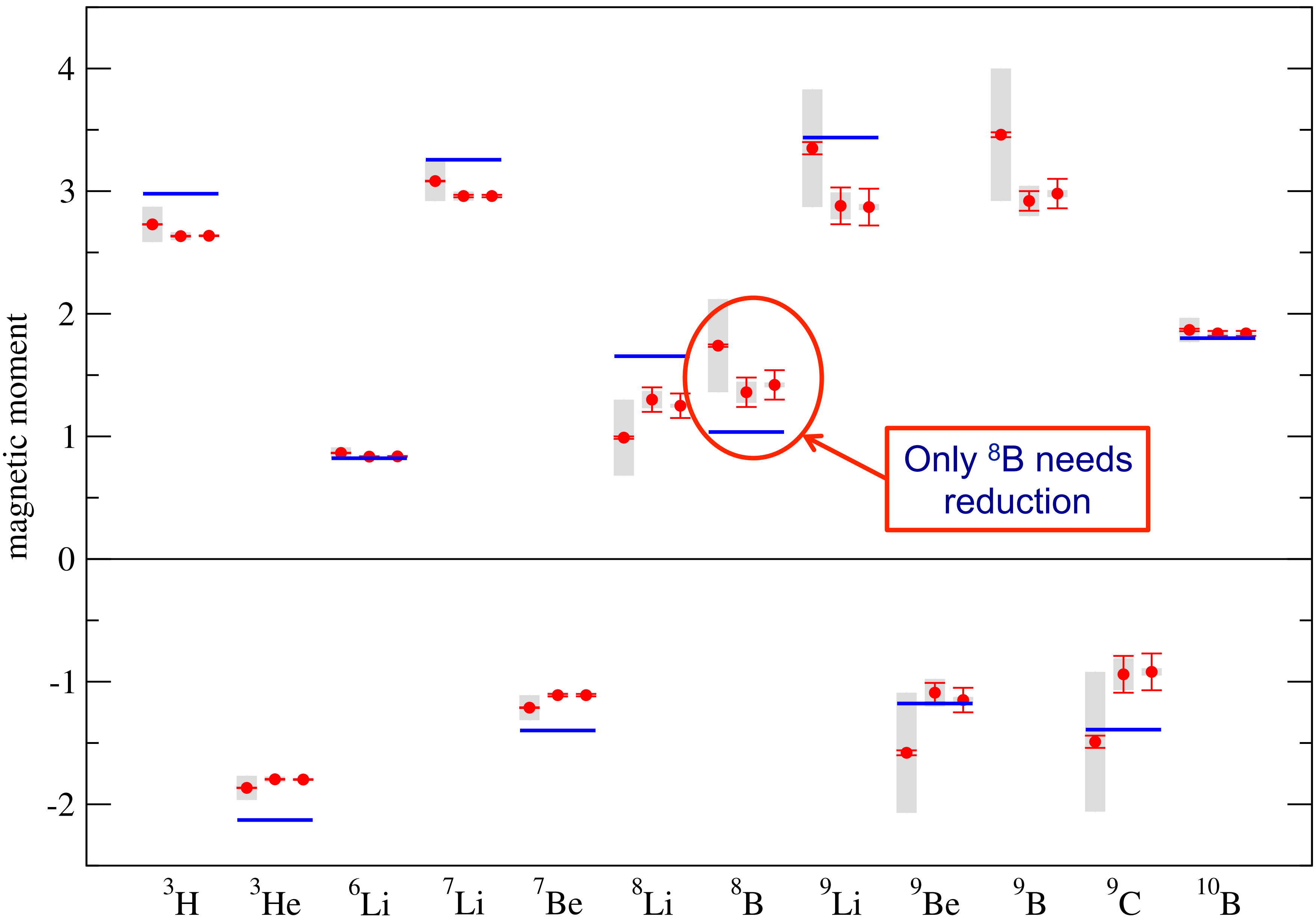


- Ground state energy similar behavior as ^{3}H and ^{4}He
- Open question:
  - Are chiral uncertainty estimates applicable to excitation energies?
- Need compatible chiral 3NFs
- Need chiral expansion conserved current operator



S. Binder, et al., LENPIC Collaboration, in preparation

Preliminary LENPIC results with Chiral NN only and R = 1.0 fm, IA for operator
S. Binder, et al., LENPIC Collaboration, in preparation



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 $$H = T + U_{\text{osc}}(\hbar\Omega_{\text{basis}}) + V$$

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

Deuteron gs energy: truncation vs OLS

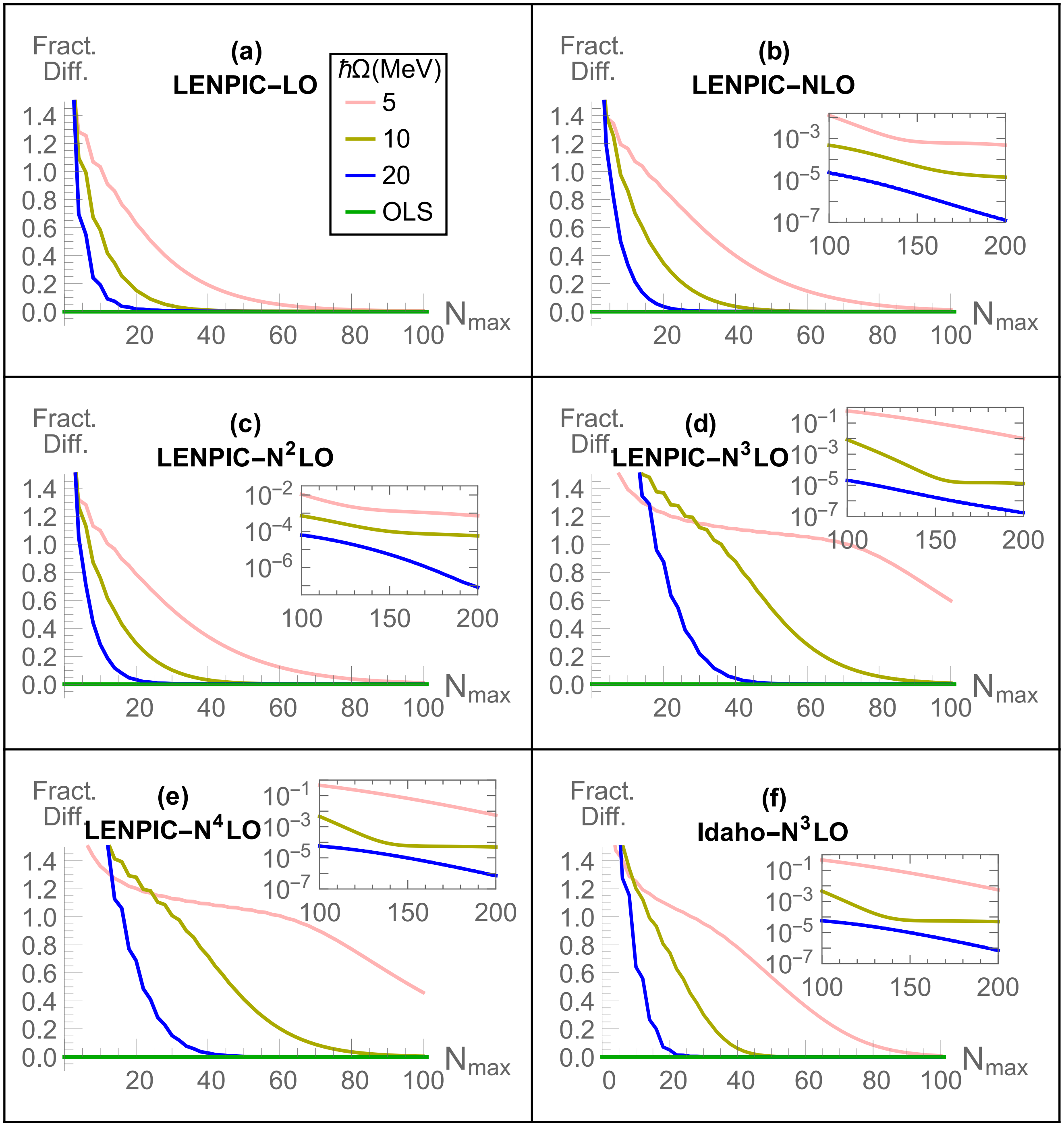
Fract. Diff. = $(E_{model} - E_{exact})/|E_{exact}|$

Insets: Semilog plots of high N_{max} region

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

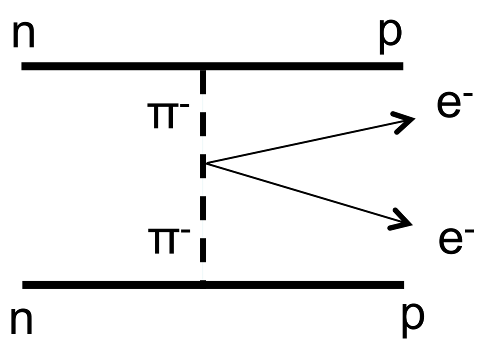
Convergence patterns sensitive to chiral order

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



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

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



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

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

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

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

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

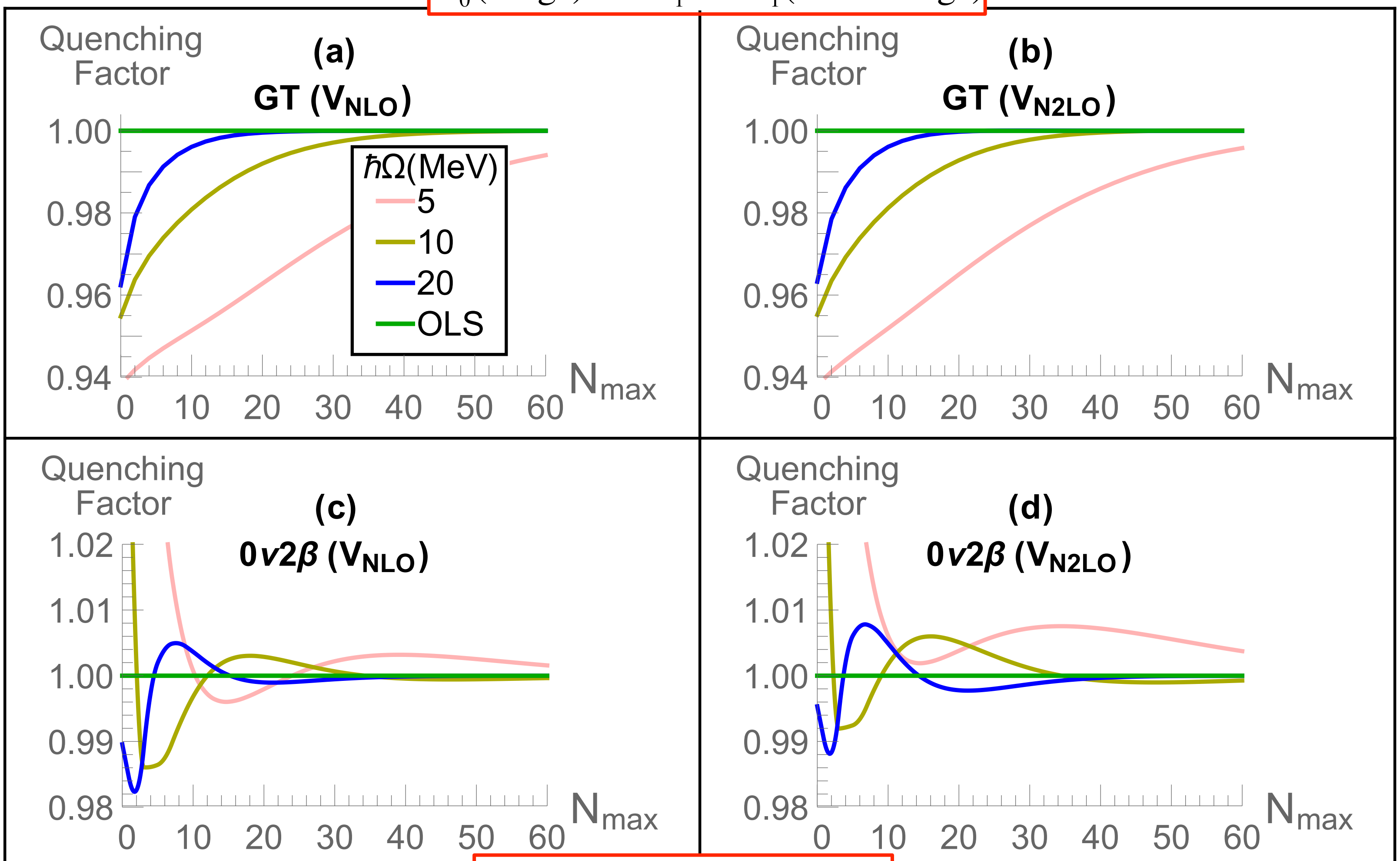
$R = 1.0$ fm for these results

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 0n2b-decay matrix elements from truncation with Exact/OLS

Recast Fract. Diff. (FD) results as a Quenching Factor (QF)
QF = Exact/Model = 1 – (FD x |Exact|)/Model

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



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

Outlook:

Implement in finite nuclei:

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

Evaluate/save density matrices (static and transition)
and use them to evaluate consistent OLS'd or SRG'd observables

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

Extend to 3-body interactions with OLS or SRG on operators at the 3-body level

Extend to medium weight nuclei with "Double OLS" approach

Partial list of projects underway – keep on your radar screens

Iteratively improved natural orbitals (with Notre Dame Univ)

Ab initio nuclear reactions
- multiple-scattering with realistic 1-body density matrices (with Ohio Univ)
- non-perturbative time-dependent Coulomb excitation (with IMP-Lanzhou)

Benchmarking neutrinoless double-beta decay (with UNC)

Consistent electroweak operators (LENPIC)
- moments
- transitions
- double-beta decay

} This talk

Valence effective interactions (with S. Korea, France, Russia)

Artificial Neural Network developments and applications to NCSM (with LBNL)

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
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
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