NN and 3N (effective) interactions for ab initio nuclear structure calculations

Pieter Maris

Dept. of Physics and Astronomy
Iowa State University
Ames, IA 50011
pmaris@iastate.edu

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Outline

Phenomenological nuclear interactions

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

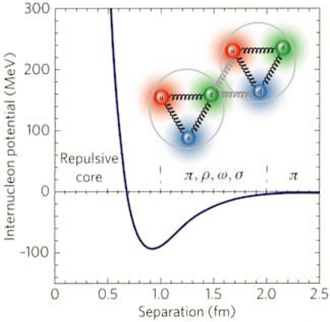
Nuclear interaction not well-determined

- In principle calculable from QCD
- Constrained by experimental (scattering) data

Alphabet of realistic NN potentials

- Argonne potentials
- Bonn potentials
- Chiral interactions
- Daejeon16
- ...

Most need 3N forces as well



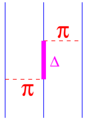
NN potential and scattering data

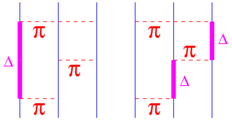
- Experimental cross-section data for *pp* and *pn* scattering, but not for *nn* scattering
  - analysis in terms of isoscalar $T = 0$ and isovector $T = 1$ channels
- Typically, cross-section data converted to phase shifts
- NN potentials fitted to phase shifts
  - propagation of experimental uncertainties?
  - fitted up to what energy?
- NN scattering data constrain only the on-shell NN potential, but not the off-shell behavior
  - many NN potentials describe NN scattering data equally well
- Additional (physics) input
  - meson exchange currents
  - chiral effective field theory
  - select observables from light nuclei (which?)
  - more or less suitable for intended computational framework (e.g. local vs. nonlocal interactions)

Argonne V18

Wiringa, Stoks and Schiavilla, PRC 51, 38 (1995)

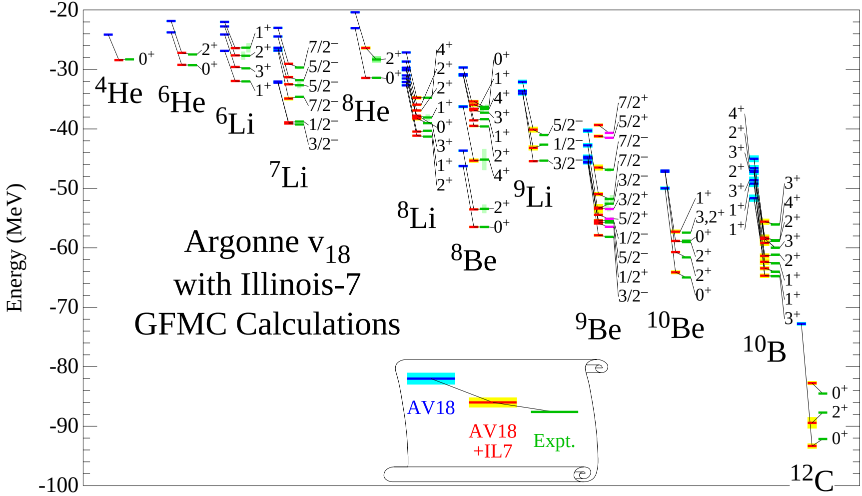
- Accurate local NN potential
  - 14 charge-independent operators (AV14)
  - 3 charge-dependent, 1 charge asymetric operator
  - 40 parameters fitted to *pp* and *np* scattering data up to 350 MeV
- Extensively used in VMC and GFMC calculations of light nuclei
- Not used much in NCSM calculations
  - slow convergence ('hard' interaction)
  - would need significant renormalization
- Additional 3-nucleon forces
  - Urbana IX – based on 2π exchange diagrams (in particular Fujita–Miyazawa term) plus short-range phenomenological terms
  - Illinois 7 – most important additional term: 3π ring diagram with one or two Δ's





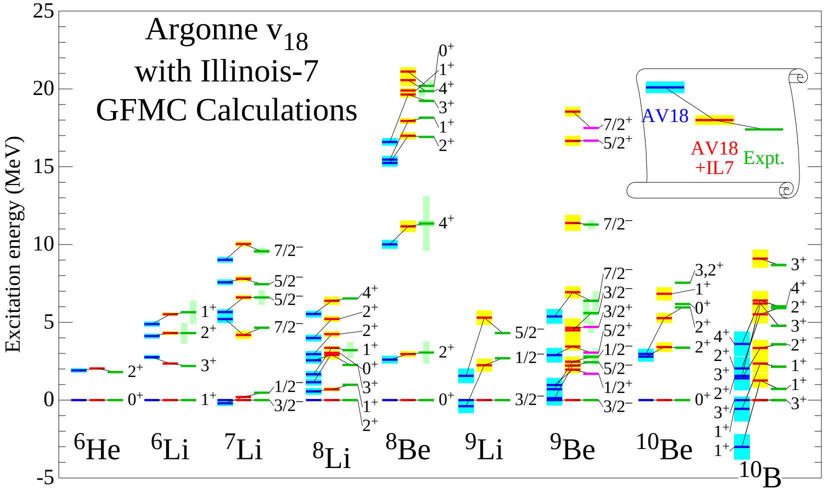
Energies with AV18 + IL7

Carlson, Gandolfi, Pederiva, Pieper, Schiavilla, Schmidt and Wiringa, RMP 87, 1067 (2015)



Spectra with AV18 + IL7

Carlson, Gandolfi, Pederiva, Pieper, Schiavilla, Schmidt and Wiringa, RMP 87, 1067 (2015)



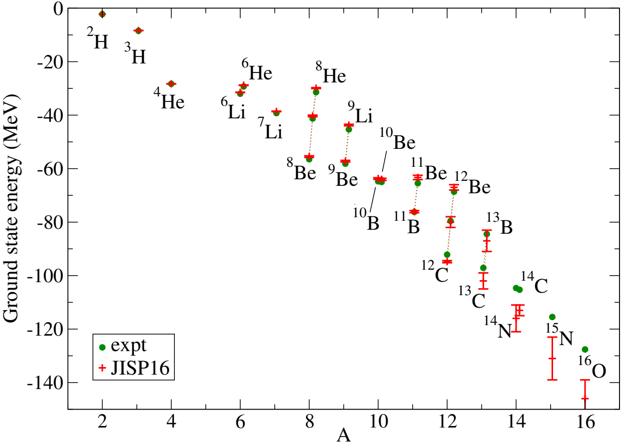
JISP16

Shirokov, Vary, Mazur and Weber, PLB 644, 33 (2007)

J-matrix Inverse Scattering Potential

- Nonlocal finite rank seperable NN potential in H.O. representation, constructed to reproduce *np* scattering data
  - $2n + l \leq 8$ for even partial waves, limited to $J \leq 4$
  - $2n + l \leq 9$ for odd partial waves, limited to $J \leq 4$
  - $\hbar\omega = 40$ MeV
  - χ^2/datum of 1.05 for the 1999 *np* data base (3058 data)
- Use Phase-Equivalent Transformations (PET) to tune off-shell interaction to
  - deuteron quadrupole moment
  - binding energy of ^{3}H and ^{4}He
  - low-lying states of ^{6}Li (JISP6, precursor to JISP16)
  - binding energy of ^{16}O
- Unfortunately, convergence insufficiently understood and basis space was limited when tuning to ^{16}O

Ground state energies of *p*-shell nuclei with JISP16

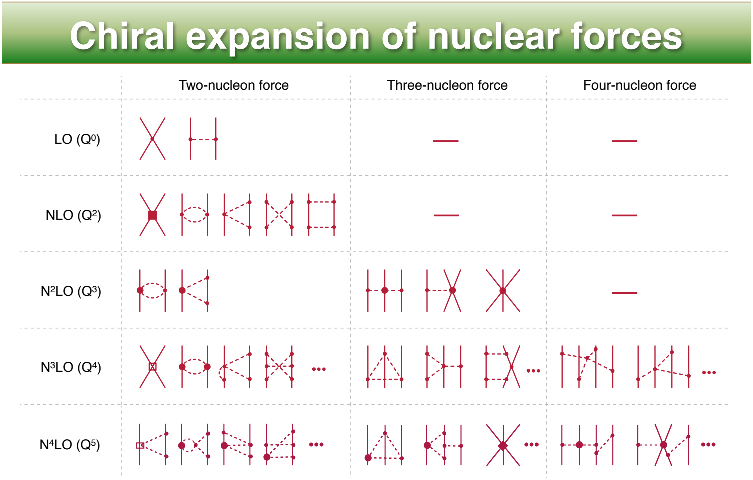


Maris and Vary,
IJMPE22, 1330016 (2013)

- ^{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

Nuclear interactions from Chiral Effective Field Theory

- Controlled power series expansion in Q/Λ
- Hierarchy for many-body forces $V_{NN} \gg V_{NNN} \gg V_{NNNN}$



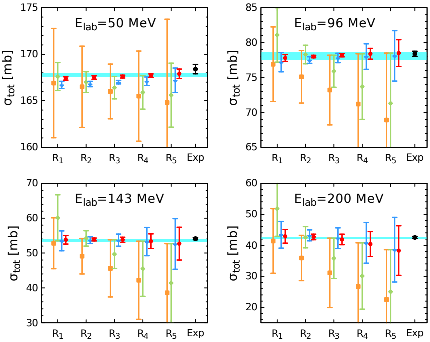
NN potential from χEFT up to N^{4}LO

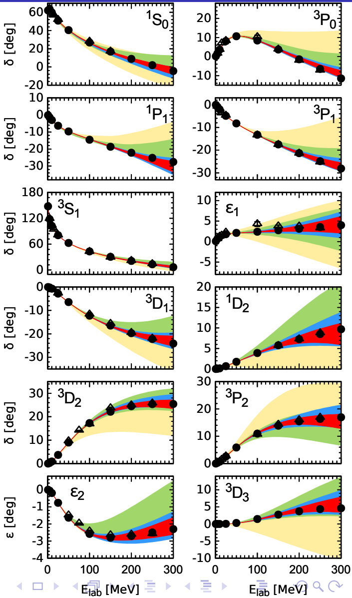
Epelbaum, Krebbs, Meißner, PRL 115 (2015); EPJ A51 (2015)

- Local regulator long-range terms

$$V(r) \to V(r)\left[1 - \exp\left(-r^2/R^2\right)\right]^6$$

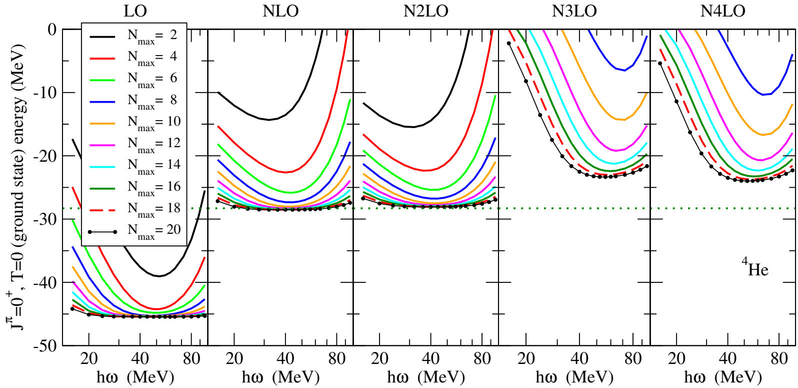
- Regulators $R_1 = 0.8$ to $R_5 = 1.2$ fm
- Reduced finite-cutoff artefacts





Ground state energy of ^{4}He

LENPIC collaboration, PRC 93, 044002 (2016)

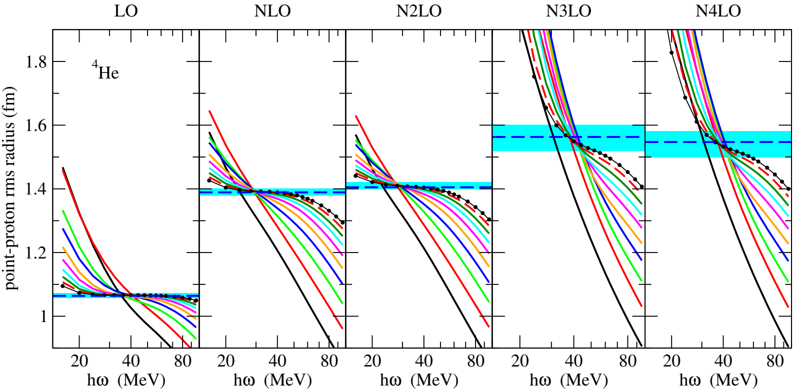


Chiral *NN* interaction with regulator $R = 1.0$ fm ($\Lambda_b = 600$ MeV)

- Many-body calc'ns converge rapidly at LO, NLO, and N^{2}LO
- Convergence significantly slower at N^{3}LO and N^{4}LO
- No 3NFs included (yet) – should be present at N^{2}LO and up

Point-proton rms radius of ^{4}He

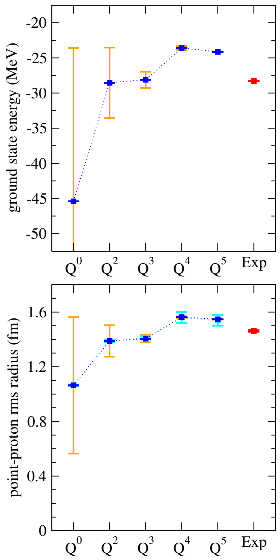
LENPIC collaboration, PRC 93, 044002 (2016)



- Convergence of many-body calculation for RMS radius slower than convergence for (ground state) energy
  - Long-range operator
  - H.O. basis function fall off like gaussians, instead of exponential
  - Nevertheless, agree with Faddeev–Yakubovsky calc'ns

Chiral EFT uncertainty estimates

LENPIC collaboration, PRC 93, 044002 (2016)



- Chiral expansion in $m_\pi/\Lambda_b \approx 0.23$

$$X^{(i)} = X^{(0)} + \Delta X^{(2)} + \ldots + \Delta X^{(i)}$$

- Expected chiral corrections at order i

$$\Delta X^{(i)} \approx \mathcal{O}\left(Q^i X^{(0)}\right)$$

- Chiral uncertainty estimates

$$\delta X^{(0)} \approx Q^2 |X^{(0)}|$$

$$\delta X^{(2)} \approx \max\left(Q\delta X^{(0)}, Q|\Delta X^{(2)}|\right)$$

- 3NF at N^{2}LO ($i = 3$) and up not yet included

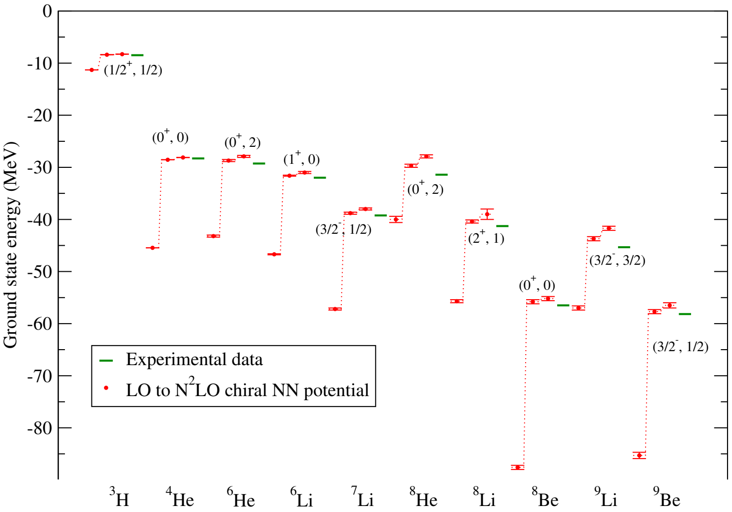
$$\delta X^{(i\geq 3)} \approx \max\left(Q\delta X^{(i-1)}, Q^{i-2}|\Delta X^{(3)}|\right)$$

- Additional condition on LO uncertainty estimate $\delta X^{(0)} \geq \max(|X^{(i)} - X^{(j)}|)$

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

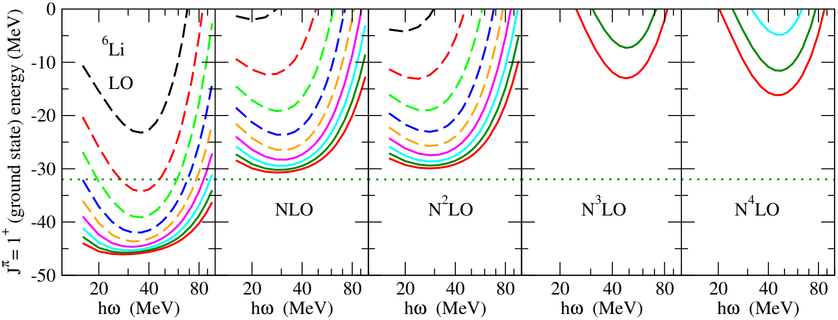
LENPIC collaboration

in preparation



Results for ^{6}Li with χEFT NN potential

LENPIC collaboration, PRC 93, 044002 (2016)



- Up to N^{2}LO good numerical convergence
- At N^{3}LO (and N^{4}LO) convergence significantly slower
- Need to use renormalization techniques to accelerate convergence

Renormalization

Challenge: achieve numerical convergence for No-Core CI calculations using a finite amount of CPU time on current HPC systems

- Use unitary transformations to renormalize interaction
  - can improve quality of results in small basis spaces
  - need to renormalize other operators as well
- Commonly used in NCSM calculations
  - Similarity Renormalization Group
  - Okubo–Lee–Suzuki
  - $V_{\mathrm{low}\,k}$, V_{UCOM}, ...
- In principle, unitary transformations change the wavefunction, but should not change physical observables
- In practice, induced many-body effects are neglected ...
  - need to study effect of induced many-body forces

Similarity Renormalization Group

Glazek, Wilson, PRD 48, 5863 (1993); PRD 49, 4214 (1994); Wegner, Ann. Phys. 3, 77 (1994)

- Consider series of unitary transformations

$$H_\alpha = U_\alpha H U_\alpha^\dagger$$

- Define anti-hermitian operators η_α

$$\eta_\alpha = \frac{dU_\alpha}{d\alpha} U_\alpha^\dagger = -\eta_\alpha^\dagger$$

  such that H_α evolves according to

$$\frac{dH_\alpha}{d\alpha} = [\eta_\alpha, H_\alpha]$$

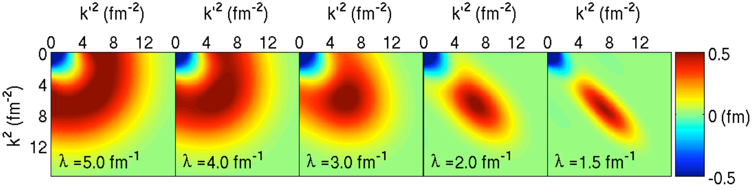
- Common choice for 'generator' η_α

$$\eta_\alpha = (2\mu)^2 [T_{\text{rel}}, H_\alpha]$$

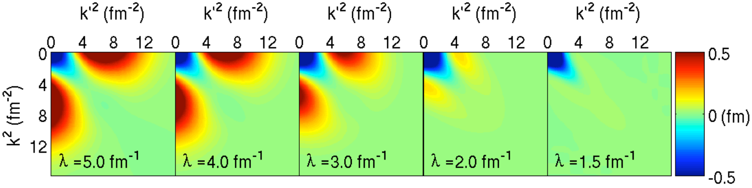
SRG evolution of Idaho χEFT at N^{3}LO(500 MeV)

Bogner, Furnstahl, Perry, PRC 75, 061001 (2007)

$^1S_0$



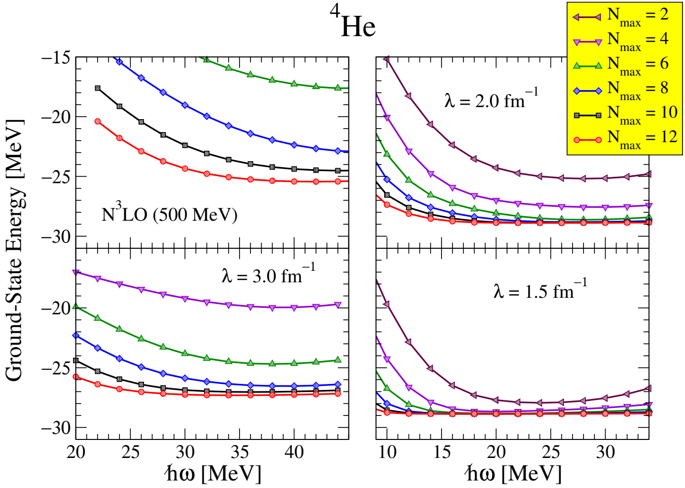
$^3S_1$



- Drives interaction to diagonal
- Decouples low and high momenta
- Note: SRG parameter $\lambda = \alpha^{-\frac{1}{4}}$

^{4}He with SRG evolved χEFT

Bogner *et al*, NPA 801, 21 (2008)

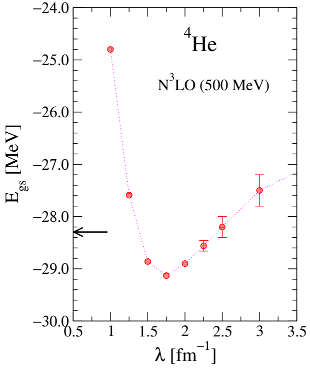


- SRG renormalization improves convergence significantly
- SRG parameter dependence indicates omitted induced 3NF

^{4}He with SRG evolved χEFT including (induced) 3NF

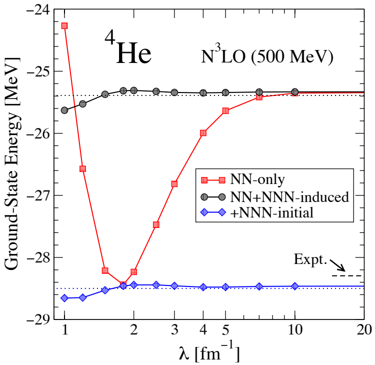
Bogner *et al*, NPA 801, 21 (2008)

(without Coulomb interaction)



Jurgenson, Navratil, Furnstahl, PRL 103, 082501 (2009)

(with Coulomb interaction)

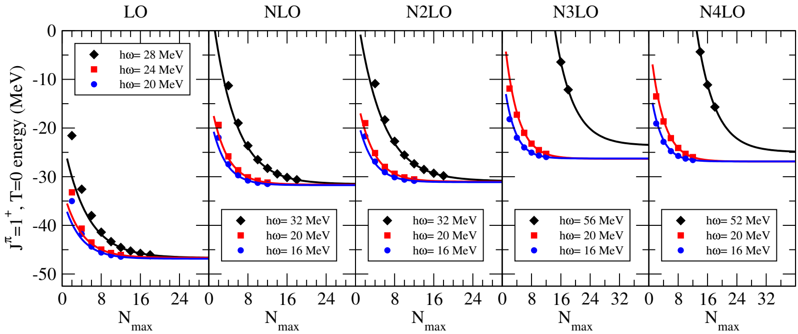


- Strong SRG parameter $\alpha = \lambda^{-4}$ dependence without induced 3NF
- Almost no SRG parameter $\alpha = \lambda^{-4}$ dependence with induced 3NF
- Explicit 3NF needed for agreement with experiment

^{6}Li with SRG evolved χEFT including induced 3NF

- Empirical extrapolation method (ground state) energies

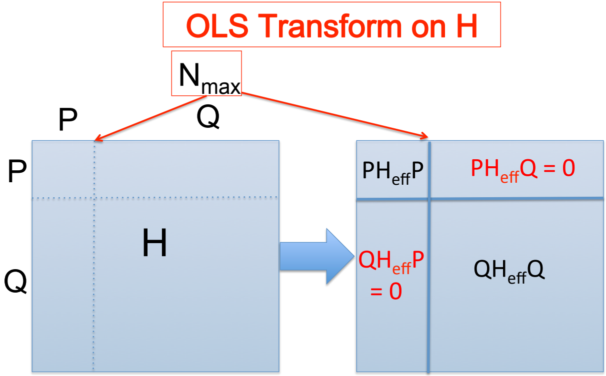
$$E(N_{\max}) \approx E_\infty + a \exp(-bN_{\max})$$



- Extrapolations at different SRG α and without SRG are consistent with each other to within estimated extrapolation uncertainty

Okubo–Lee–Suzuki renormalization

- Divide large (but finite) space into a ’P’-space and a ’Q’-space
- Construct unitary transformation that decouples ’P’- and ’Q’-space
- Effective Hamiltonian and other operators in ’P’-space
- Physical observables remain the same



Okubo–Lee–Suzuki renormalization

- Diagonalize original Hamiltonian $H = T + V$,
  to obtain D eigenvalues E_i and matrix of eigenvectors U

$$U\, H\, U^\dagger \;=\; \mathrm{diag}(E_i)$$

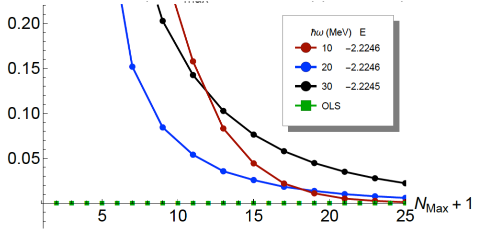
- Project U to the P-space: $U_P = P^T\, U\, P$
- Calculate the norm of $U_P^\dagger\, U_P$, that is,
  the d eigenvalues N_i of $U_P^\dagger\, U_P$ and corresponding eigenvectors W
- Iff $||U_P^\dagger\, U_P|| > 0$, that is,
  if all eigenvalues are positive, we can proceed

$$\begin{aligned} H_{\mathrm{OLS}} &= \left[W\,\mathrm{diag}(1/\sqrt{N_i})\, W^\dagger\, P^T\right]\; H\; \left[P\, W\,\mathrm{diag}(1/\sqrt{N_i})\, W^\dagger\right] \\ &= U_{\mathrm{OLS}}\, H\, U_{\mathrm{OLS}}^\dagger \;=\; P^T\, T\, P + V_{\mathrm{OLS}} \end{aligned}$$

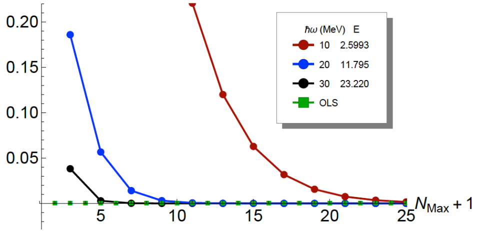
OLS renormalization for deuteron

Toy model: coupled *sd* channel in relative H.O. basis with JISP16

- Fractional difference between converged ground state energy and g.s. energy in smaller bases with $H = T + V_{\text{JISP16}}$

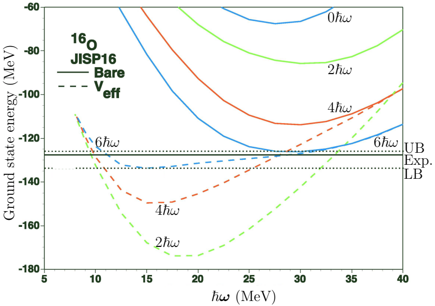


- Same, but with $H = T + V_{\text{JISP16}} + V_{\hbar\omega}^{\text{H.O.}}$

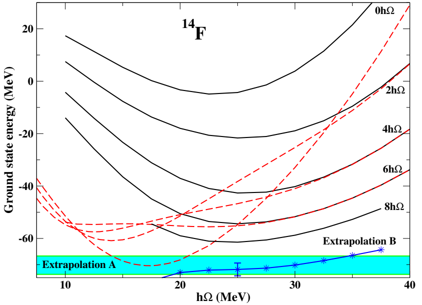


Energies for JISP16 with OLS renormalization

Shirokov, Vary, Mazur and Weber, PLB 644, 33 (2007)



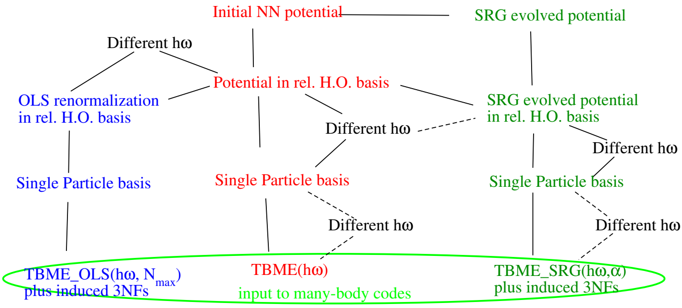
PM, Shirokov and Vary, PRC81, 021301(R) (2010)



OLS renormalized V_{OLS} without induced many-body forces

- About 10 years ago, was believed to be a lower bound
- Extrapolation to complete basis with bare potential is monotonic
- Results V_{OLS} approach bare results as N_{max} increases

Appendix: From (effective) interactions to H.O. matrix elements in single-particle coordinates



Essential H.O. transformations

- Relative $\rightarrow$ single-particle (Talmi-Moshinsky brackets)
- Transformation $\hbar\omega \rightarrow \hbar\tilde{\omega}$ (in relative basis)

Renormalization: SRG evolution and/or OLS in relative basis

For further reading

- J. Carlson, S. Gandolfi, F. Pederiva, S.C. Pieper, R. Schiavilla, K.E. Schmidt and R.B. Wiringa, *Quantum Monte Carlo methods for nuclear physics*, Rev. Mod. Phys. **87**, 1067 (2015).
- E. Epelbaum, H.-W. Hammer and U.-G. Meißner, *Modern Theory of Nuclear Forces*, Rev. Mod. Phys. **81** 1773 (2009).
- R. Machleidt and D.R. Entem, *Chiral effective field theory and nuclear forces*, Phys. Rept. 503, 1 (2011).
- S.K. Bogner, R.J. Furnstahl and A. Schwenk, *From low-momentum interactions to nuclear structure*, Prog. Part. Nucl. Phys. **65**, 94 (2010).
- R. Roth, A. Calci, J. Langhammer and S. Binder, *Evolved Chiral NN+3N Hamiltonians for Ab Initio Nuclear Structure Calculations*, Phys. Rev. C90, 024325 (2014).