Recent results for *p*-shell nuclei using χEFT NN + 3N interactions

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Ab initio nuclear strucuture calculations

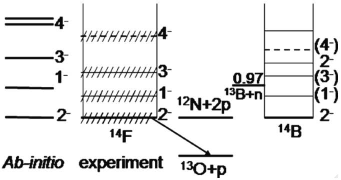
Given a Hamiltonian operator

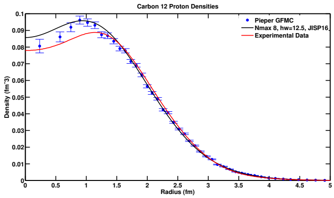
$$\hat{\mathbf{H}} = \sum_{i<j} \frac{(\vec{p}_i - \vec{p}_j)^2}{2\, m\, A} + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \ldots$$

solve the eigenvalue problem for wave function of A nucleons

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

- eigenvalues λ discrete (quantized) energy levels
- eigenvectors: $|\Psi(r_1, \ldots, r_A)|^2$ probability density for finding nucleons 1, ..., A at r_1, ..., r_A





Ab initio nuclear physics – Computational challenges

- Self-bound quantum many-body problem,
  with $3A$ degrees of freedom in coordinate (or momentum) space
- Not only 2-body interactions, but also intrinsic 3-body interactions
  and possibly 4- and higher N-body interactions
- Strong interactions,
  with both short-range and long-range pieces
- Uncertainty quantification for calculations needed
  - for comparisons with experiments
  - for comparisons between different methods
- Sources of numerical uncertainty
  - statistical and round-off errors
  - systematical errors inherent to the calculational method
    - Configuration Interaction (CI) methods: finite basis space
    - Monte Carlo methods: sensitivity to the trial wave function
    - Lattice calculations: finite volume and lattice spacing
  - uncertainty of the nuclear potential

No-Core Configuration Interaction approach

Barrett, Navrátil, Vary, *Ab initio no-core shell model*, PPNP69, 131 (2013)

- Expand wavefunction in basis states $|\Psi\rangle = \sum a_i |\Phi_i\rangle$
- Express Hamiltonian in basis $\langle\Phi_j|\hat{\mathbf{H}}|\Phi_i\rangle = H_{ij}$
- Diagonalize Hamiltonian matrix H_{ij}
- No-Core: all A nucleons are treated the same
- Complete basis $\longrightarrow$ exact result
  - caveat: complete basis is infinite dimensional

- In practice
  - truncate basis
  - study behavior of observables as function of truncation

- Computational challenge
  - construct large $(10^{10} \times 10^{10})$ sparse symmetric matrix H_{ij}
  - obtain lowest eigenvalues & -vectors corresponding to low-lying spectrum and eigenstates

NCCI approach – Basis expansion

- Expand A-body wave function in basis functions

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

- Use basis of single Slater Determinants of Single-Particle states

$$\Phi_i(r_1, \ldots, r_A) = \frac{1}{\sqrt{(A!)}} \begin{vmatrix} \phi_{i1}(r_1) & \phi_{i2}(r_1) & \ldots & \phi_{iA}(r_1) \\ \phi_{i1}(r_2) & \phi_{i2}(r_2) & \ldots & \phi_{iA}(r_2) \\ \vdots & \vdots & & \vdots \\ \phi_{i1}(r_A) & \phi_{i2}(r_A) & \ldots & \phi_{iA}(r_A) \end{vmatrix}$$

which takes care of anti-symmetrization

- Single-Particle basis states $\phi_{ik}(r_k)$
  - eigenstates of SU(2) operators $\hat{\mathbf{L}}^2$, $\hat{\mathbf{S}}^2$, $\hat{\mathbf{J}}^2 = (\hat{\mathbf{L}} + \hat{\mathbf{S}})^2$, and $\hat{\mathbf{J}}_\mathbf{z}$ with quantum numbers n, l, s, j, m
  - radial wavefunctions
    - Harmonic Oscillator
    - Wood–Saxon basis
    - Coulomb–Sturmian
    - ...

Negoita, PhD thesis 2010

Caprio, Maris, Vary, PRC86, 034312 (2012)

NCCI – Truncation schemes

- *M*-scheme: Many-Body basis states eigenstates of $\hat{\mathbf{J}}_\mathbf{z}$

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

  - single run gives entire spectrum
- $N_{\max}$ truncation: Many-Body basis states satisfy

$$\sum_{k=1}^{A} (2\, n_{ik} + l_{ik}) \quad \leq \quad N_0 + N_{\max}$$

  - exact factorization of Center-of-Mass motion
- Alternatives:
  - FCI (commonly used in nuclear shell model, quantum chemistry, ...) truncation on Single-Particle basis states only
  - 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)
  - ...

Intermezzo: Center-of-Mass motion

- Use single-particle coordinates, not relative (Jacobi) coordinates
  - straightforward to extend to many particles
  - have to separate Center-of-Mass motion from relative motion
- Center-of-Mass wavefunction factorizes for H.O. basis functions in combination with $N_{\rm max}$ truncation

$$|\Psi_{\rm total}\rangle = |\phi_1\rangle \otimes \ldots \otimes |\phi_A\rangle$$
$$= |\Phi_{\text{Center-of-Mass}}\rangle \otimes |\Psi_{\rm rel}\rangle$$

where
$$\hat{\mathbf{H}}_{\rm rel}|\Psi_{\rm i,\, rel}\rangle = E_{\rm i}|\Psi_{\rm i,\, rel}\rangle$$

- Add Lagrange multiplier to Hamiltonian (Lawson term)

$$\hat{\mathbf{H}}_{\rm rel} \longrightarrow \hat{\mathbf{H}}_{\rm rel} + \Lambda_{\rm CM}\left(\hat{\mathbf{H}}^{\rm H.O.}_{\rm CM} - \frac{3}{2}\hbar\omega\right)$$

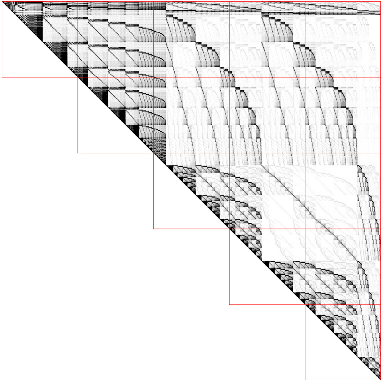
with $\hat{\mathbf{H}}_{\rm rel} = \hat{\mathbf{T}}_{\rm rel} + \hat{\mathbf{V}}_{\rm rel}$ the relative Hamiltonian
  - separates states with CM excitations from states with 0s CM motion $|\Phi_{\rm CM}\rangle = |\Phi_{0s}\rangle$

Hamiltonian – Large sparse matrix

- Express Hamiltonian in basis $\langle \Phi_j | \hat{\mathbf{H}} | \Phi_i \rangle = H_{ij}$
- A-body problem with 2-body interaction

$$H_{ij}^{(A)} = (-1)^{\text{permutations}} \; \delta_{i_1, j_1} \ldots \delta_{i_{(A-2)}, j_{(A-2)}} \; \langle a\, b | \hat{\mathbf{H}} | c\, d \rangle$$

- Sparse symmetric matrix

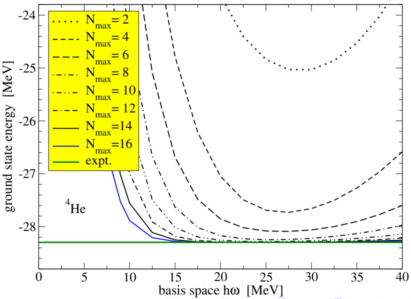


- Obtain lowest eigenvalues using Lanczos algorithm
  - Eigenvalues: bound state spectrum
  - Eigenvectors: wavefunctions

No-Core Configuration Interaction approach

- Expand wave function in basis states $|\Psi\rangle = \sum a_i|\psi_i\rangle$
- Express Hamiltonian in basis $\langle\psi_j|\hat{\mathbf{H}}|\psi_i\rangle = H_{ij}$
- Diagonalize Hamiltonian matrix H_{ij}
- Variational: for any finite truncation of the basis space, eigenvalue is an upper bound for the ground state energy
- Smooth approach to asymptotic value with increasing basis space

- Convergence: independence of both $N_{\max}$ and H.O. basis $\hbar\omega$
  - different methods (NCCI, CC, IM-SRG, GFMC, . . .) using the same interaction should give same results within (statistical plus systematic) numerical uncertainties



Extrapolating to complete basis

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

- Perform a series of calculations with increasing $N_{\rm max}$ truncation
- Extrapolate to infinite model space $\longrightarrow$ exact results
  - Empirical: binding energy exponential in $N_{\rm max}$

$$E^{N}_{\rm binding} = E^{\infty}_{\rm binding} + a_1 \exp(-a_2 N_{\rm max})$$

  - use 3 or 4 consecutive $N_{\rm max}$ values to determine $E^{\infty}_{\rm binding}$
  - use $\hbar\omega$ and $N_{\rm max}$ dependence to estimate numerical error bars

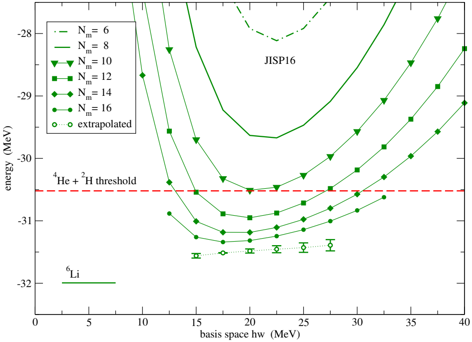
Maris, Shirokov, Vary, PRC79, 014308 (2009)

- Recent studies of IR and UV behavior based on S.P. asymptotics: exponentials in $\sqrt{\hbar\omega/N}$ and $\sqrt{\hbar\omega N}$

Coon *et al*, PRC86, 054002 (2012);
Furnstahl, Hagen, Papenbrock, PRC86, 031301(R) (2012);
More, Ekstrom, Furnstahl, Hagen, Papenbrock, PRC87, 044326 (2013);
Wendt, Forssén, Papenbrock and Sääf, PRC91, 061301 (2015);

Extrapolating to complete basis – in practice

- Perform a series of calculations with increasing N_{max} truncation



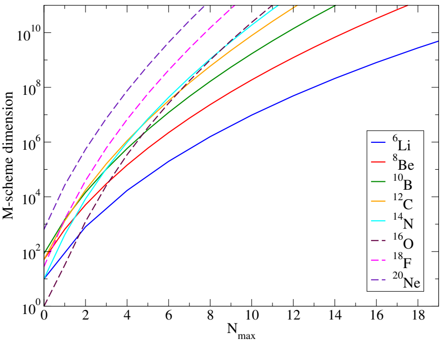
- H.O. basis up to $N_{\text{max}} = 16$ and exponential extrapilation $E_b = -31.49(3)$ MeV

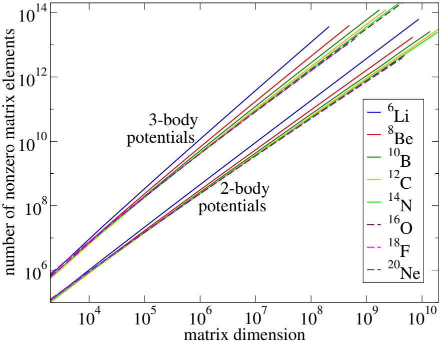
Cockrell, Maris, Vary, PRC86, 034325 (2012)

- Hyperspherical harmonics up to $K_{\text{max}} = 14$: $E_b = -31.46(5)$ MeV

Vaintraub, Barnea, Gazit, PRC79, 065501 (2009)

NCCI approach – Main Challenge

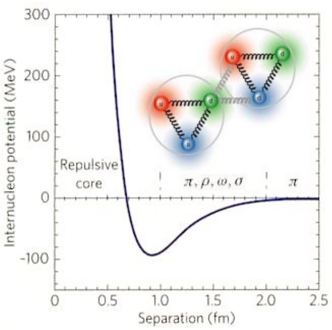




- Increase of basis space dimension with increasing A and N_{max}
  - need calculations up to at least $N_{max} = 8$ for meaningful extrapolation and numerical error estimates
- More relevant measure for computational needs
  - number of nonzero matrix elements
  - current limit 10^{13} to 10^{14} (Edison, Mira, Titan)

Nuclear interaction

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



Nuclear interaction not well-determined

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

Alphabet of realistic NN potentials

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

Most NN potentials need 3N forces for good agreement with data

Nuclear interactions from Chiral Effective Field Theory

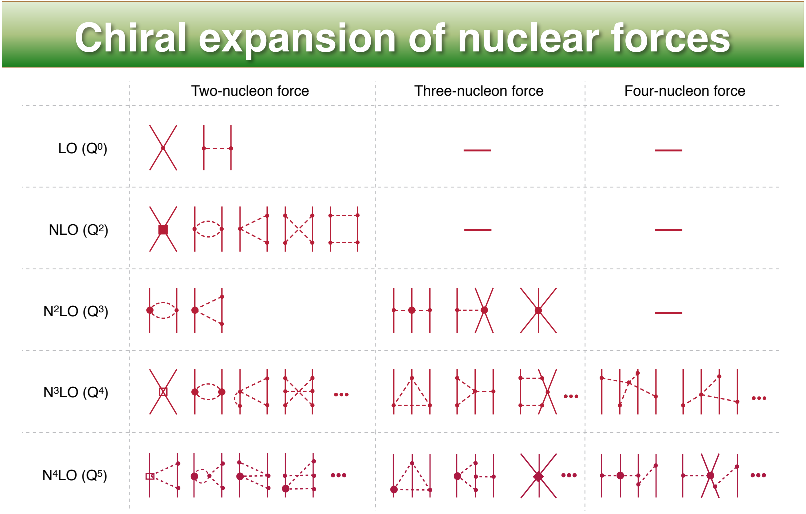
- Strong interaction in principle calculable from lattice QCD
- Use chiral perturbation theory to obtain effective A-body interaction from QCD — Entem and Machleidt, PRC68, 041001 (2003)
  - controlled power series expansion in Q/Λ_χ with $\Lambda_\chi \sim 1$ GeV
  - natural hierarchy for many-body forces

$$V_{NN} \gg V_{NNN} \gg V_{NNNN}$$

- In principle no free parameters
  in practice a few undetermined LEC's, fitted to
  - NN scattering data (plus $A = 3$ systems for 3NFs)
  - select light nuclei NNLO_{opt} — Ekström *et al*, PRL110, 192502 (2013)
  - select nuclei and nuclear matter NNLO_{sat} — Ekström *et al*, PRC91, 051301 (2015)
  - NN scattering data, plus nuclei using PETs — Shirokov *et al*, PLB761, 87 (2016)
- Not unique
  - different choices for regulators
  - different formulations: pionless χEFT, explicit Δ's, ...

Nuclear interaction from Chiral Effective Field Theory

- Controlled power series expansion in Q/Λ



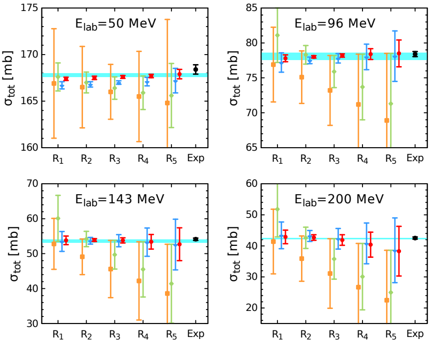
NN potential from χEFT up to N^{4}LO

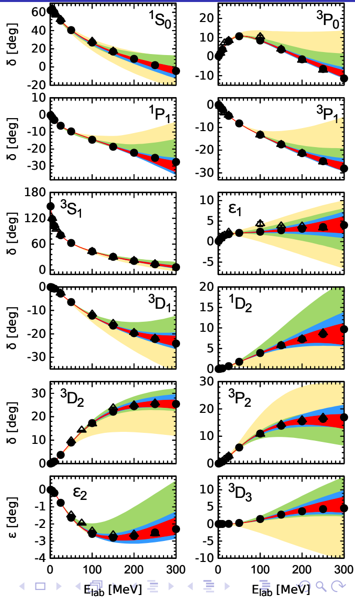
Epelbaum, Krebbs, Meißner, PRL 115 (2015); EPJ A51 (2015)

- Local regulator long-range terms

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

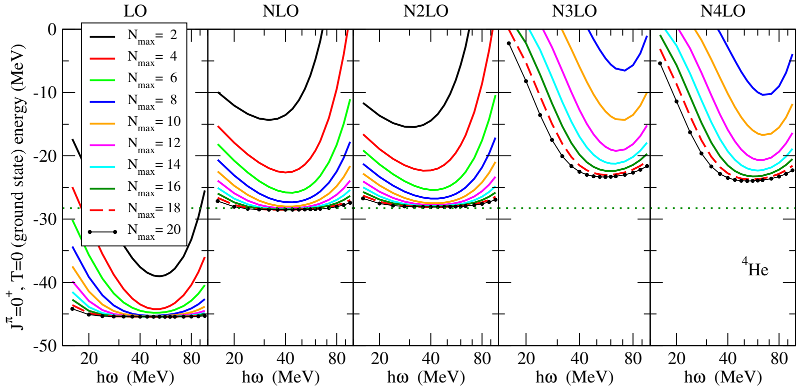
- Regulators $R_1 = 0.8$ to $R_5 = 1.2$ fm
- Reduced finite-cutoff artefacts





Ground state energy of ^{4}He

LENPIC collaboration, PRC 93, 044002 (2016)

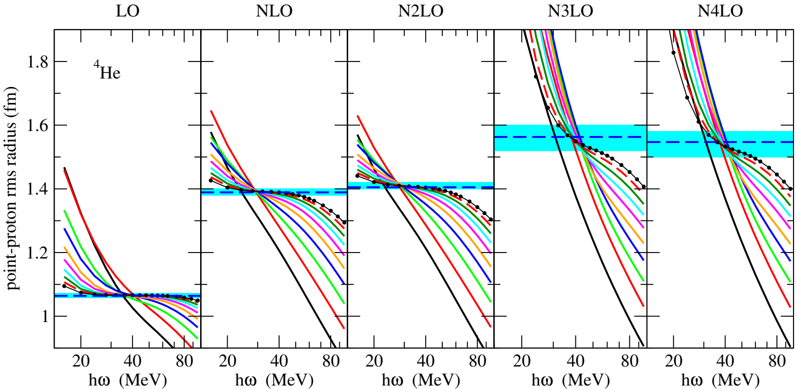


Chiral *NN* interaction with regulator $R = 1.0$ fm ($\Lambda = 600$ MeV)

- 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

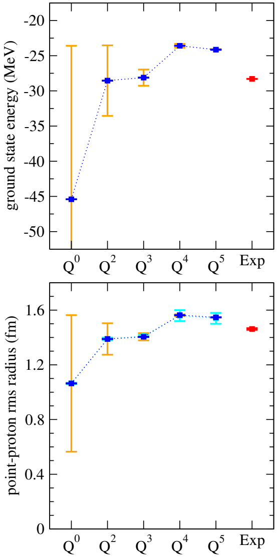
LENPIC collaboration, PRC 93, 044002 (2016)



- 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 $m_\pi/\Lambda \approx 0.23$

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

- Expected chiral corrections at order i

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

- Chiral uncertainty estimates

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

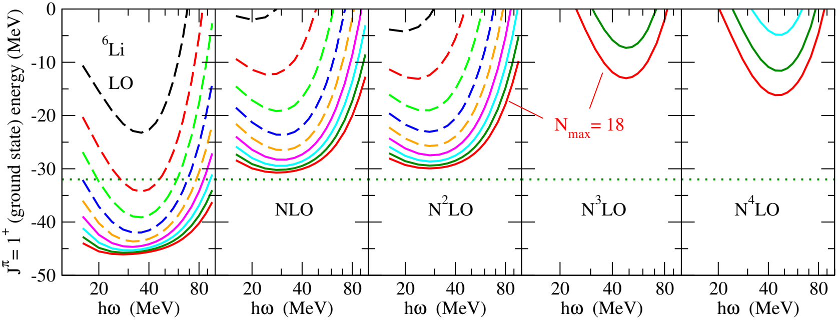
- 3NF at N^{2}LO ($i = 3$) and up not yet included

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

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

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 Similarity Renormalization Group (SRG) to accelerate convergence

Renormalization

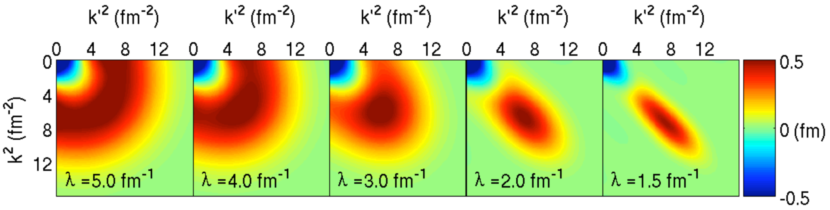
Challenge: achieve numerical convergence for No-Core CI calculations using a finite amount of CPU time on current HPC systems

- 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 (SRG)
  - Okubo–Lee–Suzuki (OLS)
  - $V_{\mathrm{low}\,k}$, 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 – NN interaction

- SRG evolution

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



  - drives interaction towards band-diagonal structure
  - SRG shifts strength between 2-body and many-body forces

- Initial χEFT Hamiltonian power-counting hierarchy

$$V_{NN} \gg V_{NNN} \gg V_{NNNN}$$

  - key issue: preserve hierarchy of many-body forces

Bogner, Furnstahl, Maris, Perry, Schwenk, Vary, NPA801, 21 (2008)
Jurgenson, Nagratil, Furnstahl, PRL 103, 082501 (2009)

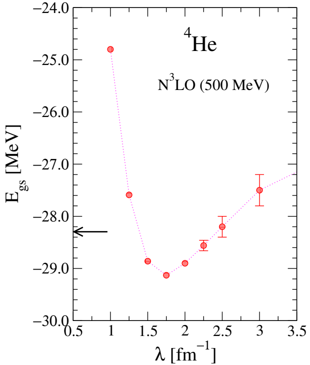
^{4}He with SRG evolved χEFT including (induced) 3NF

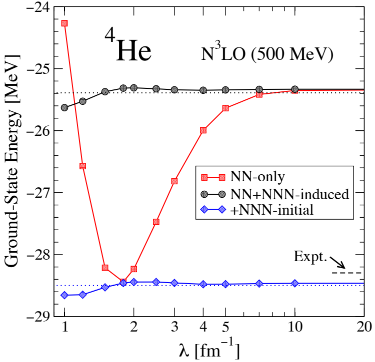
Bogner *et al*, NPA 801, 21 (2008)

(without Coulomb interaction)

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

(with Coulomb interaction)



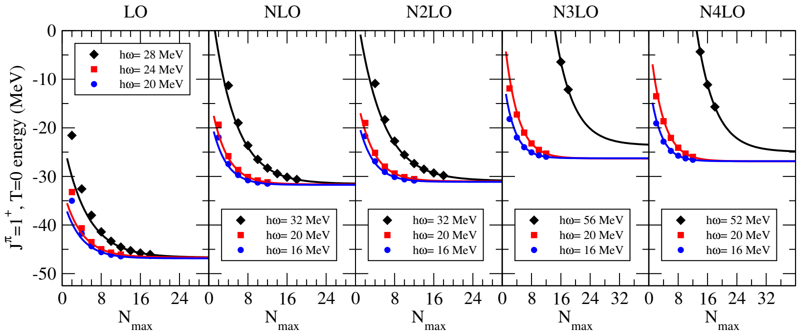


- Strong SRG parameter $\alpha = \lambda^{-4}$ dependence without induced 3NF
- Almost no SRG parameter $\alpha = \lambda^{-4}$ dependence with induced 3NF
- Explicit 3NF needed for agreement with experiment

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

- Empirical extrapolation method (ground state) energies

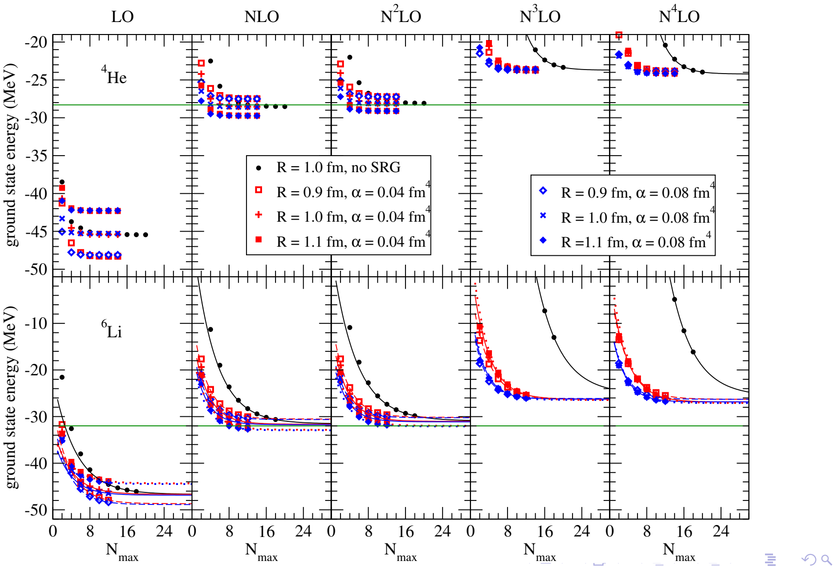
$$E(N_{max}) \approx E_\infty + a \exp(-b N_{max})$$



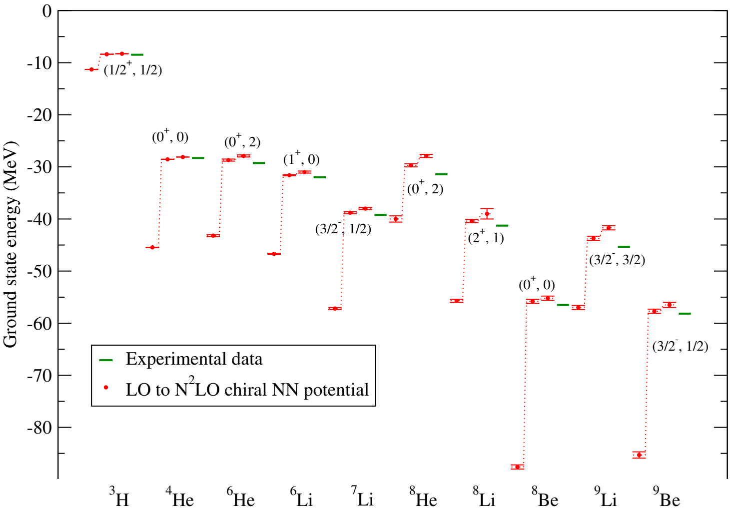
- Extrapolations at different SRG α and without SRG are consistent with each other to within estimated extrapolation uncertainty

Dependence on regulator *R* and SRG parameter α

LENPIC collaboration, in preparation



Ground state energies up to N^{2}LO for $A = 3$ to $A = 9$

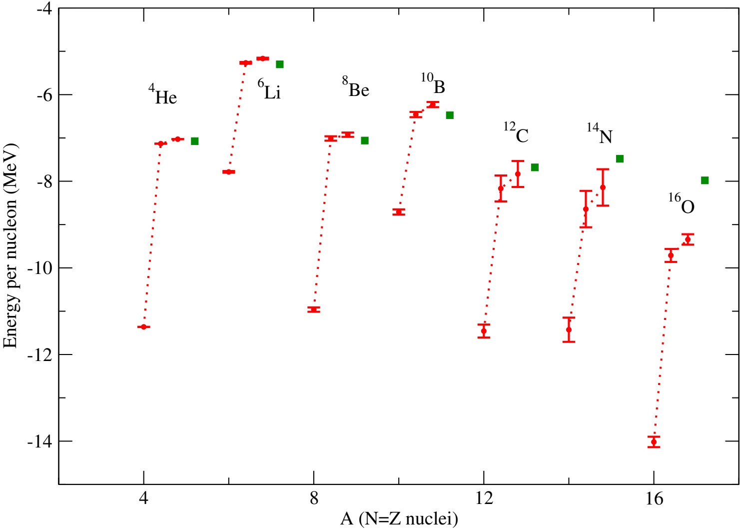


- NN only
- $R = 1.0$ fm
- many-body uncertainties shown

LENPIC collaboration

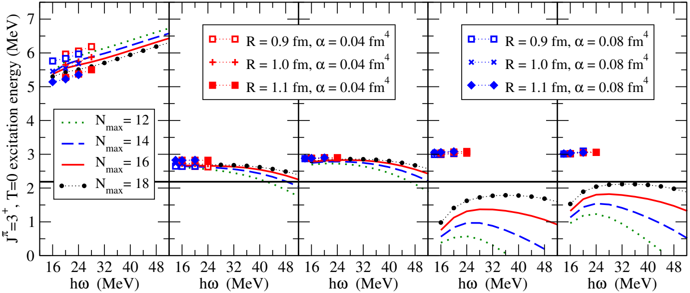
in preparation

$N = Z$ Ground state energies up to N^{2}LO



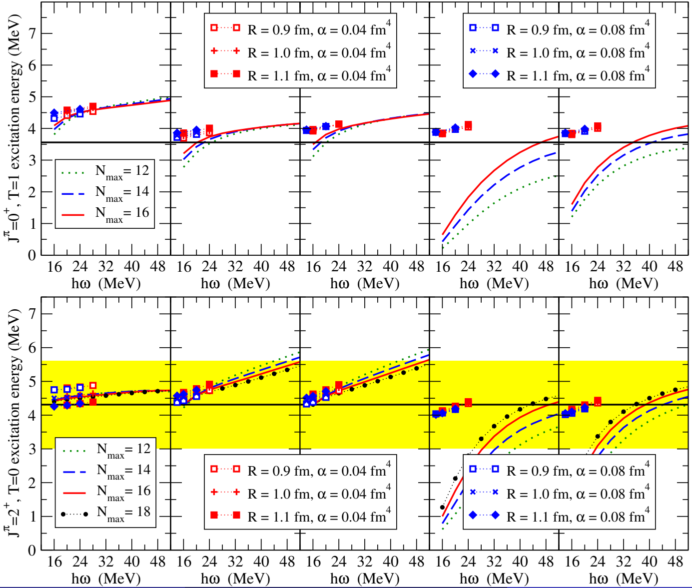
Excitation energies ^{6}Li

LENPIC collaboration, in preparation



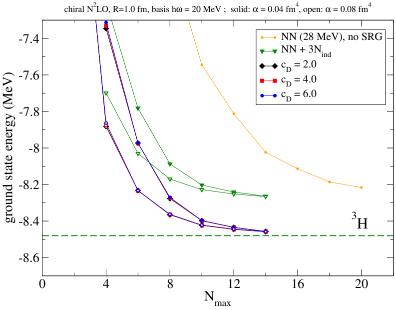
- NLO and N^{2}LO well converged
- SRG evolved N^{3}LO and N^{4}LO SRG also converged
- NLO and higher converged in chiral expansion?
  - reasonable agreement with data
  - only weakly dependent on regulator *R*

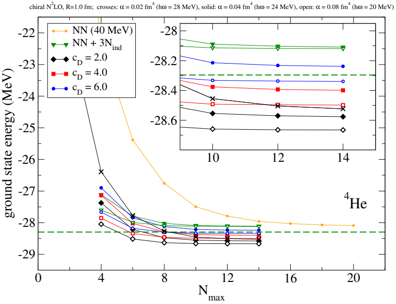
Excitation energies ^{6}Li



Including N^2LO 3N interaction

LENPIC collaboration, work in progress

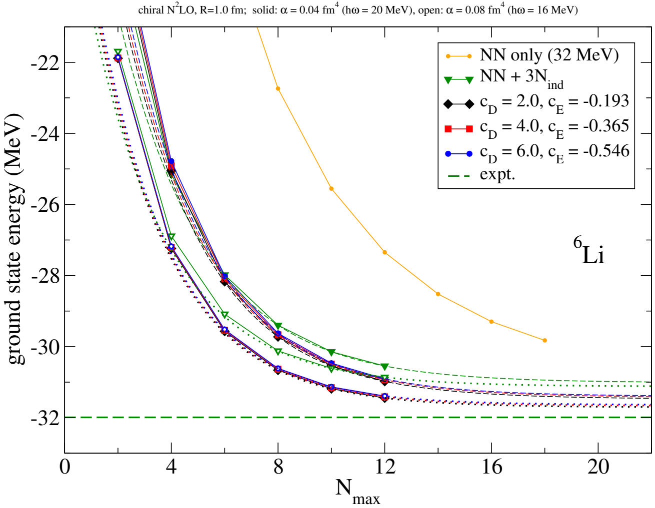




- (c_D, c_E) fitted to reproduce ground state energy ^{3}H
- $A = 3$: no SRG parameter dependence
- $A = 4$: weak ($\sim$ 0.1 MeV) SRG parameter with explicit 3NF (negligible SRG parameter dependence without explicit 3NF)

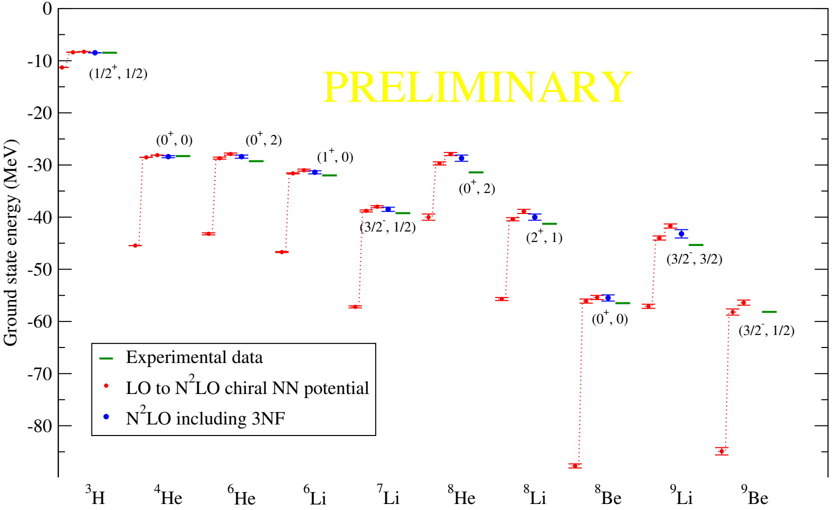
Including N^2LO 3N interaction

LENPIC collaboration, work in progress

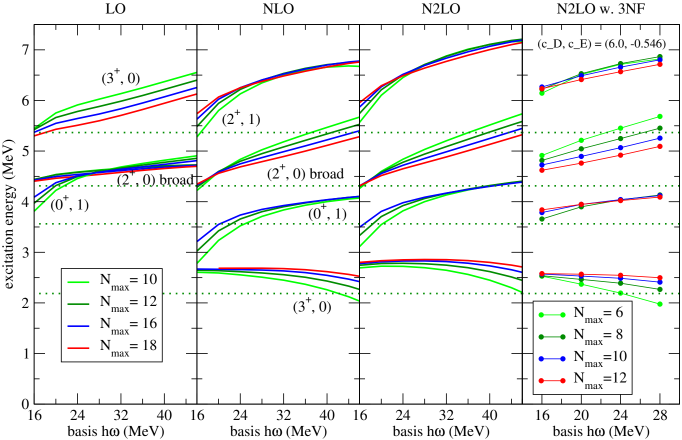


- extrapolation uncertainty ~ 0.1 MeV
- dependence on SRG α ~ 0.2 MeV
- dependence on (c_D, c_E) ~ 0.1 MeV
- gs energy NN only -31.0 ± 0.2 MeV with 3NF -31.4 ± 0.3 MeV

Ground state energies up to N^{2}LO including 3NF



Spectrum ^{6}Li up to N^{2}LO including 3NF



$T = 1$ states

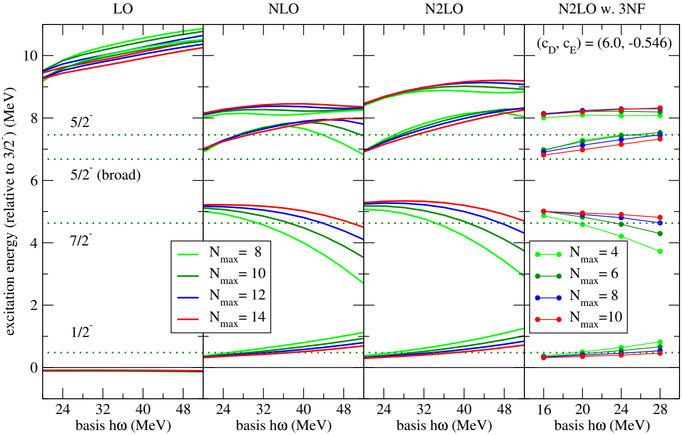
- analog states of ^{6}He
- not very well converged

Broad 2^+

- not converged
- need to include continuum

- Excitation energy of 3^+ state reasonably well converged, seems insensitive to higher chiral orders
- Question: does deviation from experiment decrease at N^{3}LO?

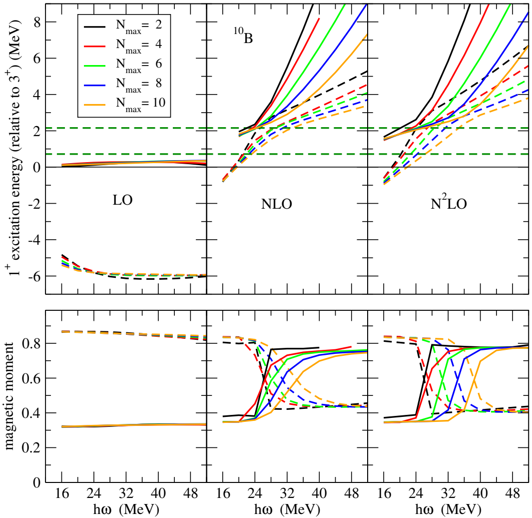
Spectrum ^{7}Li up to N^{2}LO



- $\frac{1}{2}^-$ and $\frac{3}{2}^-$: α plus triton in $L = 1$ state
- $\frac{5}{2}^-$ and $\frac{7}{2}^-$: α plus triton in $L = 3$ state
- second $\frac{5}{2}^-$ different structure

- LO: $\frac{1}{2}^-$ just below $\frac{3}{2}^-$ and $\frac{5}{2}^-$ just below $\frac{7}{2}^-$
- Second (narrow) $\frac{5}{2}^-$ sensitive 3NF

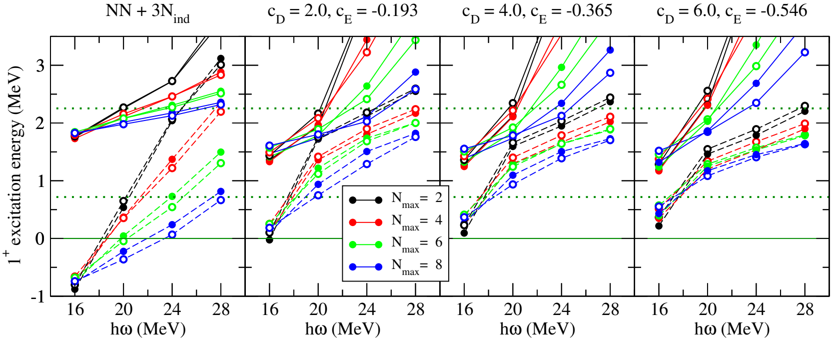
Spectrum ^{10}B: 1^+ states



- Two low-lying 1^+ levels
  - LO: well seperated
  - NLO (and higher): mix and cross, depending on basis parameters ($N_{\text{max}}, \hbar\omega$)
- Can be distinguished by e.g. magnetic moments
  - state with $\mu \sim 0.4$ and $E_x \sim 2$ to 3 MeV
  - state with $\mu \sim 0.8$ and E_x strongly dependent on basis

Jurgenson et al. PRC87 (2013)

Spectrum ^{10}B at N^{2}LO: influence of 3NFs



- At N^{2}LO without 3NF's: lowest 1^+ below 3^+
- With 3NF's correct 3^+ ground state
- Preferred LEC's: $(c_D, c_E) = (6.0, -0.546)$
- Numerical uncertainties hard to estimate due to mixing ...

Conclusions and Outlook

- Systematic calculations for *p*-shell nuclei
  - order-by-order in χEFT
- Same interactions also used for $A = 3$ and $A = 4$
  - Faddeev and Faddeev–Yakubovsky calculations
  - benchmark for NCCI calculations
- Same interactions also used for heavier nuclei
  - IM-SRG and CC
  - benchmark with NCCI calculations for ^{16}O
- Uncertainty Quantification
  - many-body method – dependence on basis space
  - renormalization – SRG parameter dependence
  - nuclear interaction – order in χEFT expansion
- Work in progress
  - UQ of excitation energies?
  - Consistent electroweak operators
  - 3NF at N^3LO