12C and A=10 nuclei with SRG evolved chiral two- and three-nucleon interactions

NUCLEI
Nuclear Computational Low-Energy Initiative

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SciDAC project – NUCLEI
lead PI: Joe Carlson (LANL)
http://computingnuclei.org

PetaApps award
lead PI: Jerry Draayer (LSU)

INCITE award – Computational Nuclear Structure
lead PI: James P Vary (ISU)

NERSC

SciDAC
Scientific Discovery through Advanced Computing

National Science Foundation
WHERE DISCOVERIES BEGIN

Office of Science
INCITE
Advancing America's Science and Industrial Competitiveness

NERSC

Ab initio nuclear physics – Quantum many-body problem

- 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

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

  - 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
- Self-bound quantum many-body problem, with $3(A-1)$ degrees of freedom
- 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

No-Core Configuration Interaction calculations

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 Configuration Interaction
  - 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 real matrix H_{ij}
  - use Lanczos algorithm to obtain lowest eigenvalues & -vectors

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 $\phi_{ik}(r_k)$ quantum numbers n, l, s, j, m
- Radial wavefunctions: Harmonic Oscillator, Wood–Saxon, Coulomb–Sturmian, Berggren (for resonant states)
- M-scheme: Many-Body basis states eigenstates of $\hat{\mathbf{J}}_\mathbf{z}$

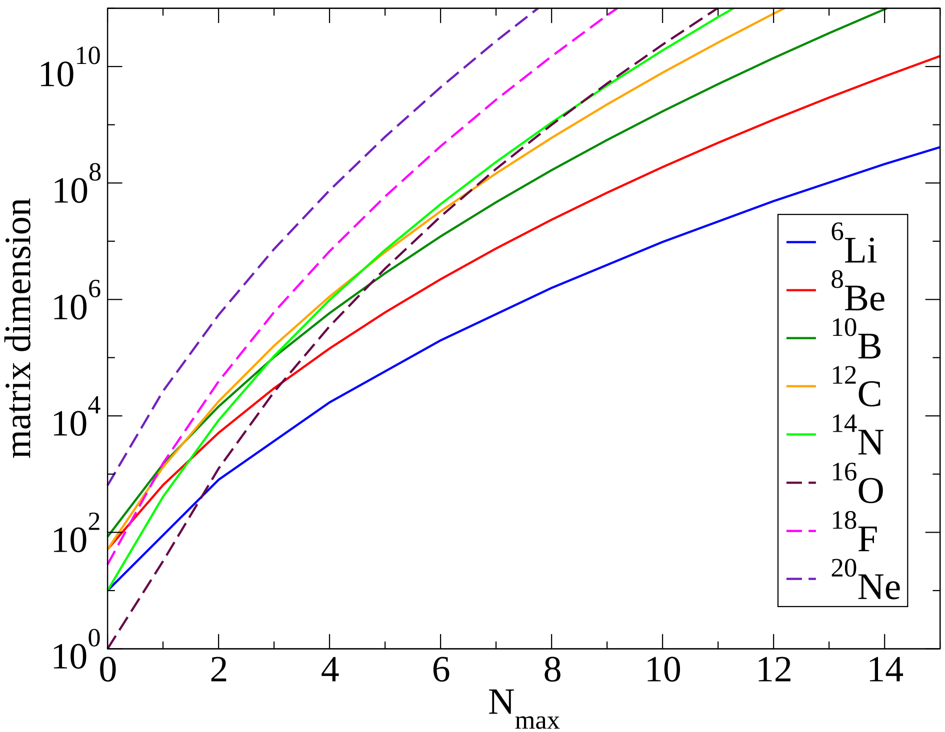
$$\hat{\mathbf{J}}_\mathbf{z}|\Phi_i\rangle = M|\Phi_i\rangle = \sum_{k=1}^{A} m_{ik}|\Phi_i\rangle$$

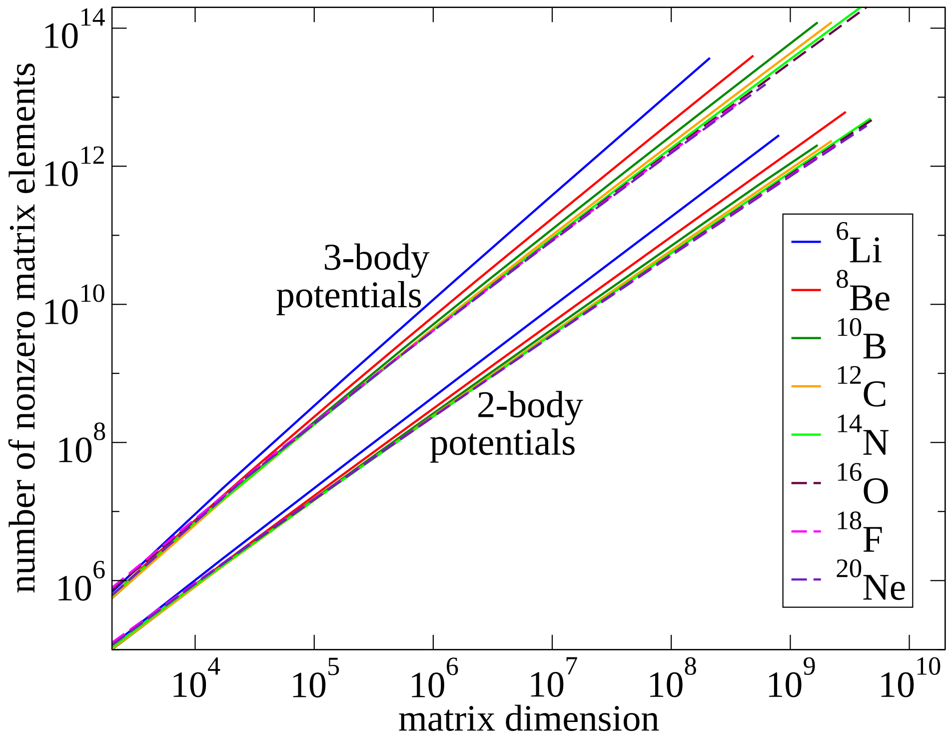
- N_{max} truncation: Many-Body basis states satisfy

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

- Alternatives:
  - 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)
  - . . .

NCCI calculations – main challenge





- Increase of basis space dimension with increasing A and N_{max}
  - need calculations up to at least $N_{\text{max}} = 8$ 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)

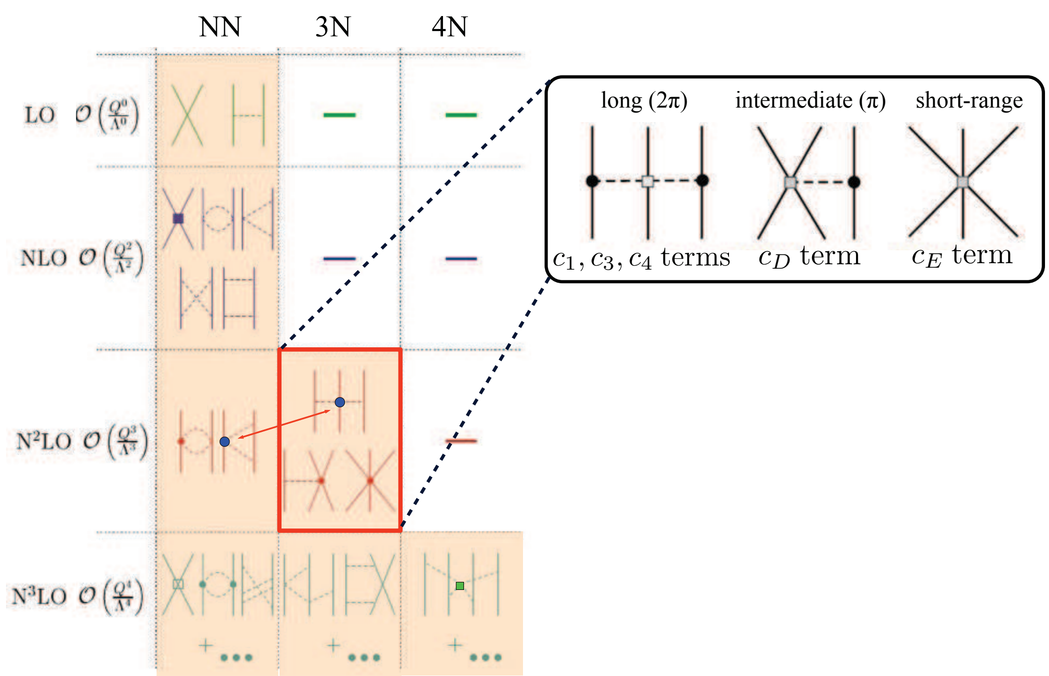
Nuclear interaction from chiral perturbation theory

- Strong interaction in principle calculable from 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 parameters
  - renormalization typically necessary

Leading-order 3N forces in chiral EFT



Intermezzo: Consistent chiral EFT 2- and 3-body interactions

Low
Energy
Nuclear
Physics
International
Collaboration

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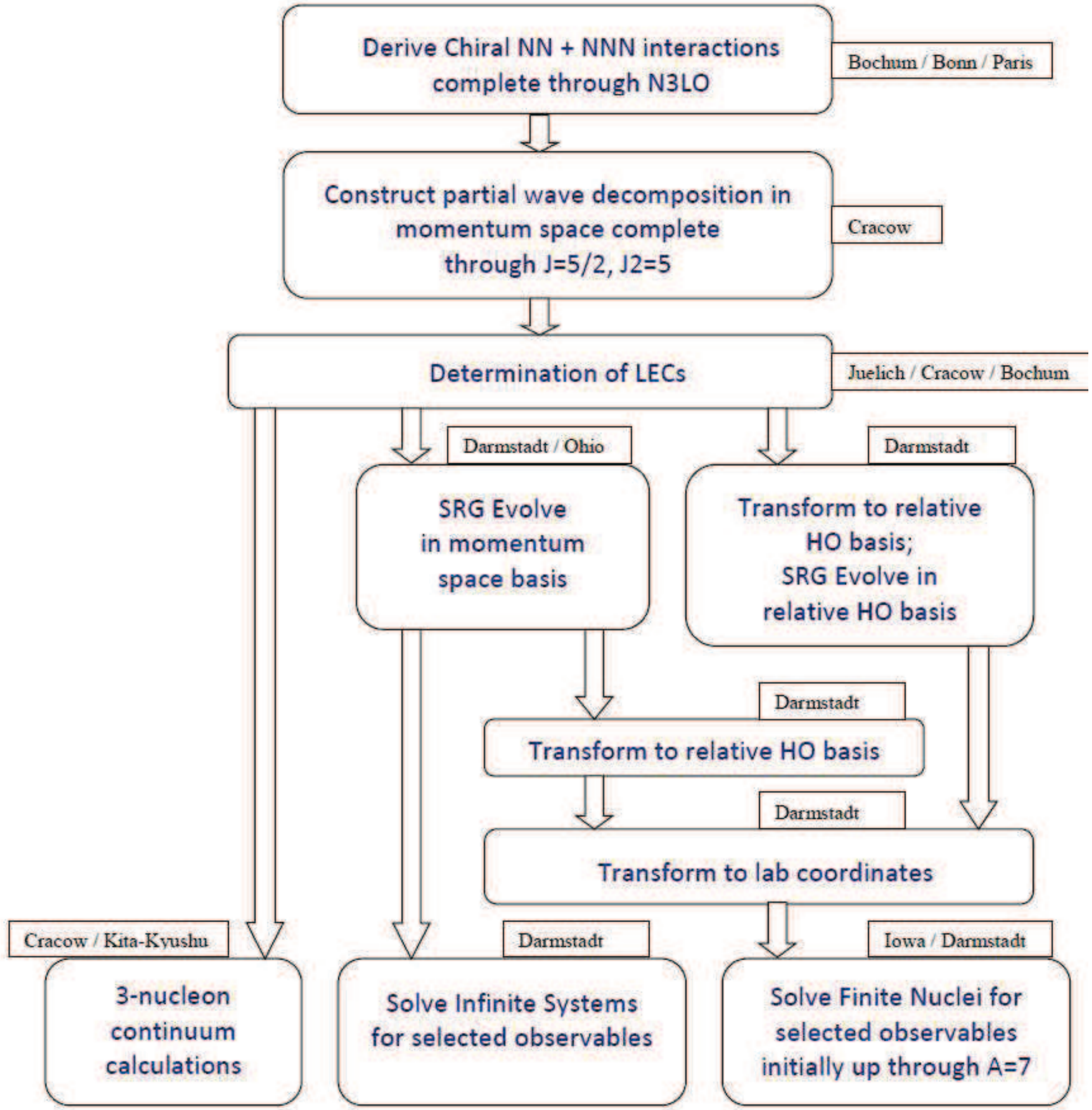
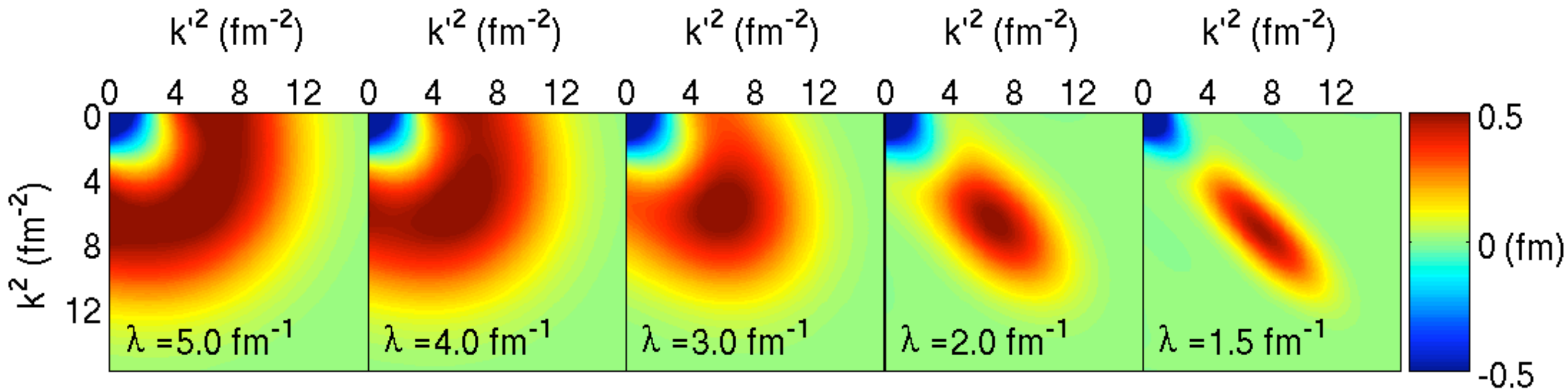


Similarity Renormalization Group – NN interaction

- 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 chiral EFT Hamiltonian
  power-counting hierarchy A-body forces

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

  - key issue: preserve hierarchy of many-body forces

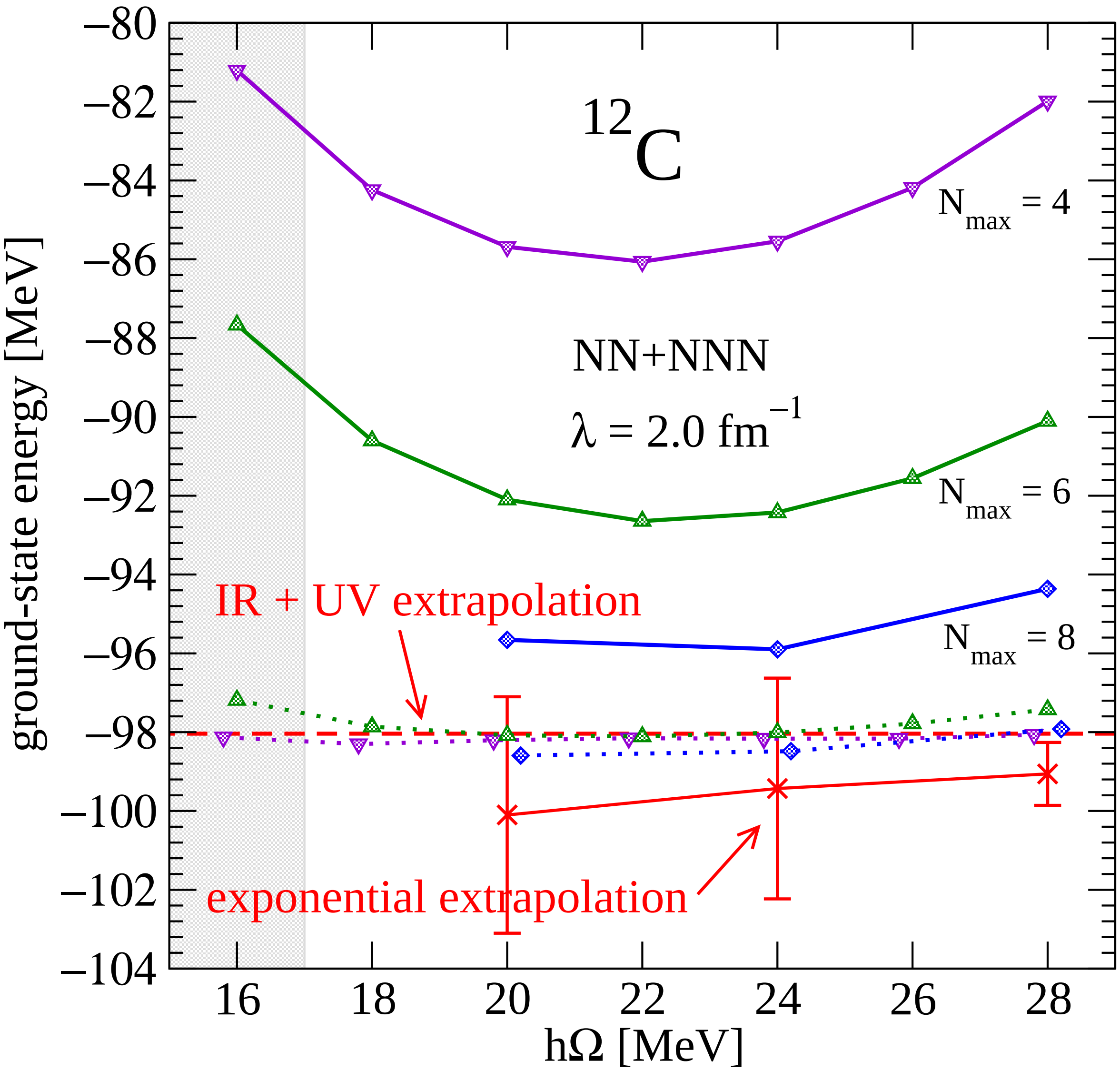
Bogner, Furnstahl, Maris, Perry, Schwenk, Vary, NPA801, 21 (2008)

Roth, Langhammer, Calci, Binder, Navrátil, PRL 107 072501 (2011)

Jurgenson, Maris, Furnstahl, Navrátil, Ormand, Vary, PRC87 054312 (2013)

Ground state energy of ^{12}C with SRG evolved chiral interaction

Jurgenson, Maris, Furnstahl, Navrátil, Ormand, Vary, PRC87, 054312 (2013)



Interaction

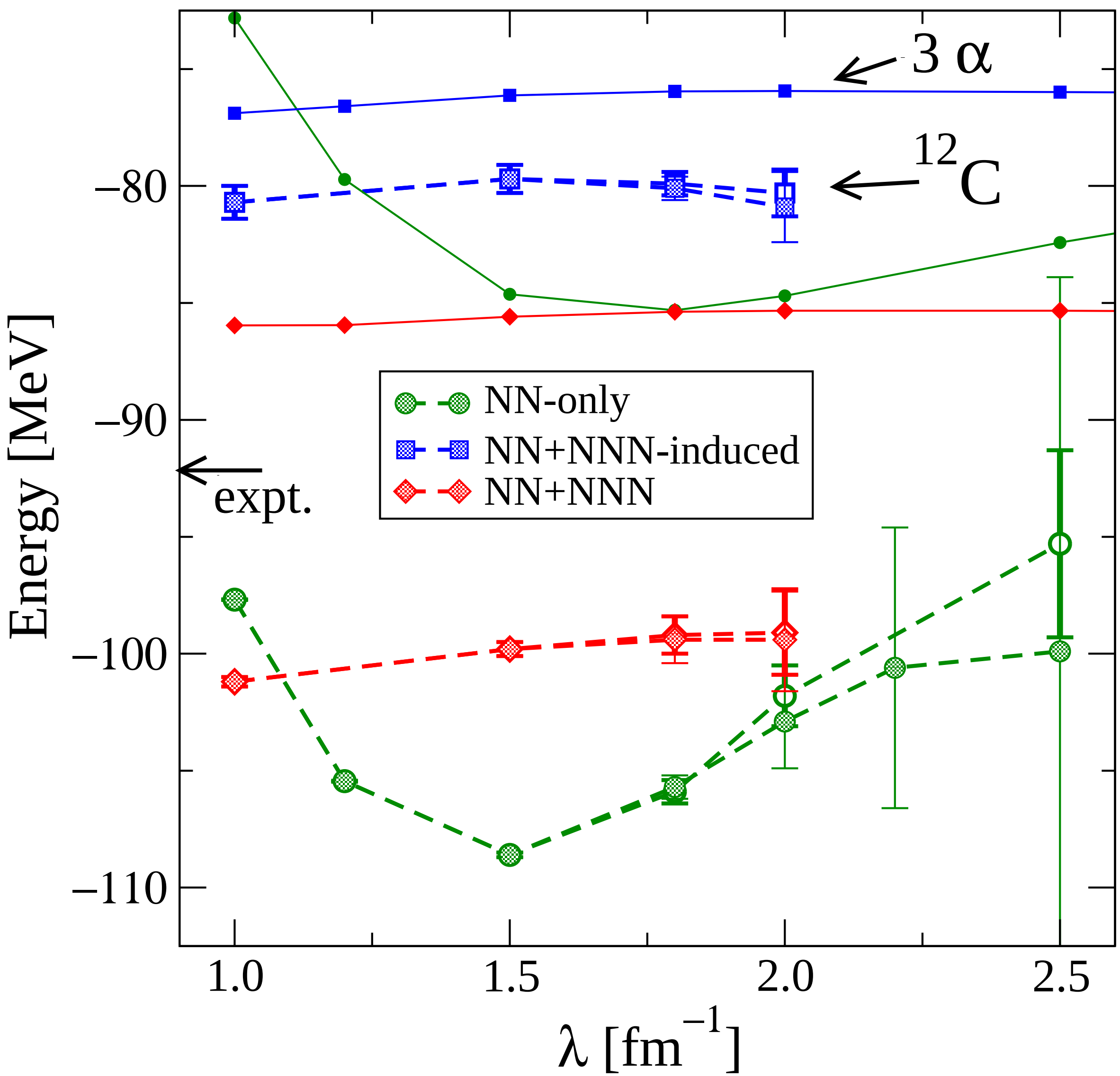
- chiral NN at N^3LO
- chiral 3NF at N^2LO
- 3NF LEC values:
  $c_D = -0.2$
  $c_E = -0.205$
- 500 MeV cutoff

SRG evolved to $\lambda = 2.0$ fm^{-1}

IR and UV extrapolations based on Furnstahl, Hagen, Papenbrock, PRC86, 031301(R) (2012); More, Ekstrom, Furnstahl, Hagen, Papenbrock, PRC87, 044326 (2013)

Running of ground state energy of ^{12}C with SRG evolution

Jurgenson, Maris, Furnstahl, Navrátil, Ormand, Vary, PRC87, 054312 (2013)



Numerical convergence

- good $\lambda < 2.0$ fm^{-1}
- slow $\lambda > 2.0$ fm^{-1}

Dependence on SRG parameter λ

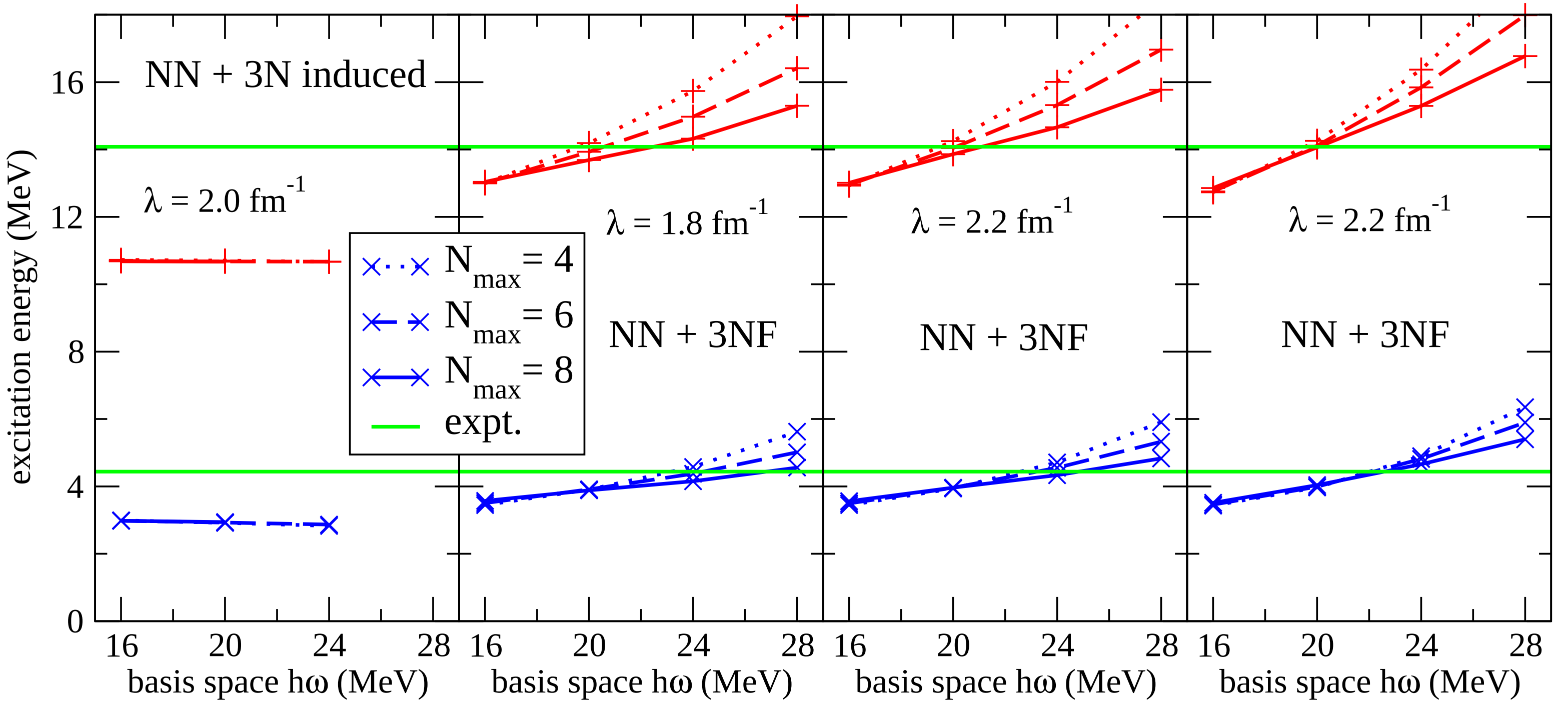
- NN only: strong
- NN + 3N induced: weak
- NN + 3NF: weak

Effect 3NF:

- increase binding energy
- increase 3α threshold

Effect of chiral 3NF – rotational 2^+ and 4^+ states

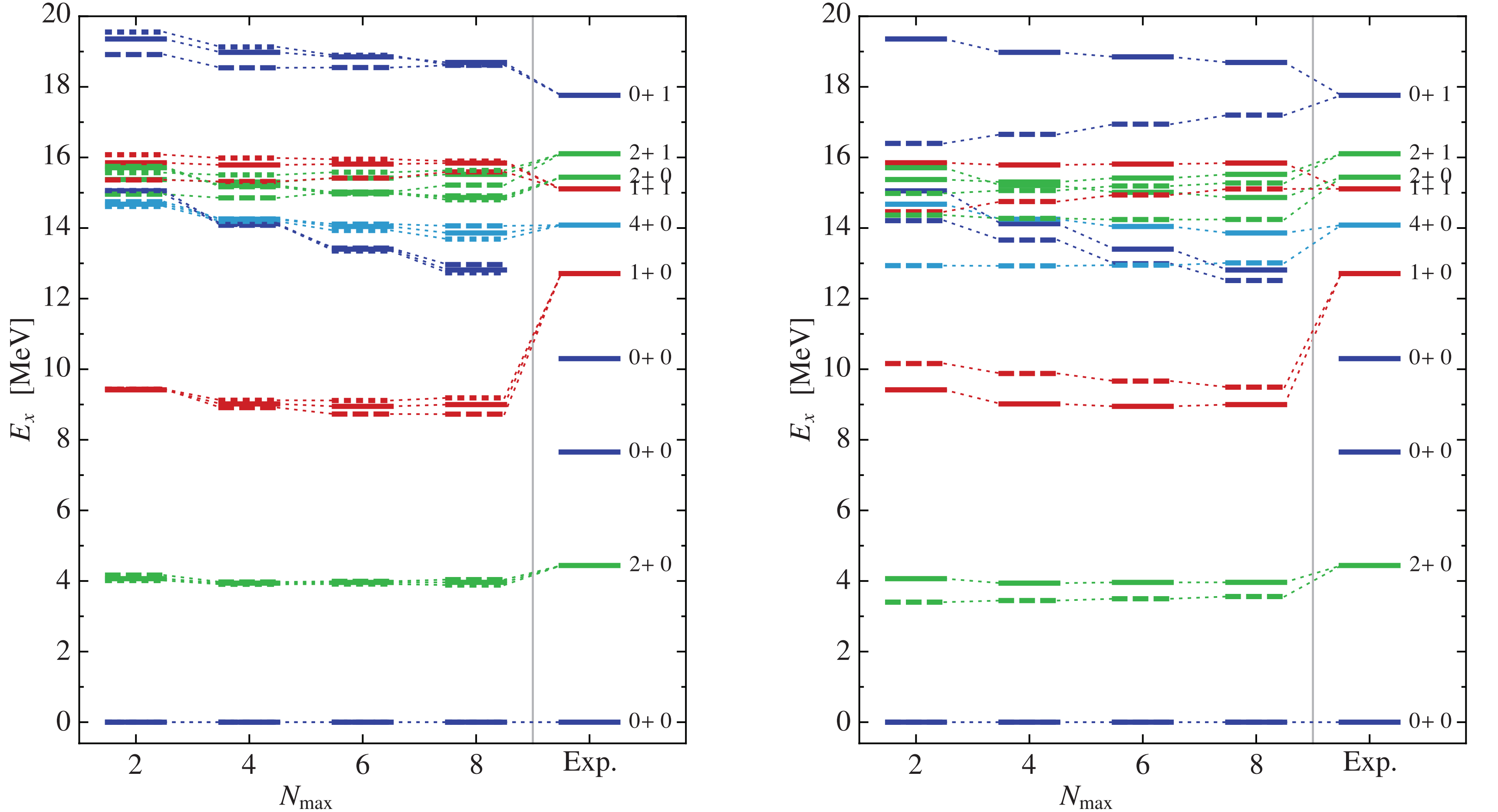
Maris, Aktulga, Binder, Calci, Catalyurek, Langhammer, Ng, Saule, Roth, Vary, Yang
J. Phys. Conf. Ser. 454, 012063 (2013)



- Chiral 3NF improves agreement with data
- Not converged with explicit 3NF, despite weak $N_{\max}$ dependence
- Increase in excitation energy of $(2^+, 0)$ and $(4^+, 0)$ rotational states likely due to increased binding of $(0^+, 0)$

Spectrum of ^{12}C: convergence

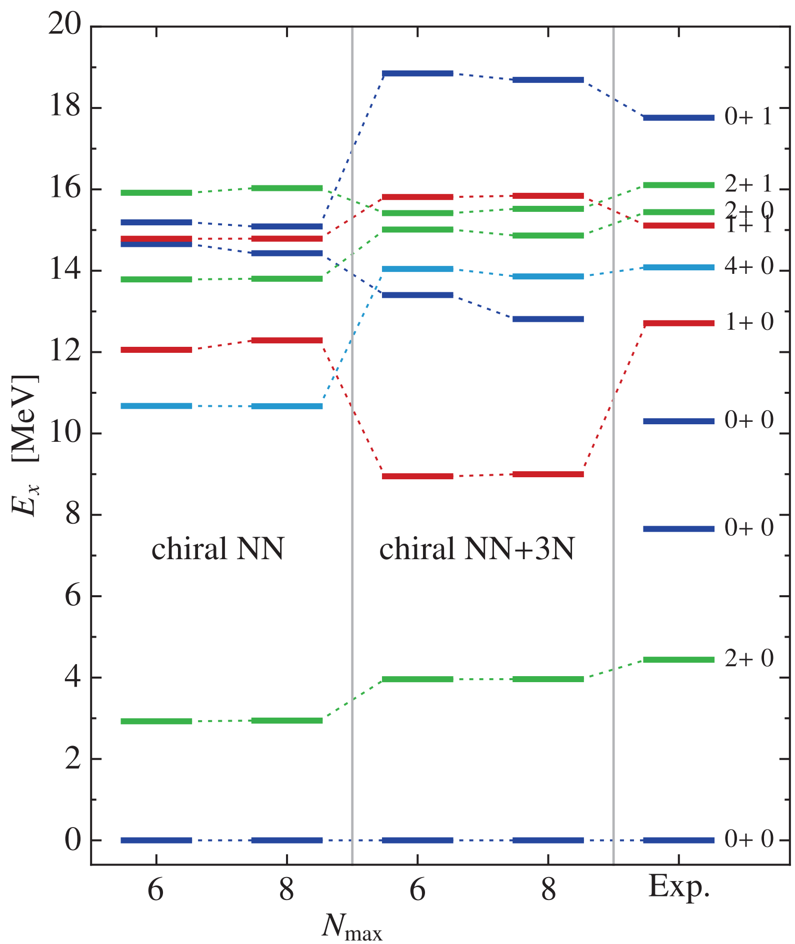
Maris, Vary, Calci, Langhammer, Binder, Roth, PRC90, 014314 (2014)



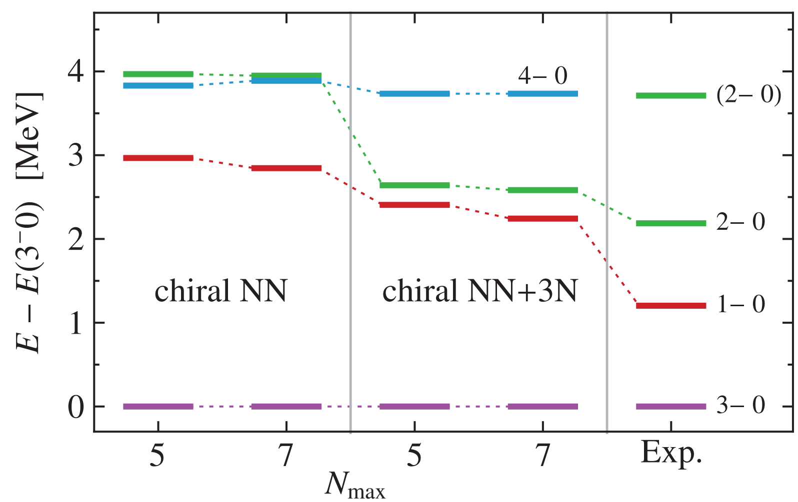
- Excitation energies better converged than total energies
- Dependence of SRG parameter (left) generally smaller than dependence on basis $\hbar\Omega$ (right)

Effect of chiral 3NF

at SRG parameter $\lambda = 2.0$ fm^{-1} and $\hbar\omega = 20$ MeV

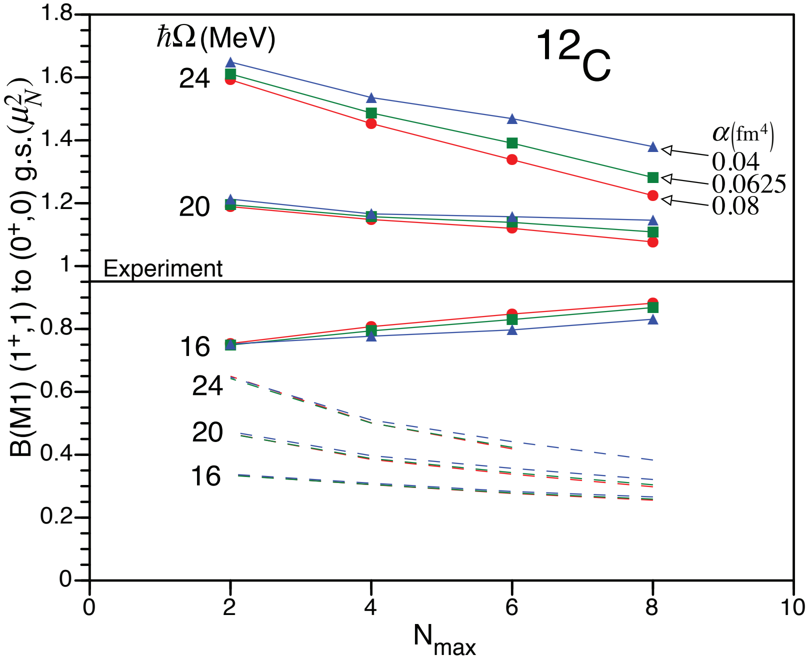


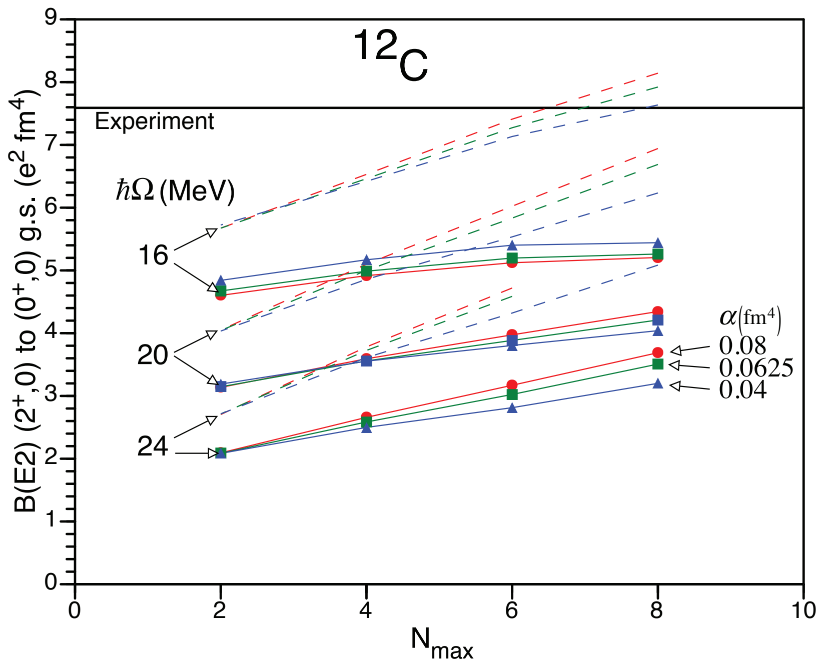
- chiral NN at N^{3}LO
- chiral 3N at N^{2}LO
- 3N LEC values: $c_D = -0.2$, $c_E = -0.205$
- 500 MeV cutoff



- Excitation energies $(1^+, 0)$ and $(0^+, 1)$ sensitive to 3NF
- Negative parity spectrum relative to lowest $(3^-, 0)$ reasonably well converged, and 3NF improves agreement with experiment

Convergence of M1 and E2 transitions

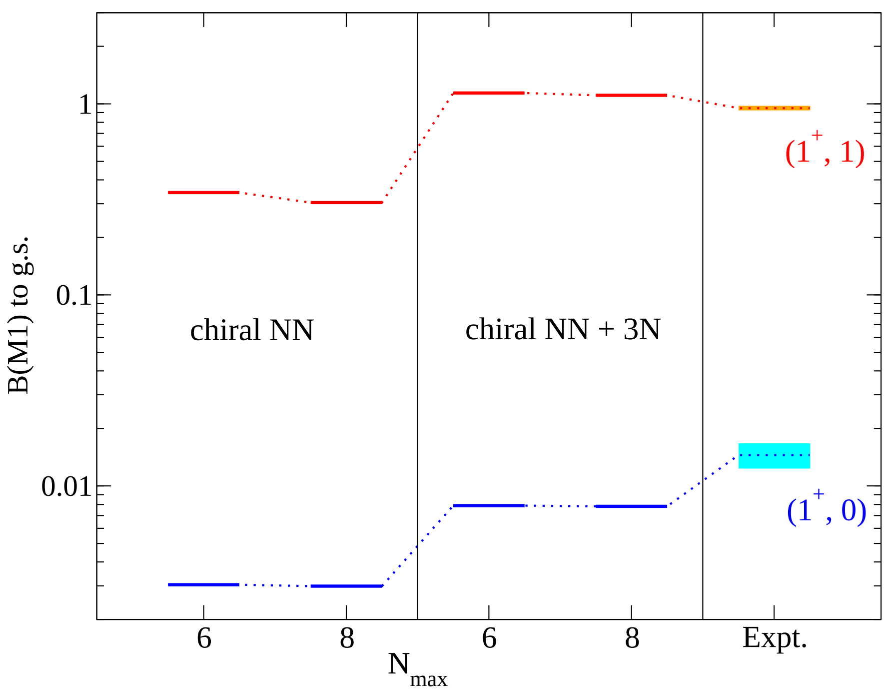


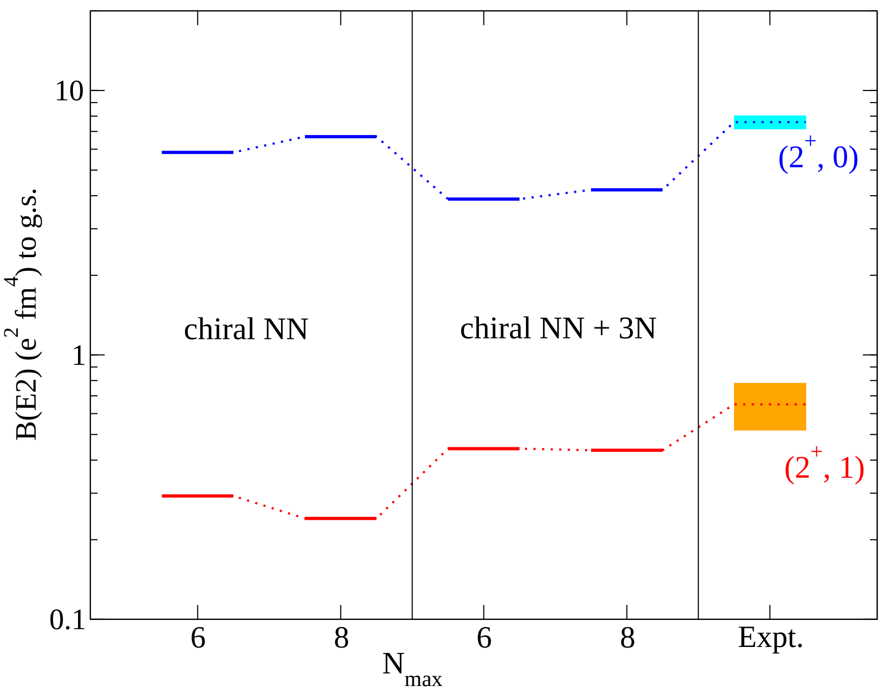


- M1 transitions reasonably converging
- B(M1)$(1^+, 1) \rightarrow (0^+, 0)$ significantly enhanced by 3NF

- E2 transitions not converged
- B(E2)$(2^+, 0) \rightarrow (0^+, 0)$
  - significantly reduced by 3NF
  - consistent with increased E_x and decreased radius and Q

Electromagnetic transitions at SRG parameter $\lambda = 2.0$ fm^{-1} and $\hbar\omega = 20$ MeV



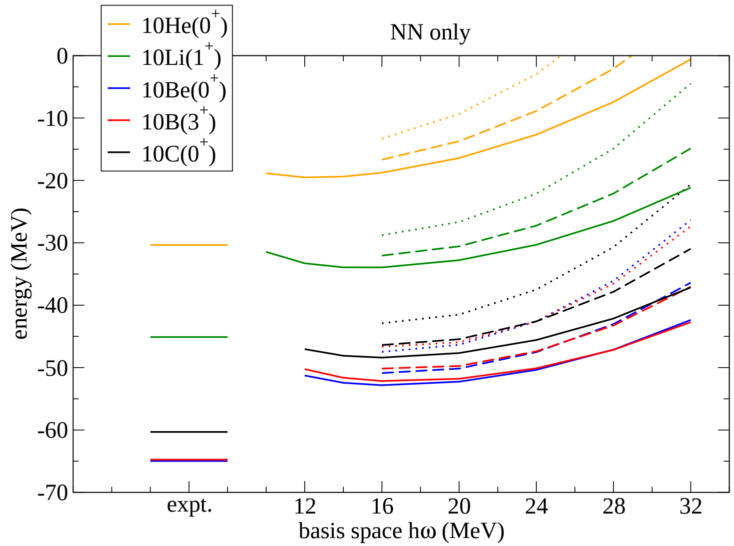


- Transition strengths in qualitative agreement with experiment
- Agreement generally improves by including chiral 3N forces, except for the B(E2)$(2^+, 0) \to (0^+, 0)$ transition
- Future
  - consistent chiral EFT current operators
  - consistent SRG evolution of operators

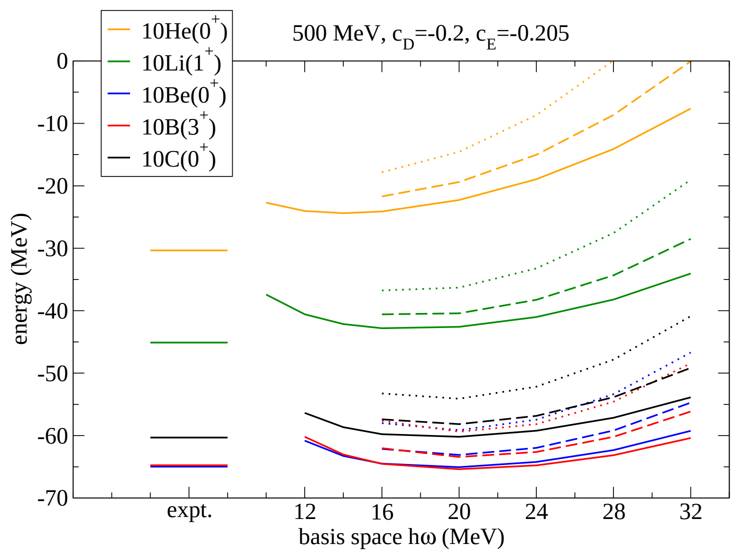
A=10 ground state energies

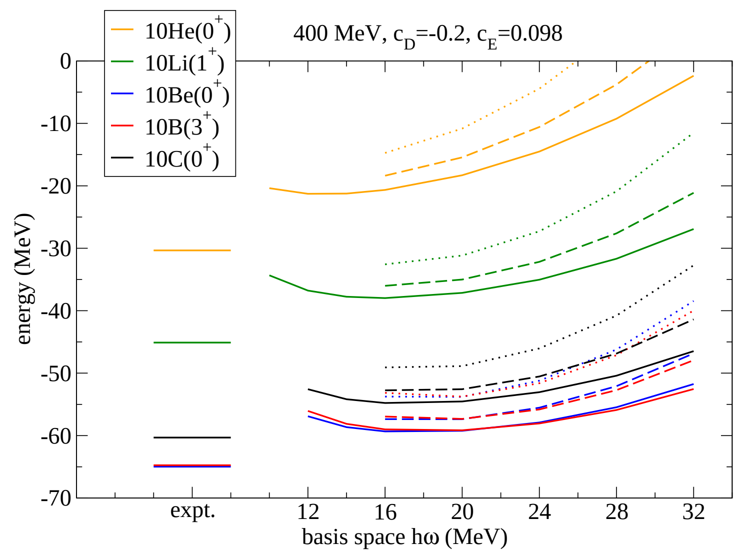
work in progress

preliminary results at SRG parameter $\lambda = 1.8$ fm^{-1}



- Clearly underbound without chiral 3NF
- With chiral 3NF
  - overbound with 500 MeV cutoff, $c_D = -0.2$, $c_E = -0.205$
  - underbound with 400 MeV cutoff, $c_D = -0.2$, $c_E = 0.098$?
- Need extrapolation to complete basis

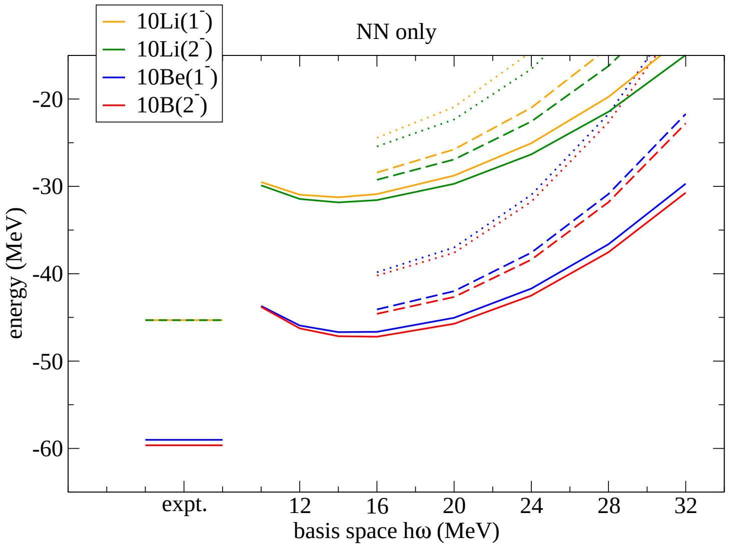




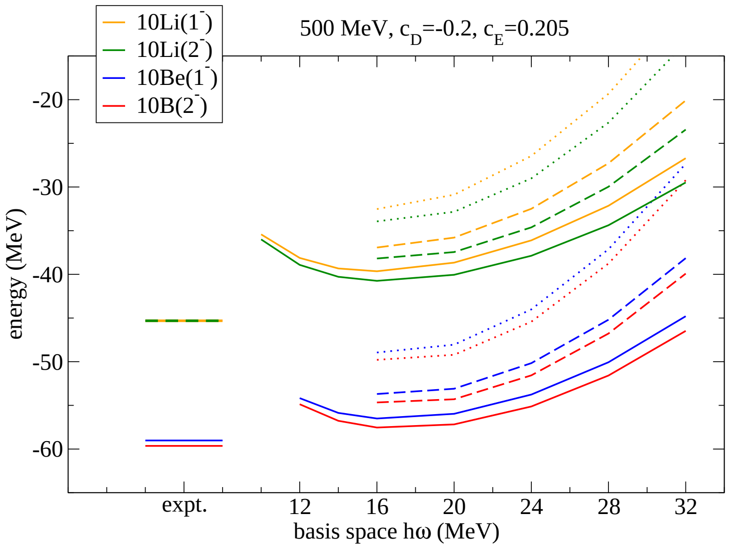
A=10 lowest negative parity states

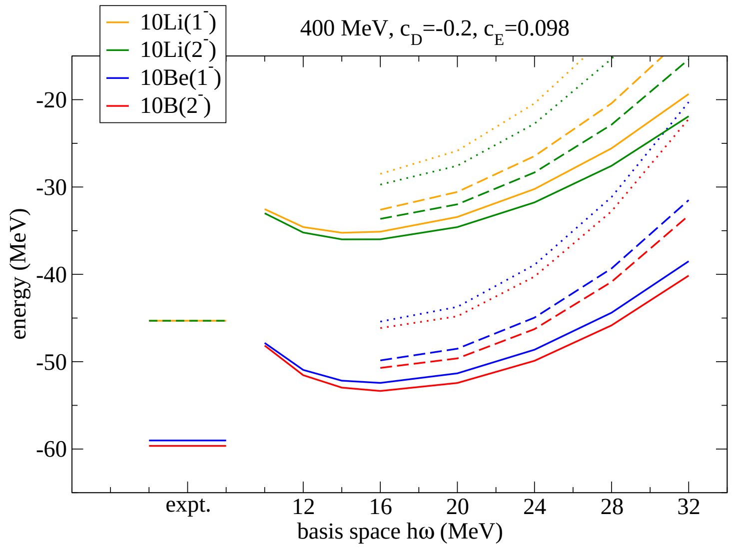
work in progress

preliminary results at SRG parameter $\lambda = 1.8$ fm^{-1}



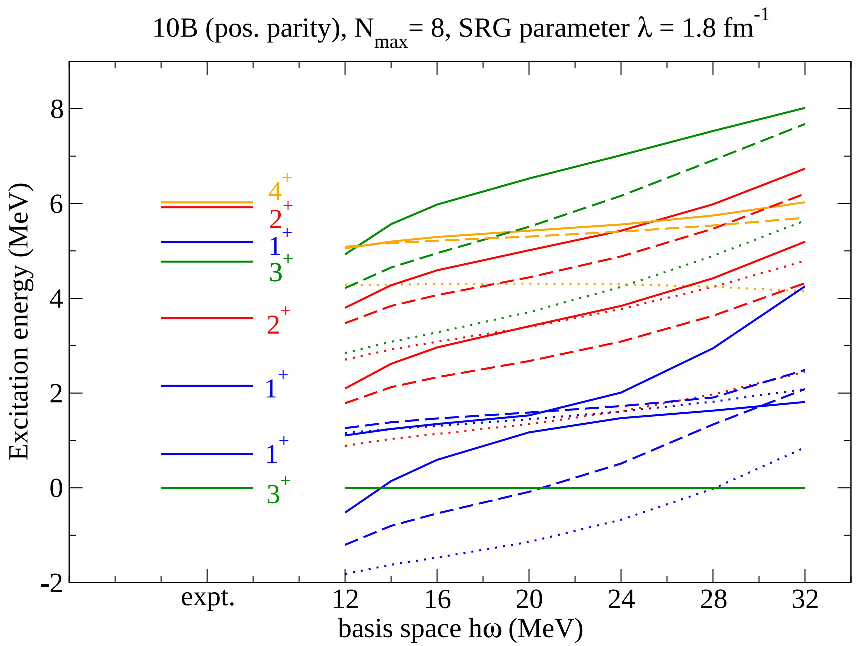
- Clearly underbound without chiral 3NF
- Need extrapolation to complete basis
- Note ^{10}Li
  - exp. ground state is 1^- or 2^-
  - calculations suggest 2^-

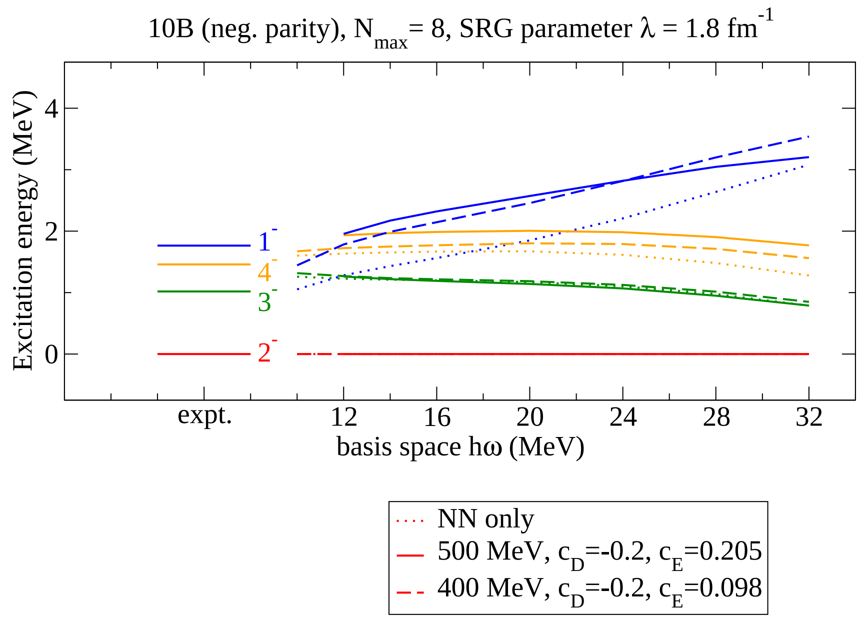




10B spectrum – $T \approx 0$ only

work in progress



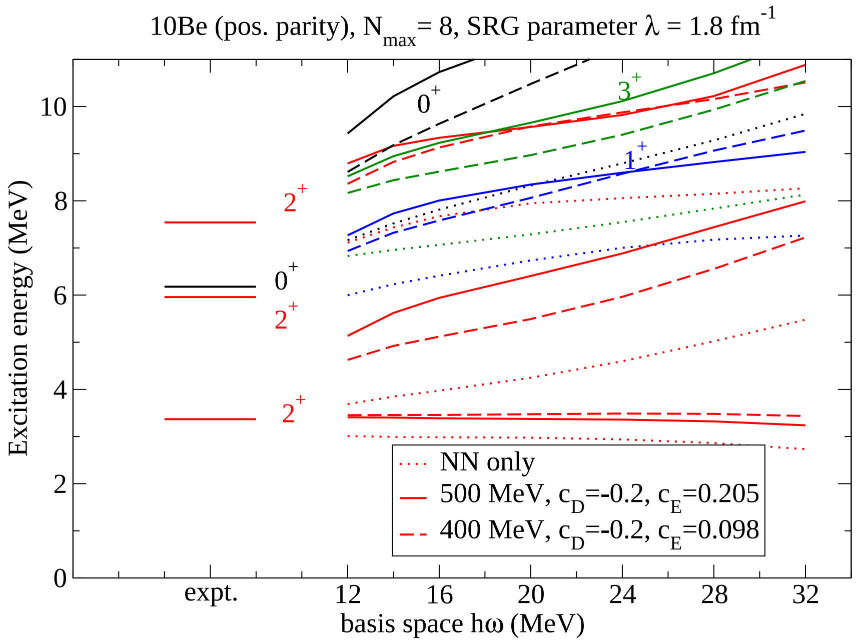


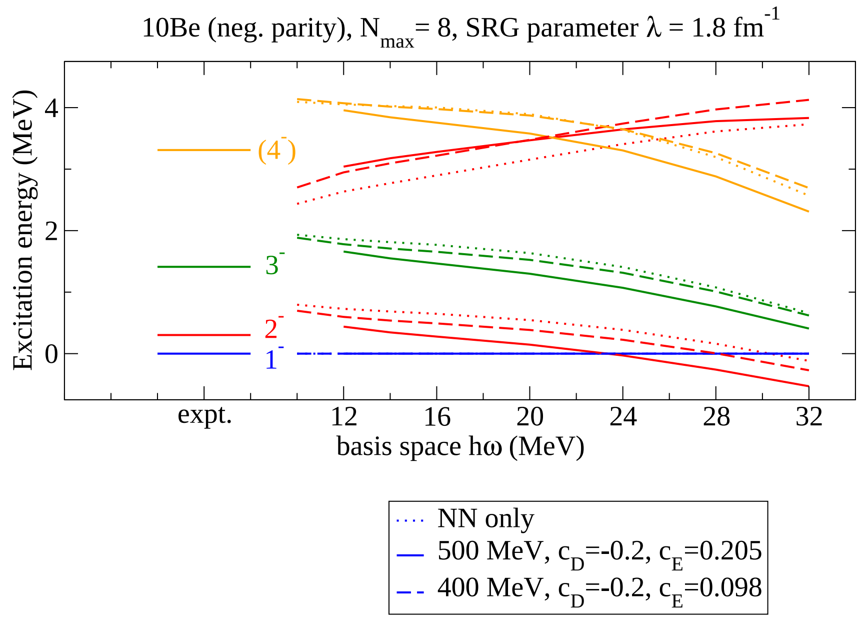
- $(1^+, 0)$ around 1.5 MeV w. $\mu \approx 0.4$
- unconverged $(1^+, 0)$ with $\mu \approx 0.8$
- lowest $(4^+, 0)$ reasonably well converged; inclusion of 3NF improves agreement with data

- negative parity spectrum reasonably well converged w.r.t. $(2^-, 0)$
- excitation energies not very sensitive to 3NF

10Be spectrum

work in progress





- first 2^+ converged, negative quadrupole moment insensitive to 3NF
- higher excited states not converged
  - sensitive to 3NF
  - $\mathcal{Q}$ second 2^+ positive
  - excited 0^+ 'missing'
  - additional 1^+ and 3^+
- negative parity spectrum reasonably well converged w.r.t. $(1^-, 1)$
- excitation energies not very sensitive to 3NF
- experimental $(4-)$ overlapping 2^- and 4^- ?

Conclusions and Outlook

- No-core Configuration Interaction nuclear structure calculations
  - Binding energy, spectrum, magnetic moments, M1 transitions
  - $\langle r^2 \rangle$, $\mathcal{Q}$, E2 transitions, wfns, one-body densities
- Main challenge: construction and diagonalization of extremely large (D $\sim 10^{10}$) sparse (NNZ $\sim 10^{14}$) matrices
- Chiral EFT interactions
  - Convergence many-body calculations, improved by SRG
    - SRG parameter dependendence under control if $N+1$-body induced interaction are incorporated
  - Need consistent NN and 3NF for description of nuclei
  - Effect 3NF on pure neutron drops surprisingly small
  - LENPIC
    - new, consistent, N^{2}LO and N^{3}LO NN + 3NF interactions
    - consistent electroweak meson-exchange currents
- Would not have been possible without collaboration with applied mathematicians and computer scientists

Ab Initio Extreme Neutron Matter

Neutrons confined in a trap

- Model for neutron-rich systems
  in particular those with closed shell protons (Oxygen, Calcium)
- Theoretical 'laboratory' to explore
  - properties of different nuclear interactions
  - effect of density and gradient
    on nuclear properties for different interactions
- Construct and/or validate Nuclear Energy Density Functionals
  using microscopic ab-initio calculations
  - Validate Density Matrix Expansion using Minnesota potential

    Bogner *et al*, arXiv:1106.3557 [nucl-th], PRC84, 044306 (2011)
  - Adjust standard Skyrme functionals
    to reproduce ab-initio neutron drop energies

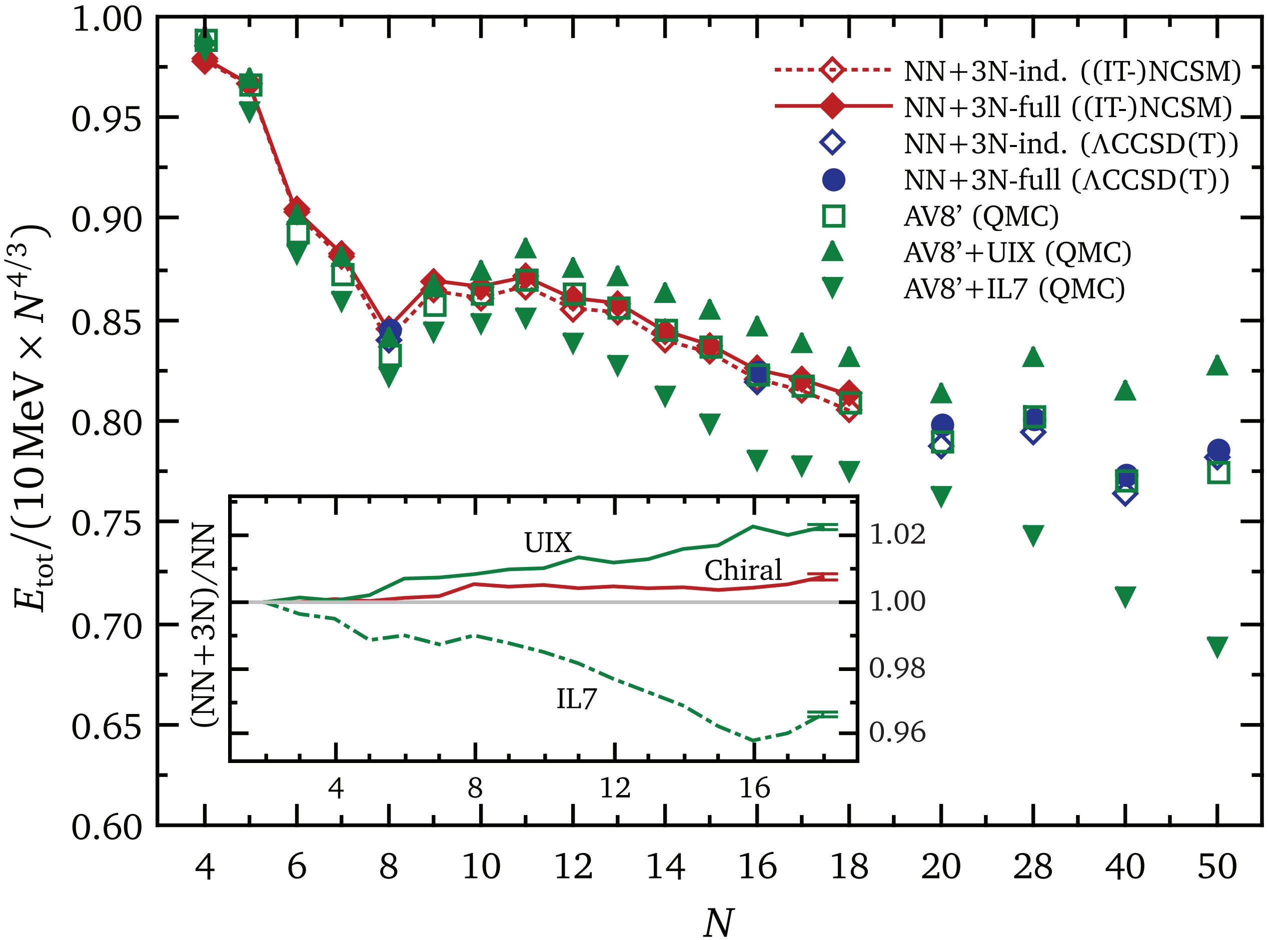
    Gandolfi, Carlson, Pieper, arXiv:1010.4583 [nucl-th], PRL106 012501 (2011)

Efficient decoupling of input coupled-J 3NF matrix elements on GPUs

Oryspayev, Potter, Maris, Sosonkina, Vary, Binder, Calci, Langhammer, Roth,
IPDPS Workshops 2013, 1365 (2013)

Neutrons confined in HO external field

Potter, Fischer, Maris, Vary, Binder, Calci, Langhammer, Roth, arXiv:1406.1160 [nucl-th]



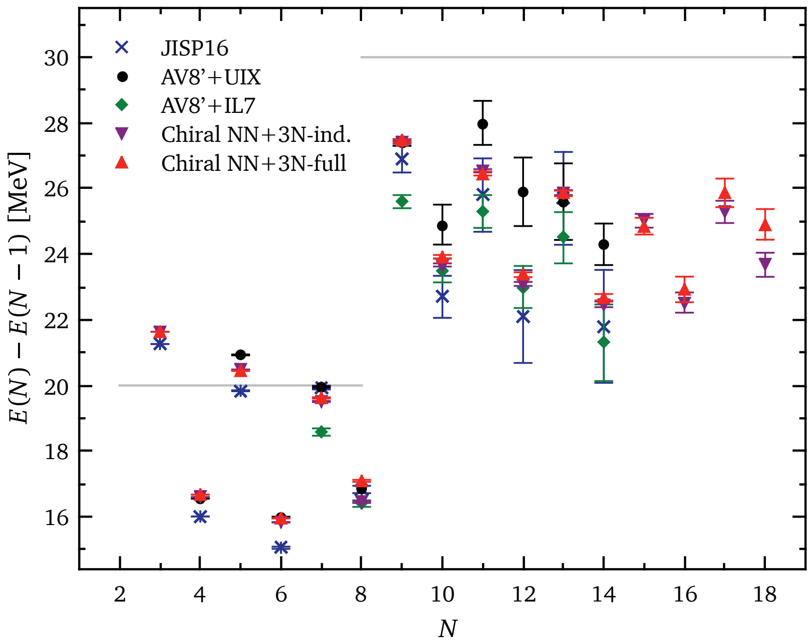
- chiral NN at N^3LO
- chiral 3N at N^2LO
- 3N LEC values:
  $c_D = -0.2,$
  $c_E = -0.205$
- 500 MeV cutoff

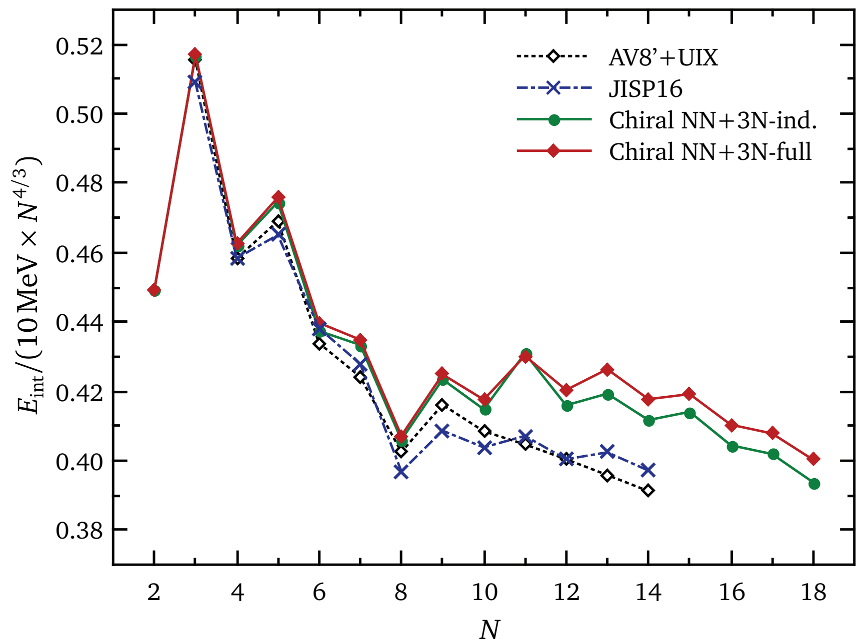
AV8'(+3NF) data from
Gandolfi, Carlson, Pieper,
PRL106 012501 (2011)

- Chiral 3NF very weak repulsive
- Chiral EFT results very similar to AV8' without 3NF

Neutrons confined in HO external field

Potter, Fischer, Maris, Vary, Binder, Calci, Langhammer, Roth, arXiv:1406.1160 [nucl-th]





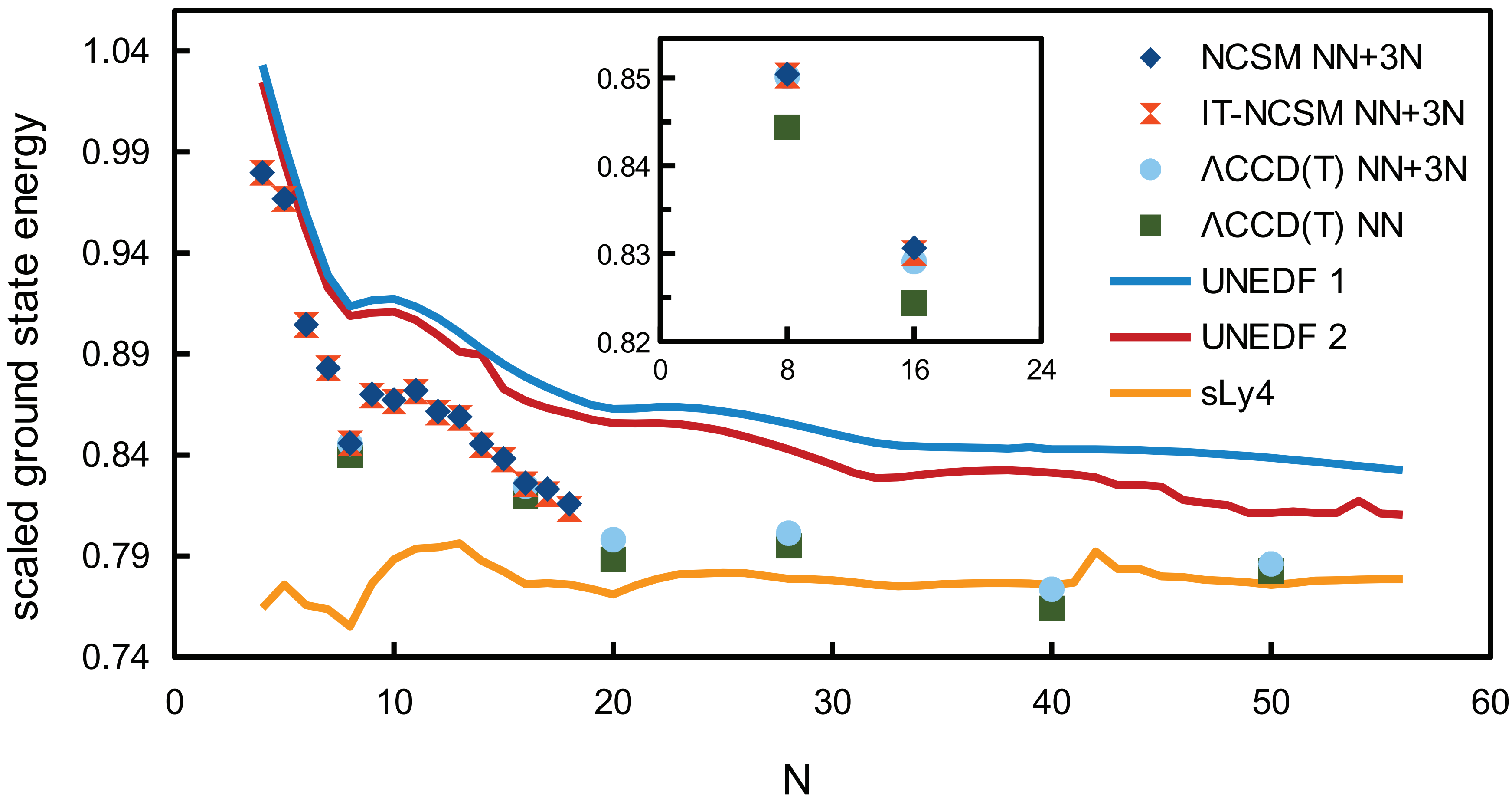
- Clear evidence for pairing with chiral EFT potential both in total energy (left) and in internal energy (right)
- GFMC results for AV8' + IUX show significantly less pairing, in particular above $N = 8$

JISP16, AV8'+3NF data from Maris, Vary, Gandolfi, Carlson, Pieper, PRC87 054318 (2013)

Comparison with Energy Density Functionals

Neutron drops in 10 MeV harmonic trap

NCSM, IT-NCSM, CC and HFB results



work in progress, Hugh Potter (PhD student)