Neutrons in a HO trap with chiral interactions

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http://computingnuclei.org

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NERSC (CPU time and code development support)

Neutrons in a trap: Why

- Theoretical ’laboratory’
  to explore properties of different nuclear interactions
- Validate ab-initio DFT approaches
  against microscopic ab-initio calculations with the same interaction
- Guide developments of Nuclear Energy Density Fuctionals
  consistent with ab-initio calculations
- Model for neutron-rich systems
  in particular those with closed shell protons (Oxygen, Calcium)

- Uncertainty quantification essential
  - For comparisons between different methods
    - statistical and round-off errors in calculation
    - systematical errors inherent to the many-body method
  - For comparisons between different interactions
    - uncertainty of the nuclear potential

Neutrons in a trap: What

Neutrons

- Confined by external potential $\hat{\mathbf{U}}_{\text{ext}}$
- Interacting via $\hat{\mathbf{V}}_{NN}, \hat{\mathbf{V}}_{3NF}, \ldots$

$$\hat{\mathbf{H}} \quad = \quad \hat{\mathbf{T}} + \hat{\mathbf{U}}_{\text{ext}} + \hat{\mathbf{V}}_{NN} + \hat{\mathbf{V}}_{3NF} + \ldots$$

Observables

- Total energy $E_{\text{tot}} = \langle \hat{\mathbf{H}} \rangle$ (per neutron)
- Internal energy $E_{\text{int}} = \langle \hat{\mathbf{H}} \rangle - \langle \hat{\mathbf{U}}_{\text{ext}} \rangle$ (per neutron)
- Spectra, energy splittings
- One-body density $\rho(r)$
  - rms radius $r = \langle \hat{\mathbf{r}}^2 \rangle^{\frac{1}{2}}$
  - Fourier transform of density: form factor $F(q)$
- . . .

Neutrons in a trap: How

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

No-Core Configuration Interaction calculations

- 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 N neutrons 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

No-Core Configuration Interaction methods

- Many-Body basis states $\Phi_i(r_1, \ldots, r_A)$ Slater Determinants
- 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 w. basis parameter $\hbar\omega$
    - Coulomb–Sturmian Caprio, Maris, Vary, PRC86, 034312 (2012)
    - . . .
- M-scheme: Many-Body basis states eigenstates of $\hat{\mathbf{J}}_\mathbf{z}$

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

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

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

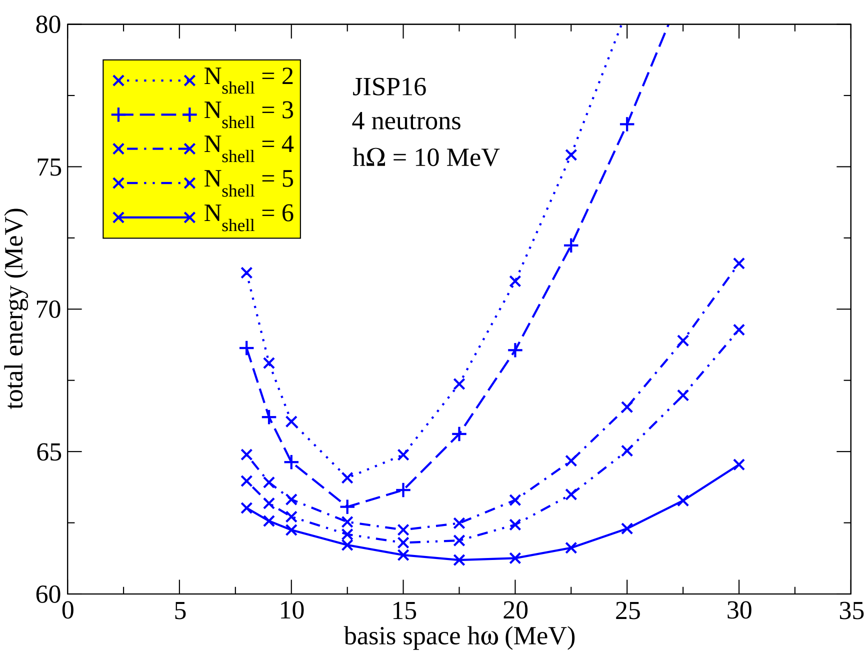
No-Core CI methods for neutrons in a trap

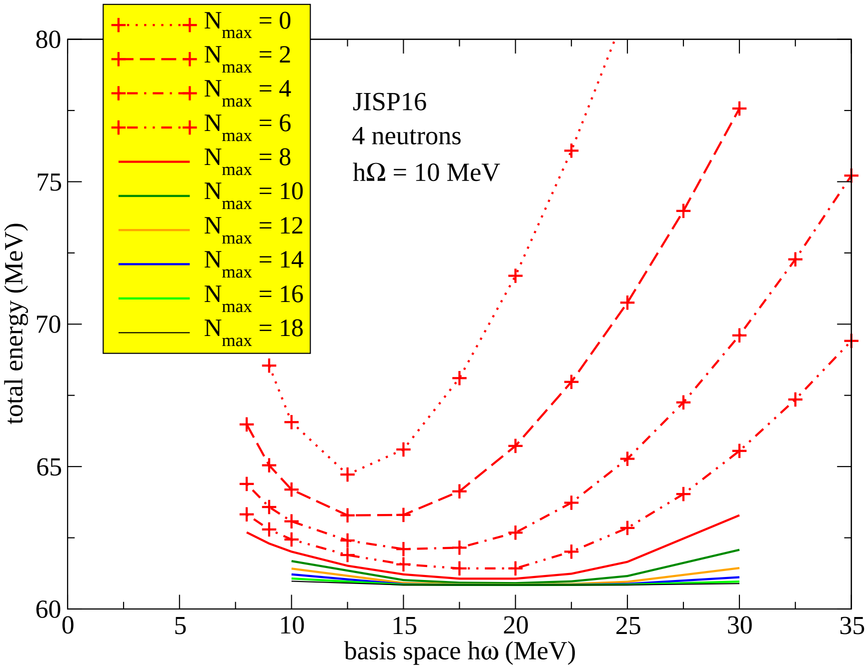
N neutrons in Harmonic Oscillator trap with strength $\hbar\Omega$

$$\hat{\mathbf{H}} = \sum_i^N \frac{\vec{p}_i^{\,2}}{2\,m} + \frac{1}{2}\sum_i^N m\,\Omega\,\vec{r}_i^{\,2} + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \ldots$$

- Trap defines coordinate system
  - Center-of-Mass motion is part of the system
  - No need to factorize out Center-of-Mass motion!
- Truncation methods
  - Many-body N_{max} truncation
  - Single-Particle basis truncation (N_{shell}) – FCI
  - Particle-hole truncation
  - SU(3) truncation — Dytrych *et al*, PRL111, 252501 (2013)
  - No-Core Monte-Carlo Shell Model — Abe *et al*, PRC86, 054301 (2012)
  - Importance Truncation — Roth, PRC79, 064324 (2009)
  - . . .
- Extrapolate to the infinite basis space

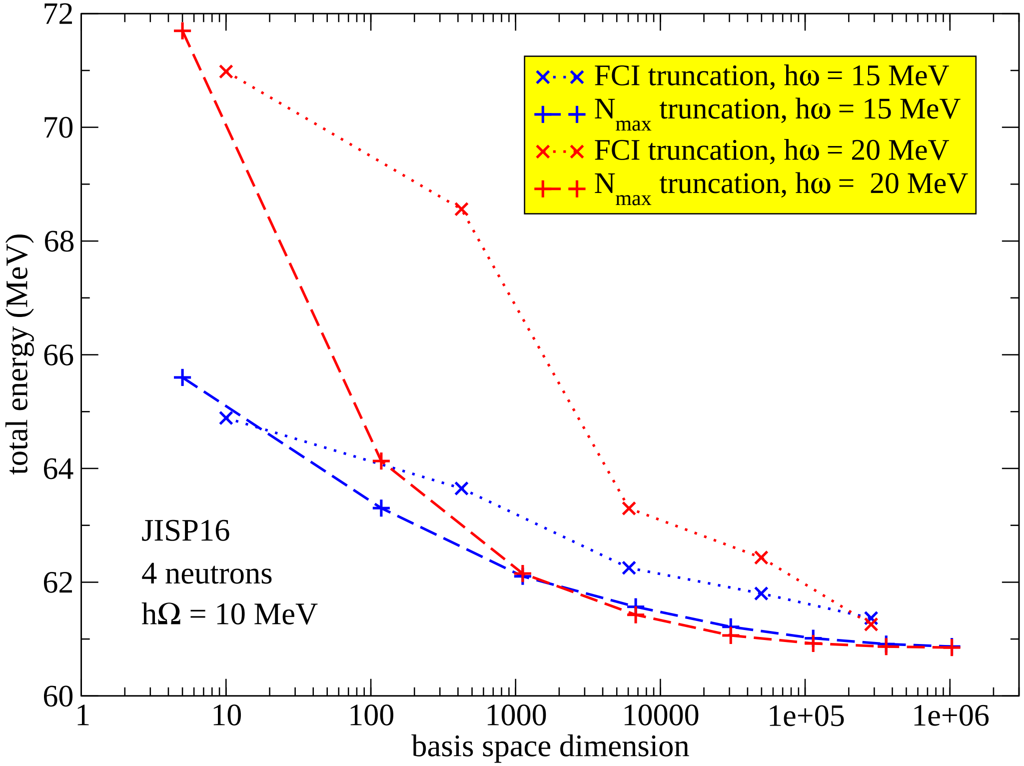
Convergence: N_{shell} truncation vs. N_{max} truncation





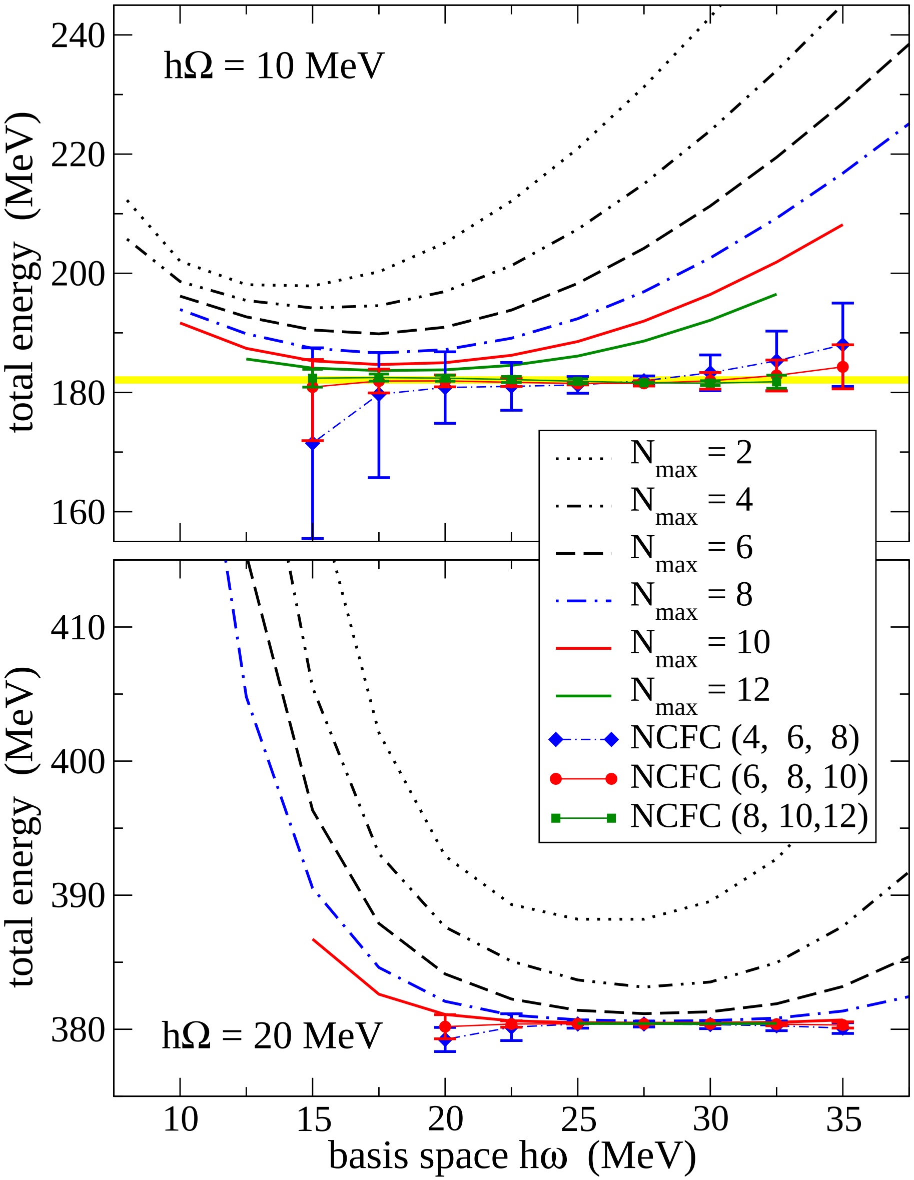
- Small model spaces
  - variational minimum for $\hbar\omega$ near H.O. trap $\hbar\Omega$
- Large model spaces
  - variational minimum for $\hbar\omega$ near optimal value for interaction
- Convergence
  - independence of basis $\hbar\omega$ and truncation parameter N

Convergence rate: N_{max} truncation vs. N_{shell} truncation



- N_{max} truncation below FCI truncation for same $\hbar\omega$ and dimension
- Smooth approach to NCFC result with N_{max} truncation
- Allows for extrapolation to exact total energy

Extrapolation to complete basis

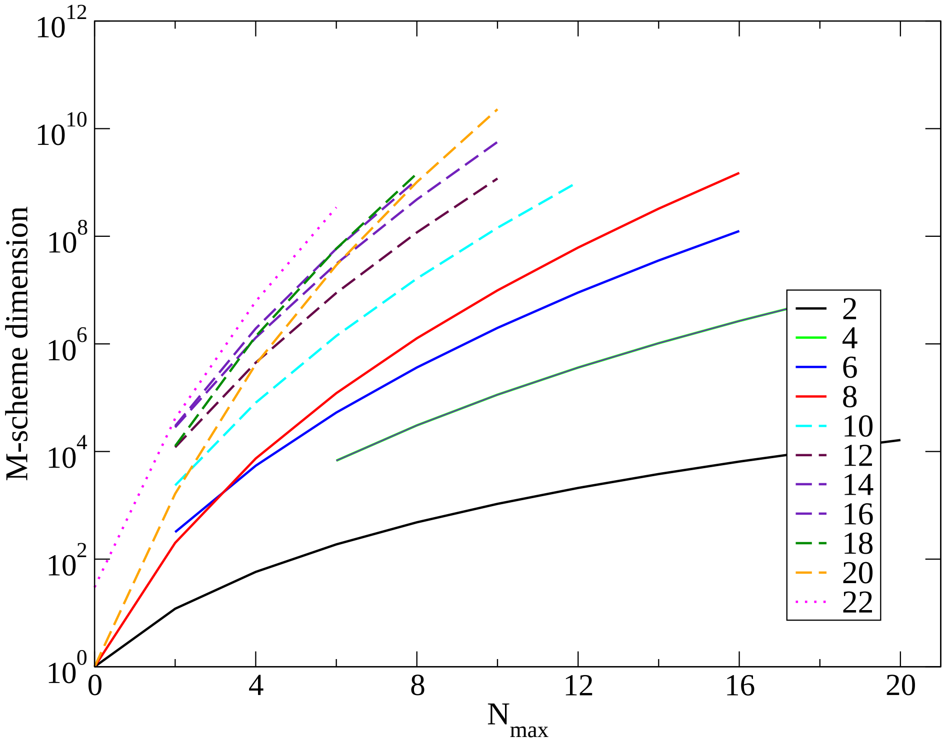


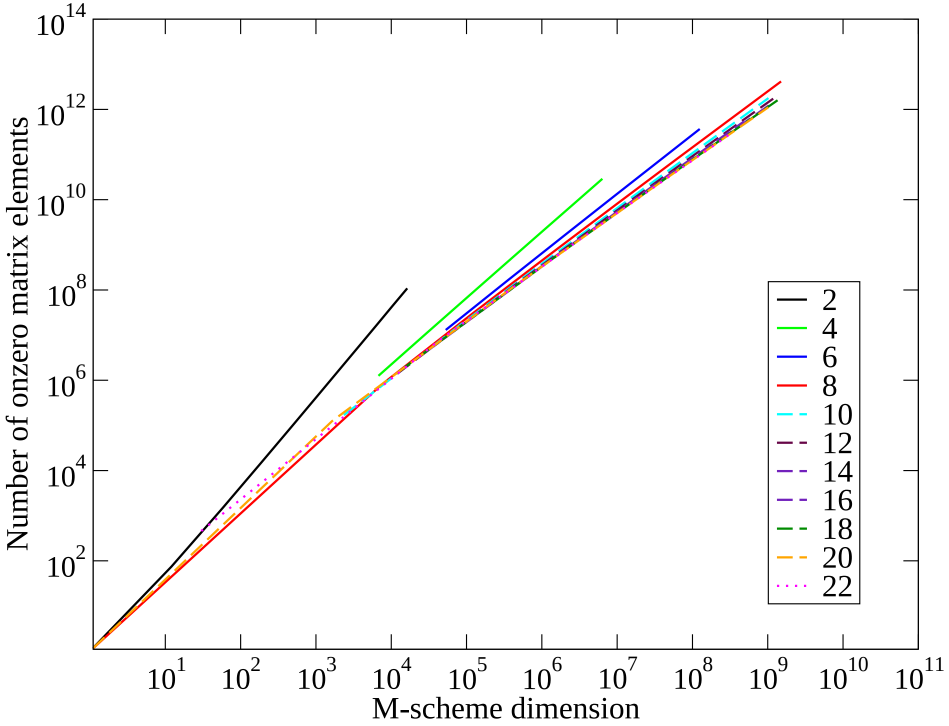
- Empirical extrapolation method (ground state) energies

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

- Error estimate: difference with result from smaller model spaces
  - errors decrease with N_{max}
  - extrapolation at N_{max} within error estimates of $N_{\text{max}} - 2$
- Need at least $N_{\text{max}} = 8$, preferably $N_{\text{max}} = 10$ for meaningfull extrapolation

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)

Many Fermion Dynamics – nuclear physics

Configuration Interaction (Shell Model) code

- Platform-independent, hybrid OpenMP/MPI, Fortran 90
- Highly parallelized, highly scalable, load-balanced
- Nonzero matrix elements stored in core
  - Lanczos iterations very fast (few seconds per iteration)
  - LOBPCG (SpMatMul instead of SpMatVec) in progress, but overall less efficient than Lanczos
- NN, 3NF implemented and fully functional
  - 4NF implemented, but no interface with input FBMEs (yet)
- One-body and scalar two-body observables fully functional
- Optimized for No-Core calculations
  - Small systems: 5 to 20 nucleons
  - Large bases: 100 to 500 S.P. orbitals ($\sim 10,000$ S.P. states)
- Capable to perform, but not optimized for, traditional shell model calculations

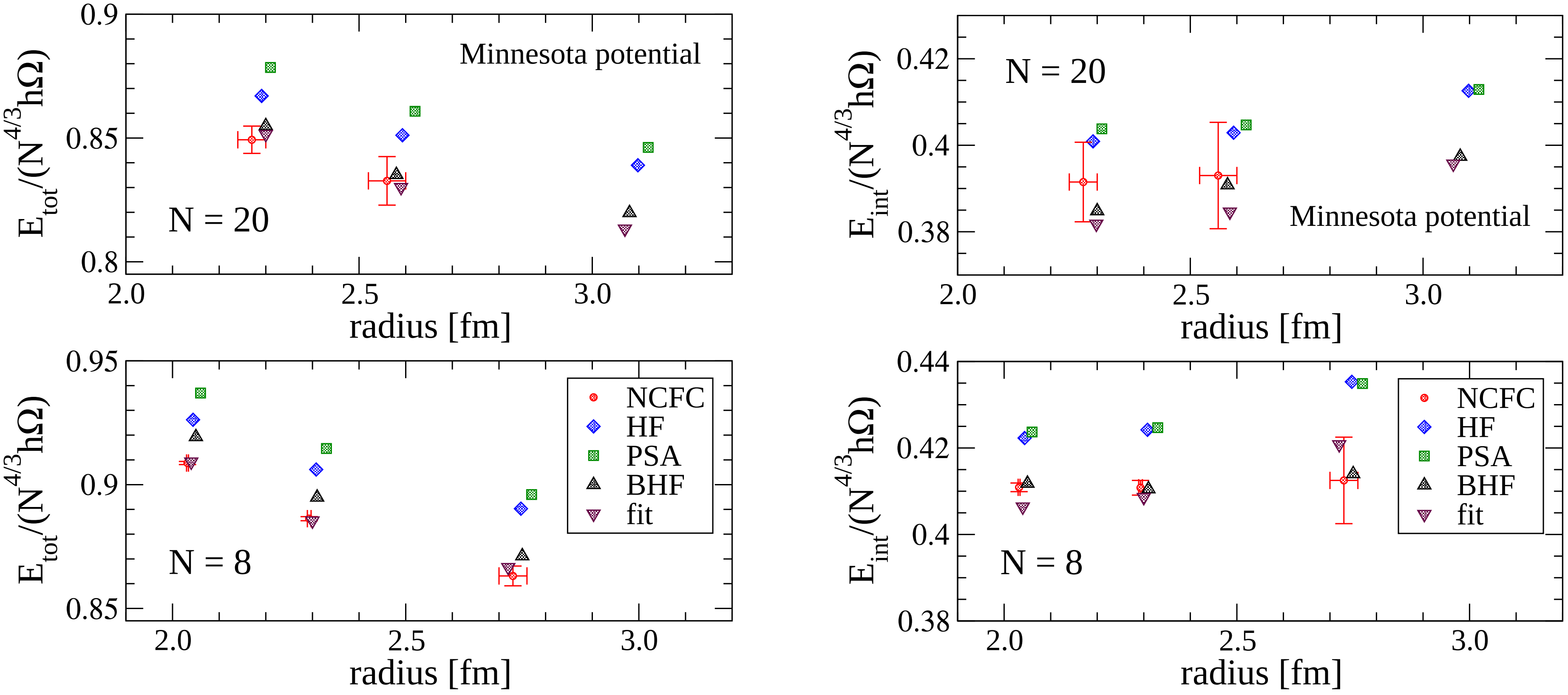
Validating ab-initio Density Functional Theory

Bogner, Furnstahl, Hergert, Kortelainen, Furnstahl, PM, Stoistov, Vary, PRC84, 044306 (2011)

- Simple model for interaction
  - Minnesota potential
- Ab-initio NCFC calculations for neutrons in H.O. potential
  - including numerical error estimates on all ’observables’
- Density Functional Theory approaches using same NN interaction
  - Hartree–Fock
  - Density Matrix Expansion / Phase–Space–Averaging with exact Hartree
  - Incorporate correlations beyond HF using Brueckner–Hartree–Fock calculations of neutron matter
    - Density-dependent terms
    - Fit surface parameters in DME functional
- Comparison for 8 and 20 neutrons
  - total and internal energy per neutron as function of radius
  - density $\rho(r)$ and form factor $F(q)$

Minnesota potential – energies and radii

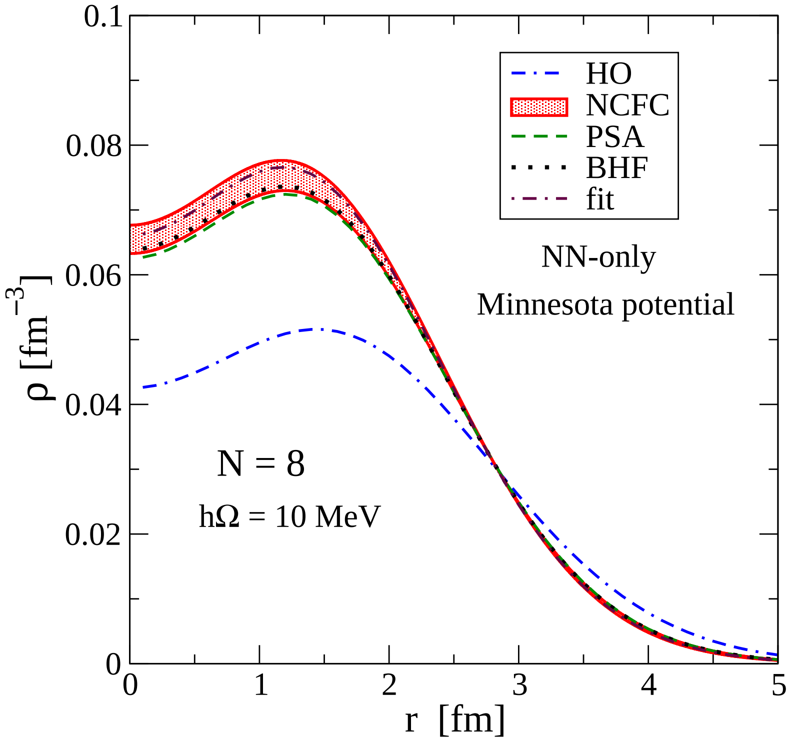
Bogner, Furnstahl, Hergert, Kortelainen, Furnstahl, PM, Stoistov, Vary, PRC84, 044306 (2011)

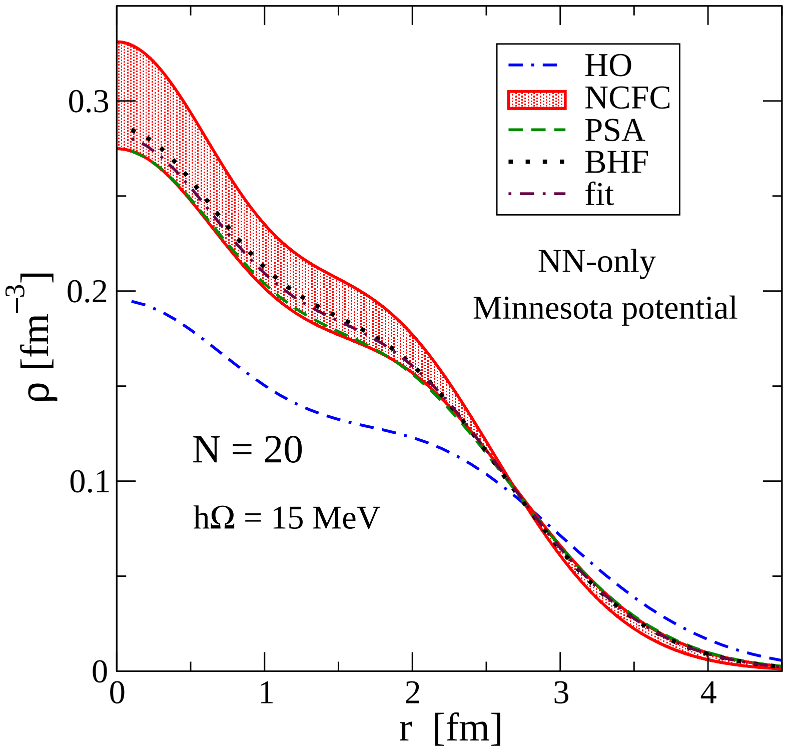


- Hartree–Fock outside error bars of ab-initio calculations
- BHF density-dependent term and fit surface terms closest to ab-initio calculations

Minnesota potential – Densities

Bogner, Furnstahl, Hergert, Kortelainen, Furnstahl, PM, Stoistov, Vary, PRC84, 044306 (2011)

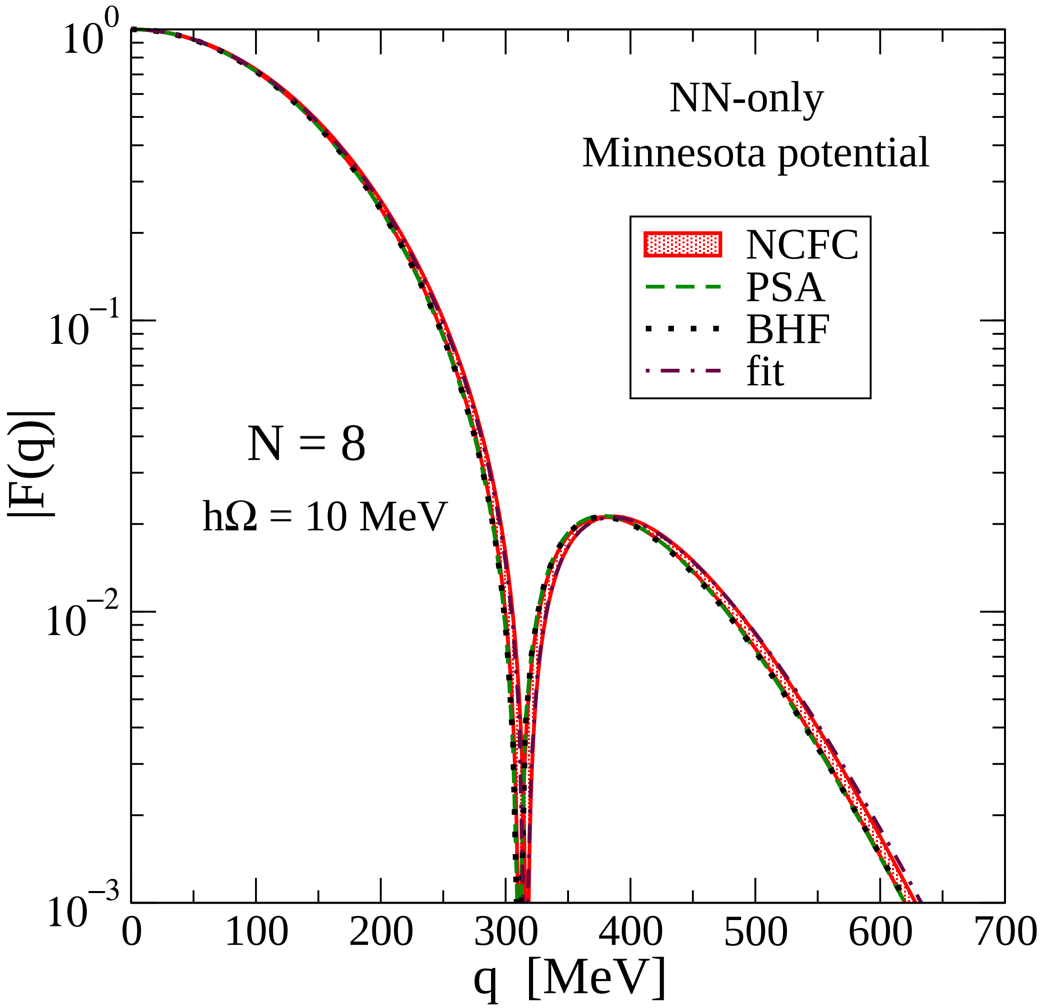




- Good agreement density profiles

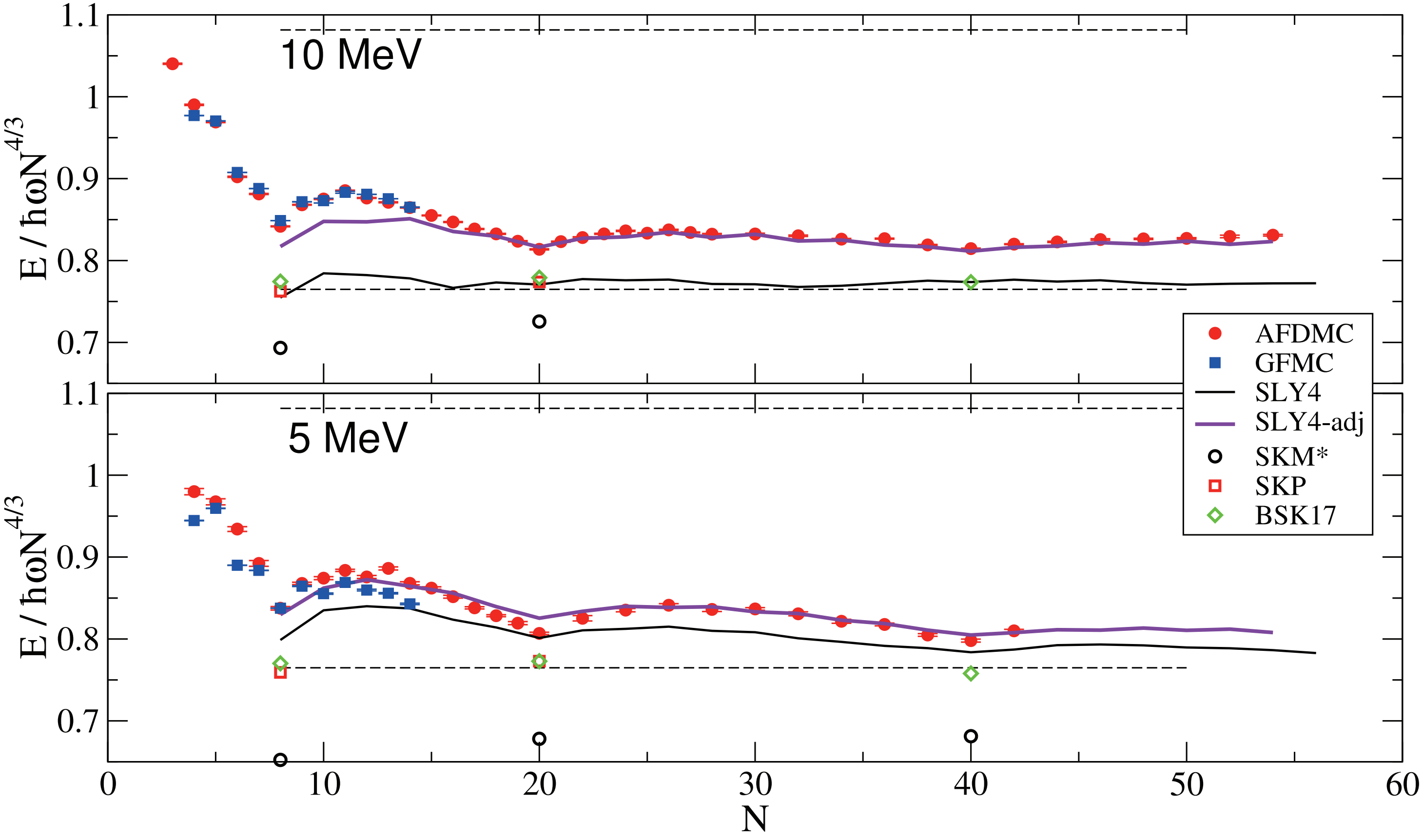
Minnesota potential – form factor

- and good agreement form factor



Results for more realistic interactions: AV8' + UIX

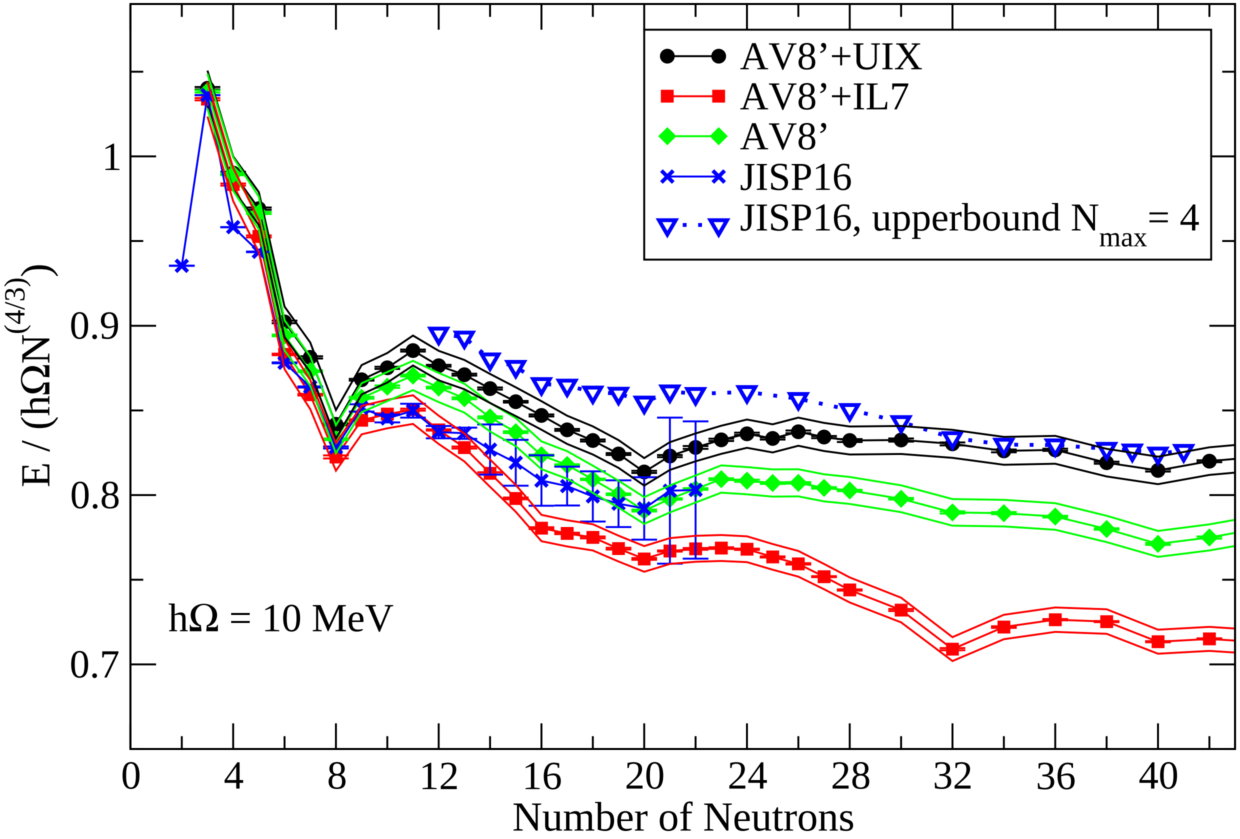
Carlson, Gandolfi, Pieper, PRL106, 012501 (2011)



- GFMC and AFDMC with AV8' + UIX
- Neutron matter EOS consistent with known neutron star masses
- Significant differences Skyrme functionals and ab-initio results

Comparing results for realistic interactions

PM, Vary, Gandolfi, Carlson, Pieper, PRC87, 054318 (2013)



- Significant difference between AV8' plus IL7 and AV8' plus UIX
- JISP16 similar to
  - AV8' plus IL7 for $N \lesssim 14$
  - AV8' without 3NF for $N \gtrsim 18$
- JISP16 and AV8'+IL7 good description of nuclei upto $A = 12 \sim 14$

- AV8': MC error bars plus estimate of systematic uncertainty (band)
- Extrapolation error estimates for JISP16

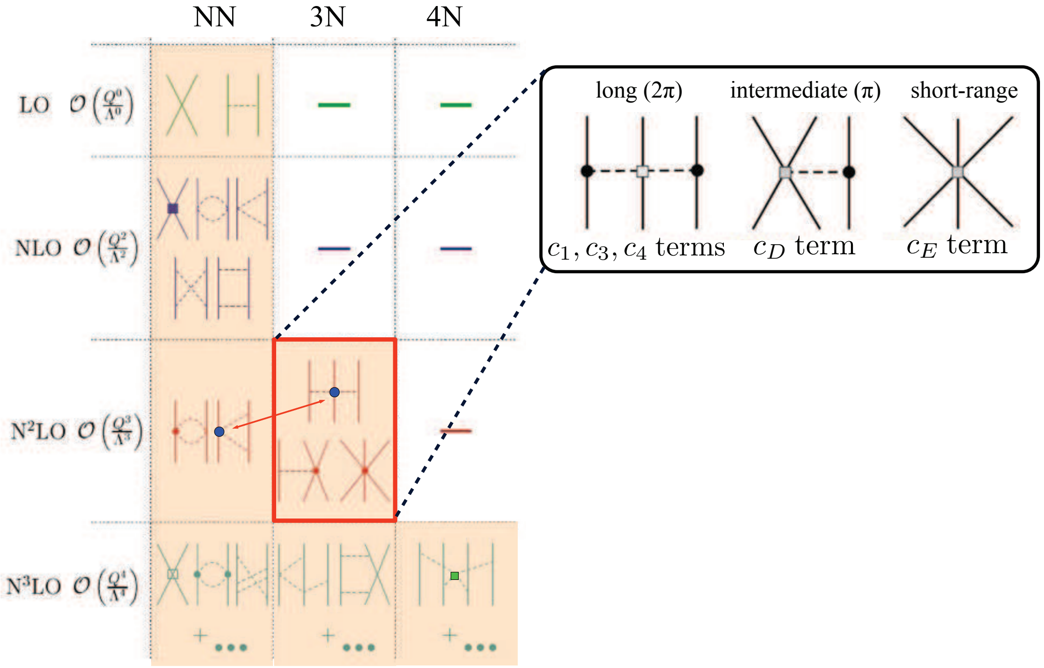
Nuclear interaction from chiral perturbation theory

- 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

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

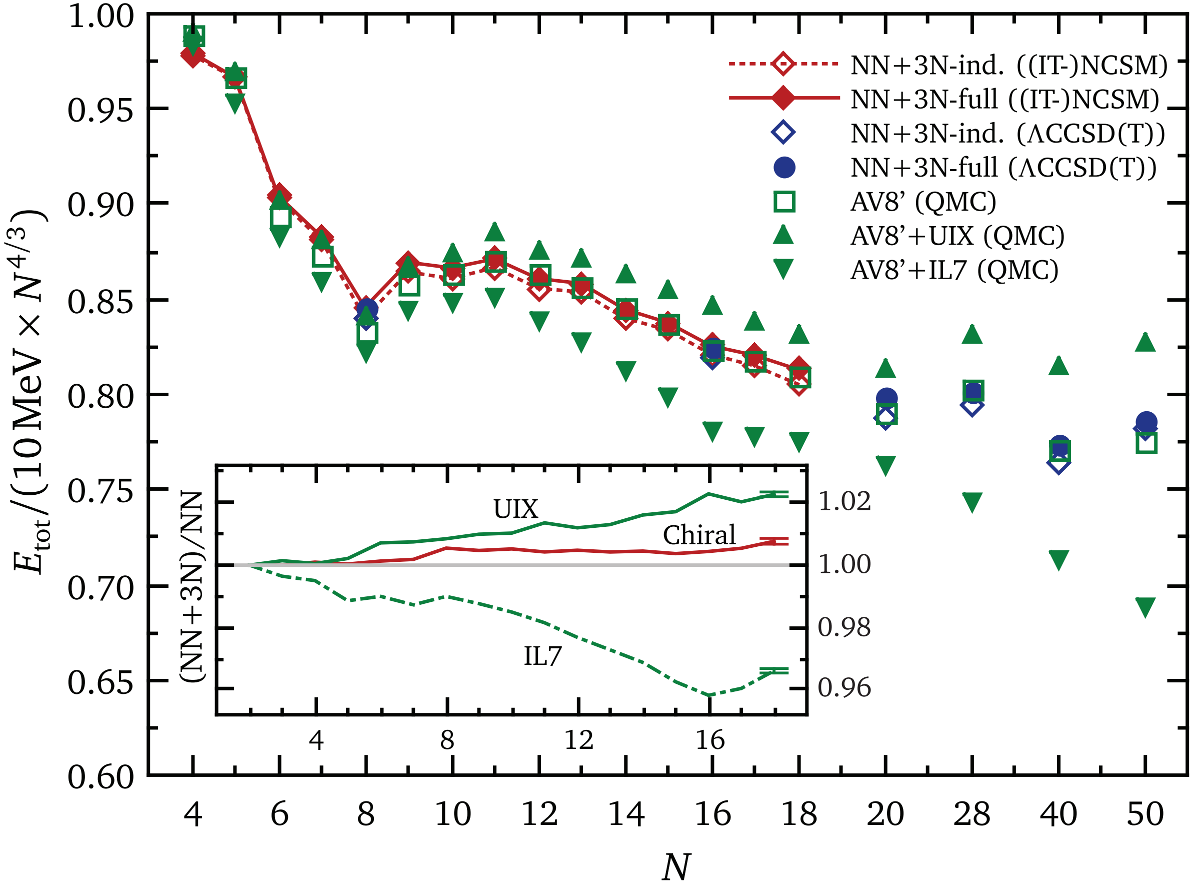
  - in principle no free parameters
    - in practice a few undetermined parameters
  - renormalization necessary

Leading-order 3N forces in chiral EFT



Argonne vs. Chiral interactions

Potter, Fischer, PM, Vary, Binder, Calci, Langhammer, Roth, PLB739, 445 (2014)

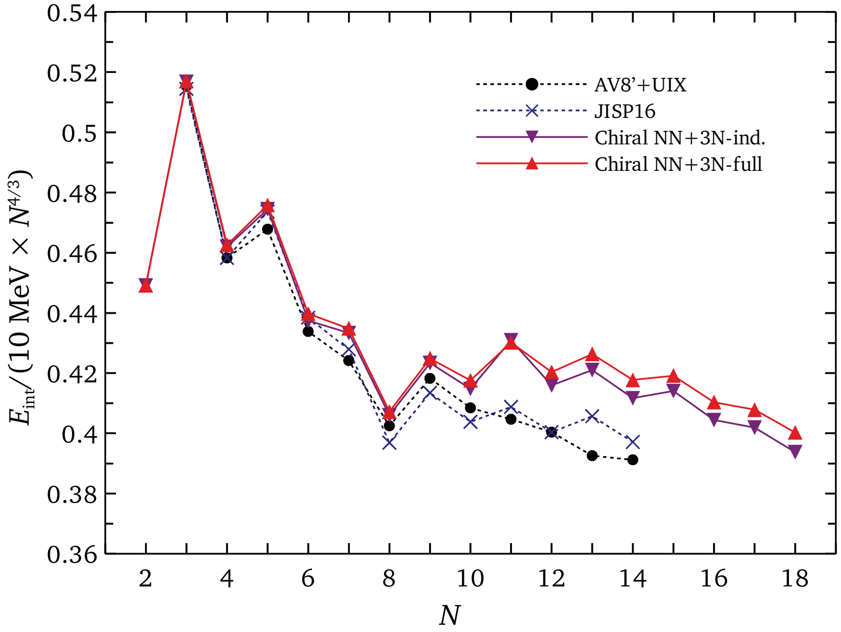


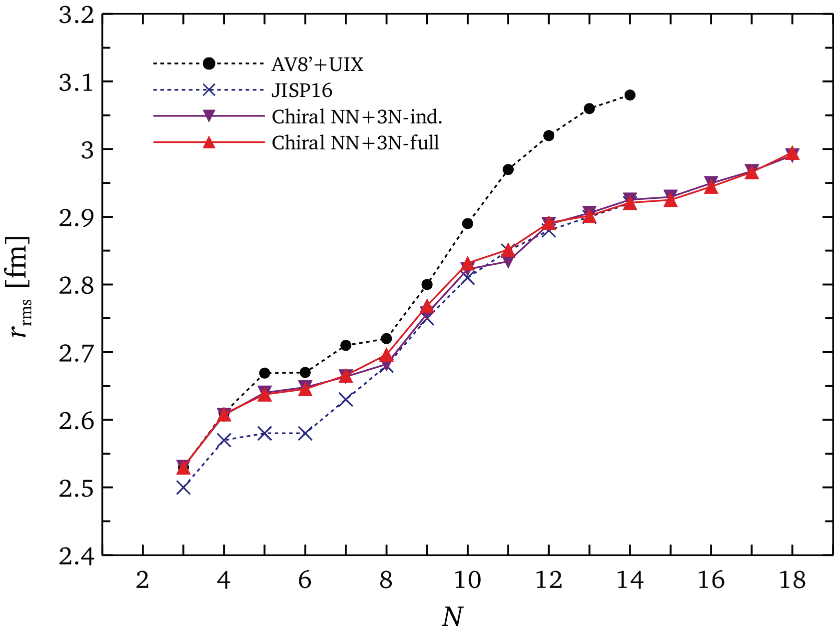
- N^3LO NN potential Entem–Machleidt with 500 MeV cutoff
- N^2LO 3NF
  $c_D = -0.2$
  $c_E = -0.205$

- Chiral N^3LO NN similar to AV8' without 3NF
- Contributions from chiral N^2LO 3NF small

Internal energies and radii

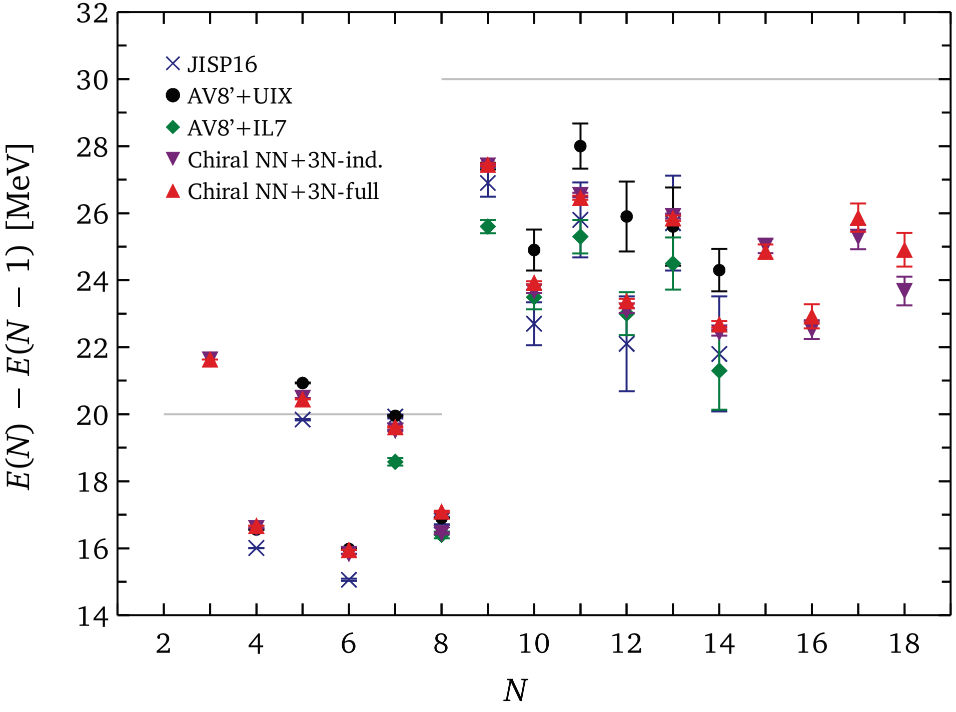
Potter, Fischer, PM, Vary, Binder, Calci, Langhammer, Roth, PLB739, 445 (2014)

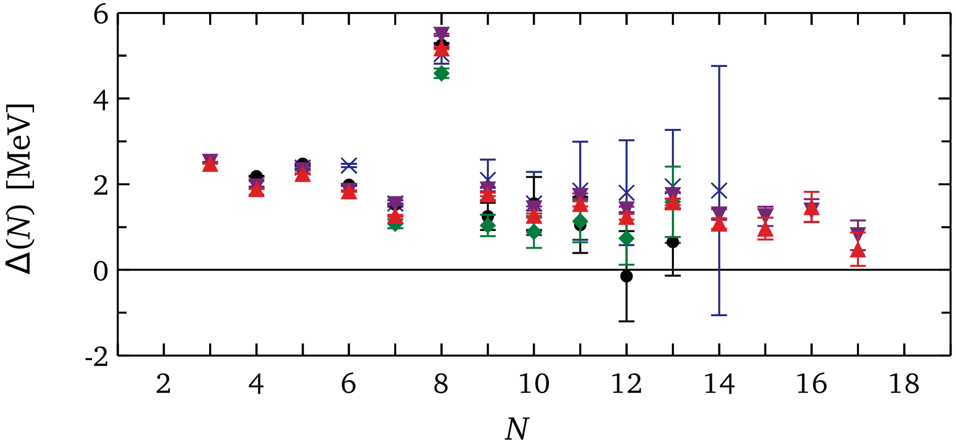




- Contributions from chiral N^{2}LO 3NF small
- Internal energies up to 10 neutrons all similar behavior, but noticable differences in radii
- Above 10 neutrons, chiral and JISP16 give similar radii, while AV8'+UIX gives larger radii
- Strong odd-even effect internal energies (also total energies)

Pairing



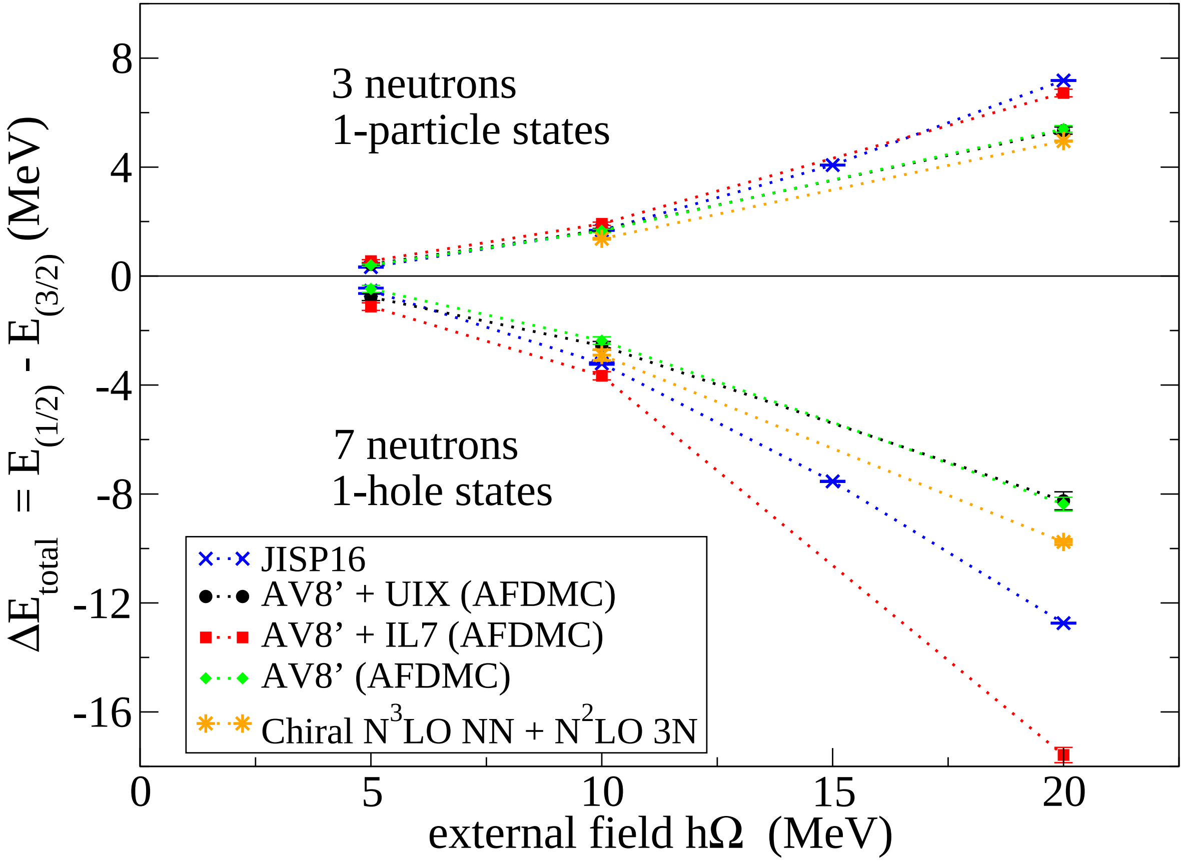


- Single differences
  - jumps at closed shell due to HO trap
  - odd-even difference indicating pairing
- Double differences $\Delta(N) = (-1)^{(N-1)}(E(N) - \frac{1}{2}(E(N-1) + E(N+1)))$
  - similar pairing effects with different interactions in p-shell
  - chiral and JISP16 lead to more pairing than AV8' interactions in sd-shell

Level splitting: p-shell

PM, Vary, Gandolfi, Carlson, Pieper, PRC87, 054318 (2013)

Chiral: work in progress (Potter, PhD student)

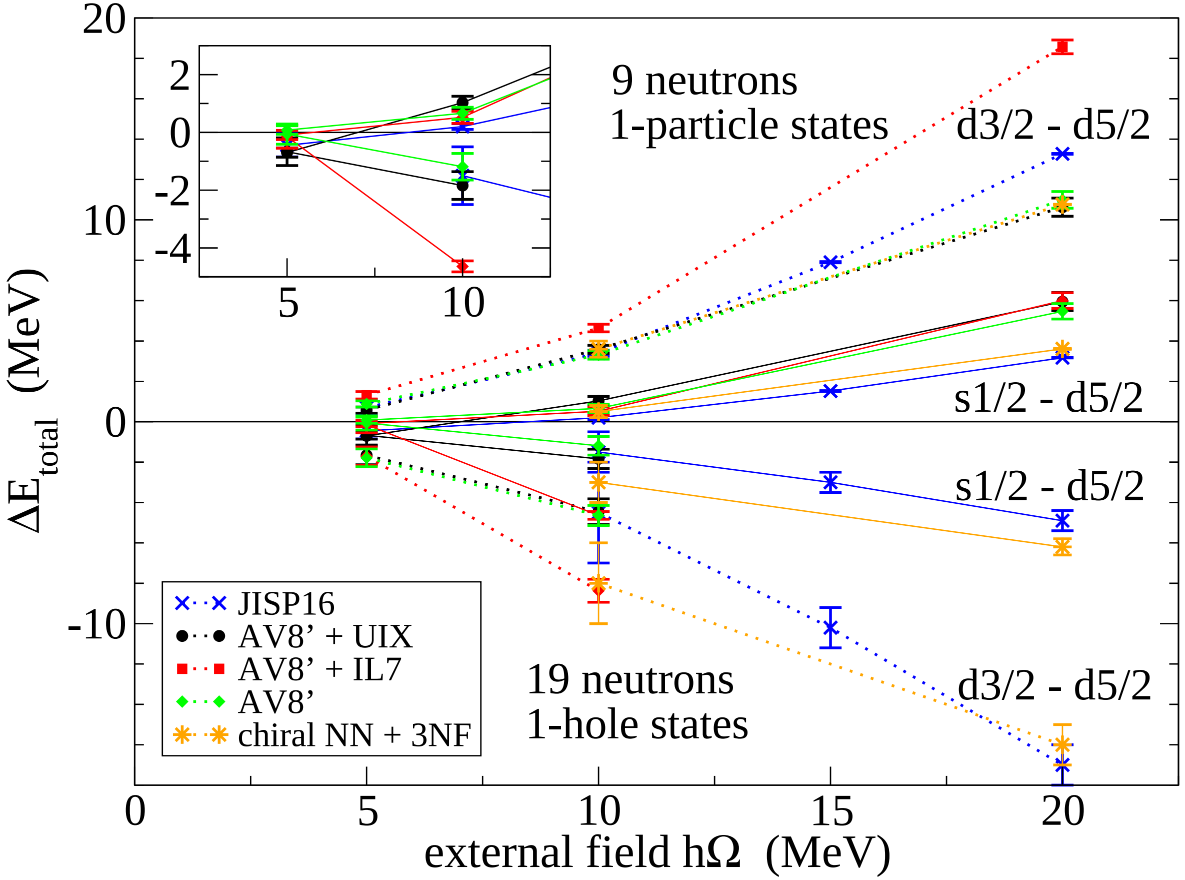


- $p\frac{1}{2} > p\frac{3}{2}$, as expected
- similar splitting for different interactions (JISP16, AV8', chiral) up to 10 MeV trap strength
- splitting larger for one-hole states than for one-particle states
- splitting increases with external field strength, due to
  - increased density?
  - steeper gradient?

Level splitting: sd-shell

PM, Vary, Gandolfi, Carlson, Pieper, PRC87, 054318 (2013)

Chiral: work in progress (Potter, PhD student)



- Level ordering
  - $d\frac{3}{2} > d\frac{5}{2}$
  - $d\frac{3}{2} > s\frac{1}{2}$
  - $s\frac{1}{2} \gtrsim d\frac{5}{2}$
- Expect subshell closures
  - weak at 14
  - strong at 16

in particular with AV8'+IL7

- Qualitatively similar splittings for different interactions

Conclusions

Microscopic ab-initio calculations of neutrons in a trap

- Compare and contrast different NN and 3N interactions
- Guide and validate ab-initio DFT approaches
- Benchmark microscopic ab-initio methods
- Simple model for neutron-rich systems

Thank you