Physics capabilities and results with Many Fermion Dynamics – nuclear physics

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Collaborators

Nuclear physics

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Computer Science/Applied Math

Ames Lab: Masha Sosonkina, Hung Le, students
LBNL: Esmond Ng, Chao Yang, Philip Sternberg

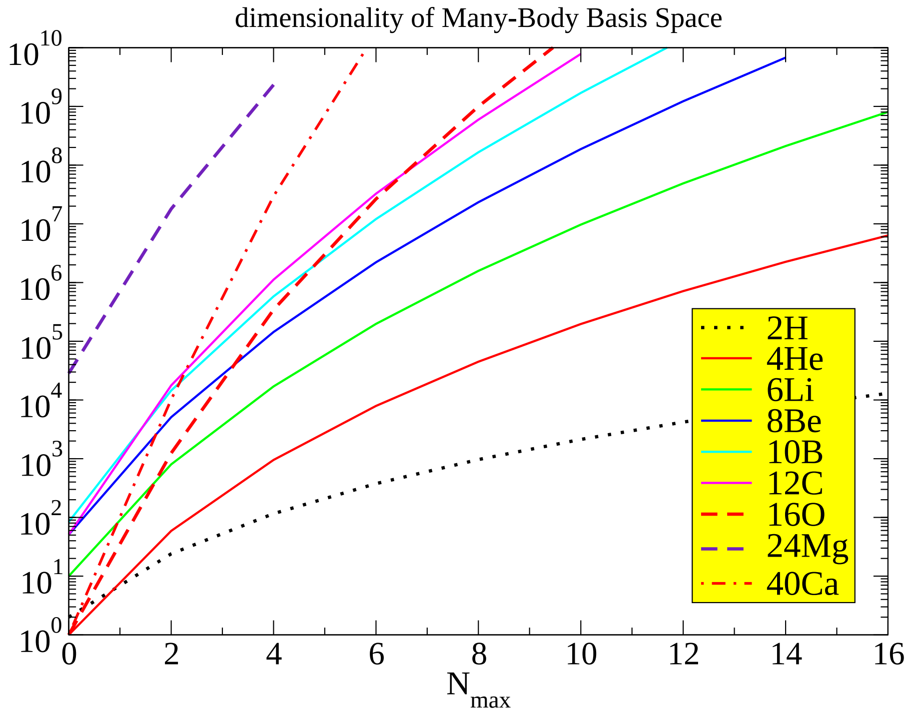
Many Fermion Dynamics – nuclear physics

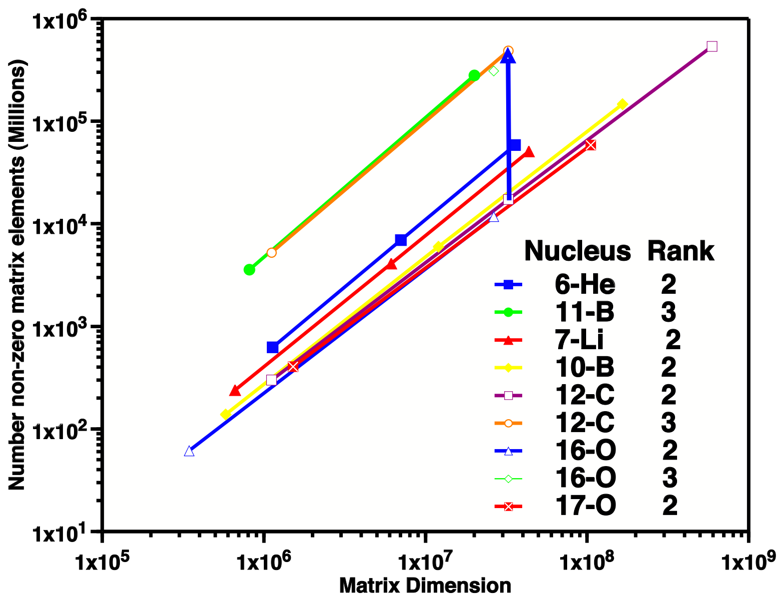
- MFDn: ab initio calculations for nuclear structure using basis space expansion methods
  - Variational: for any finite truncation of the basis space, MFDn gives an upper bound for the ground state energy
  - Smooth approach to asymptotic values with increasing basis space: no-core Full Configuration method
- Construct Many–Body Basis States in an m-scheme H.O. basis that eliminates spurious center of mass motion effects
- Construct the many-nucleon Hamiltonian in this basis
  - Determine which matrix elements are nonzero
  - Evaluate nonzero matrix elements
- Solve the many-nucleon Hamiltonian for lowest eigenvalues to obtain spectrum and wavefunctions (input for TRDENS)
- Evaluate selected 1-body and 2-body observables to compare with experiment and for use with energy-density functionals

Many Fermion Dynamics – challenges

Single most important computational issue:

- How to deal with the exponential increase
  of the Many–Body Basis Space with increasing H.O. levels





- Memory constrictions

^{14}F in $N_{\rm m} = 8$: dimension $\sim 2 \cdot 10^9$, $\#$ nonzero m.e. $\sim 2 \cdot 10^{12}$, storage matrix $\sim$ 16 TB

- Speed of execution

Many Fermion Dynamics – challenges

Single most important computational issue:

- How to deal with the exponential increase of the Many–Body Basis Space with increasing H.O. levels

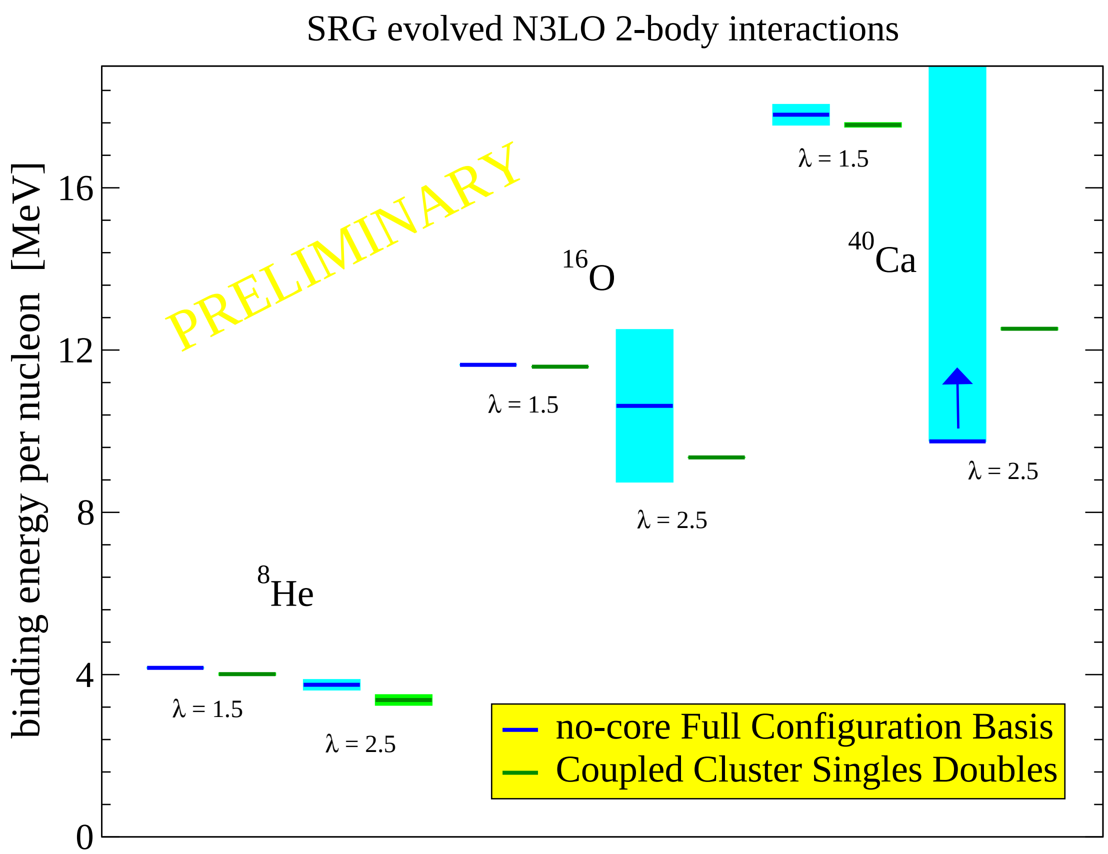
Additional challenges

- Construction of Many-Body Basis States and determination of nonzero matrix elements: all combinatorics, no flops
  (i.e. branching statements, integer operations, boolean masking operations)
  $\Longrightarrow$ performance tools based on flop rates not useful
- I/O burden with 3-body input files
  - need alternative scheme for 3-body interactions
- Limitations of H.O. basis and m-scheme inefficiencies
  - need more general basis spaces
  - need coupled J basis capability

  will result in more compute-intensive inner loops for generating matrix elements and lead to denser matrices

Accomplishments – physics results

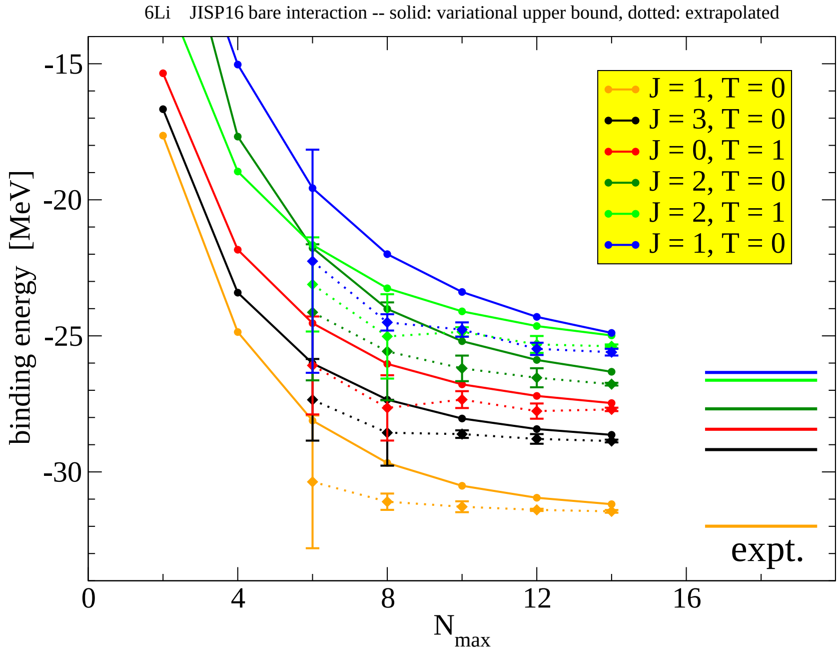
Comparison with Coupled Cluster for chiral interactions

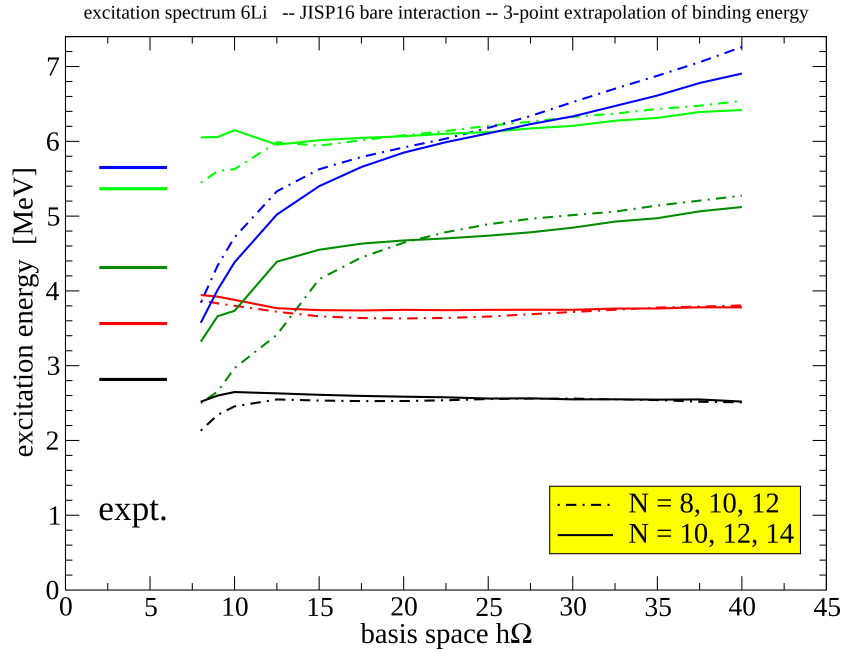


- systematic differences due to alt. Coulomb treatments
- contribution of triples small at $\lambda = 2.5$, virtually zero at $\lambda = 1.5$

Accomplishments – physics results

Established extrapolation for ground state and excited states



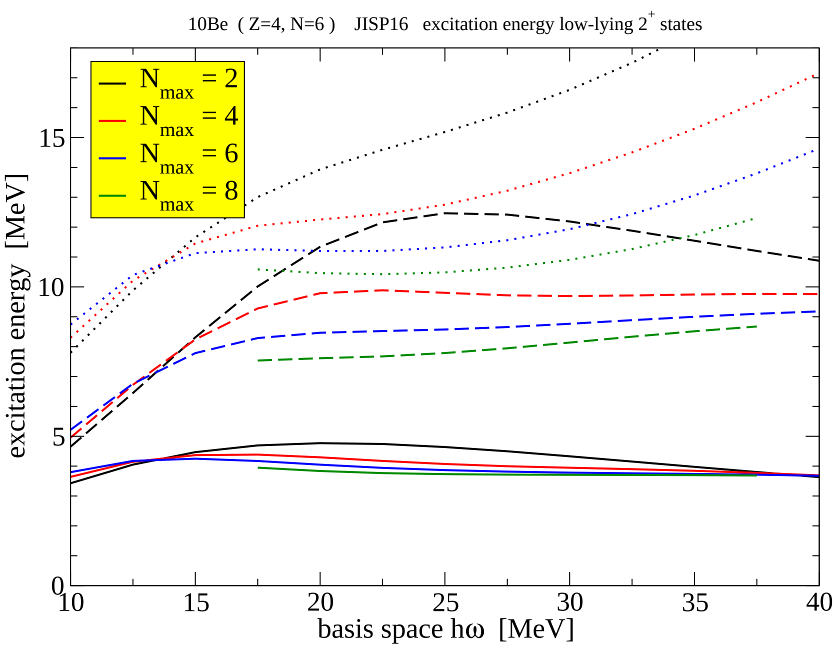


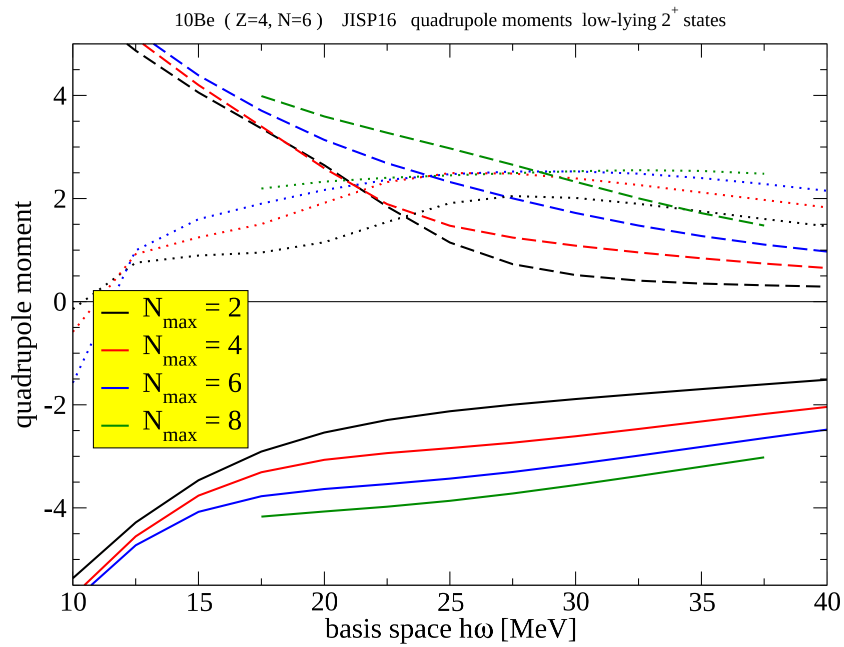
Results for ^{6}Li with JISP16

- spectrum in good agreement with experimental data
- extrapolated spectrum nearly independent of basis space $\hbar\Omega$ except for radially excited $J^\pi = 1^+$, $T = 0$ state
- ground state quadrupole moment Q also in good agreement

Work in progress: ^{10}Be

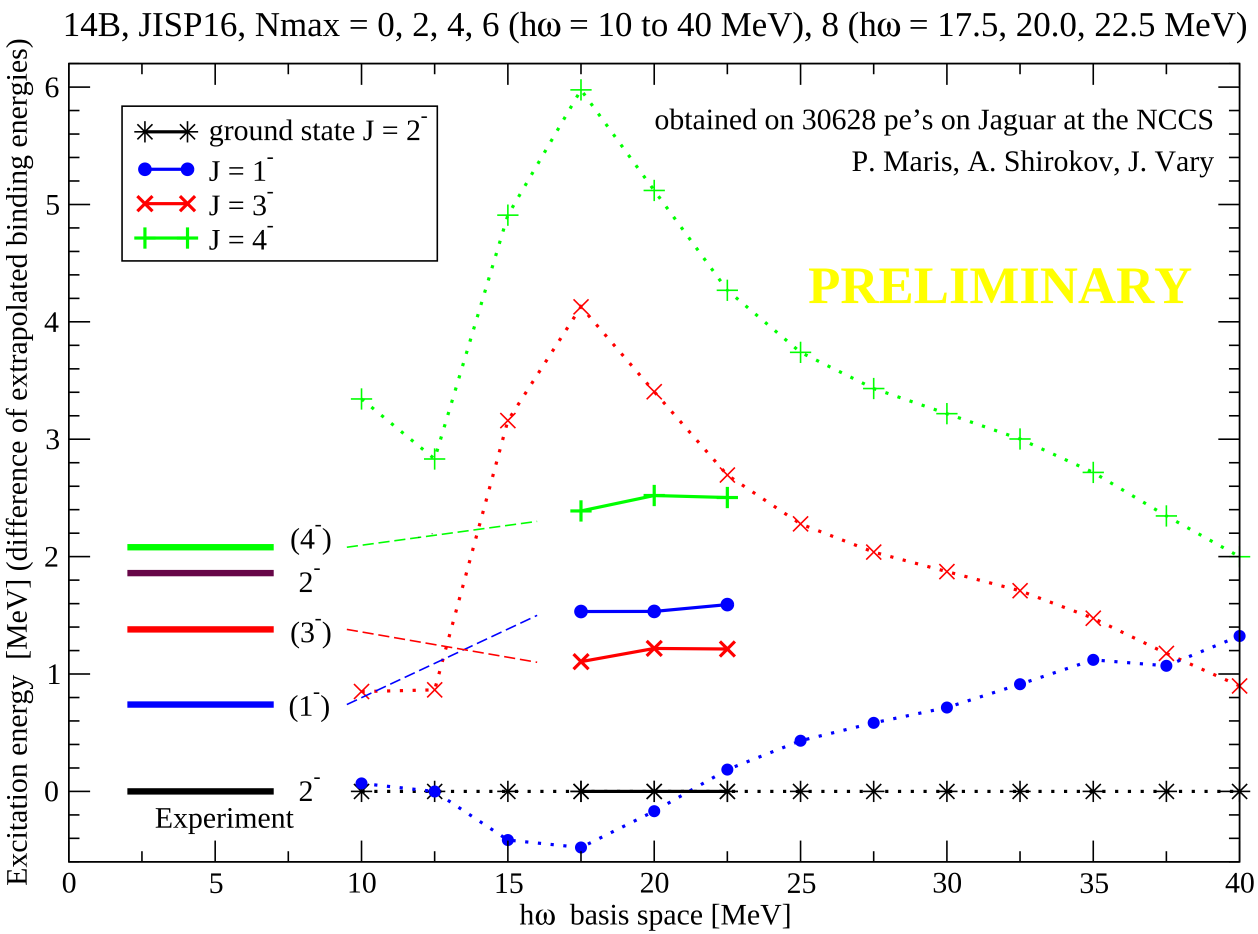
- Motivated by GFMC results
  - without 3-body forces: $\mathcal{Q}$ of lowest 2^+ state is positive but with 3-body forces: $\mathcal{Q}$ of lowest 2^+ state is negative and vice-versa for first excited 2^+ state





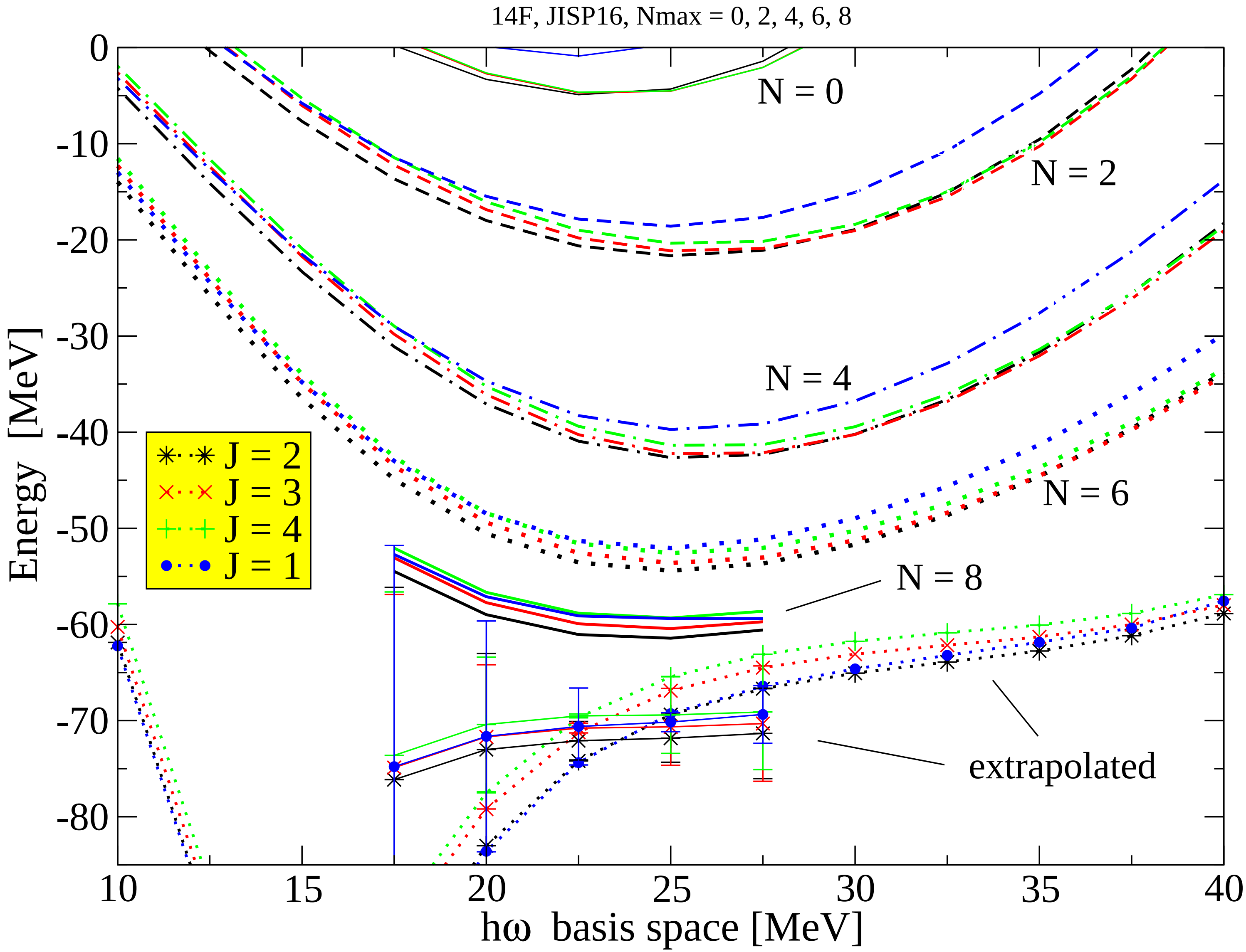
- JISP16 agrees qualitatively with AV18 plus 3-body forces
- Might be checked by experiments at ANL?

Work in progress: A = 14 nuclei

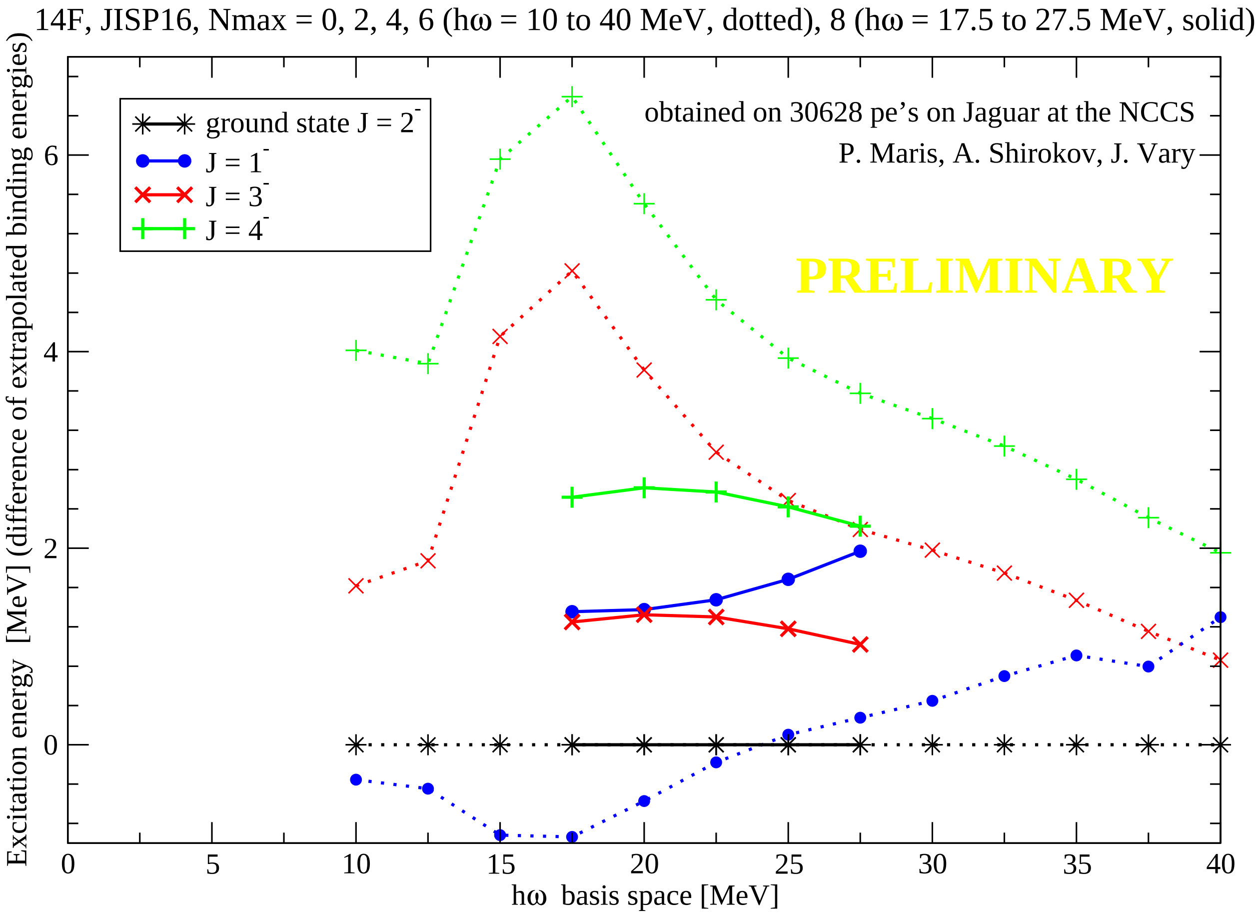


- 9 hours on 30,628 cores (Jaguar) for 3 $\hbar\omega$ values
- w/o recent CS/AM improvements: 18 hrs / $\hbar\omega$ value

Work in progress: A = 14 nuclei



Work in progress: A = 14 nuclei



- ^{14}F: mirror nucleus of ^{14}B
- experiments planned by Texas A&M

New capabilities – external fields

- Nucleons in a trap: apply H.O. external field w. strength Ω

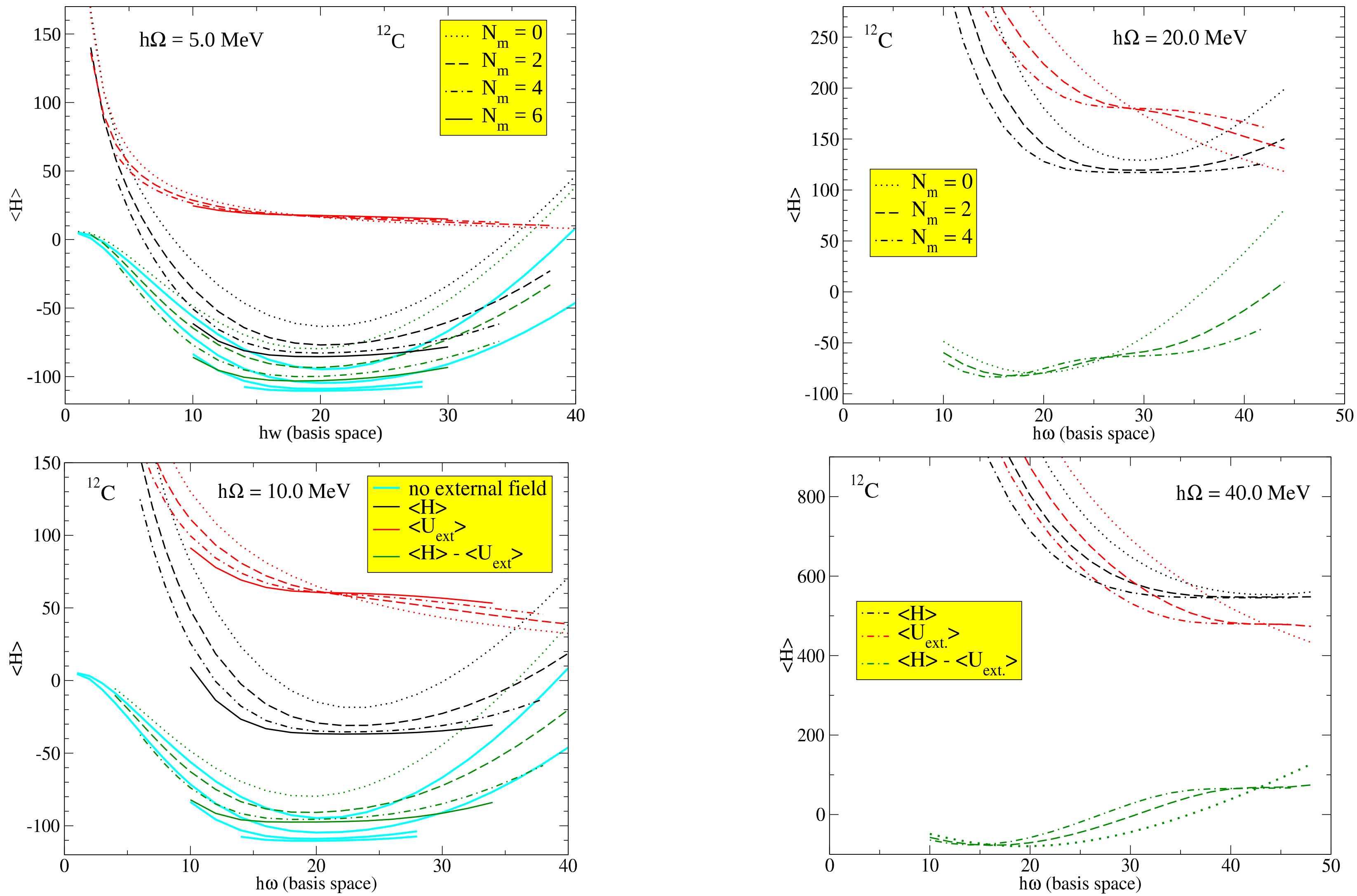
$$U_{\text{ext}} \;=\; \frac{1}{2} m \, \hbar\Omega \, \sum_i r_i^2$$

- Results shown for
  - eigenvalue, equivalent to $\langle H \rangle$
  - expectation value of external field, $\langle U_{\text{ext}} \rangle$
  - expectation value internal energy, $\langle H \rangle - \langle U_{\text{ext}} \rangle$
  - rms radius R, defined through $R^2 = \frac{1}{A} \sum_i \langle r_i^2 \rangle$

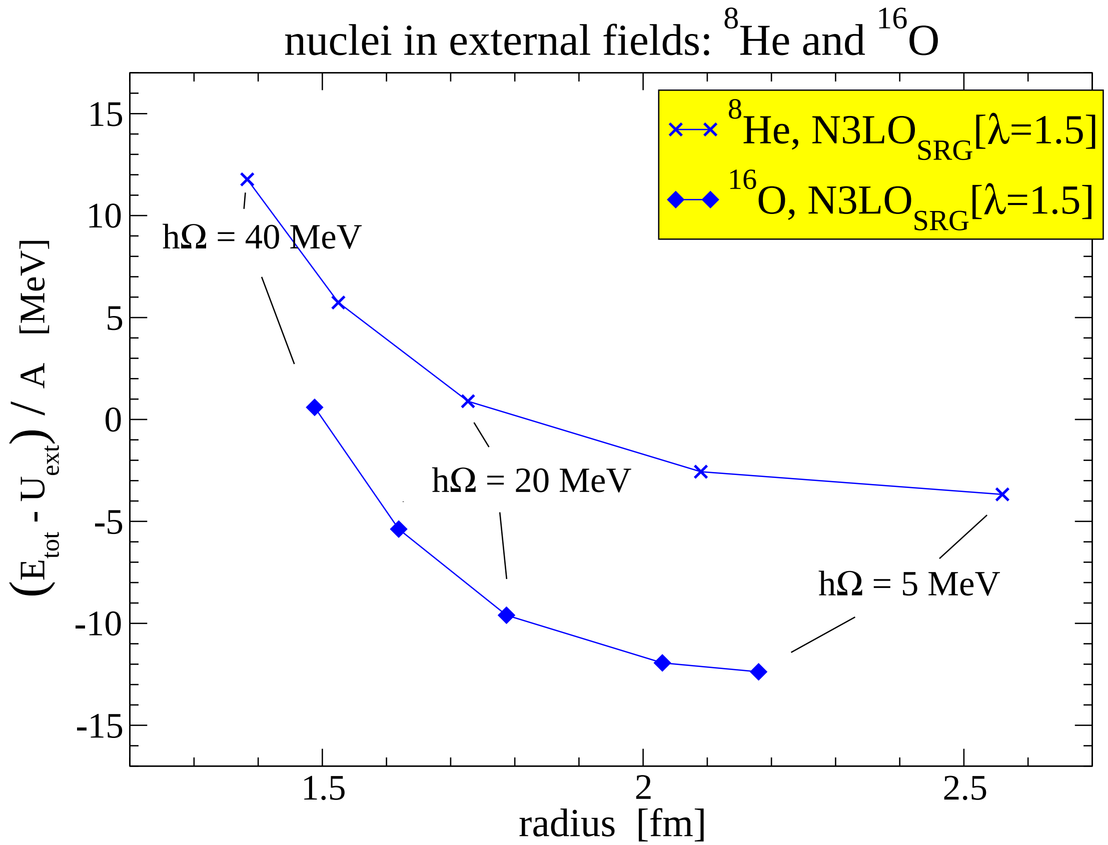
  as function of basis space $\hbar\omega$ for several $N_{\max}$ values
- Internal energy vs. radius plots:
  $\langle H \rangle - \langle U_{\text{ext}} \rangle$ per nucleon as function of R
- Results shown for ground state only
  but MFDn calculates properties of excited states as well

External fields – initial results

N3LO$(\lambda = 1.5)$ potential for rapid convergence (Proof of principle)

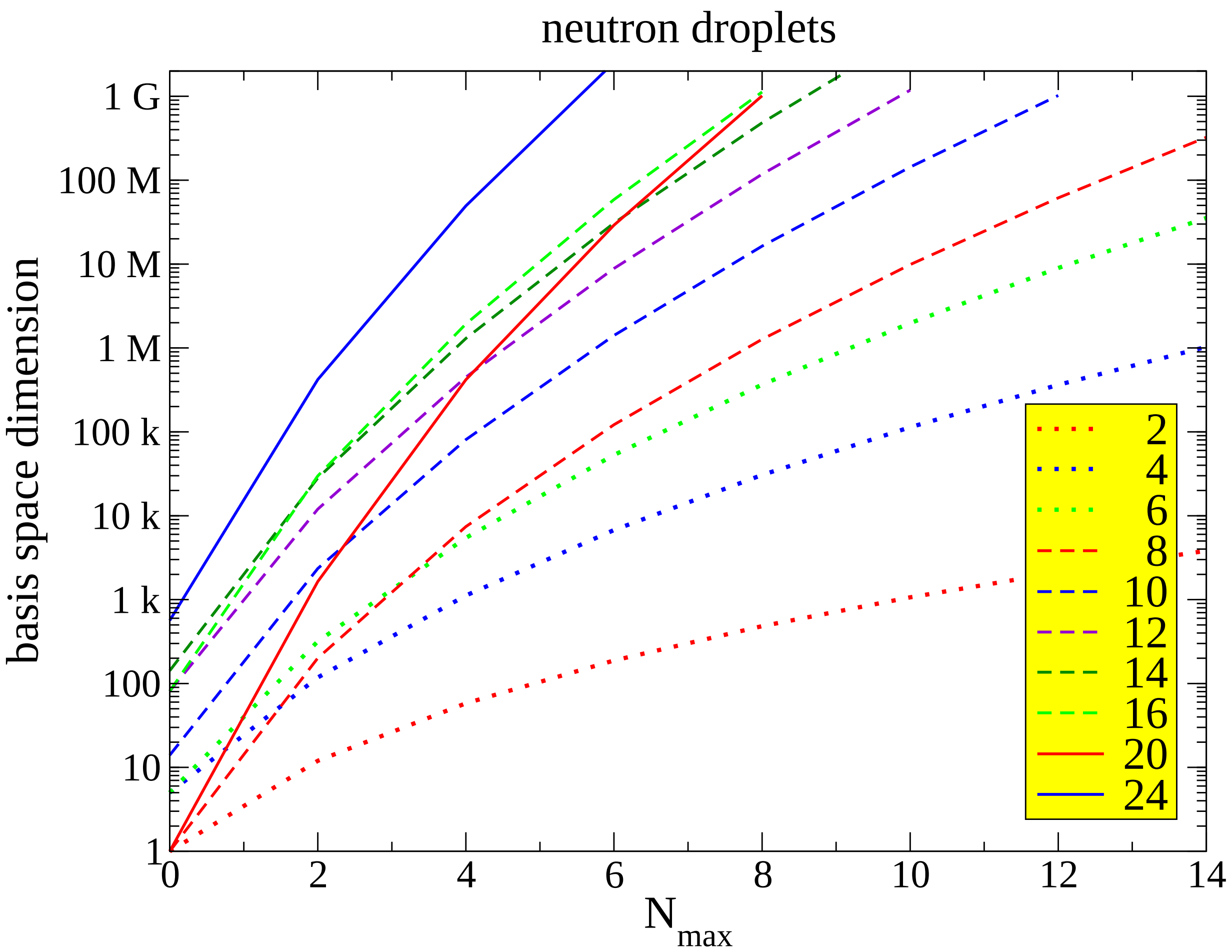


External fields – energy vs. radius



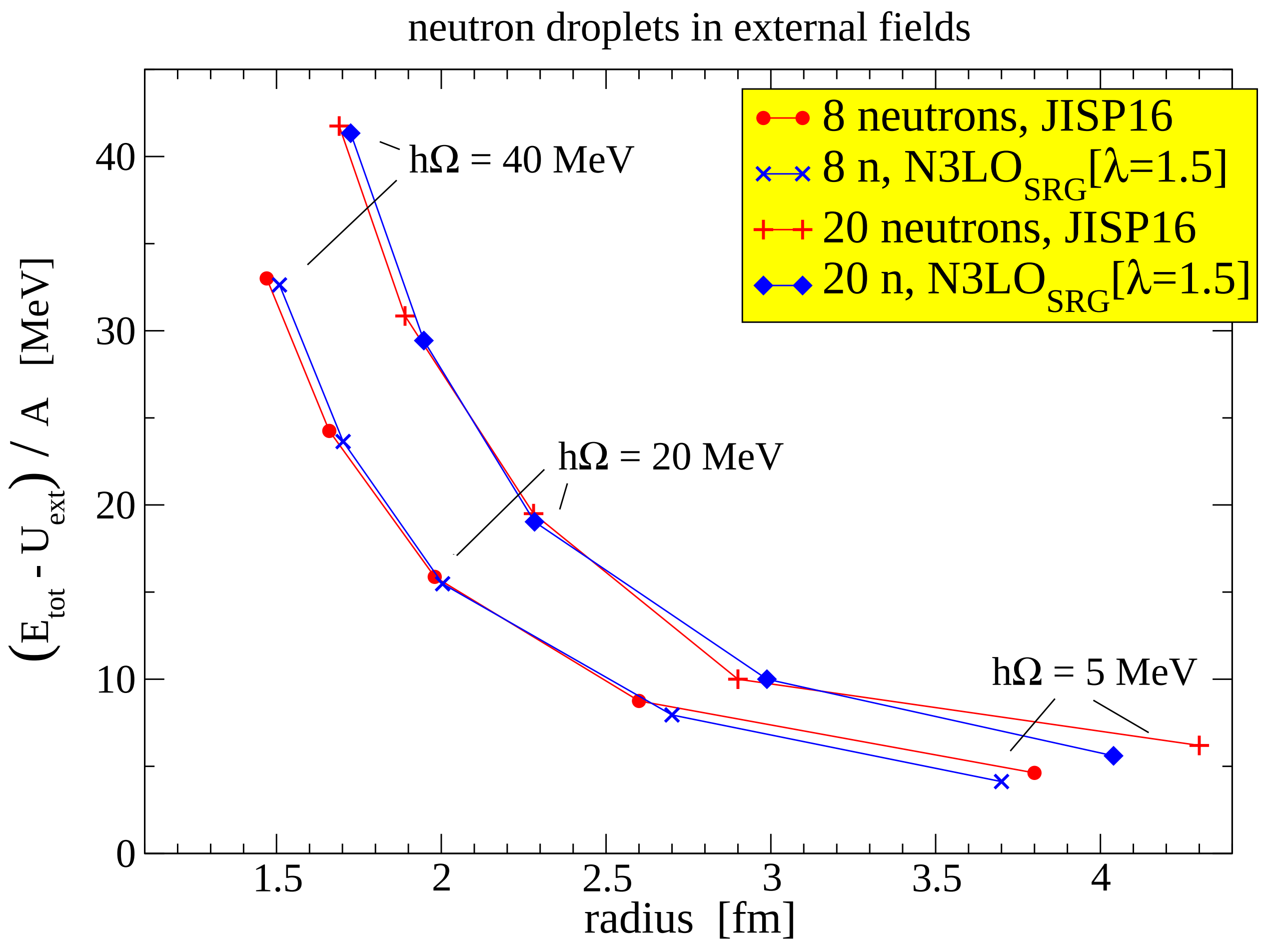
- 8He and 16O for N3LO$(\lambda = 1.5)$ potential (without Coulomb)
- 8He and 16O for JISP16 – in progress

New capabilities – neutron droplets



- Increase of dimension with N_{max} not quite as rapid as for nuclei
- 20 neutrons doable up to $N_{\mathrm{max}} = 8$

New capabilities – neutron droplets with external fields



Results virtually identical for N3LO$(\lambda = 1.5)$ and JISP16 despite different results for real nuclei (e.g. 186 vs. 144 MeV for ^{16}O)

- How does it compare with AV18 and other interactions?

MFDn – Physics Yr 2 workplan

Note: CS/AM workplan presented in next talk

- Benchmark against GFMC (SSC) and CC (N3LO, JISP16)
- External field constraints – functional
- Neutron droplets – functional
- Physics runs $A = 7 - 14$ NN potentials – in progress
  - NERSC (mostly Franklin)
  - INCITE (mostly Jaguar, starting to use Intrepid)
- Realistic chiral 3-body forces $A = 12$ – in progress (65% done)
  - Grand challenge award LLNL (Atlas, Thunder)

To be done

- Generalized single-particle basis capablity – on track

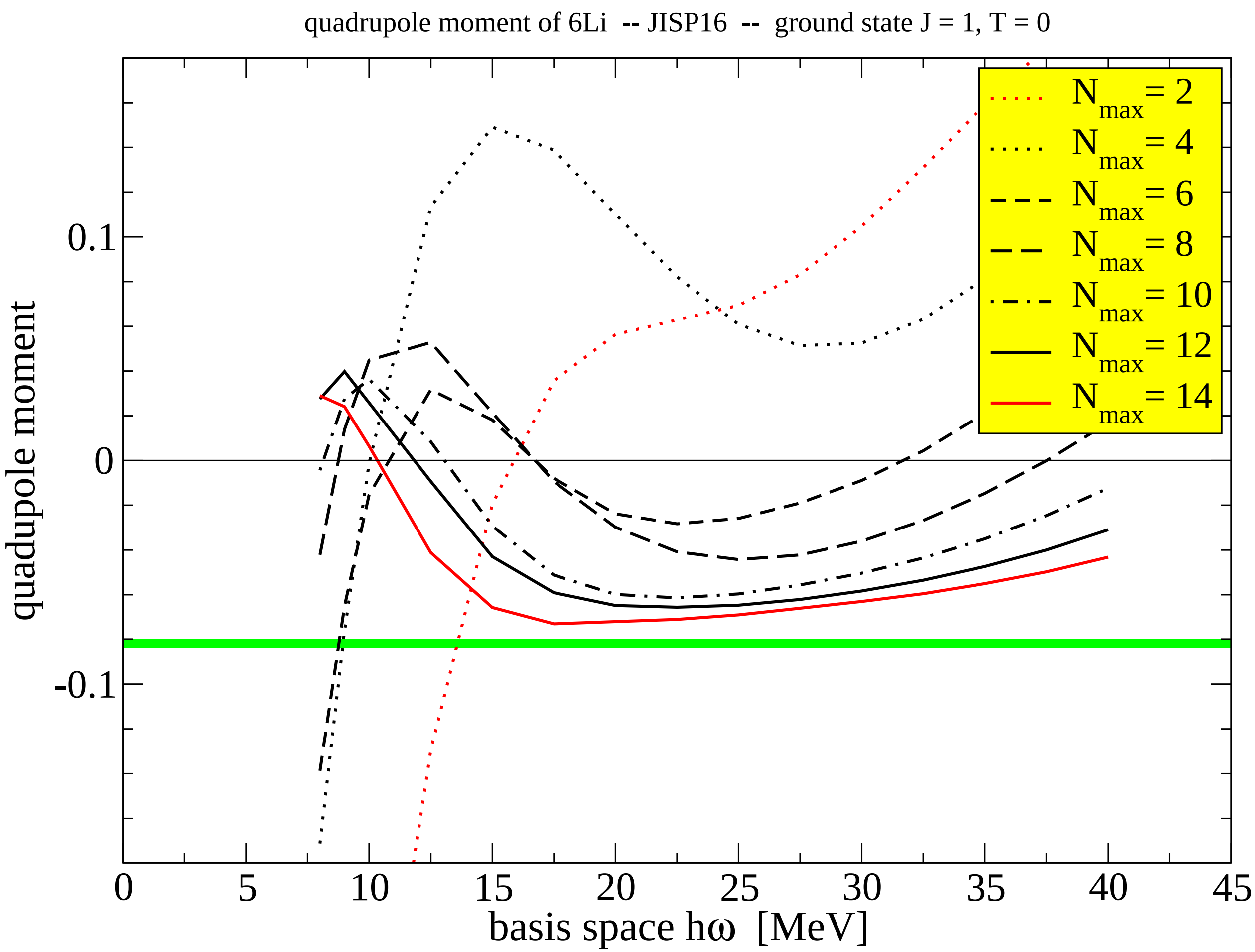
MFDn – Physics Yr 3 workplan

- Extend capability of realistic (chiral) NNN interactions
  to larger model spaces
  - currently limited to $N_{\mathrm{max}} = 6$, due to memory constraints
    $N_{\mathrm{max}} = 8$ is highly desirable for reliable extrapolations
  - requires significant improvements in performance of MFDn and/or new algorithms
- Explore realistic single-particle basis states
  - integrate MFDn with optimization techniques
- Generalize external field
  and produce 1-body density matrices in external fields
  - what type of external fields are needed?
  - what level of accuracy is needed?
  - which systems are most useful?
  - what observables?

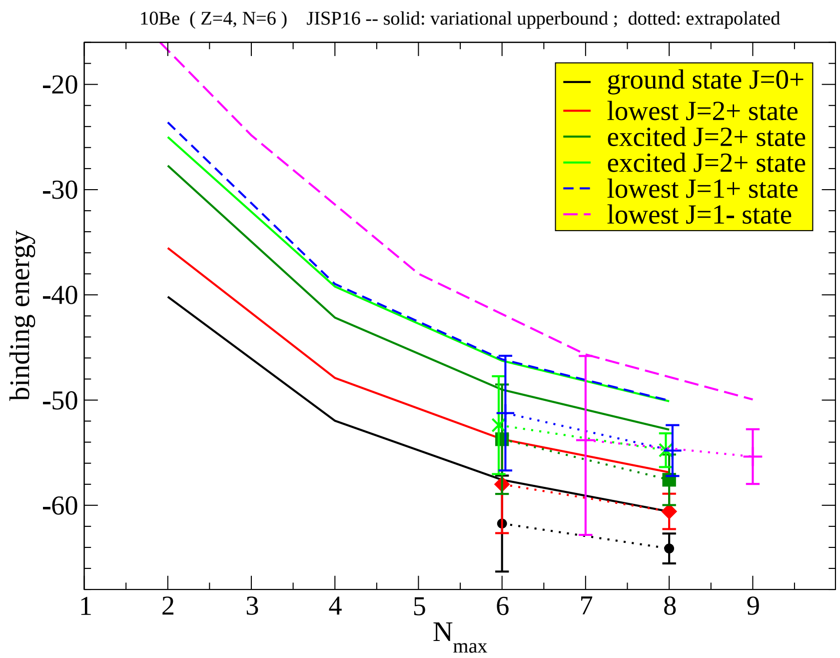
MFDn – Physics Yr 3 - 5 outlook

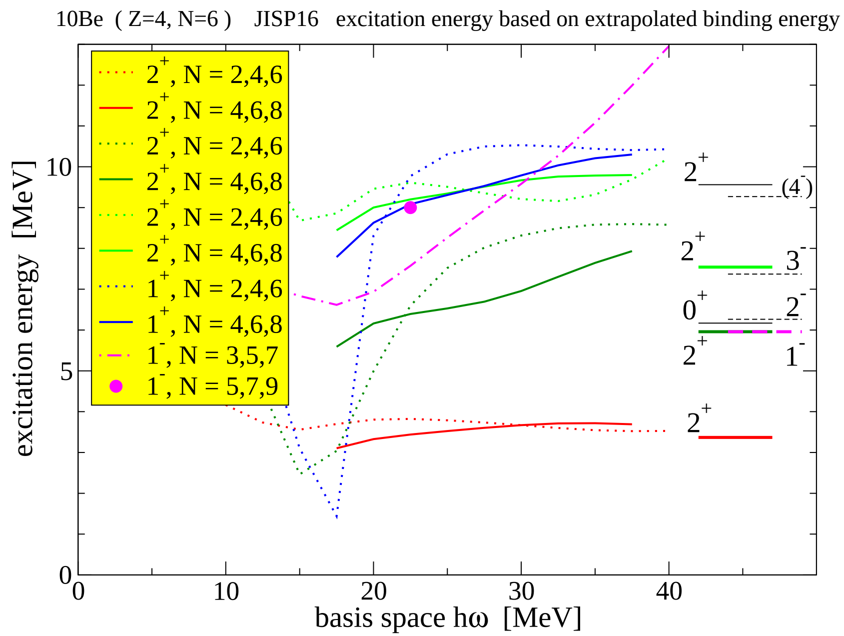
- Implement coupled J basis capability
  - Reduction of basis space for ^{16}O at $N_{\max} = 8$:
    $D \sim 10^9$ in m-scheme reduces to $30 \cdot 10^6$ for $J = 0$ states
  - In combination with realistic basis states:
    Hoyle (and Hoyle-like) states in ^{12}C and ^{16}O
- Scattering applications
  - Needs alternative eigensolvers
    (requires hundreds (thousands) of states)
- Code documentation
- Integrate MFDn with other codes to create general CI code

Quadrupole moment 6Li ground state JISP16



Work in progress: ^{10}Be – more details





- first 2^+ state converged, and agrees with experiments
- higher excited states not yet converged
- calculated spectrum: 1^+, but no 0^+ among lowest 5 states
- experimental spectrum: 0^+, but no 1^+ among lowest 5 states