No-Core CI calculations of p-shell nuclei with 2- and 3-body forces

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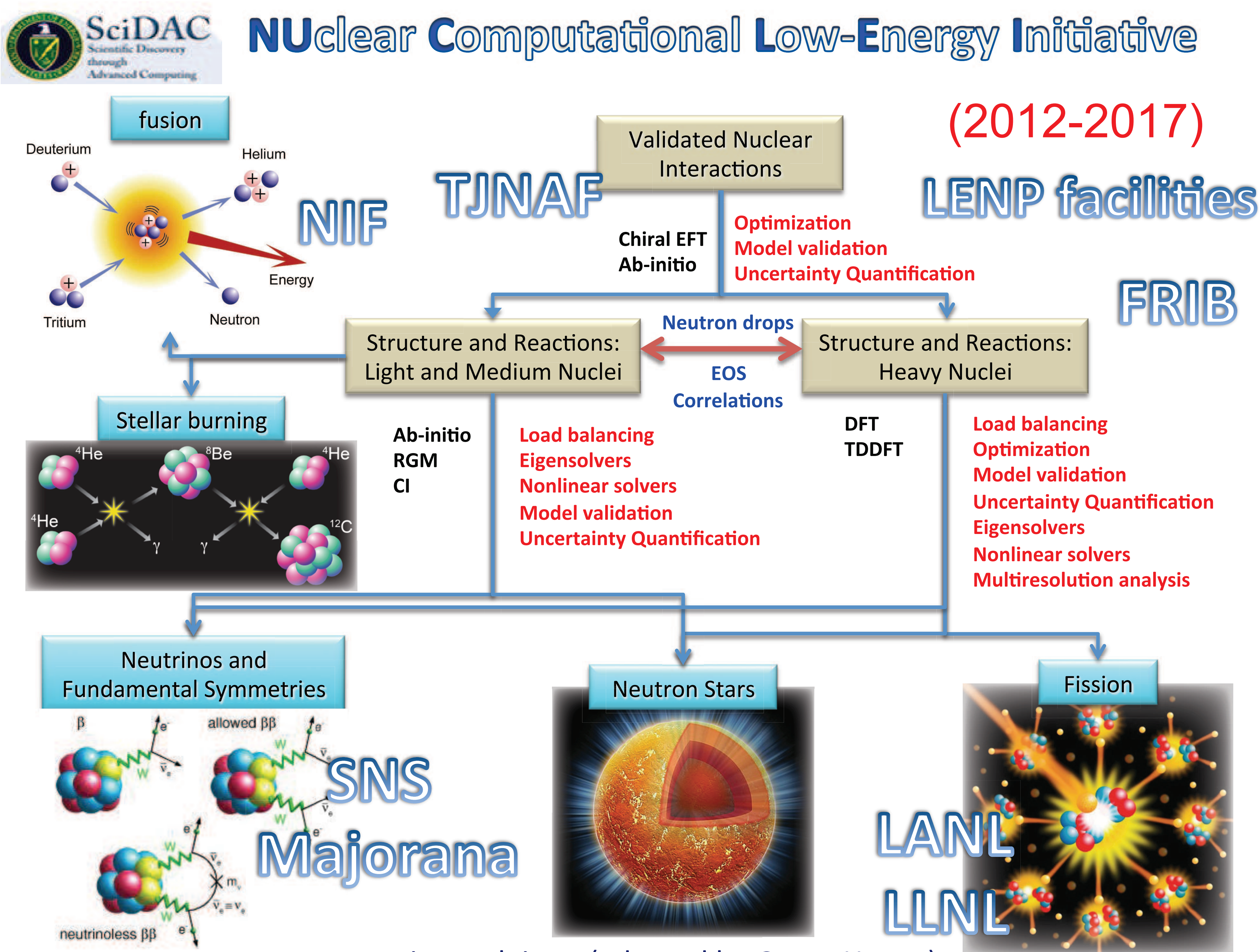
SciDAC project – NUCLEI
lead PI: Joe Carlson (LANL)
http://computingnuclei.org

PetaApps award
lead PI: Jerry Draayer (LSU)

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

NERSC

NUclear Computational Low-Energy Initiative



computingnuclei.org (adapted by Gaute Hagen)

Ab initio nuclear physics – Quantum many-body problem

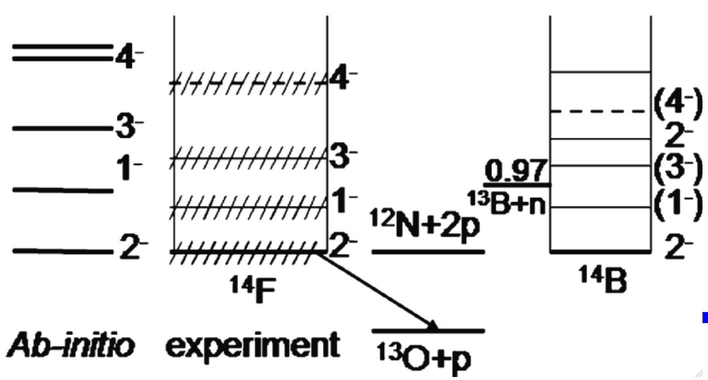
Given a Hamiltonian operator

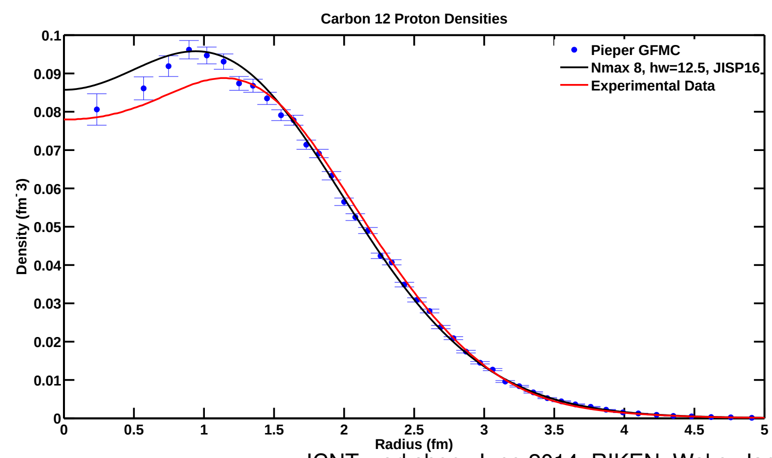
$$\hat{\mathbf{H}} = \sum_{i<j} \frac{(\vec{p}_i - \vec{p}_j)^2}{2\,m\,A} + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \ldots$$

solve the eigenvalue problem for 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 $1, \ldots, A$ at $r_1, \ldots, r_A$





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
    - 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 calculations

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

- Expand wave function 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

NCCI – Basis space expansion

- Expand wave function in basis $\Psi(r_1, \ldots, r_A) = \sum a_i \Phi_i(r_1, \ldots, r_A)$
- Many-Body basis states $\Phi_i(r_1, \ldots, r_A)$ Slater Determinants of Single-Particle states $\phi_{ik}(r_k)$

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

- 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 $\hat{\mathbf{J}}_{\mathbf{z}}$

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

  - single run gives entire spectrum
  - alternatives:
    Coupled-J scheme, Symplectic basis, . . .
- N_{max} truncation: Many-Body basis states satisfy

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

  - exact factorization of Center-of-Mass motion
- 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)
  - . . .

Intermezzo: Center-of-Mass excitations

- 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 wave function factorizes for H.O. basis functions in combination with N_{max} truncation

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

where

$$
\hat{\mathbf{H}}_{\text{rel}}|\Psi_{\text{j, rel}}\rangle = E_{\text{j}}|\Psi_{\text{j, rel}}\rangle
$$

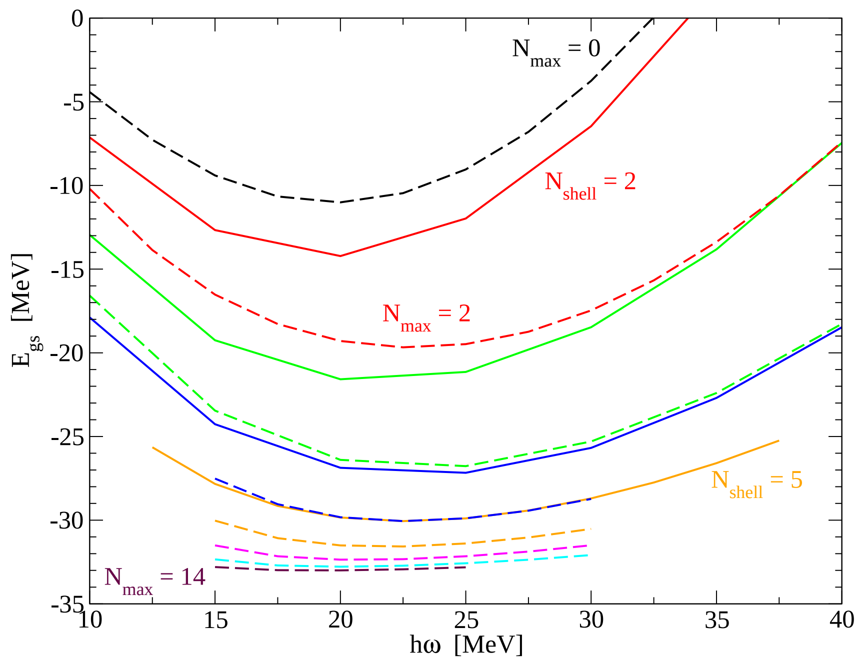
- Add Lagrange multiplier to Hamiltonian (Lawson term)

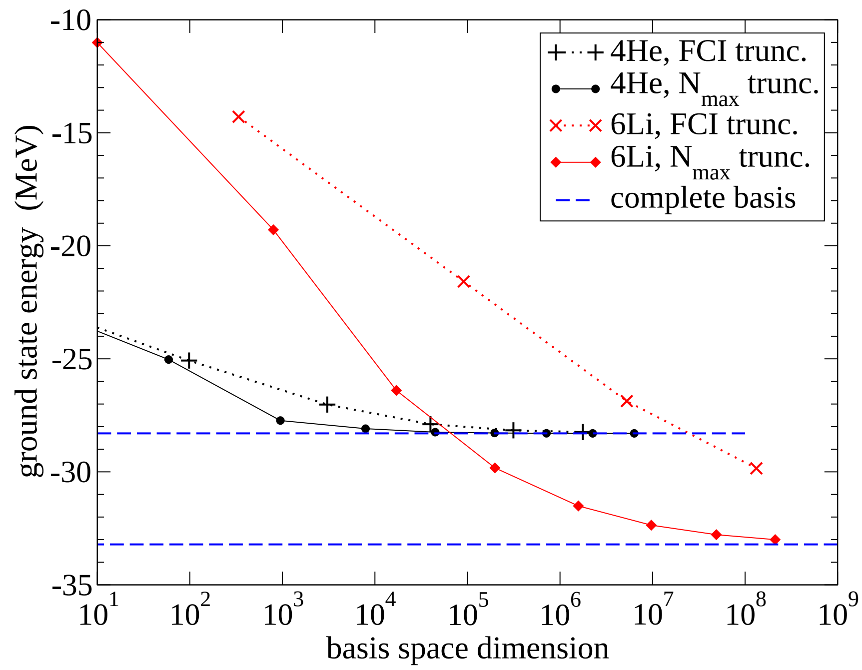
$$
\hat{\mathbf{H}}_{\text{rel}} \longrightarrow \hat{\mathbf{H}}_{\text{rel}} + \Lambda_{CM}\left(\hat{\mathbf{H}}_{CM}^{H.O.} - \frac{3}{2}\Big(\sum_i m_i\Big)\,\omega\right)
$$

with $\hat{\mathbf{H}}_{\text{rel}} = \hat{\mathbf{T}}_{\text{rel}} + \hat{\mathbf{V}}_{\text{rel}}$ the relative Hamiltonian

  - separates CM excitations from CM ground state $|\Phi_{CM}\rangle$

Intermezzo: FCI vs. Nmax truncation

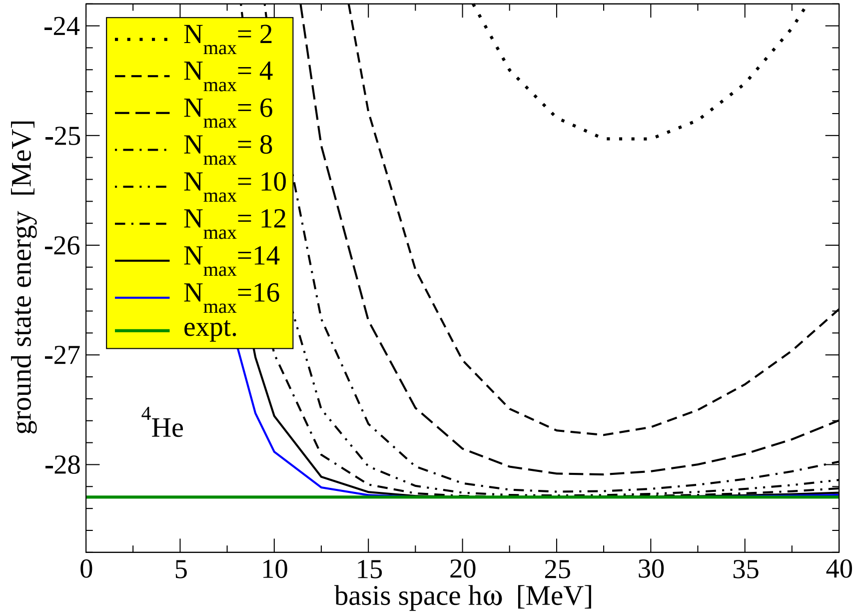




- N_{max} truncation
  - exact factorization of Center-of-Mass motion
- Infinite basis space limit: No-Core Full Configuration (NCFC)
  - both N_{max} truncation and FCI converge to the same results
  - N_{max} truncation does so much more rapidly

Configuration Interaction methods

- 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: No-Core Full Configuration calculation
- Convergence: independence of N_{max} and H.O. basis $\hbar\omega$
  - different methods (NCFC, CC, 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 Full Configuation calculations using finite model space calculations

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

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

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

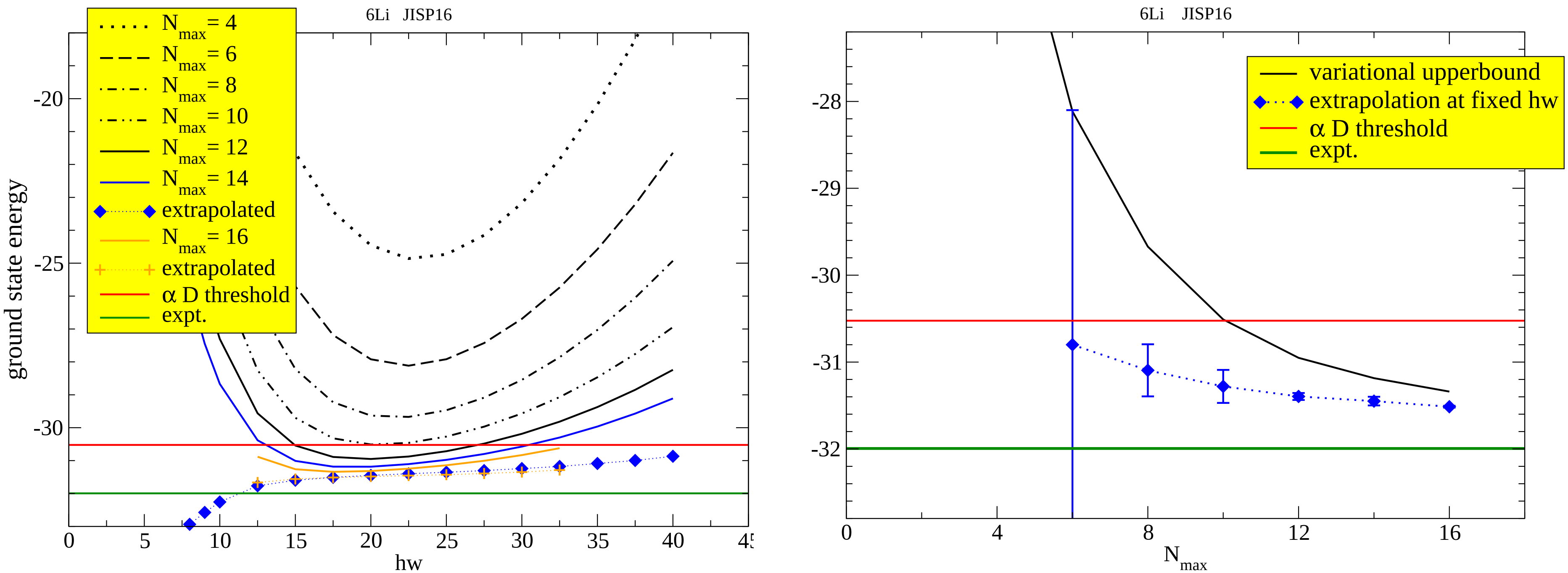
Maris, Shirokov, Vary, PRC79, 014308 (2009)

- Recent studies of IR and UV behavior:
  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)

Extrapolating to complete basis – in practice

- Perform a series of calculations with increasing N_{max} truncation
- Use empirical exponential in N_{max}:
  $E^{N}_{\text{binding}} = E^{\infty}_{\text{binding}} + a_1 \exp(-a_2 N_{\text{max}})$

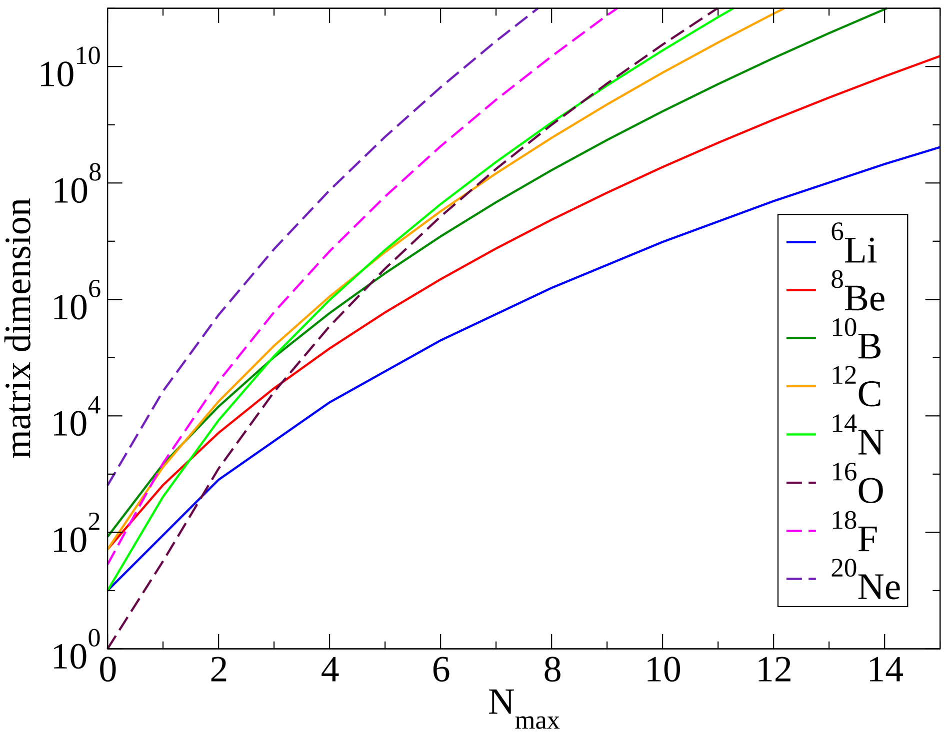


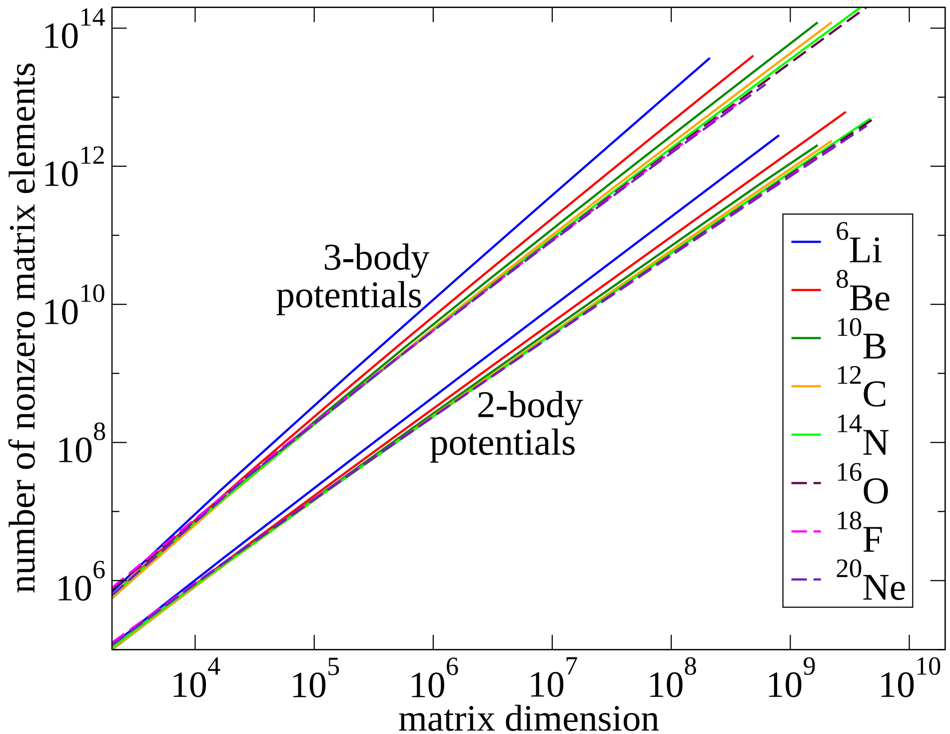
- H.O. basis up to $N_{\text{max}} = 16$: $E_b = -31.49(3)$ MeV

  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 calculations – main challenge





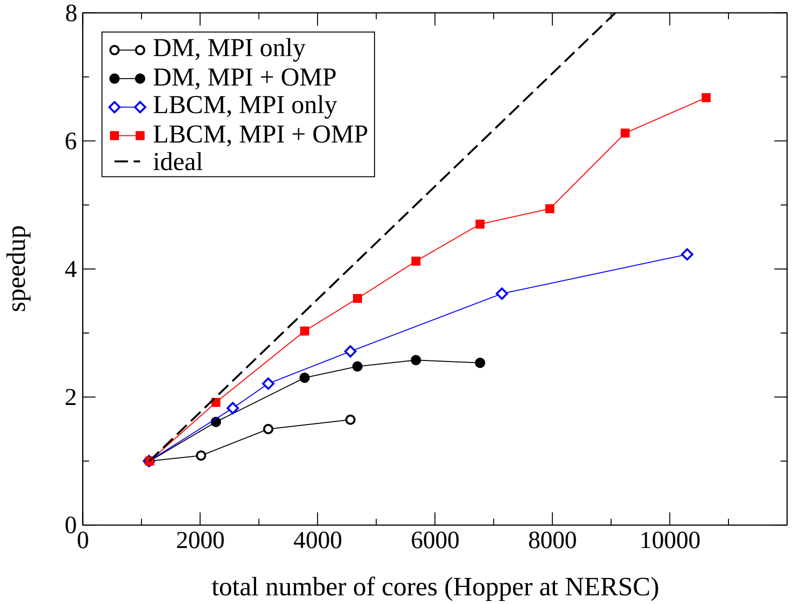
- Increase of basis space dimension with increasing A and N_{max}
  - need calculations up to at least $N_{\text{max}} = 8$ for meaningful extrapolation and numerical error estimates
- More relevant measure for computational needs
  - number of nonzero matrix elements
  - current limit 10^{13} to 10^{14}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

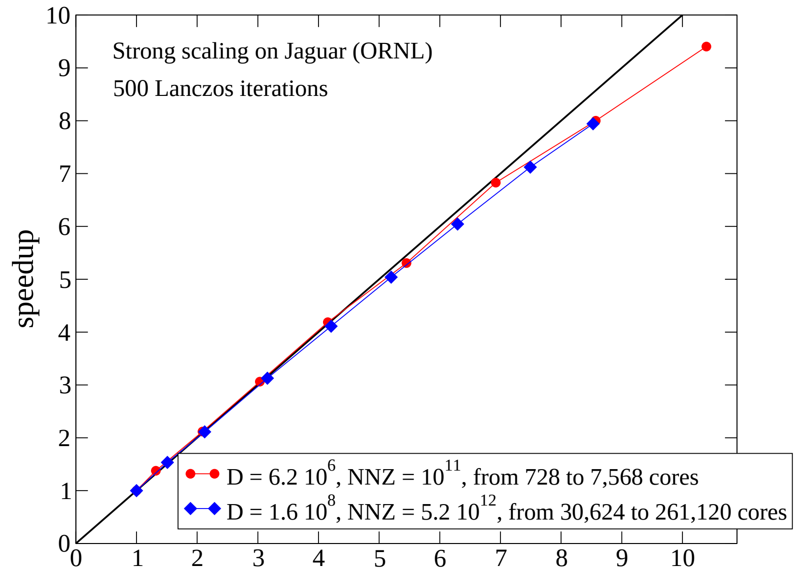
Many Fermion Dynamics – nuclear physics

Efficient Configuration Interaction code for nuclear physics as a result of collaboration with applied mathematicians and computer scientists

- Platform-independent, hybrid OpenMP/MPI, Fortran 90
- Generate many-body basis space
  subject to user-defined truncation and symmetry constraints
- Construct many-body matrix H_{ij}
  - determine which matrix elements can be nonzero
    based on quantum numbers of underlying single-particle states
  - evaluate and store nonzero matrix elements
    in compressed row/column format
- Obtain lowest eigenpairs using Lanczos algorithm
  - typical use: 10 to 20 lowest eigenvalues and eigenvectors
  - typically need $\sim$ 500 to $\sim$ 1000 Lanczos iterations
  - some applications need hundreds of eigenvalues
- Write eigenvectors to disk and calculate observables

Strong Scaling of MFDn

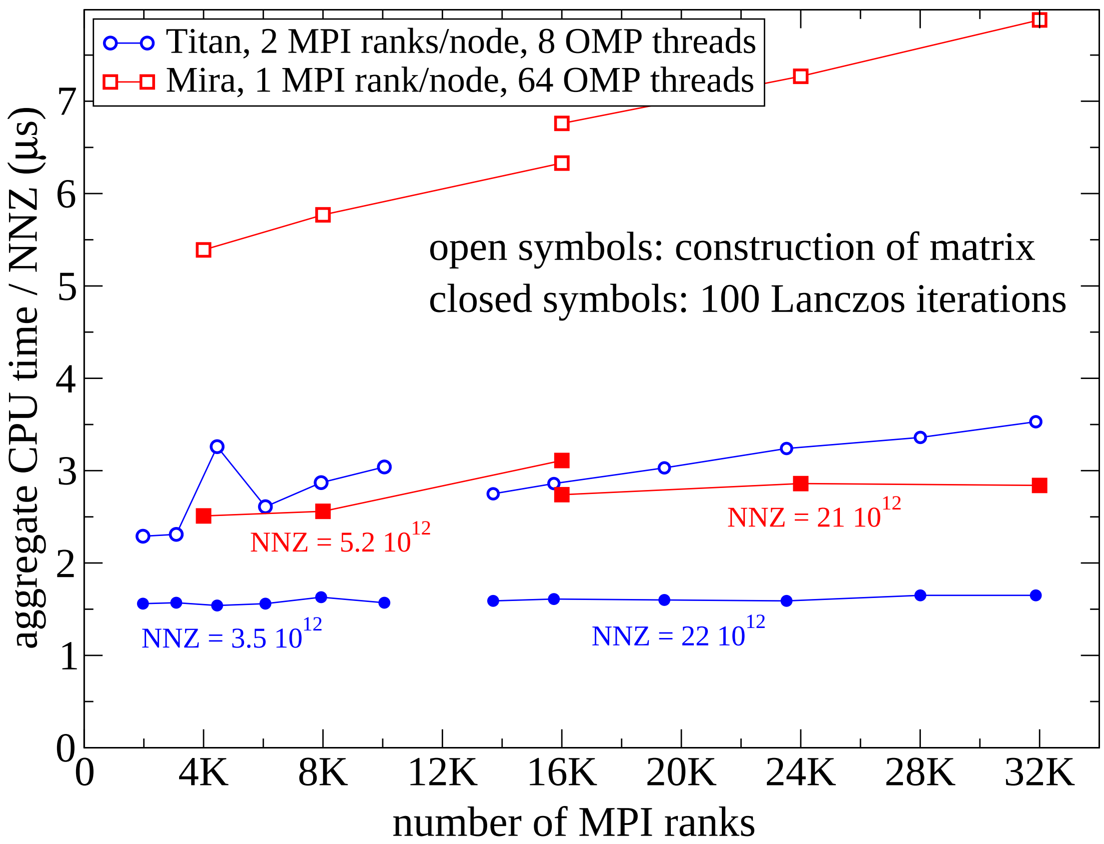




- Understand communication overheads in terms of heuristic network model based on set of compute nodes, physical links between compute nodes, and link capacity
- Hybrid OpenMP/MPI with 1 MPI processor per NUMA node performs better than MPI-only for more than few hundred cores
- Runs with 3-body forces scale better than NN-only runs

Aktulga, Yang, Ng, Maris, Vary, Concurrency Computat.: Pract. Exper. (2013)

Scaling of MFDn on Leadership Class Facilities



- Version14 Beta03, June 2013
- 2-body + 3-body forces
- 100 Lanczos iterations

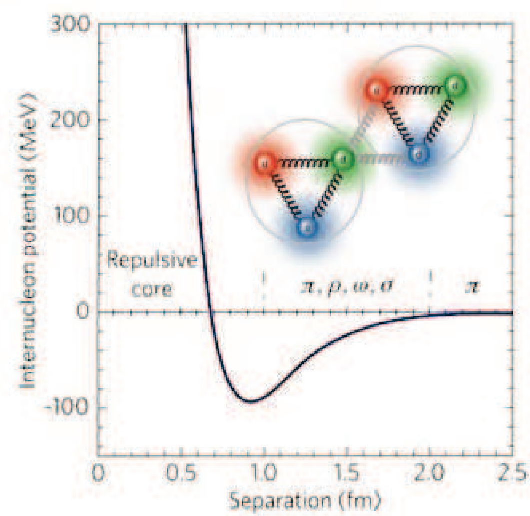
- Titan: Cray XK7 with 2.2 GHz AMD Opteron 16-core CPU with 32 GB per node (plus NVIDIA Kepler GPUs)
- Mira: IBM BG/Q with 1.6 GHz 16-core CPU with 16 GB per node (supporting up to 64 threads)

Nuclear interaction

Nuclear potential not well-known,

though in principle calculable from QCD

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



In practice, alphabet of realistic potentials

- Argonne potentials: AV8′, AV18
  - plus Urbana 3NF (UIX)
  - plus Illinois 3NF (IL7)
- Bonn potentials
- Chiral NN interactions
  - plus chiral 3NF, ideally to the same order
- ...
- JISP16
- ...

Phenomeological NN interaction: JISP16

JISP16 tuned up to ^{16}O

- Constructed to reproduce np scattering data
- Finite rank seperable potential in H.O. representation
- Nonlocal NN-only potential
- Use Phase-Equivalent Transformations (PET) to tune off-shell interaction to
  - binding energy of ^{3}H and ^{4}He
  - low-lying states of ^{6}Li (JISP6, precursor to JISP16)
  - binding energy of ^{16}O

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Realistic nuclear Hamiltonian: Ab exitu approach

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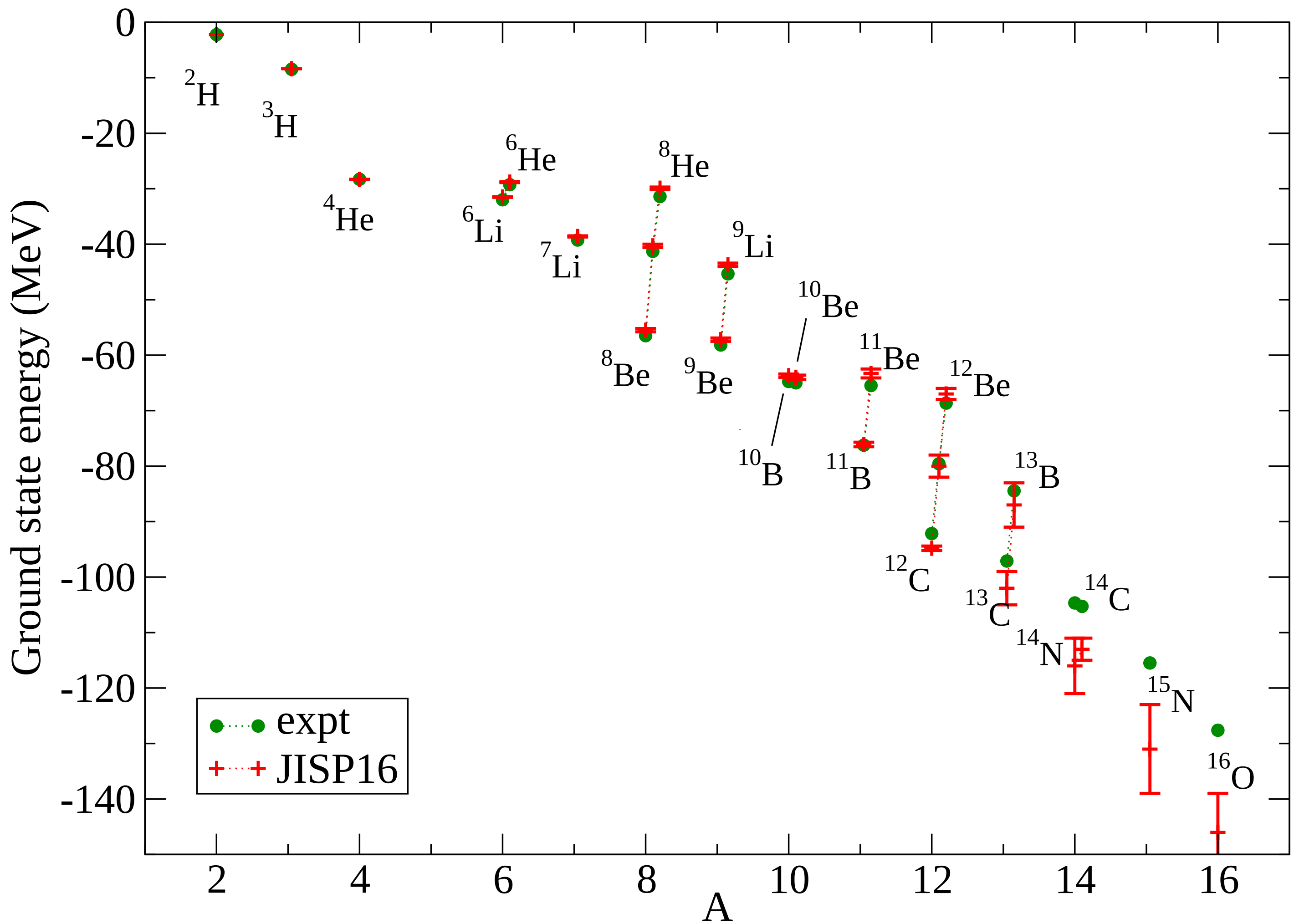
Ground state energy of p-shell nuclei with JISP16

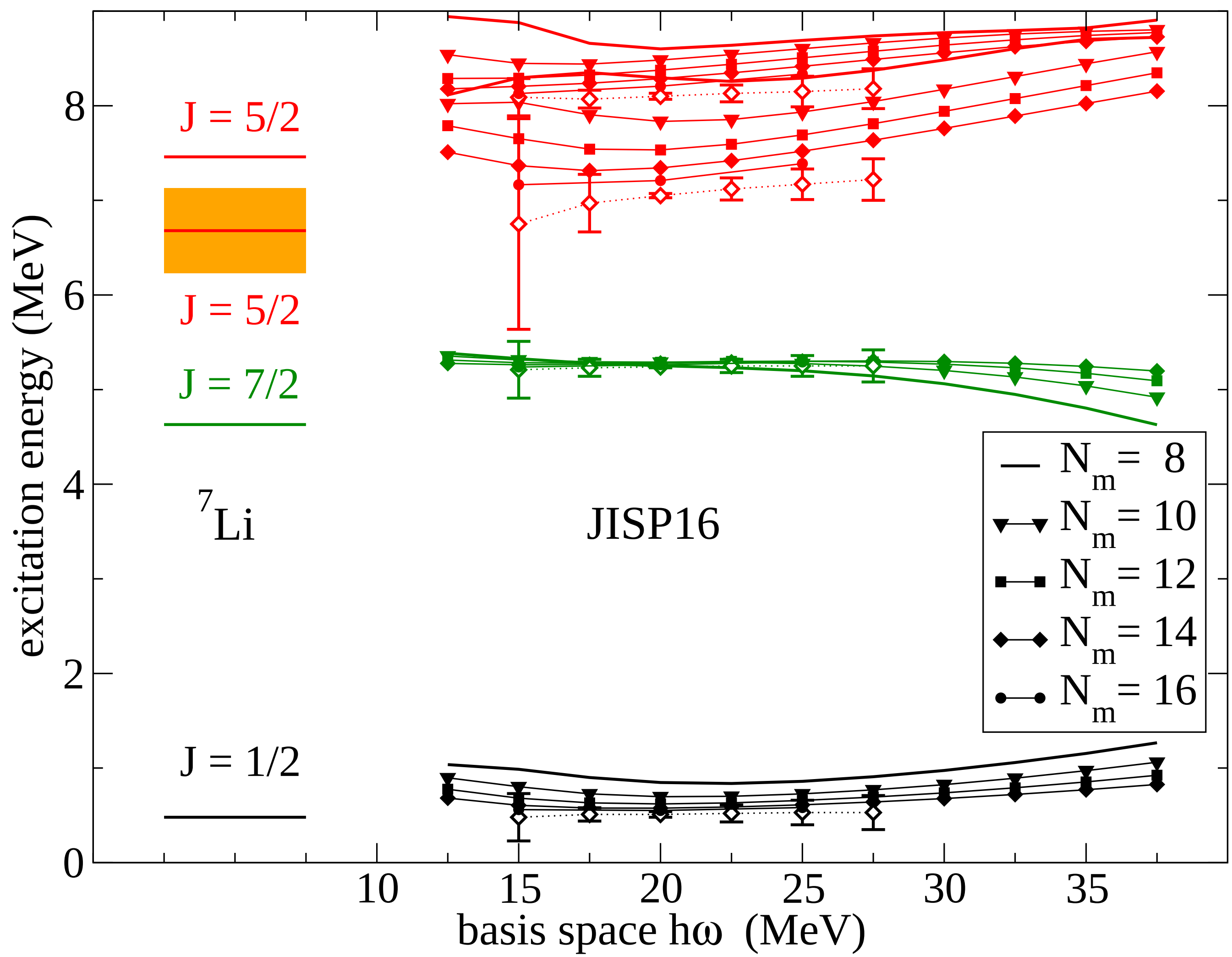
Maris, Vary, IJMPE22, 1330016 (2013)



- ^{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

Excitation spectrum 7Li

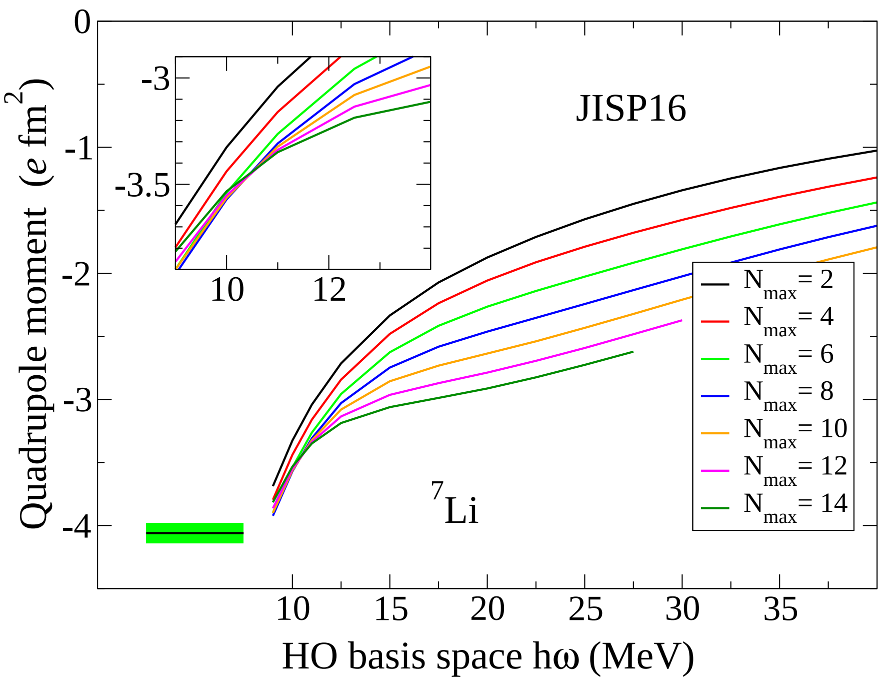
Cockrell, Maris, Vary, PRC86 034325 (2012)

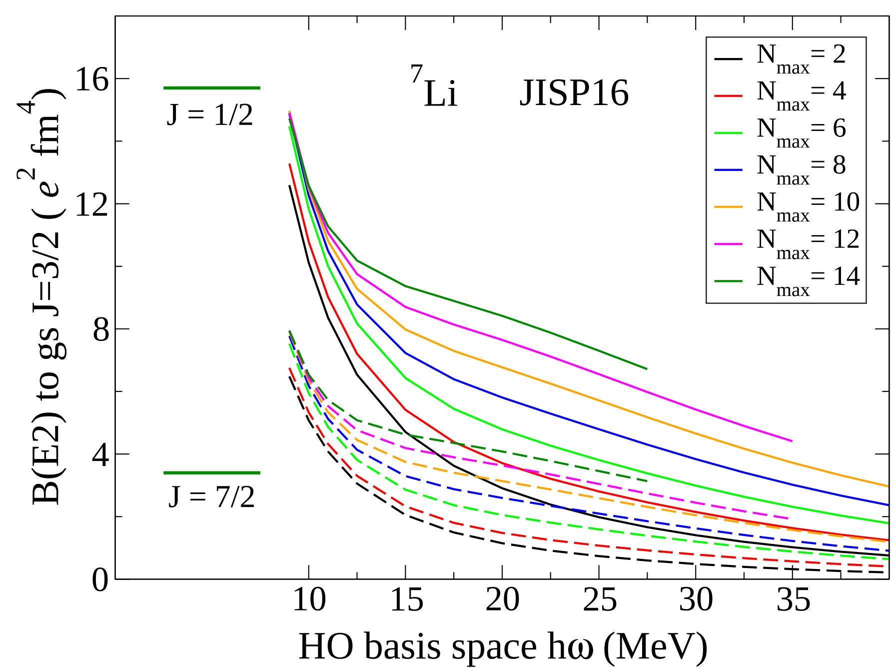


- Narrow states well converged, no extrapolation needed
- Broad resonances generally not as well converged; may need to incorporate continuum?

Quadrupole moment and B(E2) transition strengths 7Li

Cockrell, Maris, Vary, PRC86 034325 (2012)



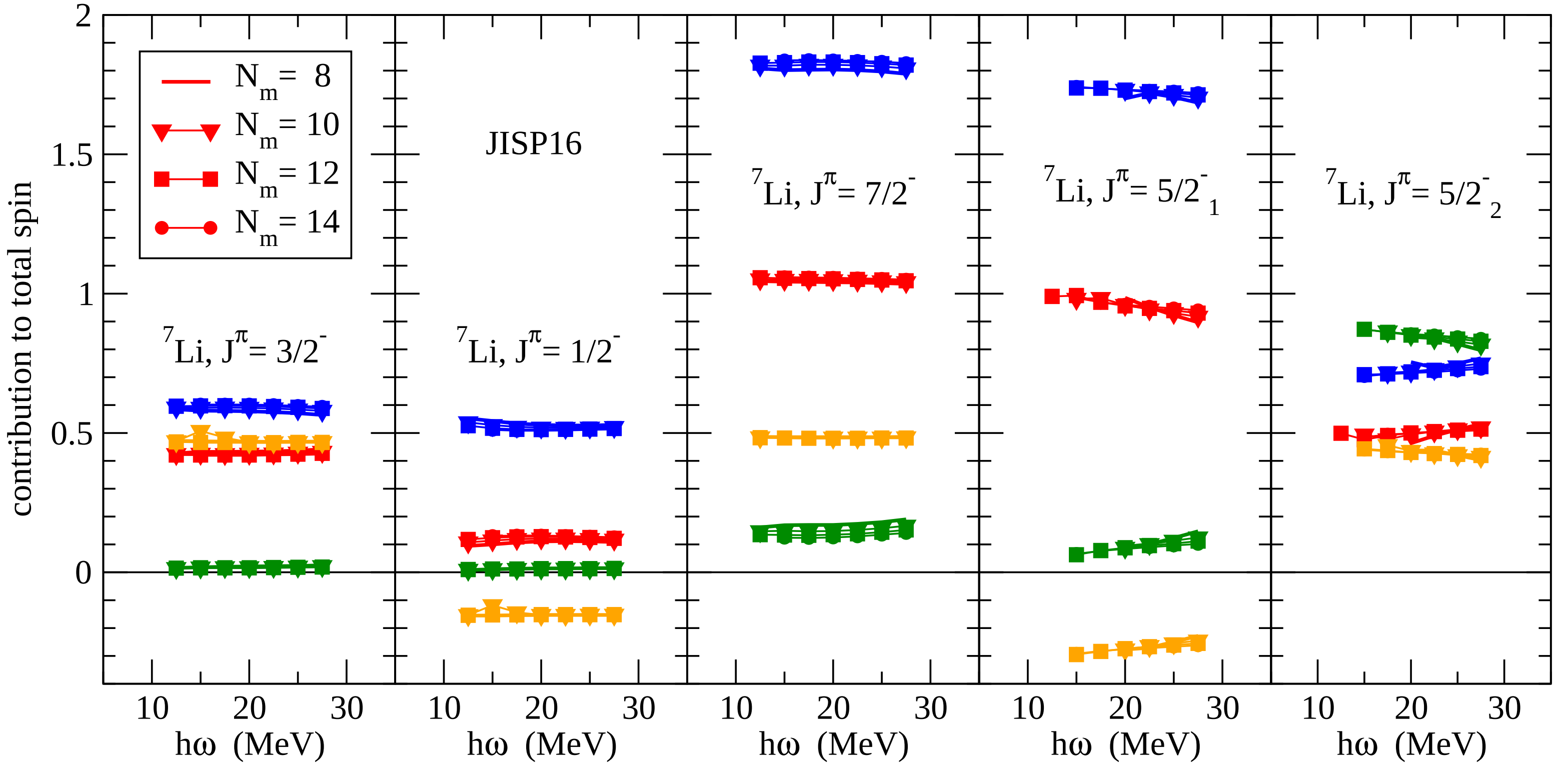


- E2 observables not converged,
  due to gaussian fall-off of HO wavefunction
- Nevertheless, qualitative agreement of $\mathcal{Q}$ and B(E2) with data

Details: spin components of 7Li

Maris, Vary, IJMPE22, 1330016 (2013)

$$J = \frac{1}{J+1}\left(\langle \vec{J}\cdot\vec{L}_p\rangle + \langle \vec{J}\cdot\vec{L}_n\rangle + \langle \vec{J}\cdot\vec{S}_p\rangle + \langle \vec{J}\cdot\vec{S}_n\rangle\right)$$

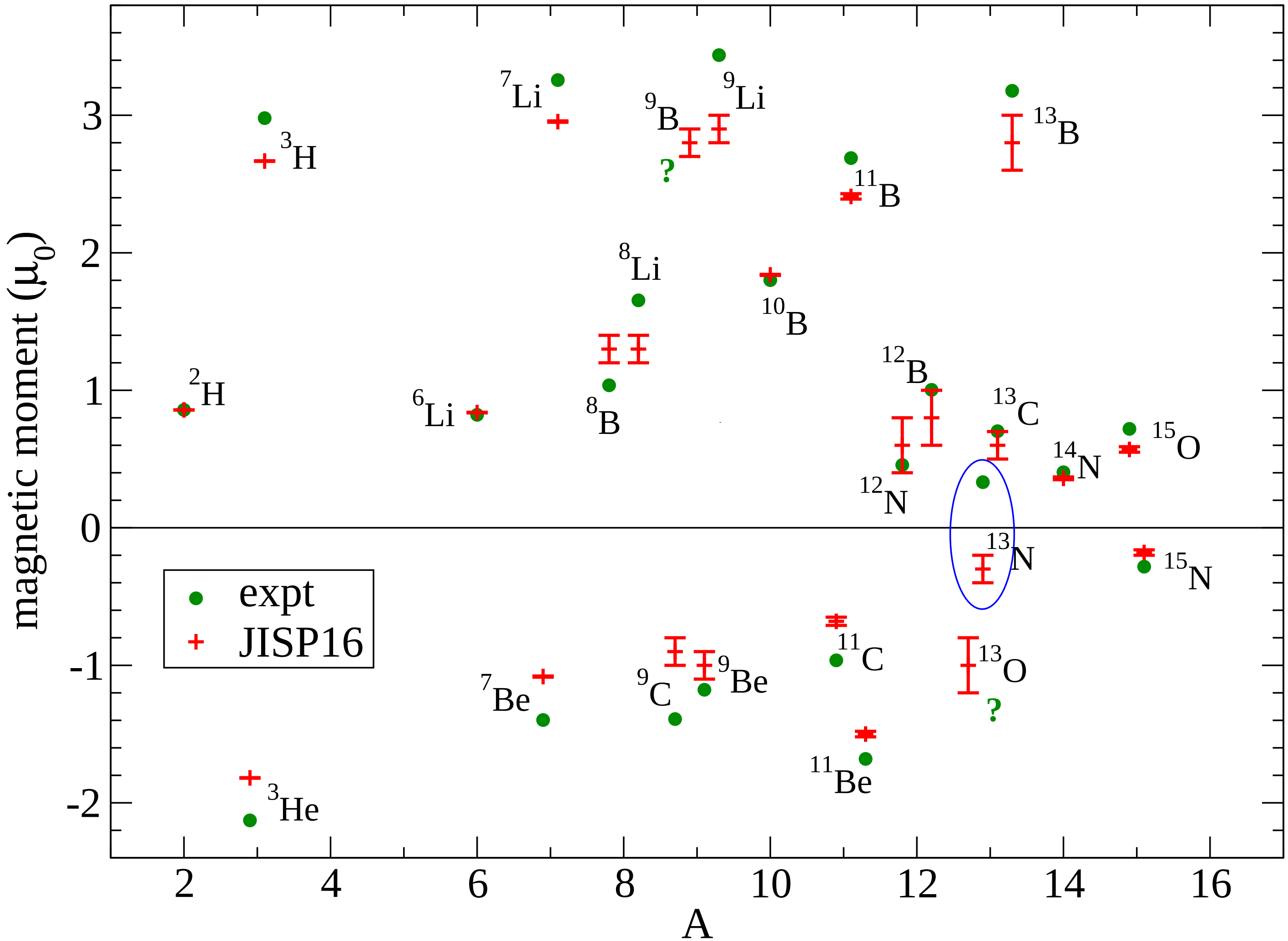


- Converged with $N_{\rm max}$, persistent weak $\hbar\omega$ dependence $\frac{5}{2}^-$ states
- Two $\frac{5}{2}^-$ states have very different structure

Magnetic moments of p-shell nuclei with JISP16

Maris, Vary, IJMPE22, 1330016 (2013)

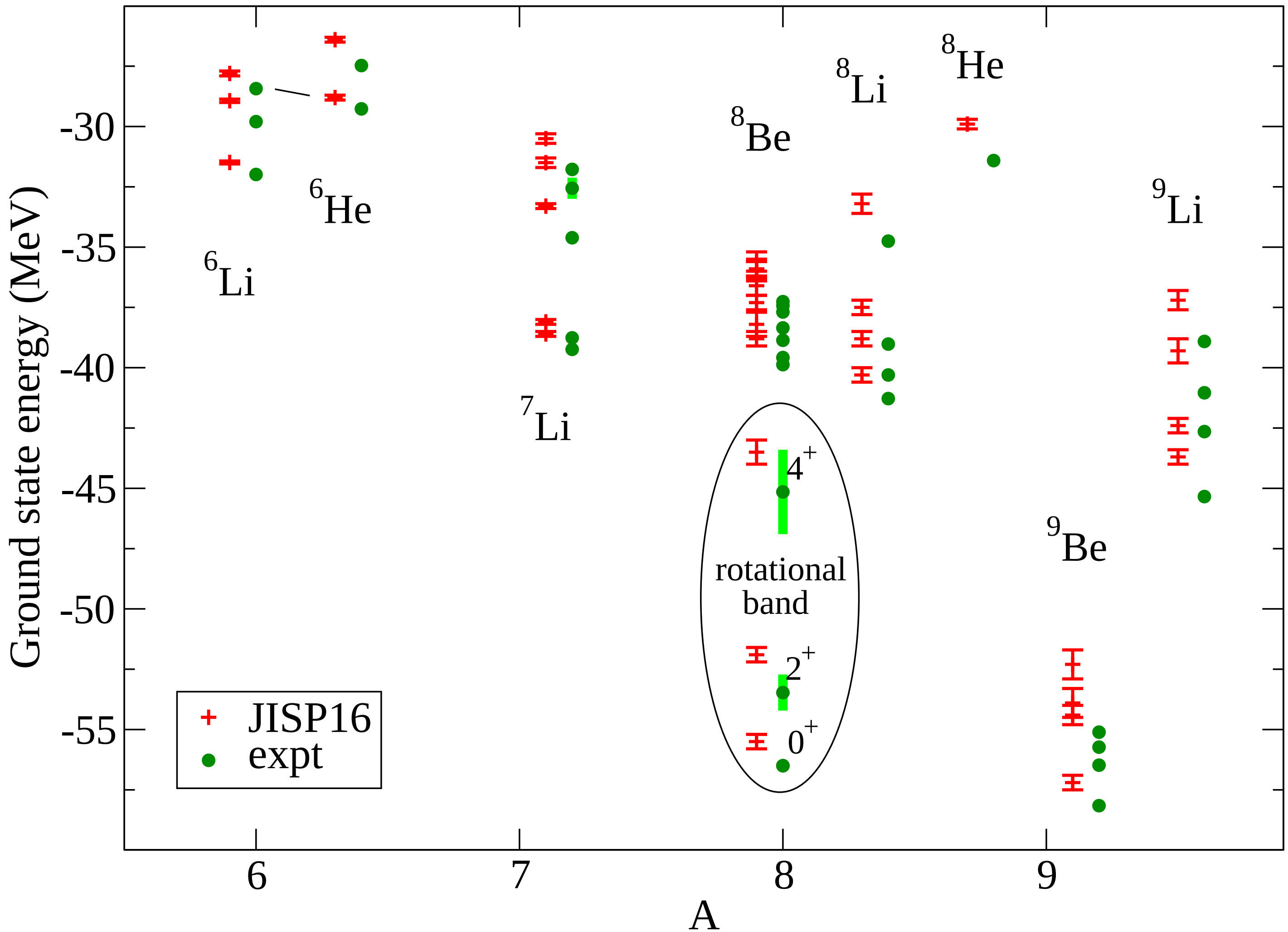
$$\mu = \frac{1}{J+1}\left(\langle \vec{J}\cdot\vec{L}_p\rangle + 5.586\langle \vec{J}\cdot\vec{S}_p\rangle - 3.826\langle \vec{J}\cdot\vec{S}_n\rangle\right)\mu_0$$



- Good agreement with data,
  given that we do not have any meson-exchange currents

Energies of narrow A=6 to A=9 states with JISP16

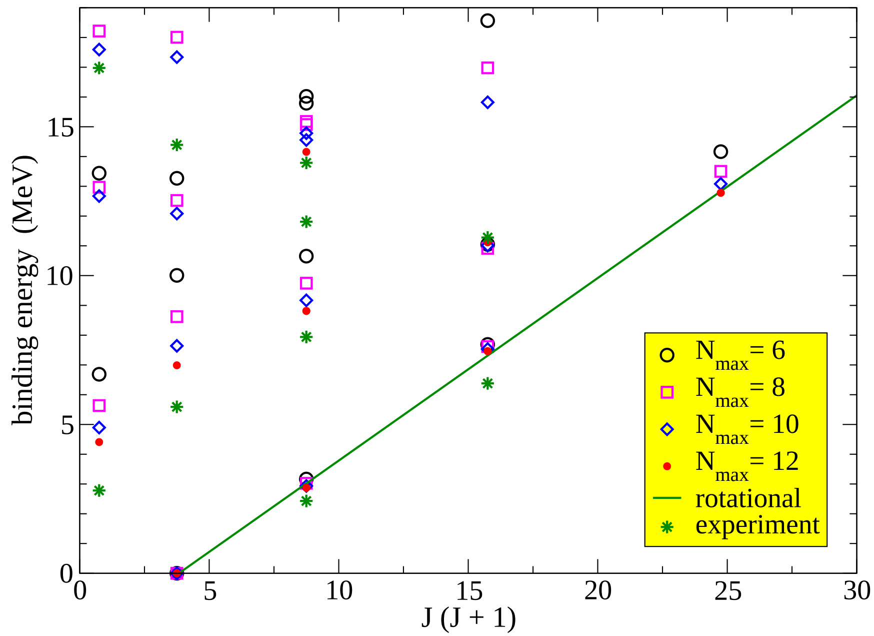
Cockrell, Maris, Vary, PRC86 034325 (2012); Maris, Vary, IJMPE22, 1330016 (2013)

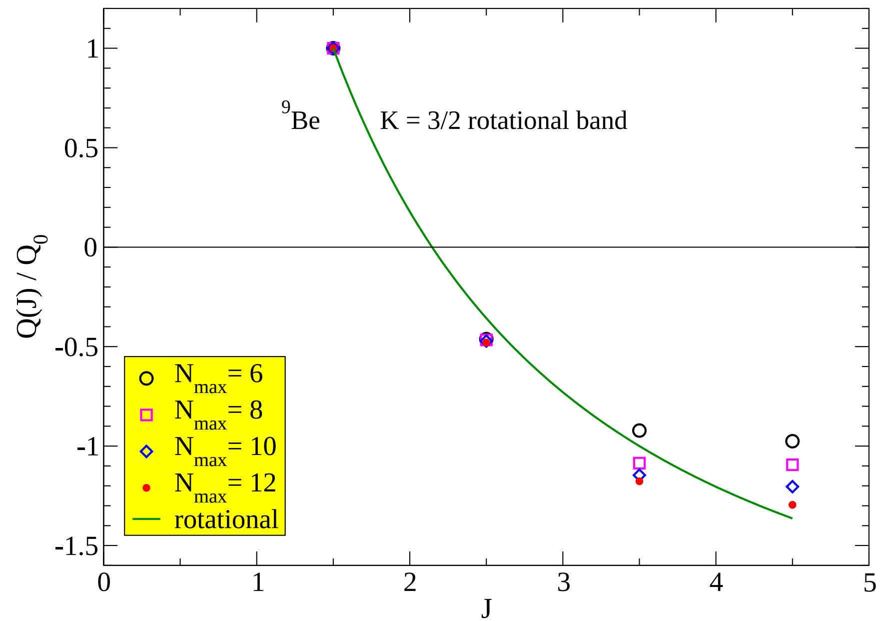


- Excitation spectrum narrow states in good agreement with data

Emergence of rotational bands

Caprio, Maris, Vary, PLB719 (2013) 179





- Rotational energy for states with axial symmetry $E(J) \propto J(J+1)$
- Quadrupole moments for rotational band

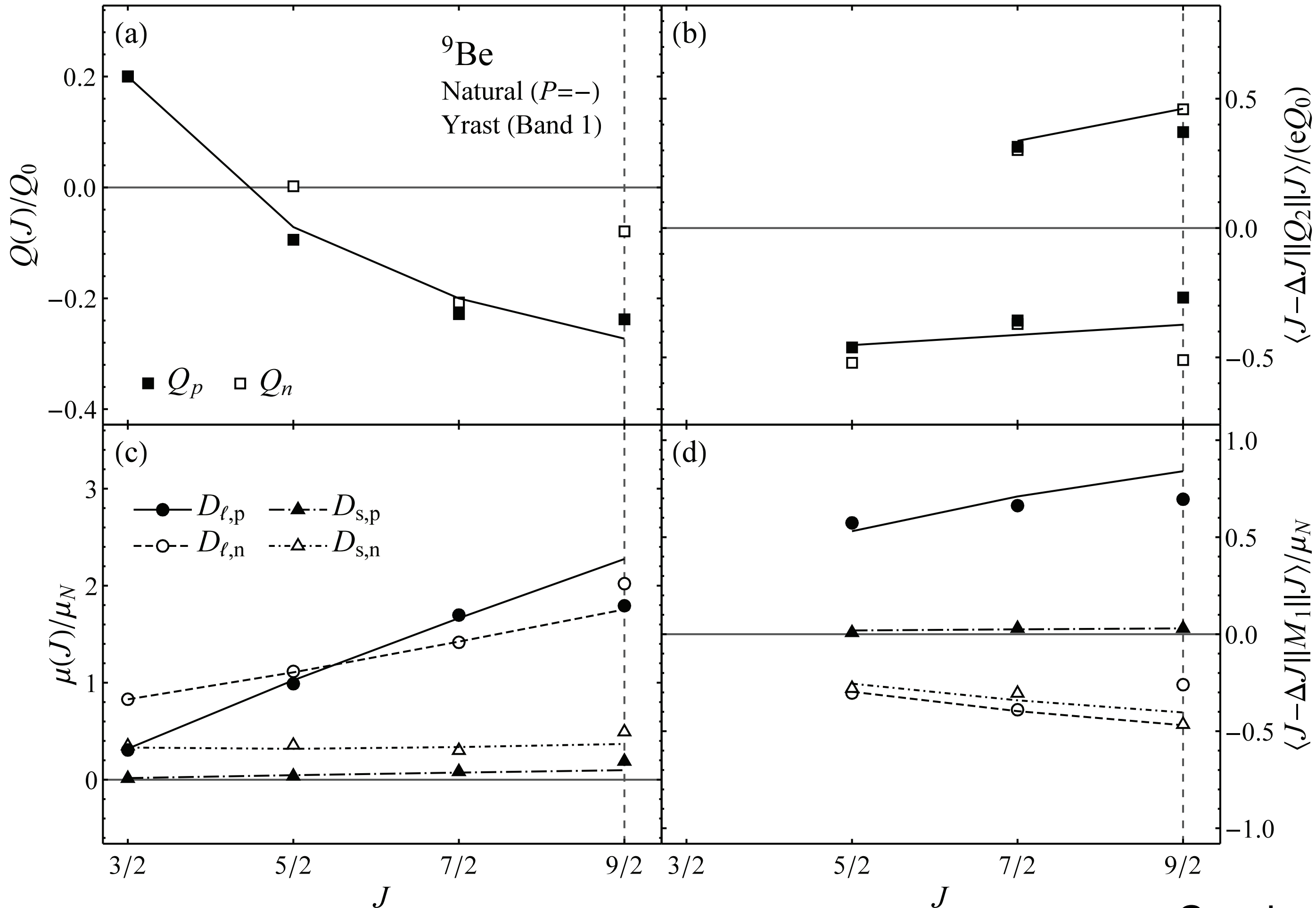
$$Q(J) = \frac{3\,K^2 - J(J+1)}{(J+1)(2J+3)}\,Q_0$$

- Large B(E2) transition rates between members rotational band

$$\langle J_f||E2||J_i\rangle = \sqrt{\frac{5}{16\pi}}\,\sqrt{2J_i+1}\,(J_i K 2 0|J_f K)\,\mathcal{Q}_0$$

Emergence of rotational bands

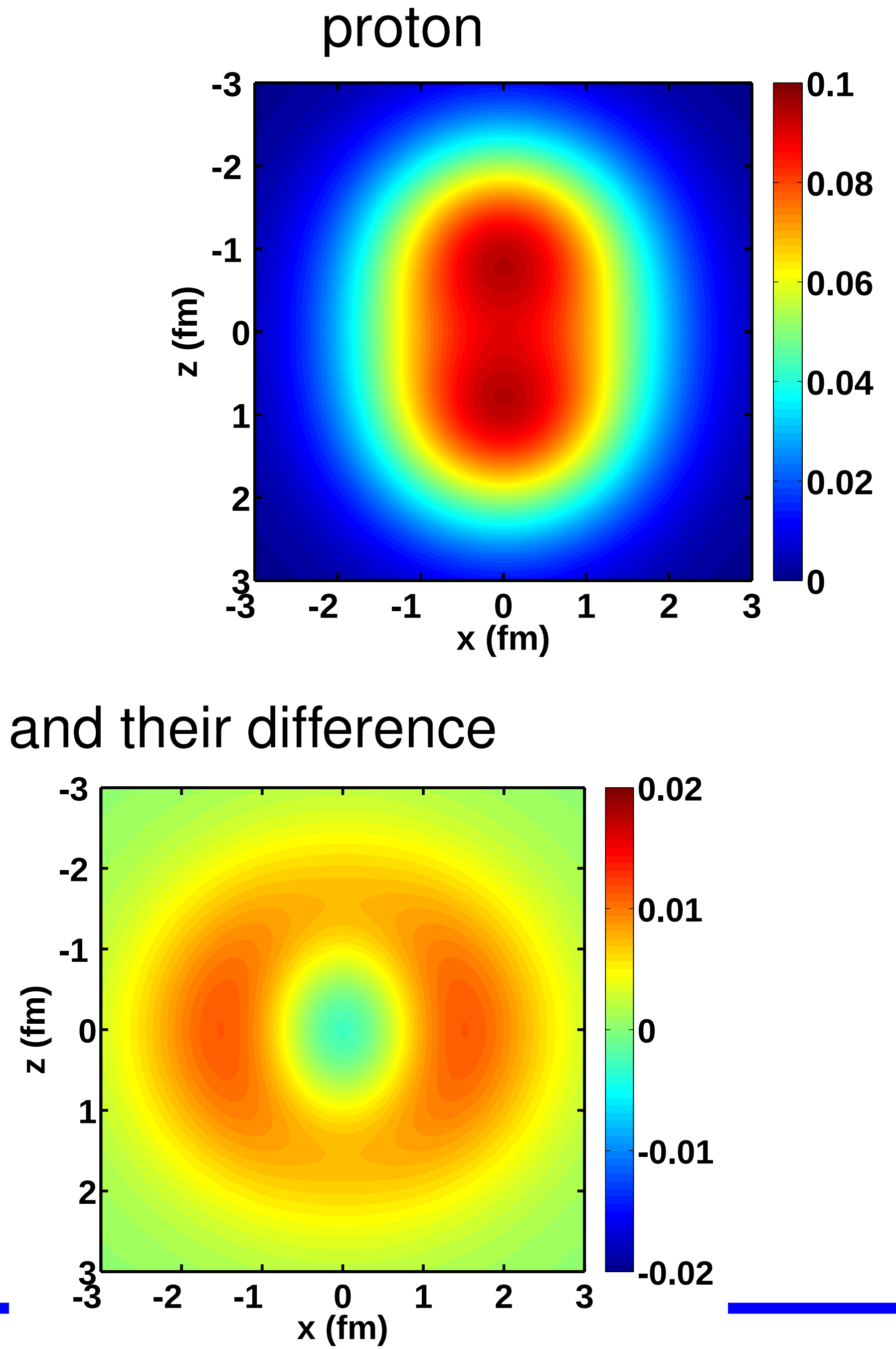
- Magnetic moments $\mu(J) = a_0\, J + a_1\, \frac{K}{J+1}$
- Magnetic transitions $\langle J-1||M1||J\rangle = -\sqrt{\frac{3}{4\pi}}\,\sqrt{\frac{J^2-K^2}{J}}\; a_1$



- Both proton and neutron $\mathcal{Q}$ and $\langle J_f||E2||J_i\rangle$
- Dipole terms: proton and neutron orbital motion and intrinsic spin contributions

Caprio, Maris, Vary, in preparation

Details: one-body density of 9Be ground state $(\frac{3}{2}^-, \frac{1}{2})$

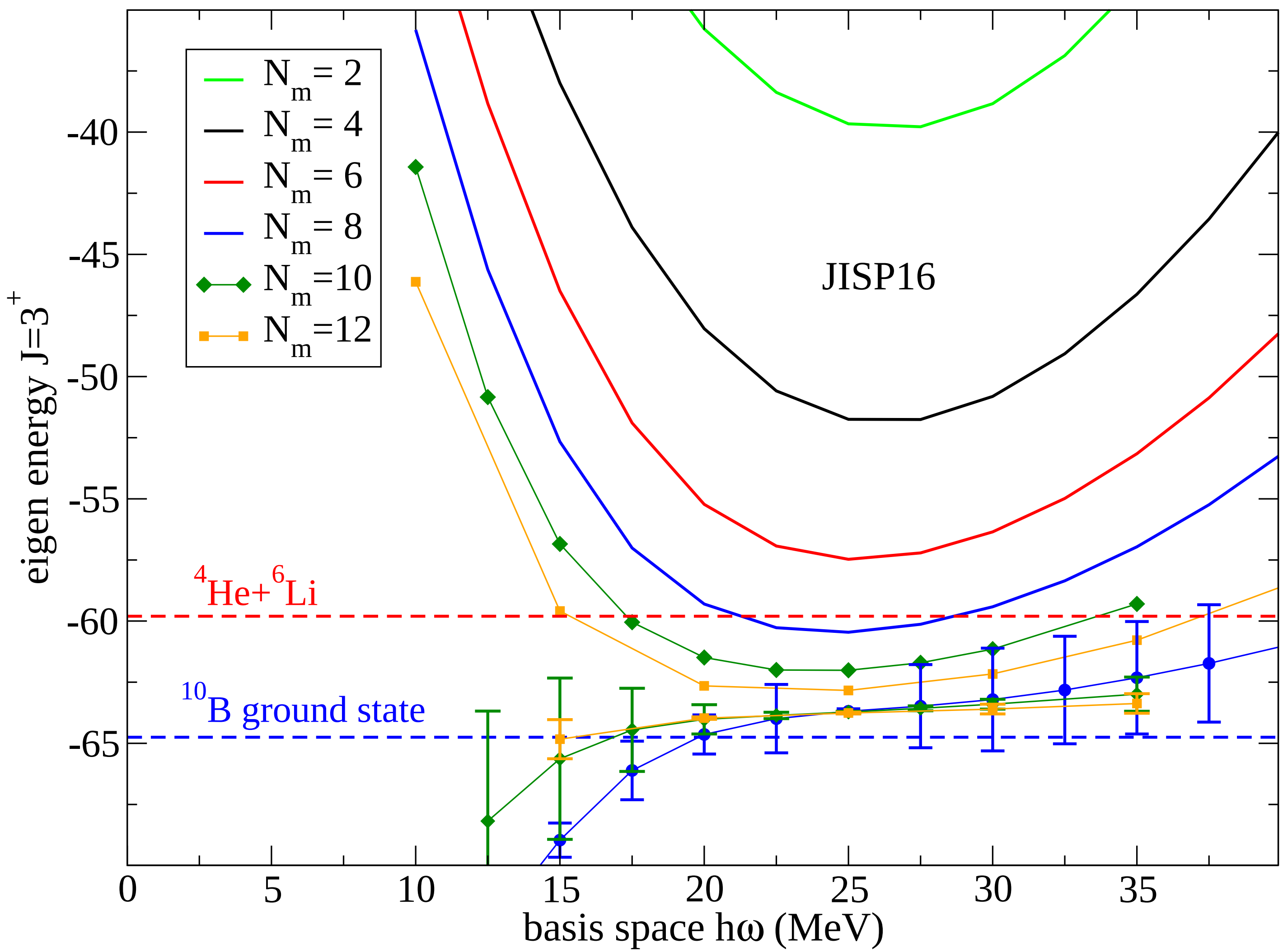


Translationally-invariant proton and neutron densities

Cockrell, PhD thesis, 2012

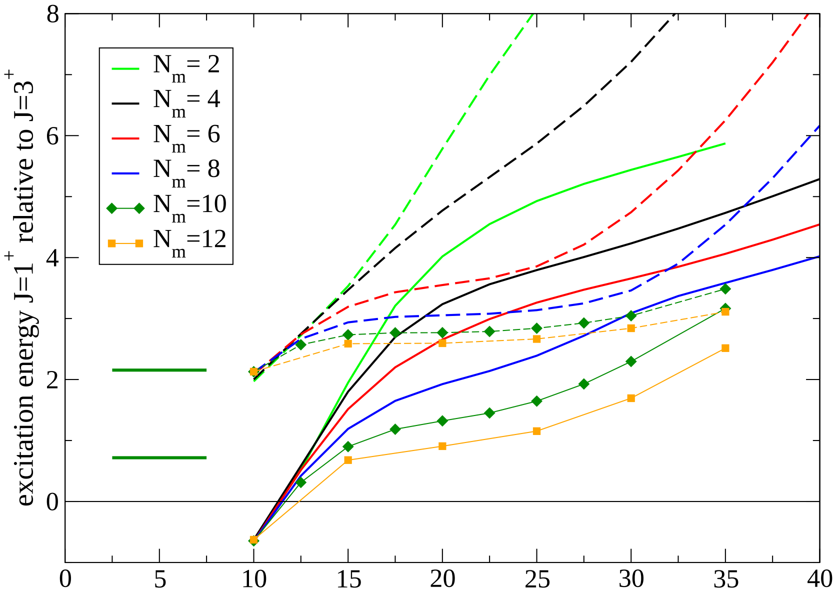
- Emergence of α clustering
  - extra neutron appears to be in π orbital

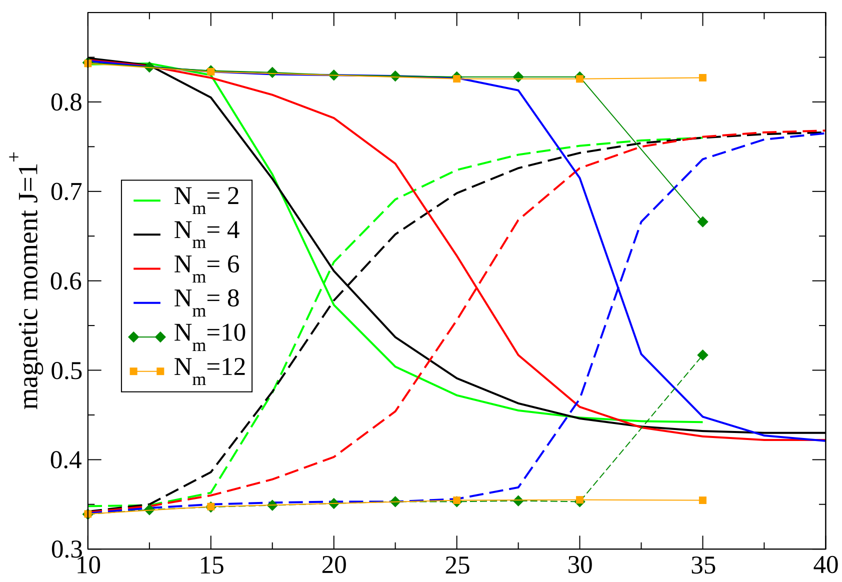
Ground state energy 10B

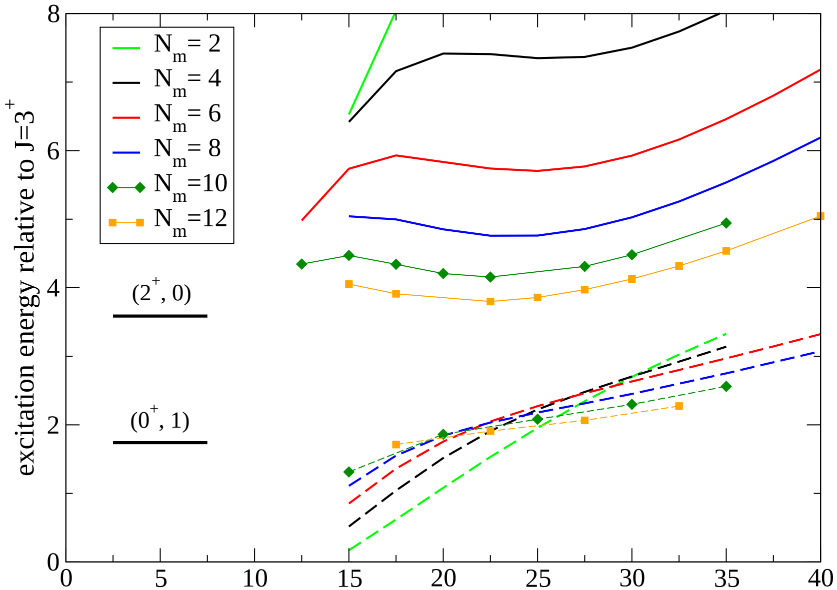


- Extrapolated energy 3^+ state in reasonable agreement with data

Low-lying spectrum of 10B



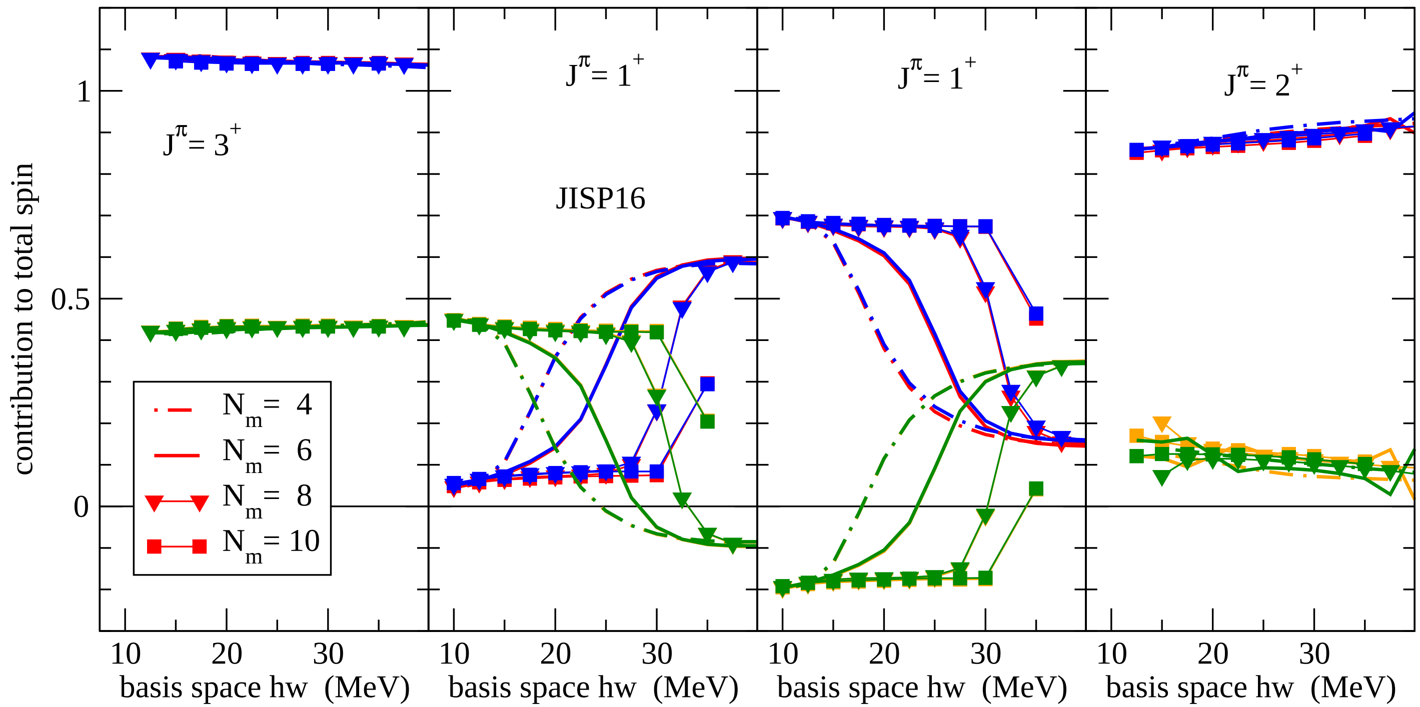




- Two low-lying 1^+ states
  - different convergence patterns
  - level crossing hinders extrapolation
  - magnetic moments converged
- Slow convergence for 2^+ state
- Good convergence for $(0^+, 1)$ state

Details: spin components 10B

$$J = \frac{1}{J+1}\left(\langle\vec{J}\cdot\vec{L}_p\rangle + \langle\vec{J}\cdot\vec{L}_n\rangle + \langle\vec{J}\cdot\vec{S}_p\rangle + \langle\vec{J}\cdot\vec{S}_n\rangle\right)$$



- Converged with $N_{\max}$, same spin structure protons and neutrons
- Two 1^+ states have very different structure
- Clear evidence of level crossing

Predictions for ^{14}F confirmed by experiments at Texas A&M

Theory published PRC: Feb. 4, 2010

Physics Letters B 692 (2010) 307–311

Experiment published: Aug. 3, 2010

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First observation of ^{14}F

V.Z. Goldberg [a,*], B.T. Roeder [a], G.V. Rogachev [b], G.G. Chubarian [a], E.D. Johnson [b], C. Fu [c], A.A. Alharbi [a,1], M.L. Avila [b], A. Banu [a], M. McCleskey [a], J.P. Mitchell [b], E. Simmons [a], G. Tabacaru [a], L. Trache [a], R.E. Tribble [a]

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[b] Department of Physics, Florida State University, Tallahassee, FL 32306-4350, USA
[c] Indiana University, Bloomington, IN 47408, USA

NCFC predictions (JISP16) in close agreement with experiment

TAMU Cyclotron Institute

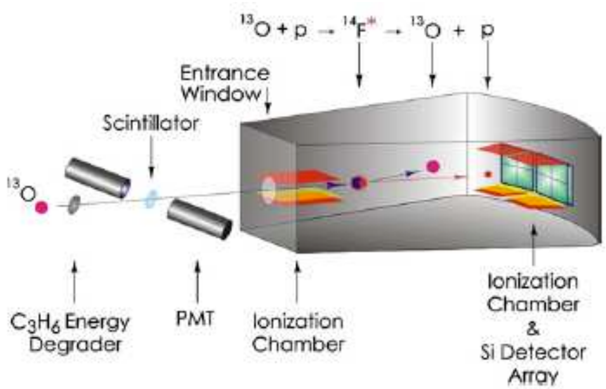


Fig. 1. (Color online.) The setup for the ^{14}F experiment. The "gray box" is the scattering chamber. See explanation in the text.

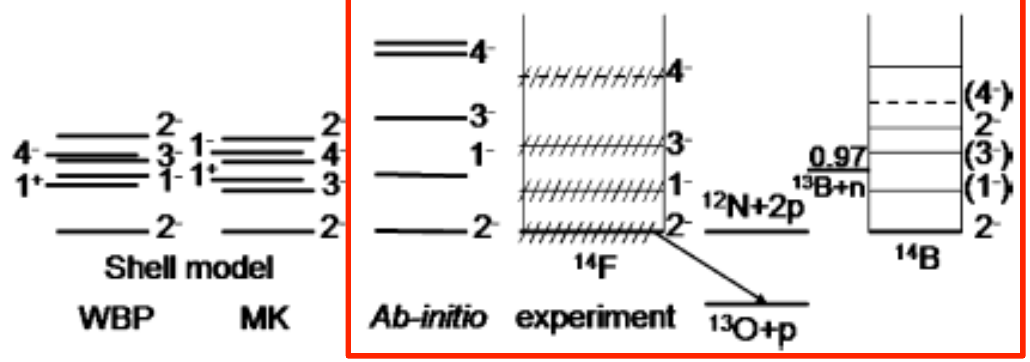


Fig. 6. ^{14}F level scheme from this work compared with shell-model calculations, *ab-initio* calculations [3] and the ^{14}B level scheme [16]. The shell model calculations were performed with the WBP [21] and MK [22] residual interactions using the code COSMO [23].

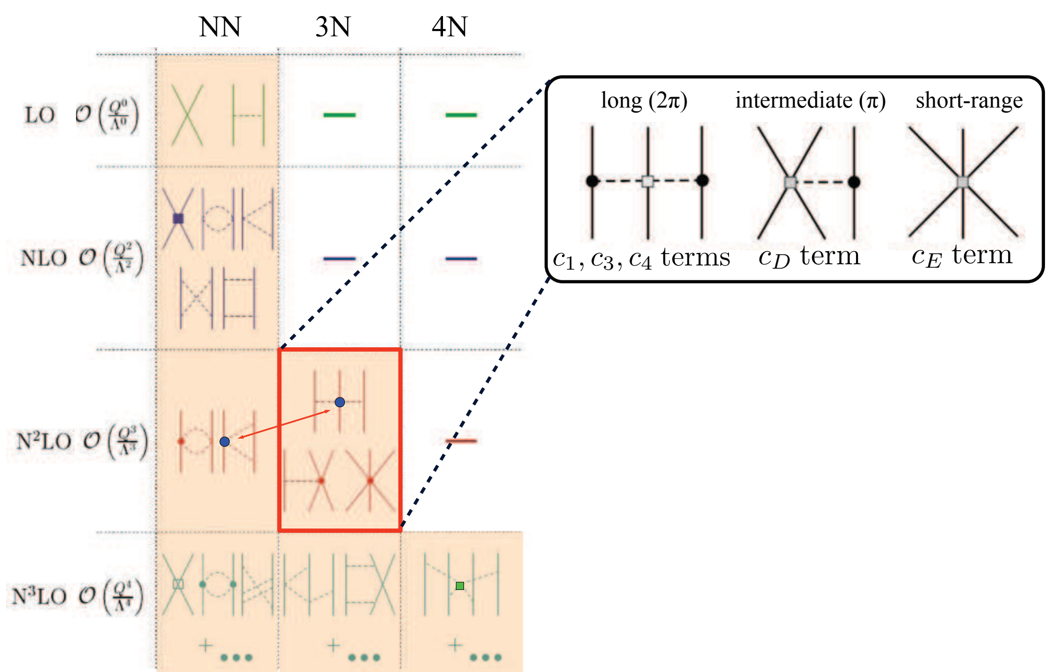
Nuclear interaction from chiral perturbation theory

- Strong interaction in principle calculable from QCD
- Use chiral perturbation theory to obtain effective A-body interaction from QCD   Entem and Machleidt, Phys. Rev. C**68**, 041001 (2003)
  - controlled power series expansion in Q/Λ_χ with $\Lambda_\chi \sim 1$ GeV
  - natural hierarchy for many-body forces

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

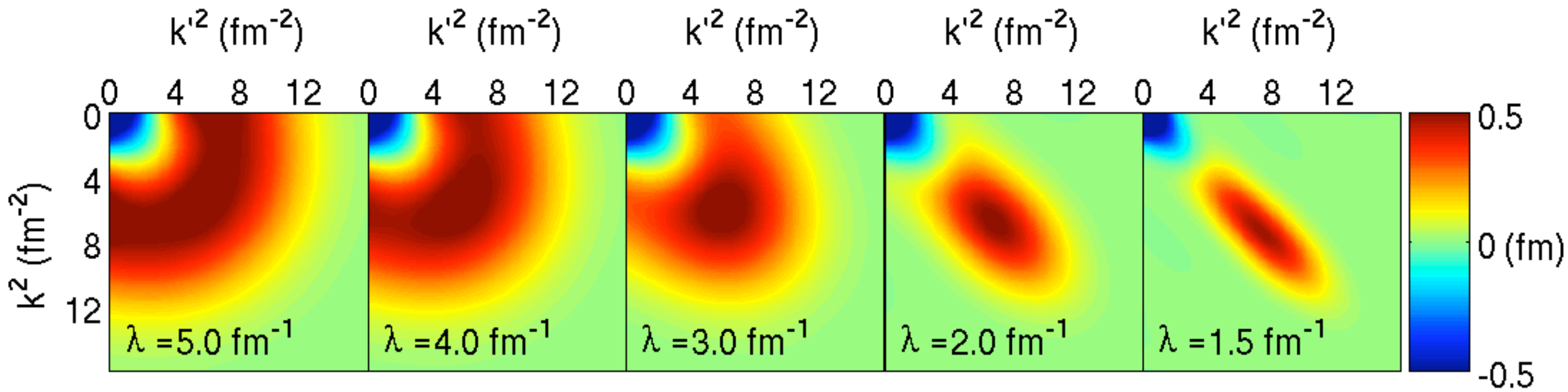
  - in principle no free parameters
    - in practice a few undetermined parameters
  - renormalization necessary

Leading-order 3N forces in chiral EFT



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

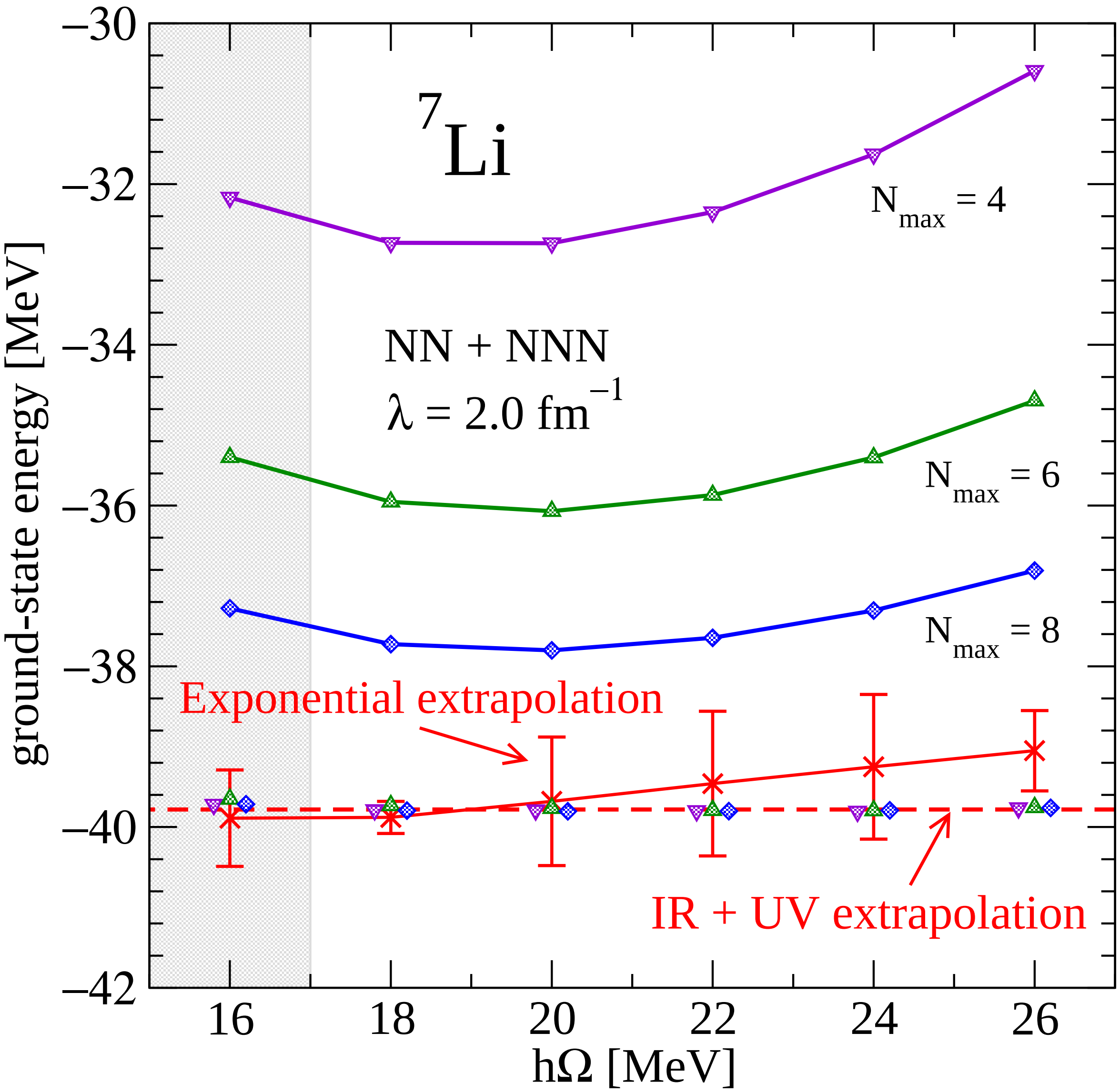
Bogner, Furnstahl, Maris, Perry, Schwenk, Vary, NPA801, 21 (2008)

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

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

Ground state energy of 7Li with SRG evolved chiral interaction

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



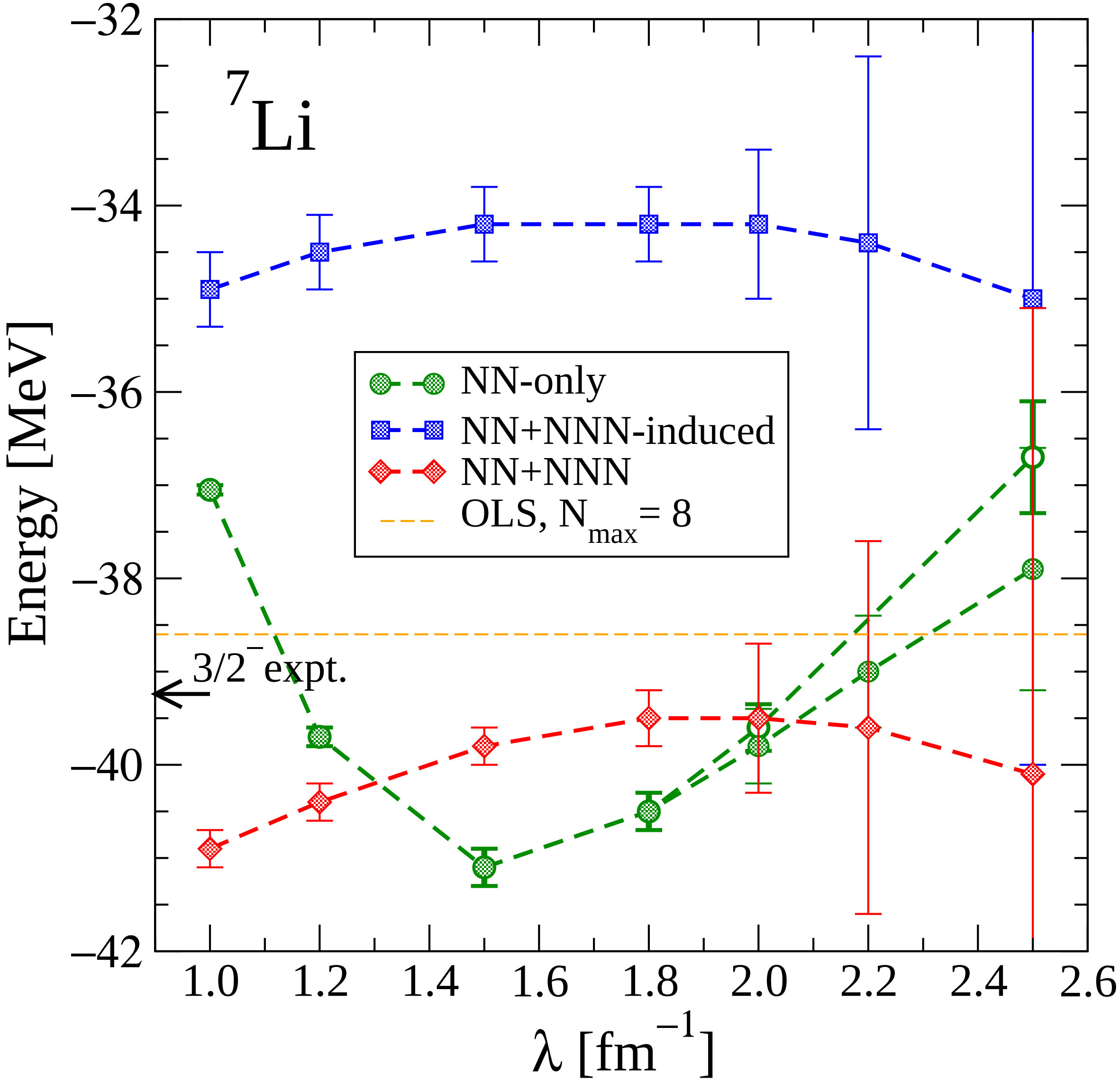
Interaction

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

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

Running of ground state energy of 7Li with SRG evolution

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



Numerical convergence

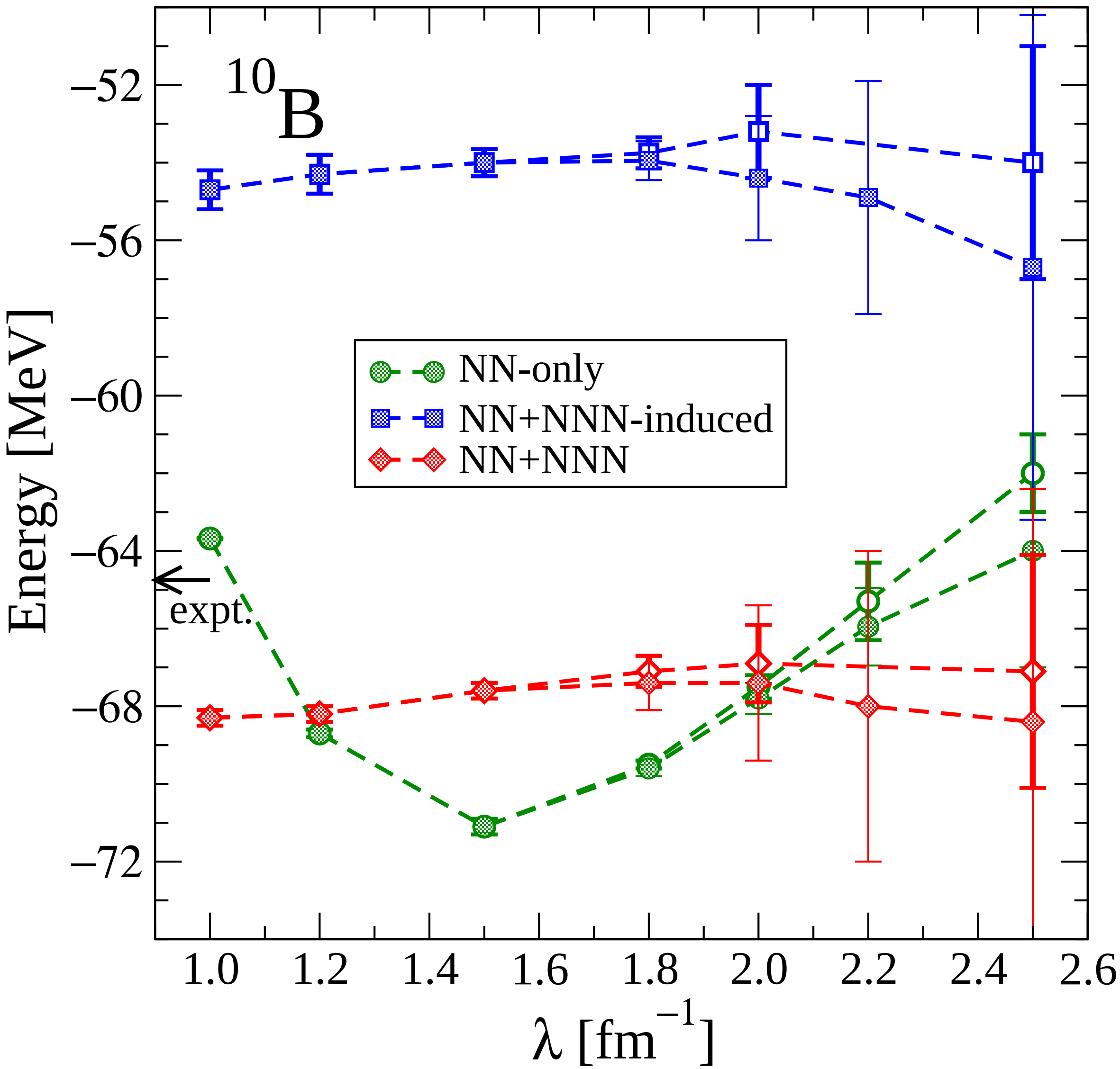
- good $\lambda < 2.0$ fm^{-1}
- slow $\lambda > 2.0$ fm^{-1}

Dependence on SRG parameter λ

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

Running of ground state energy of 10B with SRG evolution

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



Numerical convergence

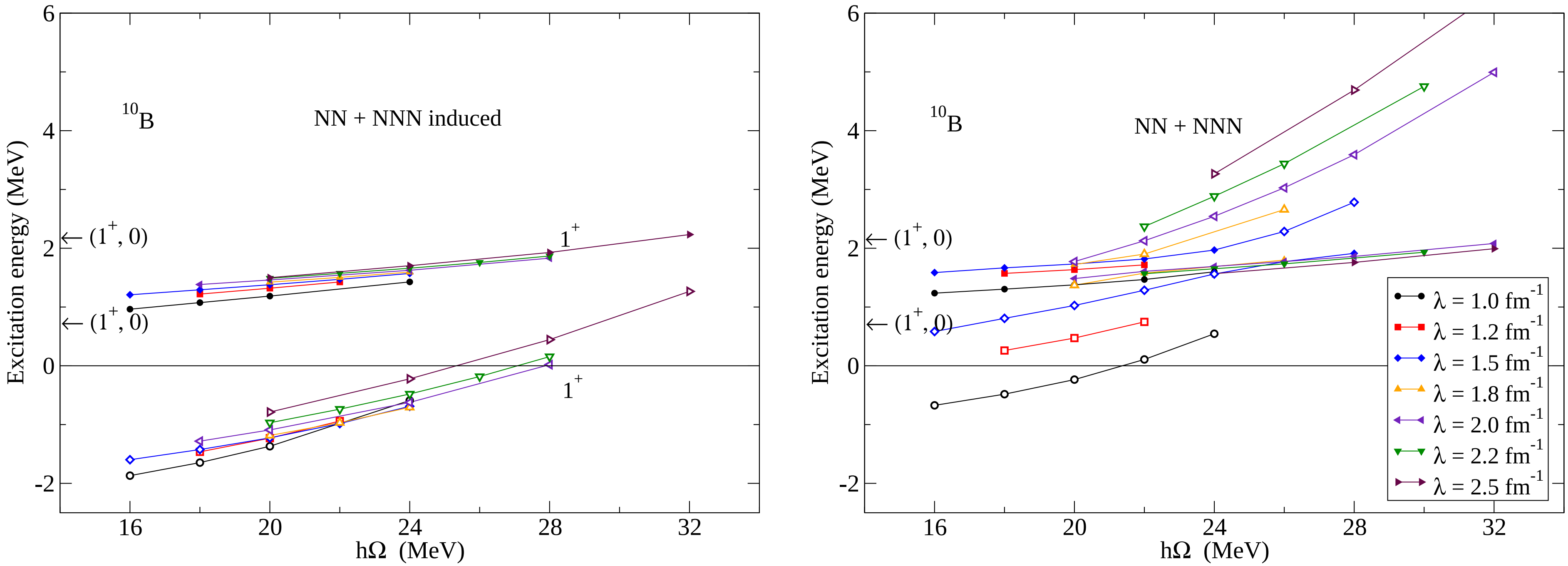
- good $\lambda < 2.0$ fm^{-1}
- slow $\lambda > 2.0$ fm^{-1}

Dependence on SRG parameter λ

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

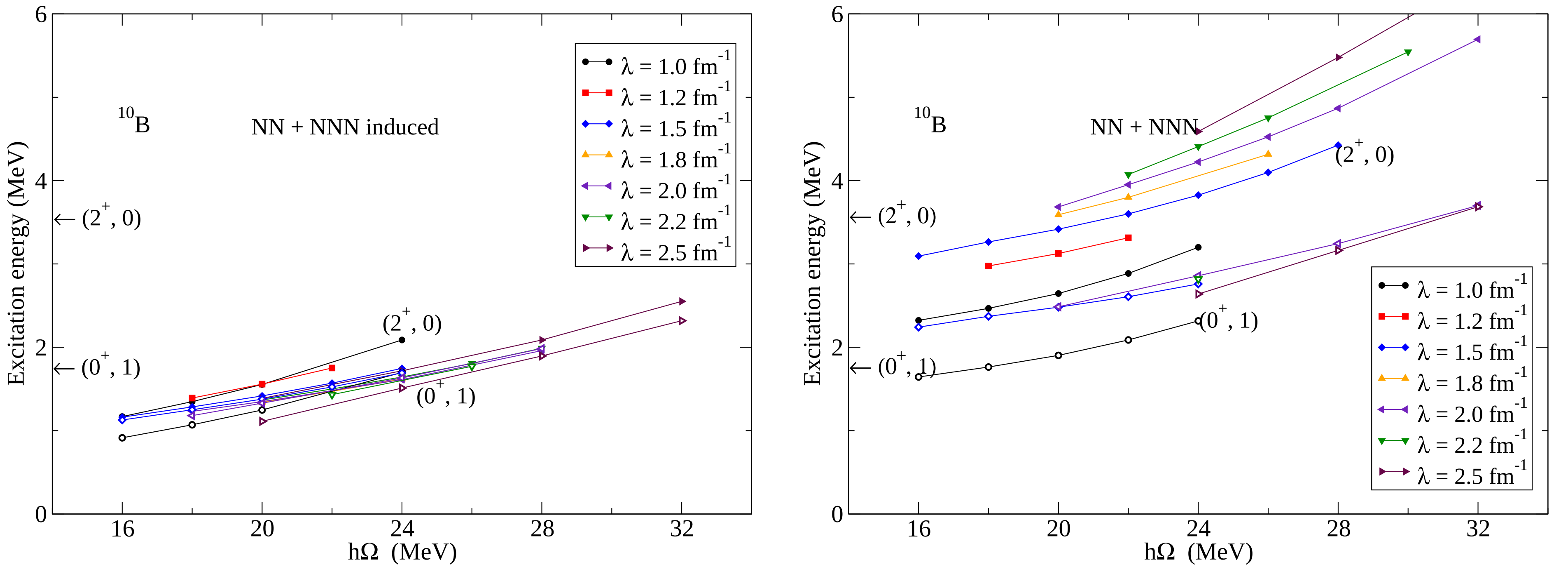
Running of spectrum of 10B

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



- $(1^+, 0)$ at about 1.6(4) MeV with $\mu \approx 0.4$ (solid symbols)
  - reasonably well converged, weak λ-dependence
- unconverged $(1^+, 0)$ with $\mu \approx 0.8$ (open symbols)
  - without 3NF: weak λ-dependence but strong $\hbar\Omega$-dependence
  - with 3NF: not converged, very strong λ- and $\hbar\Omega$-dependence

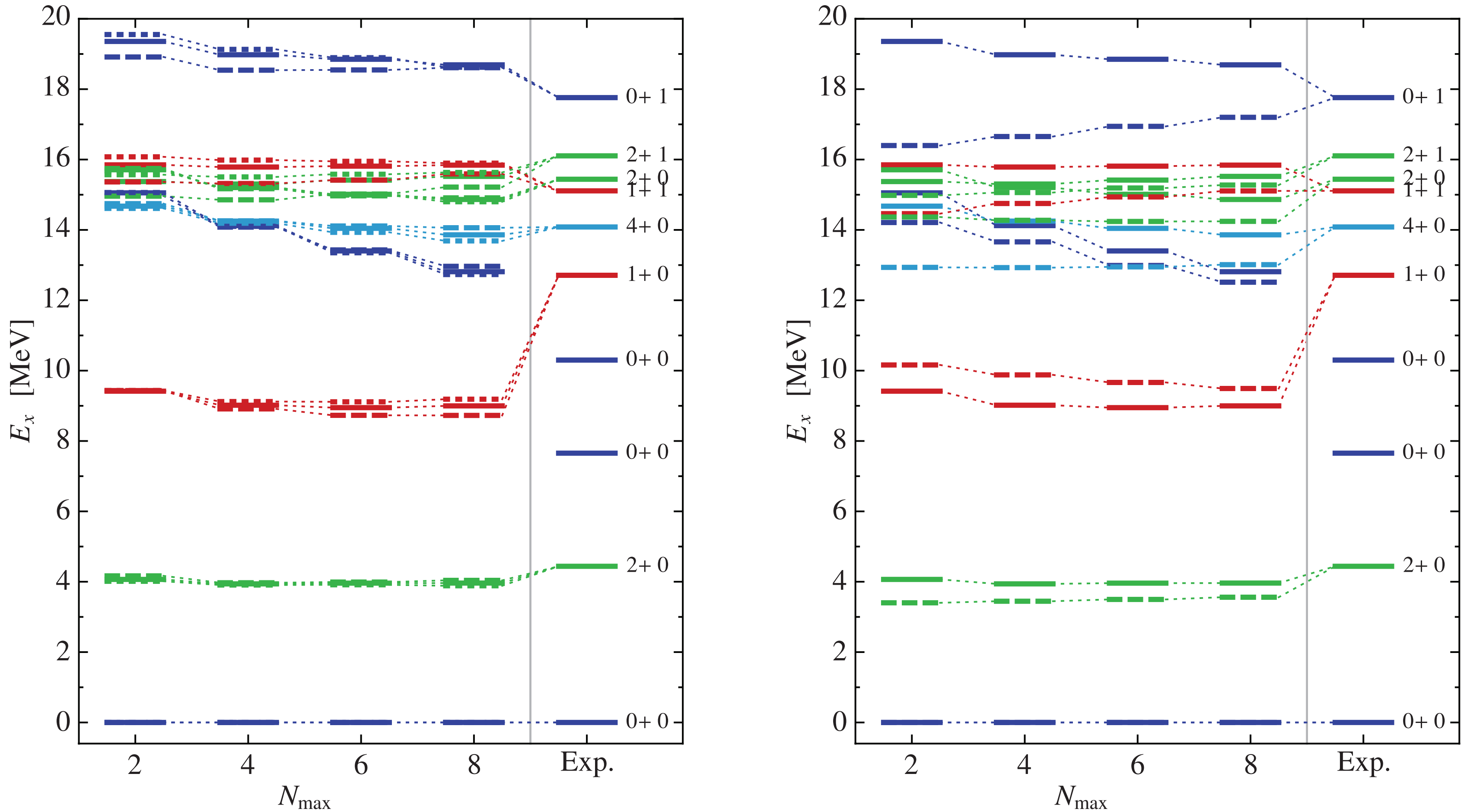
Running of spectrum of 10B



- $(0^+, 1)$ at 1 to 3 MeV (open symbols)
  - weak λ-dependence but moderate $\hbar\Omega$-dependence
- $(2^+, 0)$ (solid symbols)
  - without 3NF: weak λ-dependence, moderate $\hbar\Omega$-dependence, but too low in excitation energy
  - with 3NF: not converged, strong λ- and $\hbar\Omega$-dependence

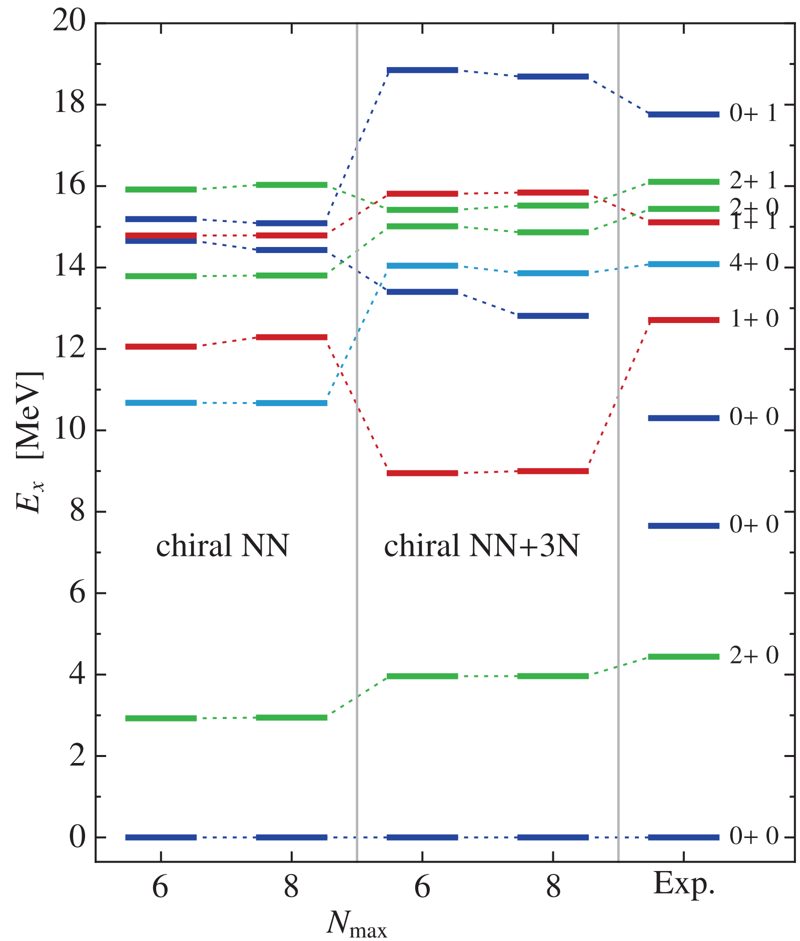
Spectrum of ^{12}C

Maris, Vary, Calci, Langhammer, Binder, Roth, arXiv:1405:1331 [nucl-th]

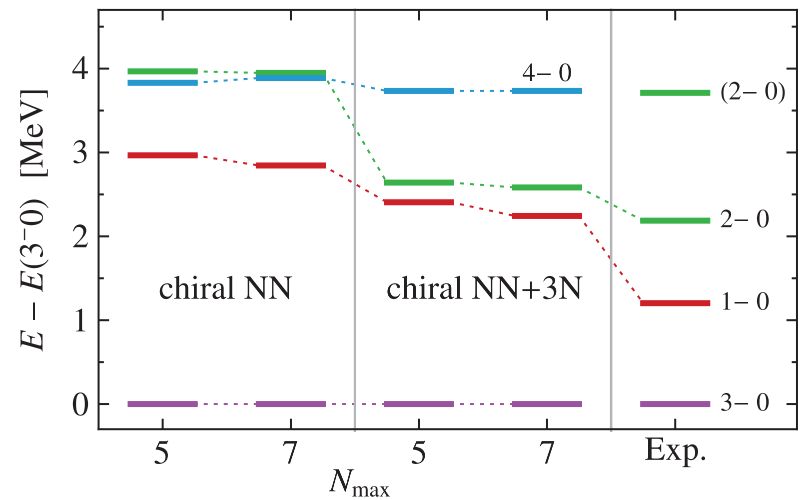


- excitation energies reasonably well converged
- dependence of SRG parameter (left) generally smaller than dependence on basis $\hbar\Omega$ (right)

Spectrum of ^{12}C



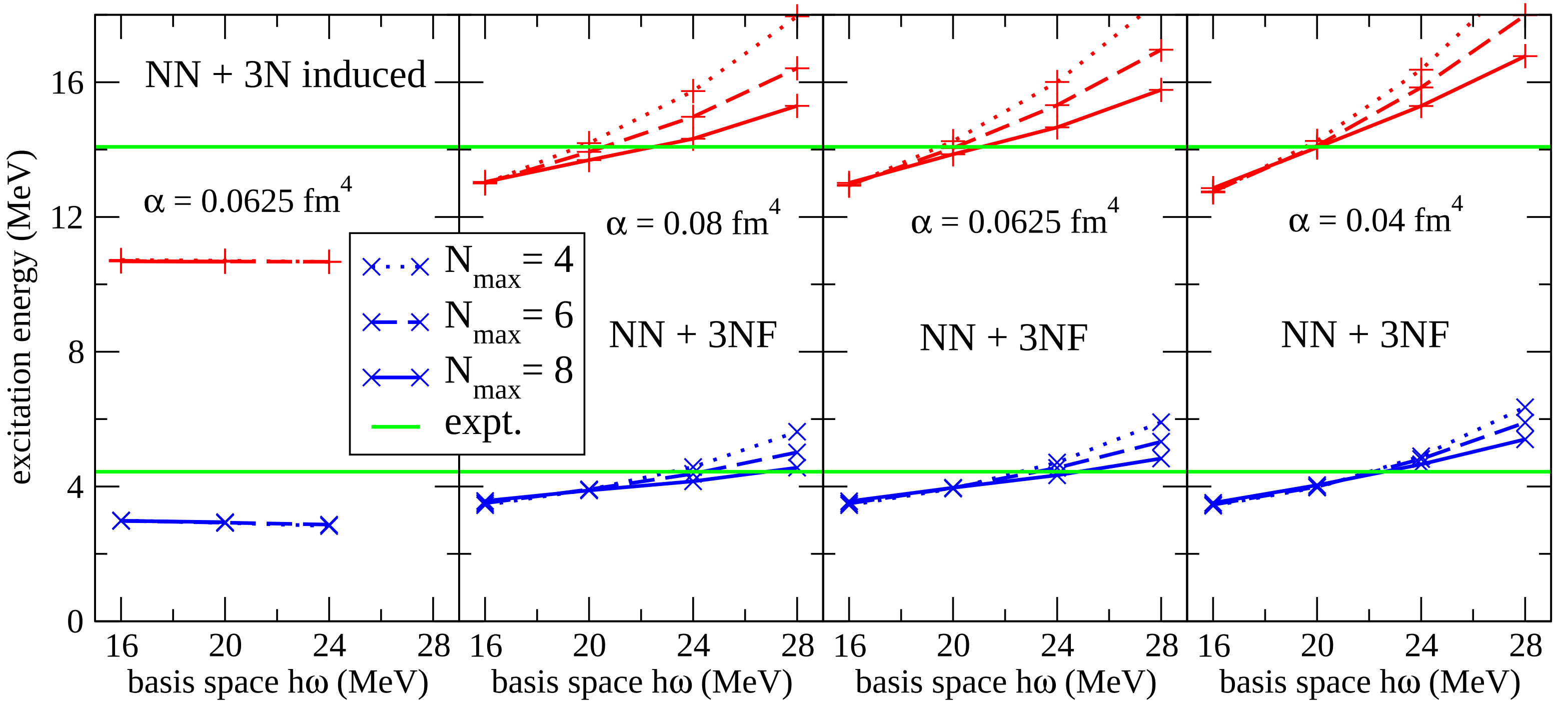
- chiral NN at N^{3}LO
- chiral 3N at N^{2}LO
- 3N LEC values:
  $c_D = -0.2$, $c_E = -0.205$
- 500 MeV cutoff



- 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

Effect of 3-body forces on rotational excited states ^{12}C

Maris *et al* J. Phys. Conf. Ser. 454, 012063 (2013)



- Qualitative agreement with data
- Not converged with explicit 3NF, despite weak $N_{\max}$ dependence
- Ratio's of excitation energies, quadrupole moments and B(E2)'s in agreement with rotational model

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

Calculation of three-body forces at N^3LO

Low
Energy
Nuclear
Physics
International
Collaboration

J. Golak, R. Skibinski, K. Tolponicki, H. Witala

RUB — E. Epelbaum, H. Krebs

JÜLICH — A. Nogga

The Ohio State University — R. Furnstahl

Technische Universität Darmstadt — S. Binder, A. Calci, K. Hebeler, J. Langhammer, R. Roth

State — P. Maris, J. Vary

Kyutech — H. Kamada

Goal

Calculate matrix elements of 3NF in a partial-wave decomposed form which is suitable for different few- and many-body frameworks

Challenge

Due to the large number of matrix elements, the calculation is extremely expensive.

Strategy

Develop an efficient code which allows to treat arbitrary local 3N interactions.
(Krebs and Hebeler)

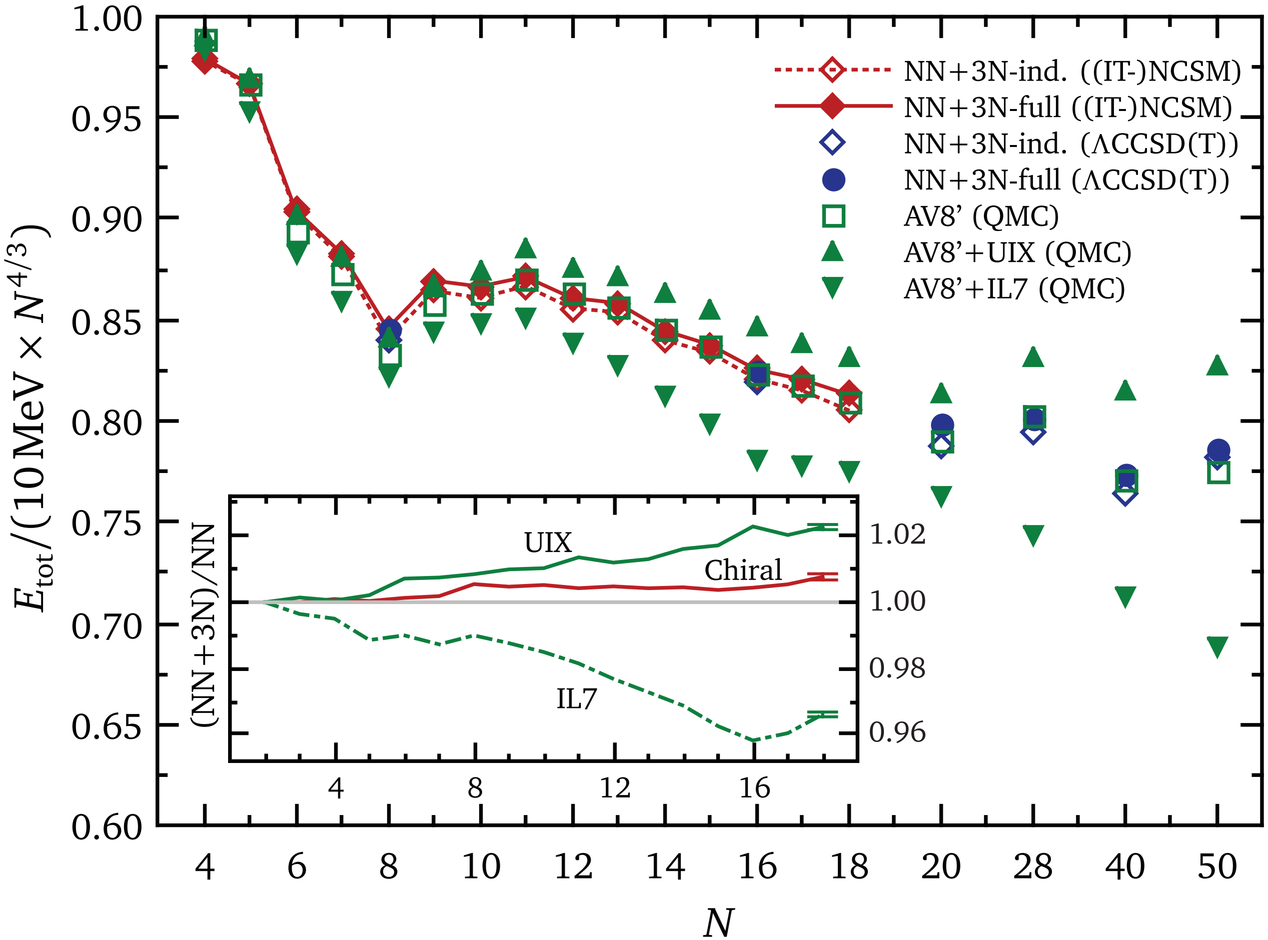
Something different: Ab Initio Extreme Neutron Matter

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)

Neutrons confined in HO external field

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



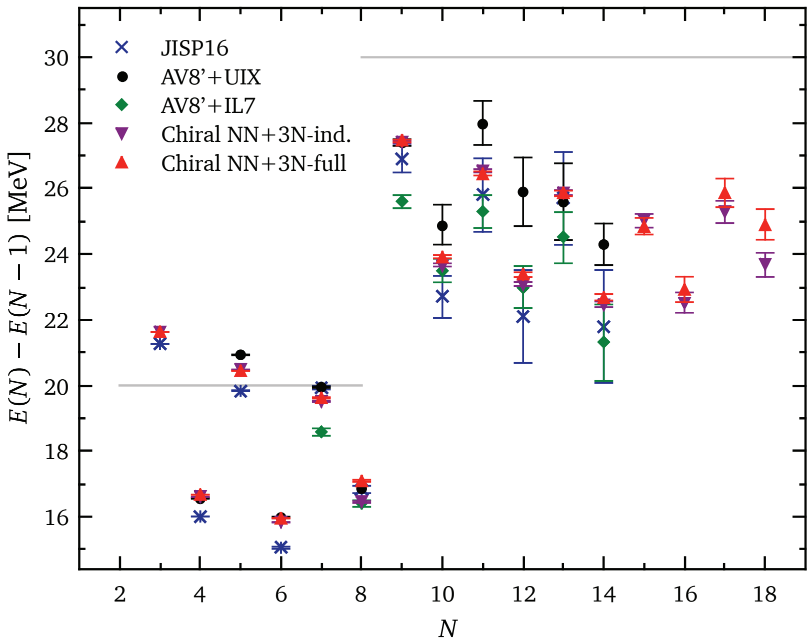
- chiral NN at N^{3}LO
- chiral 3N at N^{2}LO
- 3N LEC values:
  $c_D = -0.2,$
  $c_E = -0.205$
- 500 MeV cutoff

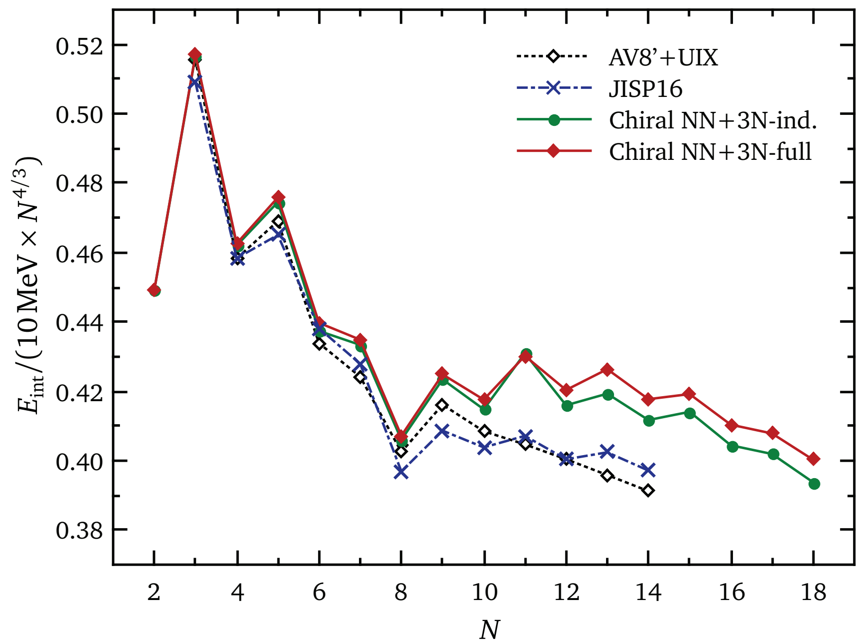
AV8'(+3NF) data from Gandolfi, Carlson, Pieper, PRL106 012501 (2011)

- 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]



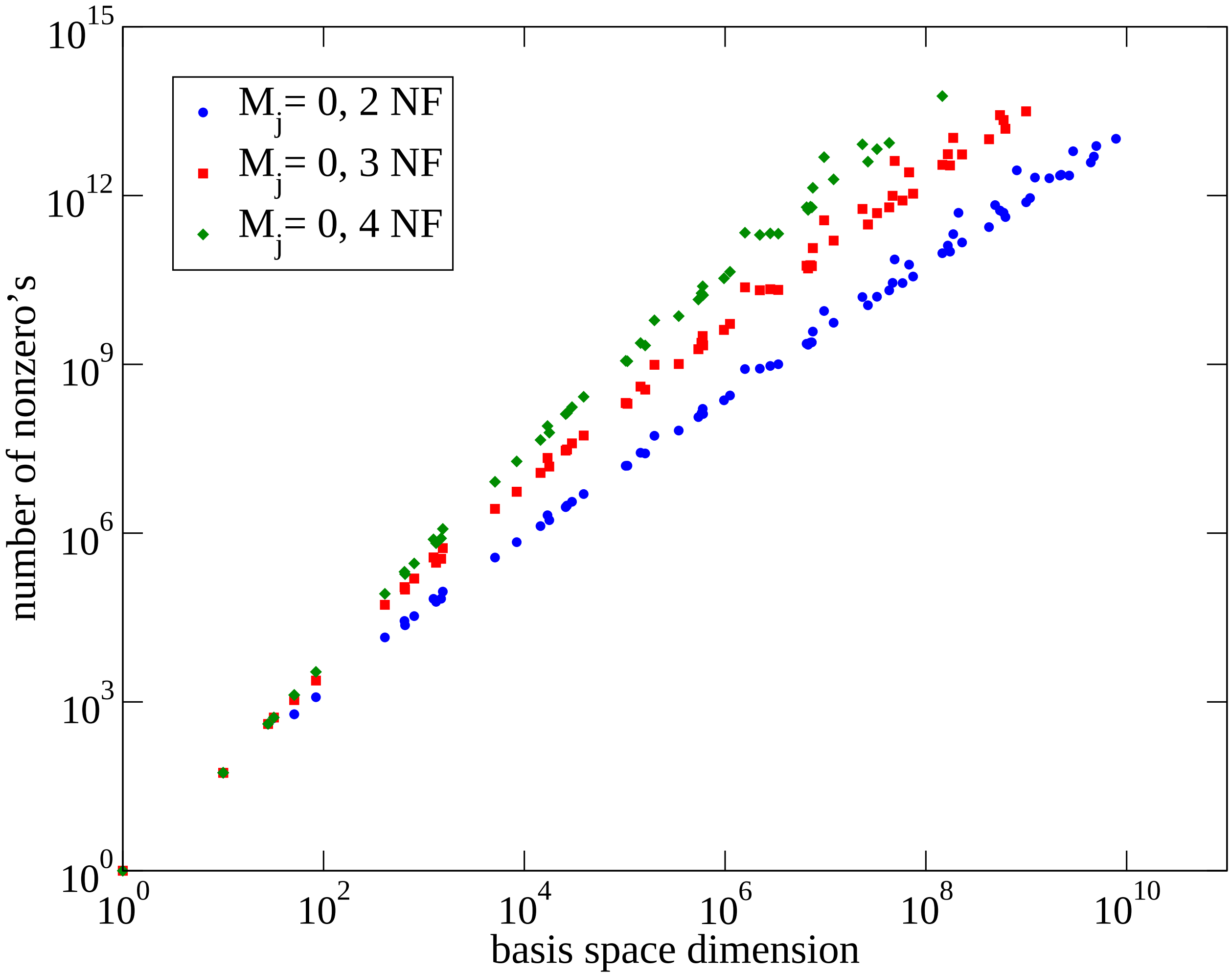


- Clear evidence for pairing with chiral EFT potential both in total energy (left) and in internal energy (right)
- GFMC results for AV8' + IUX show significantly less pairing, in particular above $N = 8$

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

Looking forward: Taming the scale explosion

- Reaching the limit of M-scheme $N_{\max}$ truncation
  - extremely large, extremely sparse matrices

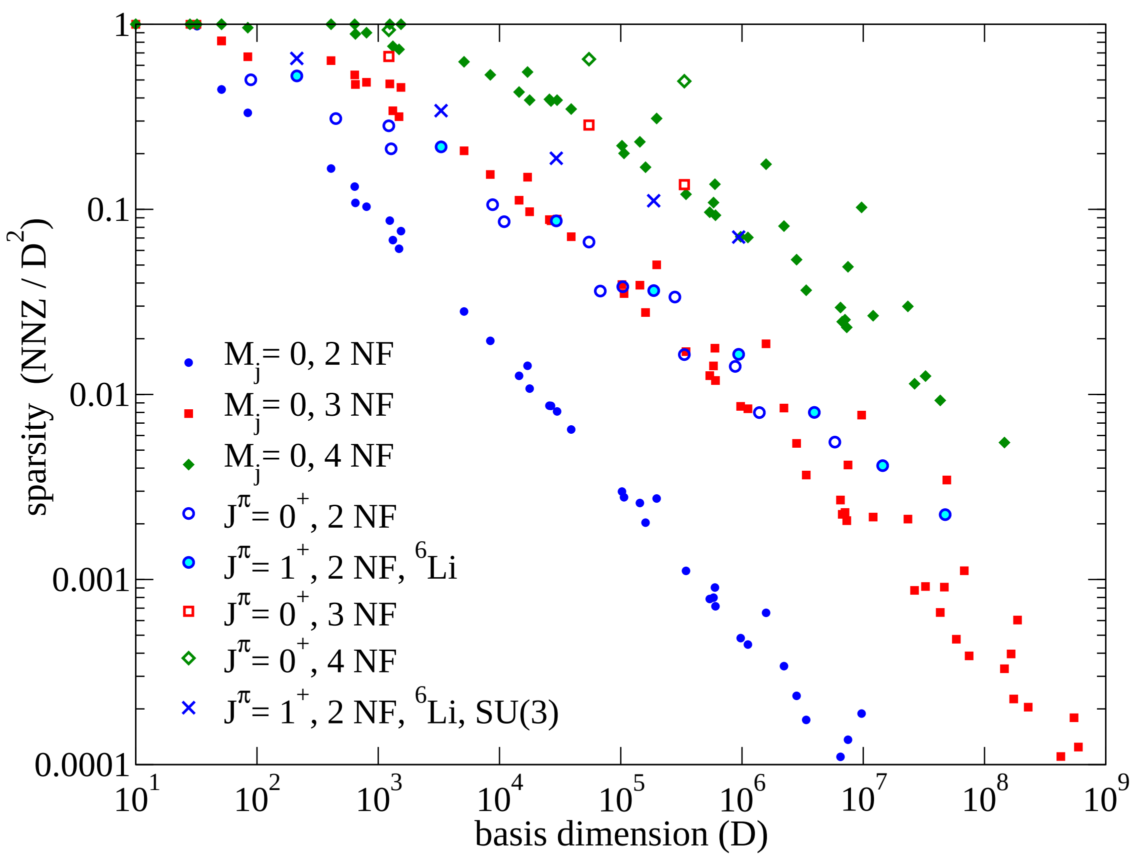


number of nonzero's in M-scheme, $M_j = 0$ for $N = Z$ nuclei from ^{6}Li to ^{20}Ne

- Hopper: 212 TB
  $26 \cdot 10^{12}$
- Edison: 333 TB
  $41 \cdot 10^{12}$
- Titan: 600 TB (CPUs)
  $75 \cdot 10^{12}$
- Mira: 768 TB
  $95 \cdot 10^{12}$

Looking forward: *Taming the scale explosion*

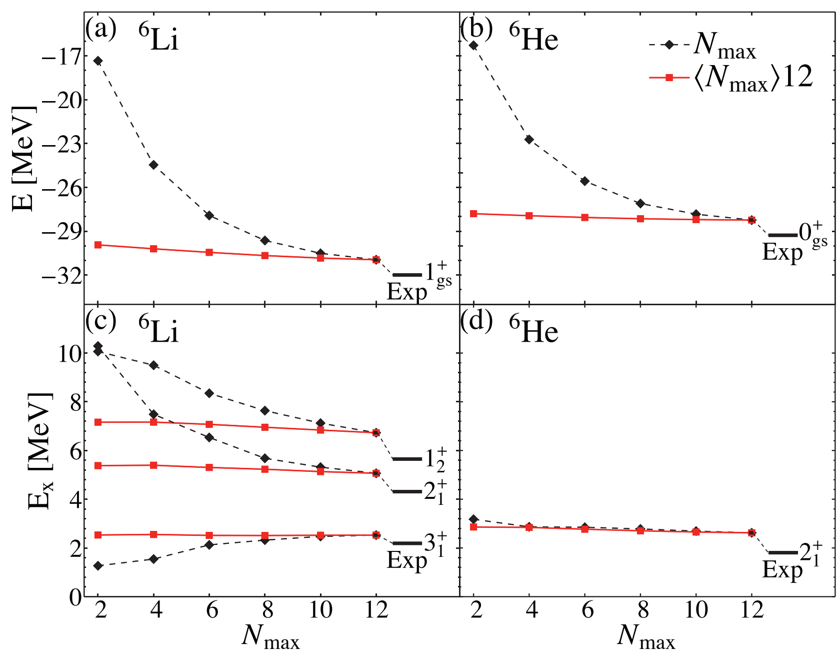
- Reaching the limit of M-scheme N_{max} truncation
- Exploit symmetries to reduce basis dimension
  - SU(3) basis — Dytrych *et al*, PRL111, 252501 (2013)
  - Coupled-J basis — Aktulga, Yang, Ng, Maris, Vary, HPCS2011

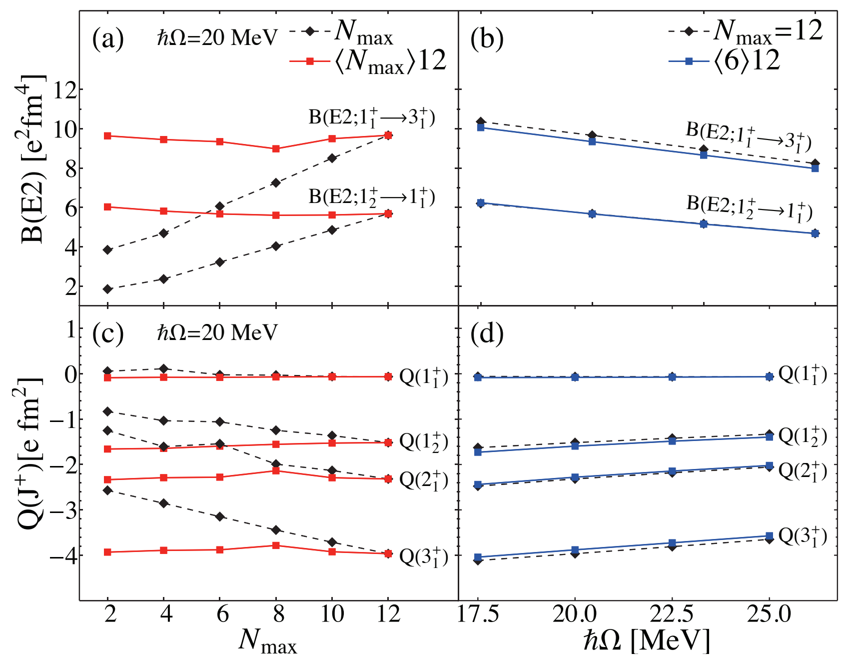


- smaller,
  but less sparse matrices
- number of nonzero matrix elements often (significantly) larger than in M-scheme
- construction of matrix more costly
- diagonalization cheaper than in M-scheme

Looking forward: Taming the scale explosion

- Reaching the limit of M-scheme N_{max} truncation
- Exploit symmetries to reduce basis dimension
- Reduce basis dim. by keeping only most important basis states
  - Symmetry Adapted No-Core Shell Model





$\langle N_{\text{max}} \rangle 12$ complete basis up to N_{max},
dominant SU(3) irreps up to $N_{\text{max}} = 12$

Dytrych *et al*, PRL111, 252501 (2013)

Looking forward: Taming the scale explosion

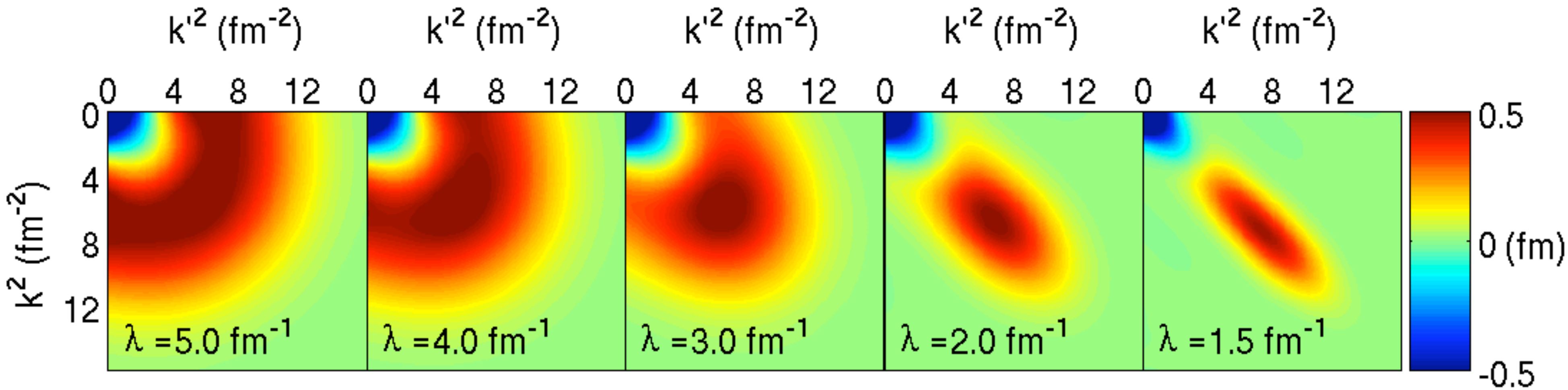
- Reaching the limit of M-scheme N_{max} truncation
- Exploit symmetries to reduce basis dimension
- Reduce basis dim. by keeping only most important basis states
  - Symmetry Adapted NCSM — Dytrych *et al*, PRL111, 252501 (2013)
  - Importance Truncated NCSM — Roth, PRC79, 064324 (2009)
    - reduce basis dimension by (several) order(s) of magnitude
    - many-body states single Slater Determinants in M-scheme
  - No-Core Monte-Carlo Shell Model
    Abe, Maris, Otsuka, Shimizu, Utsuno, Vary, PRC86, 054301 (2012)
    - reduce basis to (few) hundred highly optimized states
    - many-body states linear combination of Slater Deteminants
    - hotspot:
      construction of optimized basis and of many-body matrix

Caveat: Uncertainty Quantification

- can the numerical errors due to reduced basis dimension be quantified within the computation framework?

Looking forward: Taming the scale explosion

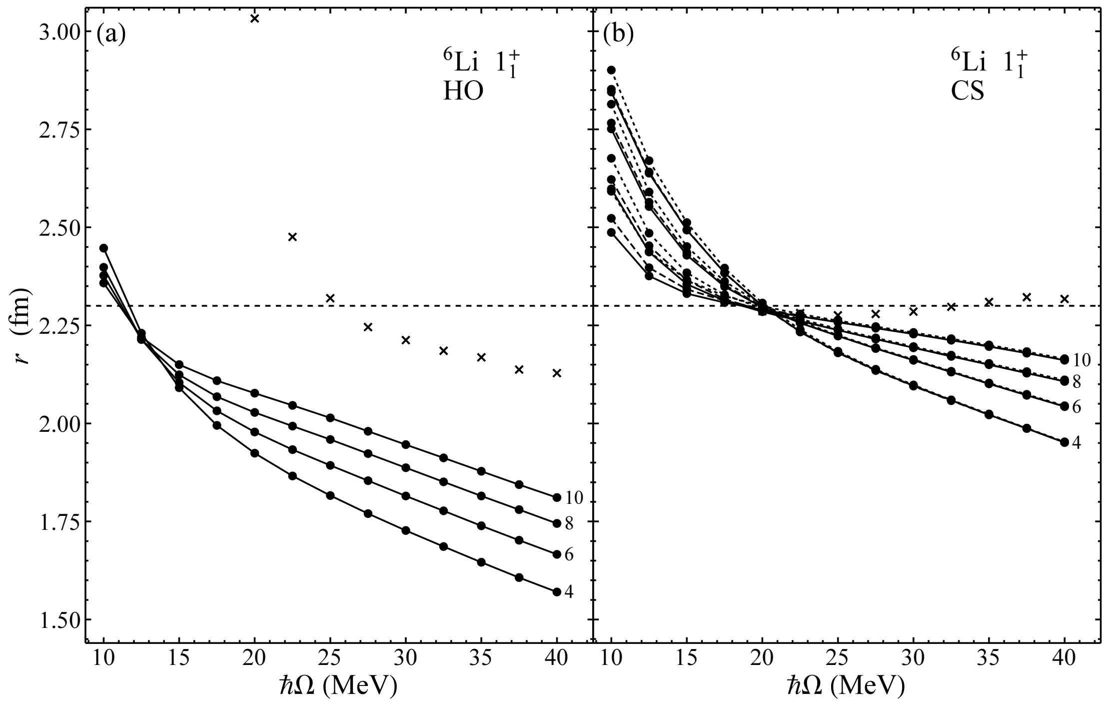
- Reaching the limit of M-scheme $N_{\rm max}$ truncation
- Exploit symmetries to reduce basis dimension
- Reduce basis dim. by keeping only most important basis states
- Accelerate convergence rate with $N_{\rm max}$
  - Similarity Renormalization Group



  - construction of renormalized input Hamiltonian
  - need to transform operators as well as Hamiltonian
  - include induced many-body interactions and operators?

Looking forward: Taming the scale explosion

- Reaching the limit of M-scheme N_{max} truncation
- Exploit symmetries to reduce basis dimension
- Reduce basis dim. by keeping only most important basis states
- Accelerate convergence rate with N_{max}
  - Similarity Renormalization Group
  - More flexible / realistic (radial) basis functions



e.g. Coulomb–Sturmian basis
to improve convergence
of RMS radius,
Caprio, Maris, Vary,
PRC86, 034312 (2012)

Conclusions

- No-core Configuration Interaction nuclear structure calculations
  - Binding energy, spectrum, magnetic moments
  - $\langle r^2 \rangle$, $\mathcal{Q}$, transitions, wfns, one-body densities
- Main challenge: construction and diagonalization of extremely large (D $\sim 10^{10}$) sparse (NNZ $\sim 10^{14}$) matrices
- JISP16
  - Nonlocal phenomenological 2-body interaction
  - Good convergence for energies and magnetic moments
  - Good description of p-shell nuclei
- Chiral EFT interactions
  - Slower convergence than JISP16, improved by SRG
  - Need consistent NN and 3NF for description of nuclei
  - Effect 3NF on pure neutron drops very small
- Would not have been possible without collaboration with applied mathematicians and computer scientists