Ab initio calculations of p-shell nuclei with the JAmes Iowa State Potential 16

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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 computer time

Ab initio nuclear physics – Quantum many-body problem

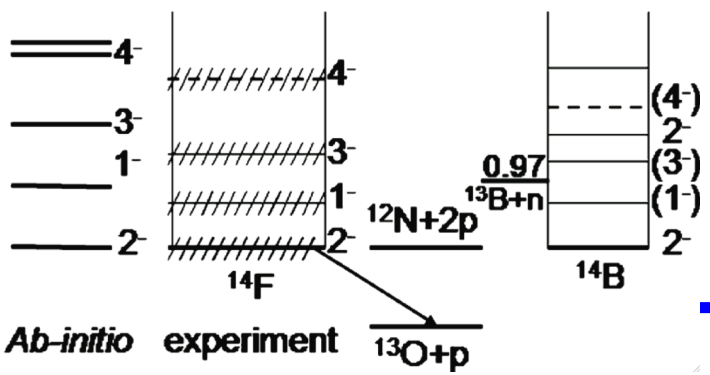
Given a Hamiltonian operator

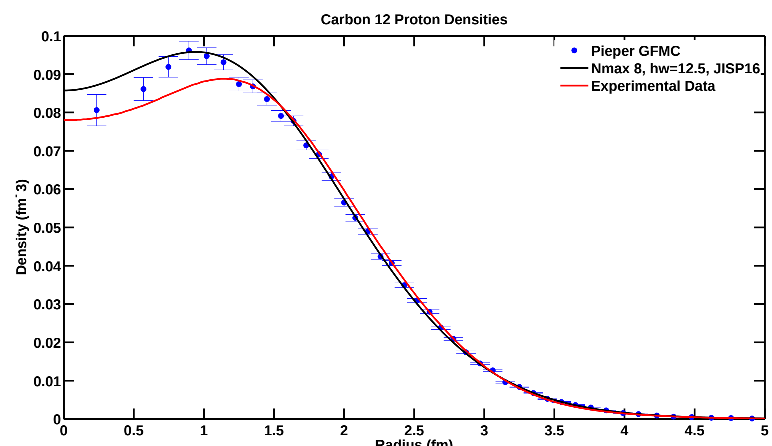
$$\hat{\mathbf{H}} \;=\; \sum_{i<j} \frac{(\mathbf{p}_i - \mathbf{p}_j)^2}{2\,m\,A} + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \ldots$$

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 $r_1, \ldots, r_A$

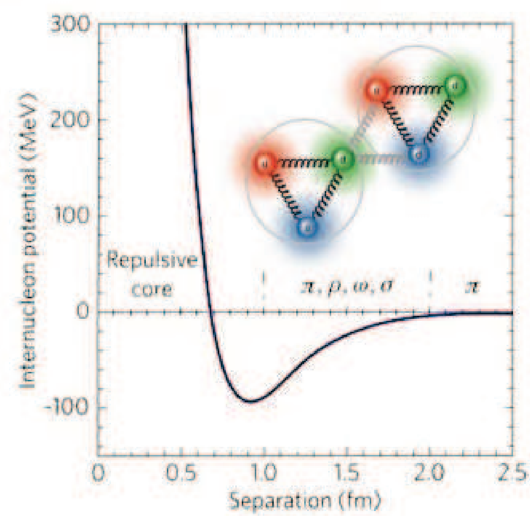




Nuclear interaction

Nuclear potential not well-known,
though in principle calculable from QCD (more on Tuesday)

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



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 (more on Friday)
- ...
- JAmes Iowa State Potential
- ...

Phenomeological NN interaction: JISP16

JAmes Iowa State Potential 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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J-matrix Inverse Scattering Potentials

- Constructed as matrix in H.O. basis
  - $2n + l \le 8$ for even partial waves, limited to $J \le 4$
  - $2n + l \le 9$ for odd partial waves, limited to $J \le 4$
  - $\hbar\omega = 40$ MeV
- χ^2/datum of 1.05 for the 1999 np data base (3058 data)
- No charge symmetry breaking
- Use PET to improve
  - deuteron quadrupole moment
  - ^{3}H and ^{4}He binding energies
  - binding energies low-lying states of ^{6}Li: JISP6

    Shirokov, Vary, Mazur, Zaystev, Weber, PLB **621**, 96 (2005)
  - binding energy of ^{16}O: JISP16

    Shirokov, Vary, Mazur, Weber, PLB **644**, 33 (2007)
  - additional tuning, more accurate calculations: JISP16$_{2010}$ reproduces ^{16}O within numerical error estimates of 3%

    Shirokov, Kulikov, Maris, Mazur, Mazur, Vary, arXiv:0912.2967

No-Core Configuration Interaction nuclear physics 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}
- Complete basis $\longrightarrow$ exact result
  - caveat: complete basis is infinite dimensional
- No-Core Configuration Interaction
  - all A nucleons are treated the same
- In practice
  - truncate basis
  - study behavior of observables as function of truncation
- Computational challenge (more on Thursday)
  - construct large 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)

(more on Thursday)

NCCI – Sparse matrix

- Express Hamiltonian in basis

$$H_{ij} = \int_\Omega \big(\Phi_i^*(r'_1,\ldots,r'_A)\,\hat{\mathbf{H}}\,\Phi_j(r_1,\ldots,r_A)\big)\,\mathrm{d}r_1\ldots\mathrm{d}r_A\,\mathrm{d}r'_1\ldots\mathrm{d}r'_A$$

- Sparse matrix

  A-body problem with N-body interaction: nonzero matrix elements iff at least $A-N$ nucleons are in identical SP states

  - many-body problem with 2-body (and 3-body) interactions
  - each many-body basis states is single Slater Determinant

$$\begin{aligned} H_{ij}^{(A)} &= (-1)^{\text{permutations}}\,\delta_{i_1,j_1}\ldots\delta_{i_{(A-2)},j_{(A-2)}} \\ &\quad \int_\Omega \big(\Phi_i^*(r_c,r_d)\,\hat{\mathbf{H}}^{(\mathbf{2})}_{\mathbf{cd}\leftarrow\mathbf{ab}}\,\Phi_j(r_a,r_b)\big)\,\mathrm{d}r_a\mathrm{d}r_b\mathrm{d}r_c\mathrm{d}r_d \\ &= (-1)^{\text{permutations}}\,\delta_{i_1,j_1}\ldots\delta_{i_{(A-2)},j_{(A-2)}}\,H^{(2)}_{cd\leftarrow ab} \end{aligned}$$

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:
    - No-Core Monte-Carlo Shell Model (more on Thursday)
      Abe, Maris, Otsuka, Shimizu, Utsuno, Vary, PRC86, 054301 (2012)
    - Importance Truncation Roth, PRC79, 064324 (2009) (Friday)
    - SU(3) Truncation NSF PetaApps collaboration (Draayer & Dytrych next)
    - . . .

Extrapolating to complete basis

Challenge: achieve numerical convergence for No-Core Full Configuation calculations using finite basis 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}

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

  - 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)

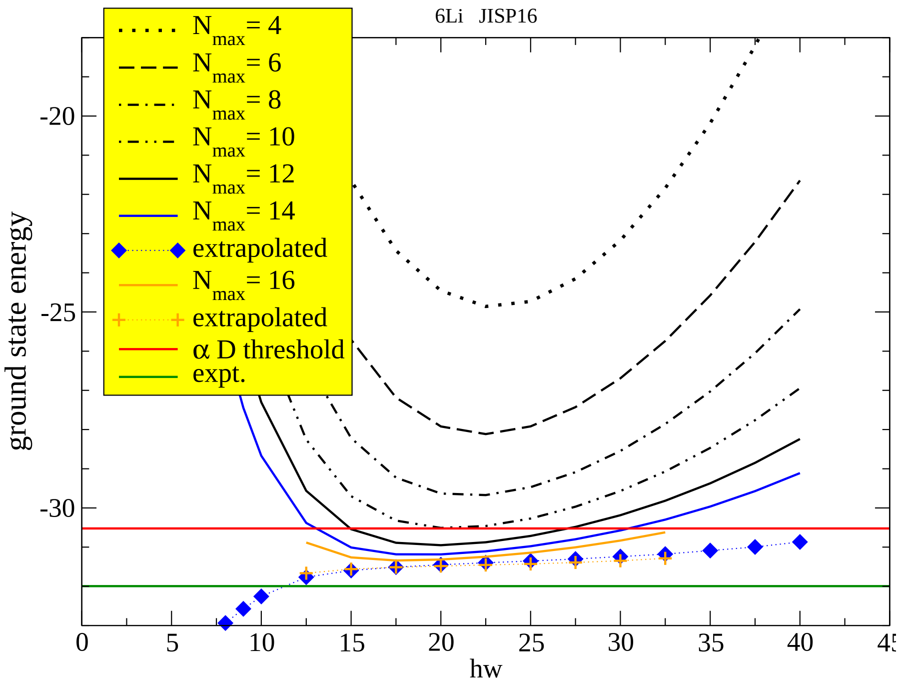
- Recent studies of IR and UV behavior
  - exponentials in $\sqrt{\hbar\omega/N}$ and $\sqrt{\hbar\omega N}$ Coon *et al*, PRC86, 054002 (2012)

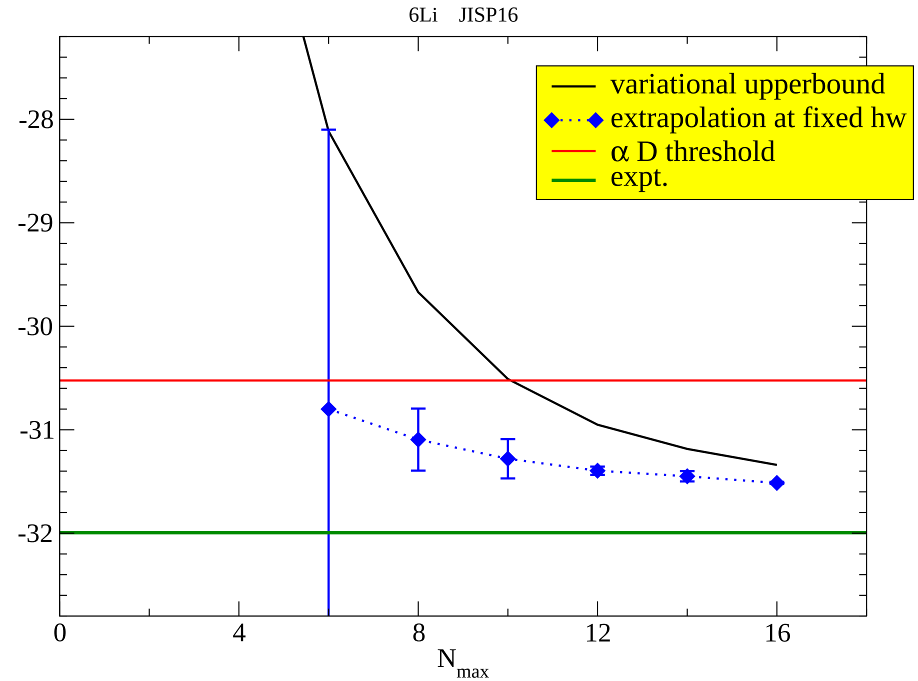
Furnstahl, Hagen, Papenbrock, PRC86, 031301(R) (2012)

(more on Thursday)

Extrapolating to complete basis – in practice

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



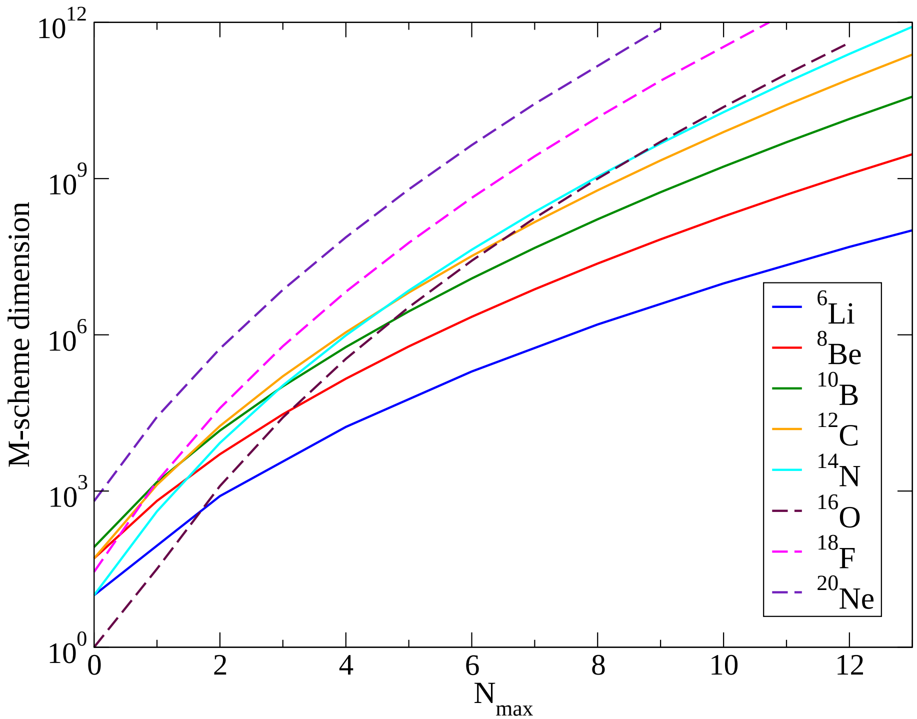


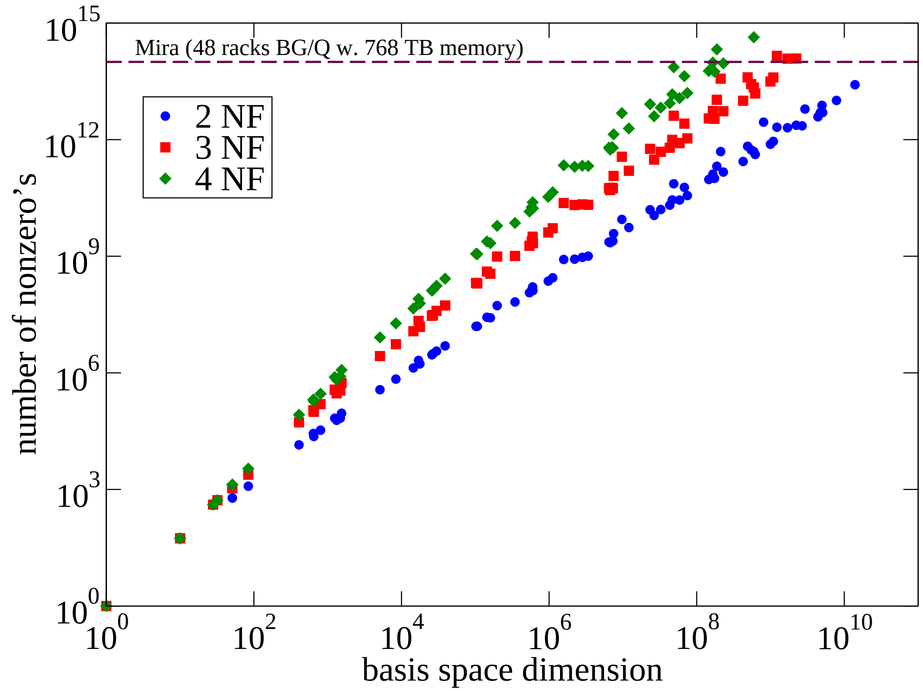
- H.O. basis up to $N_{\mathsf{max}} = 16$: E$_b = -31.49(3)$ MeV

  Cockrell, Maris, Vary, PRC86 034325 (2012)
- Hyperspherical harmonics up to $K_{\mathsf{max}} = 14$: E$_b = -31.46(5)$ MeV

  Vaintraub, Barnea, Gazit, PRC79 065501 (2009)

NCCI calculations – main challenge

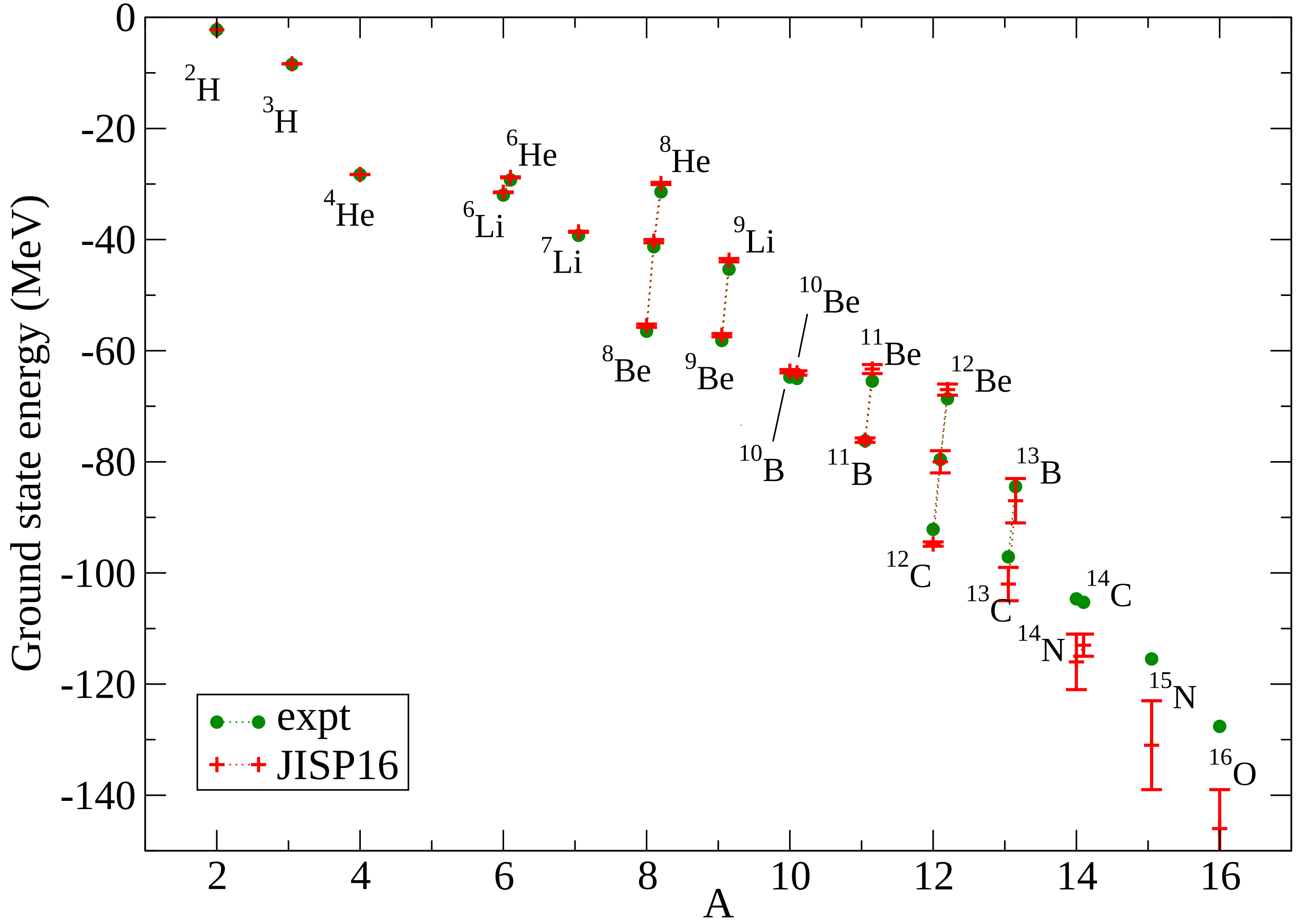




- Increase of basis space dimension with increasing A and N_{max}
  - need calculations up to at least $N_{\text{max}} = 8$ for meaningful extrapolation and numerical error estimates
- More relevant measure for computational needs
  - number of nonzero matrix elements
  - current limit 10^{13} to 10^{14}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

Ground state energy of p-shell nuclei with JISP16

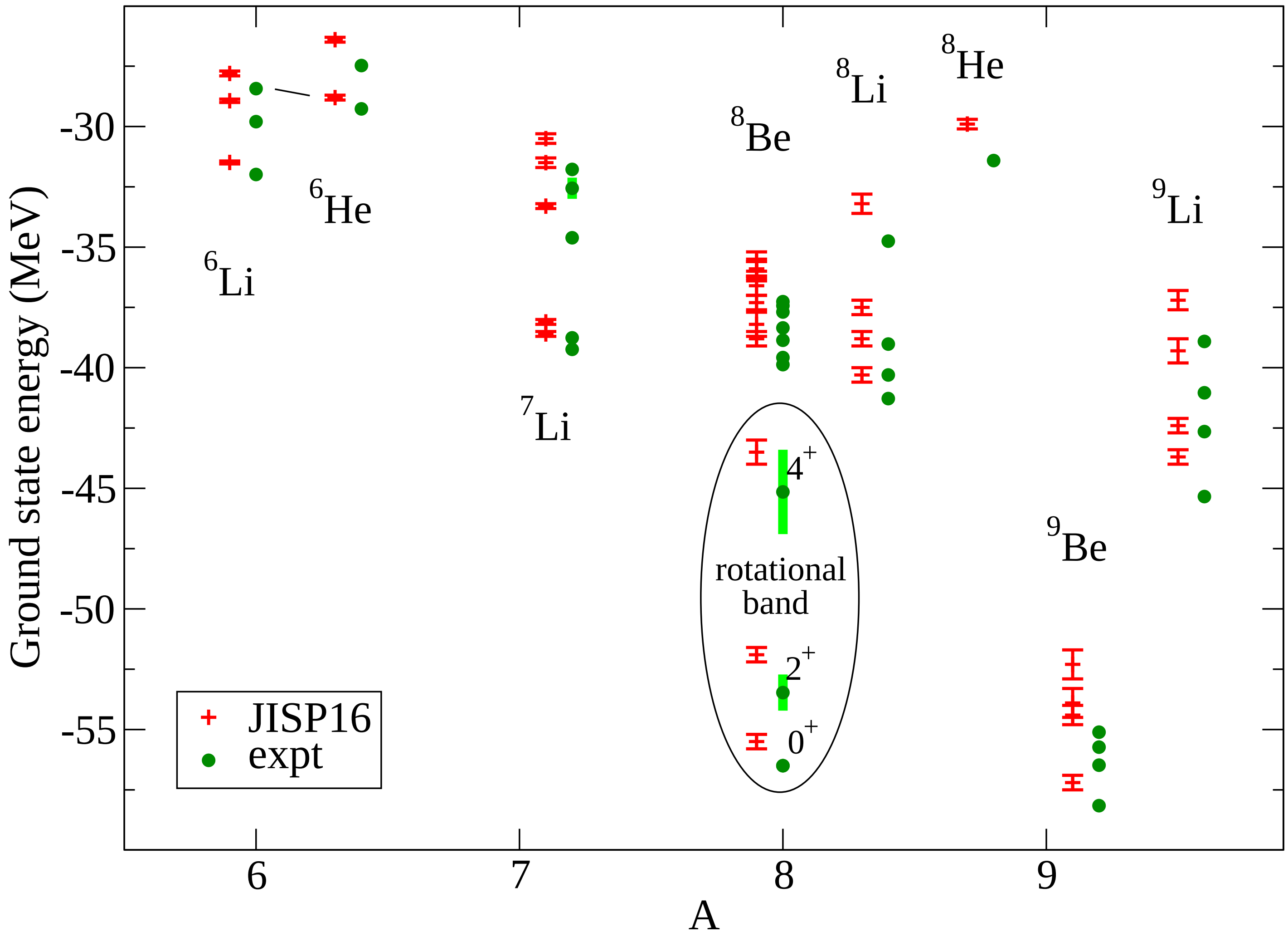
Maris, Vary, IJMPE, to appear



- ^{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

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

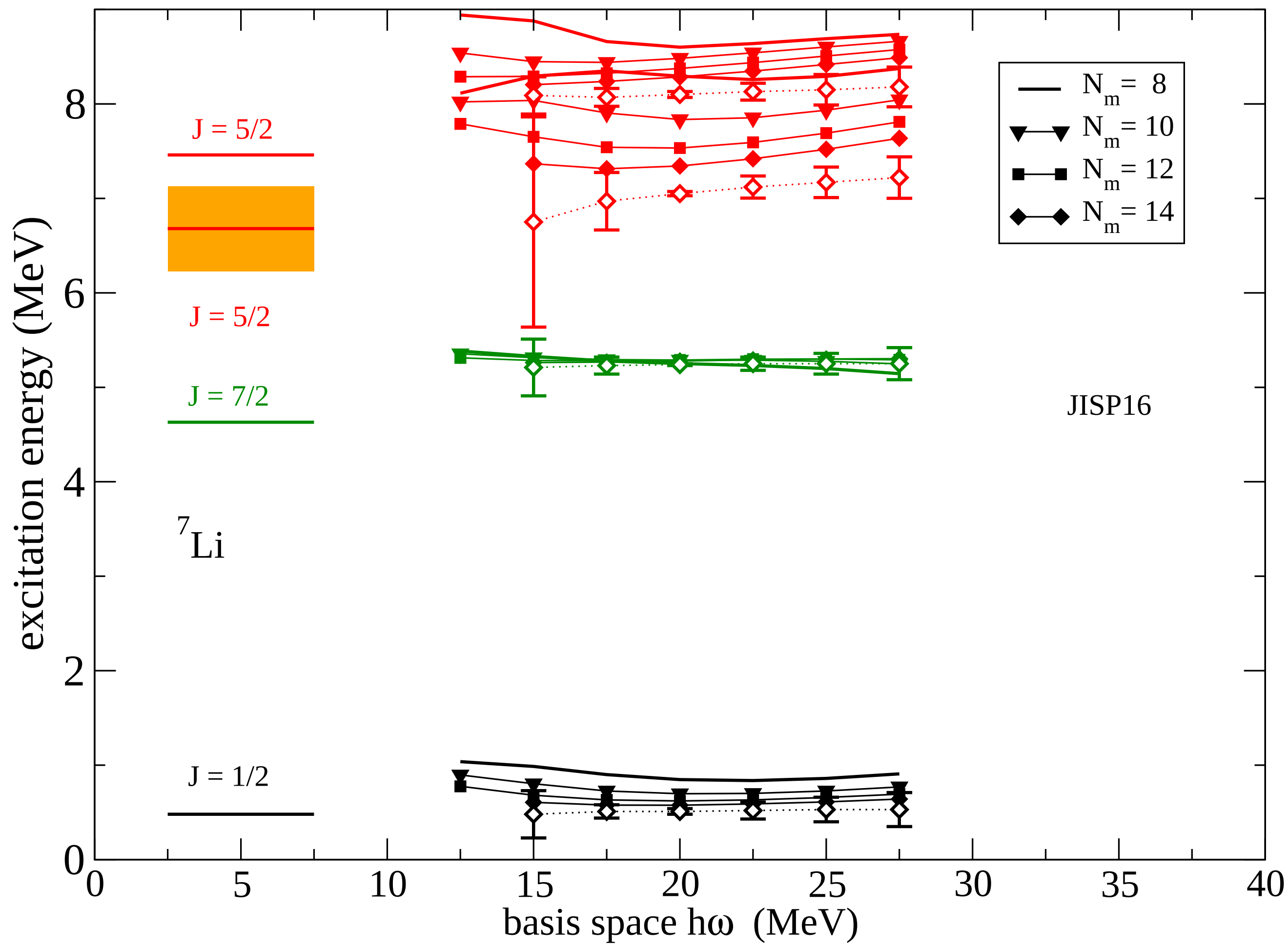
Cockrell, Maris, Vary, PRC86 034325 (2012); Maris, Vary, IJMPE, to appear



- Excitation spectrum narrow states in good agreement with data

Details: excitation spectrum 7Li

Cockrell, Maris, Vary, PRC86 034325 (2012)

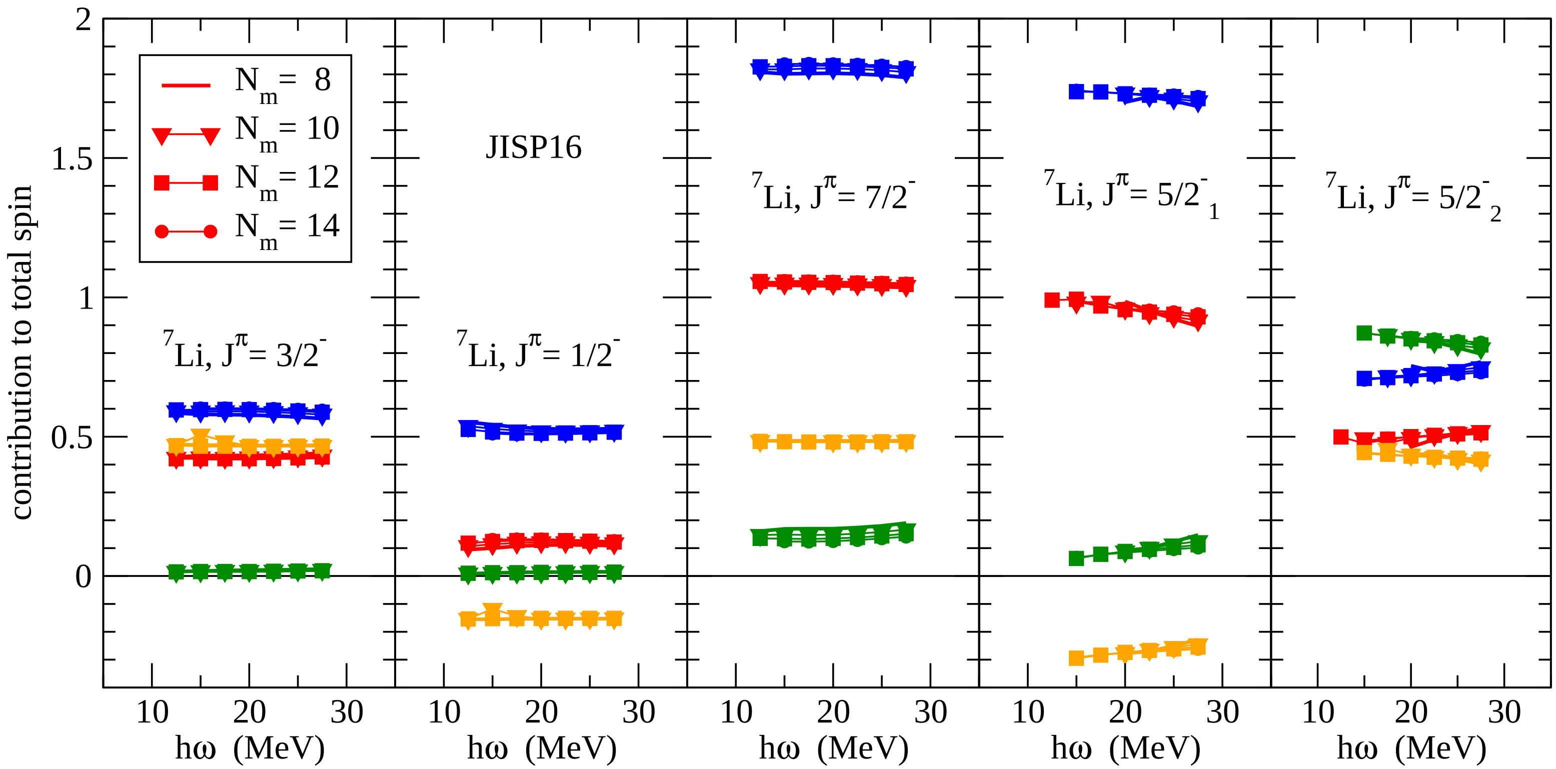


- Narrow states well converged, no extrapolation needed
- Broad resonances generally not as well converged; may need to incorporate continuum (more on Wednesday)

Details: spin components of 7Li

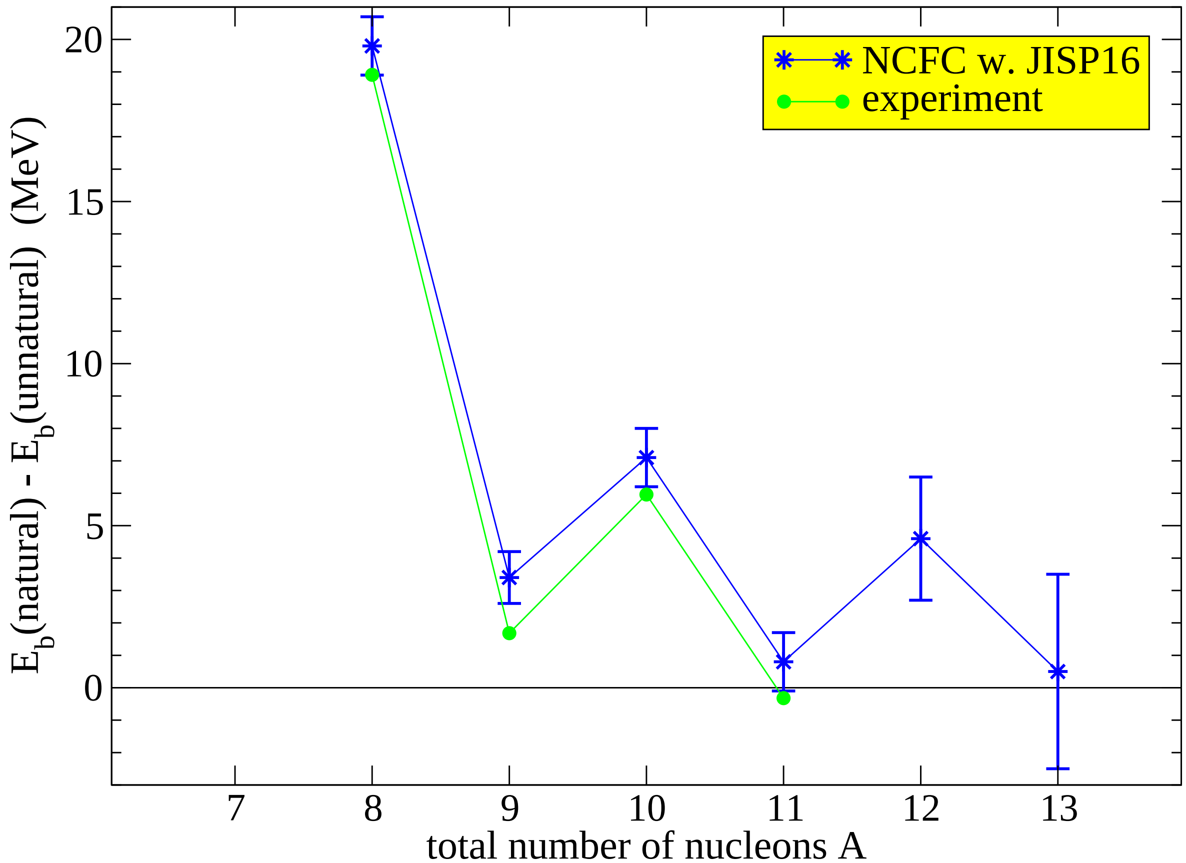
Maris, Vary, IJMPE, to appear

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



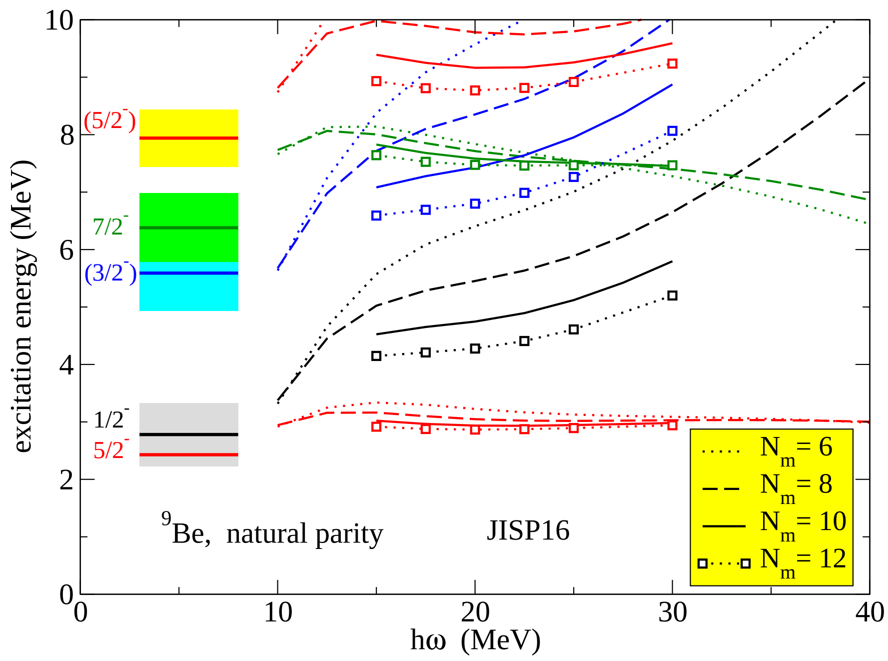
- Converged with $N_{\max}$, persistent weak $\hbar\omega$ dependence $\frac{5}{2}^-$ states
- Two $\frac{5}{2}^-$ states have very different structure

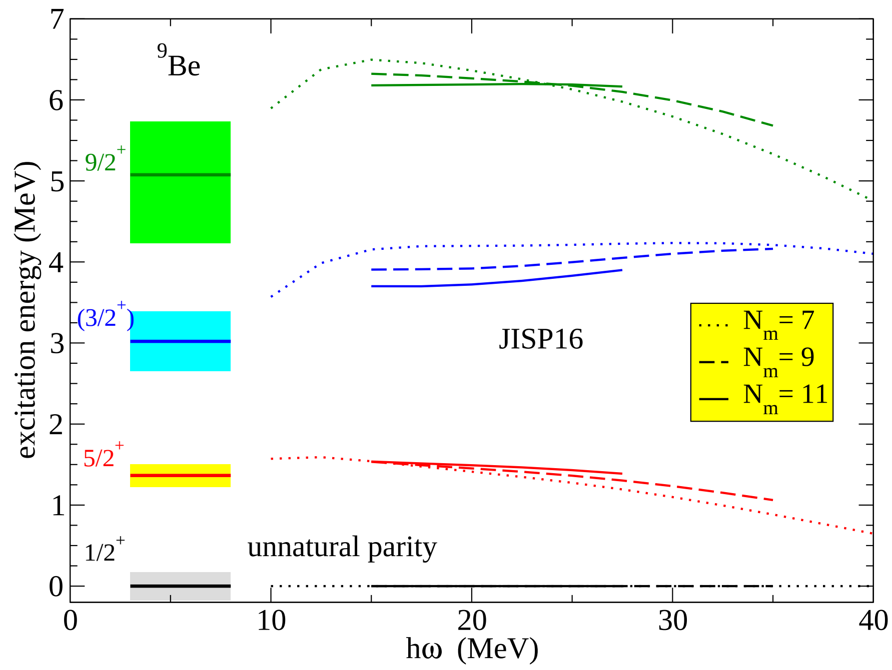
Positive vs. negative parity states of Be-isotopes



- Unnatural parity states systematically underbound by about one MeV compared to lowest natural parity states
  - interaction JISP16 not good enough?
  - difference in convergence of pos. and neg. parity states?

Details: Positive and negative spectrum of 9Be

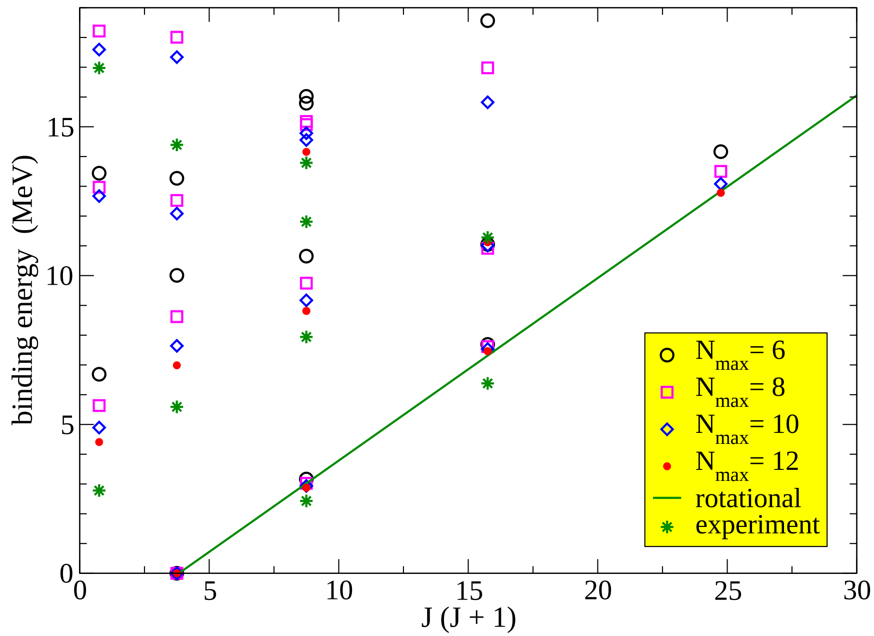


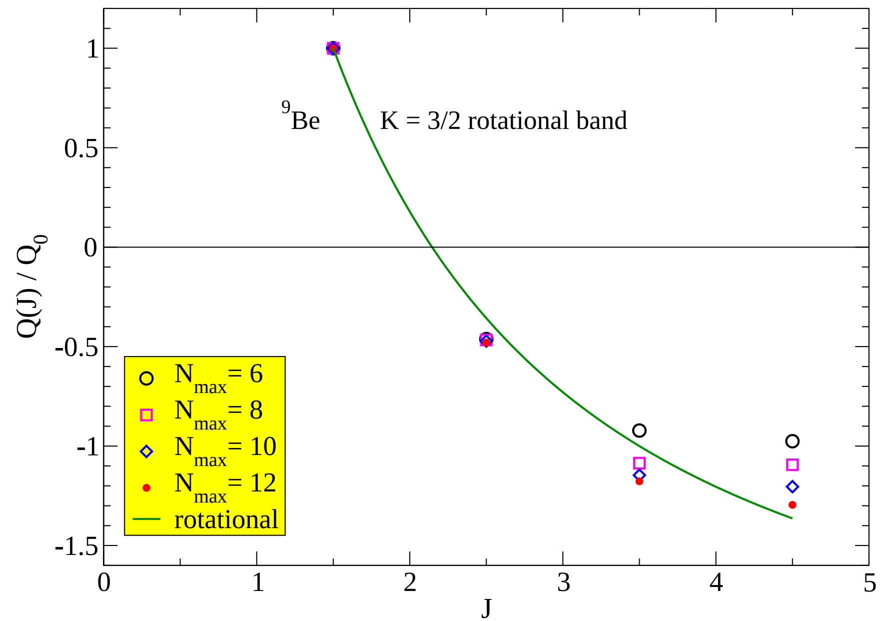


- Excitation energy $\frac{5}{2}^-$ at 3 MeV well converged (narrow)
- Excitation energy $\frac{7}{2}^-$ reasonably converged
- Excitation energies broad neg. parity not well converged
- Excitation energies pos. parity well converged

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

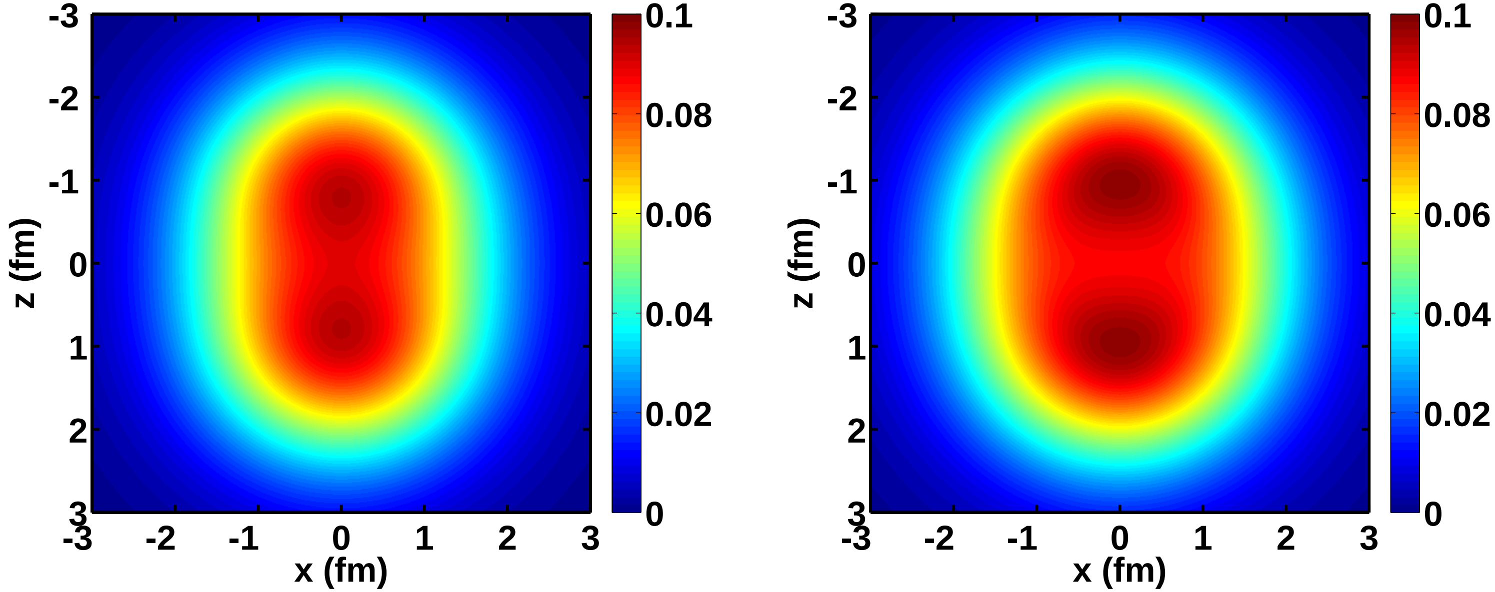
$$Q(J) = \frac{3\,K^2 - J(J+1)}{(J+1)(2J+3)}\;Q_0^K$$

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

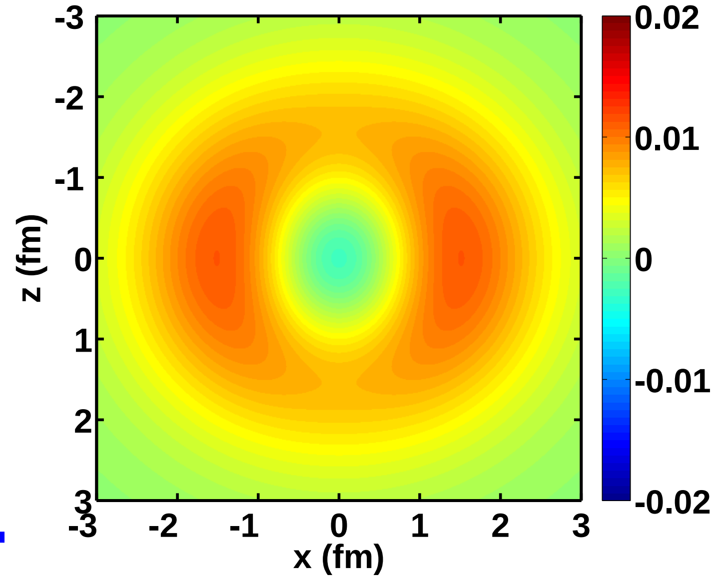
$$\mathrm{B(E2;}i \to f) = \frac{5}{16\pi}\,\left(Q_0^K\right)^2\,\left(J_i, 2; K, 0\middle|J_f, K\right)^2$$

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

proton neutron



and their difference



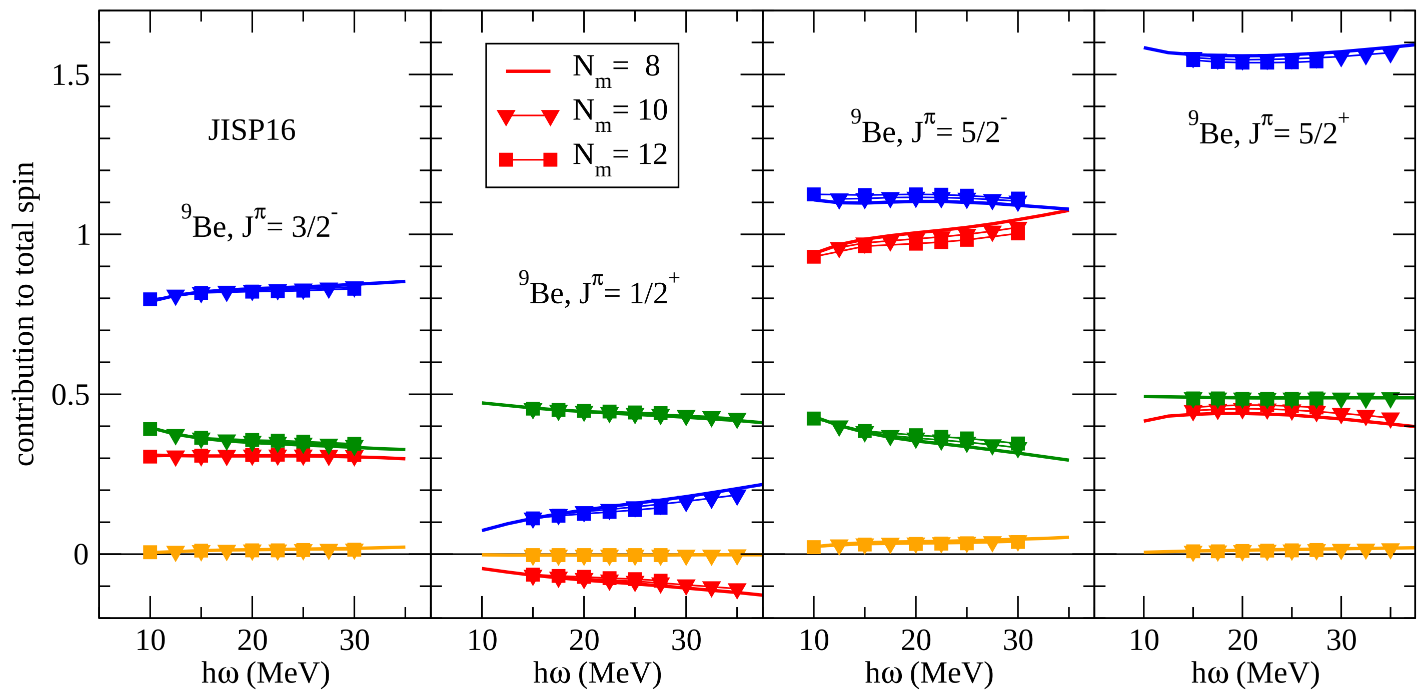
Translationally-invariant proton and neutron densities

Cockrell, PhD thesis, 2012

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

Details: spin components of 9Be

$$J = \frac{1}{J+1}\Big(\langle \mathbf{J}\cdot\mathbf{L}_p\rangle + \langle \mathbf{J}\cdot\mathbf{L}_n\rangle + \langle \mathbf{J}\cdot\mathbf{S}_p\rangle + \langle \mathbf{J}\cdot\mathbf{S}_n\rangle\Big)$$

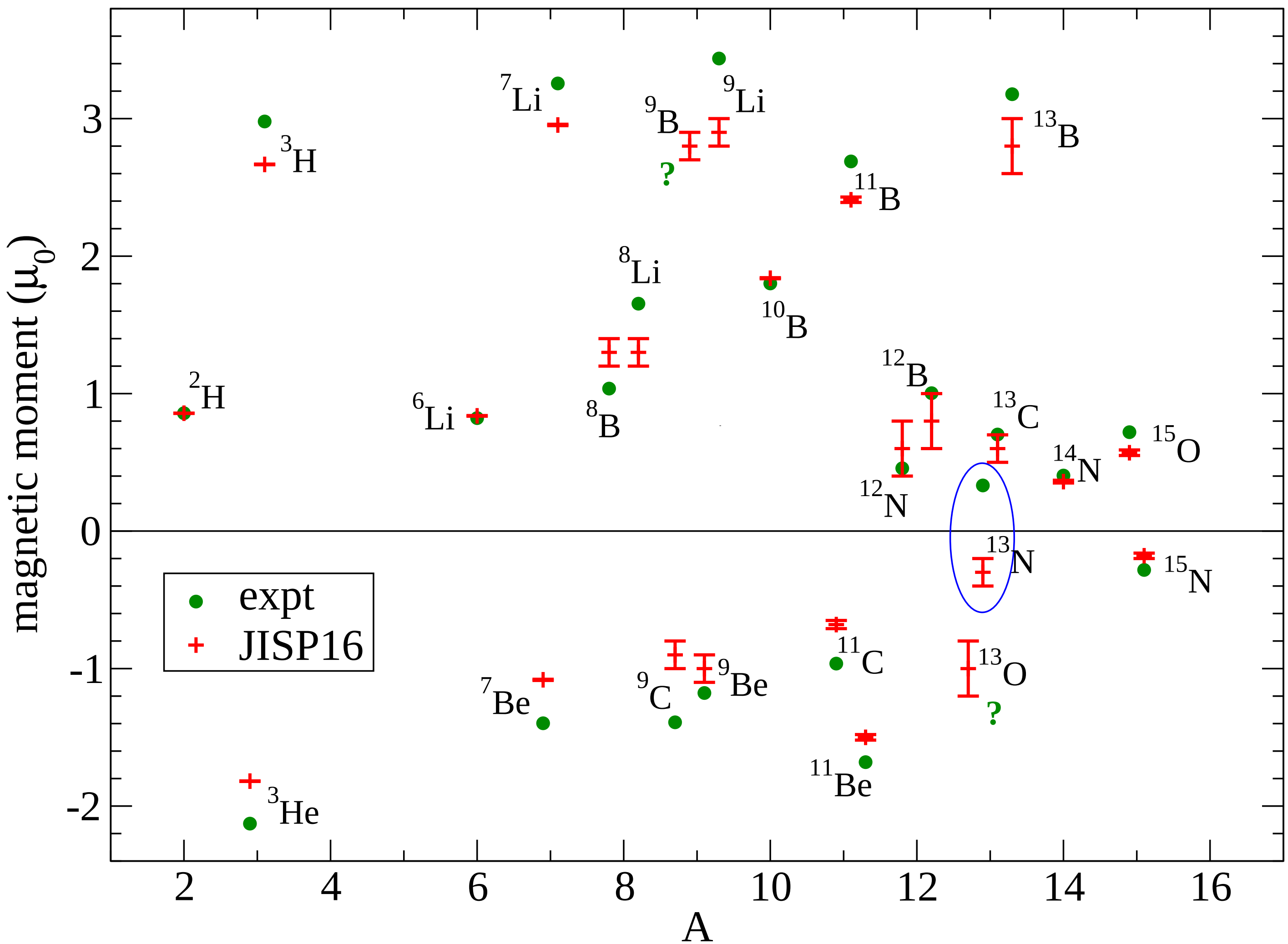


- Consistent with picture of two α particles plus a neutron
  - contribution intrinsic spin neutron approximately $\frac{1}{2}$
  - contribution intrinsic spin proton approximately 0
- Consistent with neutron $\frac{3}{2}^-$ in π orbital, neutron $\frac{1}{2}^+$ in σ orbital

Magnetic moments of p-shell nuclei with JISP16

Maris, Vary, IJMPE, to appear

$$\mu \quad = \quad \frac{1}{J+1}\Big(\langle \mathbf{J}\cdot\mathbf{L}_p\rangle + 5.586\langle \mathbf{J}\cdot\mathbf{S}_p\rangle - 3.826\langle \mathbf{J}\cdot\mathbf{S}_n\rangle\Big)\,\mu_0$$



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

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
- JAmes Iowa State Potential
  - Nonlocal phenomenological 2-body interaction
  - Good description of p-shell nuclei
  - Good convergence for energies and magnetic moments
  - Slower convergence for $\langle r^2 \rangle$, $\mathcal{Q}$, B(E2), ...
    - improved extrapolation methods?
    - basis functions w. realistic asymptotic behavior instead of HO basis?
    - include selection of additional basis states from higher $N_{\max}$ spaces?
- Would not have been possible without collaboration with applied mathematicians and computer scientists
  Aktulga, Yang, Ng (LBNL); Çatalyürek, Saule (OSU); Sosonkina (ODU/AL)