Ab inito calculations of Be isotopes with JISP16

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SciDAC project – NUCLEI
lead PIs: Joe Carlson (LANL) and Rusty Lusk (ANL)

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

NERSC CPU time

Ab initio nuclear physics – Quantum many-body problem

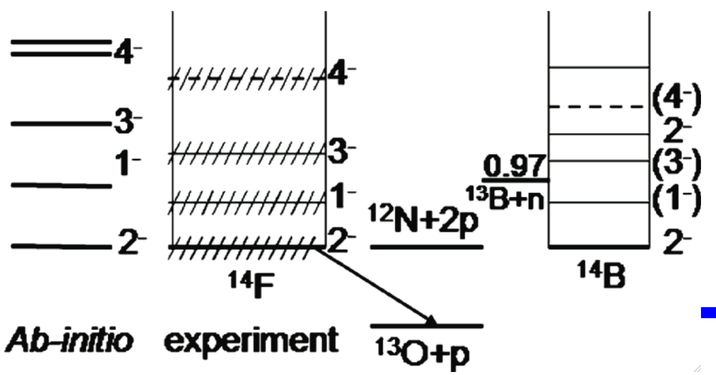
Given a Hamiltonian operator

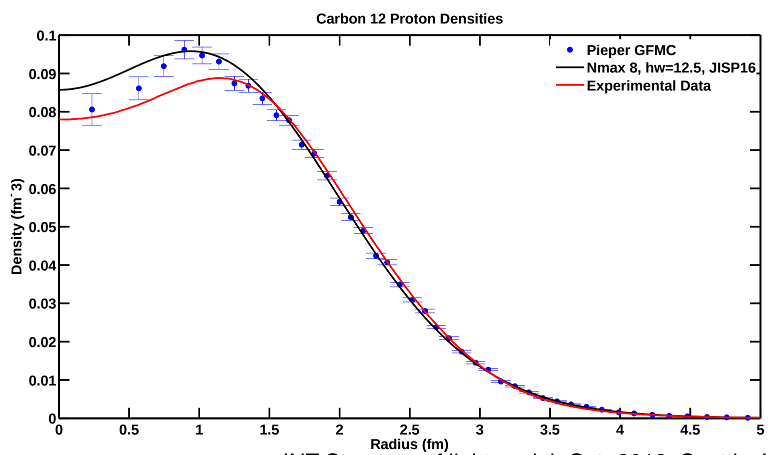
$$\hat{\mathbf{H}} \;=\; \sum_{i<j} \frac{(\vec{p_i} - \vec{p_j})^2}{2\,m\,A} + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \ldots$$

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, ..., A at r_1, ..., r_A





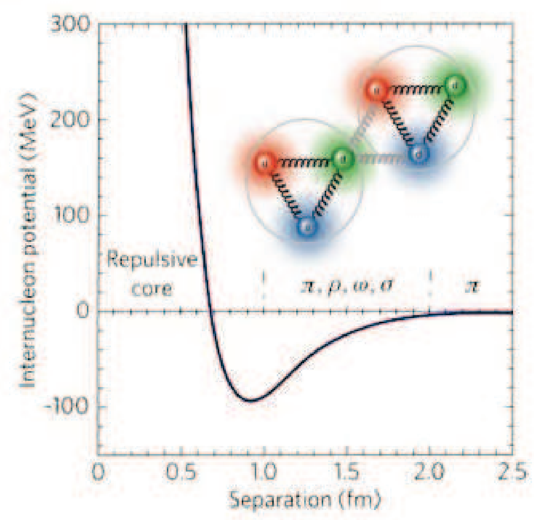
Ab initio nuclear physics – Computational challenges

- 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

Nuclear interaction

Nuclear potential not well-known . . .
though in principle calculable from Quantum Chromo Dynamics

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



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

J-matrix Inverse Scattering 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
  - $2n + l \leq 8$ for even partial waves, limited to $J \leq 4$
  - $2n + l \leq 9$ for odd partial waves, limited to $J \leq 4$
  - $\hbar\omega = 40$ 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

JISP16 results for few-body systems

deuteron properties

	E (MeV)	r_p (fm)	$\mathcal{Q}$ (e fm^2)	$\mathcal{A}_s$ (fm$^{-\frac{1}{2}}$)	$\mathcal{A}_d/\mathcal{A}_s$
expt.	-2.224575	1.971(6)	0.2859(3)	0.8846(9)	0.0256(4)
JISP16	-2.224575	1.964	0.2886	0.8629	0.0252
AV18	-2.224575	1.967	0.270	0.8850	0.0250

selected $A = 3$ and 4 results

	E$_b$(^{3}H	) μ(^{3}H)	μ(^{3}He)	E$_b$(^{4}He)
expt.	8.482	2.979	-2.128	28.296
JISP16	8.369(2)	2.667	-1.819	28.299
AV18	7.61(1)			24.07(4)
AV18+IL2	8.43(1)	2.568(1)	-1.762(1)	28.37(3)

Pieper, Wiringa, Annu. Rev. Nucl. Part. Sci. 51, 53 (2001)

Many-Body systems

Configuration Interaction methods

- 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

- 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 & eigenvectors

Basis space expansion

- Expand wave function in basis states $|\Psi\rangle = \sum a_i |\Phi_i\rangle$
- Many-Body basis states $|\Phi_i\rangle$ Slater Determinants of Single-Particle states $|\phi\rangle$

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

- Single-Particle basis states
  - eigenstates of $\hat{\mathbf{L}}^2$, $\hat{\mathbf{S}}^2$, $\hat{\mathbf{J}}^2$, and $\hat{\mathbf{J}}_{\mathbf{z}}$
    labelled by quantum numbers $|n, l, s, j, m\rangle$
  - radial wavefunctions
    - Harmonic Oscillator
    - Wood–Saxon basis (Negoita, PhD thesis 2010)
    - Coulomb–Sturmian (Caprio, Maris, Vary, PRC86, 034312 (2012))
    - Berggren Rotureau, last week
    - . . .

Truncation scheme

- M-scheme: Many-Body basis states eigenstates of $\hat{\mathbf{J}}_{\mathbf{z}}$

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

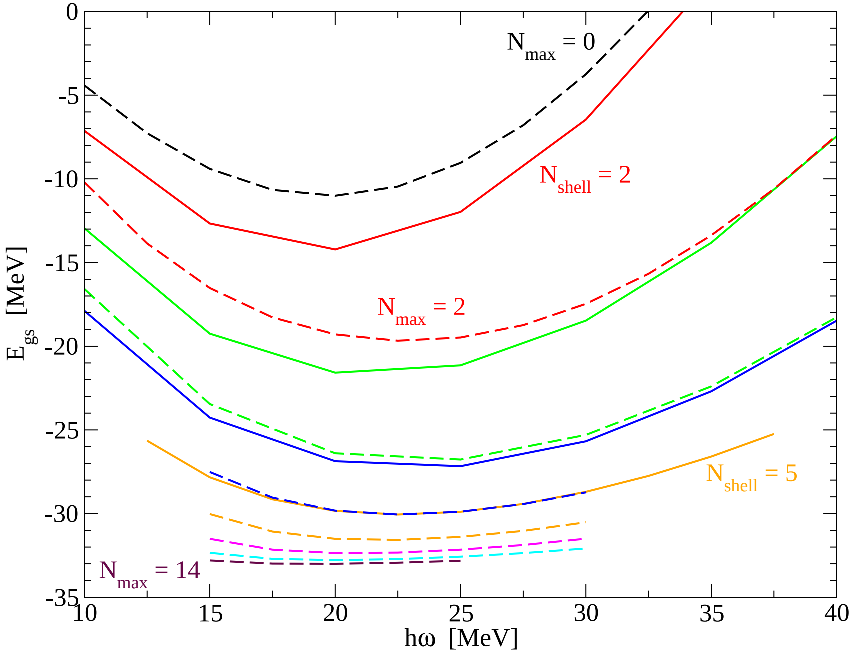
  - single run gives spectrum
  - alternatives:
    LS scheme, Coupled-J scheme, Symplectic basis, . . .

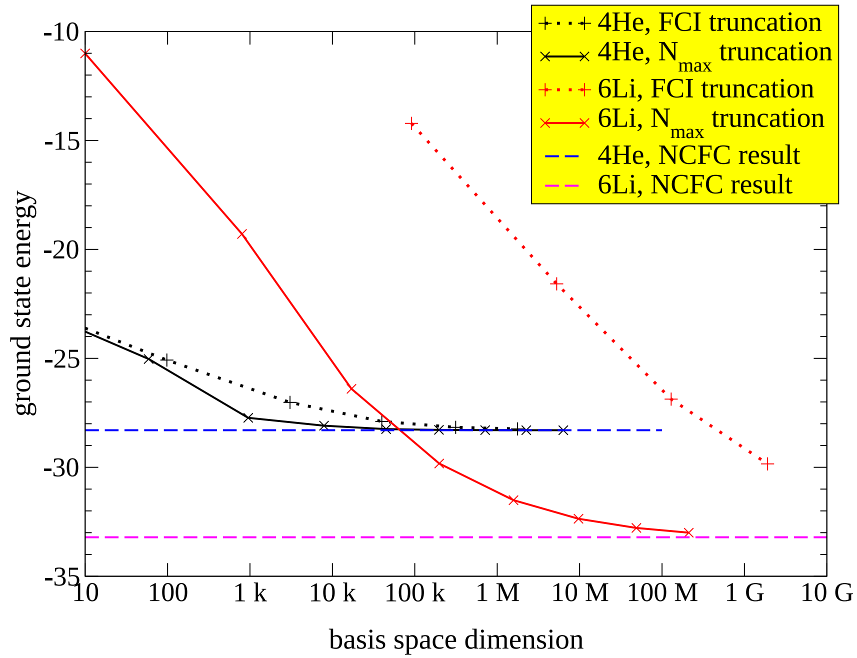
- N_{max} truncation: Many-Body basis states satisfy

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

  - exact factorization of Center-of-Mass motion
  - alternatives:
    No-Core Monte-Carlo Shell Model, Importance Truncation,
    FCI (truncation on single-particle basis only), . . .

Intermezzo: FCI vs. Nmax truncation





- N_{max} truncation
  - exact factorization of Center-of-Mass motion
  - converges much more rapidly than FCI truncation with basis space dimension
- Infinite basis space limit: No-Core Full Configuration (NCFC)

Intermezzo: Center-of-Mass excitations

- Use single-particle coordinates, not relative (Jacobi) coordinates
  - straightforward to extend to many particles
  - have to seperate Center-of-Mass motion from internal motion
- Center-of-Mass wave function factorizes for
  H.O. basis functions in combination with N_{max} truncation

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

where

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

- Add Lagrange multiplier to Hamiltonian (Lawson term)

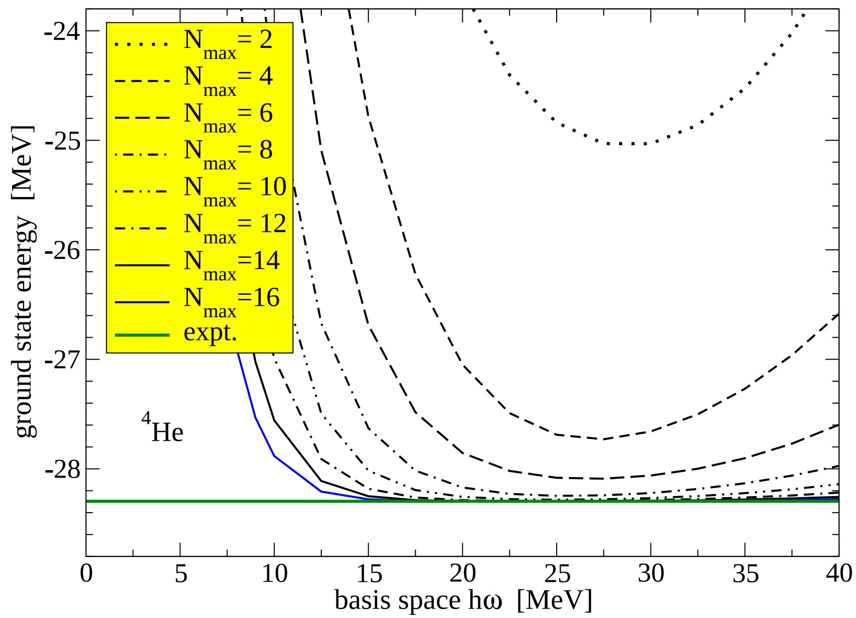
$$
\hat{\mathbf{H}}_{\text{rel}} \longrightarrow \hat{\mathbf{H}}_{\text{rel}} + \Lambda_{CM}\left(\hat{\mathbf{H}}_{CM}^{H.O.} - \frac{3}{2}\Big(\sum_i m_i\Big)\,\omega\right)
$$

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

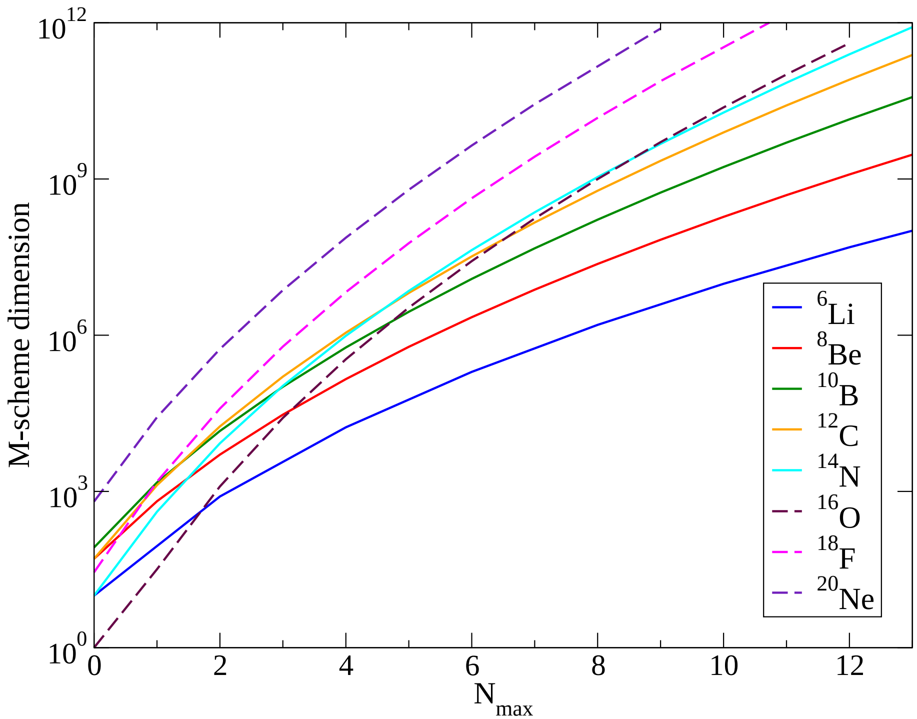
  - seperates CM excitations from CM ground state $|\Phi_{CM}\rangle$

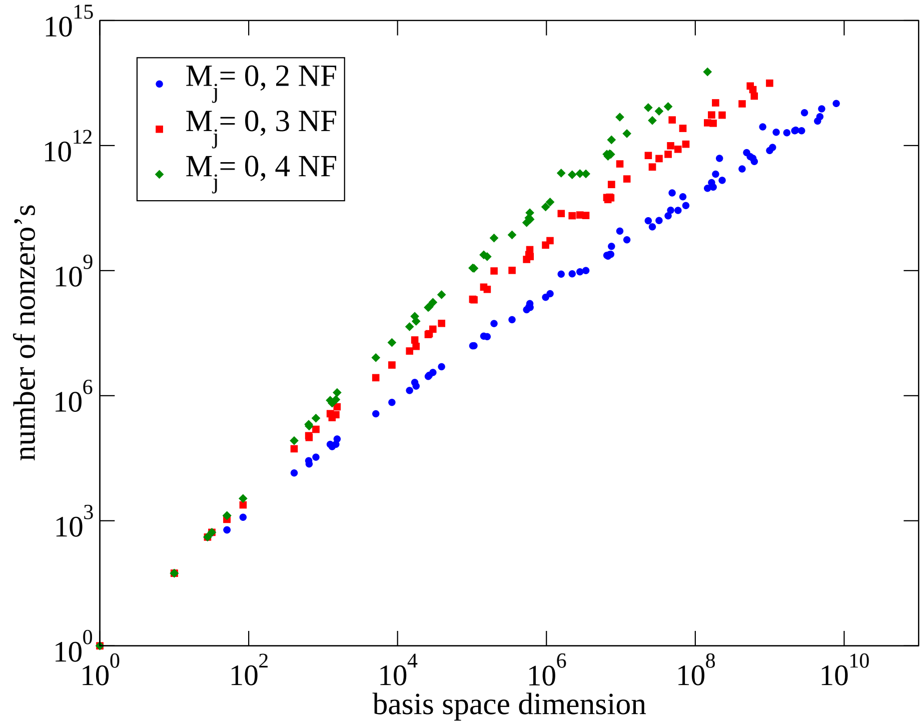
Configuration Interaction Methods

- 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



No-Core CI calculations – main challenge





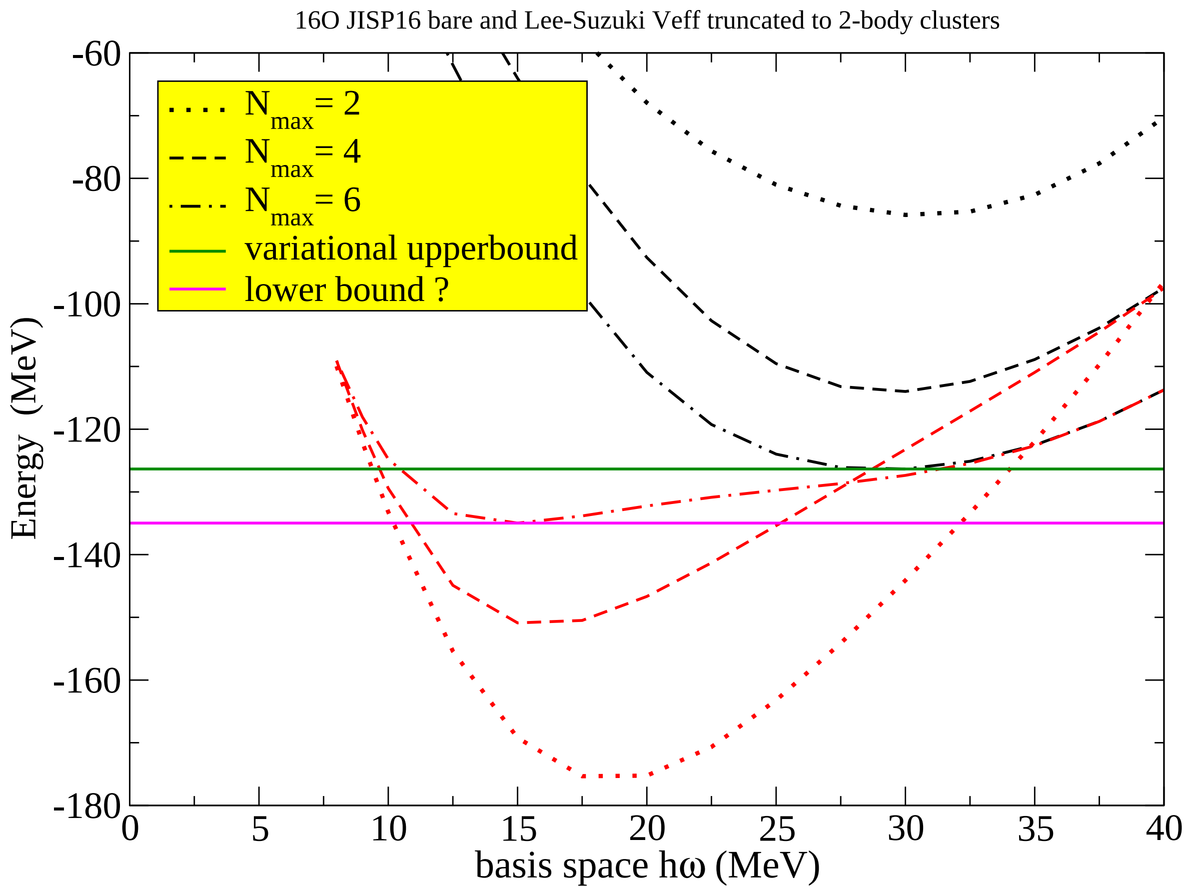
- Increase of basis space dimension with increasing A and N_{max}
- More relevant measure for computational needs
  - number of nonzero matrix elements

Accelerating convergence – renormalization techniques

Challenge: achieve numerical convergence for no-core Full Configuation calculations using finite model space calculations

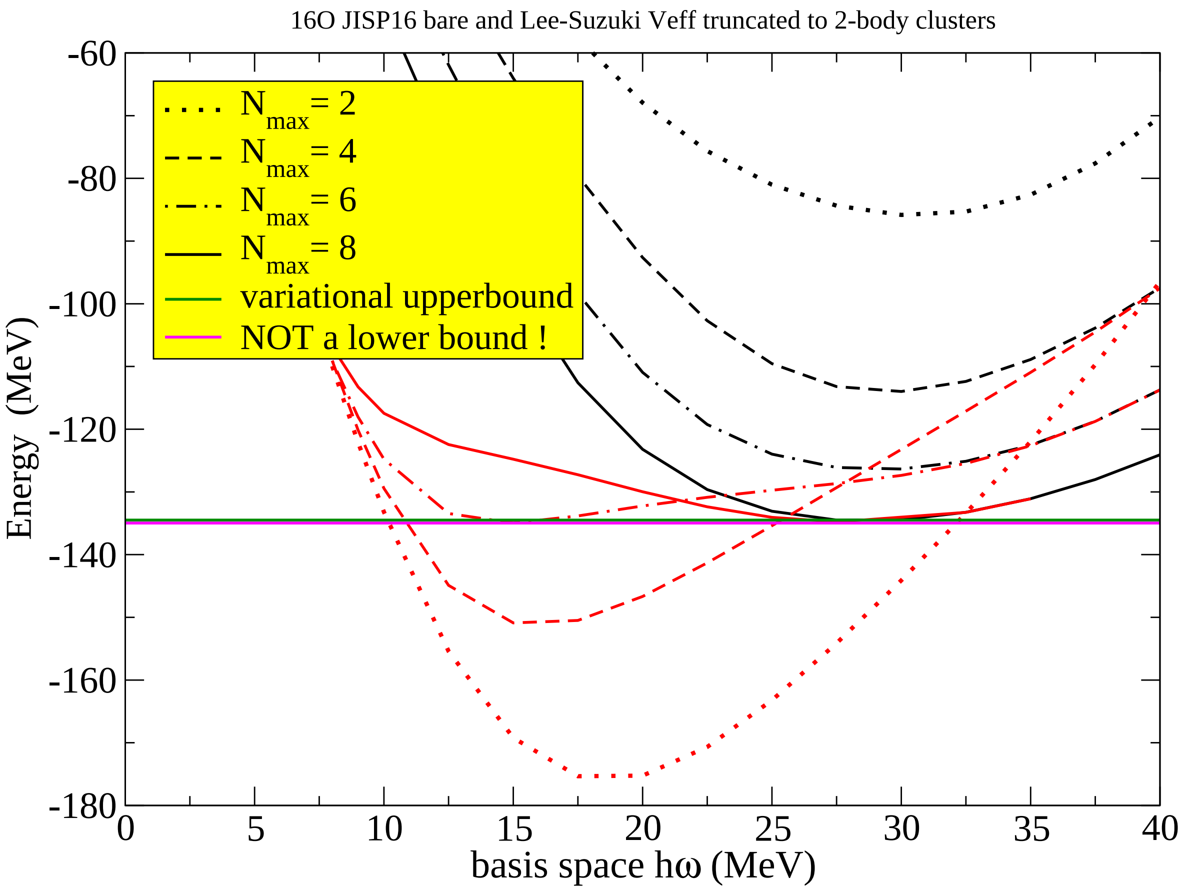
- Renormalize interaction $\longrightarrow$ effective interaction V_{eff}
  - can improve quality of results in small model spaces
- Caveats
  - induces many-body forces
    - induced 3-body forces are often neglected
    - induced 4-, 5-, ..., A-body forces are always neglected
  - variational principle applicable to renormalized Hamiltonian not to original (bare) Hamiltonian
  - often complicates extrapolation to asymptotic values
  - need to renormalize operators as well
- Commonly used renormalization procedures
  - Lee–Suzuki effective interaction
  - Similarity Renormalization Group (in particular in combination with chiral interactions)

Results with Lee–Suzuki renormalization for JISP16



- Ground state energy of ^{16}O expected to be between variational upper bound without renormalization and lower bound (?) from Lee–Suzuki renormalized interaction
- Used in tuning of JISP16 Shirokov, Vary, Mazur, Weber, PLB 644, 33 (2007)

Convergence Lee–Suzuki renormalization not monotonic



- Lee–Suzuki result for ground state energy not a lower bound
- JISP16 overbinds ^{16}O by 10% to 15%

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

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}

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

  - 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

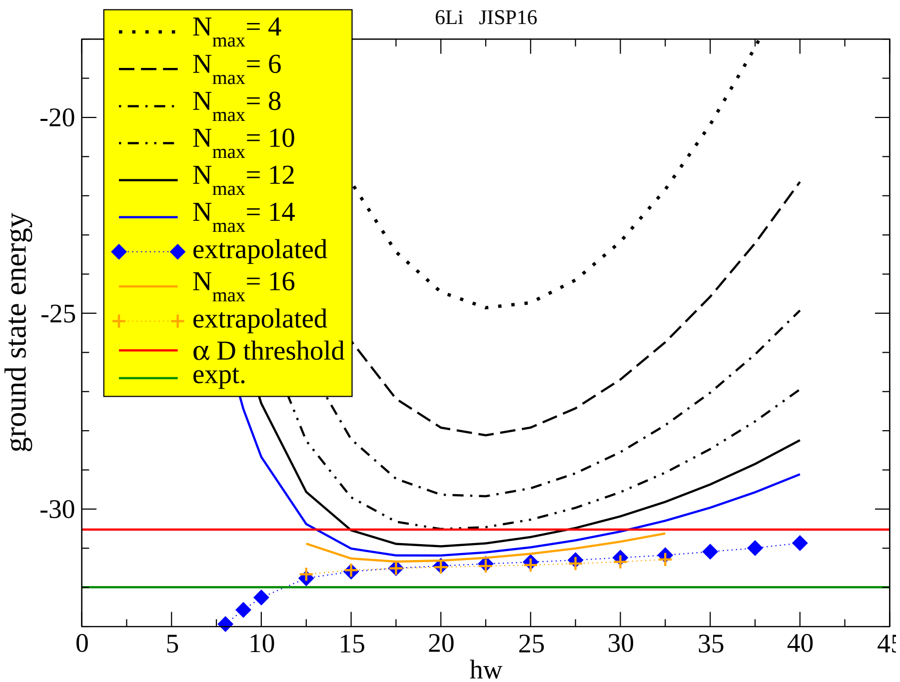
Maris, Shirokov, Vary, PRC79, 014308 (2009)

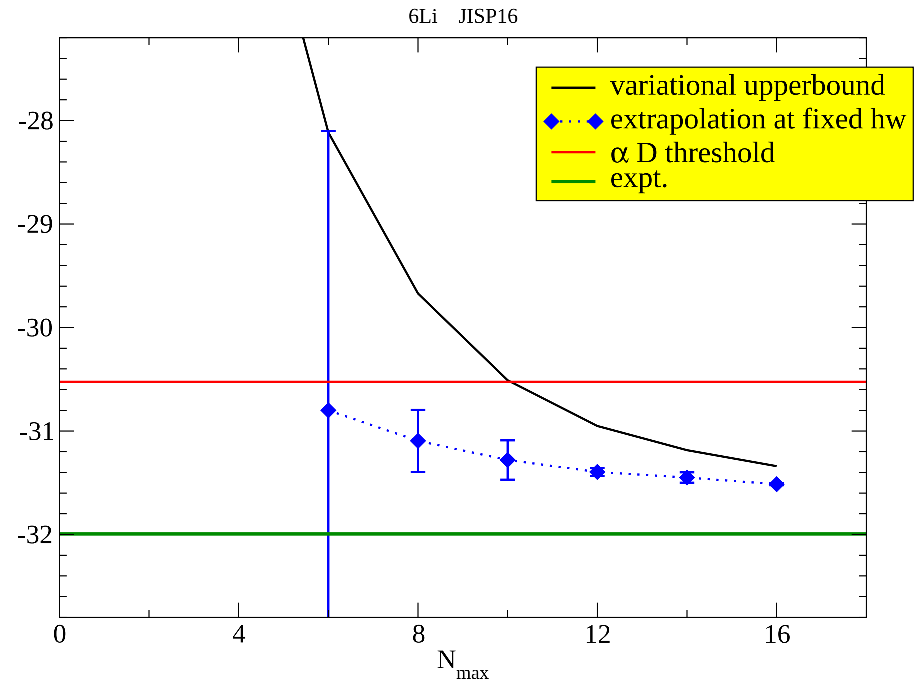
- Recent studies of IR and UV behavior
  - exponentials in $\sqrt{\hbar\omega/N}$ and $\sqrt{\hbar\omega N}$

Coon *et al*, arXiv:1205.3230;
Furnstahl, Hagen, Papen PRC86, 031301(R) (2012)

Extrapolating to complete basis – in practice

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



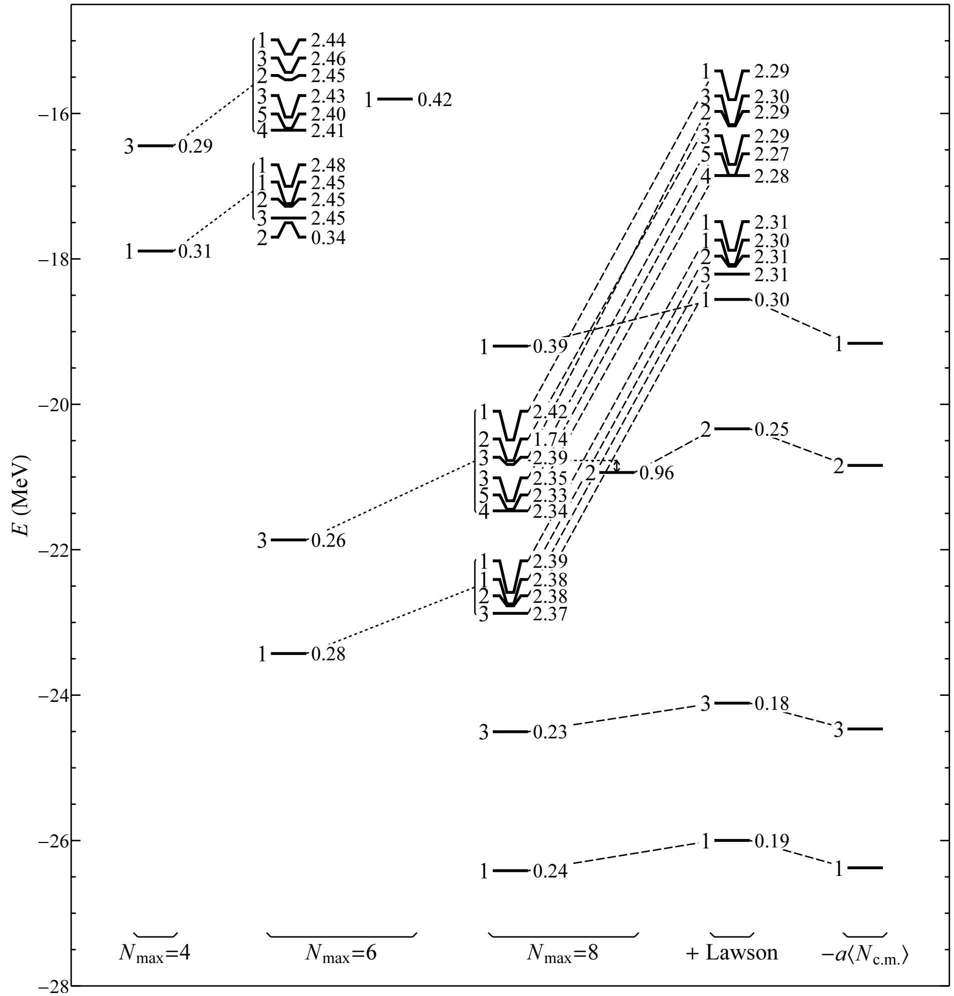


- H.O. basis up to $N_{\text{max}} = 16$: $E_b = -31.49(3)$ MeV
  Cockrell, Maris, Vary, PRC86 034325 (2012)
- Hyperspherical harmonics up to $K_{\text{max}} = 14$: $E_b = -31.46(5)$ MeV
  Vaintraub, Barnea, Gazit, PRC79 065501 (2009)

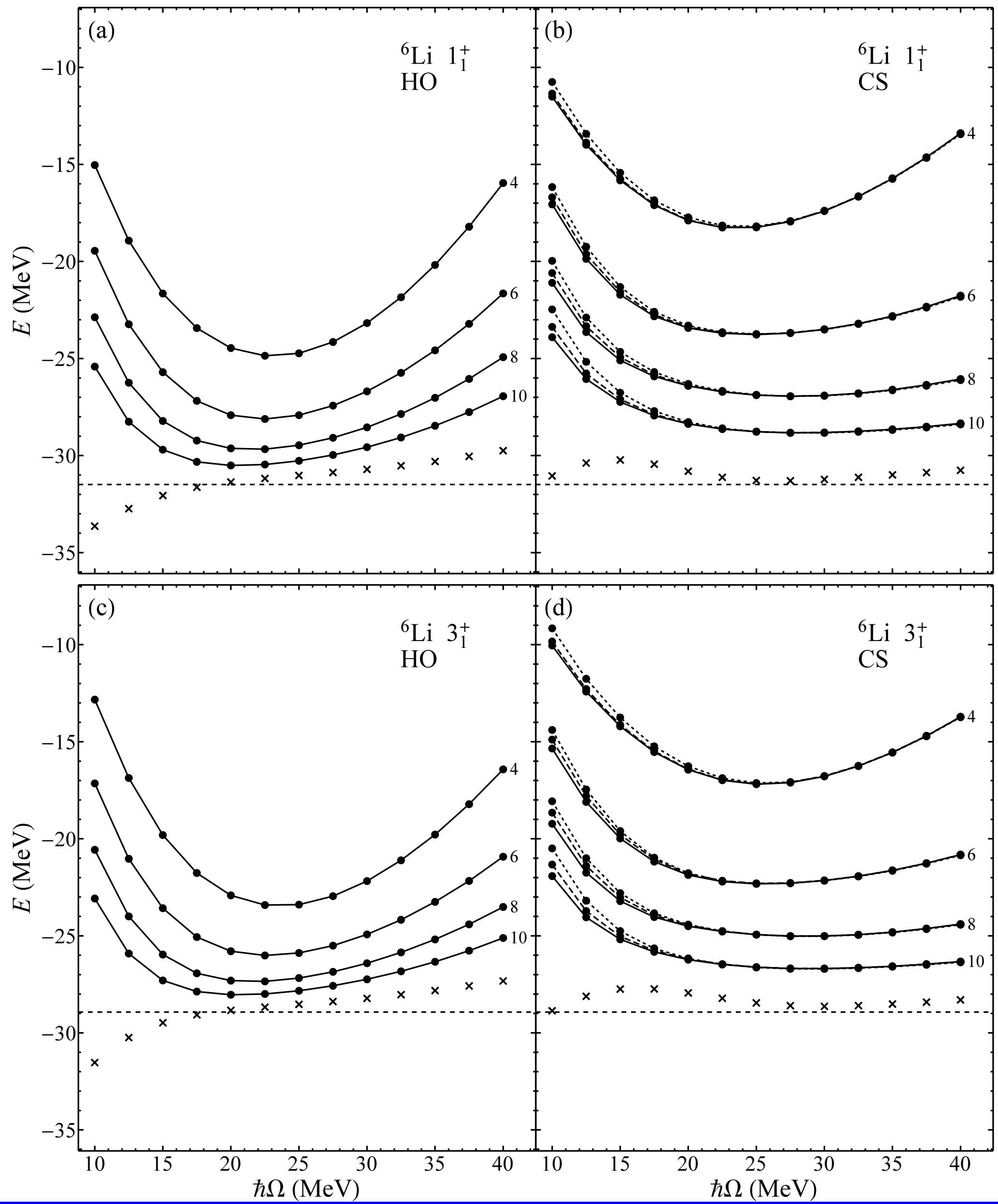
Accelerating convergence – Coulomb-Sturmian basis

Caprio, Maris, Vary, PRC86, 034312 (2012)

- Asymtotic behavior
  - H.O. basis $\exp(-a\,r^2)$
  - Coulomb–Sturmian basis $\exp(-c\,r)$
- Disadvantage
  - no exact factorization of Center-of-Mass motion
  - in practice, approximate factorization
    Hage, Papenbrock, Dean, PRL103, 062503 (2009)
  - can use Lagrange multiplier to remove spurious state



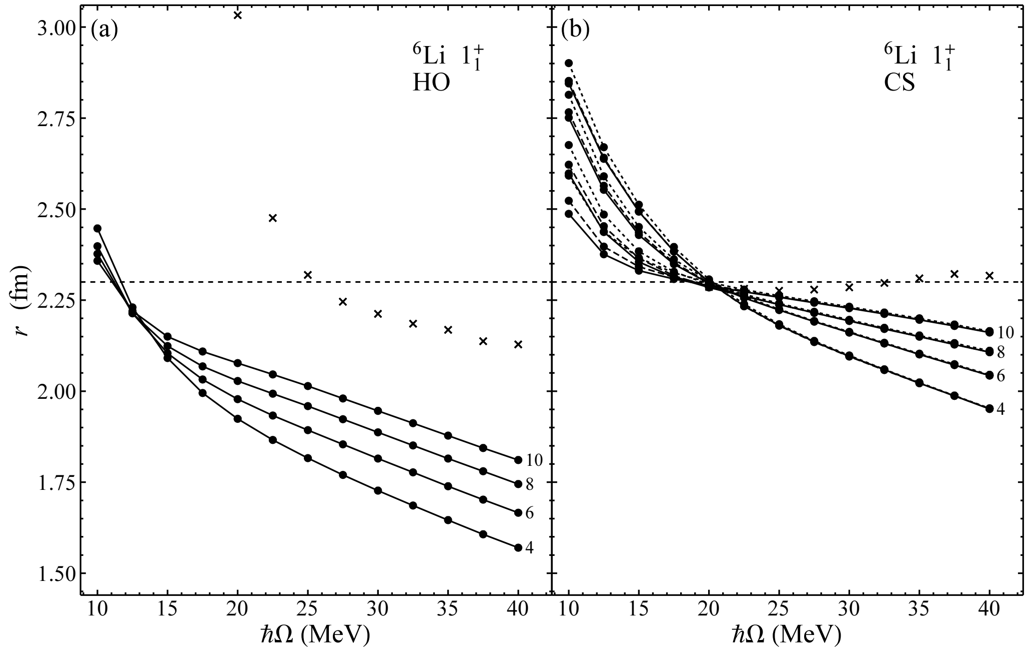
Coulomb-Sturmian – binding energies



- at $N_{\text{max}} = 4$ further from convergence than H.O. basis
- extrapolate to the same results as H.O. basis
- dashed line: extrapolated result from $N_{\text{max}} = 16$ calculations in H.O. basis
  Cockrell, Maris, Vary, PRC86 034325 (2012)

Coulomb-Sturmian – radius

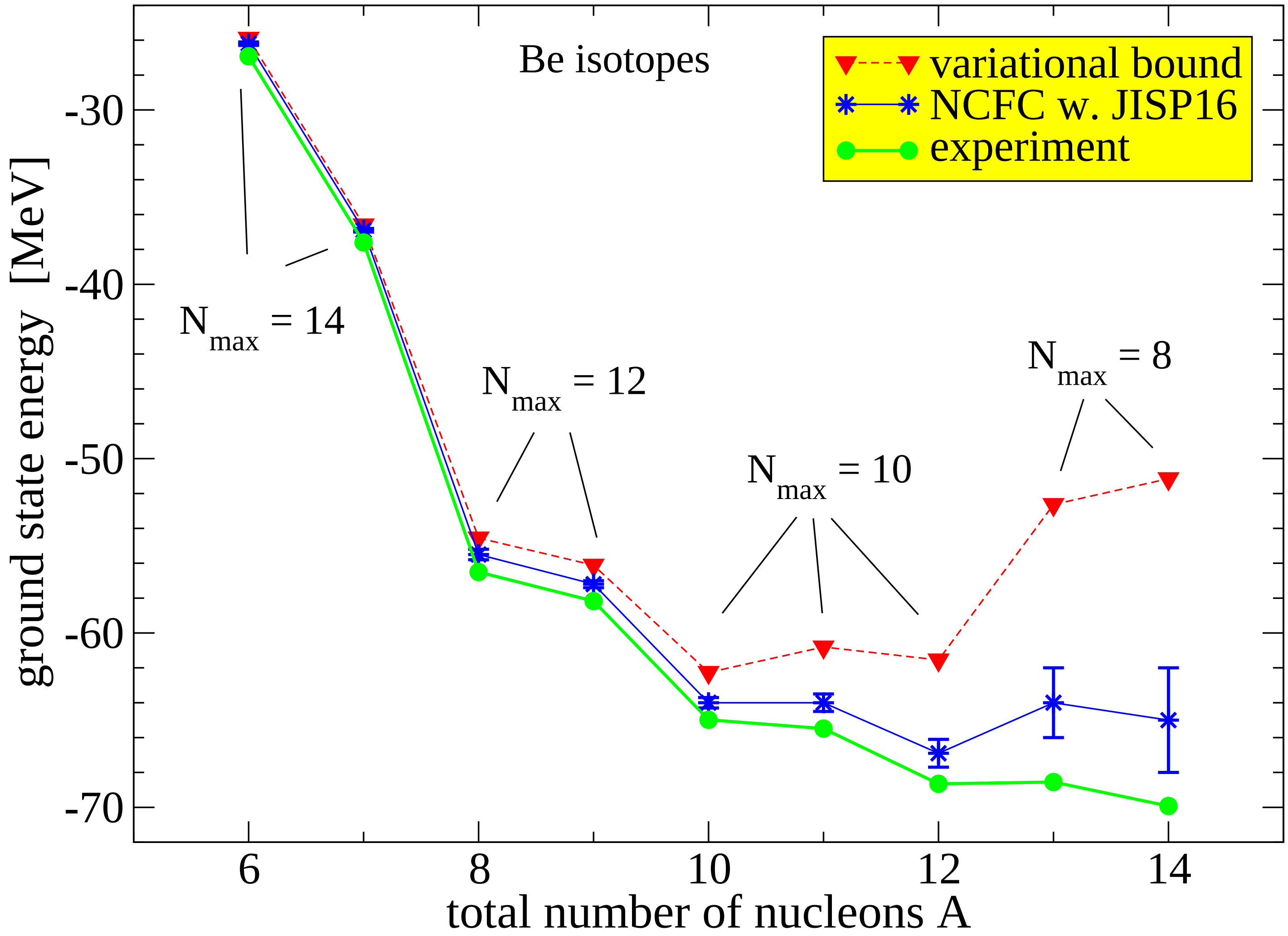
Caprio, Maris, Vary, PRC86, 034312 (2012)



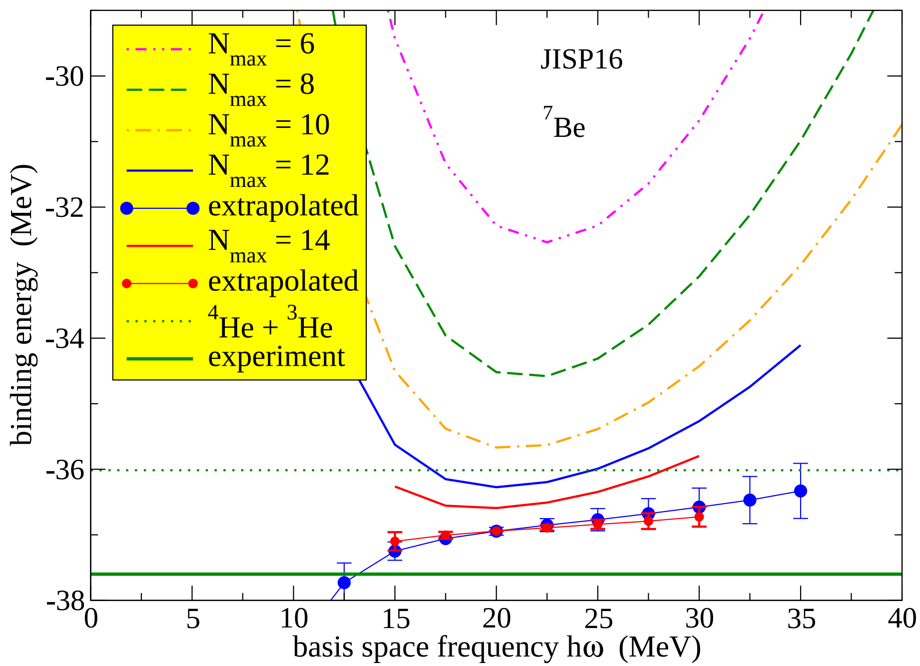
- exponential extrapolation does not work for radii in H.O. basis
- exponential extrapolation seems to work for radii in C.S. basis
- best estimate based on $N_{\text{max}} = 16$ H.O. calculations: 2.3 fm

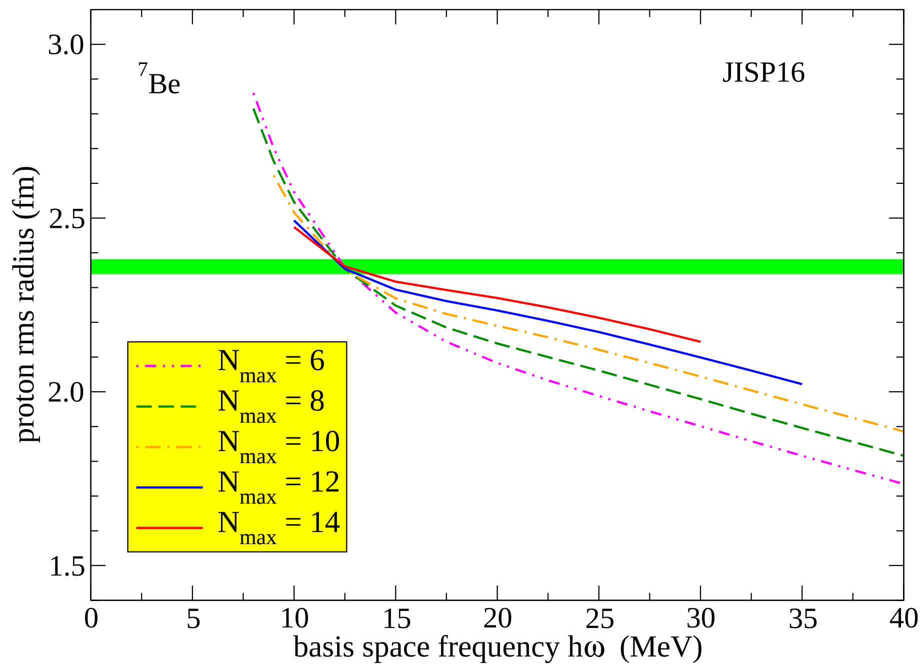
  Cockrell, Maris, Vary, PRC86 034325 (2012)
- experimental point-proton radius: 2.45 fm

Ground state energy Be-isotopes with JISP16



7Be – Ground state properties



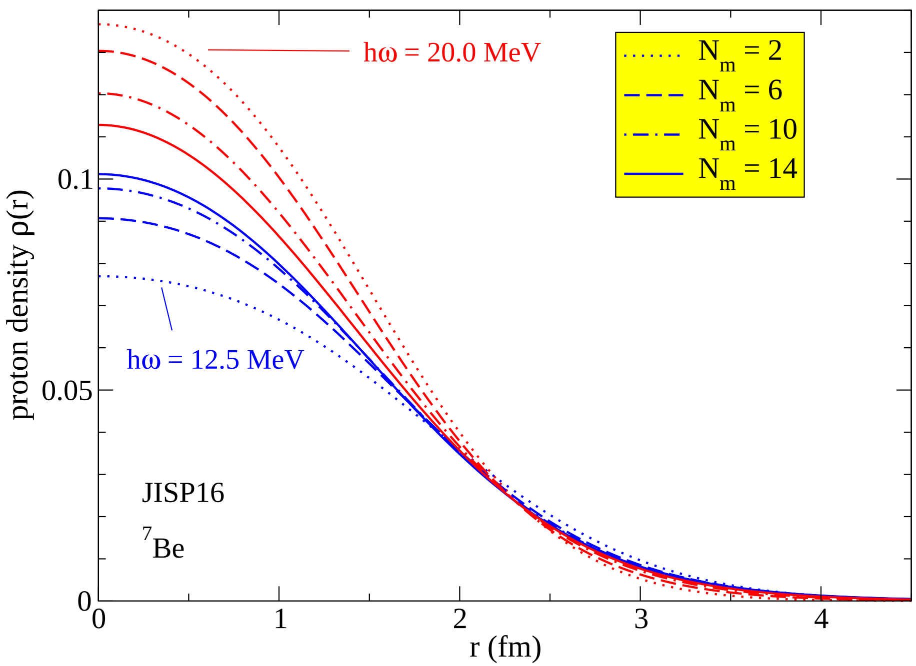


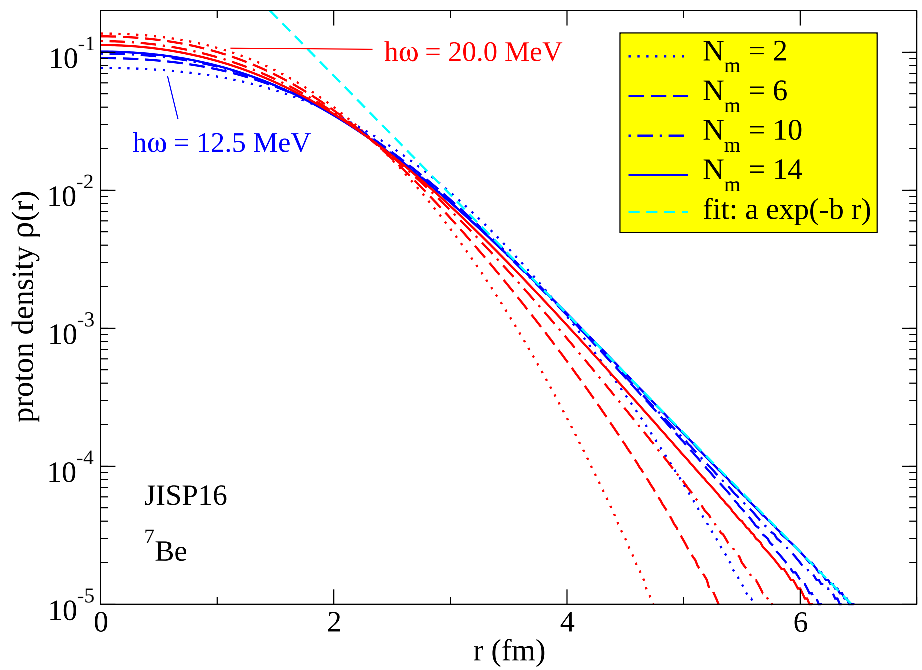
- Binding energy converges monotonically, with optimal H.O. freuqency around $\hbar\omega = 20$ MeV to 25 MeV
- Ground state about 0.7 MeV underbound with JISP16
- Proton point radius does not converge monotonically
  - Coulomb–Sturmian basis likely to improve convergence

7Be – Proton density

- Translationally-invariant density – center-of-mass motion taken out

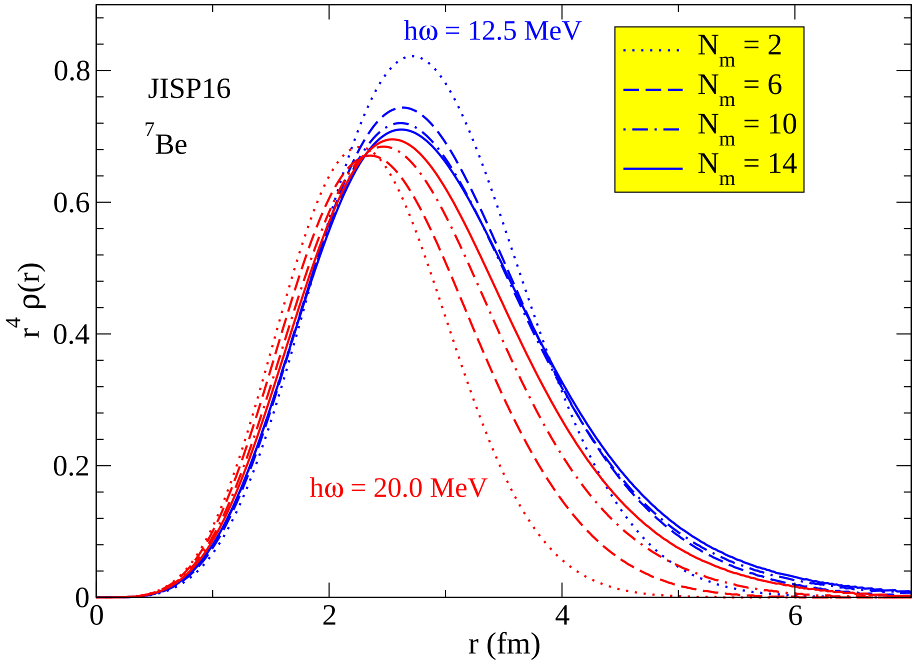
w. Cockrell, PhD thesis 2012

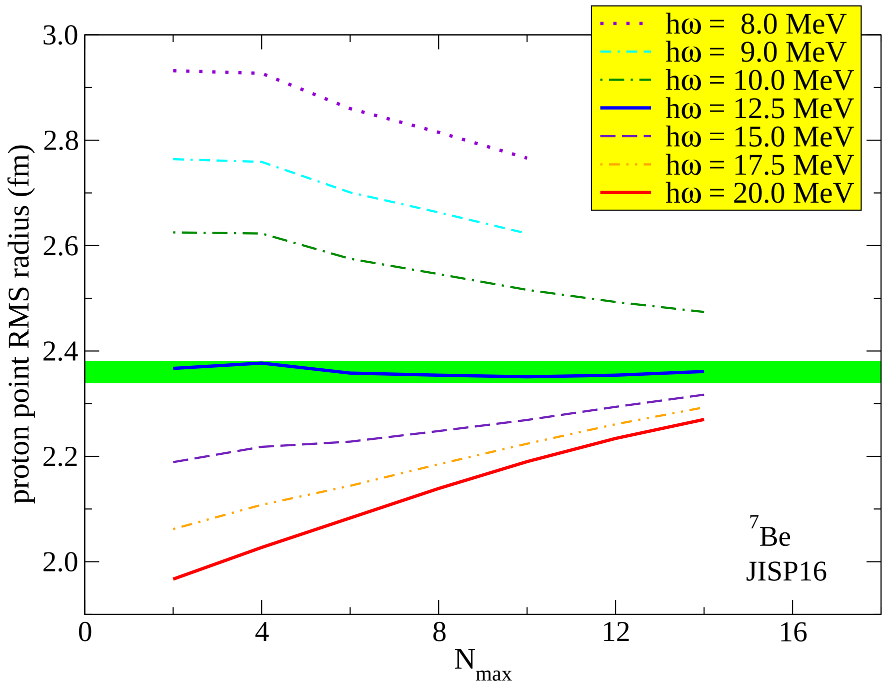




- Slow build up of asymptotic tail of wavefunction
- Proton density appears to converge more rapidly at $\hbar\omega = 12.5$ MeV than at 20 MeV because long-range part of wavefunction is better represented with smaller H.O. parameter

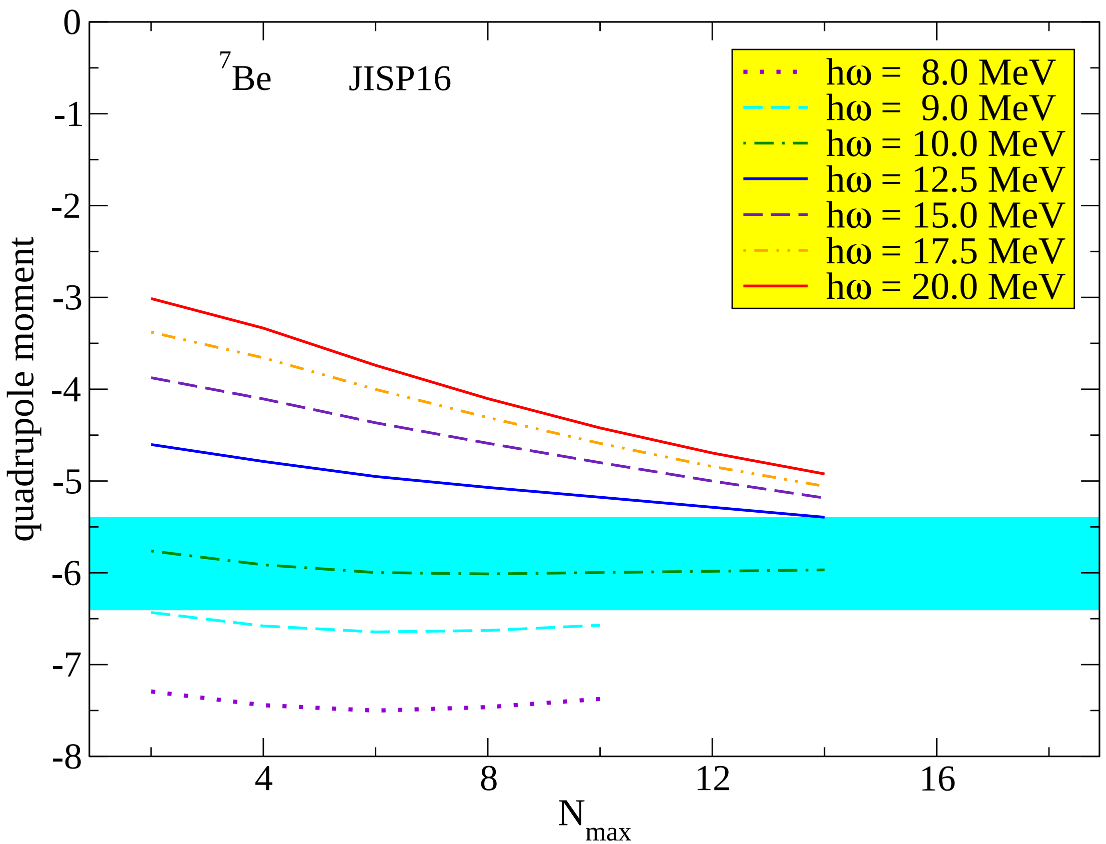
7Be – Proton radius





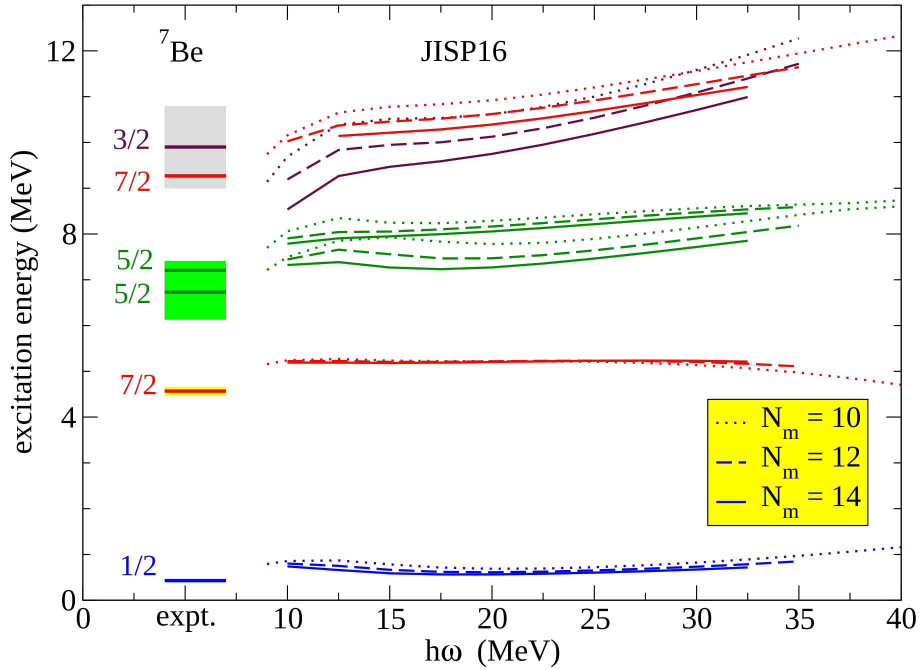
- Calculation one-body observables $\langle i|\mathcal{O}|j\rangle \sim \int \mathcal{O}(r)\, r^2\, \rho_{ij}(r)\, dr$
- RMS radius: $\mathcal{O}(r) = r^2$
- Slow convergence of RMS radius due to slow build up of asymptotic tail
- Ground state RMS radius in agreement with data

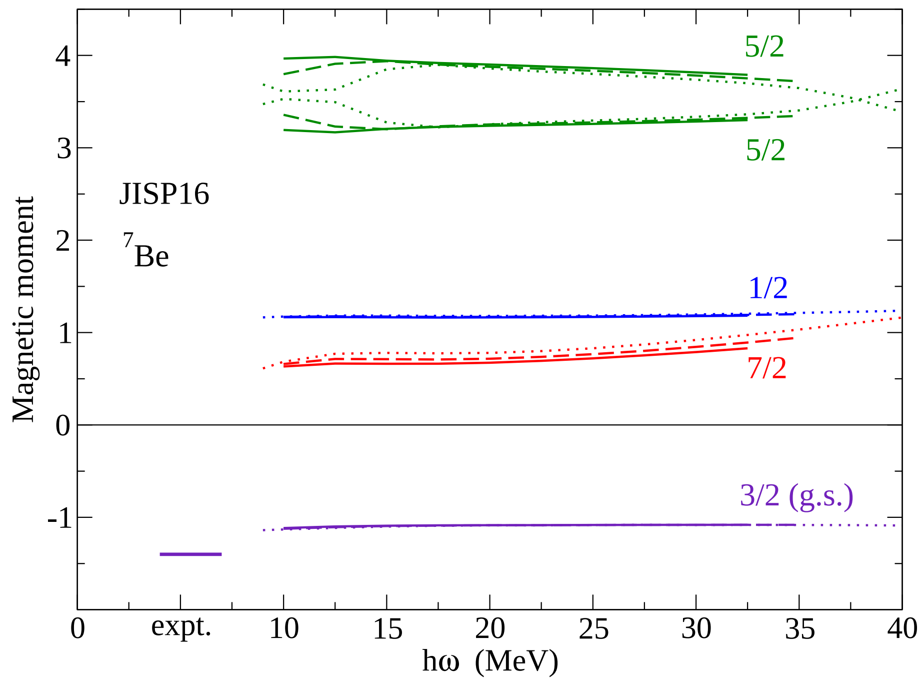
7Be – Quadrupole moment



- Ground state quadrupole moment in agreement with data
- Optimal basis space around $\hbar\omega = 10$ MeV to 12 MeV
- Similar slow convergence for E2 transitions

7Be – Excited states

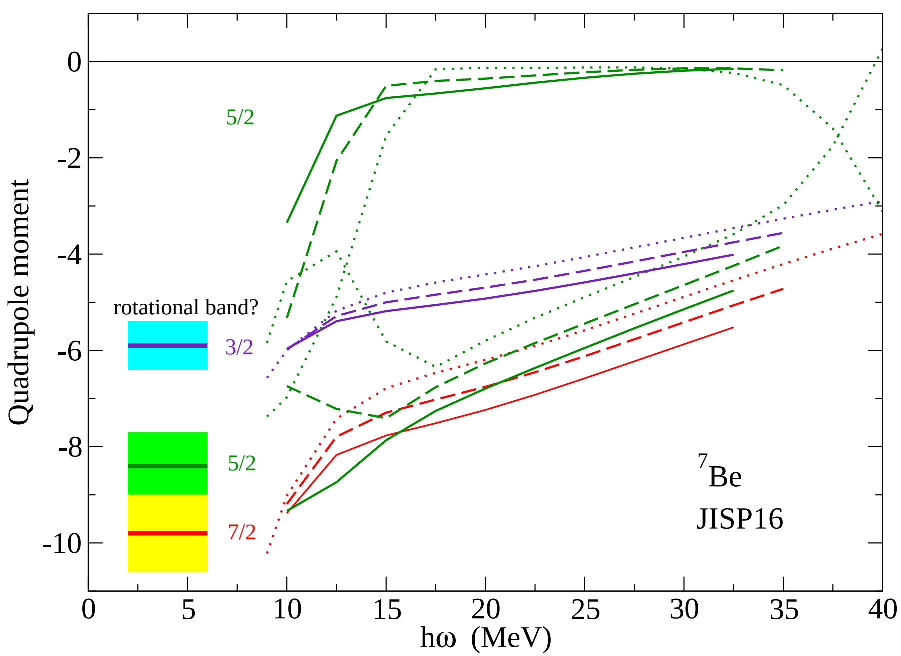


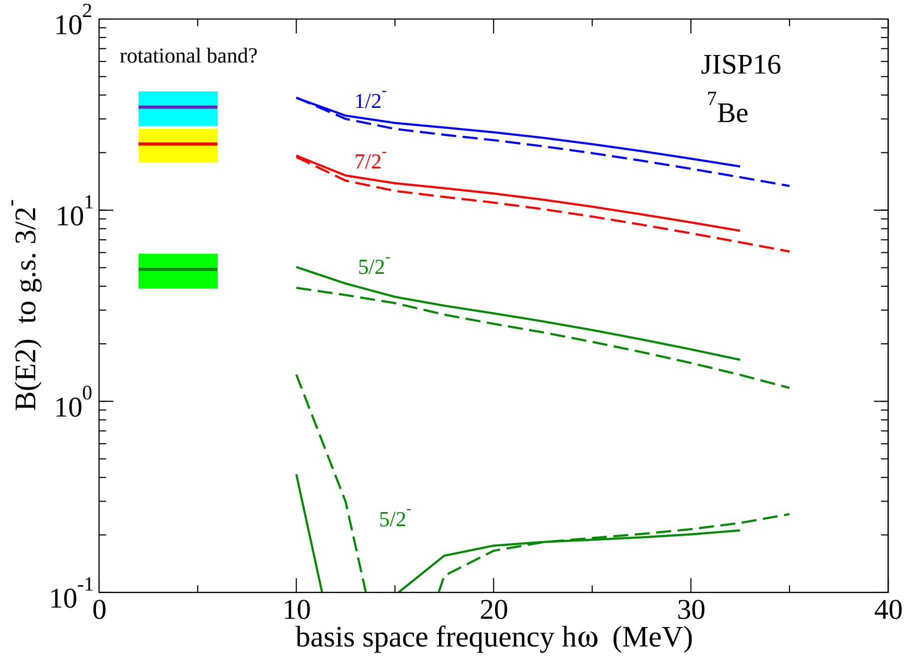


- Excitation energy of narrow states
  - converge rapidly
  - agree with experiments
- Broad resonances depend $\hbar\omega$
- Magnetic moments well converged
  - 2-body currents needed for agreement with data (meson-exchange currents)

7Be – Emergence of rotational band? *in progress, w. M. Caprio*

E2 observables suggest rotational structure for $\frac{3}{2}$, $\frac{1}{2}$, $\frac{7}{2}$, $\frac{5}{2}$ states





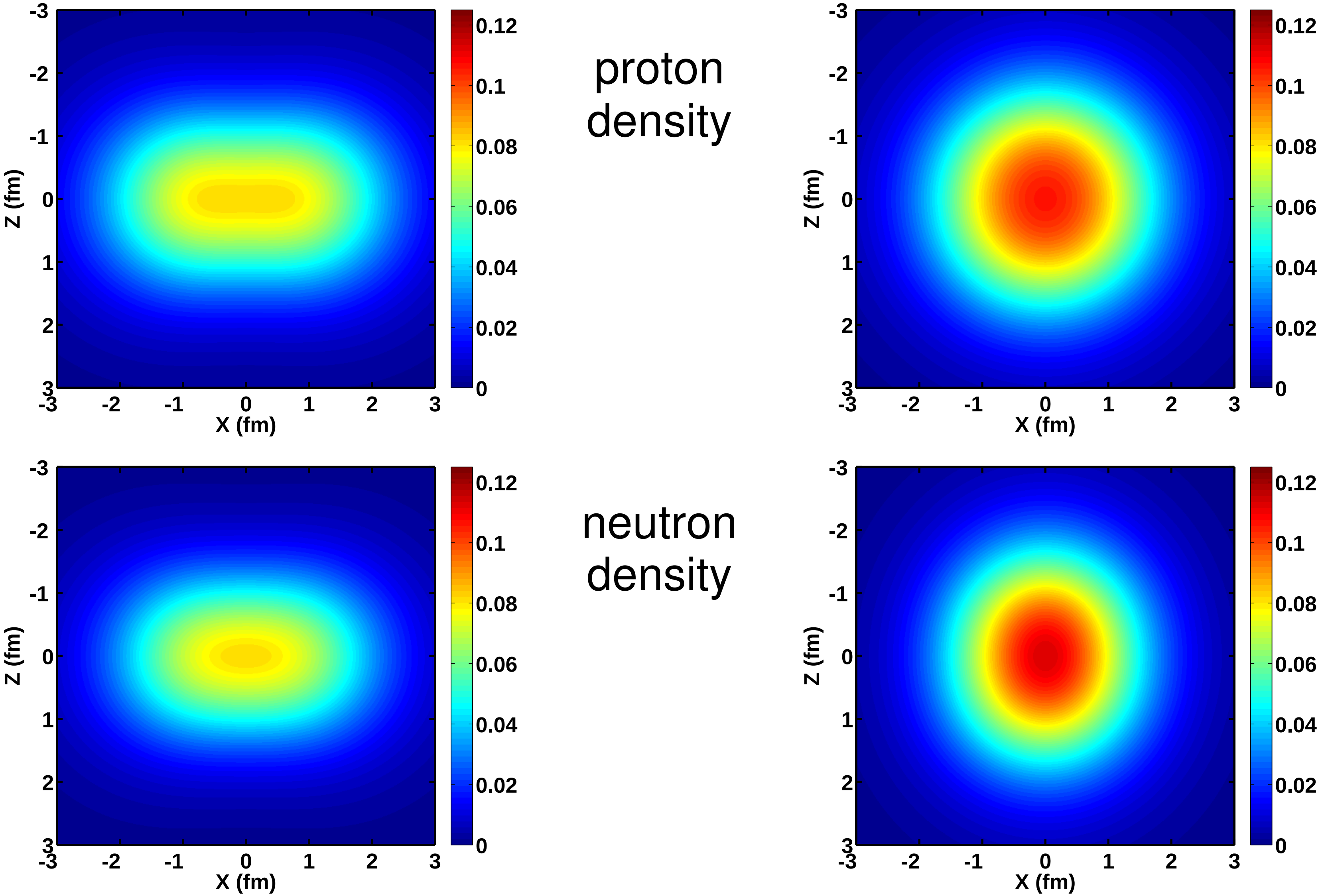
$$Q(J) = \frac{\frac{3}{4} - J(J+1)}{(J+1)(2J+3)} Q_0$$

$$B(E2; i \to f) = \frac{5}{16\pi} Q_0^2 \left(J_i, \frac{1}{2}; 2, 0 \middle| J_f, \frac{1}{2} \right)^2$$

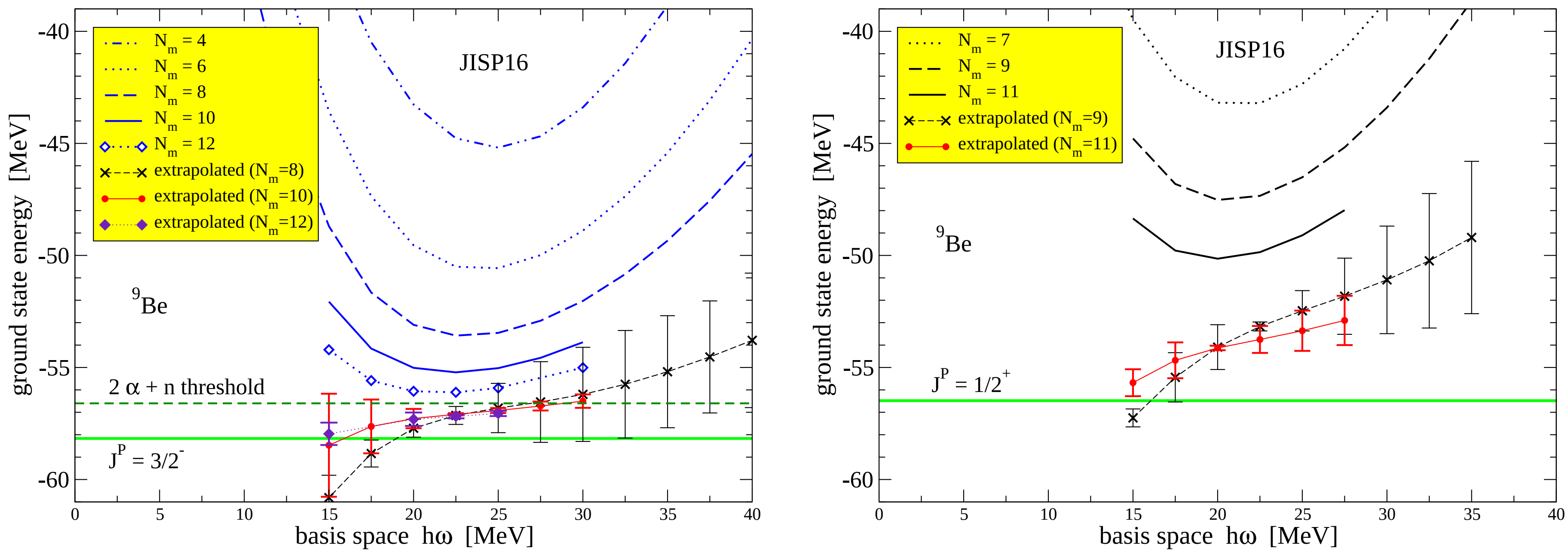
7Be – Structure of $(\frac{5}{2}^-, \frac{1}{2})_1$ (broad) and $(\frac{5}{2}^-, \frac{1}{2})_2$ (narrow) states

Translationally-invariant nucleon densities

Cockrell, PhD thesis 2012

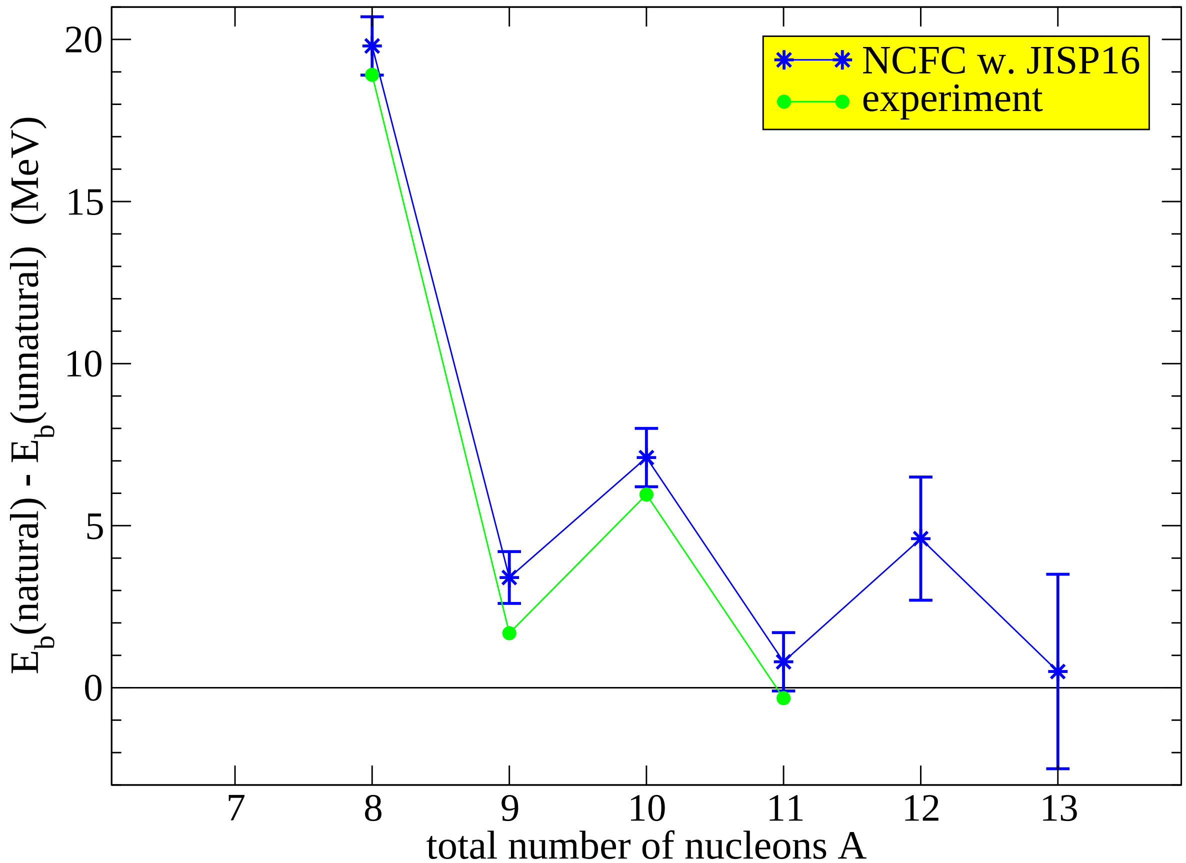


9Be – Ground state properties



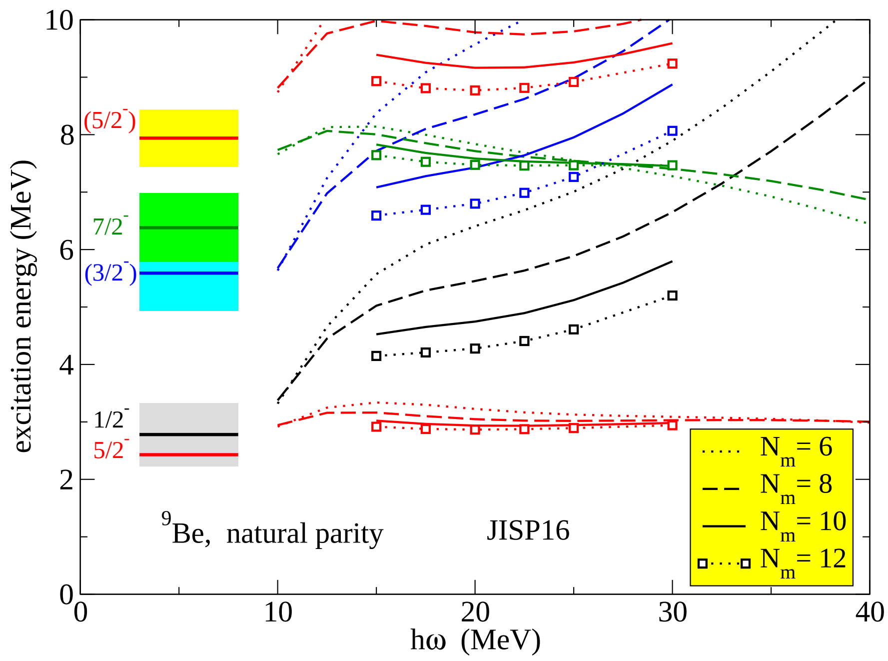
- Convergence pattern natural and unnatural parity looks similar
- Ground state about 1.0 ± 0.2 MeV underbound with JISP16
- Lowest unnatural parity state underbound by about 2.7 ± 0.8 MeV
  - need next basis space for unnatural parity
  - need improved interaction?

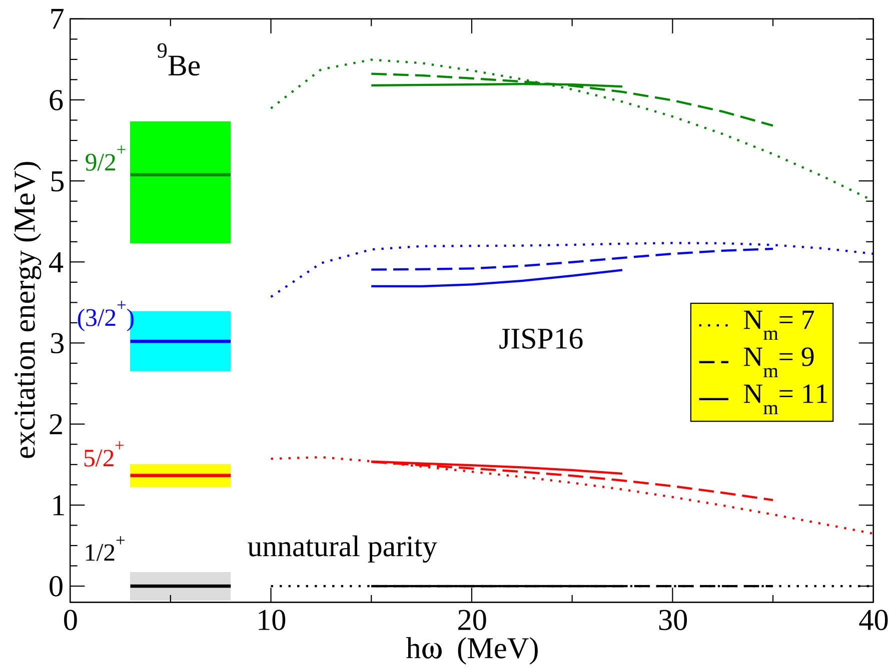
Positive vs. negative parity states of Be-isotopes



- Unnatural parity states systematically underbound by about 1 MeV to 2 MeV compared to lowest natural parity states
  - interaction JISP16 not good enough?
  - difference in convergence of pos. and neg. parity states?

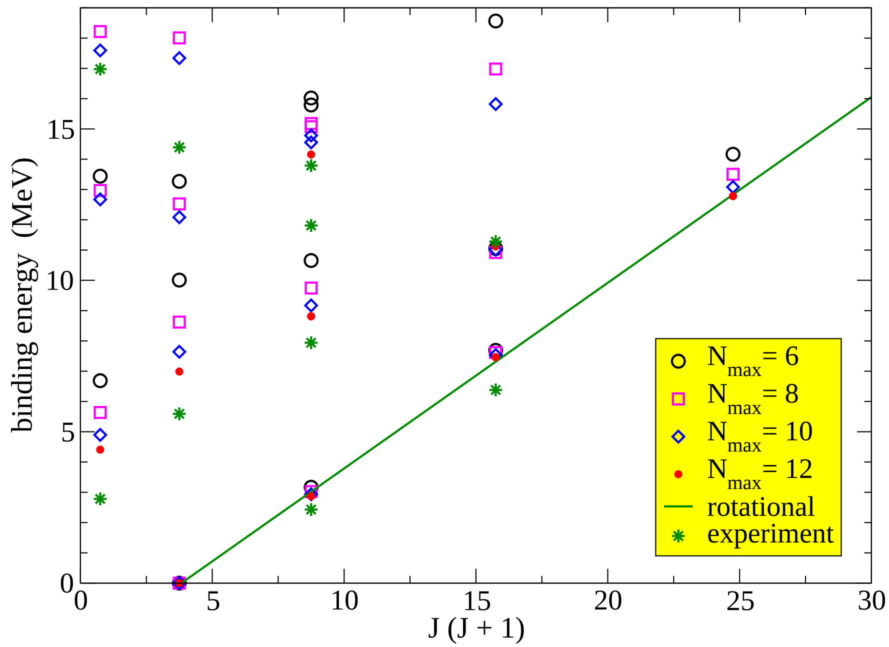
9Be – Positive and negative spectrum

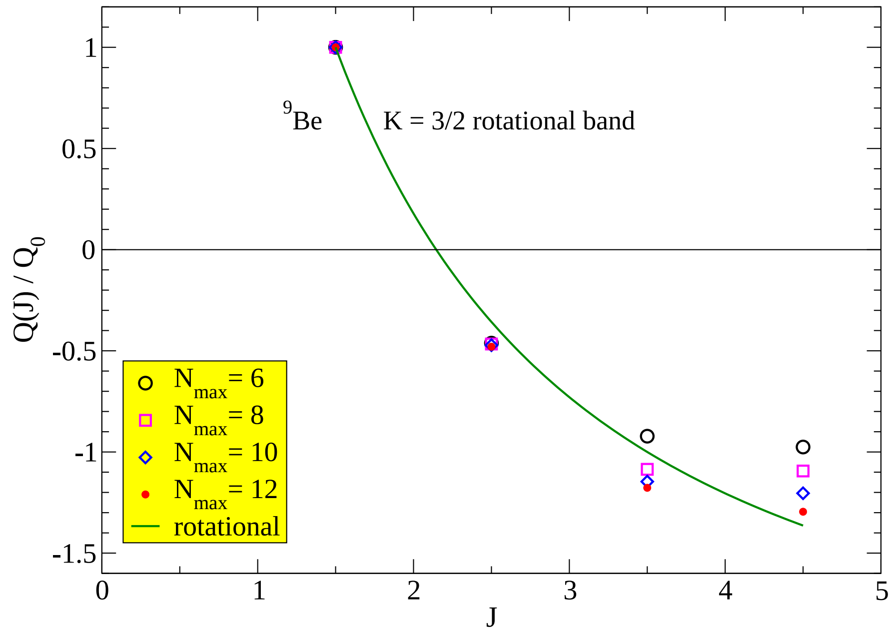




- Excitation energy $\frac{5}{2}^-$ at 3 MeV well converged (narrow)
- Excitation energy $\frac{7}{2}^-$ reasonably converged
- Excitation energies broad neg. parity not well converged
- Excitation energies pos. parity well converged

9Be – Emergence of rotational bands *in progress, w. M. Caprio*



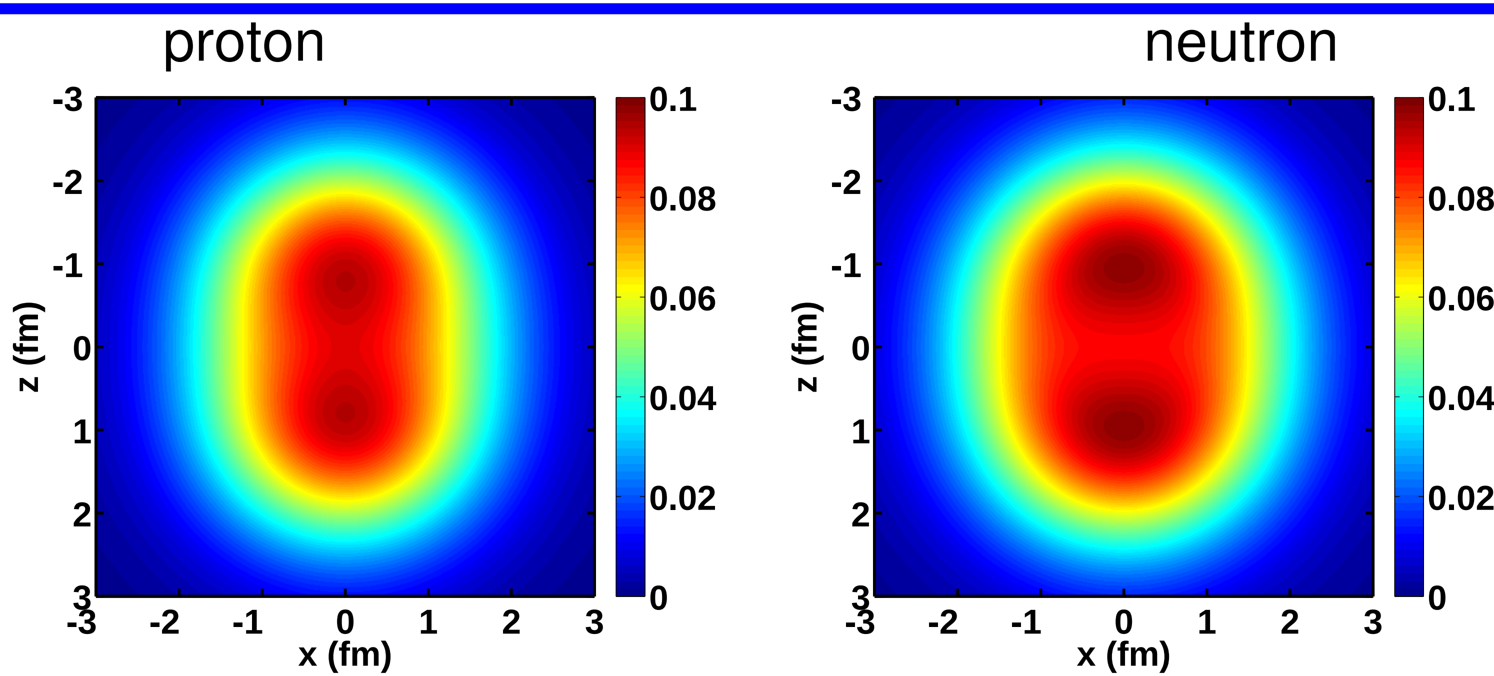


- Rotational energy for states with axial symmetry $E(J) \propto J(J+1)$
- Quadrupole moments for rotational band

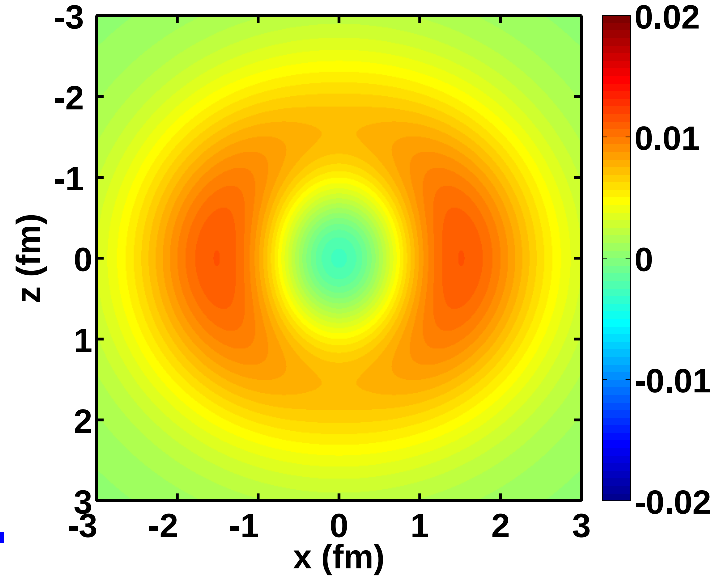
$$Q(J) \quad = \quad \frac{3\,K^2 - J(J+1)}{(J+1)(2J+3)}\,Q_0$$

- Quadrupole moments not converged, but ratio of quadrupole moments agree with rotational band structure

9Be – Structure: Density $(\frac{3}{2}^-, \frac{1}{2})$ ground state



and their difference

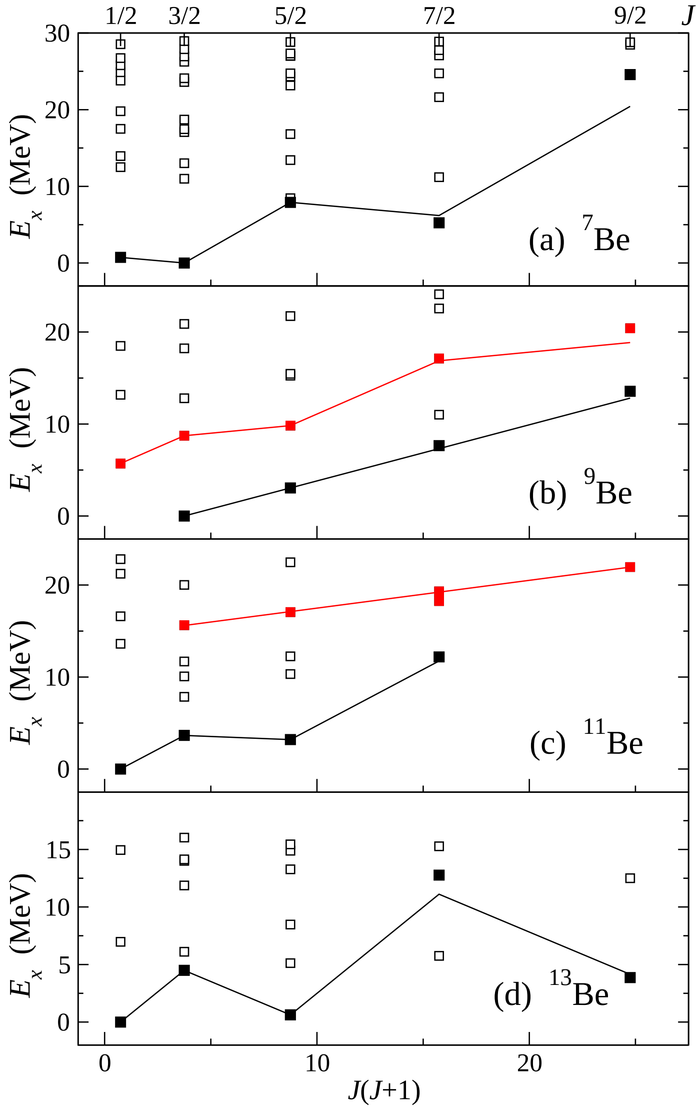


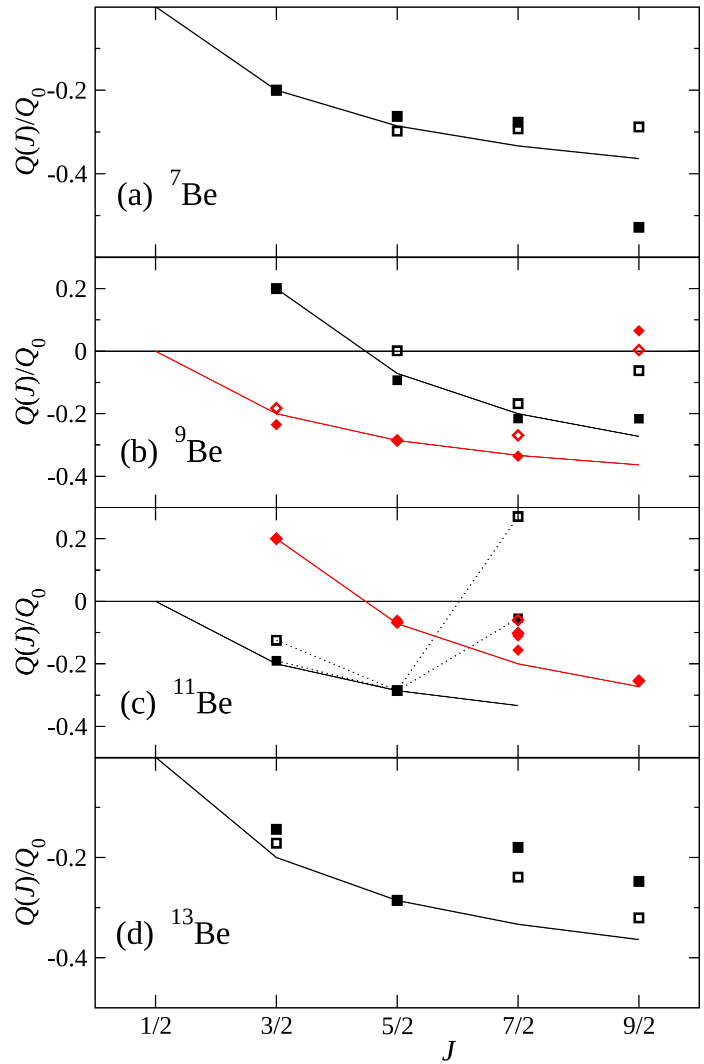
Translationally-invariant proton and neutron densities

Chase Cockrell, PhD thesis, 2012

- Emergence of α clustering?

Rotational bands odd Be isotopes *in preparation, w. M. Caprio*

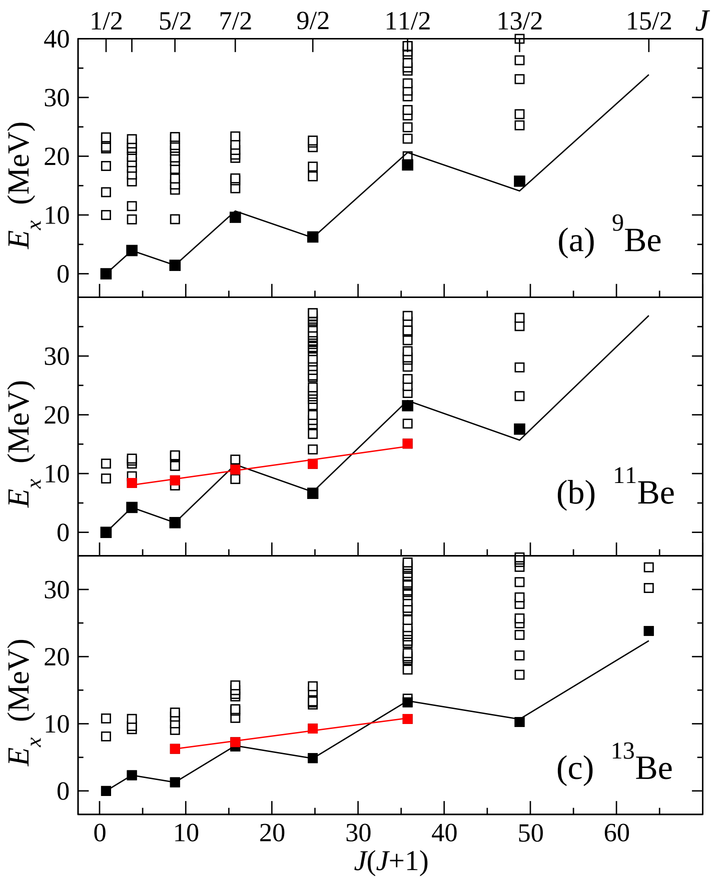


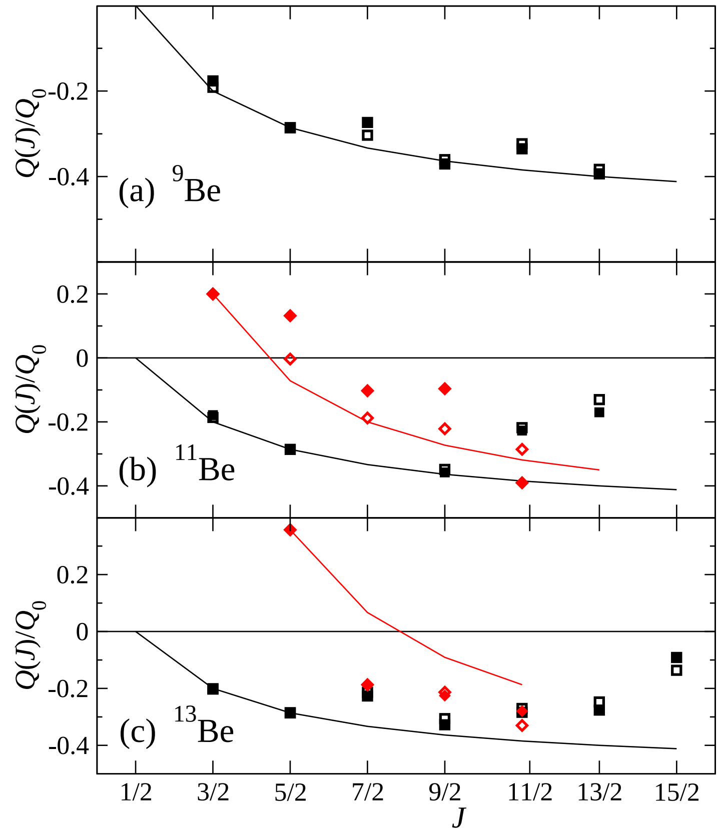


- Quadrupole moments not converged, but ratio of quadrupole moments agree with rotational band structure

Rotational bands odd Be isotopes *in preparation, w. M. Caprio*

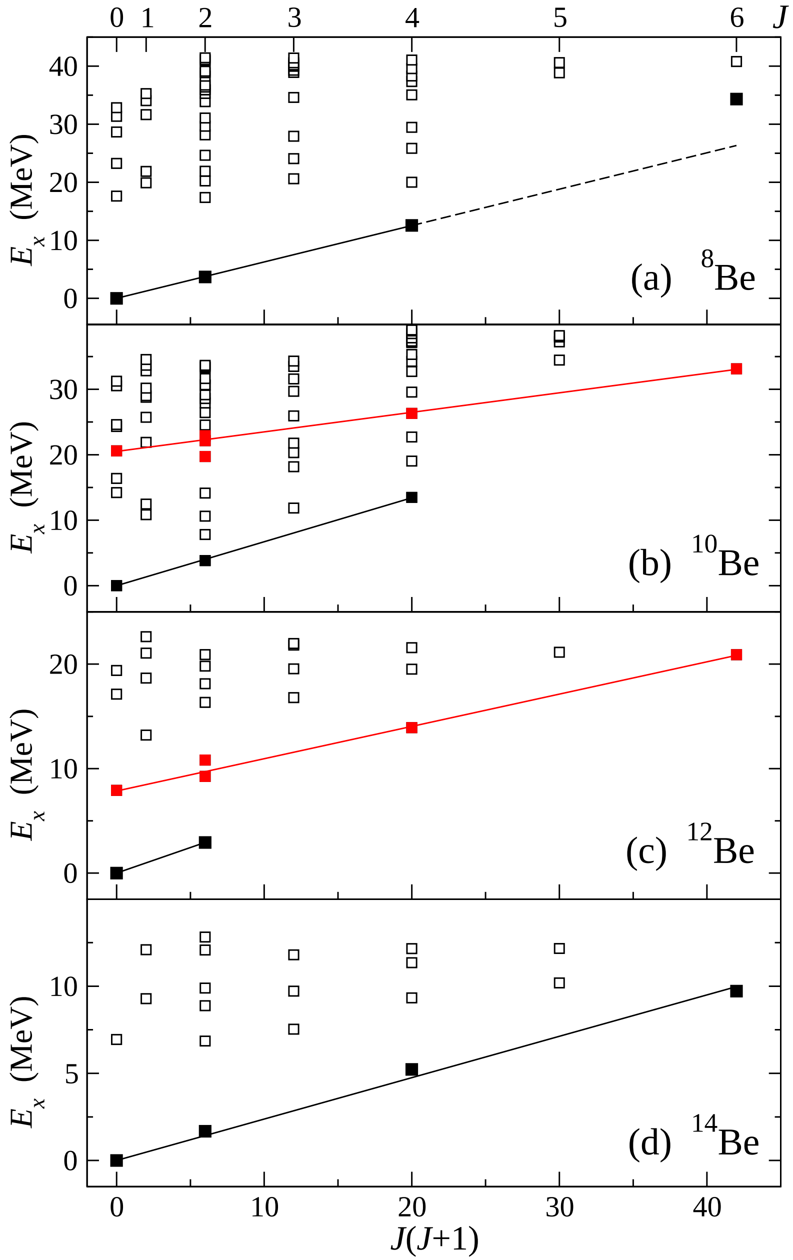
- Also for the unnatural parity states

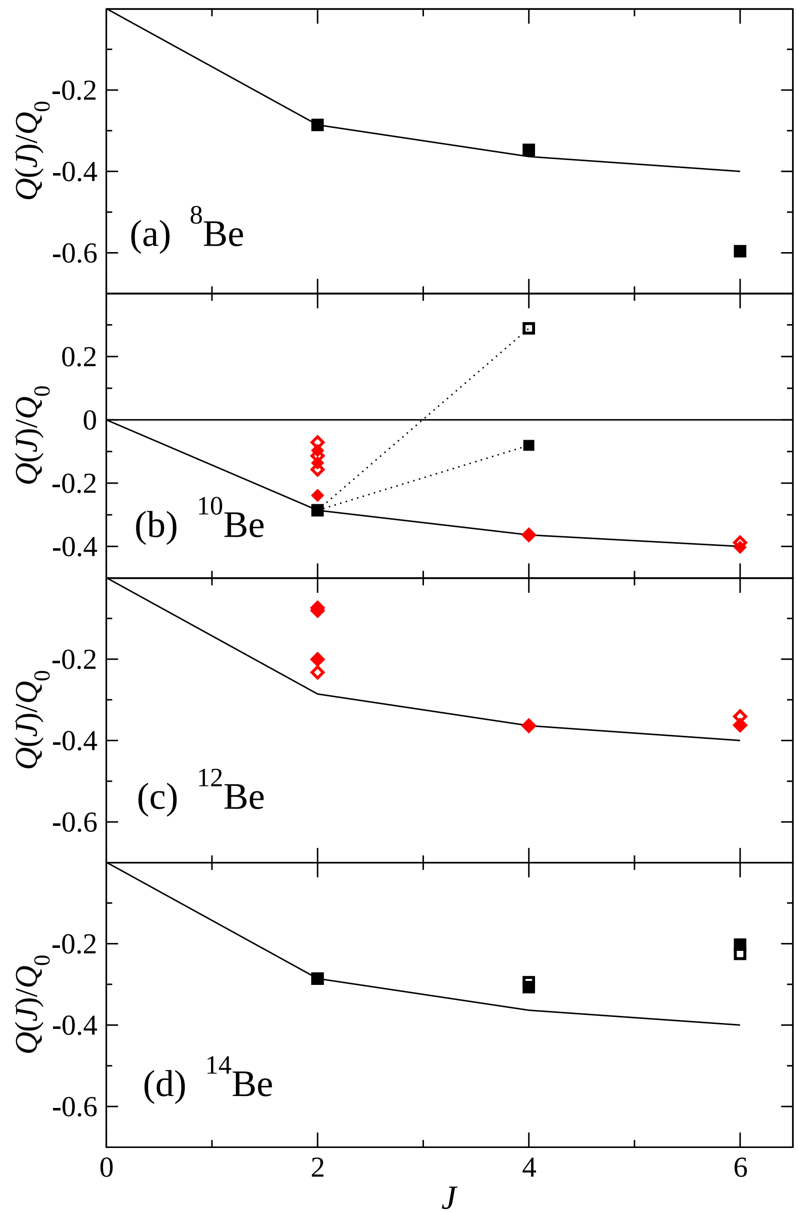




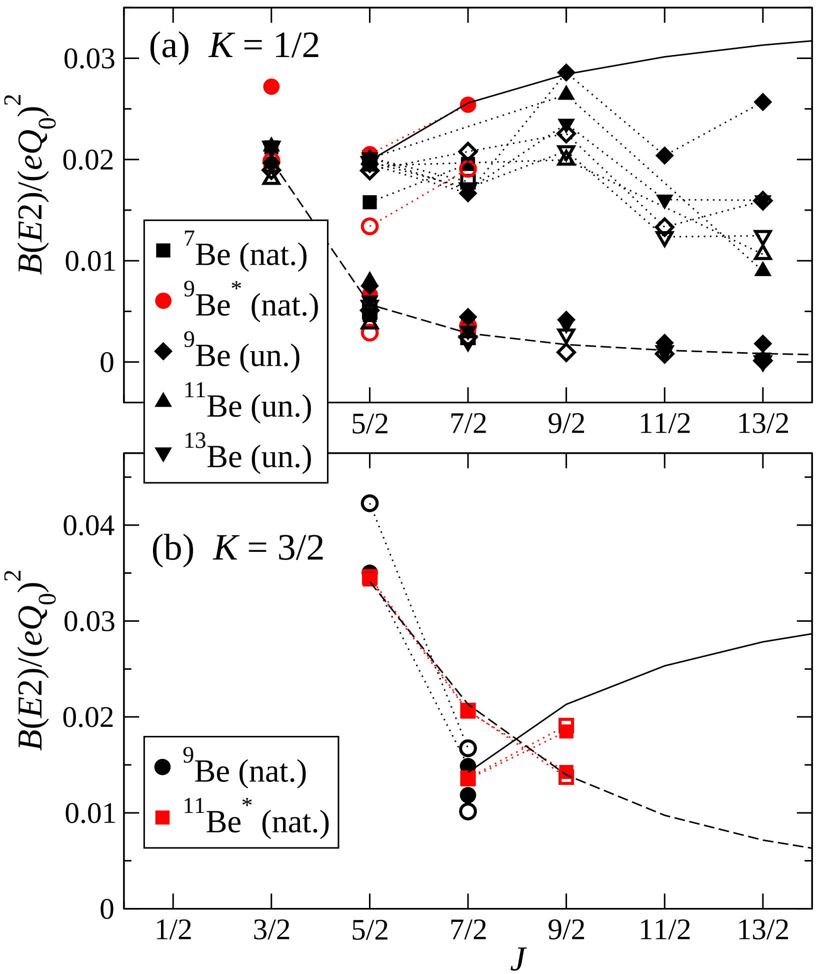
- Quadrupole moments not converged, but ratio of quadrupole moments agree with rotational band structure

Rotational bands even Be isotopes *in preparation, w. M. Caprio*

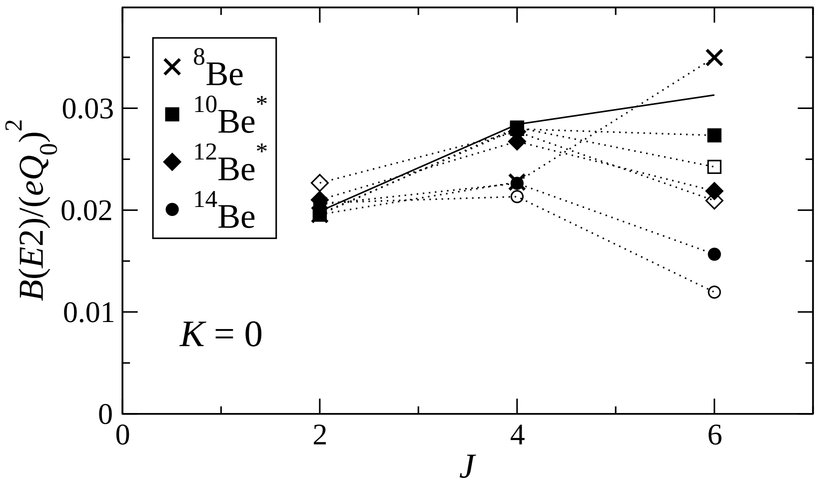




B(E2) transistions Be isotopes *in preparation, w. M. Caprio*



- Rotor prediction
  - $\Delta_J = 1$: dashed
  - $\Delta_J = 2$: solid



- Ratio's B(E2)/Q^2 in agreement with rotational structure as well

Conclusions

- No-core Configuration Interaction nuclear structure calculations
  - Binding energy, spectrum
  - $\langle r^2 \rangle$, μ, $\mathcal{Q}$, transitions, wfns, one-body densities
- Main challenge: construction and diagonalization of extremely large (D > 1 billion) sparse matrices
- Need realistic basis function to improve convergence $\langle r^2 \rangle$, $\mathcal{Q}$
- JISP16
  - Nonlocal phenomenological 2-body interaction
  - Good description of a range of light nuclei
  - Rapid convergence for binding energies
  - Emergence of rotational bands and clustering in Be-isotopes
- Would not have been possible without collaboration with applied mathematicians and computer scientists
  Aktulga, Yang, Ng (LBNL); Çatalyürek, Saule (OSU); Sosonkina (ODU/AL)