Emergence of rotational bands in light nuclei from No-Core CI calculations

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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

No-Core Configuration Interaction calculations

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

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 wavefunction of A nucleons

$$\hat{\mathbf{H}}\,\Psi(r_1, \ldots, r_A) = \lambda\,\Psi(r_1, \ldots, r_A)$$

- Expand wavefunction in basis states $|\Psi\rangle = \sum a_i |\Phi_i\rangle$
- Diagonalize Hamiltonian matrix $H_{ij} = \langle\Phi_j|\hat{\mathbf{H}}|\Phi_i\rangle$
- No-Core CI: all A nucleons are treated the same
- Complete basis $\longrightarrow$ exact result
- In practice
  - truncate basis
  - study behavior of observables as function of truncation

Basis expansion $\Psi(r_1, \ldots, r_A) = \sum a_i \Phi_i(r_1, \ldots, r_A)$

- Many-Body basis states $\Phi_i(r_1, \ldots, r_A)$ Slater Determinants
- Single-Particle basis states $\phi_{ik}(r_k)$ quantum numbers n, l, s, j, m_j
- Radial wavefunctions: Harmonic Oscillator, Wood–Saxon, Coulomb–Sturmian, Berggren (for resonant states)
- M-scheme: Many-Body basis states eigenstates of $\hat{\mathbf{J}}_\mathbf{z}$

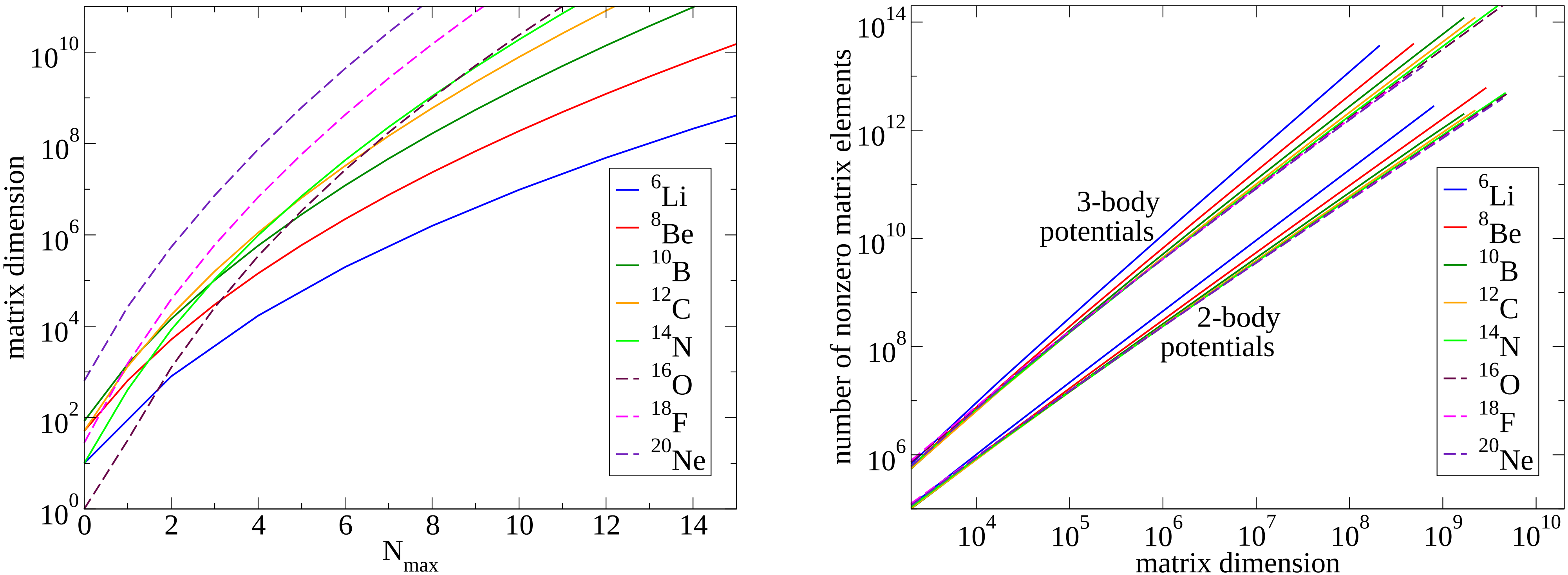
$$\hat{\mathbf{J}}_\mathbf{z}|\Phi_i\rangle \quad = \quad M|\Phi_i\rangle \quad = \sum_{k=1}^{A} m_{ik}|\Phi_i\rangle$$

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

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

- Alternatives:
  - Full Configuration Interaction (single-particle basis truncation)
  - 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)

NCCI calculations – main challenge



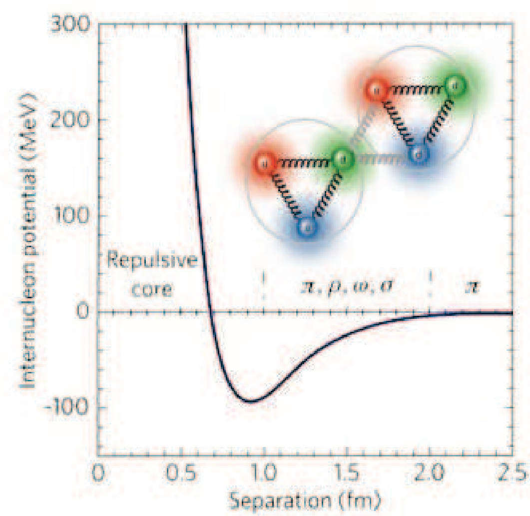
- Increase of basis space dimension with increasing A and N_{max}
  - need calculations up to at least $N_{\text{max}} = 8$ for meaningful extrapolation and numerical error estimates
- More relevant measure for computational needs
  - number of nonzero matrix elements
  - current limit 10^{13} to 10^{14}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

Nuclear interaction

Nuclear potential not well-known,

though in principle calculable from QCD

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



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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Physics Letters B 644 (2007) 33–37

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Realistic nuclear Hamiltonian: Ab exitu approach

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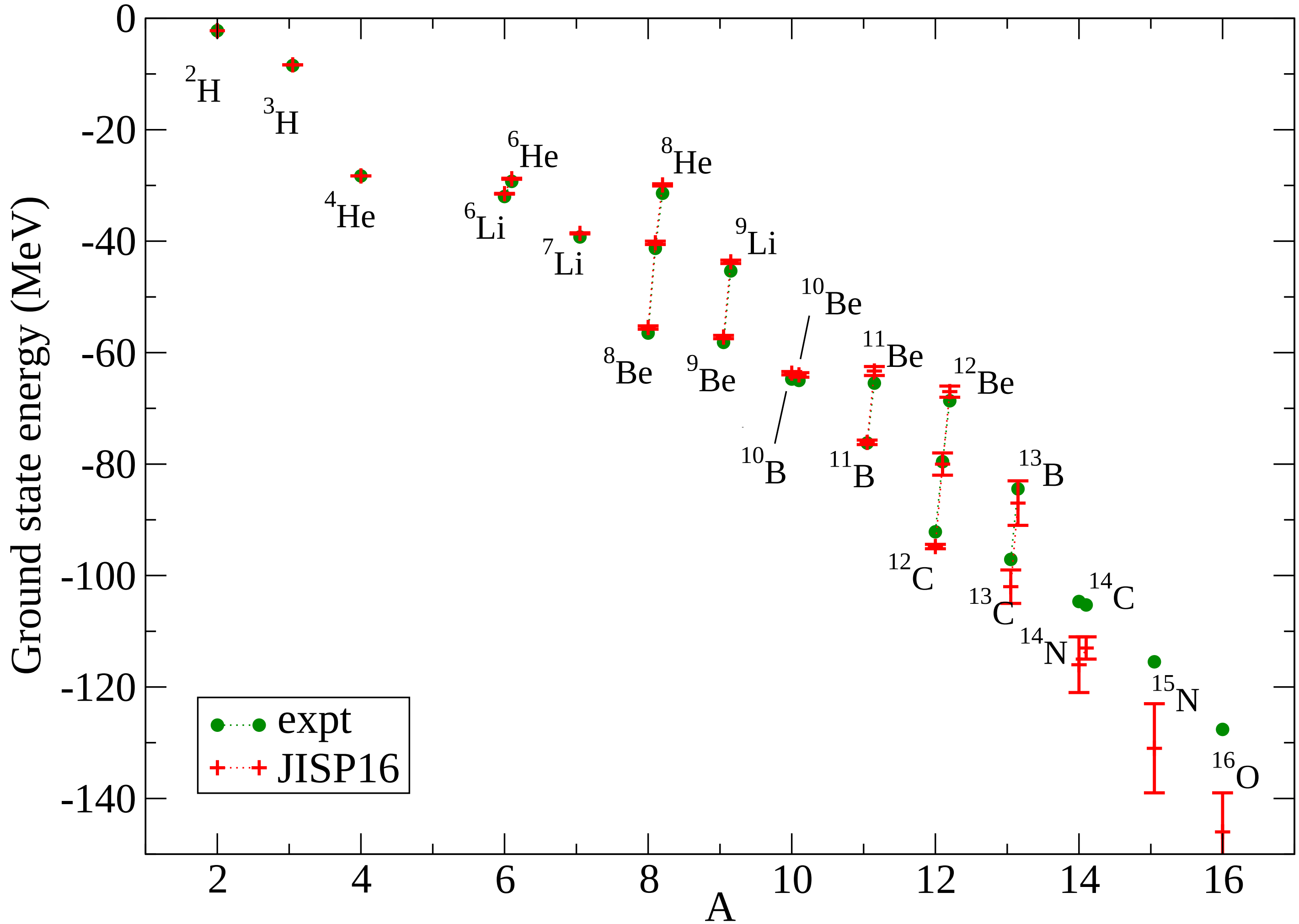
Received 6 March 2006; received in revised form 11 September 2006; accepted 30 October 2006

Ground state energy of p-shell nuclei with JISP16

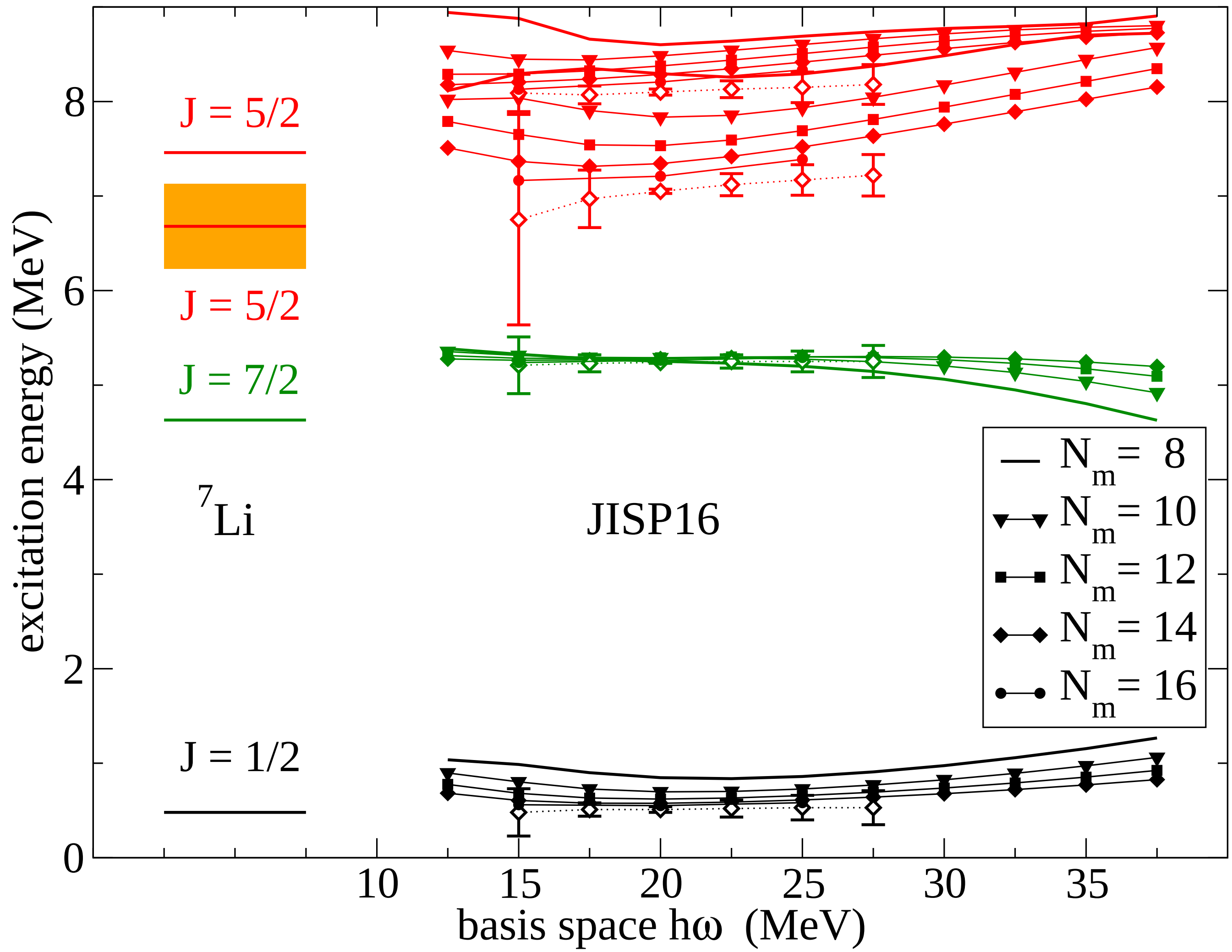
Maris, Vary, IJMPE22, 1330016 (2013)



- ^{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

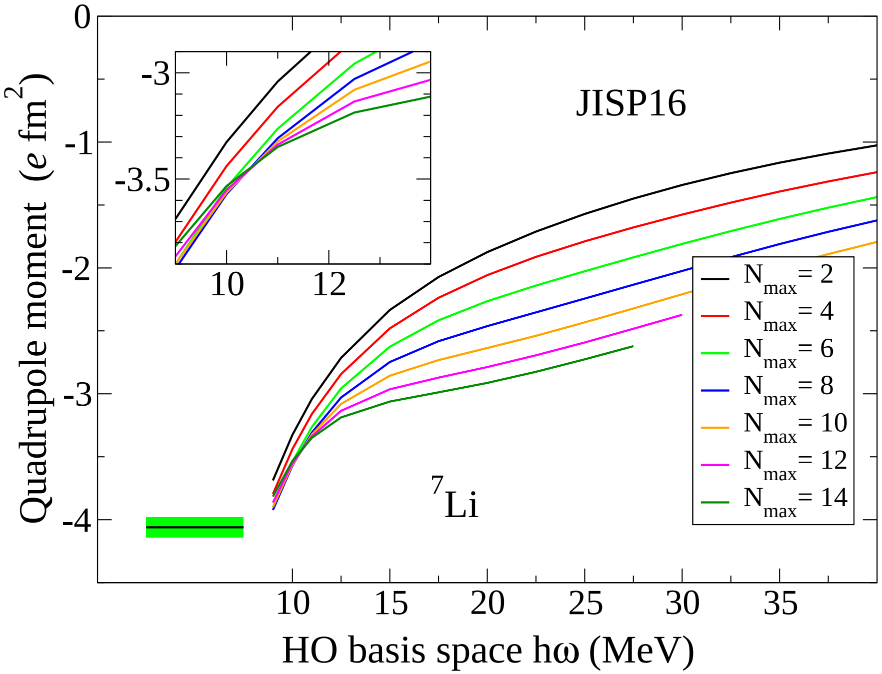
Cockrell, Maris, Vary, PRC86 034325 (2012)

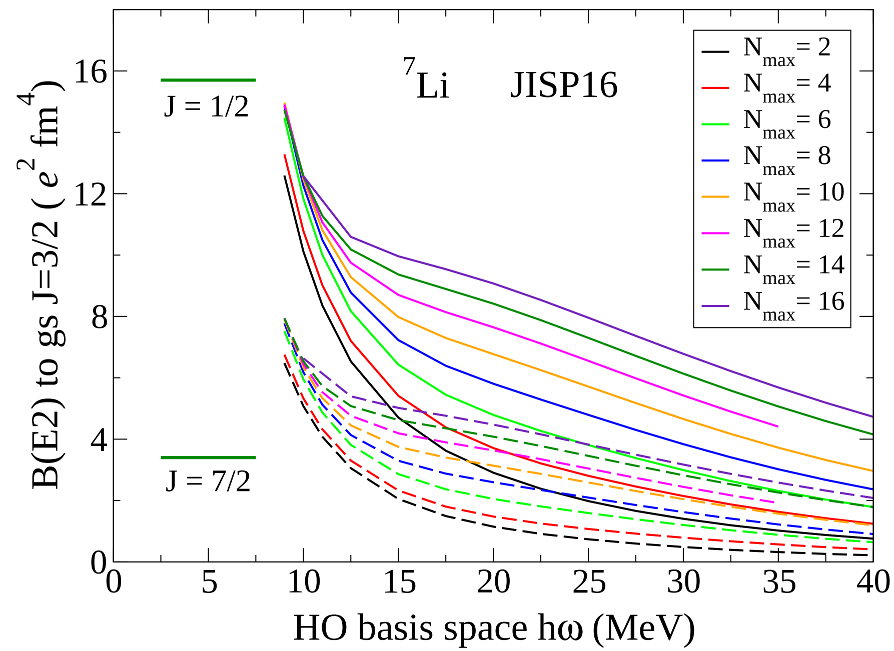


- Narrow states well converged, no extrapolation needed
- Broad resonances generally not as well converged; may need to incorporate continuum?

Quadrupole moment and B(E2) transition strengths 7Li

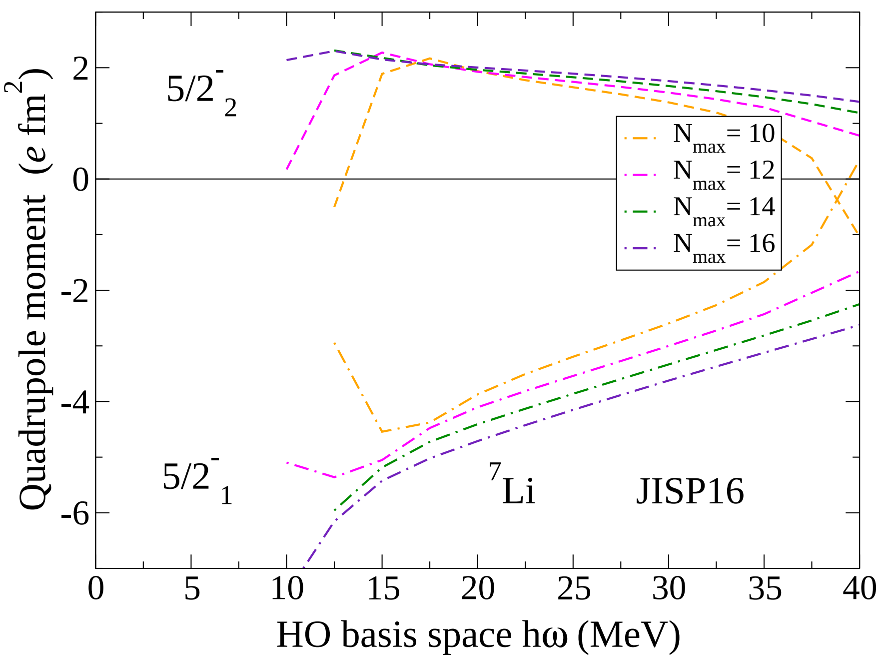
Cockrell, Maris, Vary, PRC86 034325 (2012)

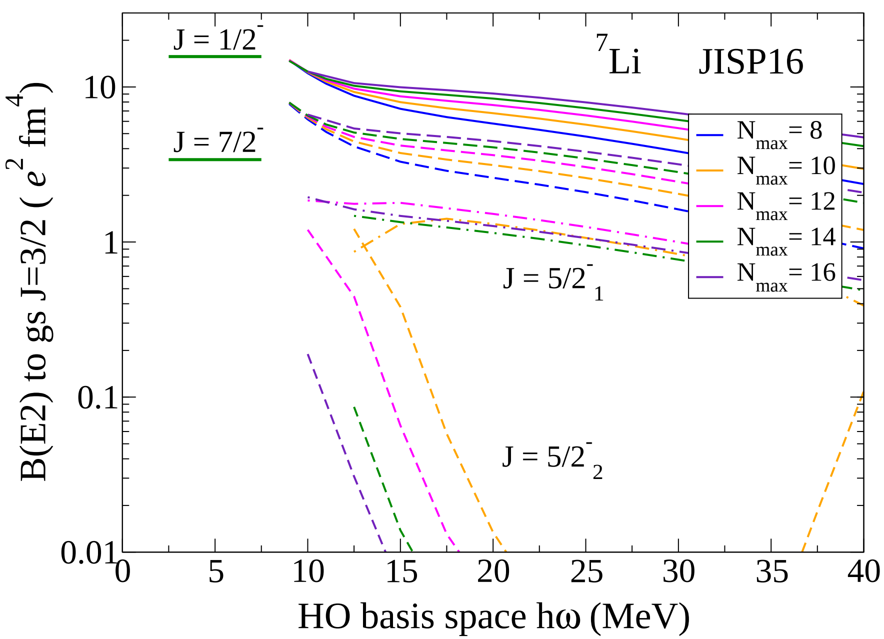




- E2 observables not converged,
  due to gaussian fall-off of HO wavefunction
- Nevertheless, qualitative agreement of $\mathcal{Q}$ and B(E2) with data

Quadrupole moments and B(E2) transitions for $J^\pi = \frac{5}{2}^-$ states

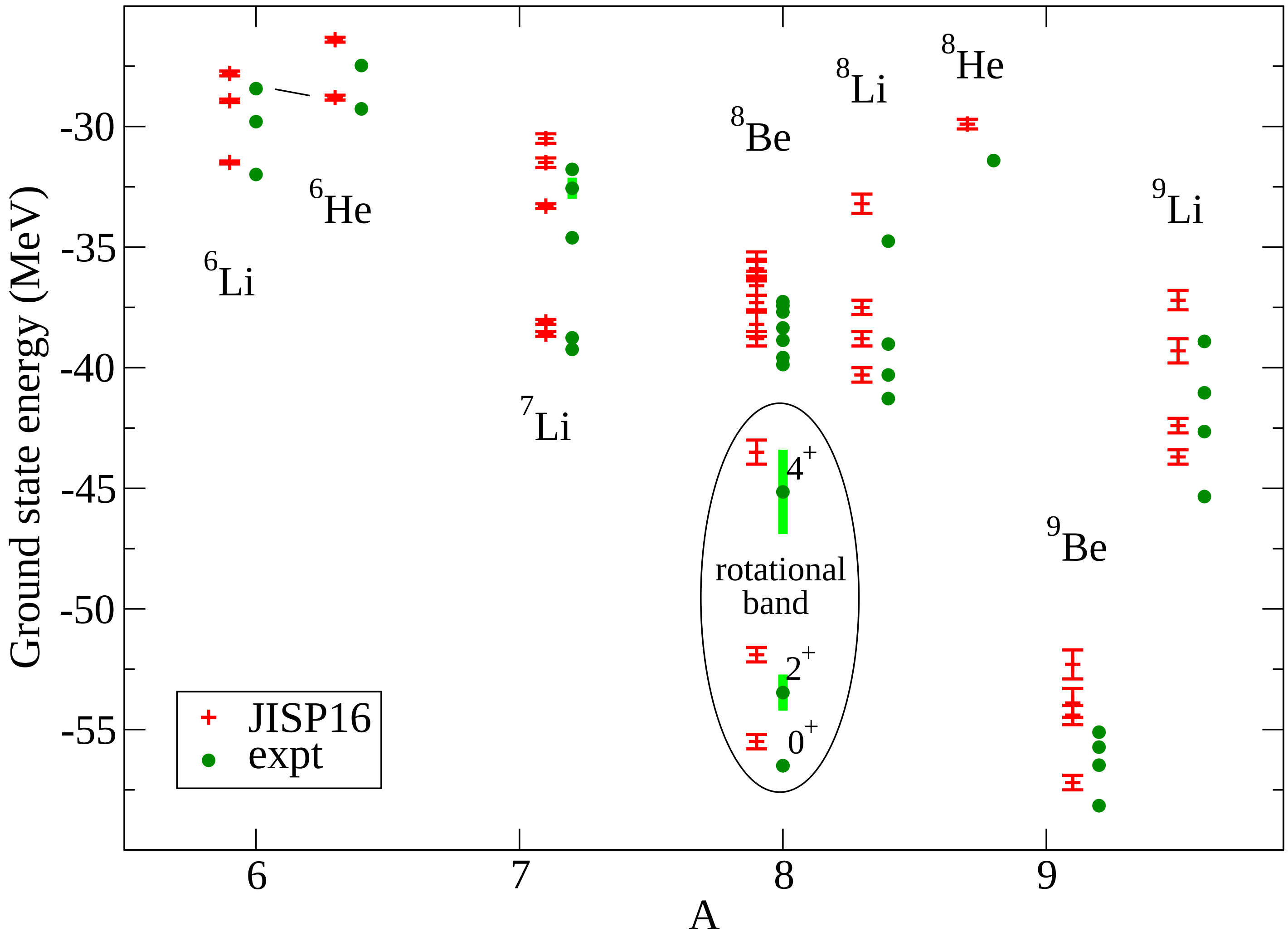




- E2 observables not converged, but nevertheless
  - $J^\pi = \left(\frac{5}{2}^-\right)_1$ large negative quadrupole moment
  - $\frac{1}{2}^-$, $\frac{7}{2}^-$, and $\left(\frac{5}{2}^-\right)_1$ relatively strong B(E2) to g.s.
  - $J^\pi = \left(\frac{5}{2}^-\right)_2$ small positive quadrupole moment, $Q \sim 2\ e$ fm^2, and very small B(E2) to g.s.

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

Maris, Vary, IJMPE22, 1330016 (2013)



- Excitation spectrum narrow states in good agreement with data

Intermezzo: Rotational states

Assuming adiabatic separation of rotational and internal degrees of freedom, a rotational nuclear state $|\psi_{JKM}\rangle$ can be described in terms of an intrinsic state $|\phi_K\rangle$ in a non-inertial frame, combined with the rotational motion of this non-inertial frame

$$|\psi_{JKM}\rangle = \mathcal{N}_{JK} \int d\vartheta \left[\mathscr{D}^J_{MK}(\vartheta)|\phi_K;\vartheta\rangle + (-)^{J+K} \mathscr{D}^J_{M-K}(\vartheta)|\phi_{\bar{K}};\vartheta\rangle \right]$$

- Rotational energy

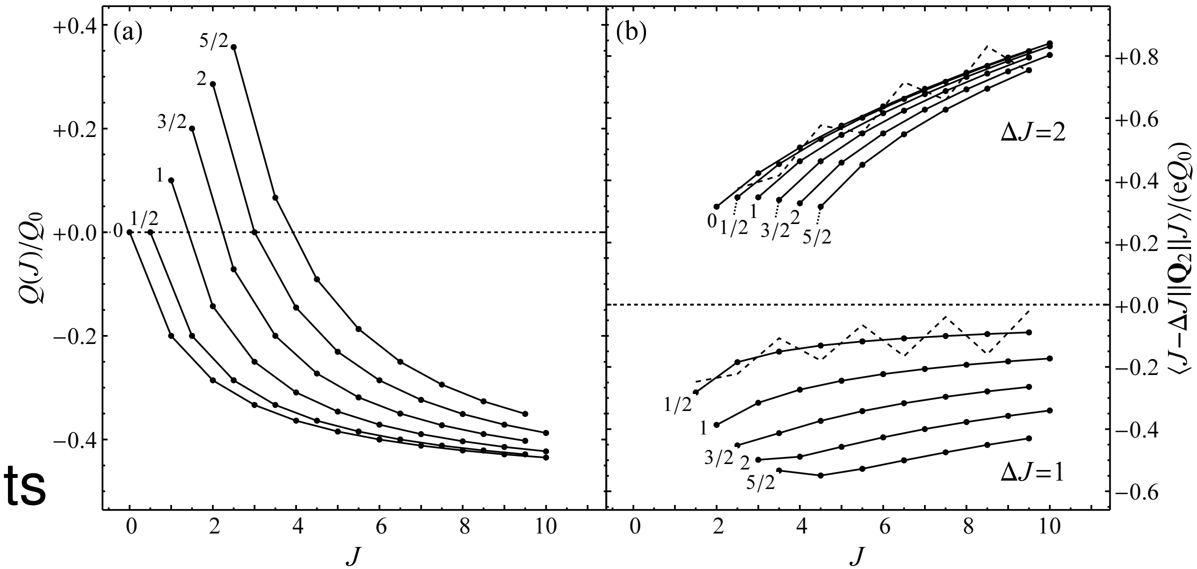
$$E(J) = E_0 + \frac{\hbar^2}{2\mathcal{I}} \left(J(J+1)\right)$$

for $K = \frac{1}{2}$ bands staggering due to Coriolis term

$$E(J) = E_0 + \frac{\hbar^2}{2\mathcal{I}} \left(J(J+1) + a\,(-1)^{J+\frac{1}{2}}\,(J+\tfrac{1}{2}) \right)$$

Rotational states: Quadrupole matrix elements

$$\langle \psi_{J_f K} || E_2 || \psi_{J_i K} \rangle = \frac{(2J_i+1)^{1/2}}{1+\delta_{K0}} \Big((J_i, K, 2, 0 | J_f, K) \, \langle \phi_K || E_{2,0} || \phi_K \rangle + (-)^{J_i+K} (J_i, -K, 2, 2K | J_f, K) \, \langle \phi_K || E_{2,2K} || \phi_{\bar{K}} \rangle \Big)$$



- Quadrupole moments

$$\mathcal{Q}(J) = \frac{3K^2 - J(J+1)}{(J+1)(2J+3)} \, \mathcal{Q}_0$$

- Transition matrix elements

$$\langle \psi_{J_f K} || E_2 || \psi_{J_i K} \rangle = \sqrt{\frac{5}{16\pi}} \sqrt{2J_i+1} \, (J_i K 2 0 | J_f K) \, \mathcal{Q}_0$$

- Consider both proton and neutron quadrupole tensors

Rotational states: Dipole matrix elements

- Magnetic moments

$$\mu(J) = a_0\, J + a_1 \frac{K}{J+1} + a_2\, \delta_{K,\frac{1}{2}} \frac{(-1)^{J-\frac{1}{2}}}{2\sqrt{2}} \frac{2J+1}{J+1}$$

- Magnetic transition matrix elements

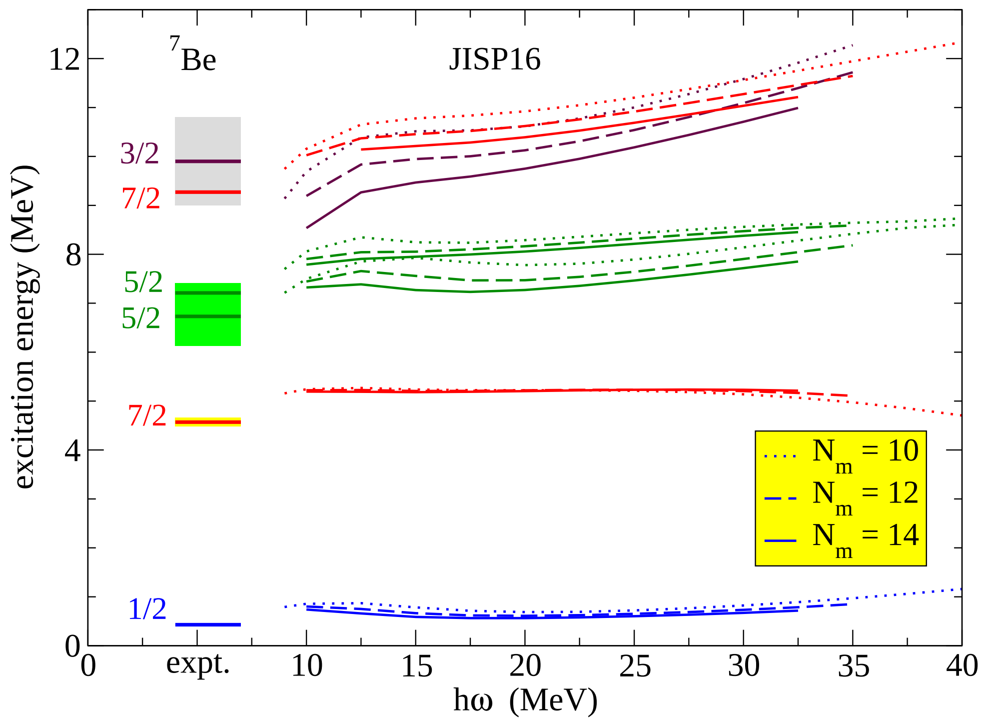
$$\langle \psi_{J-1,K} || M_1 || \psi_{J,K} \rangle = -\sqrt{\frac{3}{4\pi}} \sqrt{\frac{J^2-K^2}{J}} \left(a_1 + a_2\, \delta_{K,\frac{1}{2}} \frac{(-1)^{J-\frac{1}{2}}}{\sqrt{2}} \right)$$

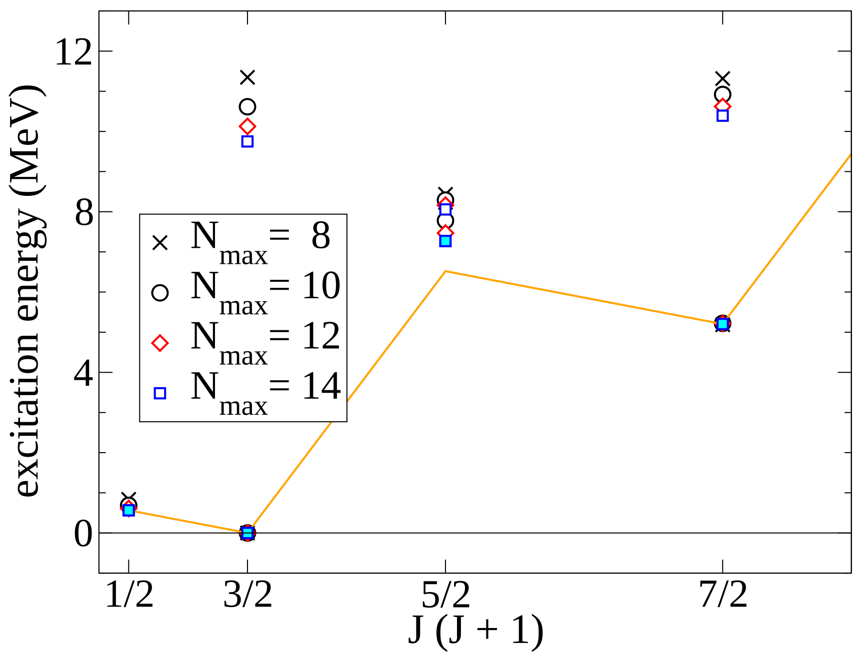
- Define dipole terms $D_{l,p}$, $D_{l,n}$, $D_{s,p}$, and $D_{s,n}$
  for both the magnetic moments and for the M_1 transitions

$$M_1 = g_{l,p}\, D_{l,p} + g_{l,n}\, D_{l,n} + g_{s,p}\, D_{s,p} + g_{s,n}\, D_{s,n}$$

  with $g_{l,p} = 1$, $g_{l,n} = 0$, $g_{s,p} = 5.586$, and $g_{s,n} = -3.826$

Excitation spectrum 7Be – Emergence of rotational band?

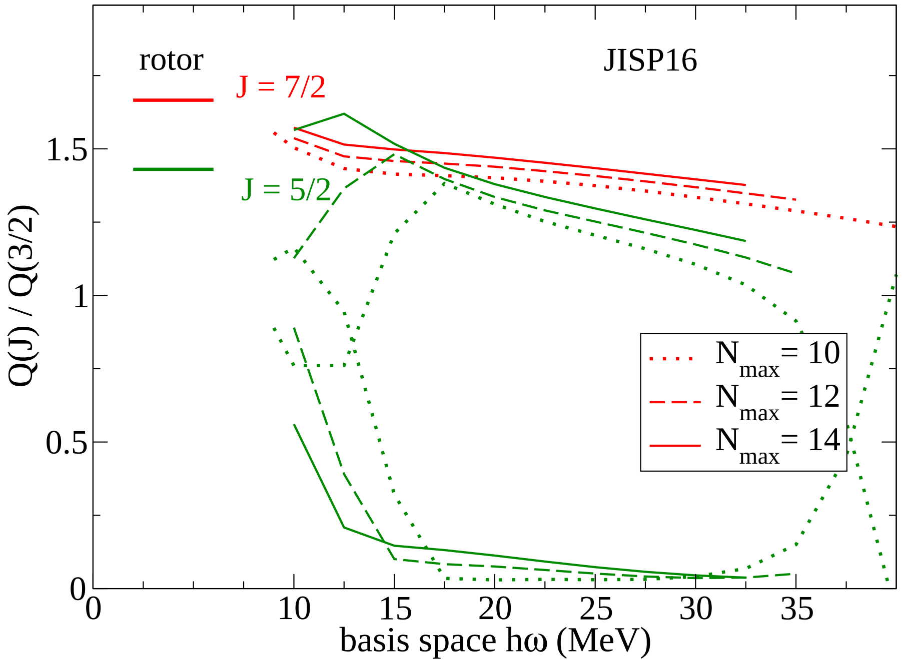


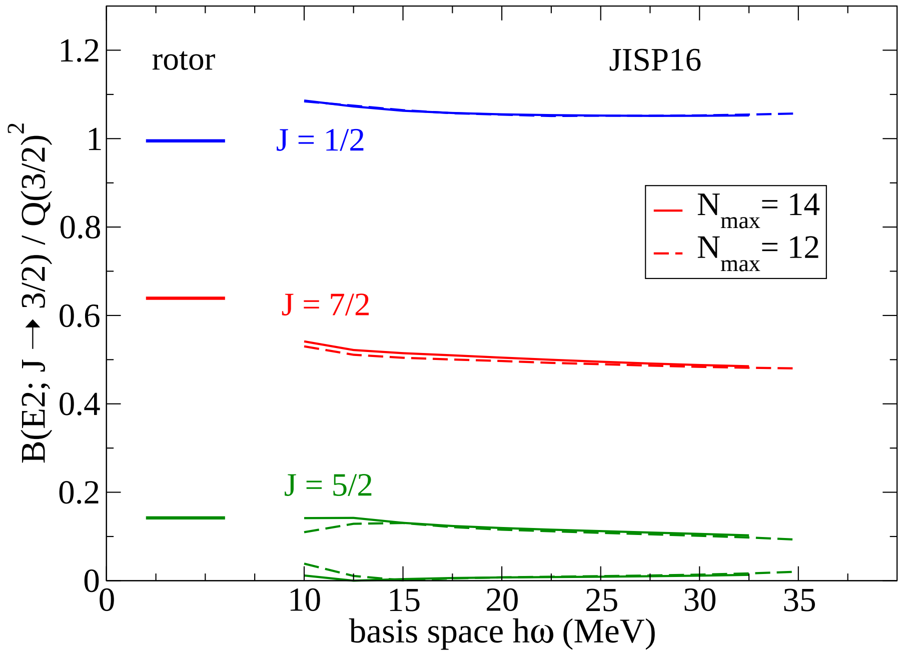


- Spectrum in reasonable agreement with data
  - lowest two excited states converged
  - broad resonances not as well converged
- Excitation energies of lowest J states consistent with $K = \frac{1}{2}$ rotational band

Emergence of $K = \frac{1}{2}$ rotational band

Ratio of electric quadrupole moments and B(E2)'s
over ground state quadrupole moment $\mathcal{Q}(3/2)$



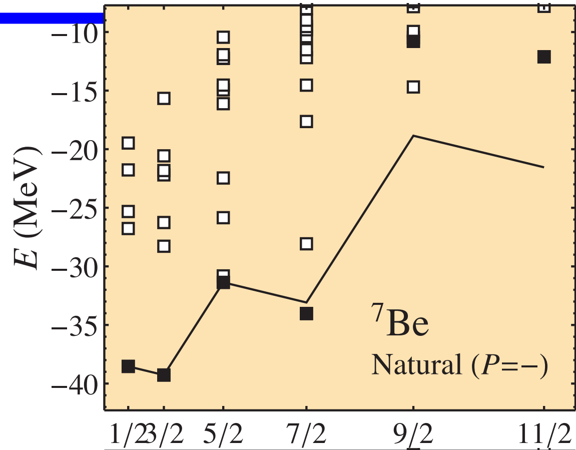


Rotor model

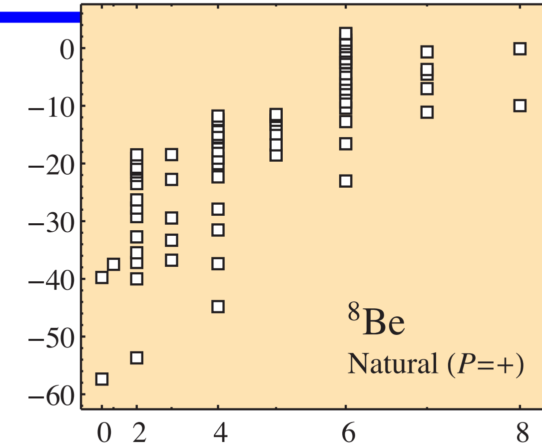
$$\mathcal{Q}(J) = \frac{\frac{3}{4} - J(J+1)}{(J+1)(2J+3)}\,\mathcal{Q}_0$$

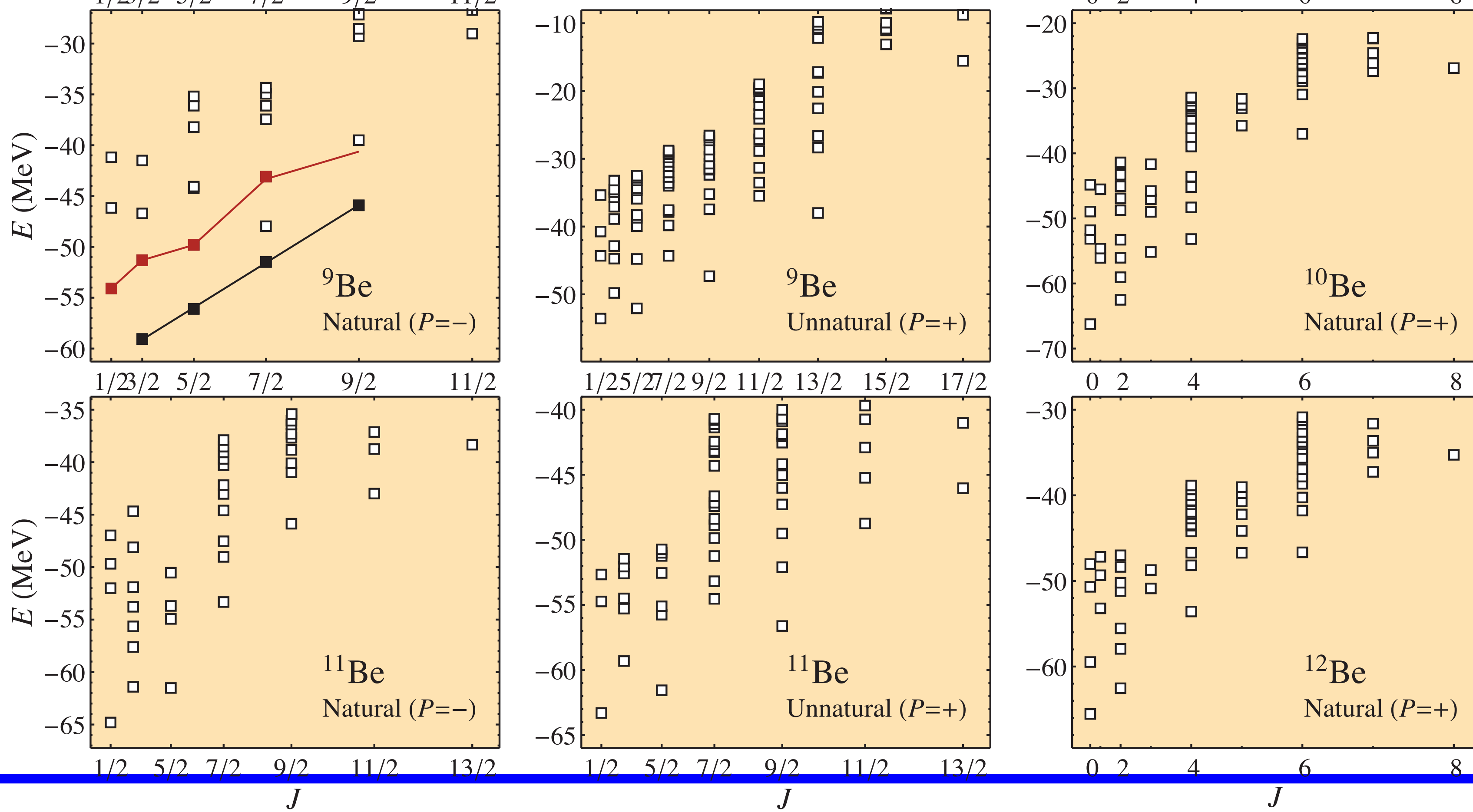
$$B(E2; i \to f) = \frac{5}{16\pi}\left(J_i, \frac{1}{2}; 2, 0 \middle| J_f, \frac{1}{2}\right)^2 \mathcal{Q}_0^2$$

Candidate rotational bands: ^{7}Be–^{12}Be



Caprio, Maris, Vary,
PLB719, 179 (2013)
PRC91, 014310 (2015)





Candidate rotational bands: ^{7}Be–^{12}Be

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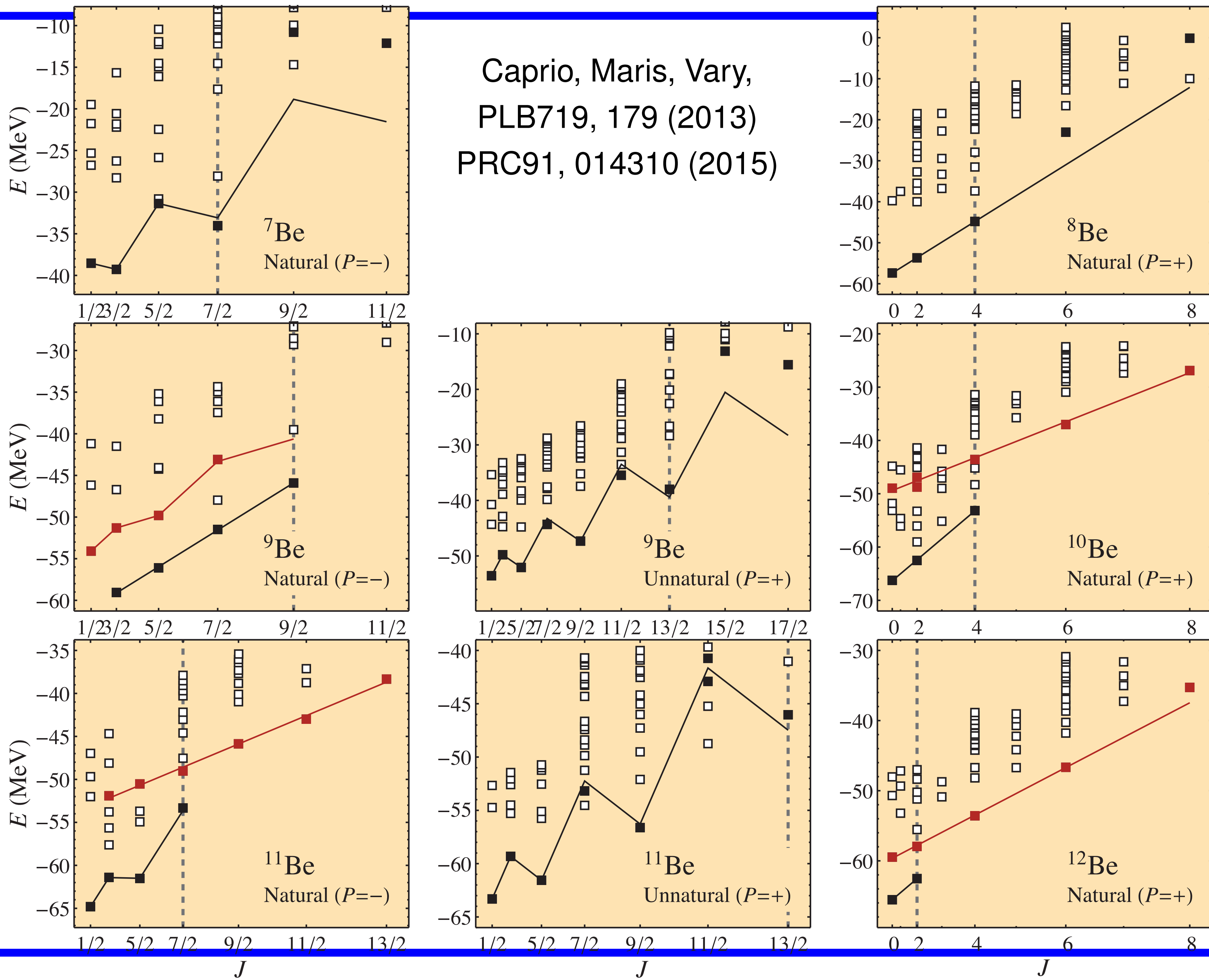
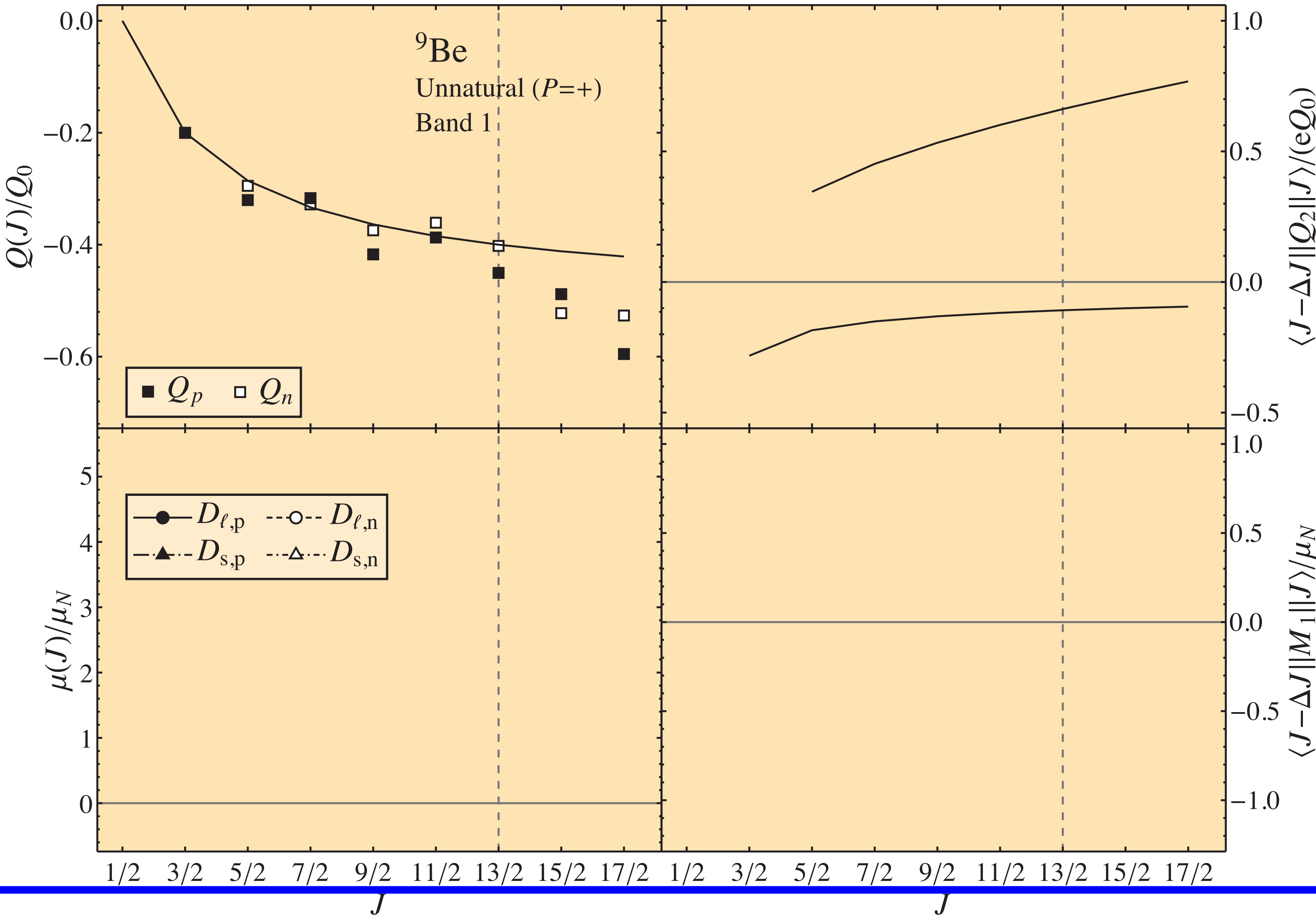
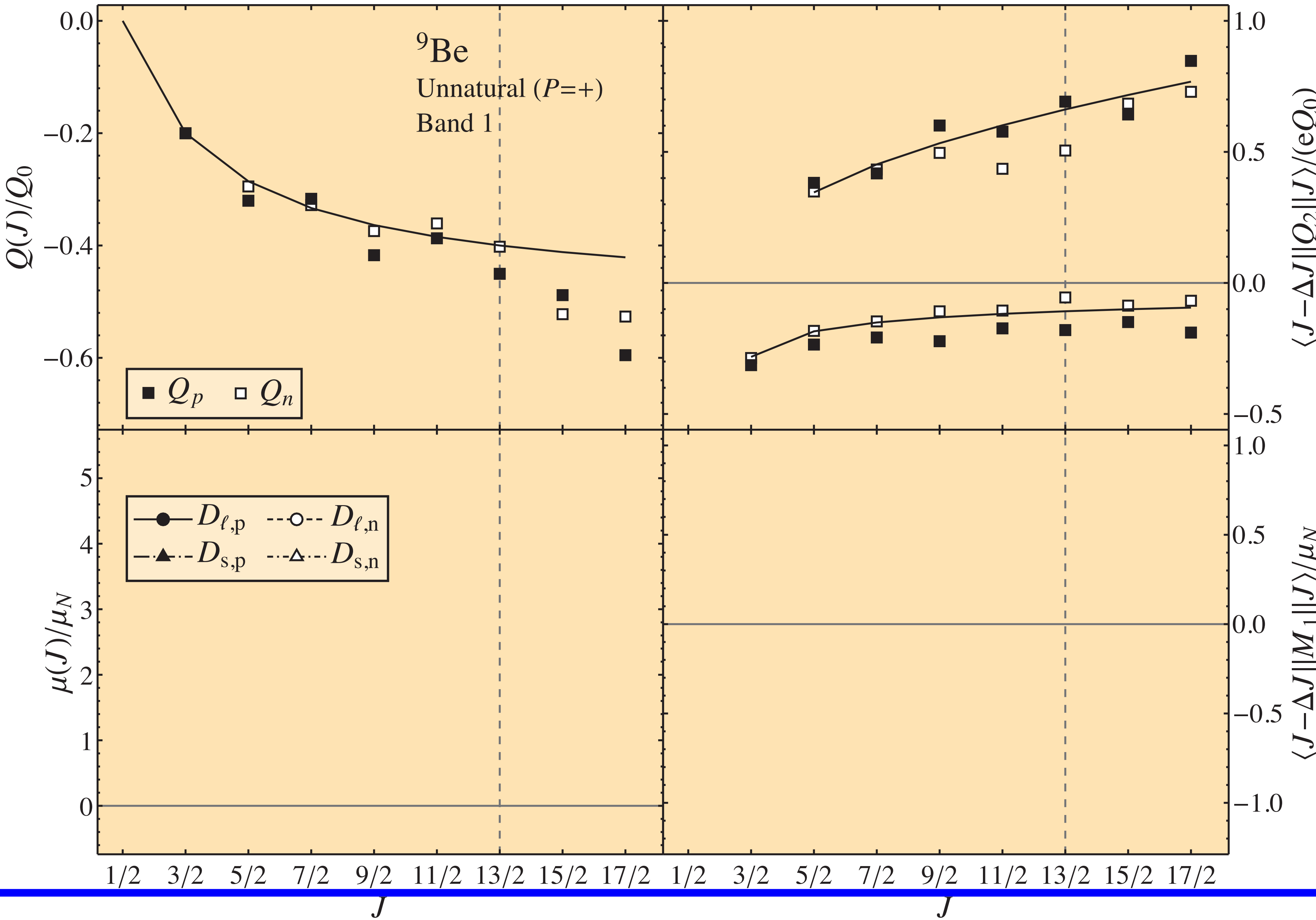
PRC91, 014310 (2015)



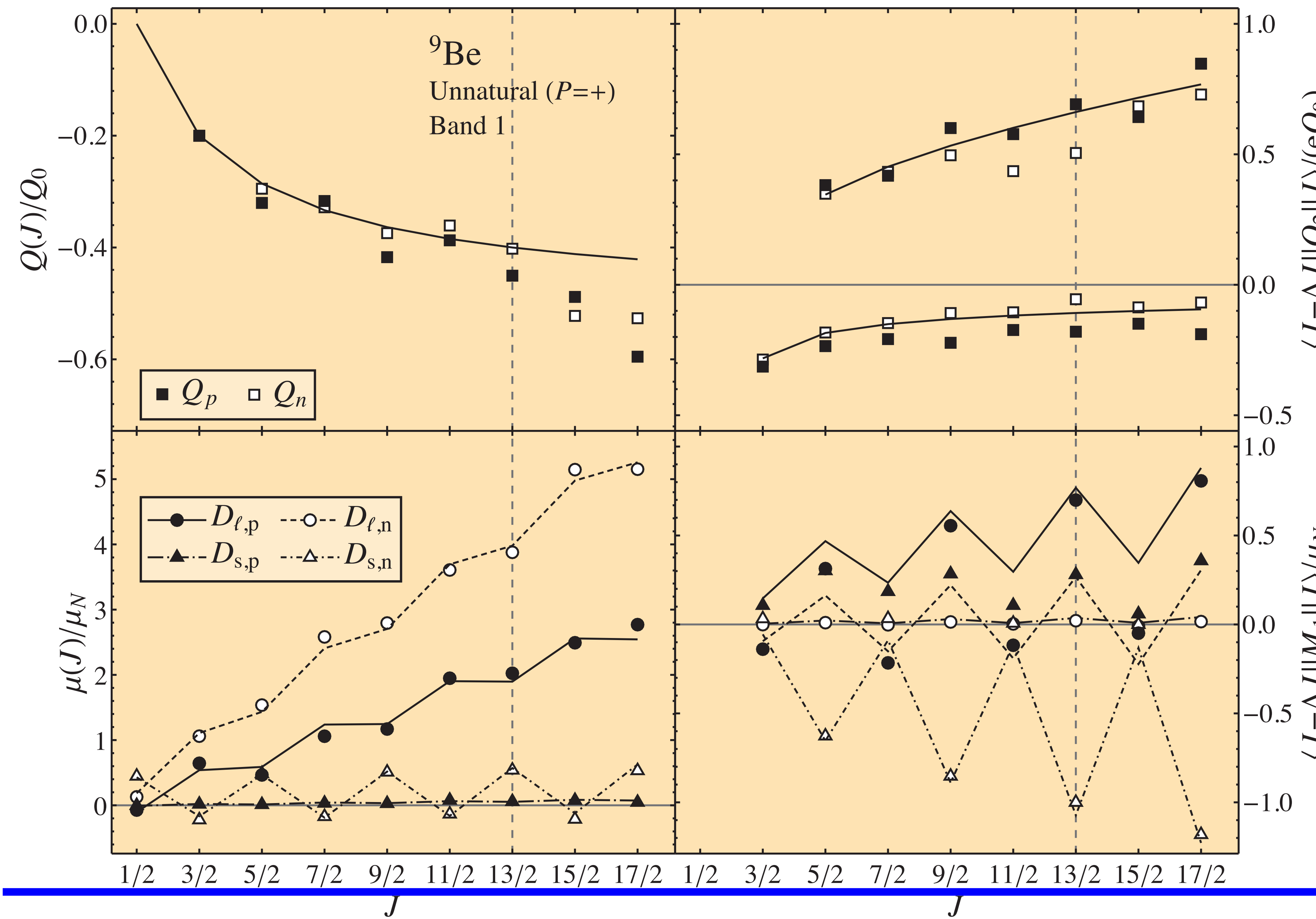
Electromagnetic moments and transitions



Electromagnetic moments and transitions



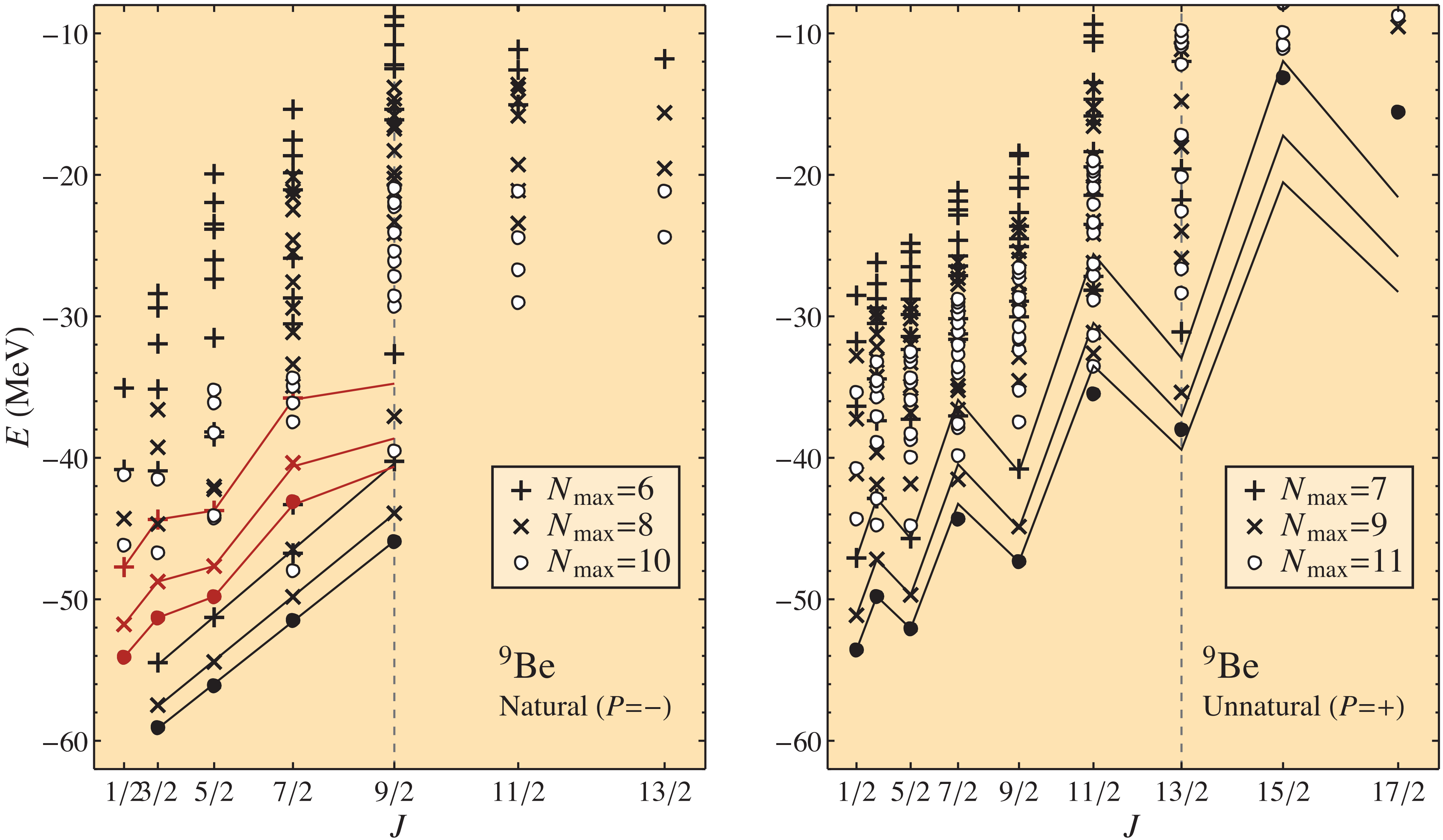
Electromagnetic moments and transitions



Convergence with basis size? ^{9}Be

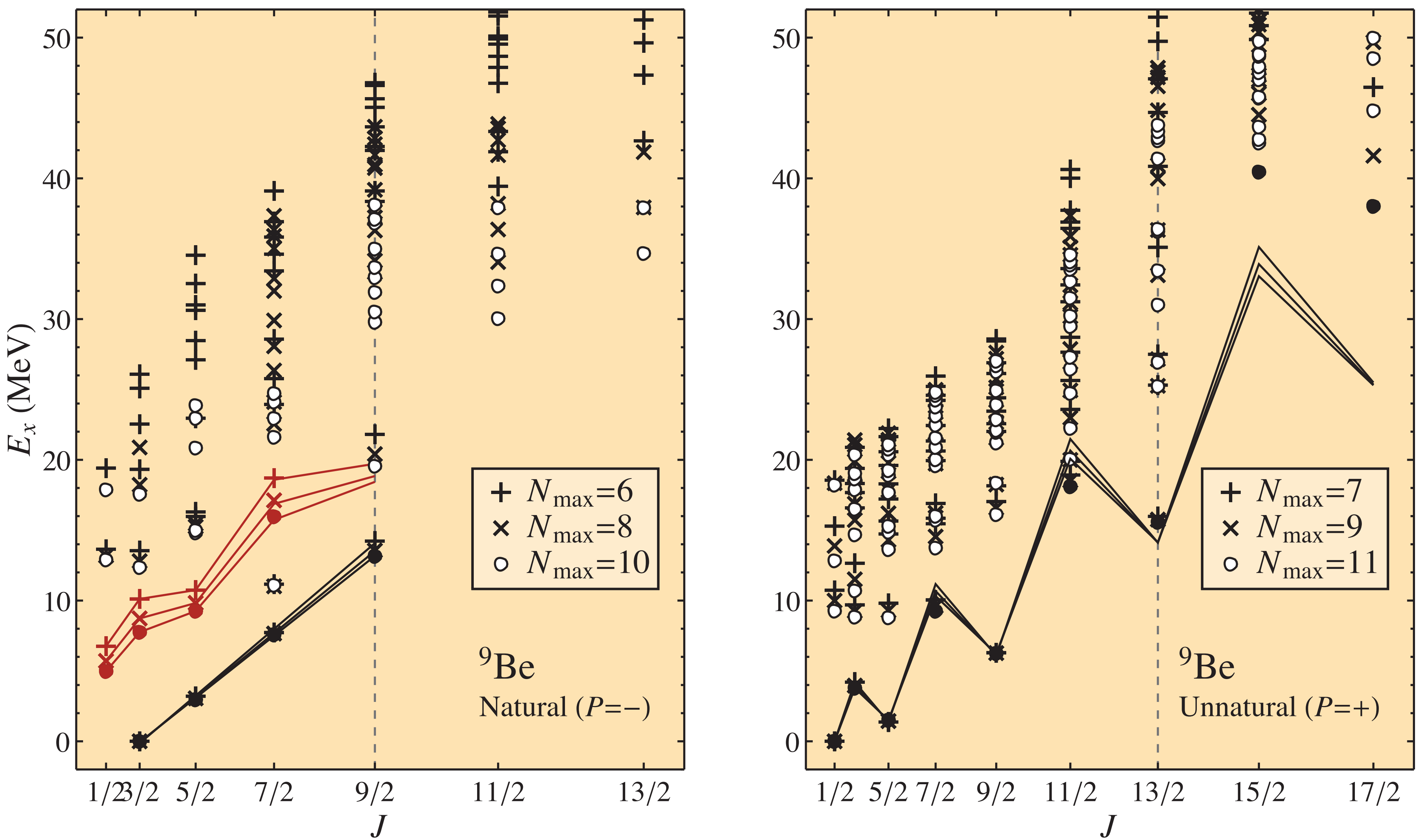
Absolute binding energy? NO!

Maris, Caprio, Vary, PRC91, 014310 (2015)



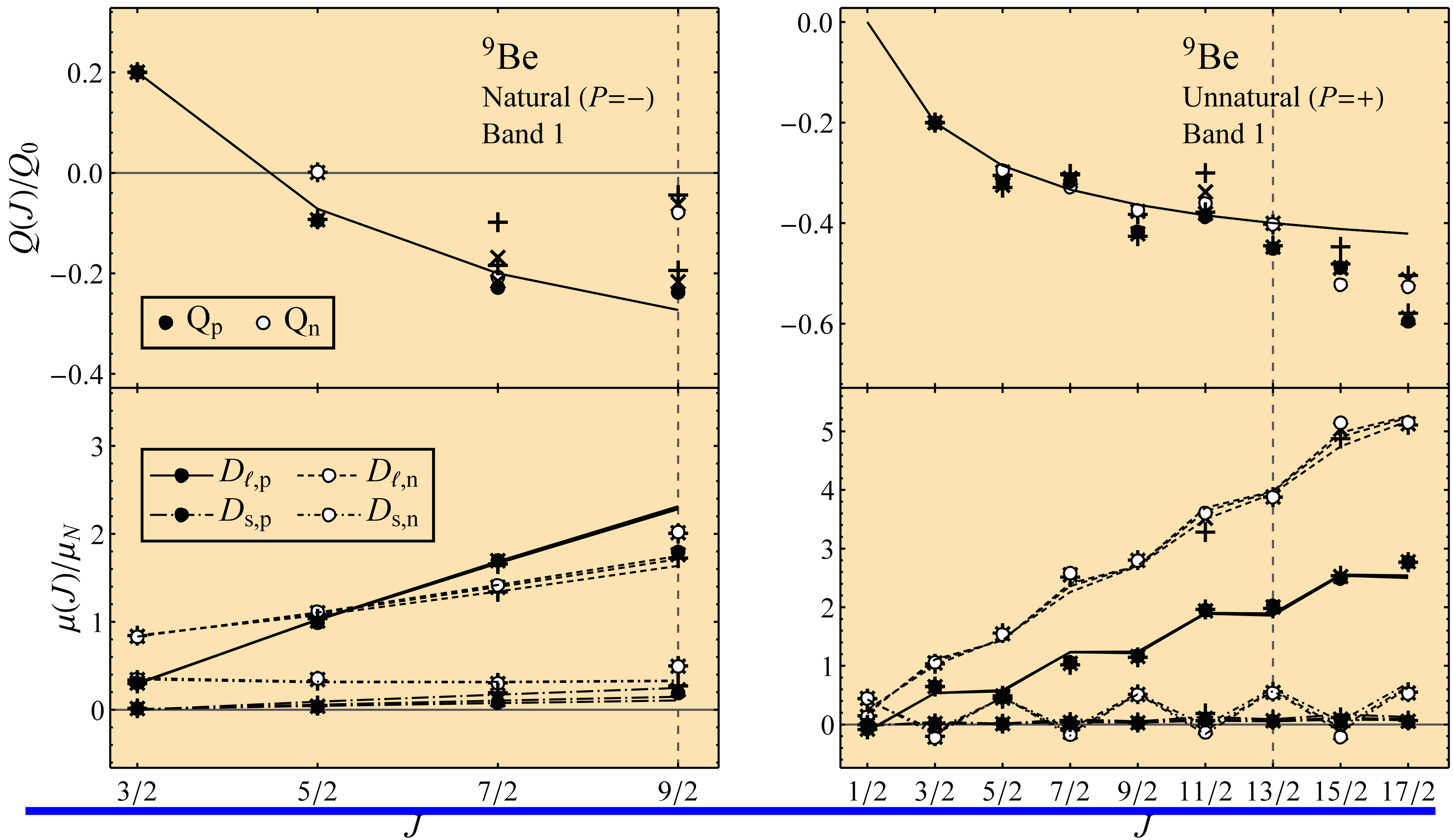
Convergence with basis size? ^{9}Be

Absolute binding energy? NO! Excitation within band? ~YES



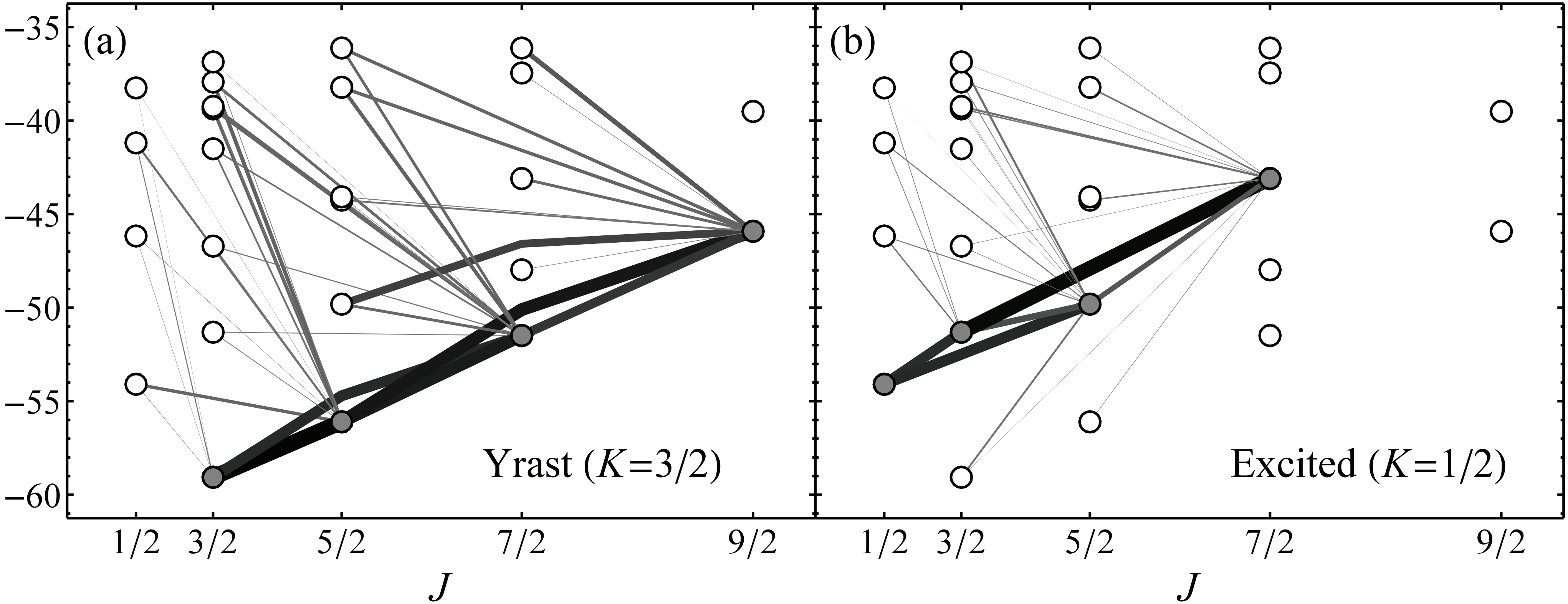
Convergence with basis size? ^{9}Be

Absolute $E2$? NO! Ratio of $E2$? ~YES Absolute $M1$? ~YES



Intra-band E2 transition strength

Caprio, Maris, Vary, Smith, arXiv:1502.01083

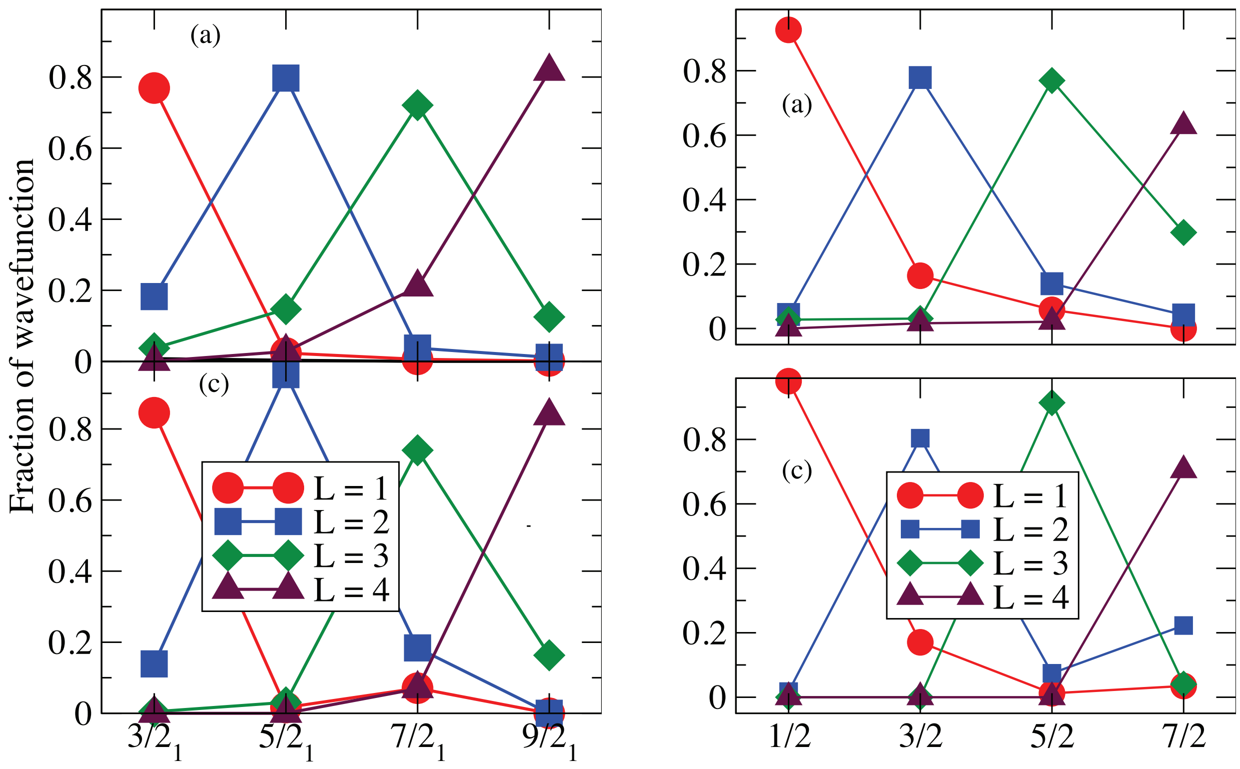


E2 transition strenght between natural (negative) parity states in ^{9}Be

- Transitions within g.s. $(K = 3/2)$ and $(K = 1/2)$ bands significantly enhanced over typical E2 transition strenght

LS decomposition rotational bands ^{9}Be

Johnson, arXiv:1409.7355



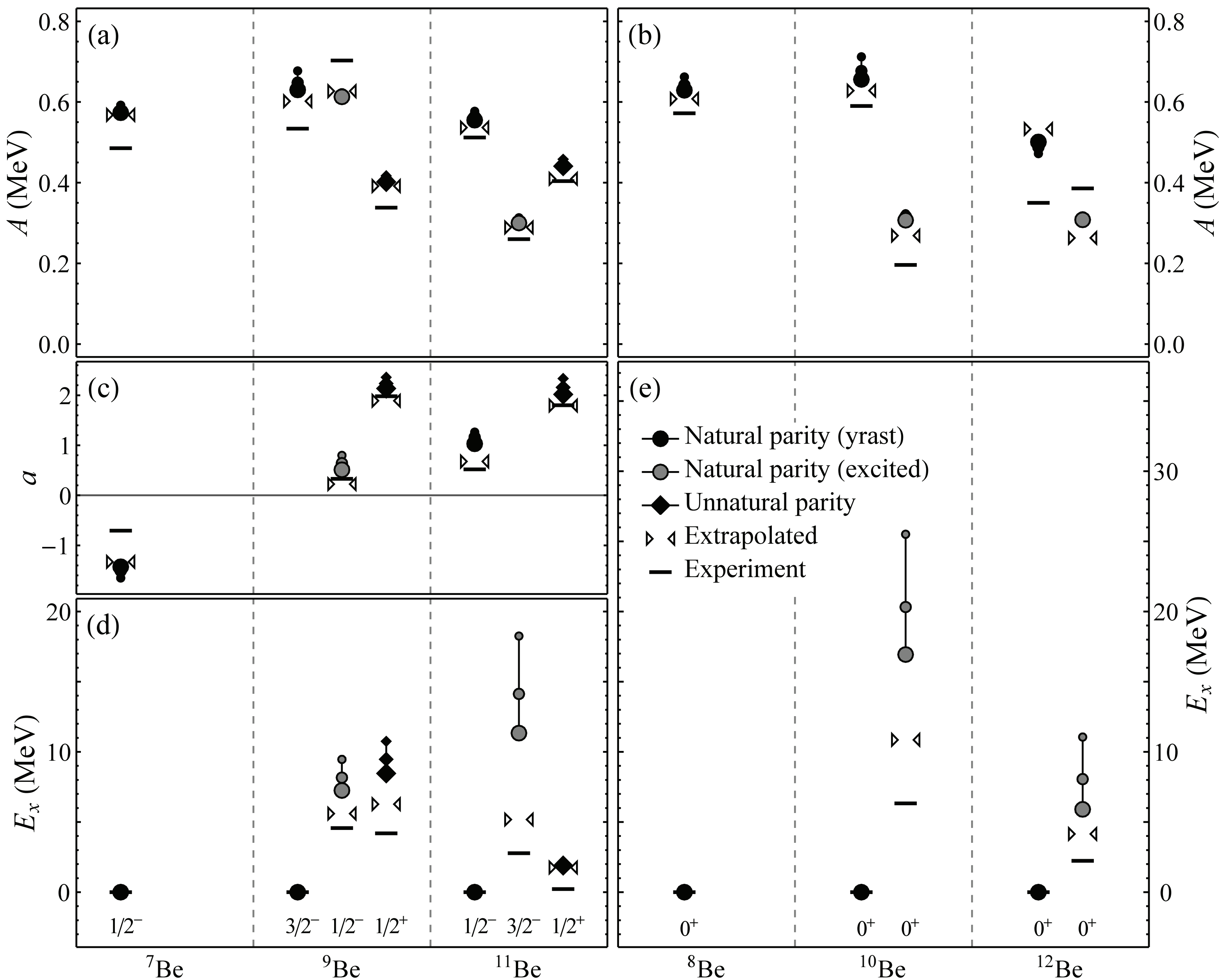
L decomposition with SRG-evolved chiral N3LO NN-only interaction

with Cohen–Kurath shell model

- g.s. $(K = 3/2)$ (left):
  $\frac{3}{2}^-$, $\frac{5}{2}^-$, $\frac{7}{2}^-$, and $\frac{9}{2}^-$ states dominated by $L = 1$, 2, 3, and 4
- excited $(K = 1/2)$ (right):
  $\frac{1}{2}^-_1$, $\frac{3}{2}^-_2$, $\frac{5}{2}^-_2$, and $\frac{7}{2}^-_3$ states dominated by $L = 1$, 2, 3, and 4

Comparison with experiment

Caprio, Maris, Vary, Smith, arXiv:1502.01083



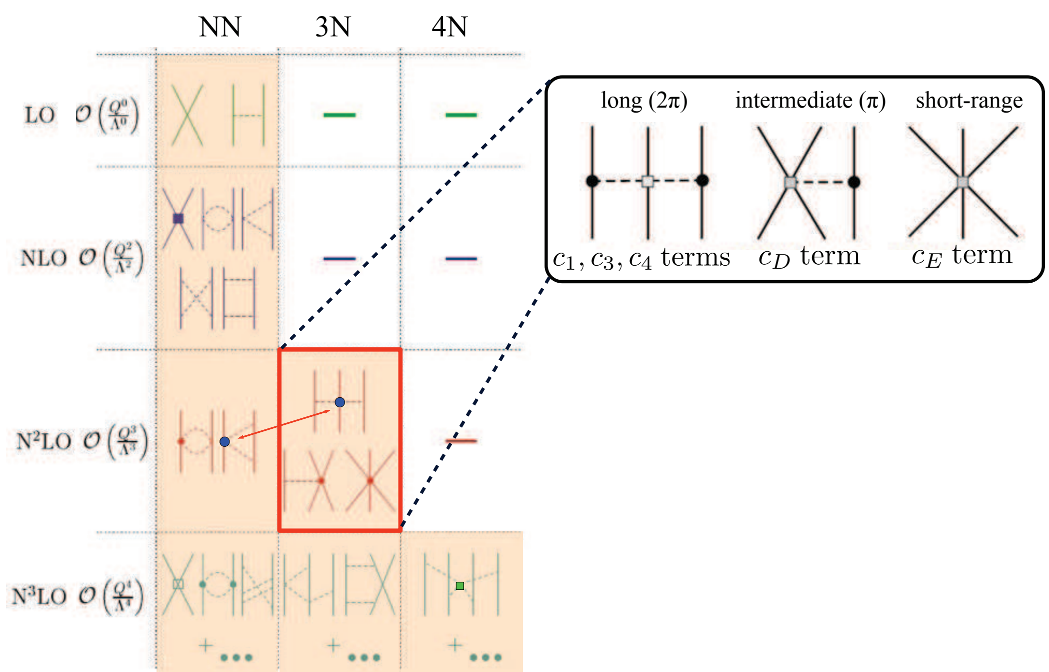
Nuclear interaction from chiral perturbation theory

- 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

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

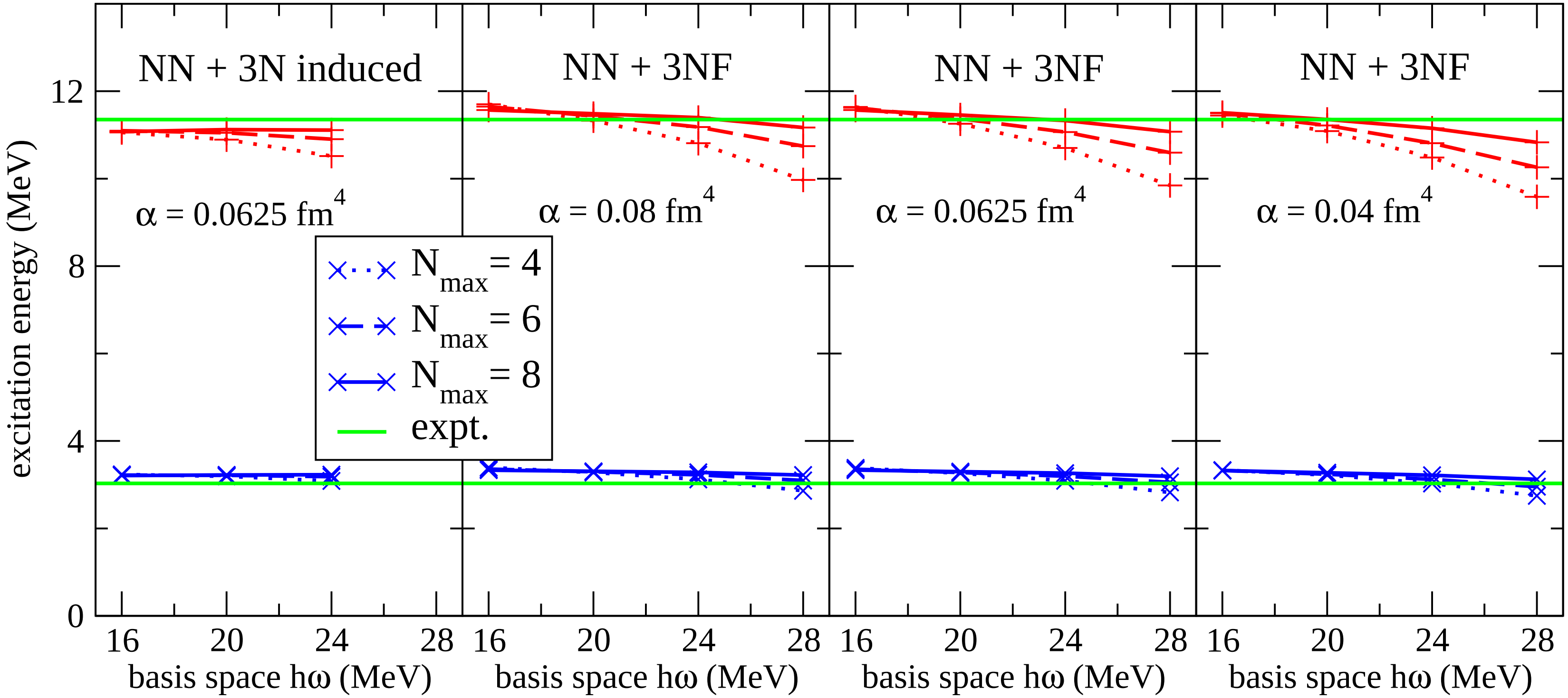
  - in principle no free parameters
    - in practice a few undetermined parameters
  - renormalization necessary

Leading-order 3N forces in chiral EFT



Effect of 3-body forces on lowest excited states ^{8}Be

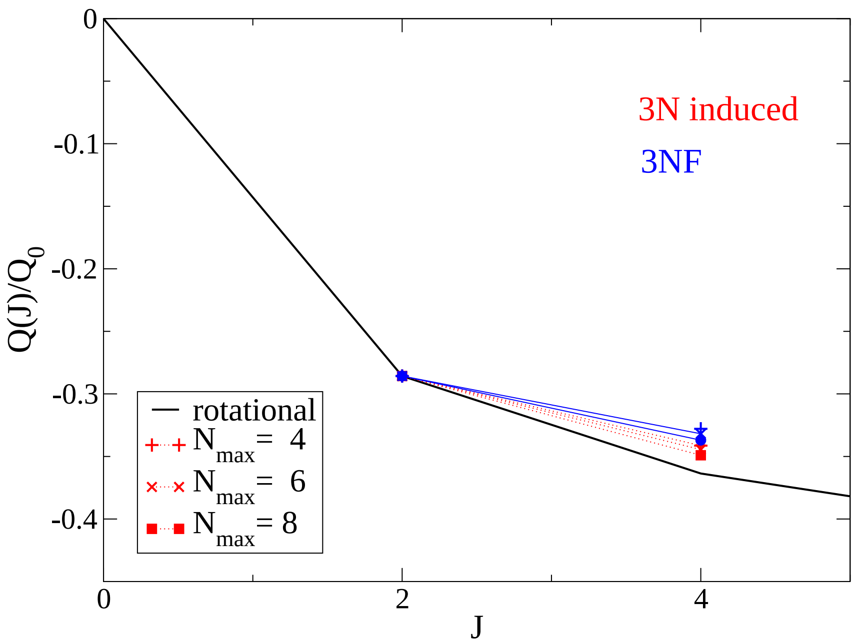
Maris, Aktulga, Binder, Calci, Catalyurek, Langhammer, Ng, Saule, Roth, Vary, Yang
J. Phys. Conf. Ser. 454, 012063 (2013)

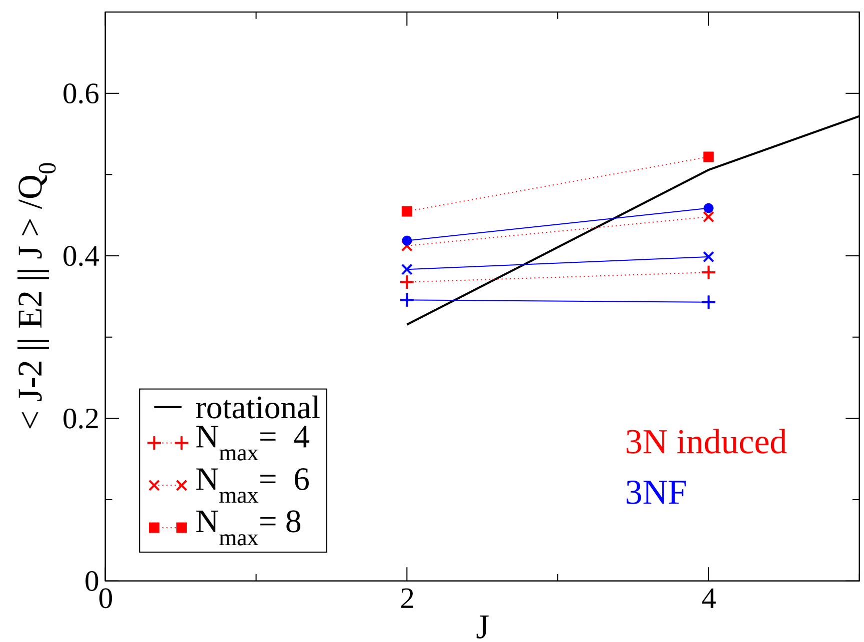


- Very well converged without explicit 3NF
- Reasonably well converged with explicit 3NF
- In agreement with data

Rotational nature of 2^+ and 4^+ of ^{8}Be

results at SRG parameter $\lambda = 2.0$ fm^{-1}, basis $\hbar\omega = 20$ MeV

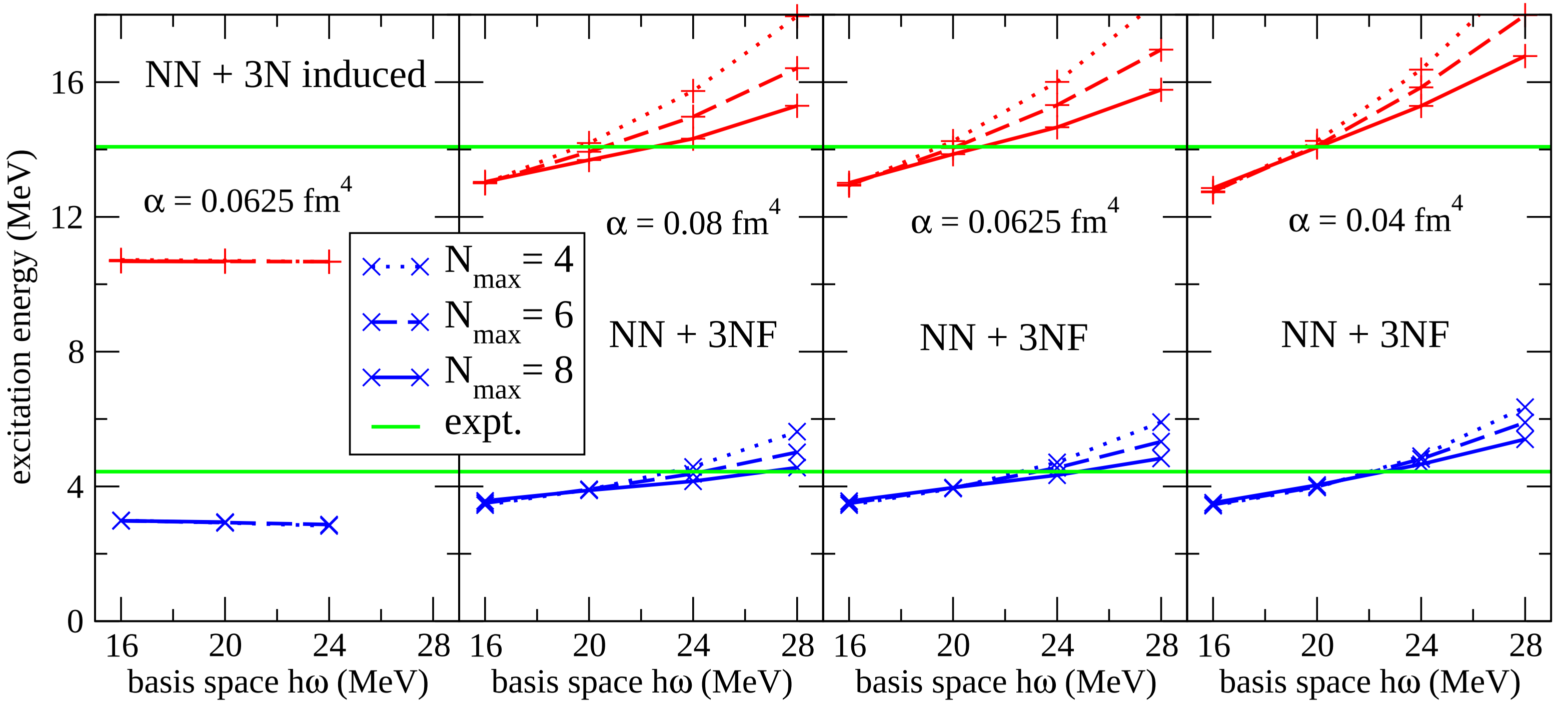




- Excitation energies in agreement with rotational model
- $\mathcal{Q}$ and E2 transition matrix elements not converged
- ratios $\mathcal{Q}/\mathcal{Q}_0$ and $M_{\mathrm{E2}}/\mathcal{Q}_0$ reasonably converged
  and in semi-quantitative agreement with rotational model
  (note: these are broad resonances, for which we cannot obtain true convergence)

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

Maris, Aktulga, Binder, Calci, Catalyurek, Langhammer, Ng, Saule, Roth, Vary, Yang
J. Phys. Conf. Ser. 454, 012063 (2013)

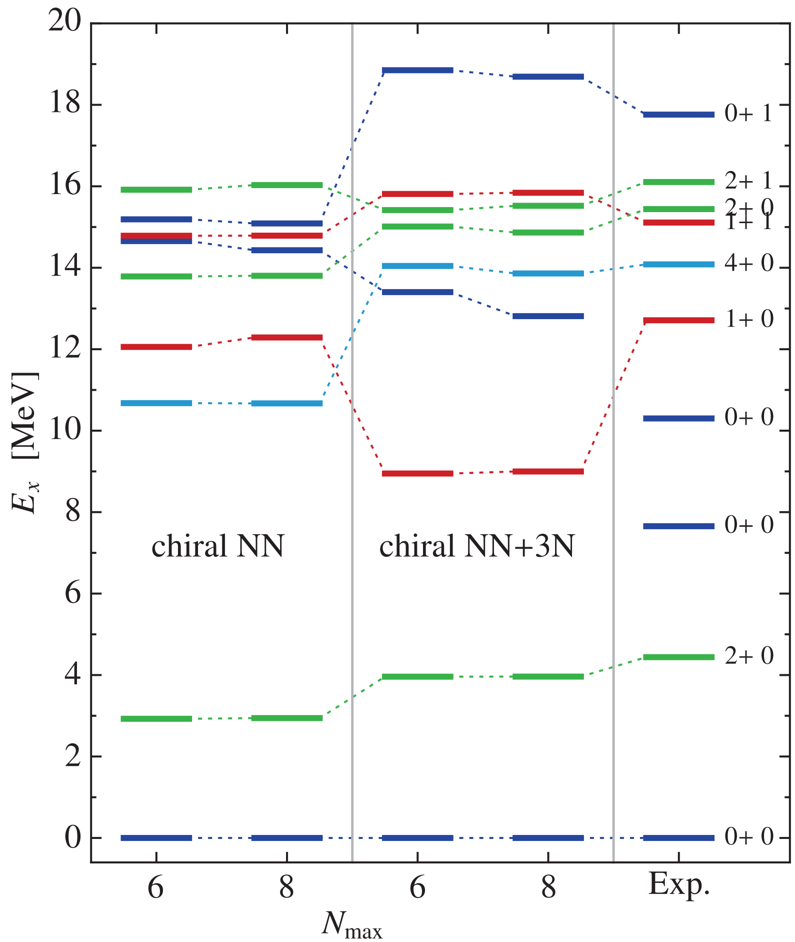


- Chiral 3NF improves agreement with data
- Not converged with explicit 3NF, despite weak N_{max} dependence
- Increase in excitation energy of $(2^+, 0)$ and $(4^+, 0)$ rotational states likely due to increased binding of $(0^+, 0)$

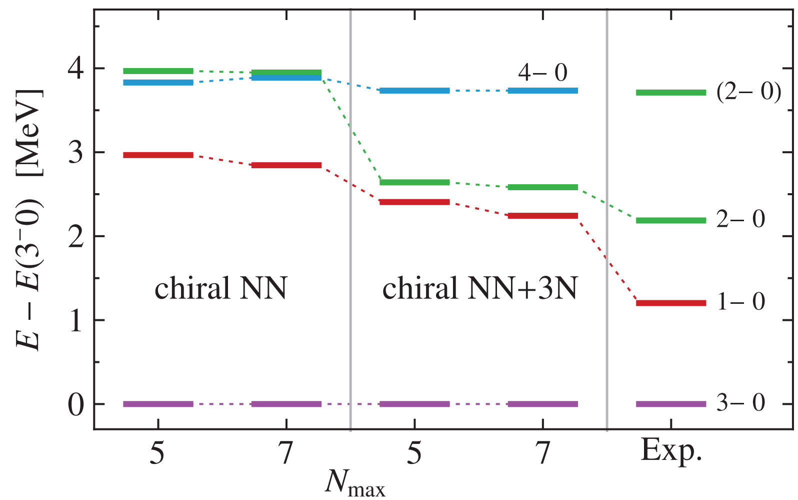
Spectrum of ^{12}C

at SRG parameter $\lambda = 2.0$ fm^{-1} and $\hbar\omega = 20$ MeV

Maris, Vary, Calci, Langhammer, Binder, Roth, Phys. Rev. C90, 014314 (2014)



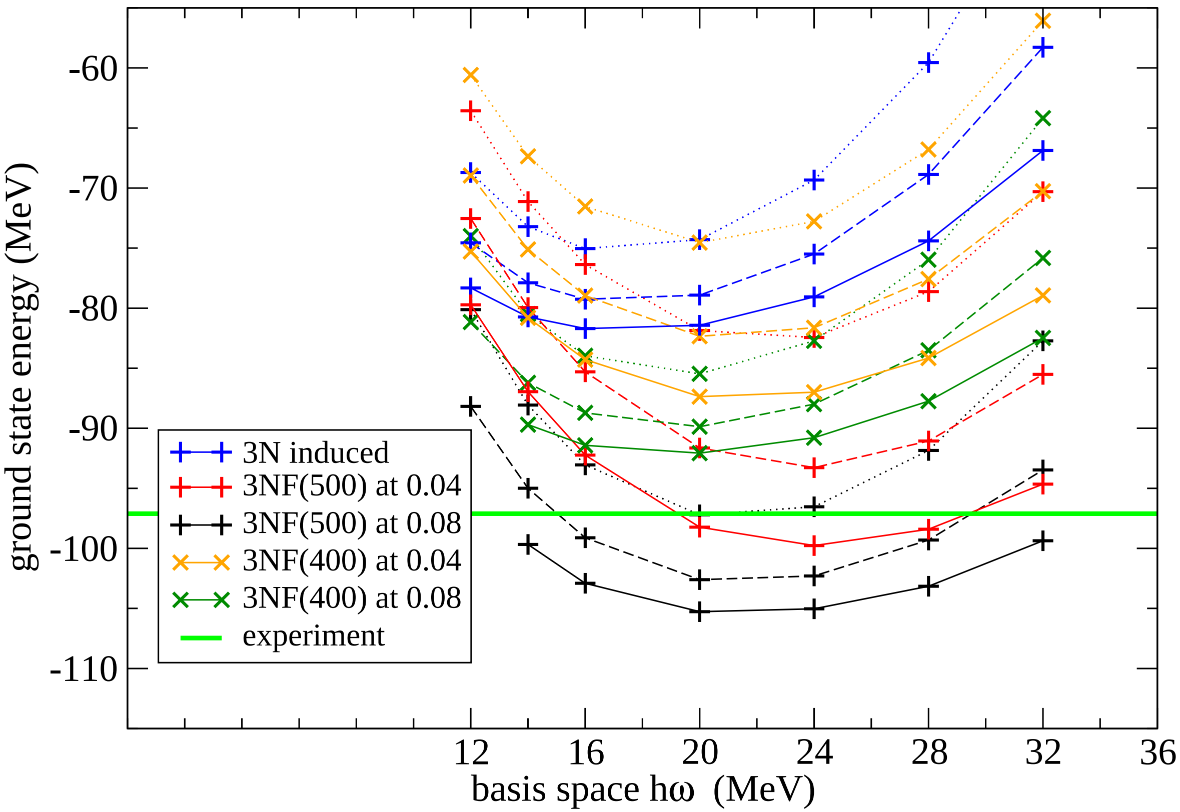
- chiral NN at N^{3}LO
- chiral 3N at N^{2}LO
- 3N LEC values:
  $c_D = -0.2,\ c_E = -0.205$
- 500 MeV cutoff



- 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

Ground state in ^{13}C – work in progress

preliminary results with SRG evolved N^{3}LO NN plus N^{2}LO 3NF

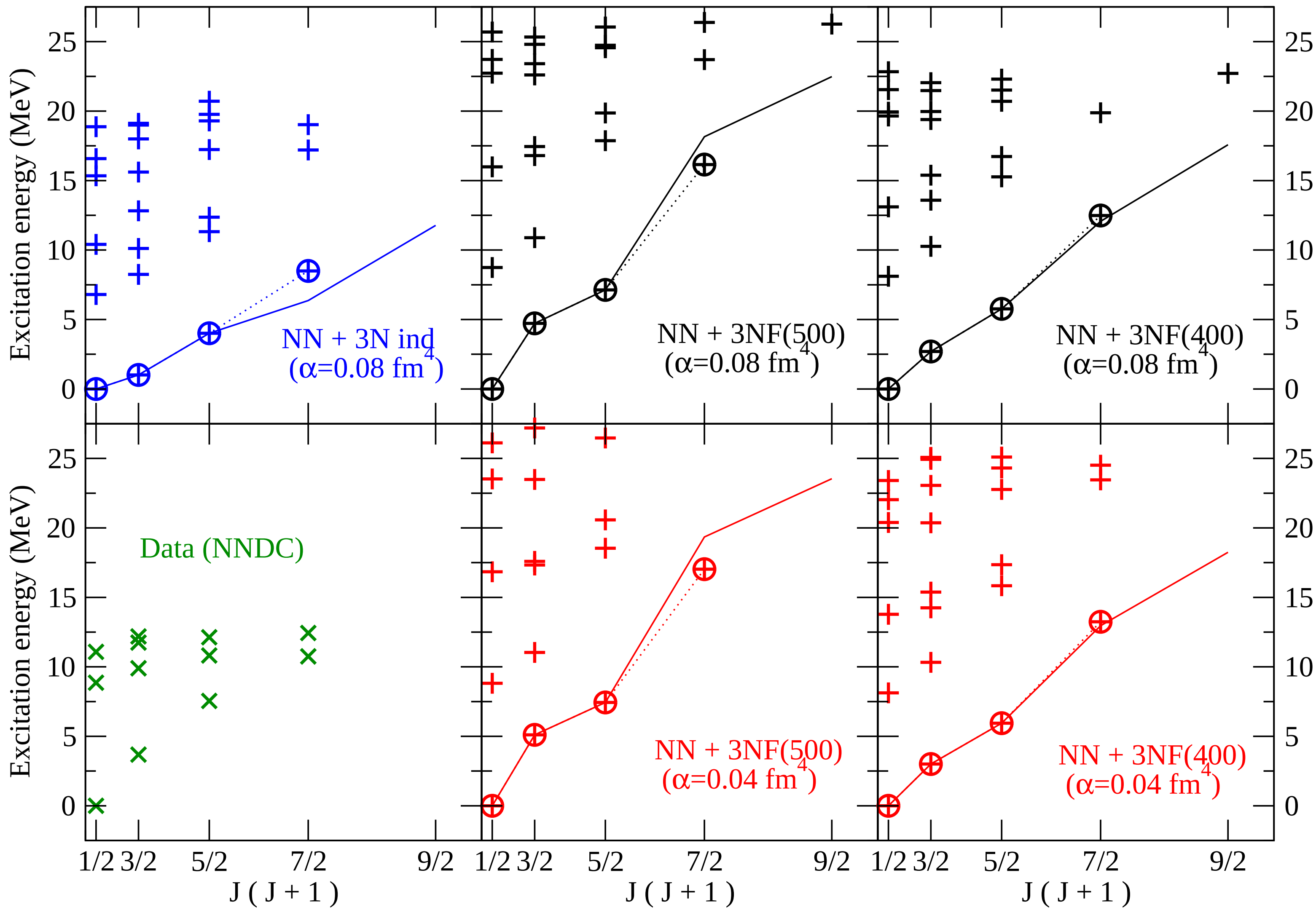


- Clearly underbound without chiral 3NF
- With chiral 3NF
  - overbound with 500 MeV cutoff, $c_D = -0.2$, $c_E = -0.205$
  - (slightly) underbound with 400 MeV cutoff, $c_D = -0.2$, $c_E = 0.098$?
- Need extrapolation to complete basis

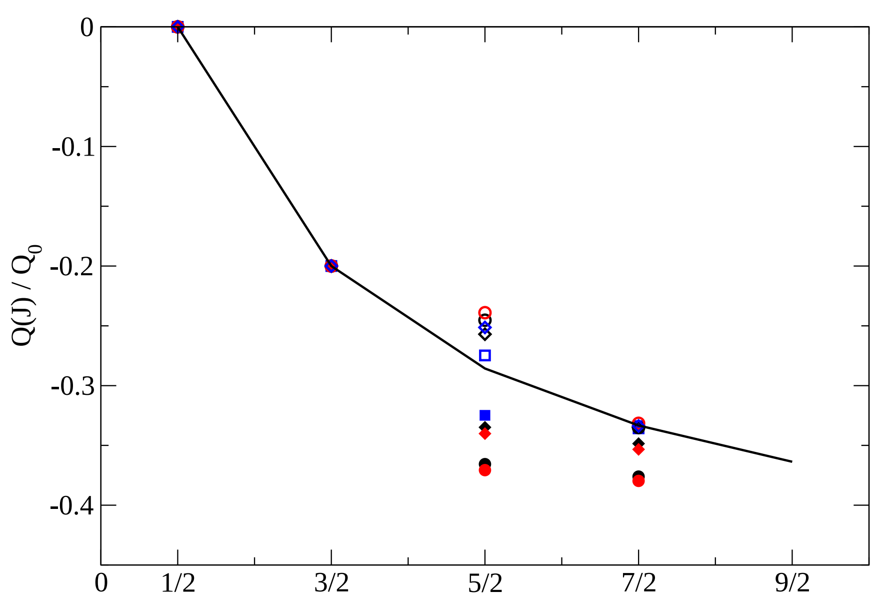
Ground state energies at $N_{\max} = 4$, 6, and 8

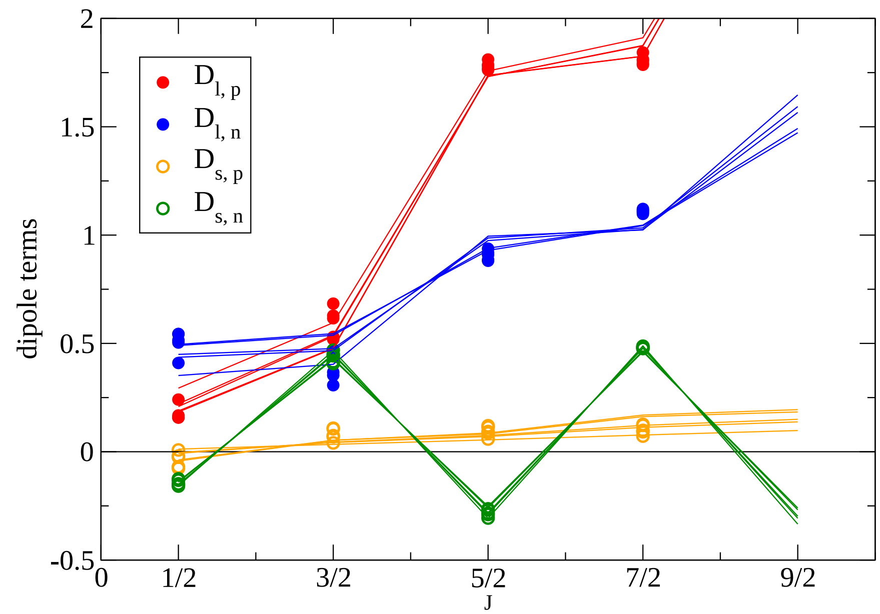
Rotational band(s) in ^{13}C ? – work in progress

Excitation energies at $N_{\max} = 8$, basis parameter $\hbar\omega = 20$ MeV



Rotational band(s) in ^{13}C ? – work in progress





- Quadrupole moments relative to Q_0 agree with rotational band predictions, but lowest $9/2^-$ does not belong to this rotational band
- Magnetic moments in agreement with rotational band predictions
- Need to look at E2 and M1 transitions

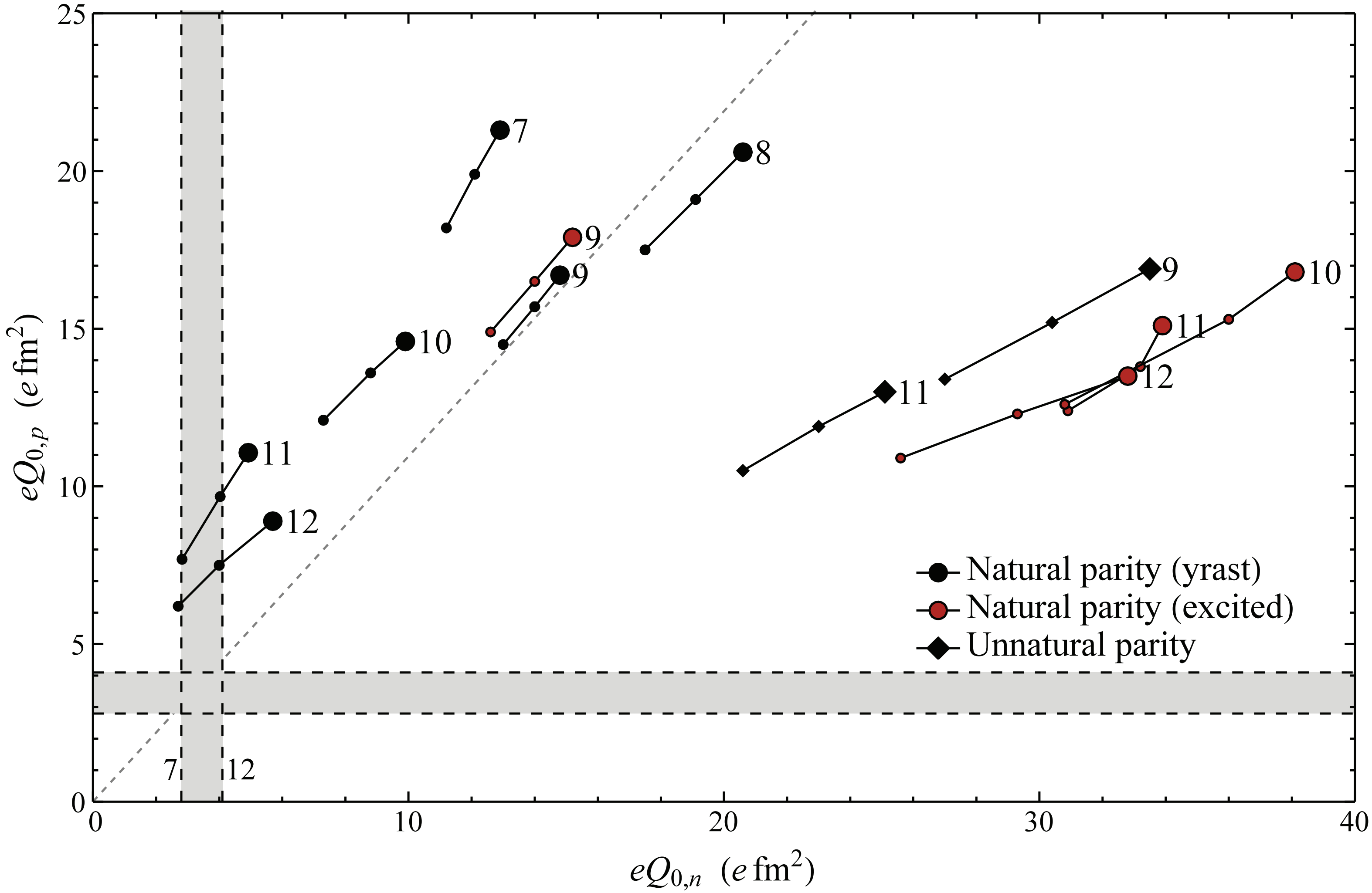
Conclusions

- No-core Configuration Interaction nuclear structure calculations
  - Main challenge: construction and diagonalization of extremely large (D $\sim 10^{10}$) sparse (NNZ $\sim 10^{14}$) matrices
- Emergence of rotational structure
  - Excitation energies (i.e. energy differences)
  - Ratios of $\mathcal{Q}$ moments and E2 transition matrix elements
  - Dipole moments and M1 transition matrix elements
- Perspectives and plans
  - Convergence of long-range observables remains a challenge
    - extrapolation tools
    - efficient truncation schemes w. uncertainty estimates
    - realistic basis functions w. correct asymptotic behavior
  - Resonance state: incorporating continuum
- Would not have been possible without collaboration with applied mathematicians and computer scientists

  NESAP award – early science project on Cori NERSC (Xeon Phi)

Intrinsic quadrupole moments

Maris, Caprio, Vary, arXiv:1409.0881



Although quadrupole moments themselves are not converged

- Significantly larger than Weisskopf estimates
- Ratio of proton over neutron quadupole moments converged

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)

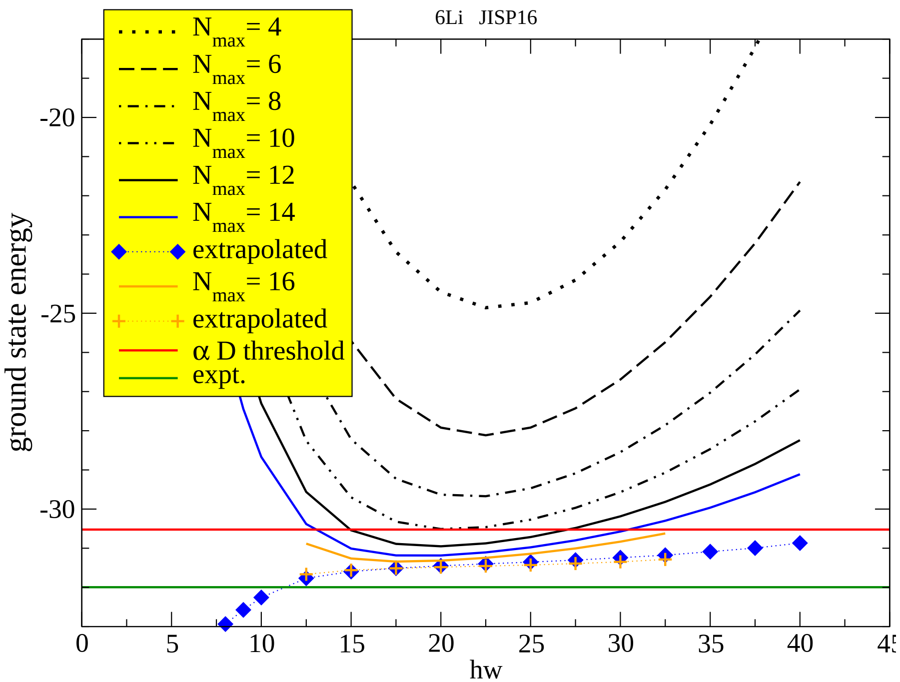
- Recent studies of IR and UV behavior:
  exponentials in $\sqrt{\hbar\omega/N}$ and $\sqrt{\hbar\omega N}$ Coon *et al*, PRC86, 054002 (2012);

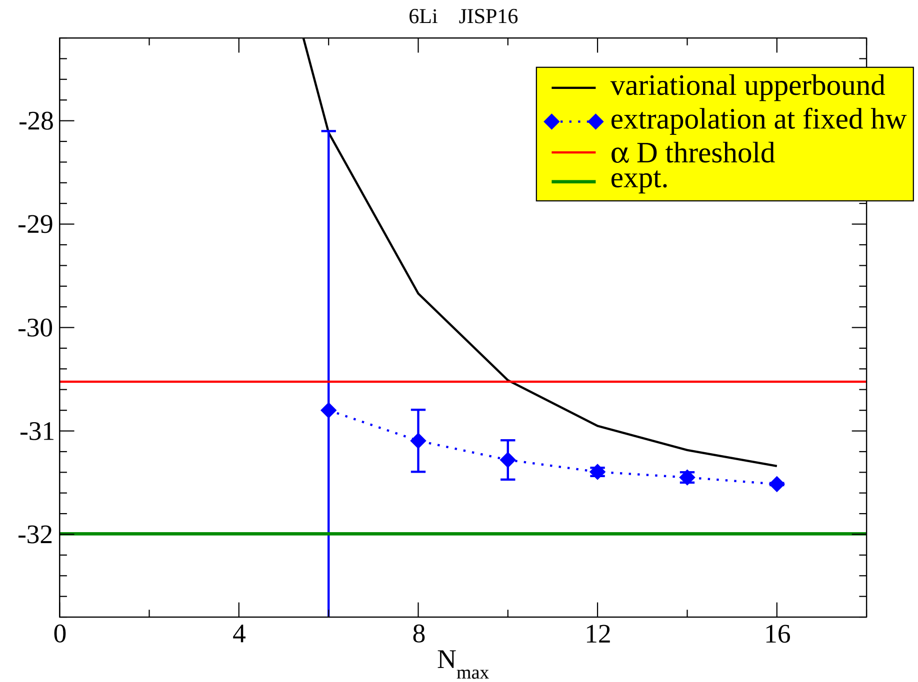
Furnstahl, Hagen, Papenbrock, PRC86, 031301(R) (2012);

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}:
  $E^N_{\text{binding}} = E^\infty_{\text{binding}} + a_1 \exp(-a_2 N_{\text{max}})$





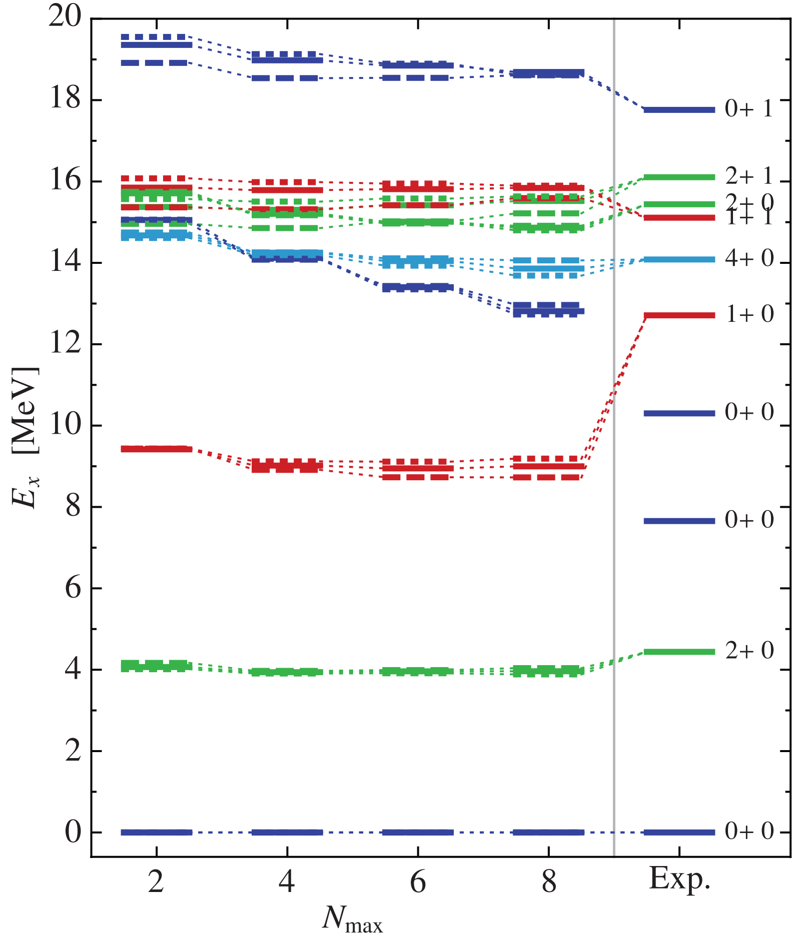
- H.O. basis up to $N_{\text{max}} = 16$: $E_b = -31.49(3)$ MeV

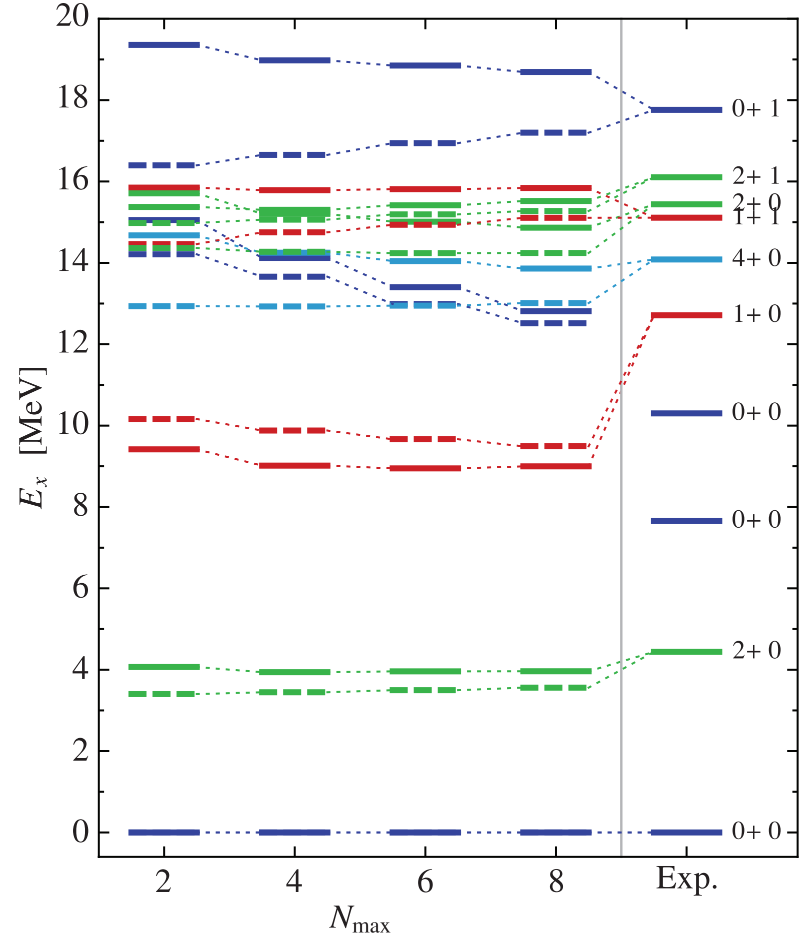
  Cockrell, Maris, Vary, PRC86, 034325 (2012)
- Hyperspherical harmonics up to $K_{\text{max}} = 14$: $E_b = -31.46(5)$ MeV

  Vaintraub, Barnea, Gazit, PRC79, 065501 (2009)

Spectrum of ^{12}C

Maris, Vary, Calci, Langhammer, Binder, Roth, Phys. Rev. C90, 014314 (2014)

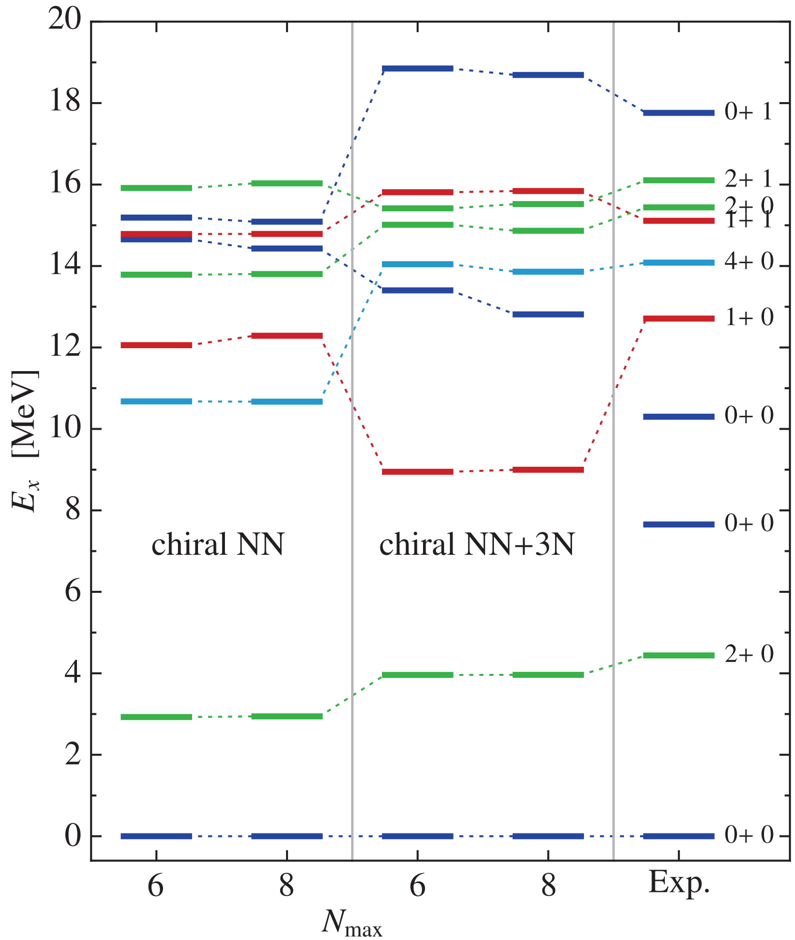




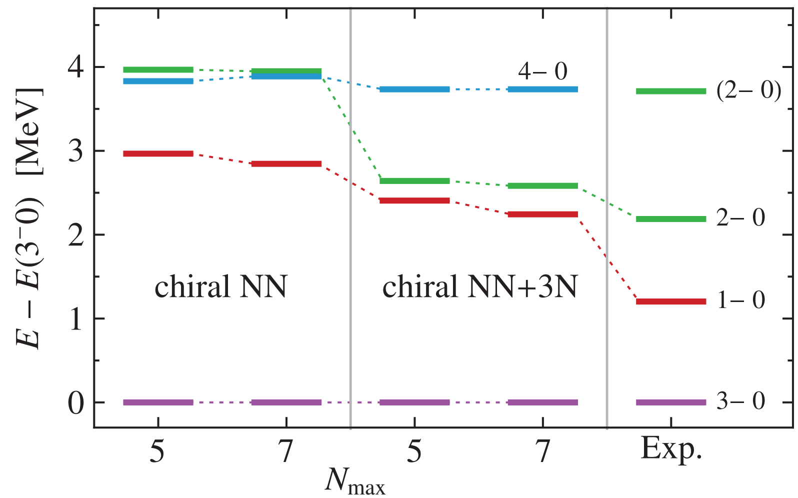
- Excitation energies reasonably well converged
- Dependence of SRG parameter (left) generally smaller than dependence on basis $\hbar\Omega$ (right)

Spectrum of ^{12}C

at SRG parameter $\lambda = 2.0$ fm^{-1} and $\hbar\omega = 20$ MeV

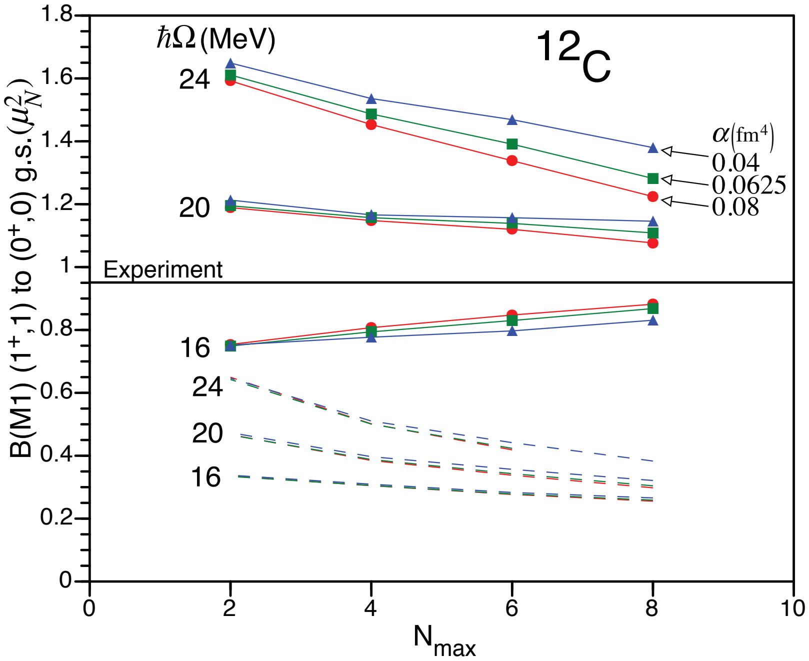


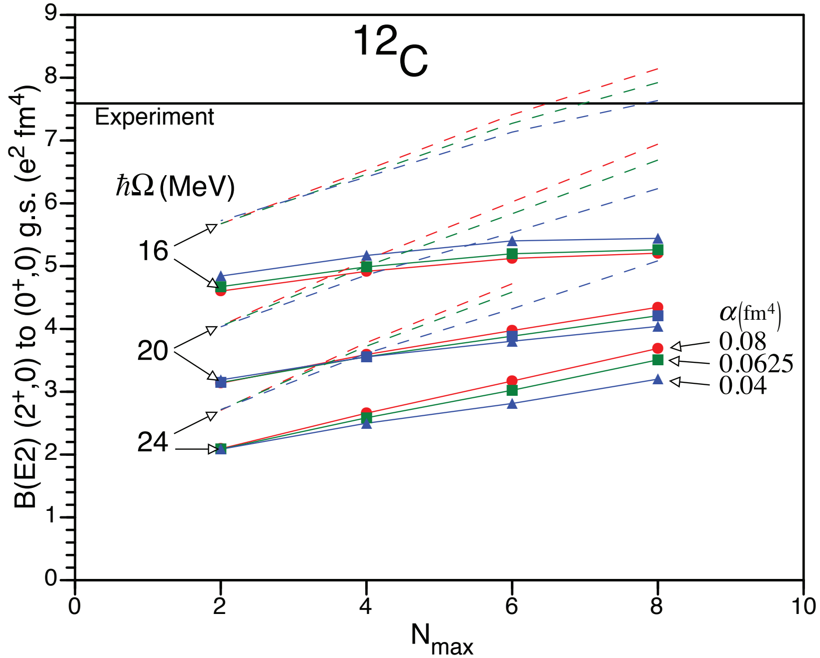
- chiral NN at N^{3}LO
- chiral 3N at N^{2}LO
- 3N LEC values:
  $c_D = -0.2$, $c_E = -0.205$
- 500 MeV cutoff



- 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

Convergence of M1 and E2 transitions

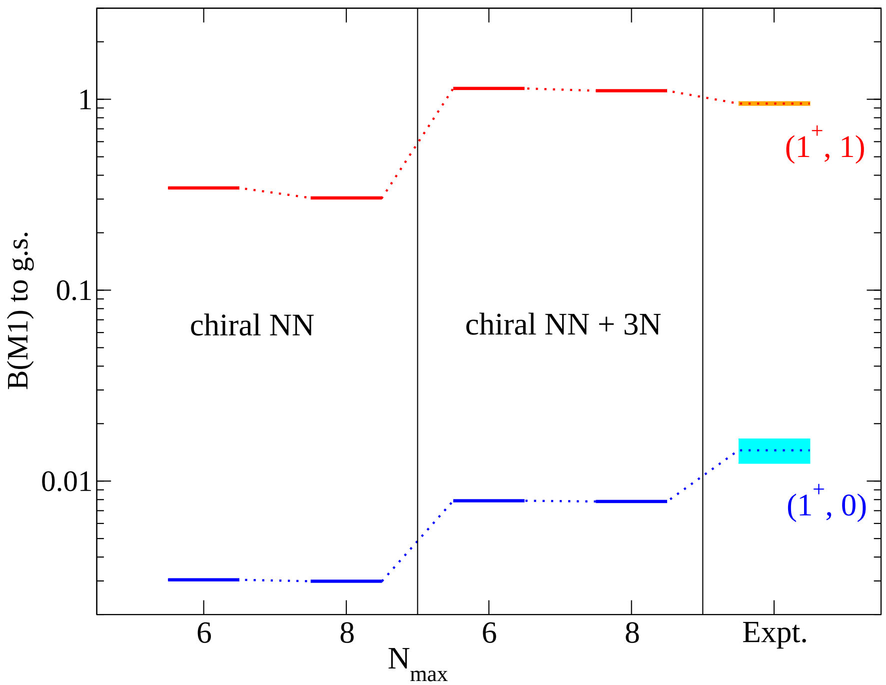


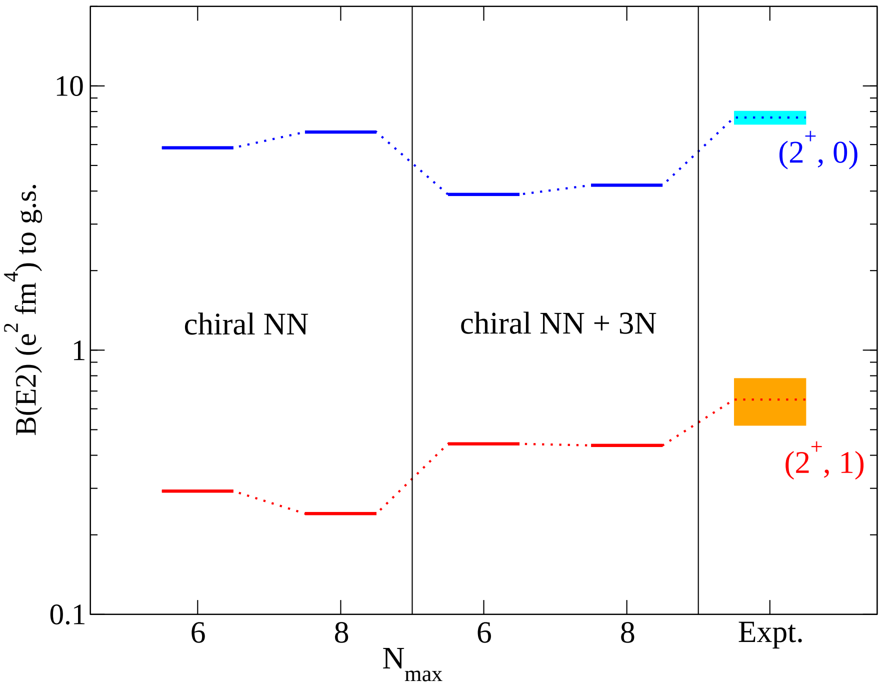


- M1 transitions reasonably converging
- B(M1)$(1^+,1) \to (0^+,0)$ significantly enhanced by 3NF

- E2 transitions not converged
- B(E2)$(2^+,0) \to (0^+,0)$
  - significantly reduced by 3NF
  - consistent with increased E_x and decreased radius and Q

Electromagnetic transitions at SRG parameter $\lambda = 2.0$ fm^{-1} and $\hbar\omega = 20$ MeV

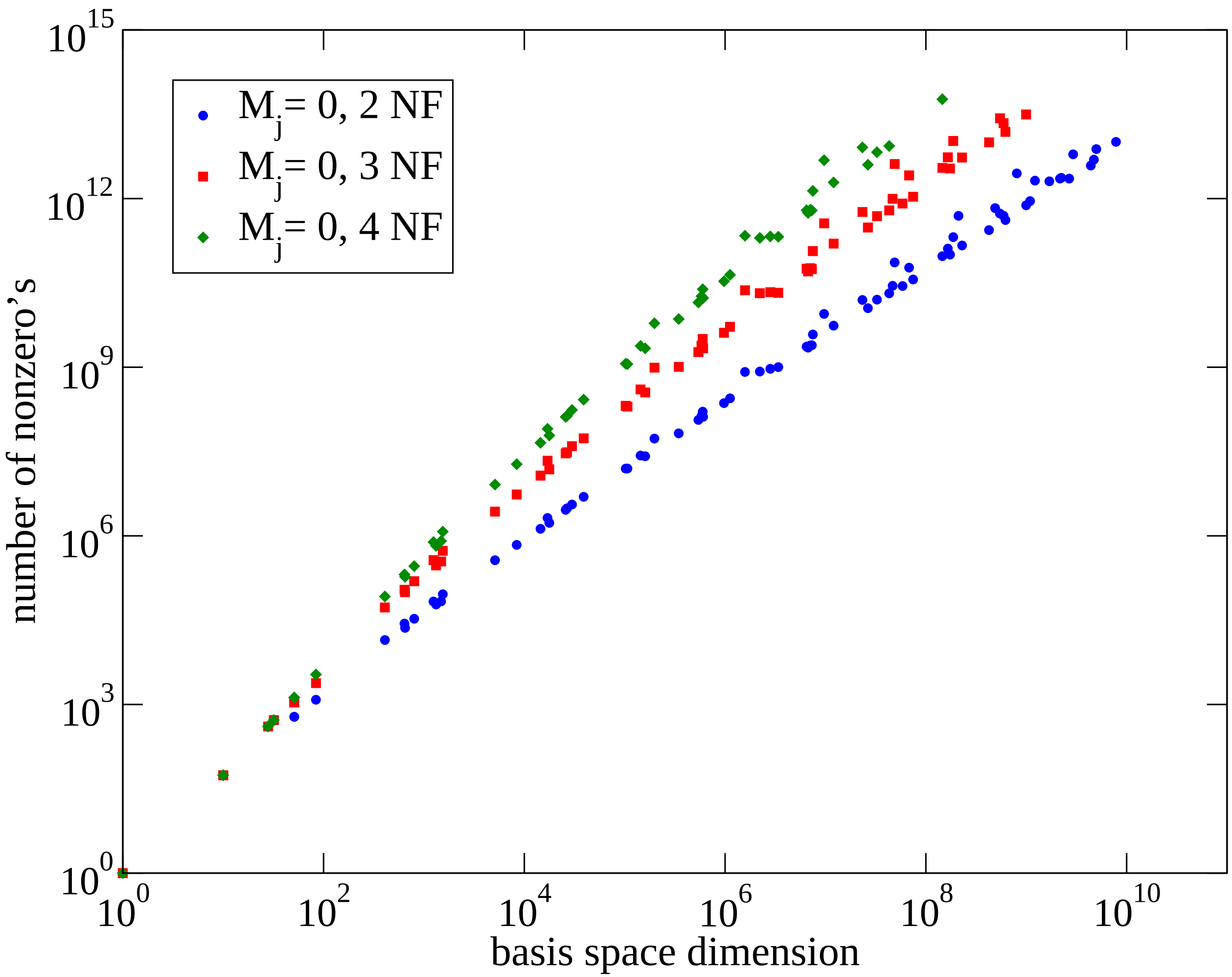




- Transition strengths in qualitative agreement with experiment
- Agreement generally improves by including chiral 3N forces, except for the B(E2)$(2^+, 0) \to (0^+, 0)$ transition
- Future
  - consistent chiral EFT current operators
  - consistent SRG evolution of operators

Looking forward: Taming the scale explosion

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

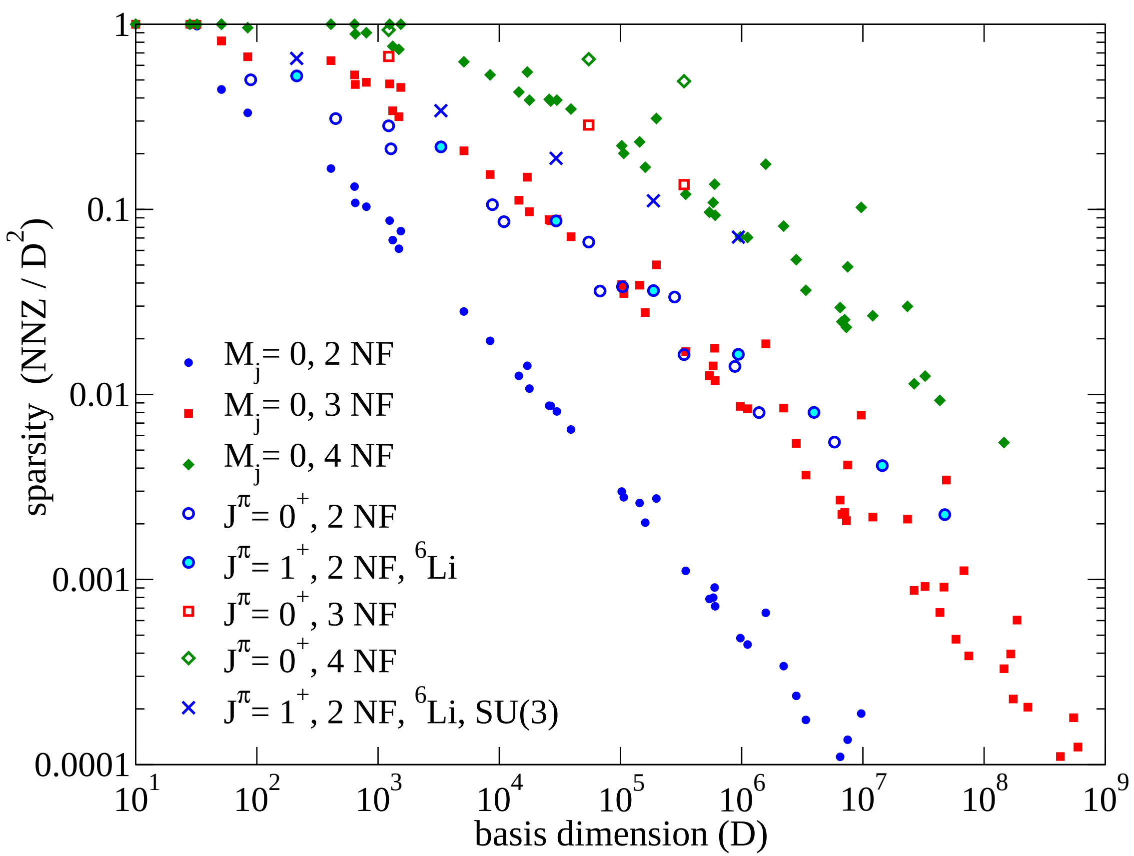


number of nonzero's in M-scheme, $M_j = 0$ for $N = Z$ nuclei from ^{6}Li to ^{20}Ne

- 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
  $95 \cdot 10^{12}$
- Blue Waters: 1.4 PB
  $170 \cdot 10^{12}$

Looking forward: Taming the scale explosion

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

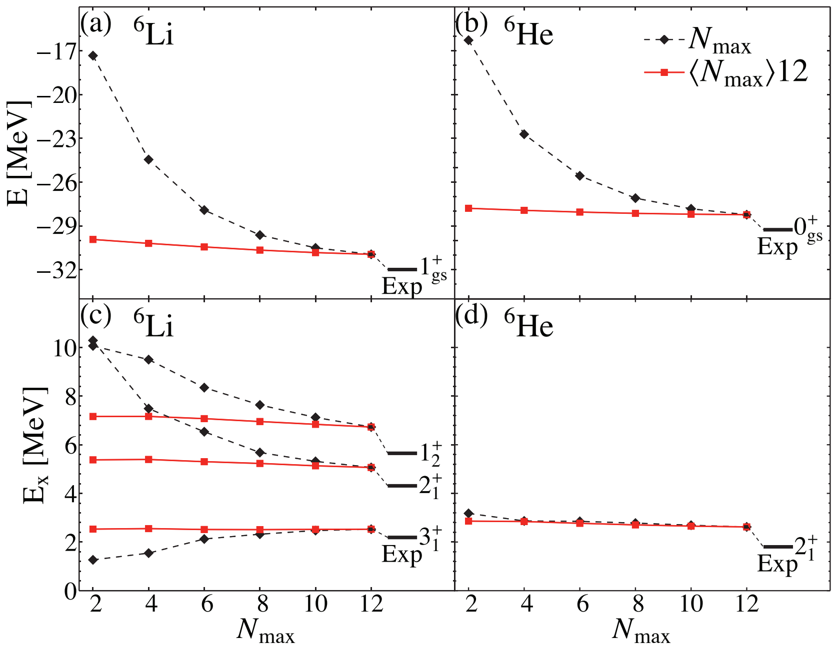


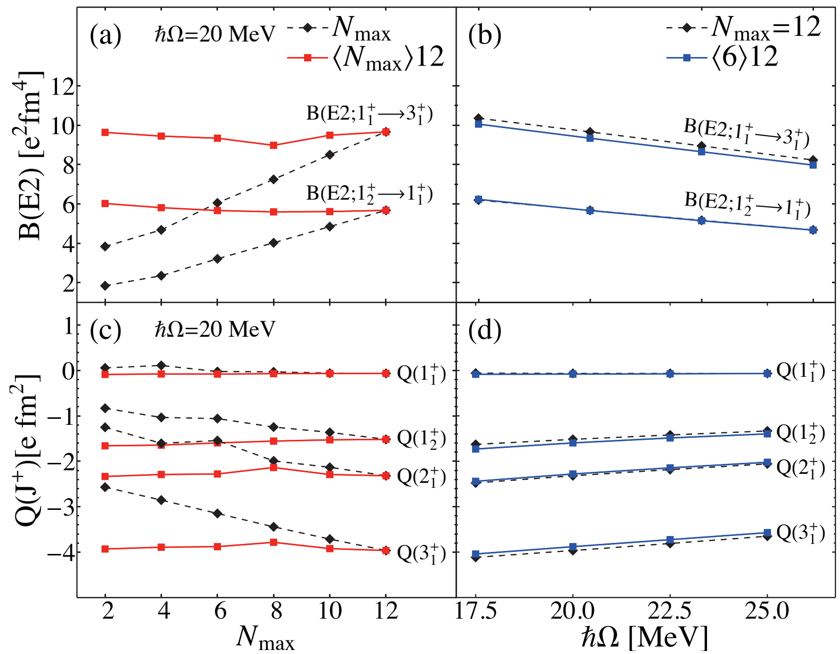
- smaller,
  but less sparse matrices
- number of nonzero matrix elements often (significantly) larger than in M-scheme
- construction of matrix more costly
- larger memory footprint than in M-scheme

Reducing the basis dimension

- Symmetry-Adapted No-Core Shell Model

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





- $\langle N_{\rm max}\rangle 12$ complete basis up to $N_{\rm max}$,
  dominant SU(3) irreps up to $N_{\rm max} = 12$
- Exact factorization (in combination with HO s.p. basis)
- Calculations for ^{12}C and ^{20}Ne in progress

Reducing the basis dimension

- Symmetry-Adapted No-Core Shell Model

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

- No-Core Monte-Carlo Shell Model

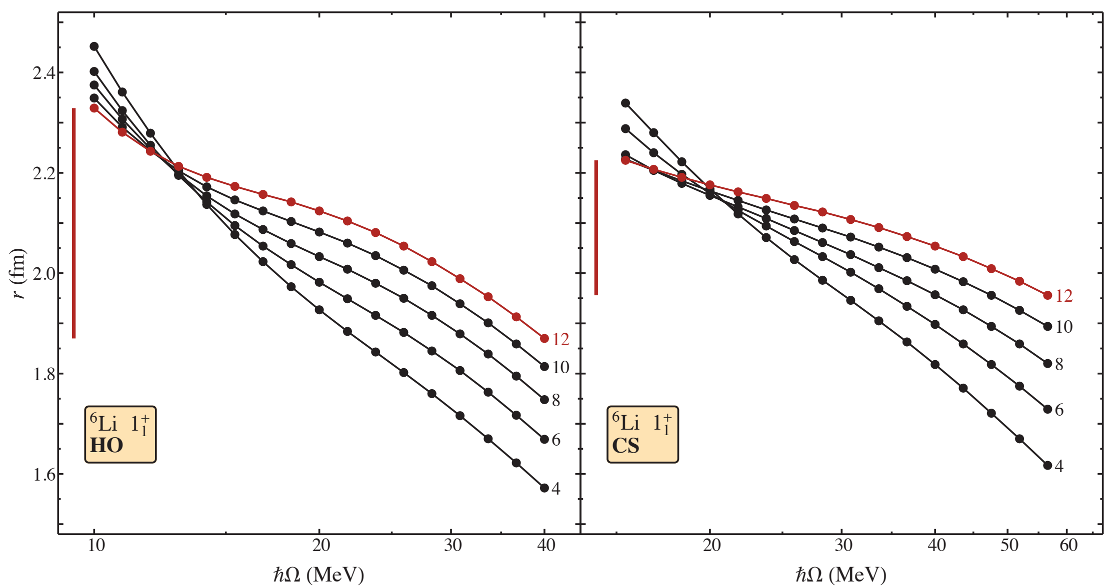
  Abe, Maris, Otsuka, Shimizu, Utsuno, Vary, PRC86, 054301 (2012)
  - based on FCI truncation, not on $N_{\rm max}$ truncation
  - reduce basis to (few) hundred highly optimized states
  - coupled-J basis
  - leads to small but dense matrix
- Importance Truncated NCSM — Roth, PRC79, 064324 (2009)
  - based on $N_{\rm max}$ truncation
  - reduce basis dimension by (several) order(s) of magnitude
  - many-body states single Slater Determinants in M-scheme

Caveat: Uncertainty Quantification

- Can the numerical errors due to reduced basis dimension be quantified within the computational framework?

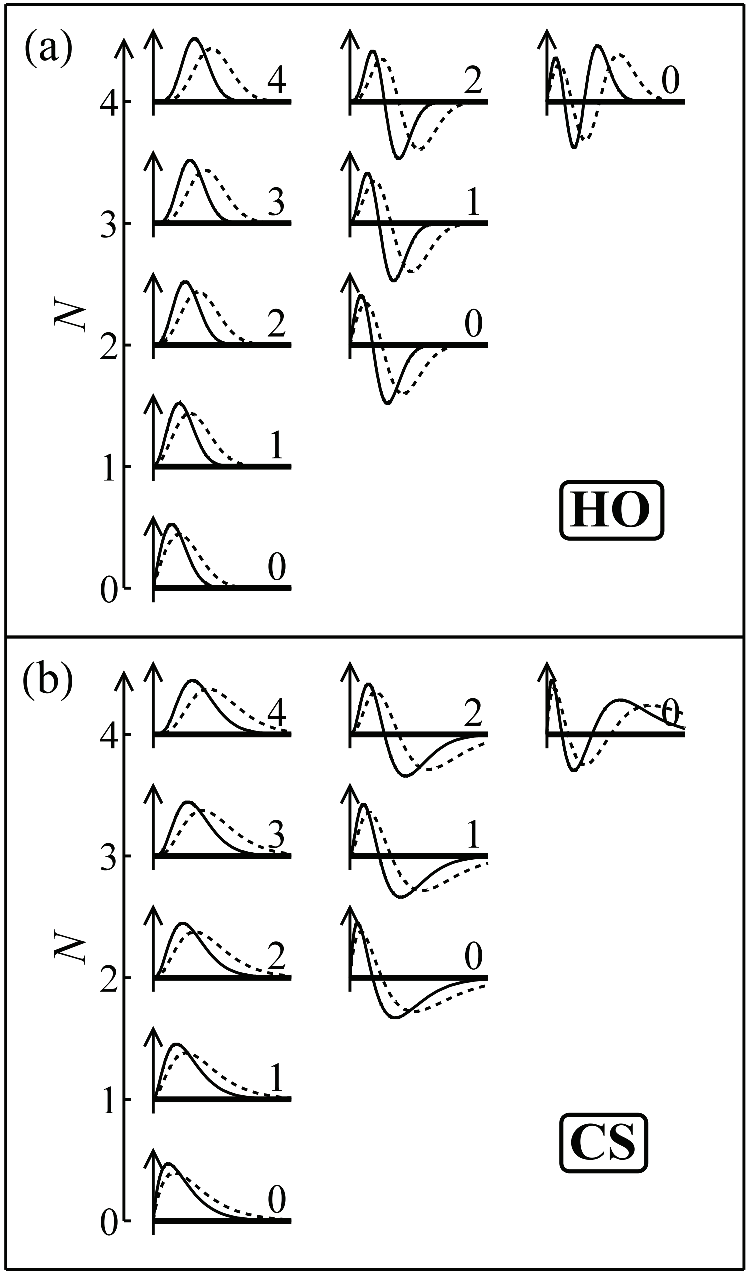
Beyond Harmonic Oscillator wavefunctions

- Berggren basis / No-Core Gamow Shell Model
  - incorporate continuum into basis
  - diagonalize complex symmetrix matrix
- Coulomb–Sturmian basis
  - radial basis functions with exponential asymptotic behavior



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

Coulomb–Sturmian basis



Caprio, Maris, Vary, PRC86, 034312 (2012);
PRCC90, 034305 (2014)

- Harmonic Oscillator radial w.f.

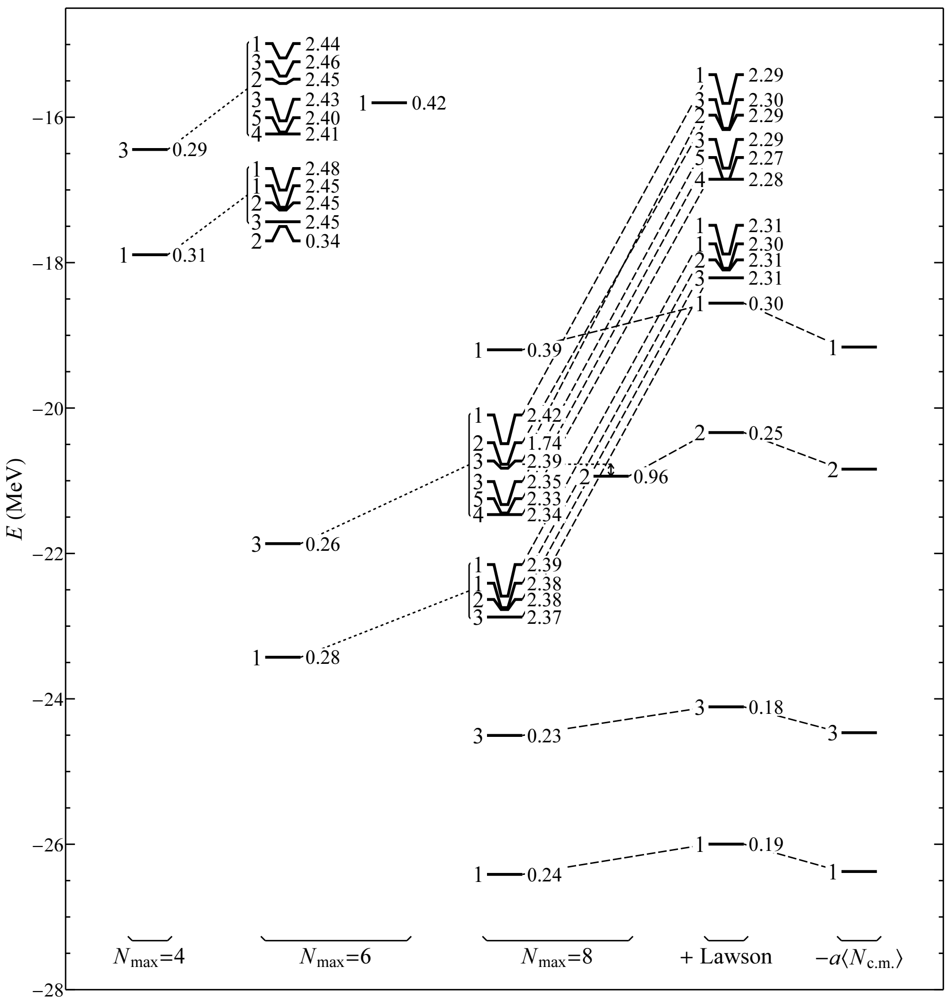
$$R_{nl}(b;r) = \left(\frac{r}{b}\right)^{l+1} L_n^{l+\frac{1}{2}}\left((r/b)^2\right) e^{-\frac{1}{2}(r/b)^2}$$

- Coulomb–Sturmian radial w.f.

$$S_{nl}(b;r) = \left(\frac{2r}{b}\right)^{l+1} L_n^{2l+2}(2r/b)\, e^{-r/b}$$

- Length scale b_l choosen such that nodes of $n = 1$ CS and HO w.f. coincide
- CS basis
  - truncation on $\sum(2n + l)$ for comparison with HO basis
  - no exact factorization of CM motion

Center-of-Mass motion



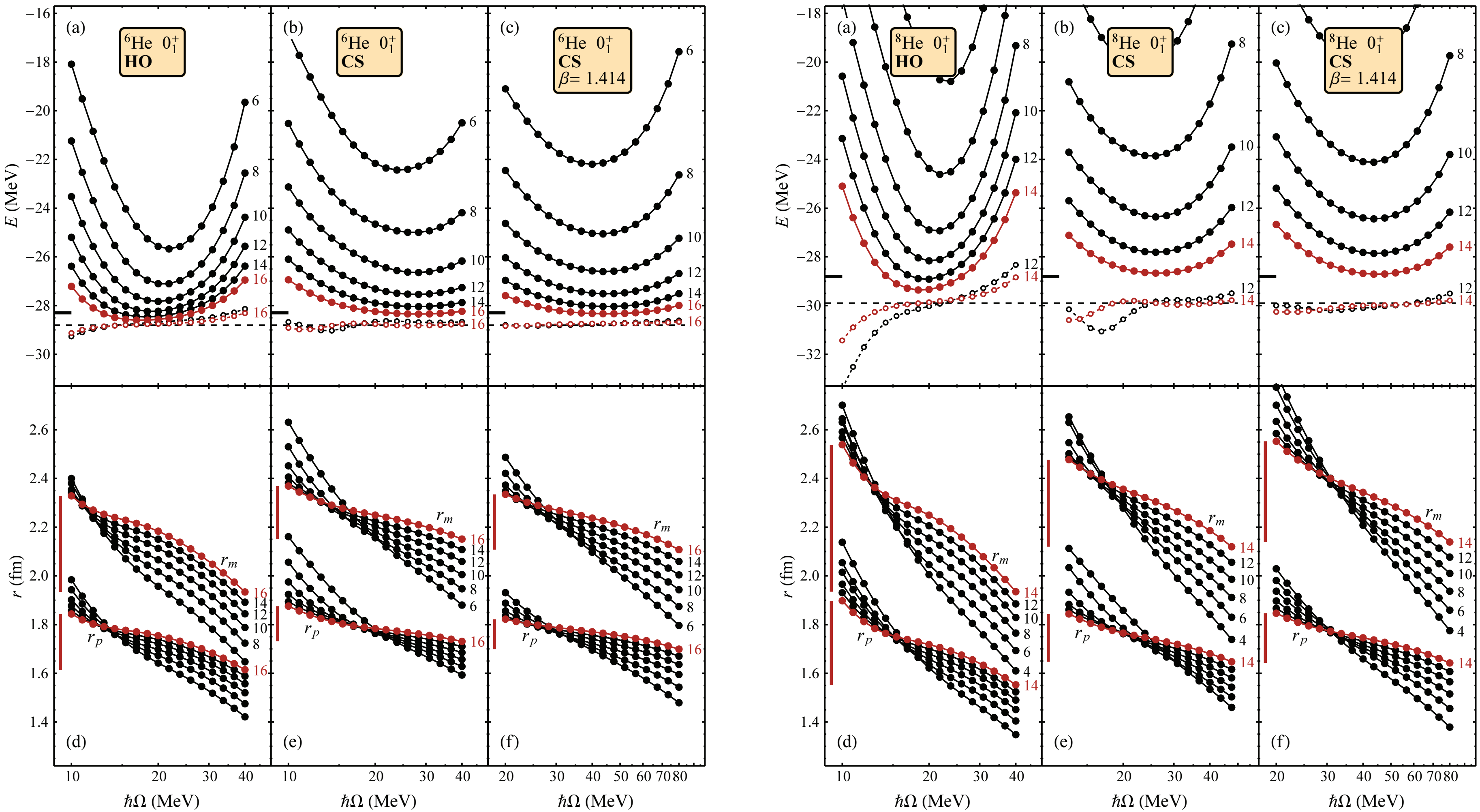
Caprio, Maris, Vary,

PRC86, 034312 (2012)

- Without Lagrange multiplier
  - at $N_{\text{max}} = 6$
    - 4 degenerate states:
      $J^\pi = 1^+$ states at $N_{\text{max}} = 4$
      with 2 quanta CM excitations
    - 6 degenerate states:
      $J^\pi = 3^+$ states at $N_{\text{max}} = 4$
      with 2 quanta CM excitations
  - degenerate states at $N_{\text{max}} = 8$:
    - 1^+ and 3^+ states at $N_{\text{max}} = 6$
      with 2 quanta CM excitations
    - 1^+ and 3^+ states at $N_{\text{max}} = 4$
      with 4 quanta CM excitations
- With Lagrange multiplier all states with CM excitations are removed from low-lying spectrum

Coulomb–Sturmian for halo nuclei

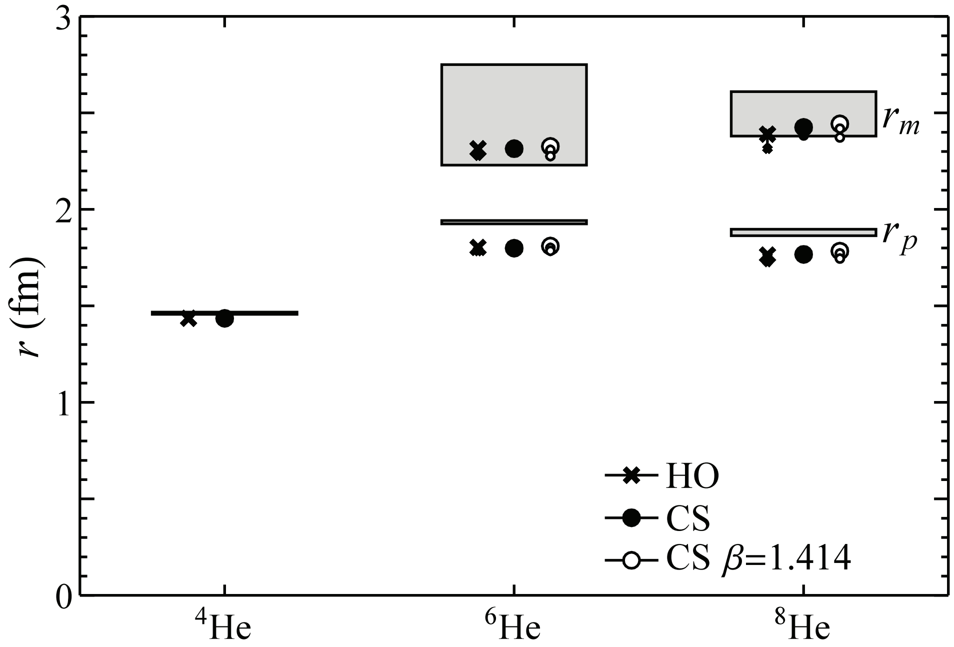
Caprio, Maris, Vary, PRC90, 034305 (2014)



- CS: different length parameters b_l for protons and neutrons

Radii of He isotopes with JISP16

Caprio, Maris, Vary, PRC90, 034305 (2014)



- Radii exctracted from crossover point for three highest N_{max} values
- HO and CS basis in good agreement with each other
- Qualitative agreement with data
- Note: matter radii in agreement with elastic scattering measurement/extraction of experimental radius

Future plans

- Explore different basis truncation schemes
- Apply to chiral NN and 3N interactions