Predictions for nuclear rotational structure from *ab initio* calculations

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Nuclear Theory in the Supercomputing Era
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Rotational structure from *ab initio* nuclear theory?

Ab initio theory should be able to describe nuclei

Light nuclei display rotational band structure

$\therefore$ *Ab initio* theory should be able to predict rotational bands

But... Convergence challenges in calculation of relevant observables

– Qualitative emergence of rotational "features"?
  Rotational energies, rotational transition patterns
– Robust quantititative prediction of rotational observables?
  Rotational energy parameters, intrinsic E2 matrix elements
– Physical nature of rotation in light nuclei — What can we learn?

Emergence of rotational patterns in Be isotopes

M. A. Caprio, P. Maris, and J. P. Vary, Phys. Lett. B **719**, 179 (2013).
P. Maris, M. A. Caprio, and J. P. Vary, Phys. Rev. C **91**, 014310 (2015).
C. W. Johnson, Phys. Rev. C **91**, 034313 (2015).
M. A. Caprio, P. Maris, J. P. Vary, and R. Smith, Int. J. Mod. Phys. E **24**, 1541002 (2015), arXiv:1509.00102.

Separation of rotational degree of freedom

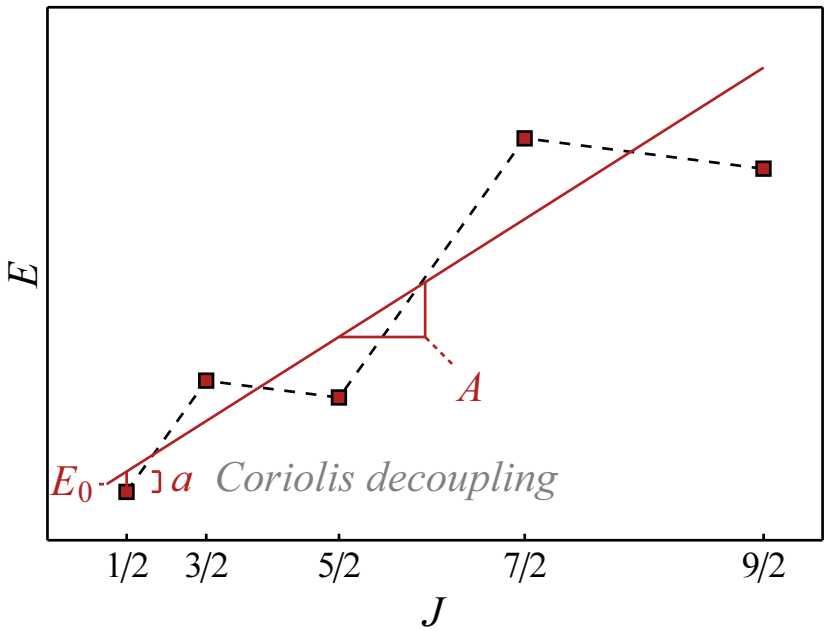
Intrinsic state $|\phi_K\rangle$ & rotation in Euler angles ϑ $\qquad (J = K, K+1, \ldots)$

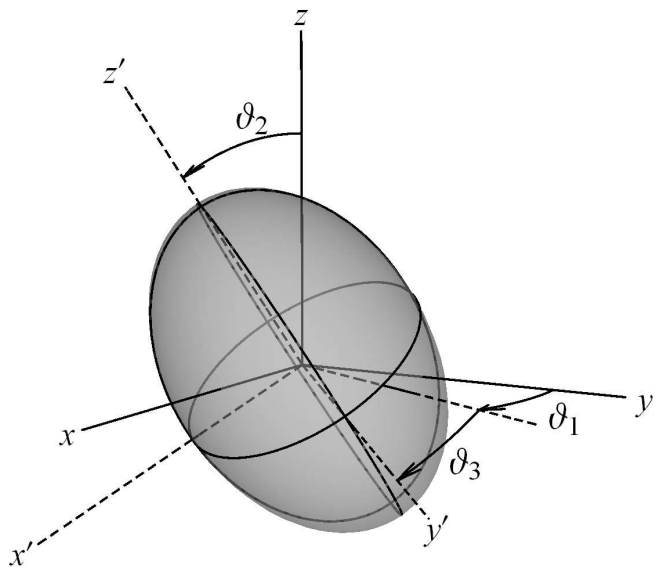
$$|\psi_{JKM}\rangle \propto \int d\vartheta \left[\mathcal{D}^J_{MK}(\vartheta)|\phi_K;\vartheta\rangle + (-)^{J+K}\mathcal{D}^J_{M-K}(\vartheta)|\phi_{\bar{K}};\vartheta\rangle \right]$$

Rotational energy

$$E(J) = E_0 + A\left[J(J+1) + \underbrace{a(-)^{J+1/2}(J+\tfrac{1}{2})}_{\text{Coriolis } (K=1/2)}\right] \qquad A \equiv \frac{\hbar^2}{2\mathcal{J}}$$

Rotational relations on electromagnetic transitions ($E2$, $M1$, ...)





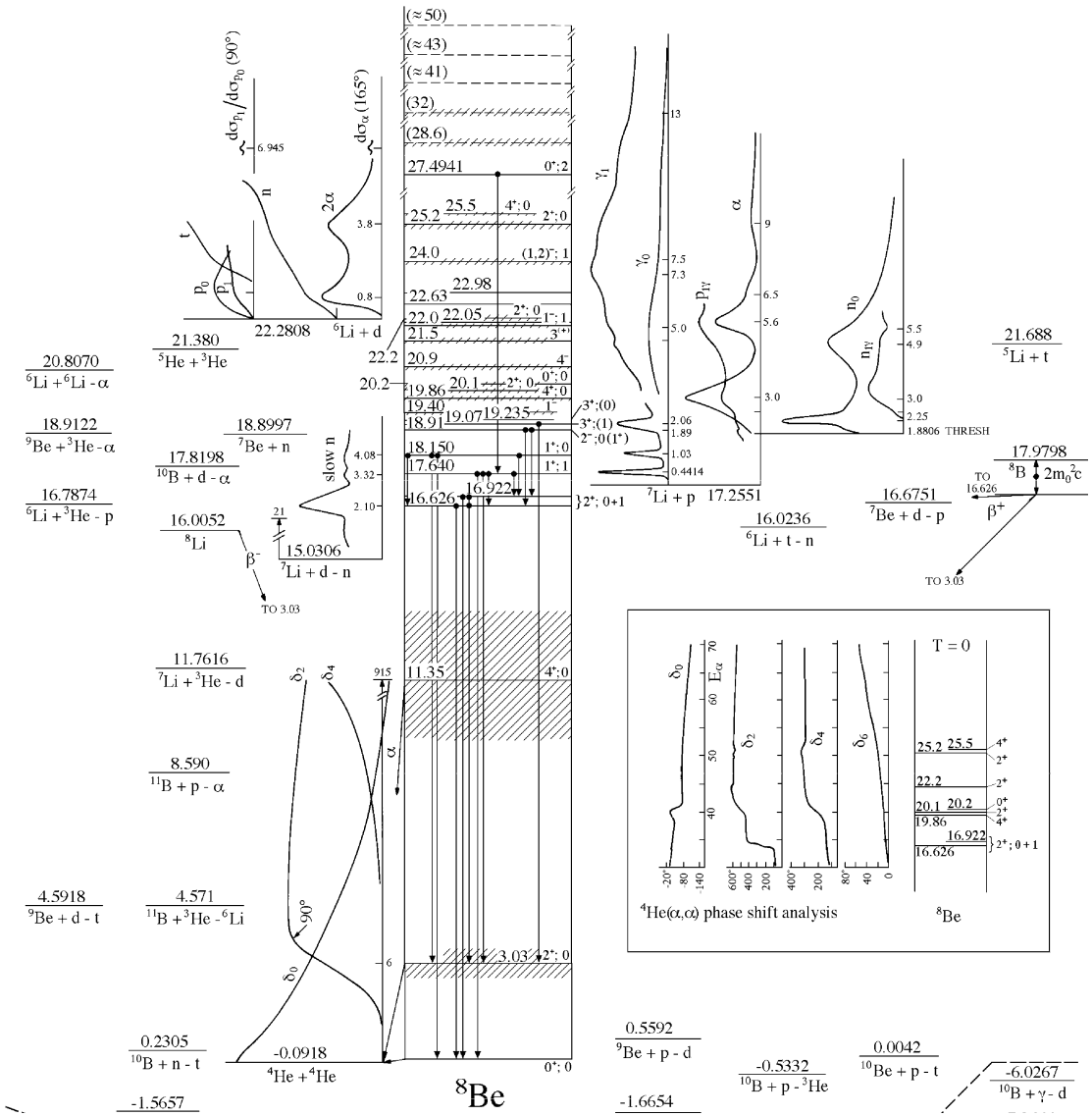


Figure from D.R. Tilley *et al.*, Nucl. Phys. A **745**, 155 (2004).

Observed energy levels for $A = 7$ nuclei

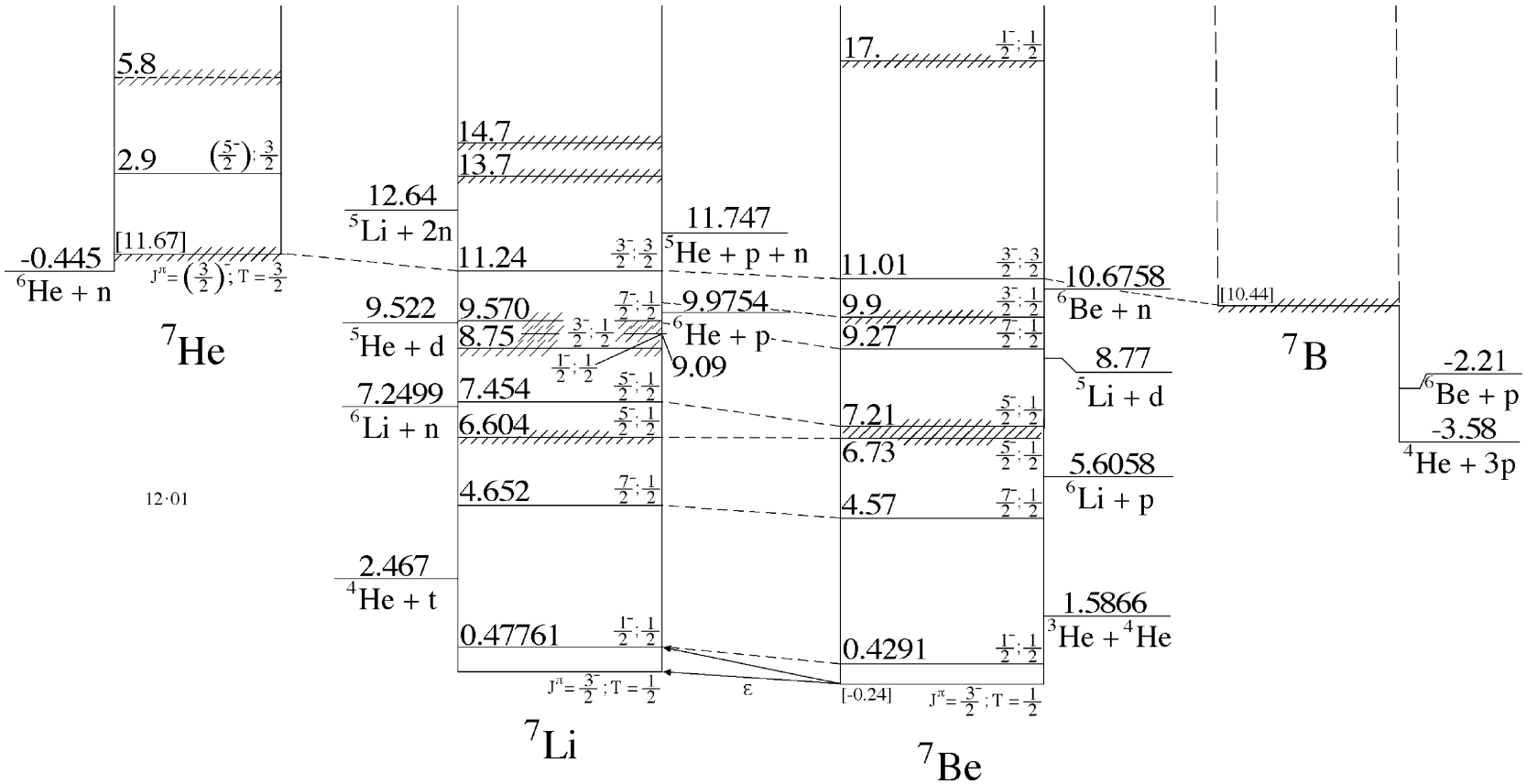
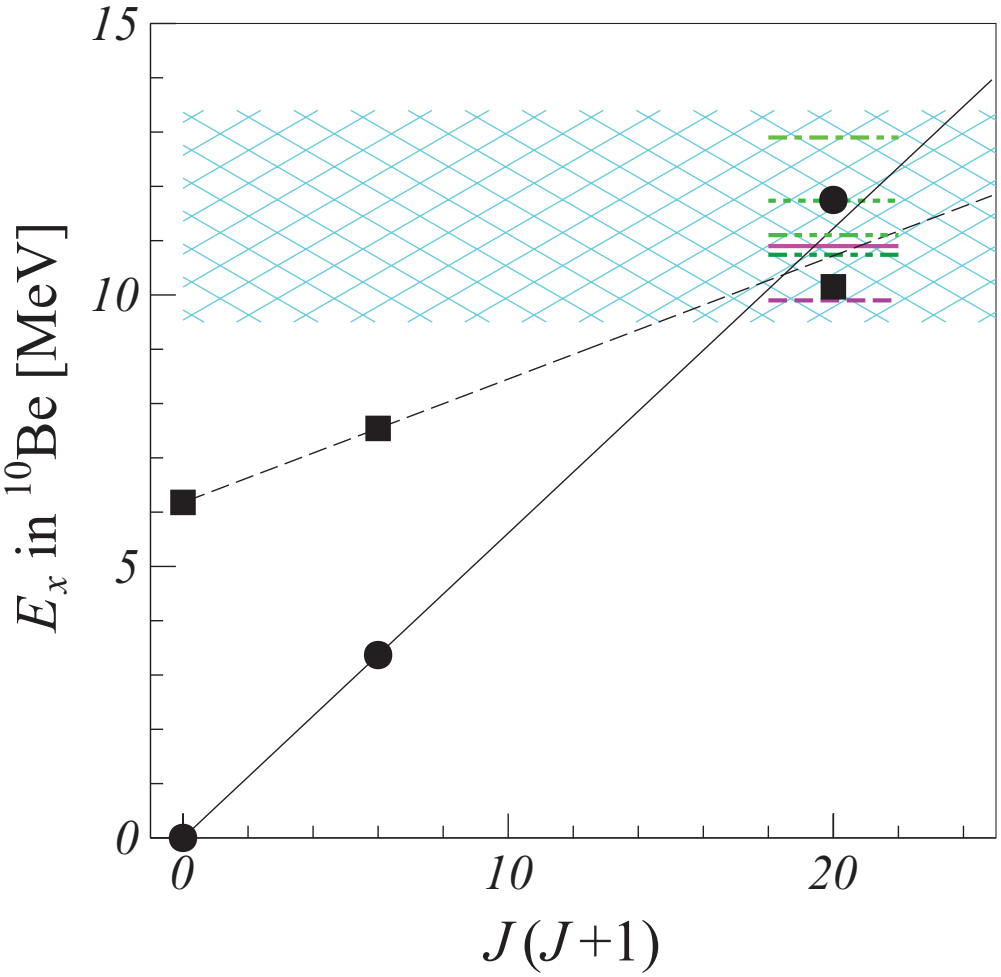
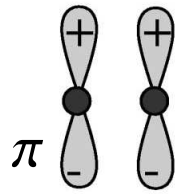


Figure from D.R. Tilley *et al.*, Nucl. Phys. A **708**, 3 (2002).

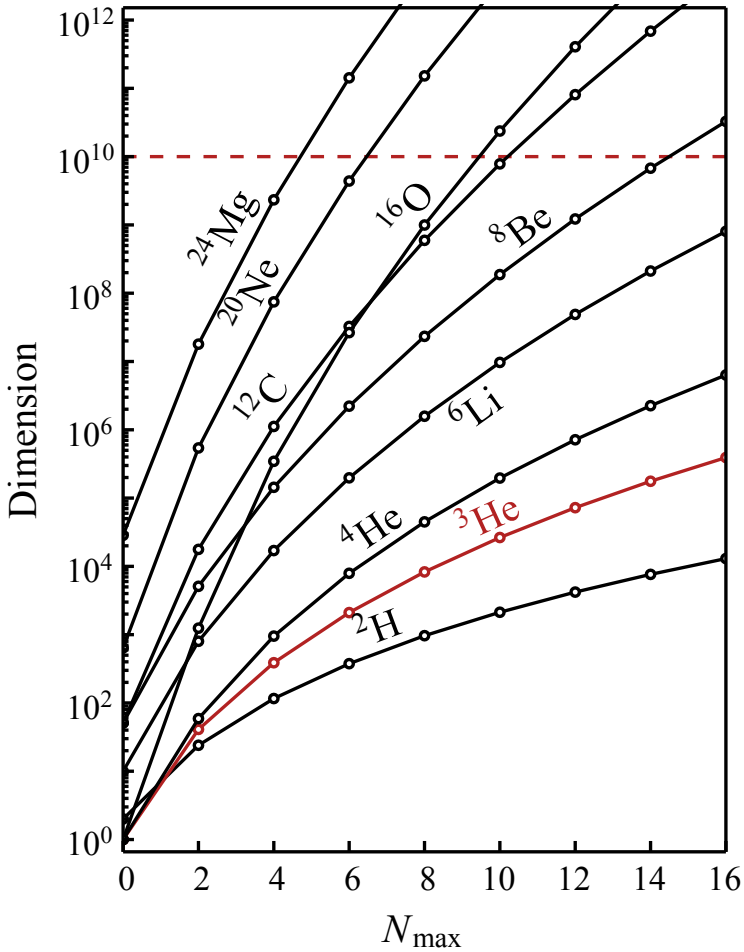
Yrast and excited bands in ^{10}Be

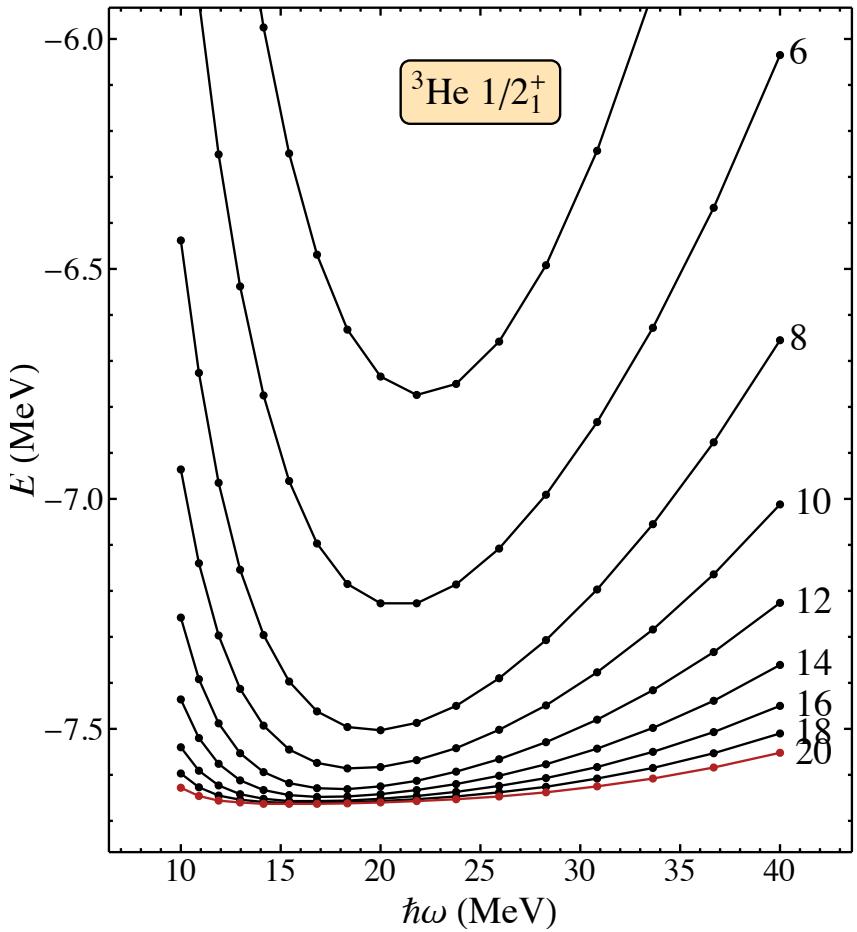




From D. Suzuki *et al.*, Phys. Rev. C **87**, 054301 (2013). Orbital schematics from Y. Kanada-En'yo, H. Horiuchi, and A. Doté, Phys. Rev. C **60**, 064304 (1999).

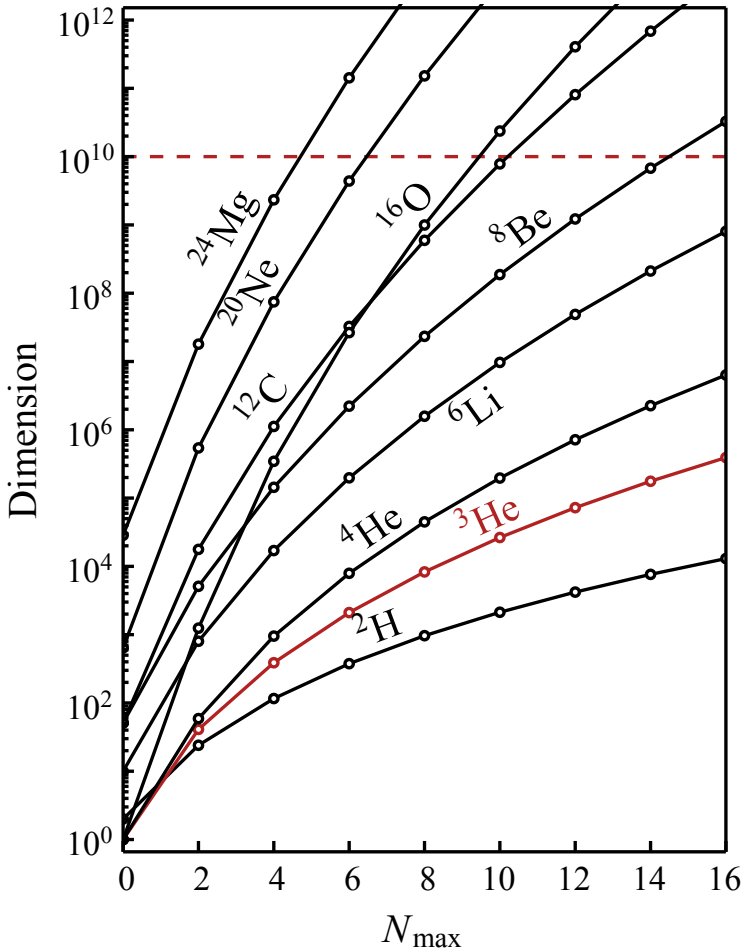
Convergence of NCCI calculations

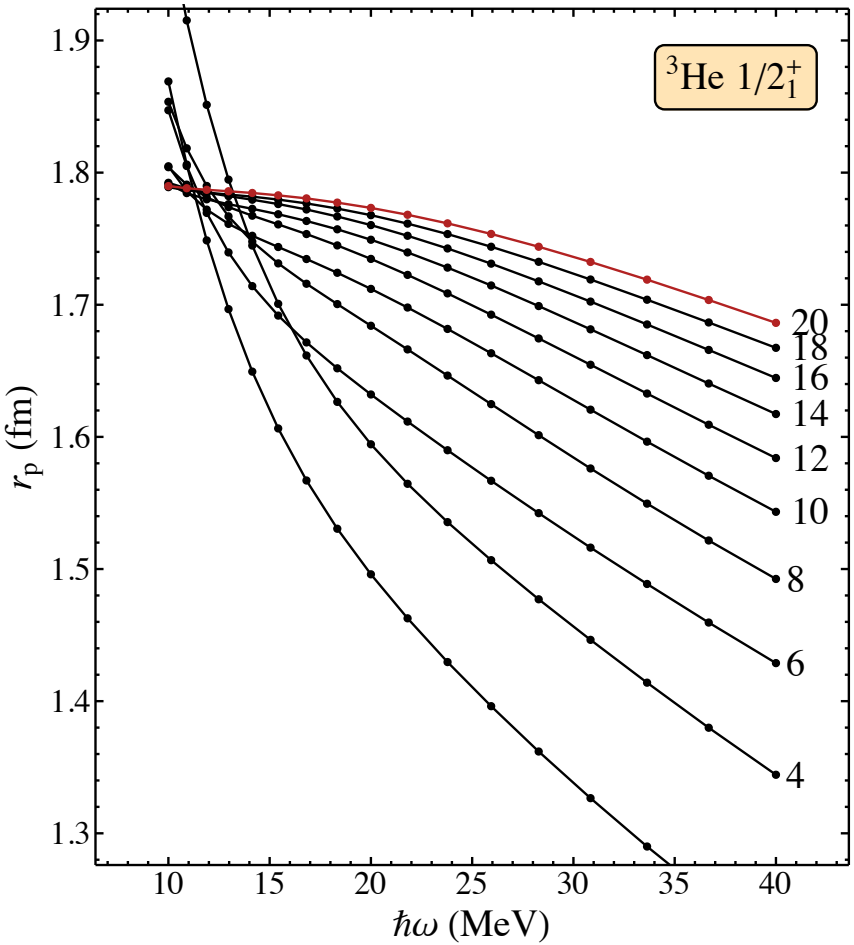




JISP16 + Coulomb interaction

Convergence of NCCI calculations





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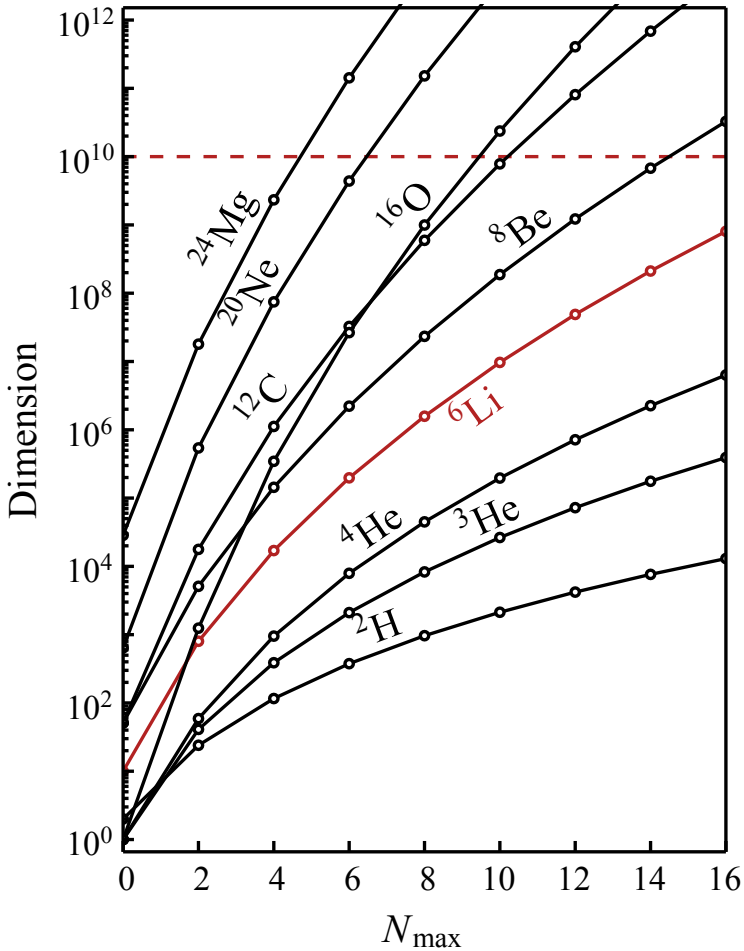

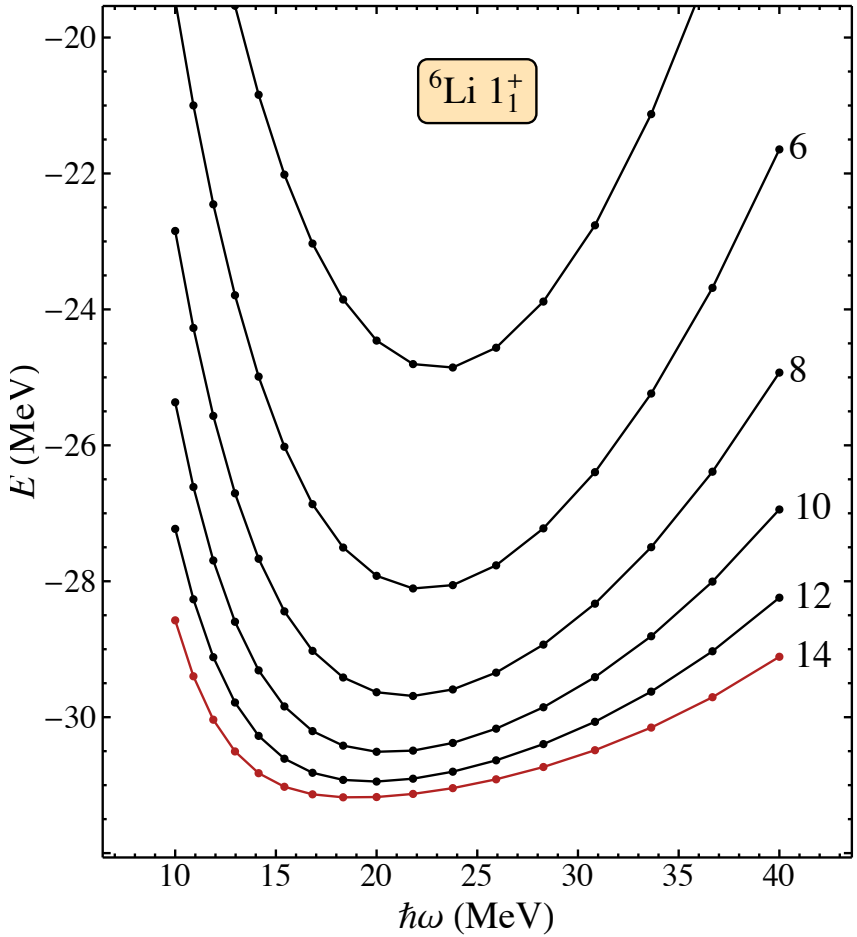

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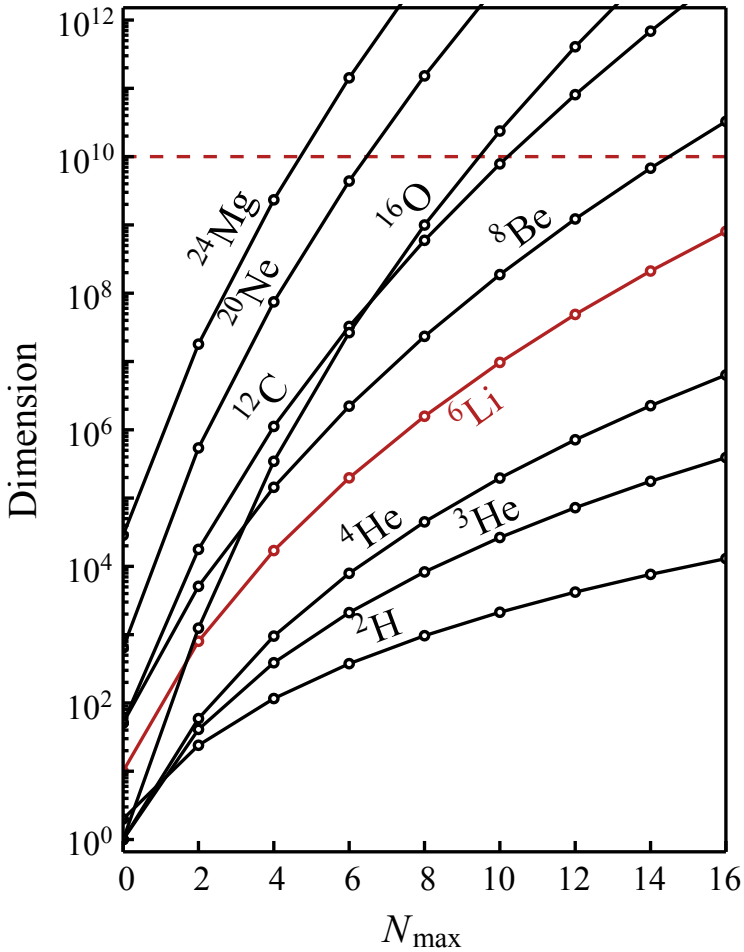

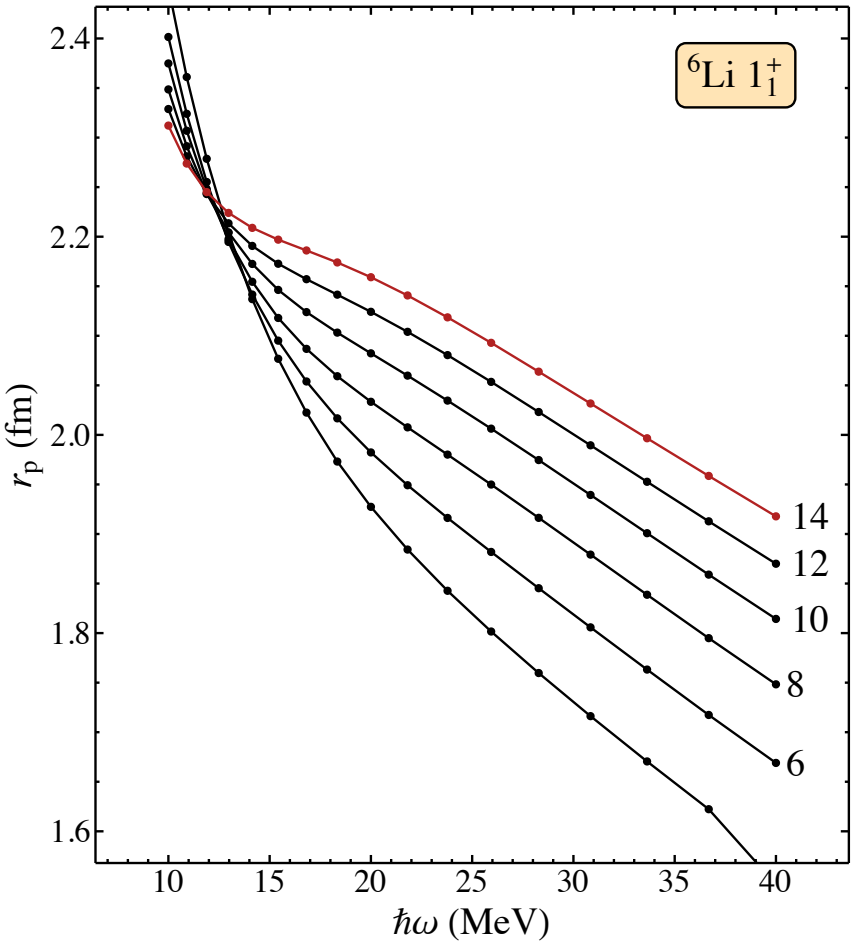

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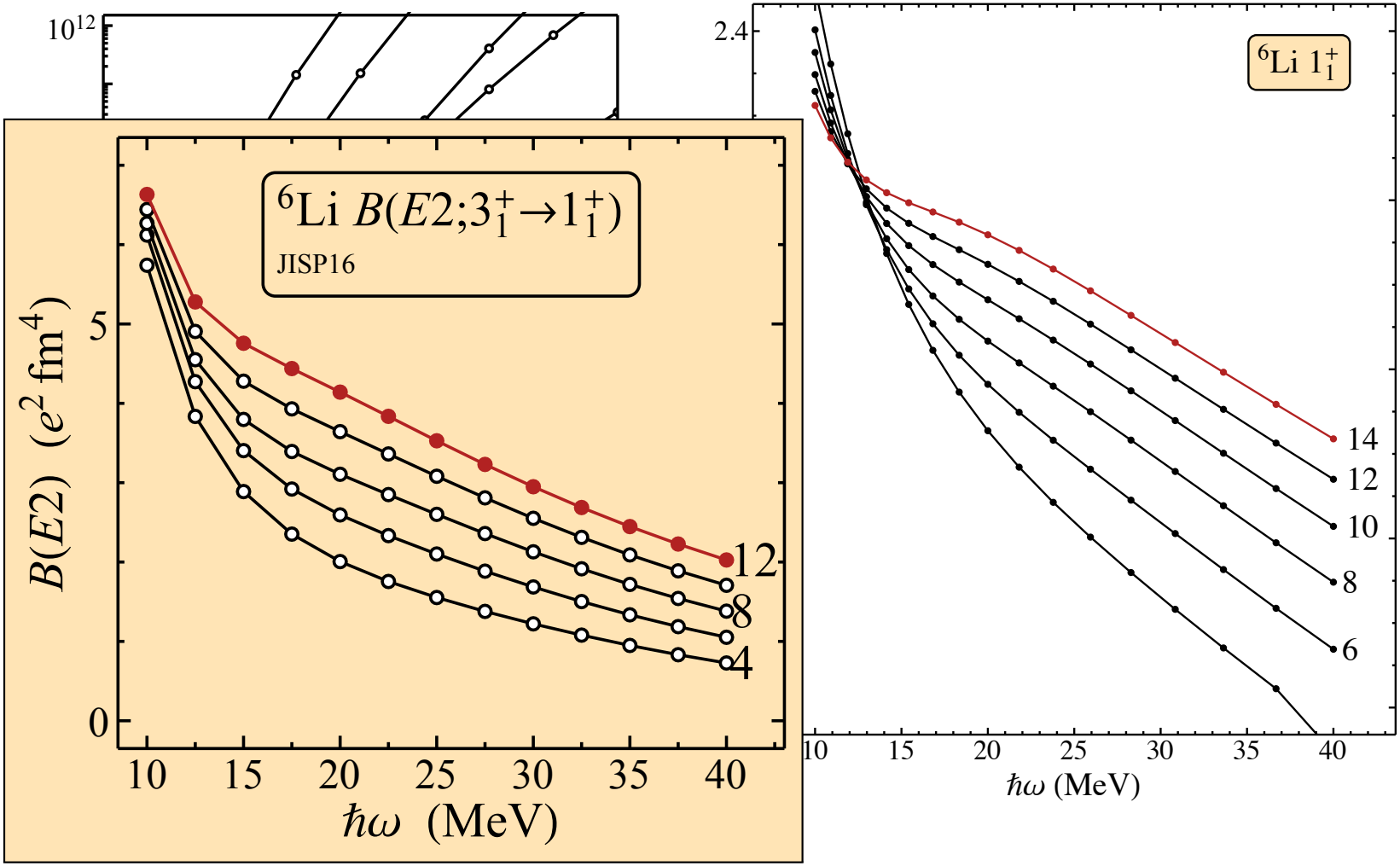
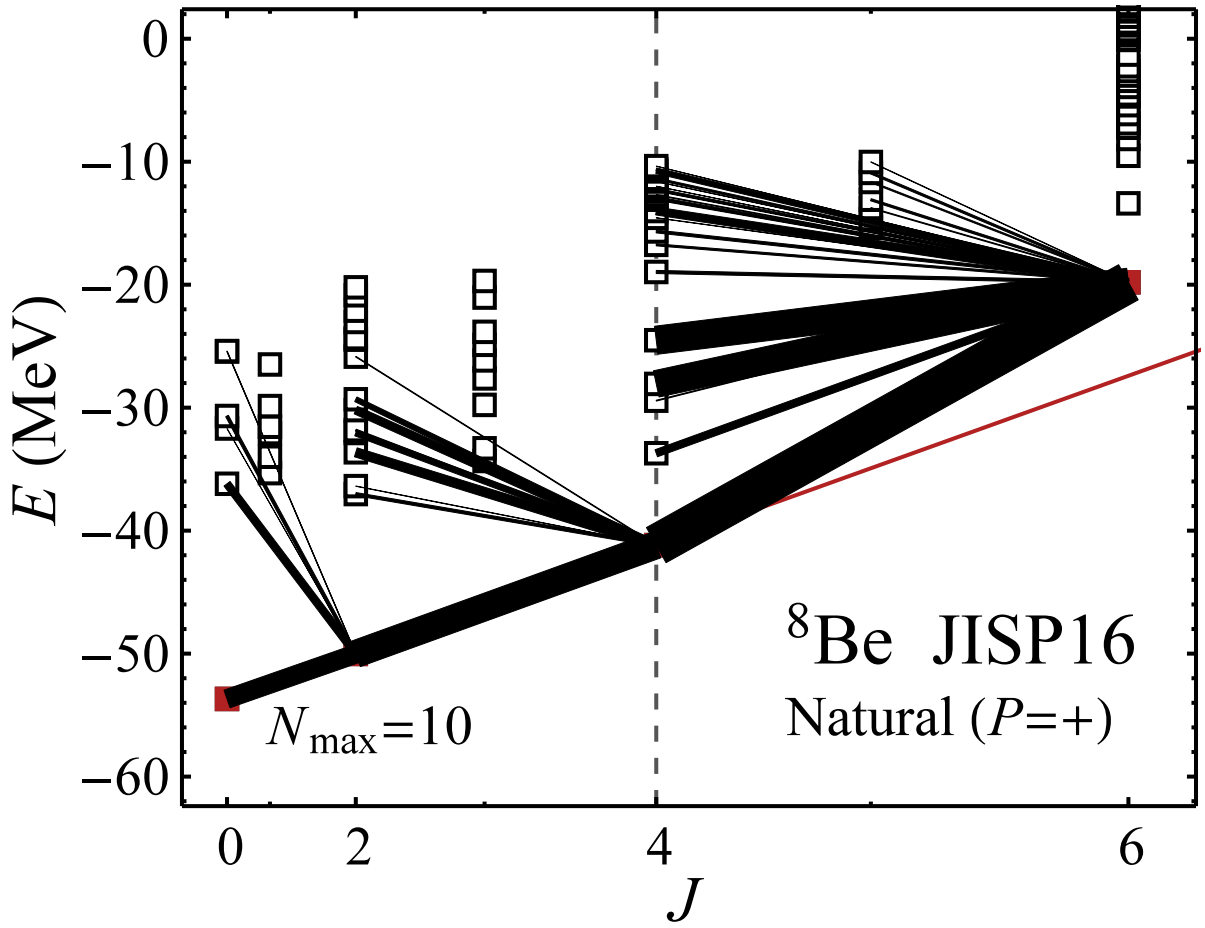


JISP16 + Coulomb interaction

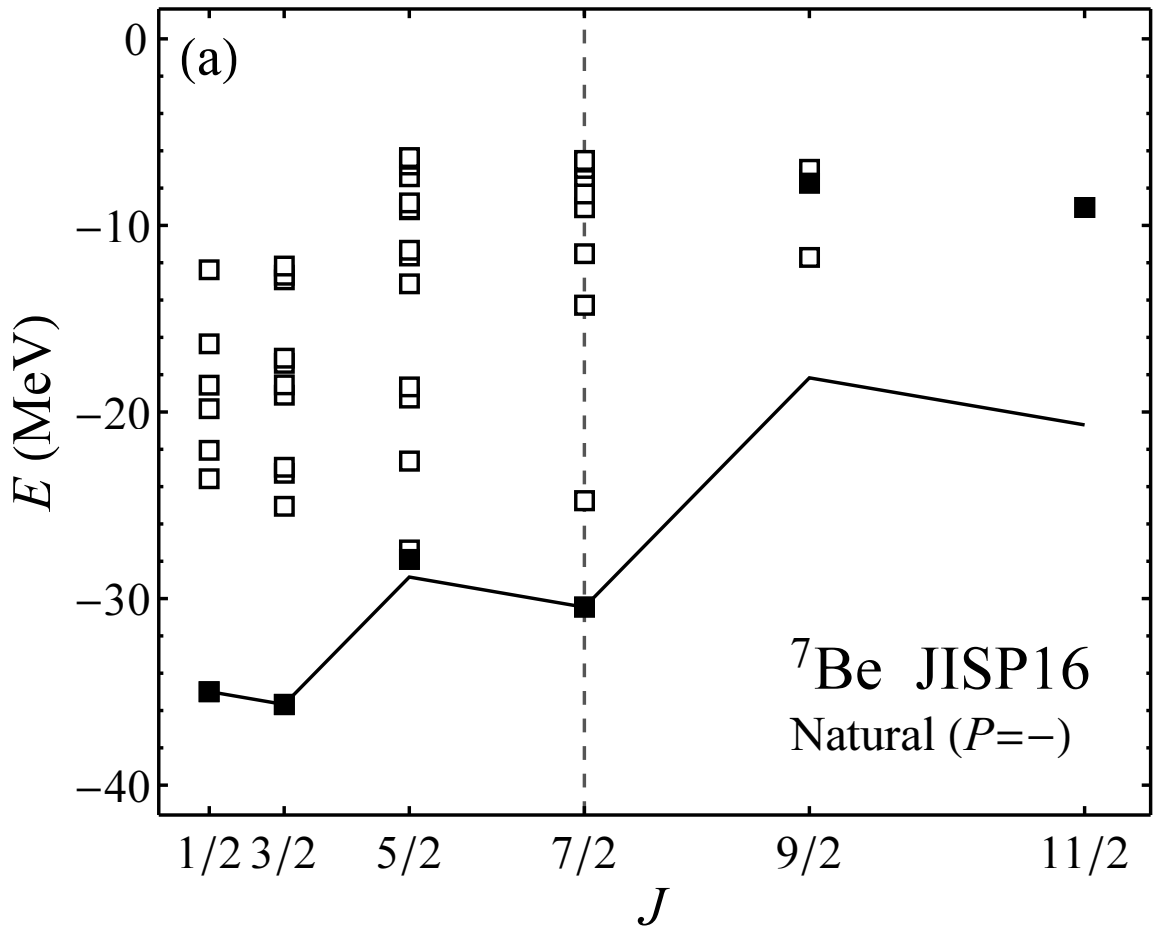
The ^{8}Be yrast band

Shell model: Valence space angular momentum $J \leq 4$

Cluster model: Molecular rotation of $\alpha + \alpha$ dimer

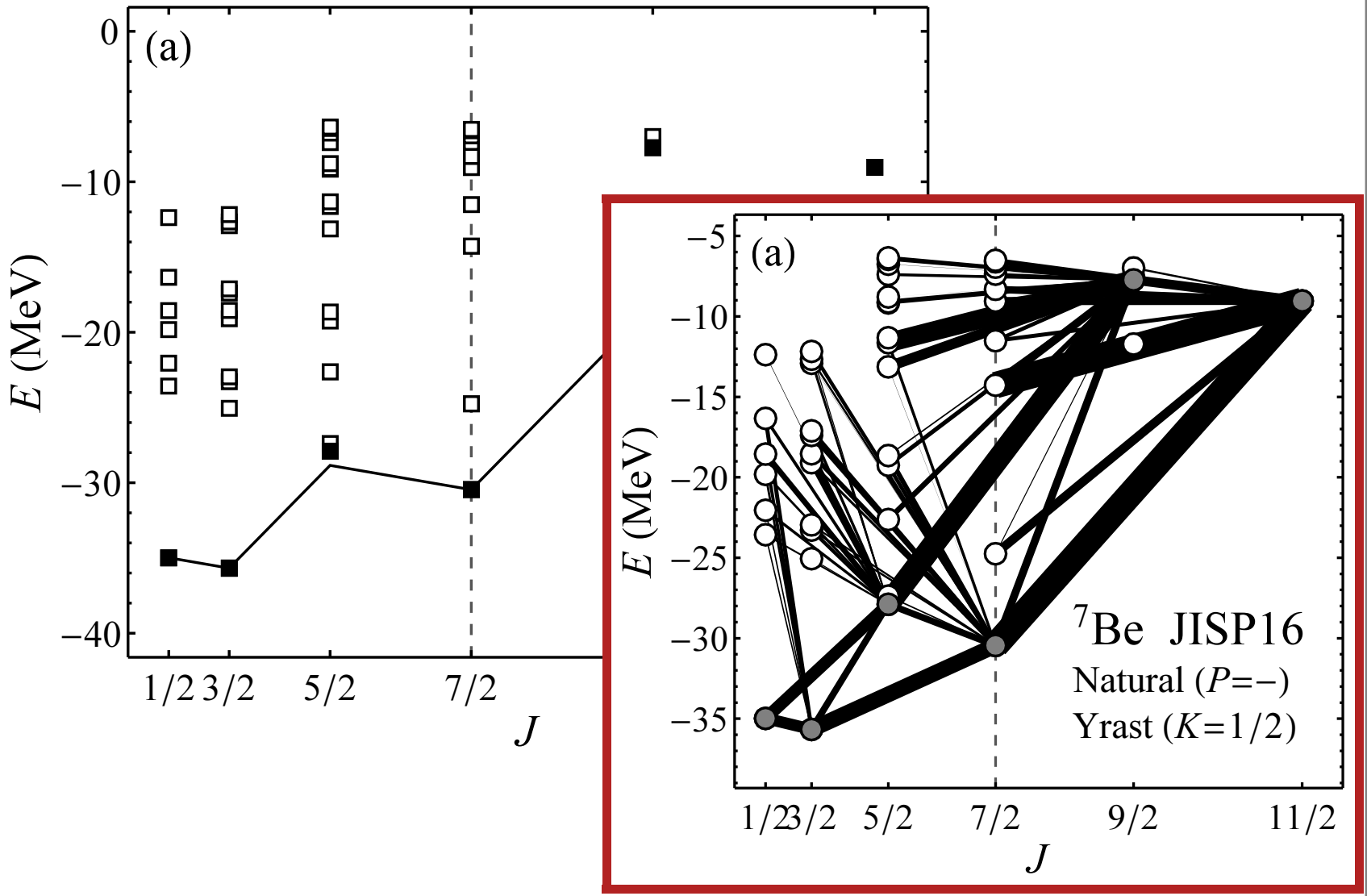


Yrast $K = 1/2$ rotational band in ^{7}Be



JISP16 + Coulomb, $N_{\max} = 10$, $\hbar\omega = 20$ MeV. [IJMPE **24**, 1541002 (2015).]

Yrast $K = 1/2$ rotational band in ^{7}Be



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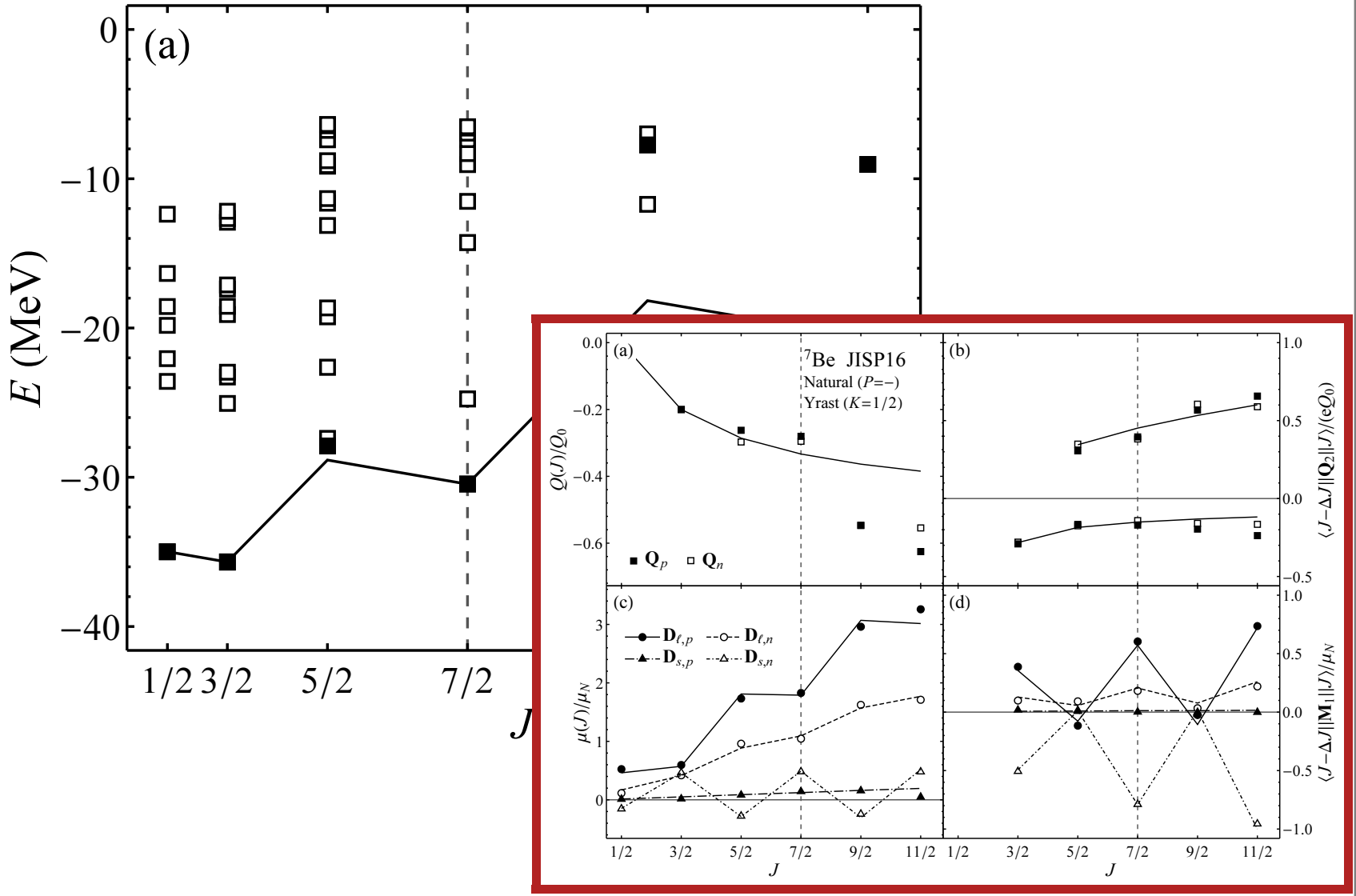
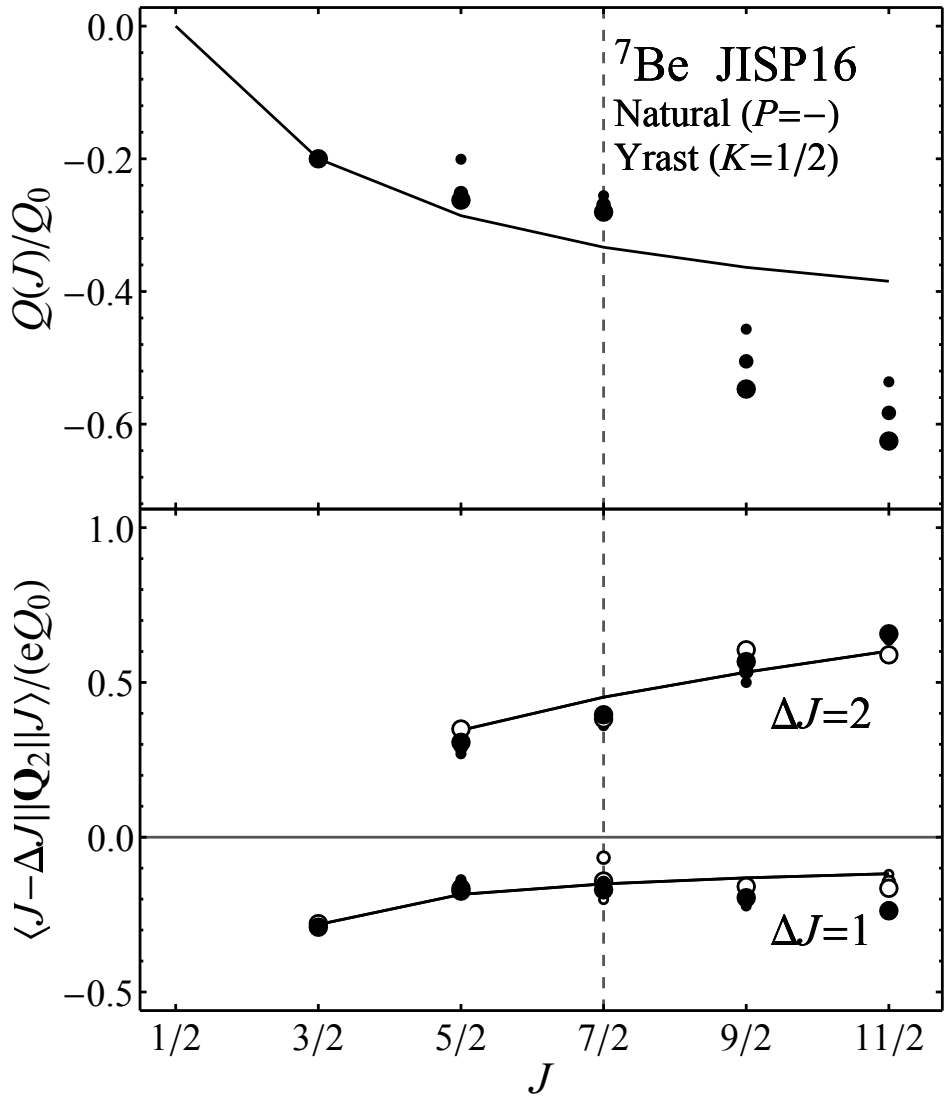
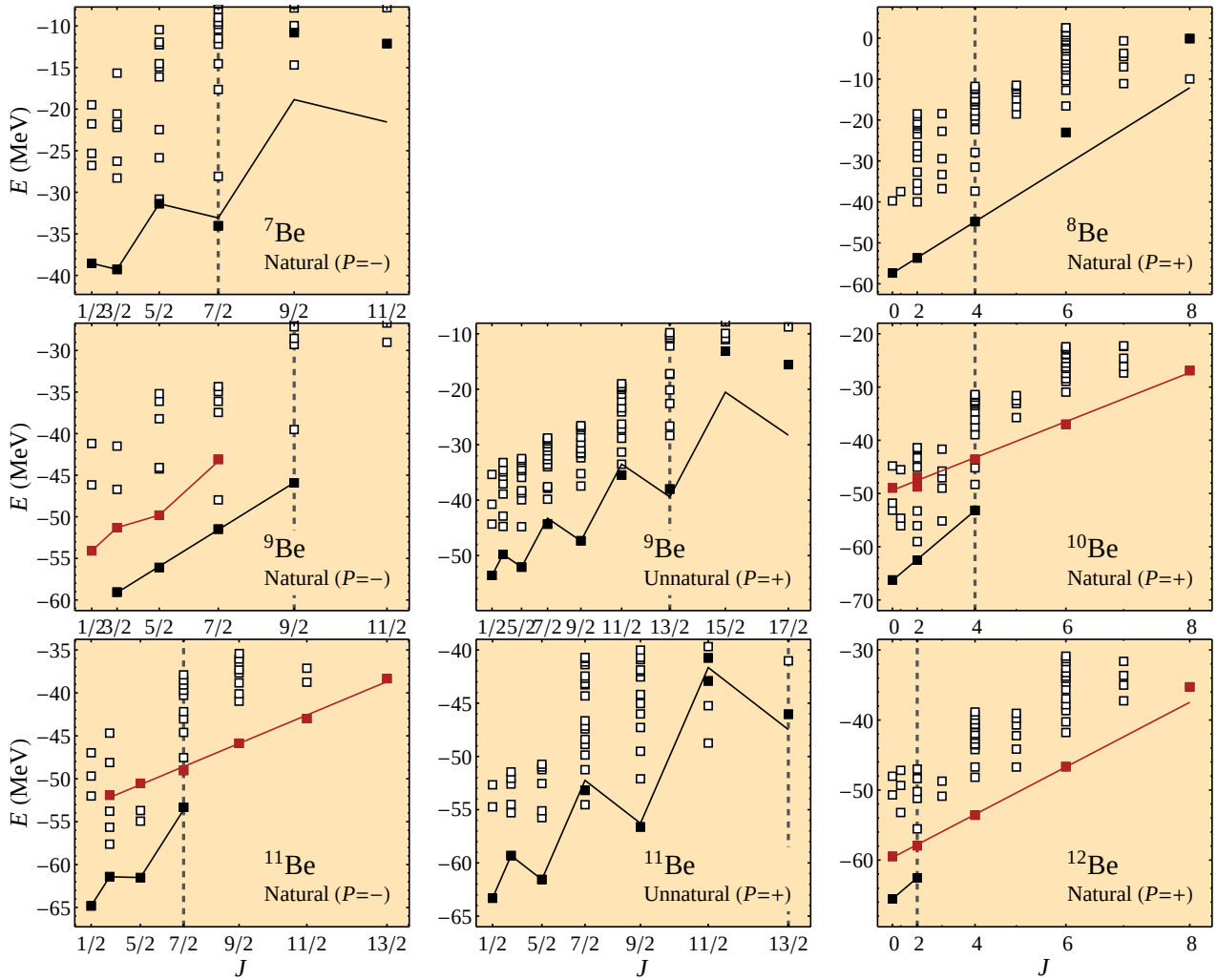


JISP16 + Coulomb, $N_{\max} = 10$, $\hbar\omega = 20$ MeV. [IJMPE **24**, 1541002 (2015).]

Convergence of in-band transition matrix elements



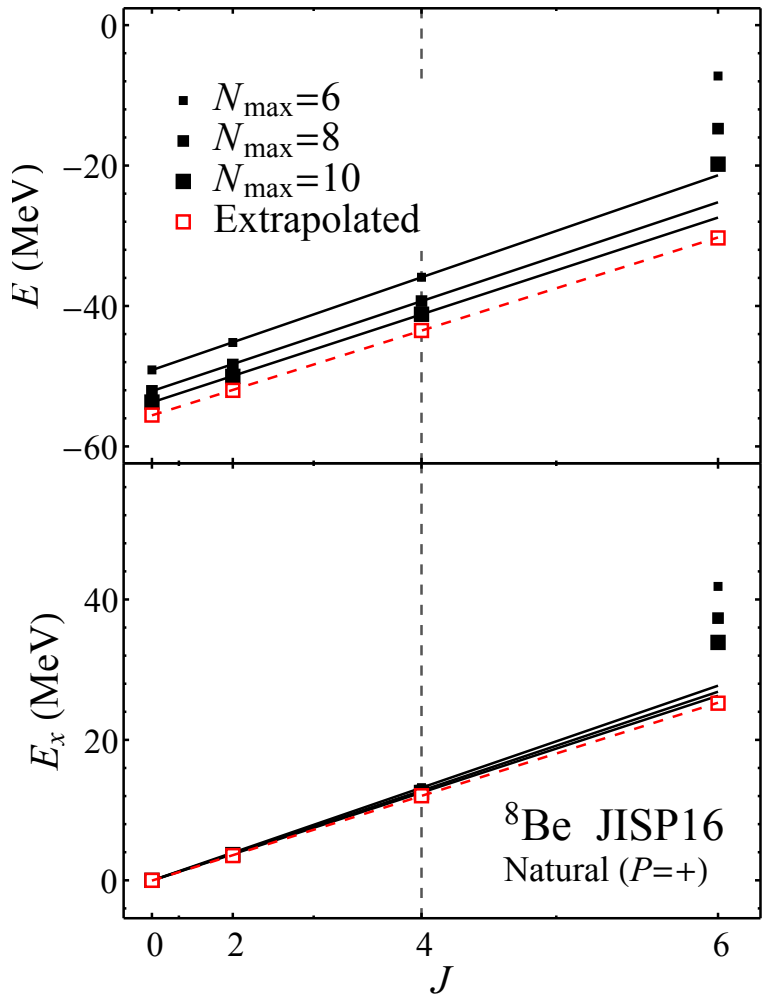
Rotational bands in $^{7-12}$Be from NCCI calculations

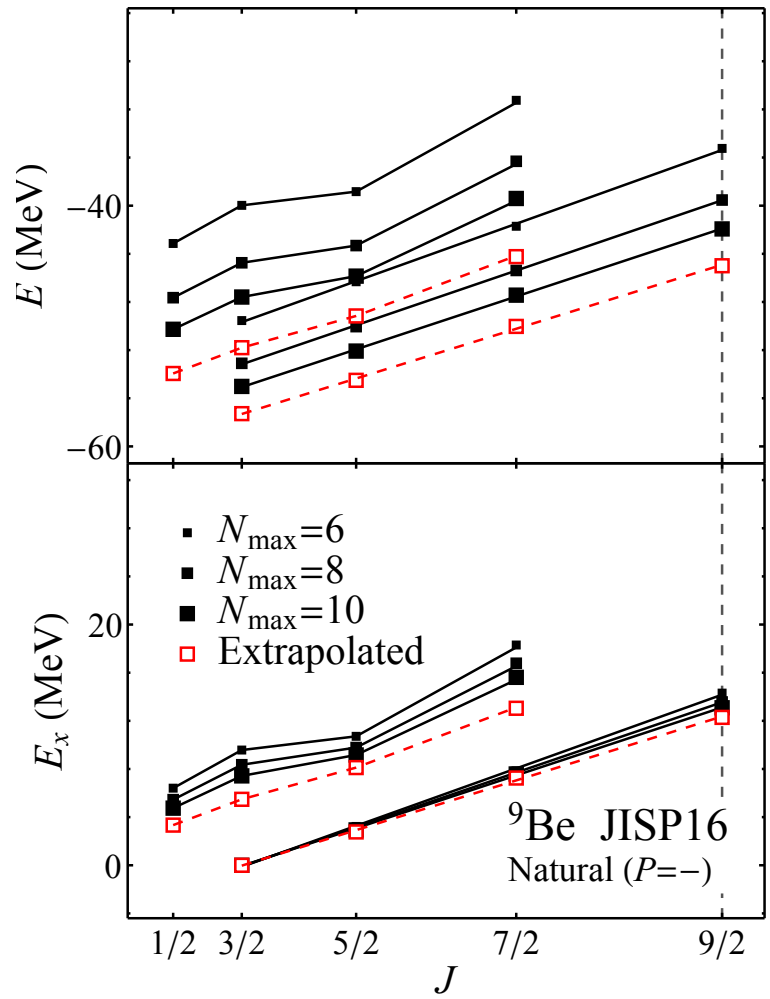


M. A. Caprio, P. Maris, and J. P. Vary, Phys. Lett. B **719**, 179 (2013).
P. Maris, M. A. Caprio, and J. P. Vary, Phys. Rev. C **91**, 014310 (2015).

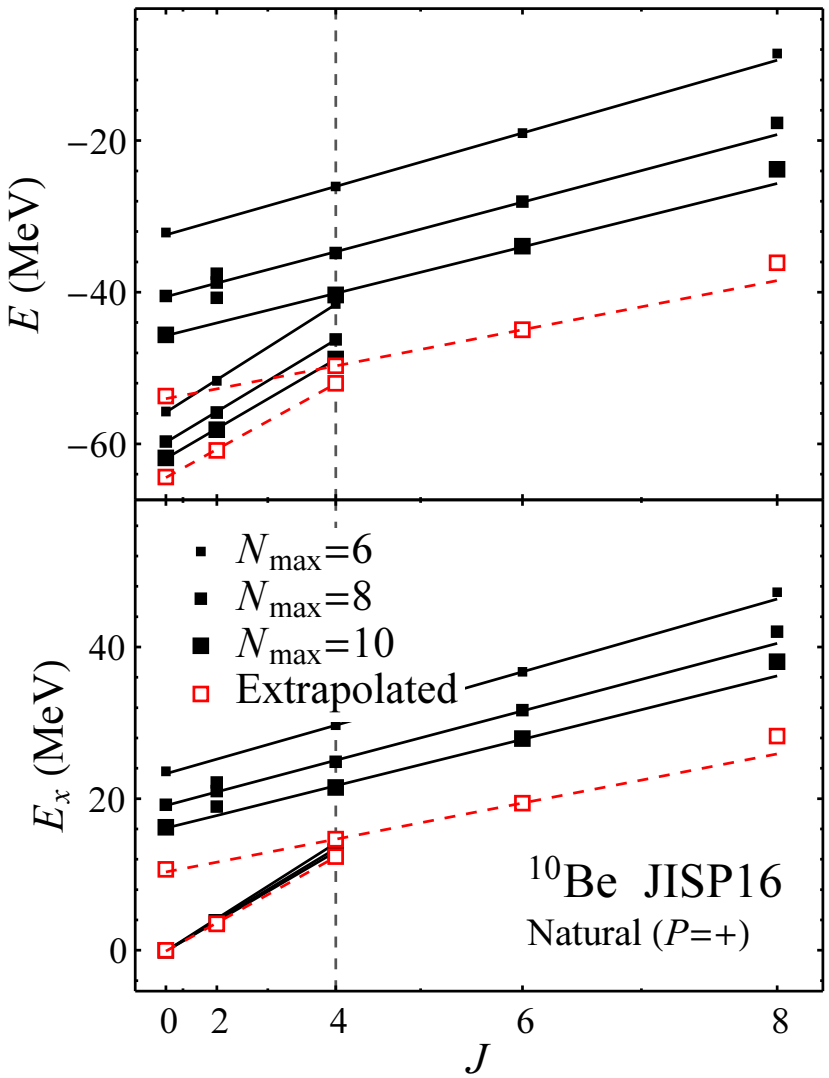
JISP16 interaction (no Coulomb), NCCI (MFDn), $N_{\max} = 10$ or 11, $\hbar\omega \approx 20$ MeV

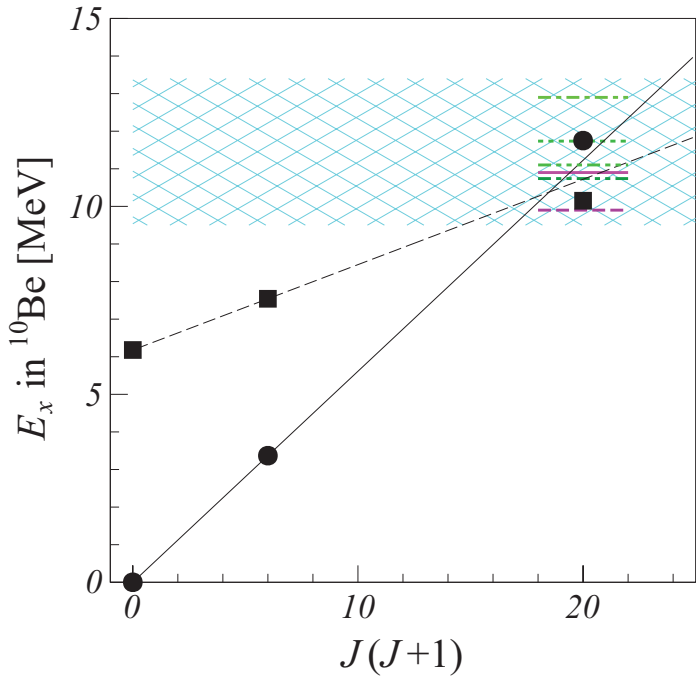
Convergence of energies for band members





Yrast and excited bands in ^{10}Be

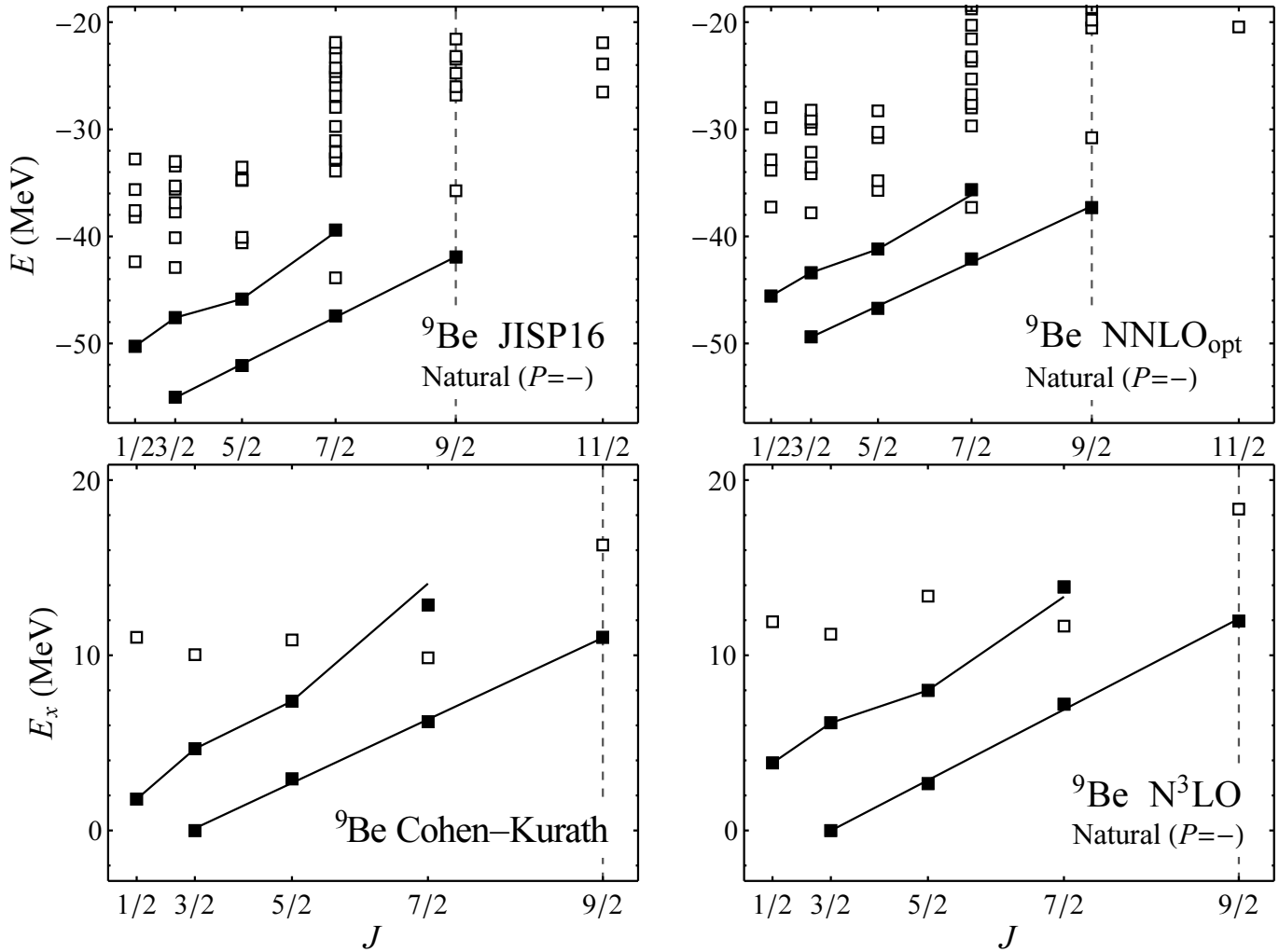




From D. Suzuki *et al.*, Phys. Rev. C **87**, 054301 (2013).

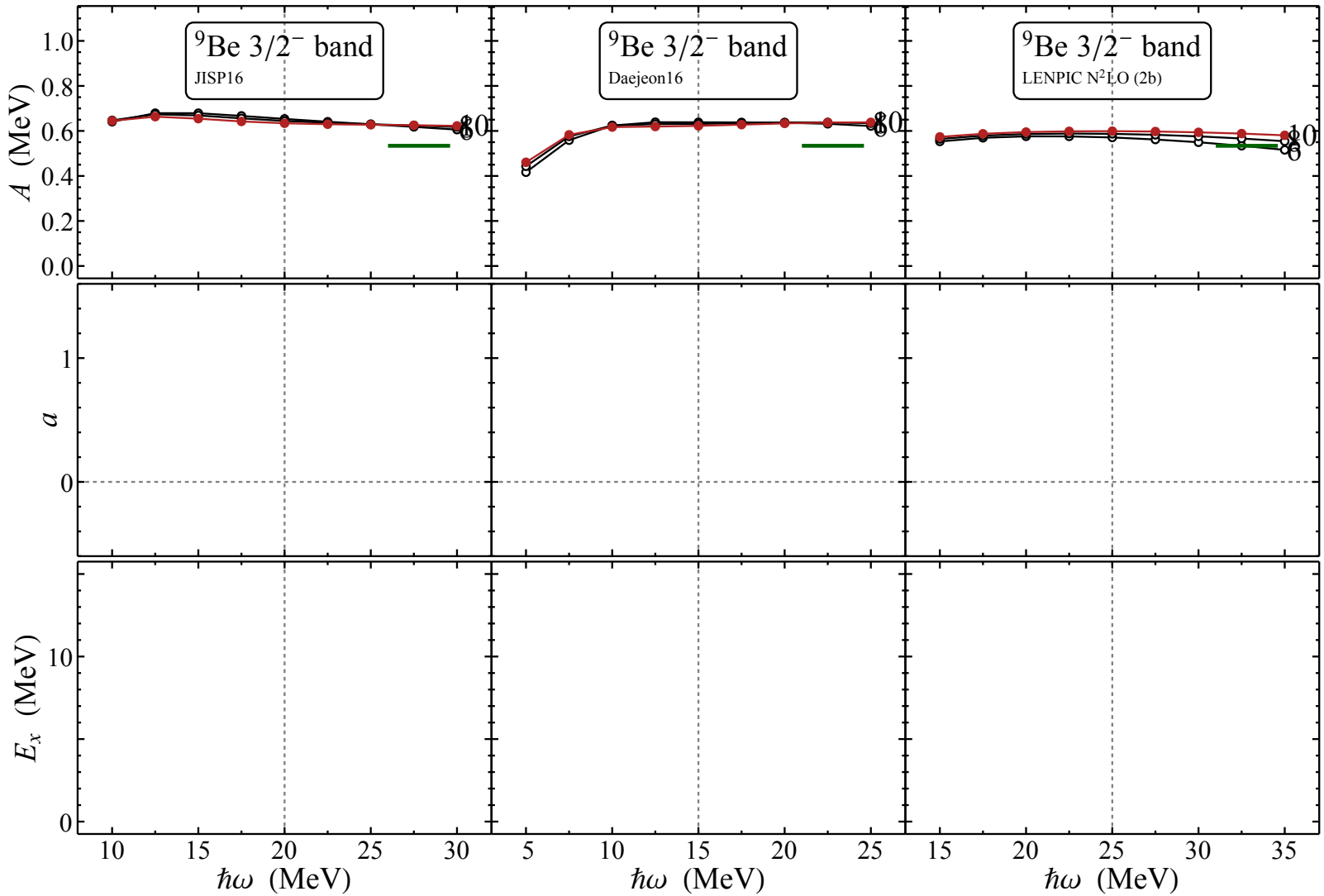
Extrapolation: Exponential in N_{max} (3-point); see P. Maris, J. P. Vary, and A. M. Shirokov, Phys. Rev. C **79**, 014308 (2009).

Rotational structure in ^{9}Be across interactions



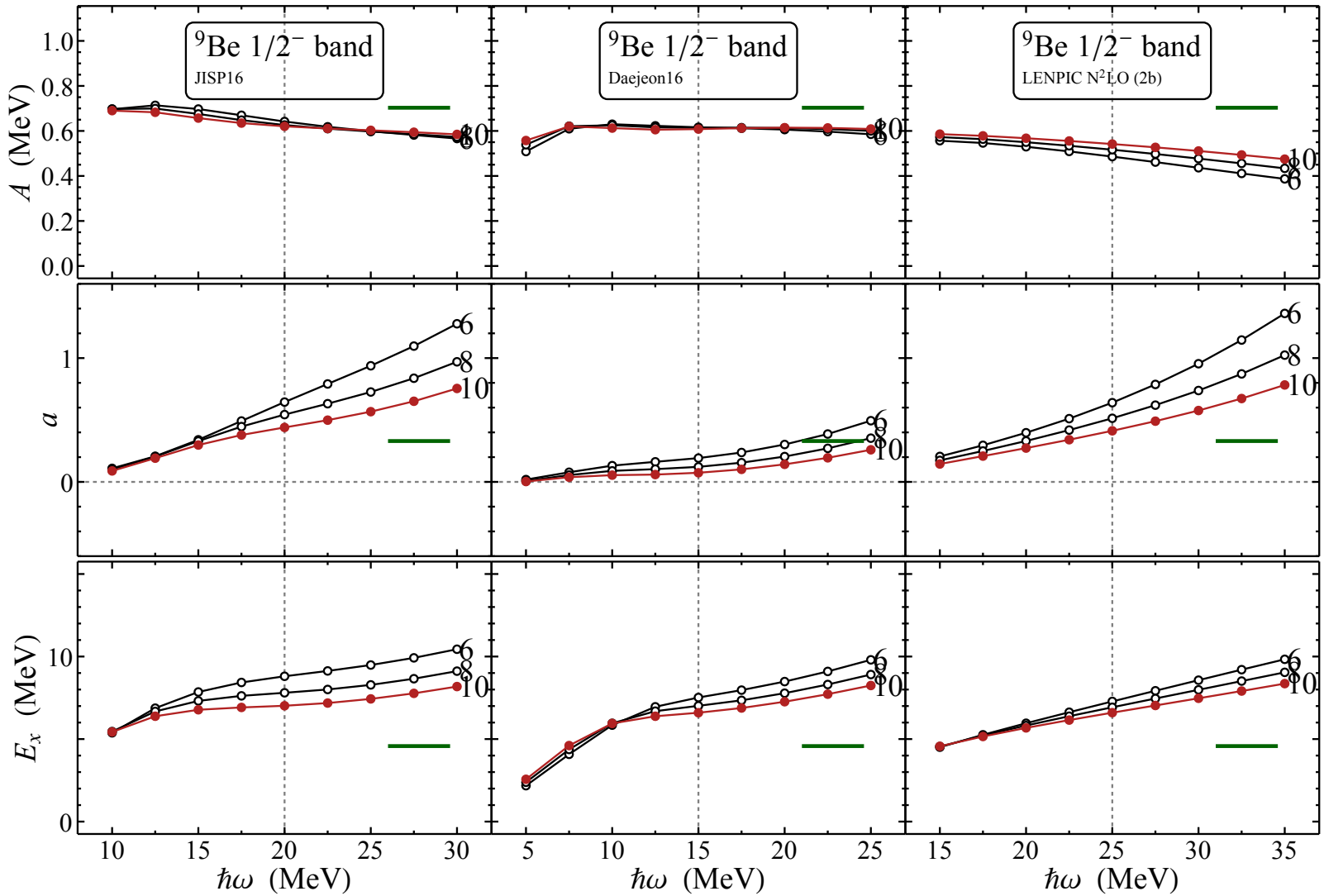
Calculations for Cohen-Kurath and N^{3}LO from C. W. Johnson, Phys. Rev. C **91**, 034313 (2015).

Convergence of band parameters?



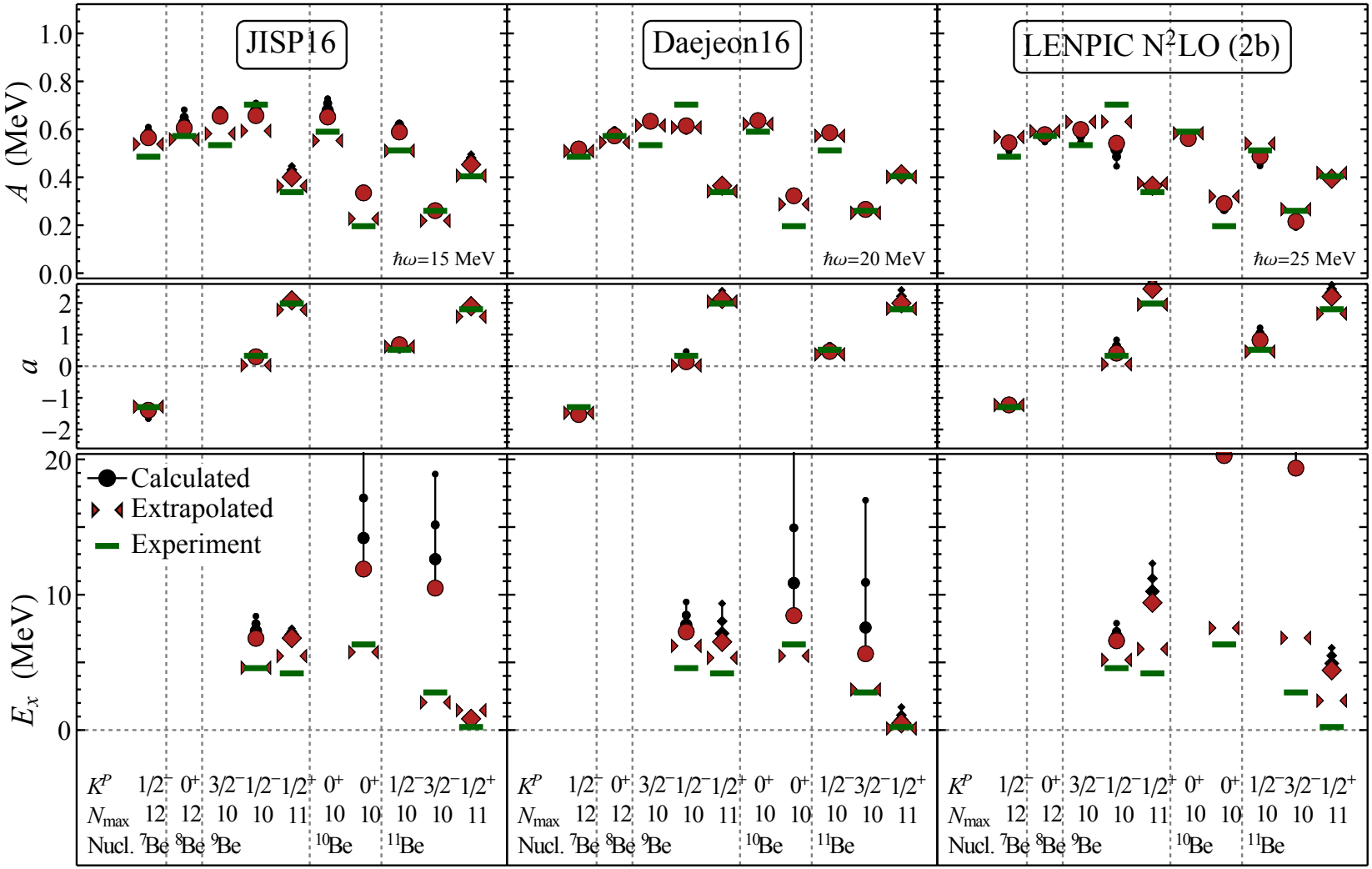
Band parameters obtained from energies of three lowest band members

Convergence of band parameters?

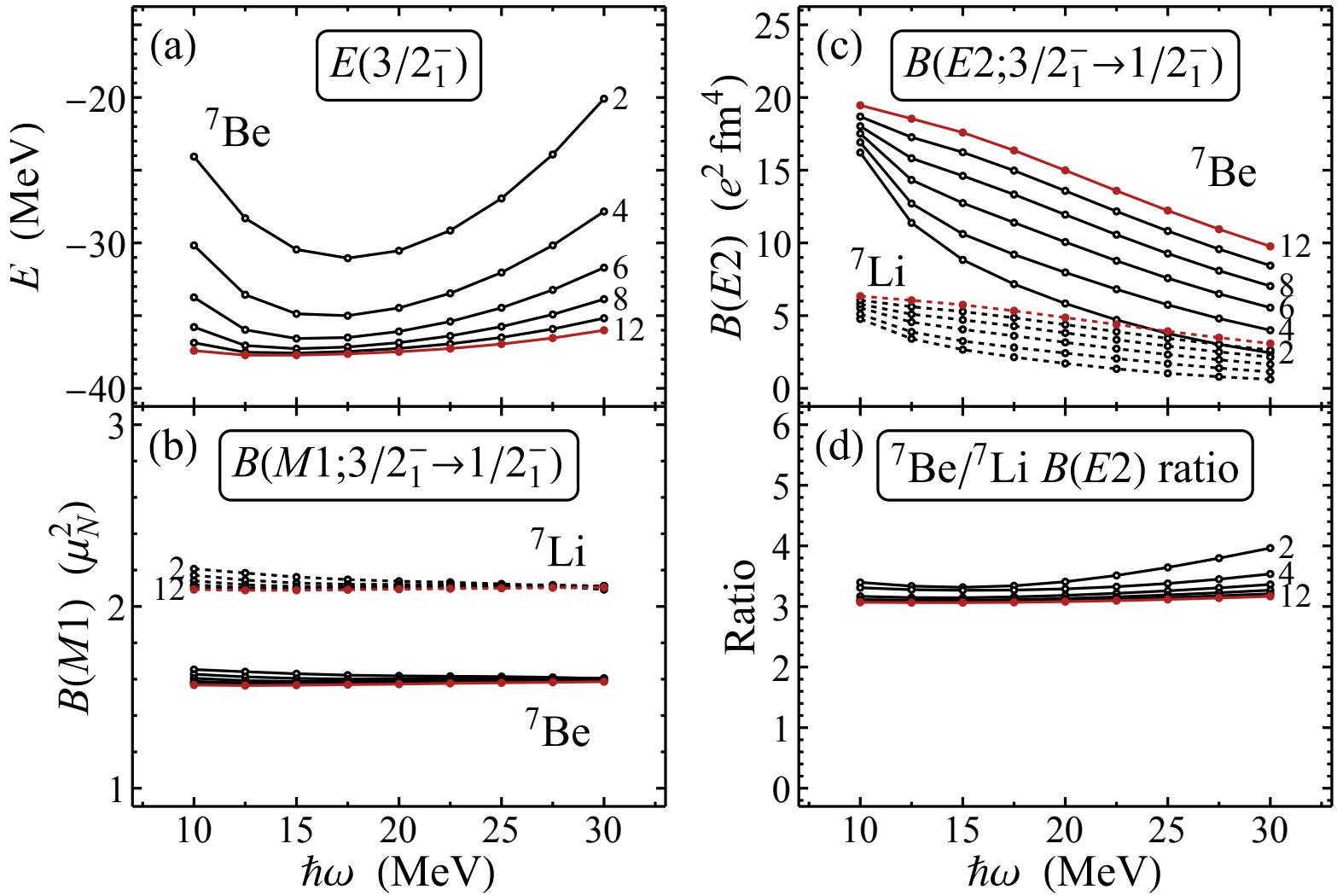


Band parameters obtained from energies of three lowest band members

Ab initio rotational band parameters for Be isotopes

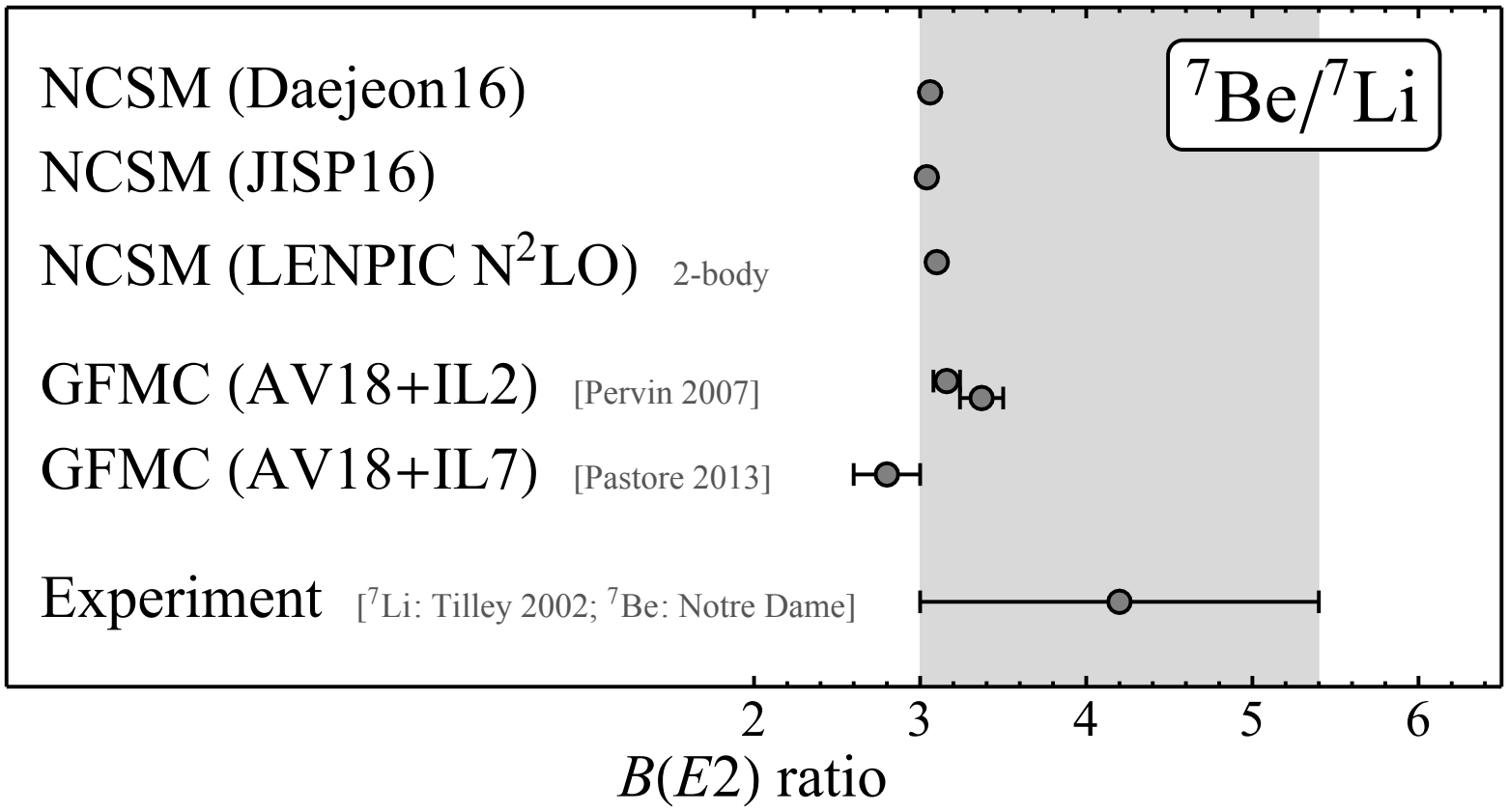


Convergence of $B(E2)$'s and their *ratio* for ^{7}Be/^{7}Li



Daejeon16 + Coulomb interaction

Comparison of calculated $E2$ ratios for ^{7}Be/^{7}Li



Summary

Can we predict nuclei *ab initio*?

Challenge: Computational scale explosion

Emergence of rotational patterns

M. A. Caprio, P. Maris, and J. P. Vary, Phys. Lett. B **719**, 179 (2013).
P. Maris, M. A. Caprio, and J. P. Vary, Phys. Rev. C **91**, 014310 (2015).
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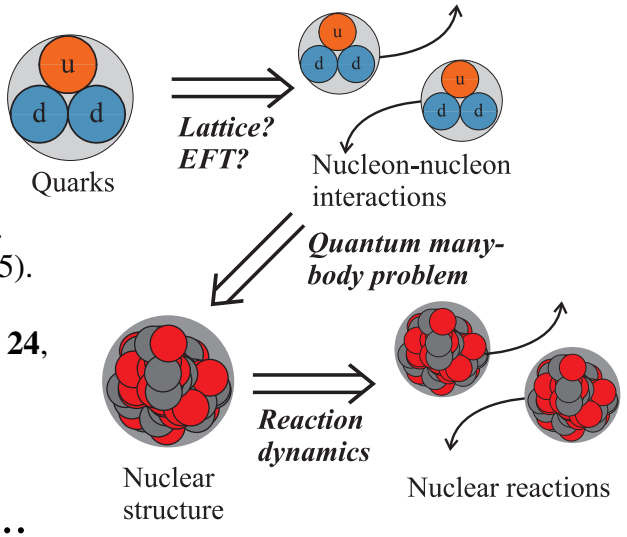

Although energies & electromagnetic moments/transitions ($E2$) are unconverged...

Ratios of observables within a band can be robustly rotational

Robustness of rotational structure across interactions?

Quantitative agreement with experiment?

Underlying structure? *Rotational separation vs. nature of intrinsic state*

- Valence shell structure? *e.g.*, SU(3) correlations
- Cluster structure? $\alpha+\alpha$ $\alpha+n+\alpha$ $\alpha+2n+\alpha$ …
- Symplectic multishell correlations?

Collaborators: Pieter Maris (ISU), James Vary (ISU), Patrick Fasano (ND)