# Predictions for nuclear rotational structure from *ab initio* calculations

Mark A. Caprio Department of Physics University of Notre Dame

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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

:. 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), <u>arXiv:1509.00102</u>.

Separation of rotational degree of freedom  
Intrinsic state 
$$|\phi_K\rangle$$
 & rotation in Euler angles  $\vartheta$   $(J = K, K + 1, ...)$   
 $|\psi_{JKM}\rangle \propto \int d\vartheta \Big[ \mathcal{D}^J_{MK}(\vartheta) |\phi_K; \vartheta \rangle + (-)^{J+K} \mathcal{D}^J_{M-K}(\vartheta) |\phi_{\bar{K}}; \vartheta \rangle \Big]$   
Rotational energy  
 $E(J) = E_0 + A[J(J+1) + a(-)^{J+1/2}(J+\frac{1}{2})] \qquad A \equiv \frac{\hbar^2}{2J}$   
Rotational relations on electromagnetic transitions (E2, M1, ...)  
Notational relations decoupling  
 $\frac{1}{J_2} \frac{1}{3J_2} \frac{1}{5J_2} \frac{1}{J_2} \frac{1}{J_2} \frac{1}{9J_2} \frac{1}$ 



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



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



Y. Kanada-En'yo, H. Horiuchi, and A. Doté, Phys. Rev. C 60, 064304 (1999).

# Convergence of NCCI calculations



JISP16 + Coulomb interaction



JISP16 + Coulomb interaction

# Convergence of NCCI calculations



JISP16 + Coulomb interaction



JISP16 + Coulomb interaction



JISP16 + Coulomb interaction

# The <sup>8</sup>Be yrast band

Shell model: Valence space angular momentum  $J \le 4$ Cluster model: Molecular rotation of  $\alpha + \alpha$  dimer





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



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



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

# Convergence of in-band transition matrix elements



# Rotational bands in <sup>7–12</sup>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).



![](_page_18_Figure_0.jpeg)

# Rotational structure in <sup>9</sup>Be across interactions

![](_page_19_Figure_1.jpeg)

Calculations for Cohen-Kurath and N<sup>3</sup>LO from C. W. Johnson, Phys. Rev. C 91, 034313 (2015).

![](_page_20_Figure_0.jpeg)

Band parameters obtained from energies of three lowest band members

M. A. Caprio, University of Notre Dame

#### Convergence of band parameters? 1.0 $^{9}\text{Be }1/2^{-}$ band $^{9}\text{Be }1/2^{-}\text{ band}$ <sup>9</sup>Be 1/2<sup>-</sup> band LENPIC N<sup>2</sup>EO (2b) W 0.8 W 0.6 W 0.4 JISP16 Dacieon16 0.2 0.0 α -*E<sub>x</sub>* (MeV) 15 25 25 20 25 30 35 10 20 30 5 10 20 ħω (MeV) ħω (MeV) $\hbar\omega$ (MeV)

Band parameters obtained from energies of three lowest band members

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## Ab initio rotational band parameters for Be isotopes

![](_page_22_Figure_1.jpeg)

## Ab initio rotational band parameters for Be isotopes

![](_page_23_Figure_1.jpeg)

# 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).
 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).

Although energies & electromagnetic moments/transitions (*E*2) are unconverged...

![](_page_24_Figure_6.jpeg)

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?  $\alpha + \alpha \quad \alpha + n + \alpha \quad \alpha + 2n + \alpha \quad \dots$
- Symplectic multishell correlations?

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