Nuclear rotation and shape coexistence from first principles

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Emergence of rotational bands in *ab initio* no-core configuration interaction calculations of light nuclei

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A B S T R A C T

The emergence of rotational bands is observed in no-core configuration interaction (NCCI) calculations for the odd-mass Be isotopes ($7 \leqslant A \leqslant 13$) with the JISP16 nucleon–nucleon interaction, as evidenced by rotational patterns for excitation energies, quadrupole moments, and $E2$ transitions. Yrast and low-lying excited bands are found. The results demonstrate the possibility of well-developed rotational structure in NCCI calculations using a realistic nucleon–nucleon interaction.

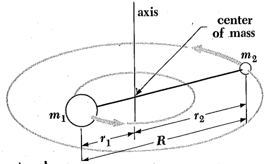
Outline

- Nuclear rotation
- *Ab initio* nuclear structure *No-core shell model*
- *Ab initio* emergence of rotation and shape coexistence

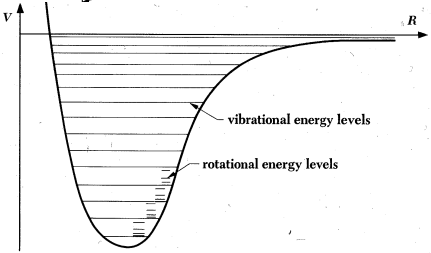
Rotation in a quantum system: Molecules

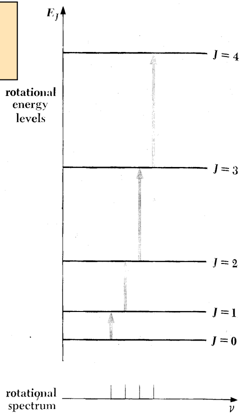
Adiabatic separation of motion (different energy scales)

- Low-energy *rotational excitations* $\approx 0.001\,\mathrm{eV}$
- Intermediate-energy *vibrational excitations* $\approx 0.1\,\mathrm{eV}$
- High-energy *electronic excitations* $\gtrsim 1\,\mathrm{eV}$



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





Figures from A. Beiser, *Concepts of Modern Physics*, 4th ed.

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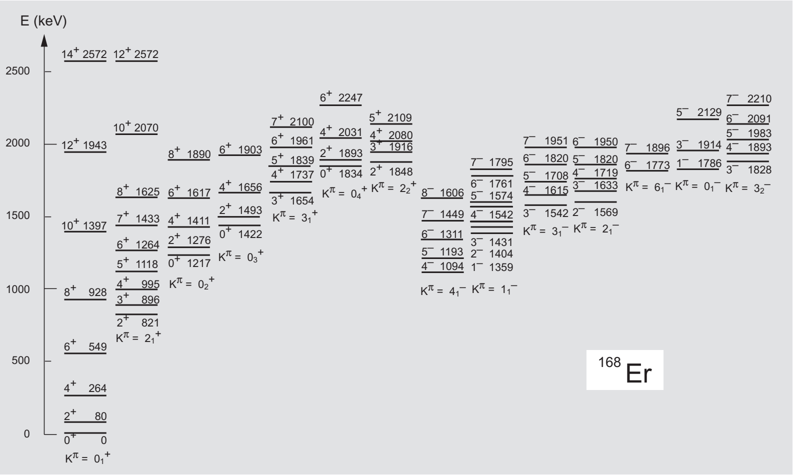

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Figure from D. J. Rowe and J. L. Wood, *Fundamentals of Nuclear Models: Foundational Models* (World Scientific, Singapore, 2010).

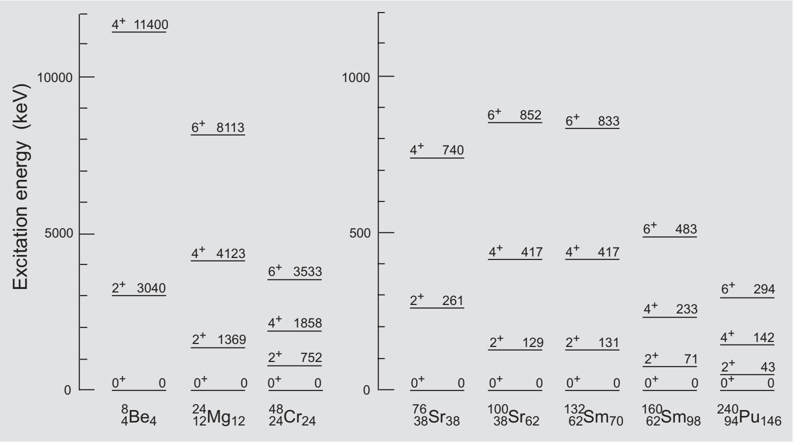
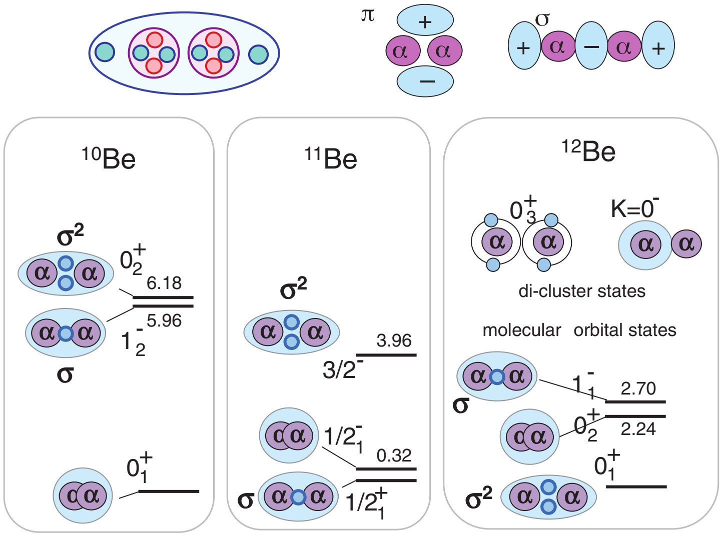


Figure from D. J. Rowe and J. L. Wood, *Fundamentals of Nuclear Models: Foundational Models* (World Scientific, Singapore, 2010).

Cluster molecular structure in light nuclei



Yoshiko Kanada-En'yo, Masaaki Kimura, and Akira Ono, PTEP 2012, 01A202 (2012).

Separation of rotational degree of freedom

Factorization of wave function $|\psi_{JKM}\rangle$ $\qquad J=K,K+1,\ldots$

$|\phi_K\rangle$ *Intrinsic structure* *($K \equiv$ a.m. projection on symmetry axis)*

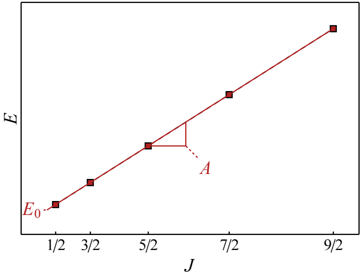
$\mathcal{D}^J_{MK}(\vartheta)$ *Rotational motion in Euler angles* ϑ

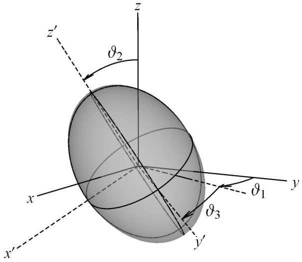
Rotational energy

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

Rotational relations (Alaga rules) on electromagnetic transitions

$$B(E2;J_i\rightarrow J_f)\propto(J_iK20|J_fK)^2(eQ_0)^2 \qquad eQ_0\propto\langle\phi_K|Q_{2,0}|\phi_K\rangle$$





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e.g., D. J. Rowe, *Nuclear Collective Motion: Models and Theory* (World Scientific, Singapore, 2010).

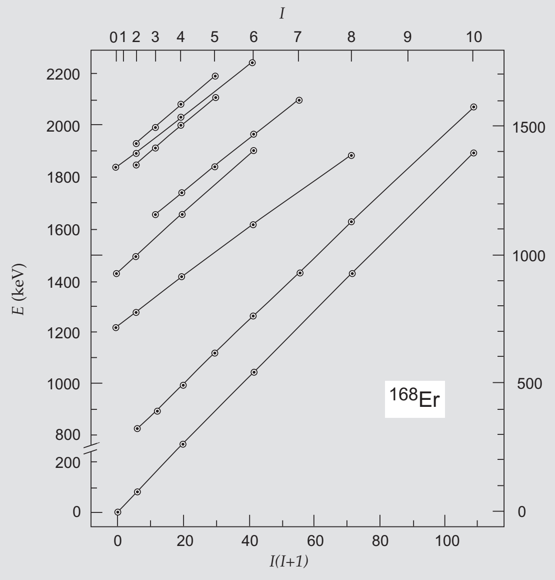

Figure from D. J. Rowe and J. L. Wood, *Fundamentals of Nuclear Models: Foundational Models* (World Scientific, Singapore, 2010).

Z \ N	1	2	3	4	5	6	7	8
O 8					^{13}O	^{14}O	^{15}O	^{16}O
N 7					^{12}N	^{13}N	^{14}N	^{15}N
C 6			^{9}C	^{10}C	^{11}C	^{12}C	^{13}C	^{14}C
B 5			^{8}B	[^{9}B]	^{10}B	^{11}B	^{12}B	^{13}B
Be 4			^{7}Be	[^{8}Be]	^{9}Be	^{10}Be	^{11}Be	^{12}Be
Li 3			^{6}Li	^{7}Li	^{8}Li	^{9}Li		^{11}Li
He 2	^{3}He	^{4}He		^{6}He		^{8}He		
H 1	^{2}H	^{3}H						

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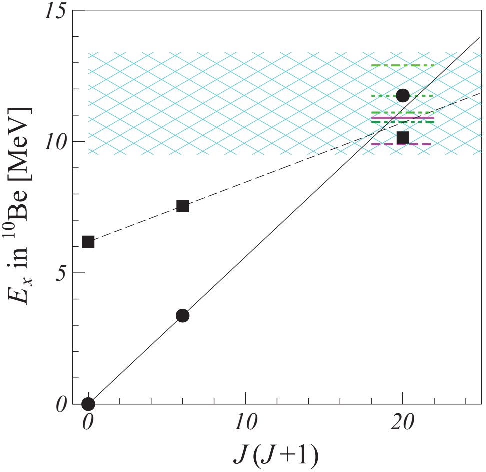
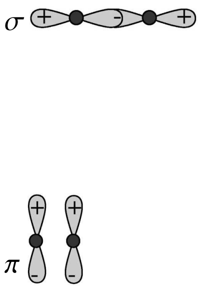
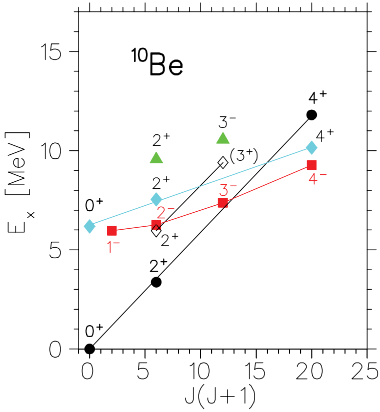
Yrast and excited bands in ^{10}Be





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).



H. G. Bohlen *et al.*, Phys. Rev. C **75**, 054604 (2007).

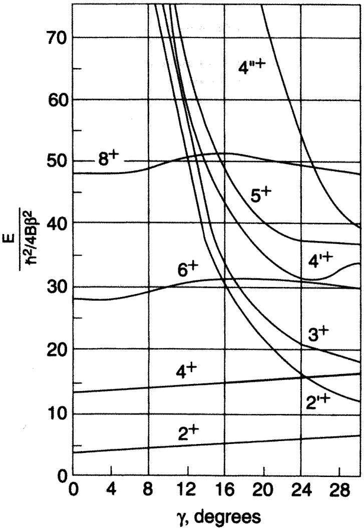


FIG. 6.24. Normal and anomalous levels of the triaxial rotor (Preston, 1975).

R. F. Casten, *Nuclear Structure from a Simple Perspective*, 2ed. (Oxford, 2000).

Outline

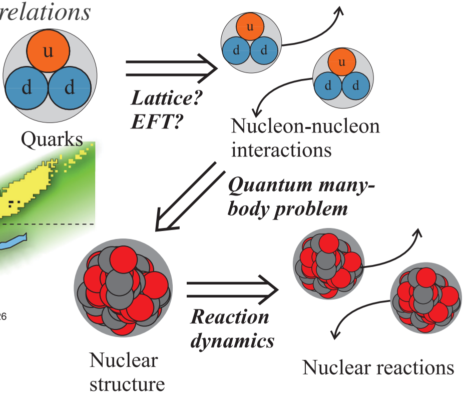
- Nuclear rotation
- *Ab initio* nuclear structure *No-core shell model*
- *Ab initio* emergence of rotation and shape coexistence

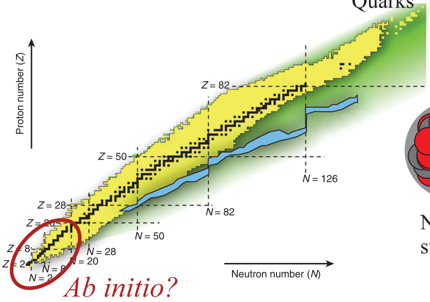
Goal of *ab initio* nuclear structure

First-principles understanding of nature *Nuclei from QCD*

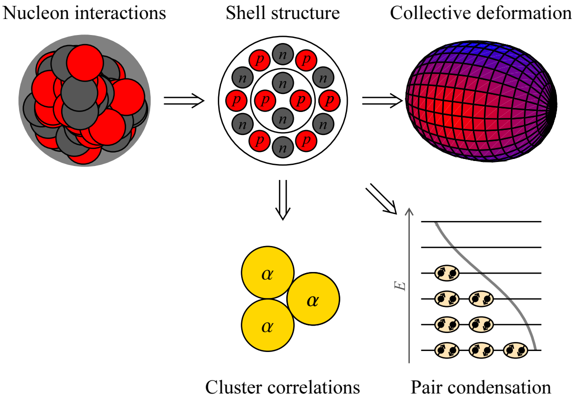
Can we understand the origin of "simple patterns in complex nuclei"?

i.e., emergent collective correlations





Adapted from B. Schwarzschild, Physics Today 63(8), 16 (2010).



Many-particle Schrödinger equation

$$\sum_{i=1}^{A}\left(-\frac{\hbar^2}{2m_i}\nabla_i^2\right)\Psi + \frac{1}{2}\sum_{i,j=1}^{A} V(|\mathbf{r}_i-\mathbf{r}_j|)\,\Psi = E\Psi$$

$$\Psi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3,\ldots,\mathbf{r}_A) \;=\; ?$$

Solution of Schrödinger equation in a basis

One particle in *one* dimension

Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

Eigenproblem

$$\hat{H}\psi(x) = E\psi(x)$$

Expand wave function in basis (unknown coefficients a_k)

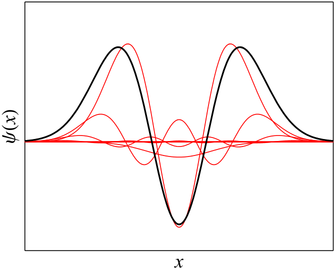
$$\psi(x) = \sum_{k=1}^{\infty} a_k \varphi_k(x)$$

Matrix elements of Hamiltonian

$$H_{ij} \equiv \langle \varphi_i | \hat{H} | \varphi_j \rangle = \int dx\, \varphi_i^*(x) \hat{H} \varphi_j(x)$$

Reduces to matrix eigenproblem

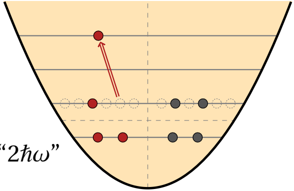
$$\begin{pmatrix} H_{11} & H_{12} & \cdots \\ H_{21} & H_{22} & \cdots \\ \vdots & \vdots & \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix} = E \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix}$$

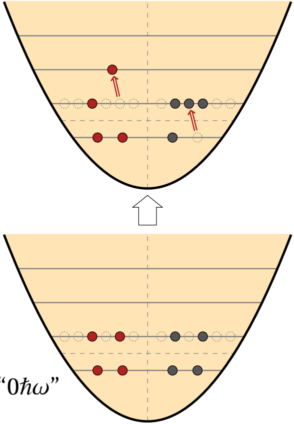


Many-body problem in an oscillator basis

No-core configuration interaction (NCCI) approach

a.k.a. no-core shell model (NCSM)





Harmonic oscillator orbitals

$\Rightarrow$ "Slater determinant" product basis

Distribute nucleons over oscillator shells

Organize basis by # oscillator excitations N_{ex}

relative to lowest Pauli-allowed filling

$N_{\text{ex}} = 0, 2, \ldots$ ("$0\hbar\omega$", "$2\hbar\omega$", ...)

Basis must be truncated: $N_{\text{ex}} \leq N_{\text{max}}$

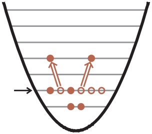
Convergence towards exact result with increasing N_{max}...

B. R. Barrett, P. Navrátil, and J. P. Vary, Prog. Part. Nucl. Phys. **69**, 131 (2013).

Convergence of NCCI calculations

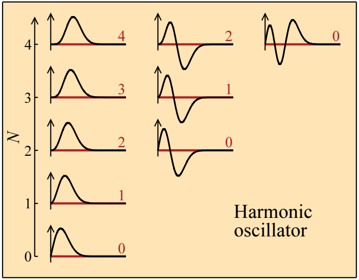
Results for calculation in finite space depend upon:

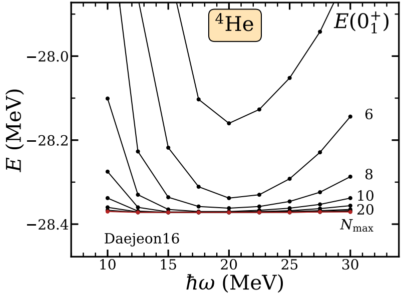
- Many-body truncation N_{max}
- Single-particle basis scale: oscillator length b (or $\hbar\omega$)



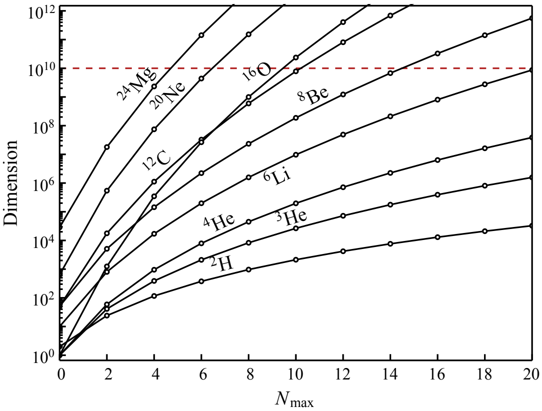
$$b = \frac{(\hbar c)}{[(m_N c^2)(\hbar\omega)]^{1/2}}$$

Convergence of calculated results signaled by independence of N_{max} & $\hbar\omega$





Dimension explosion for NCCI calculations



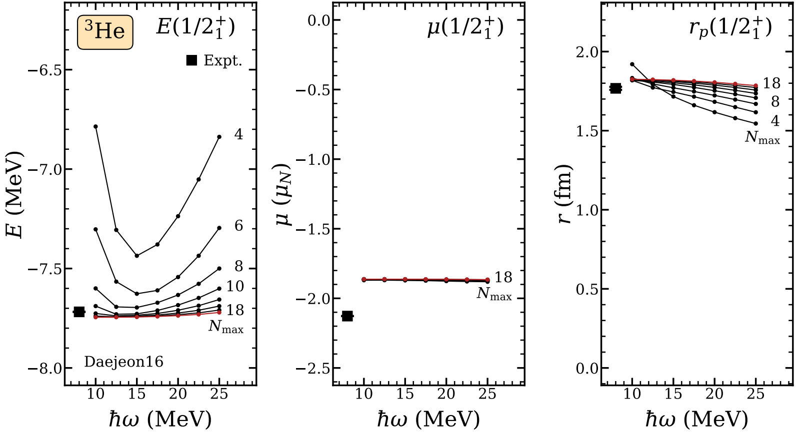
Dimension $\propto \binom{d}{Z}\binom{d}{N}$

d = number of single-particle states

Z = number of protons

N = number of neutrons

Convergence of NCCI calculations



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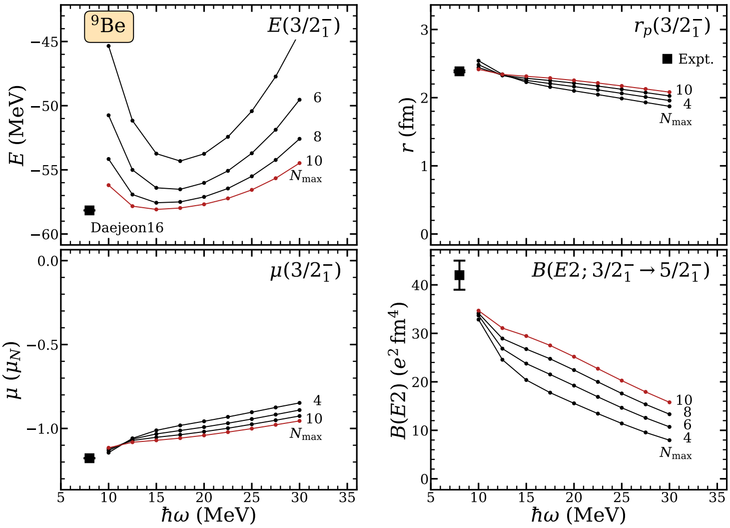
Convergence of NCCI calculations



Outline

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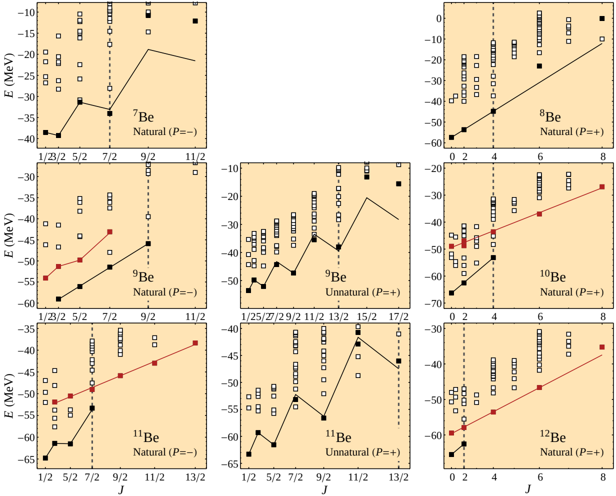
Rotational bands in $^{7\text{–}12}$Be from NCCI calculations



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, $\hbar\omega \approx 20\,\mathrm{MeV}$

Separation of rotational degree of freedom

Factorization of wave function $|\psi_{JKM}\rangle$ $\qquad J = K, K+1, \ldots$

$|\phi_K\rangle$ *Intrinsic structure* *($K \equiv$ a.m. projection on symmetry axis)*

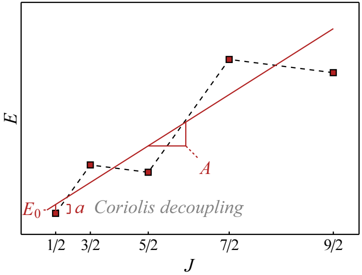
$\mathcal{D}^J_{MK}(\vartheta)$ *Rotational motion in Euler angles ϑ*

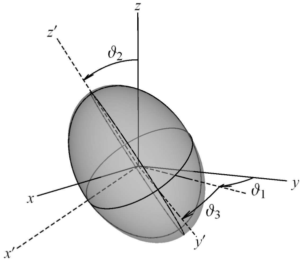
Rotational energy

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

Rotational relations (Alaga rules) on electromagnetic transitions

$$B(E2; J_i \rightarrow J_f) \propto (J_i K 20 | J_f K)^2 (eQ_0)^2 \qquad eQ_0 \propto \langle \phi_K | Q_{2,0} | \phi_K \rangle$$





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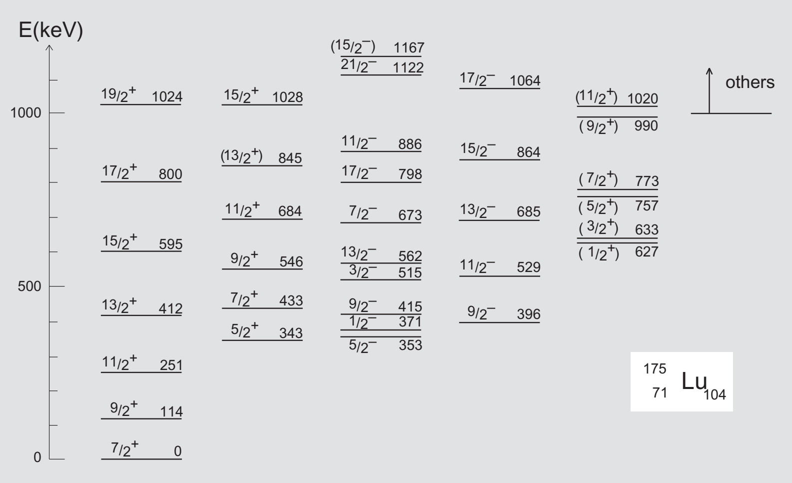
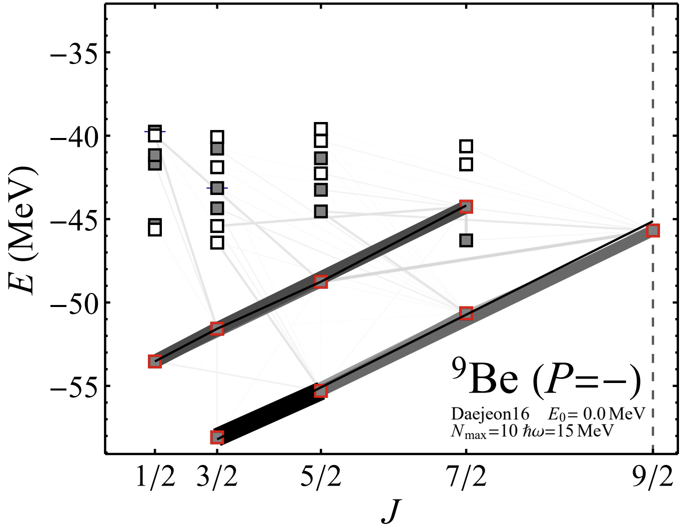
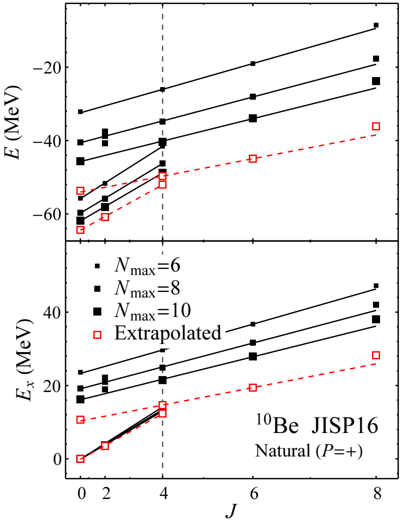


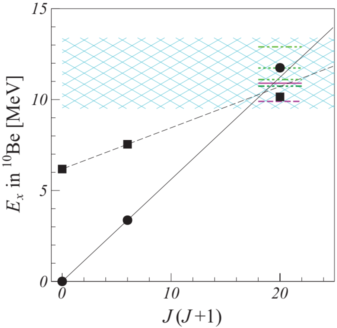
Figure from D. J. Rowe and J. L. Wood, *Fundamentals of Nuclear Models: Foundational Models* (World Scientific, Singapore, 2010).

^{9}Be: NCCI calculated energies and $E2$ transitions



Yrast and excited bands in ^{10}Be

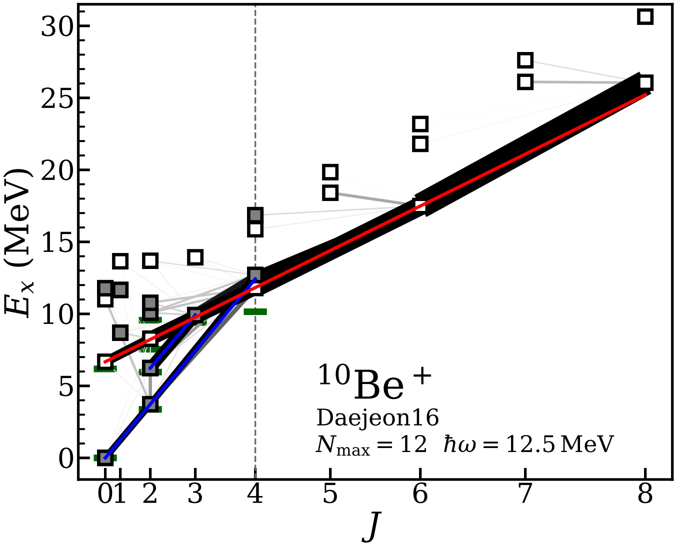


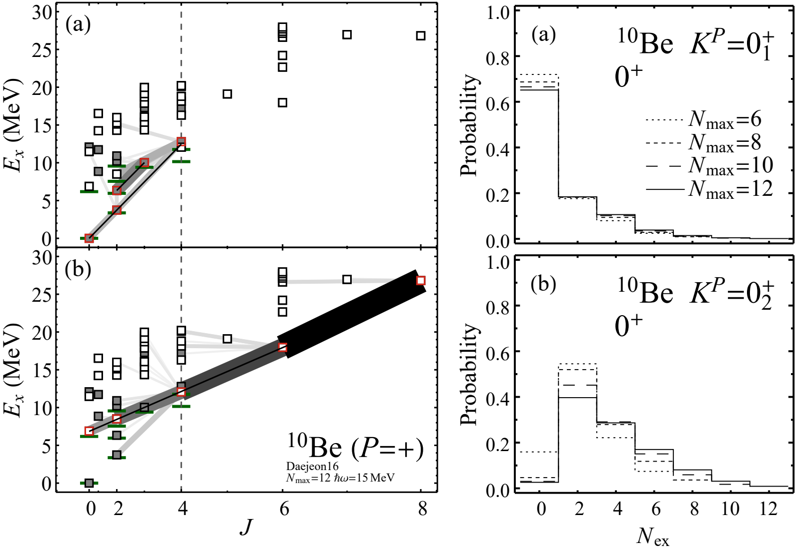


From D. Suzuki *et al.*, Phys. Rev. C **87**, 054301 (2013).

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

Convergence of bands in ^{10}Be with Daejeon16





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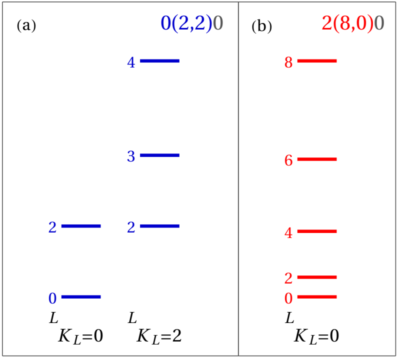
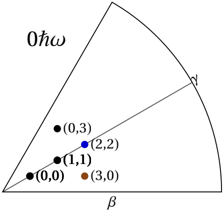
M. A. Caprio, P. J. Fasano, A. E. McCoy, P. Maris, J. P. Vary, Bulg. J. Phys. **46**, 455 (2019) (SDANCA19), `arXiv:1912.06082`.

“Leading” U(3) irreps for ^{10}Be

Intrinsic deformation for irrep (λ,μ)

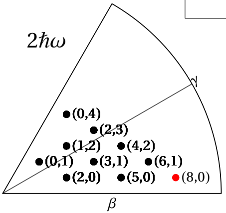
$$\beta \propto (Q\cdot Q)^{1/2}$$
$$\propto (\lambda^2+\lambda\mu+\mu^2+3\lambda+3\mu+3)^{1/2}$$
$$\gamma = \tan^{-1}\left(\frac{\sqrt{3}(\mu+3)}{2\lambda+\mu+3}\right)$$





Proton-neutron SU(3) structure

$$\underbrace{\pi(2,0)}_{\text{prolate}}\times\underbrace{\nu(0,2)}_{\text{oblate}}\Rightarrow(2,2)$$



Elliott model

$$H \propto -Q\cdot Q = -6C(\lambda,\mu)+3\mathbf{L}^2$$

M. A. Caprio, A. E. McCoy, P. J. Fasano, and T. Dytrych, Bulg. J. Phys. **49**, 57 (2022) (SDANCA21).

Summary

Simple patterns in complex nuclei

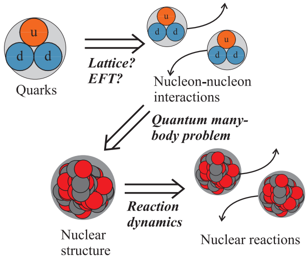
Can we predict nuclei *ab initio*?

Schrödinger ⇒ Matrix eigenproblem

Challenge: Computational scale explosion

Emergence of rotational patterns

M. A. Caprio, P. J. Fasano, P. Maris, A. E. McCoy, and J. P. Vary, Eur. Phys. J. A **56**, 120 (2020).



Coexistence of low-lying bands with different shape