(Un)welcome intruders: Getting your nucleus to come out of its shell
(in *ab initio* calculations)

Mark A. Caprio
Department of Physics and Astronomy
University of Notre Dame

Institute for Nuclear Theory
University of Washington
Seattle, WA
March 12, 2024

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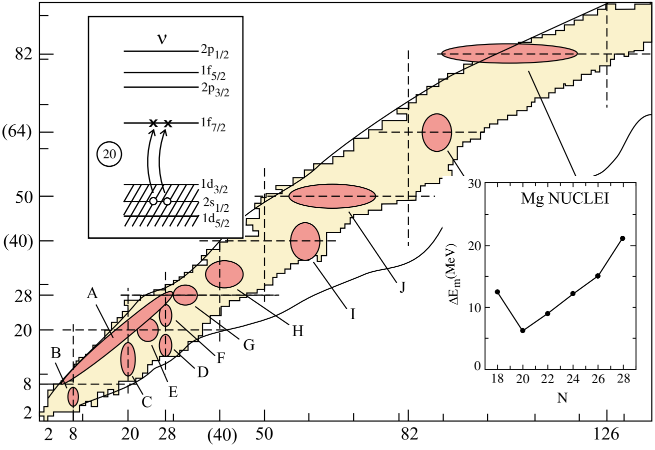
Intruder structure (and shape coexistence)

"[T]he intruder configuration ... corresponds to a more correlated state compared to the $0\hbar\omega$ states. Thus, low-lying 2p-2h intruder configurations are favored only at and near to the ... shell closure."

Normal ($0\hbar\omega$) vs. intruder ($2\hbar\omega$)



K. Heyde and J. L. Wood, Rev. Mod. Phys. **83**, 1467 (2011).

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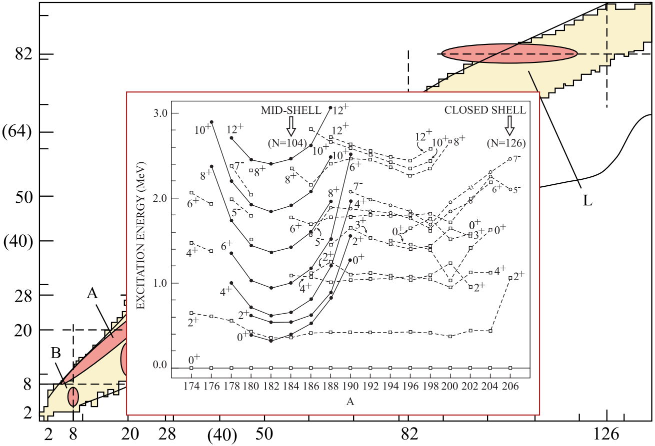


K. Heyde and J. L. Wood, Rev. Mod. Phys. **83**, 1467 (2011).

$E0$ transition as signature of shape mixing

"Transitions with E0 components are a model-independent signature of the mixing of configurations with different mean-square charge radii."
K. Heyde and J. L. Wood, Rev. Mod. Phys. **83**, 1467 (2011).

For *unmixed* ("pure") configurations $|\psi_1^{(0)}\rangle$ and $|\psi_2^{(0)}\rangle\ldots$ *Monopole moments*

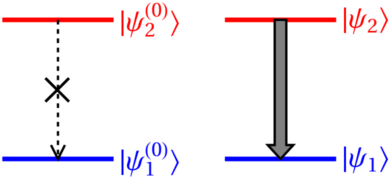
$$M_1 \equiv \langle\psi_1^{(0)}|\mathcal{M}(E0)|\psi_1^{(0)}\rangle = Ar_1^2 \quad M_2 \equiv \langle\psi_2^{(0)}|\mathcal{M}(E0)|\psi_2^{(0)}\rangle = Ar_2^2$$

$$\langle\psi_2^{(0)}|\mathcal{M}(E0)|\psi_1^{(0)}\rangle = 0$$

For *mixed* configurations $|\psi_1\rangle$ and $|\psi_2\rangle\ldots$ *Mixing angle* θ

$$\langle\psi_1|\mathcal{M}(E0)|\psi_2\rangle = \cos\theta\sin\theta\Big[\langle\psi_2^{(0)}|\mathcal{M}(E0)|\psi_2^{(0)}\rangle - \langle\psi_1^{(0)}|\mathcal{M}(E0)|\psi_1^{(0)}\rangle\Big]$$

$$= \tfrac{1}{2}(\sin 2\theta)A(r_2^2 - r_1^2)$$



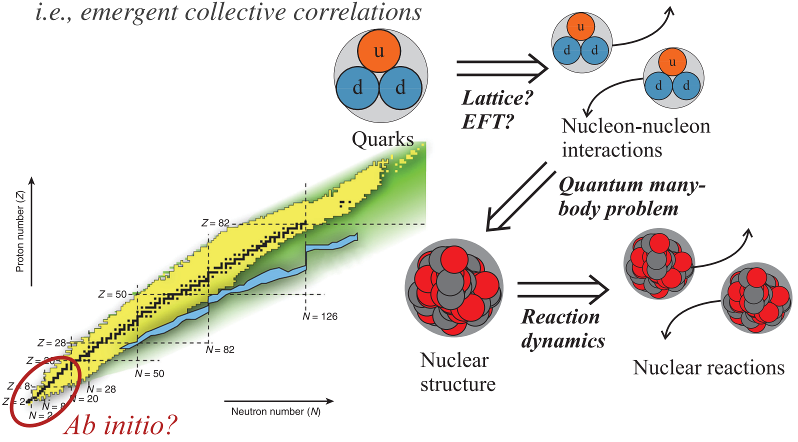
Pure states Mixed states

Goal of *ab initio* nuclear structure

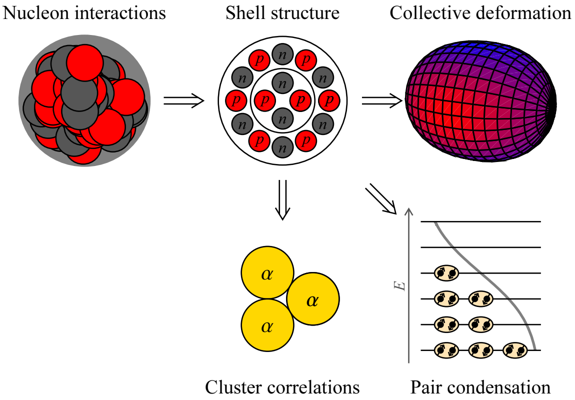
First-principles understanding of nature *Nuclei from QCD*

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

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

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

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- Emergence of rotation Be *isotopes*
- Shape coexistence, *E*0 transitions & mixing ^{10}Be, ^{14}C

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Li 3	^{6}Li 1+	^{7}Li 3/2−	^{8}Li 2+	^{9}Li 3/2−		^{11}Li 3/2−

Separation of rotational degree of freedom

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

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

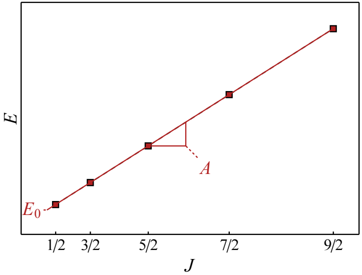
$\mathcal{D}^J_{MK}(\vartheta)$ *Rotational motion in Euler angles ϑ*

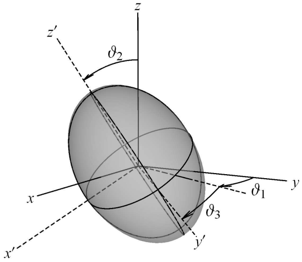
Rotational energy

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

Rotational relations (Alaga rules) on electromagnetic transitions

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





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

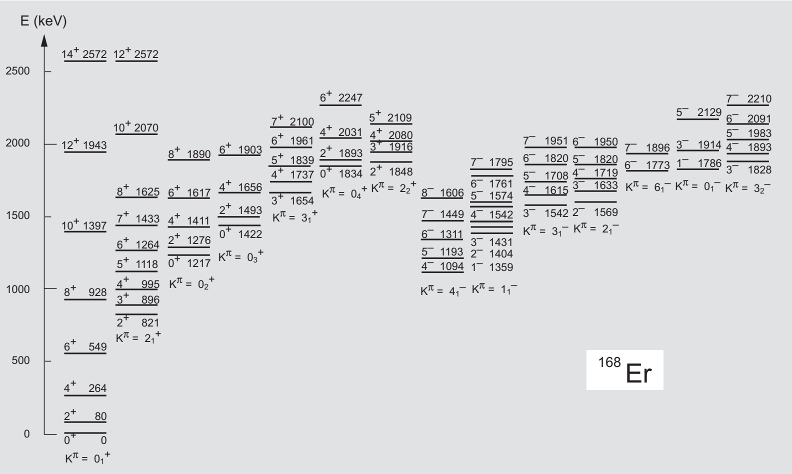

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Figure from D. J. Rowe and J. L. Wood, *Fundamentals of Nuclear Models: Foundational Models* (World Scientific, Singapore, 2010).

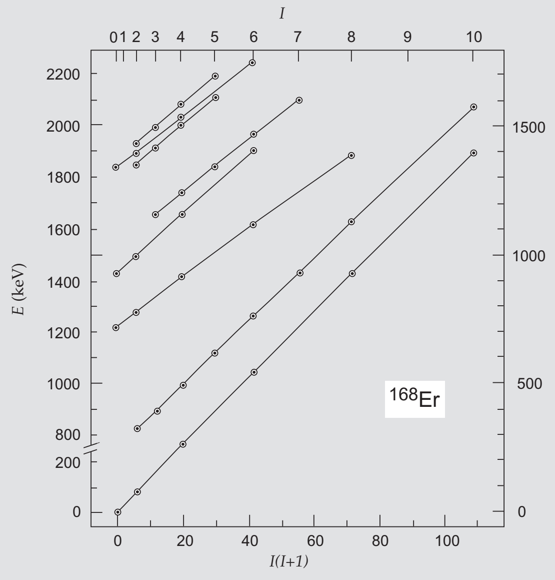

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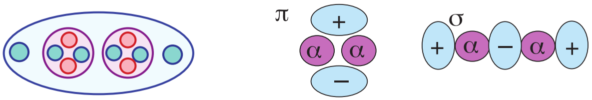
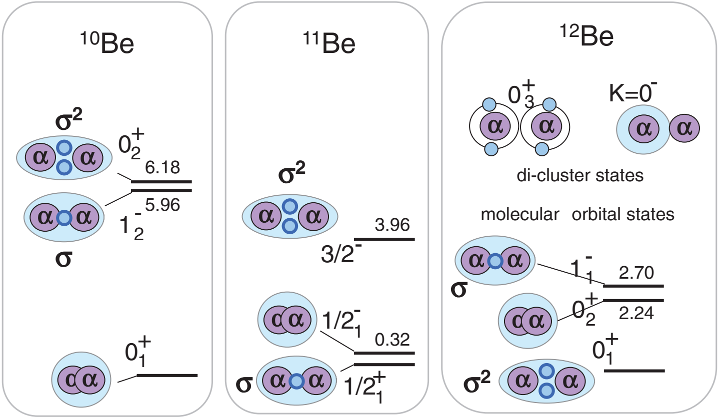
Figure from D. J. Rowe and J. L. Wood, *Fundamentals of Nuclear Models: Foundational Models* (World Scientific, Singapore, 2010).

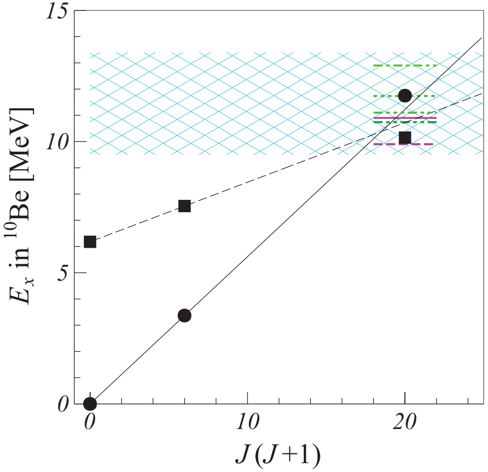
Cluster molecular structure in light nuclei

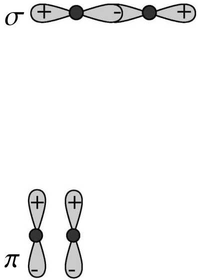




Yoshiko Kanada-En'yo, Masaaki Kimura, and Akira Ono, PTEP 2012, 01A202 (2012).

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).

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Solution of Schrödinger equation in a basis

Hamiltonian

One particle in *one* dimension

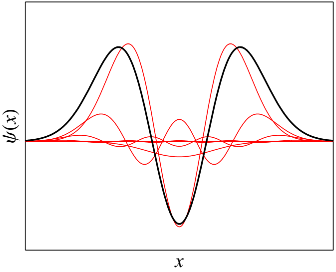
$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

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

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

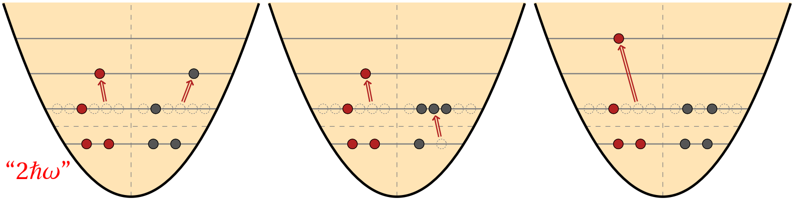
Reduces to matrix eigenproblem

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

Many-body problem in an oscillator basis

No-core configuration interaction (NCCI) approach

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



Antisymmetrized product basis *Slater determinants*

Distribute nucleons over oscillator shells

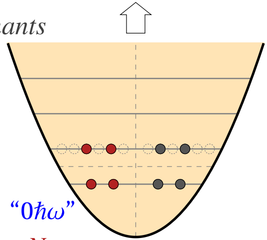
Organize basis by # oscillator excitations N_{ex}

relative to lowest Pauli-allowed filling

$N_{\mathrm{ex}} = 0, 2, \ldots$ (*i.e.*, "$0\hbar\omega$", "$2\hbar\omega$", …)

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

Convergence towards exact result with increasing N_{max}…



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

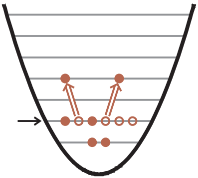
Convergence of NCCI calculations

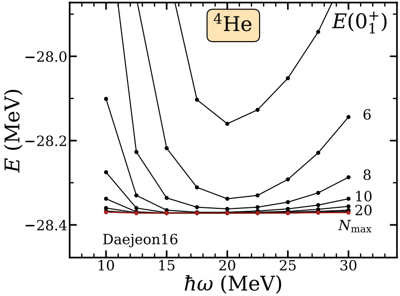
Results in finite space depend upon:

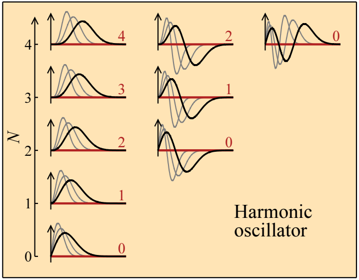
- Many-body truncation N_{max}
- Oscillator length b (or $\hbar\omega$)

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

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







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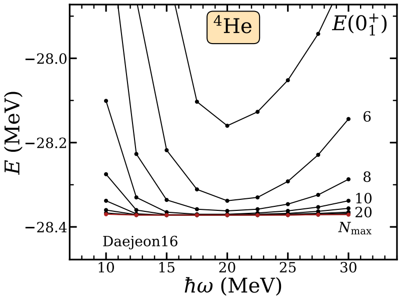

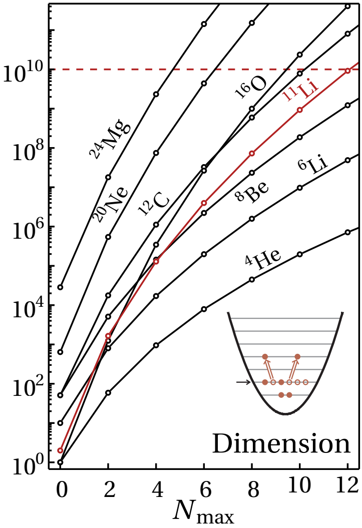

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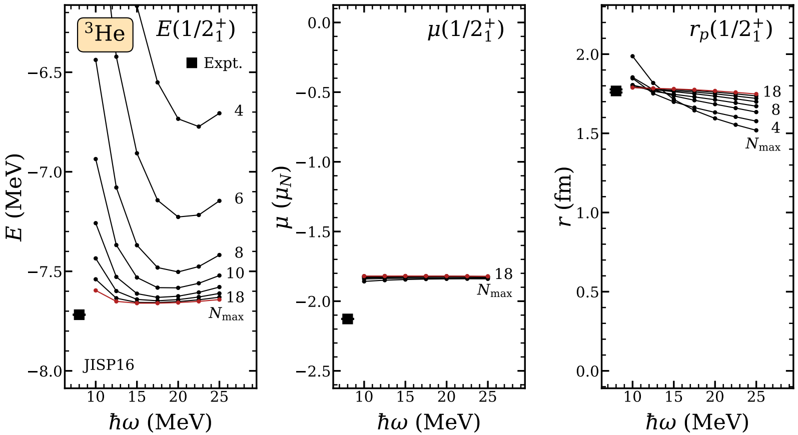

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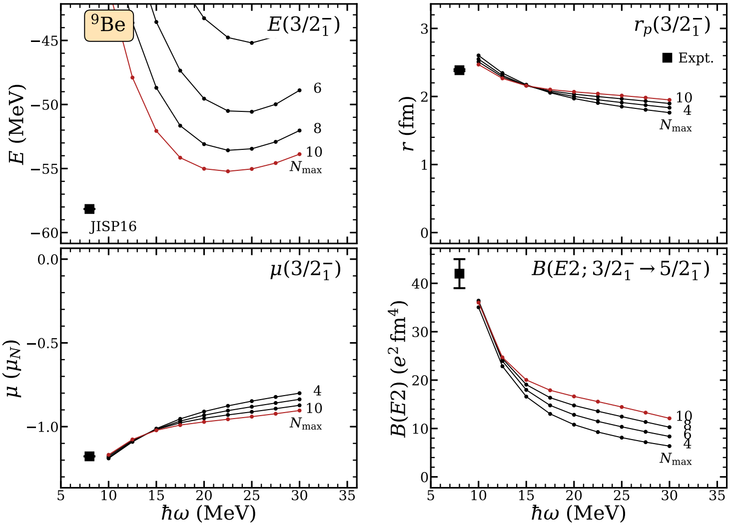

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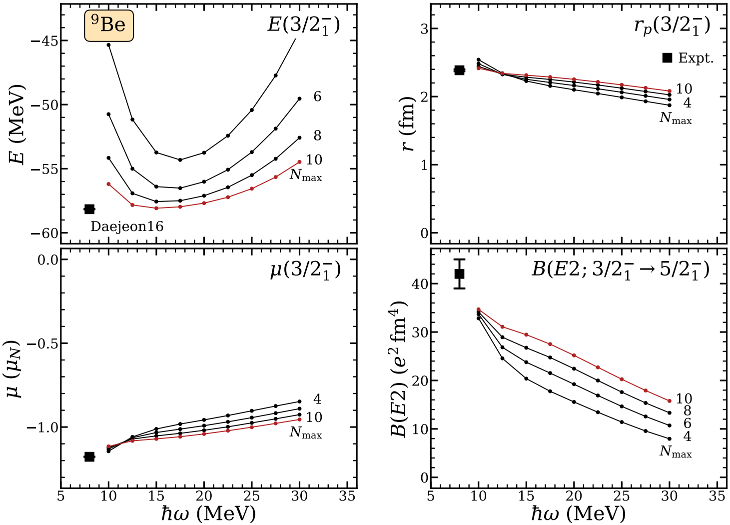

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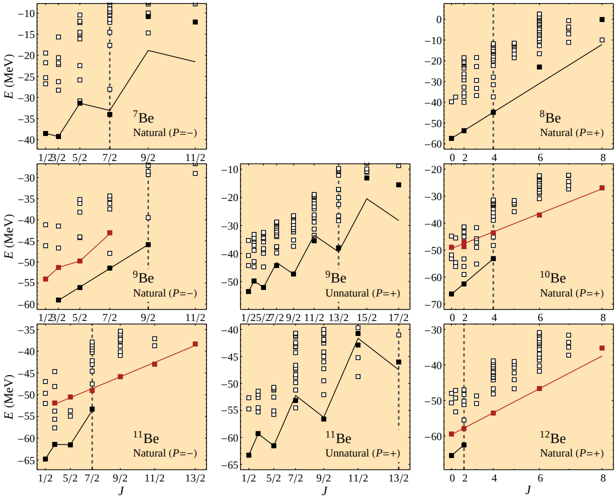
Rotational bands in $^{7-12}$Be from NCCI calculations



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

Separation of rotational degree of freedom

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

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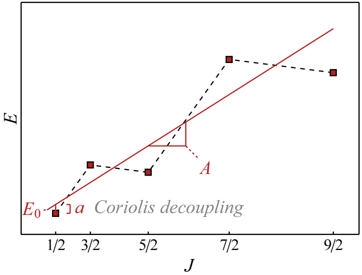

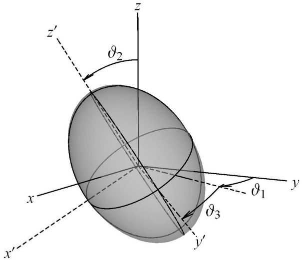

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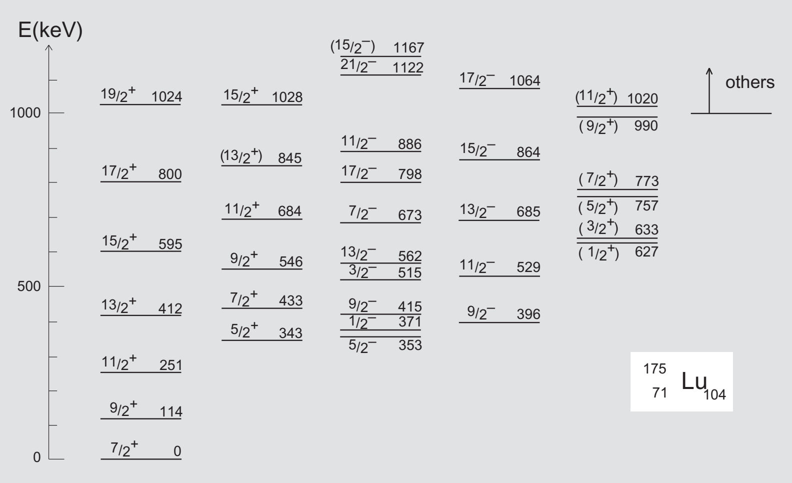
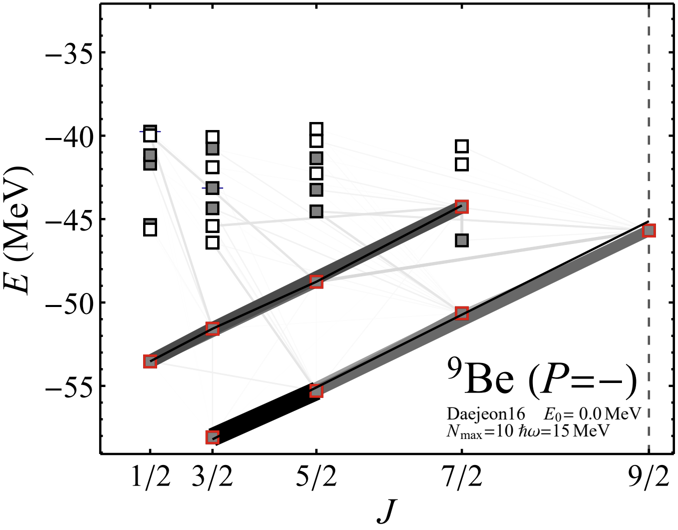


Figure from D. J. Rowe and J. L. Wood, *Fundamentals of Nuclear Models: Foundational Models* (World Scientific, Singapore, 2010).

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



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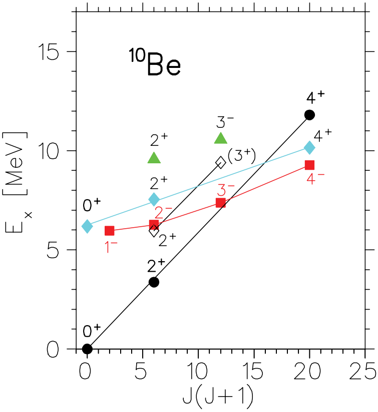


H. G. Bohlen *et al.*, Phys. Rev. C **75**, 054604 (2007).

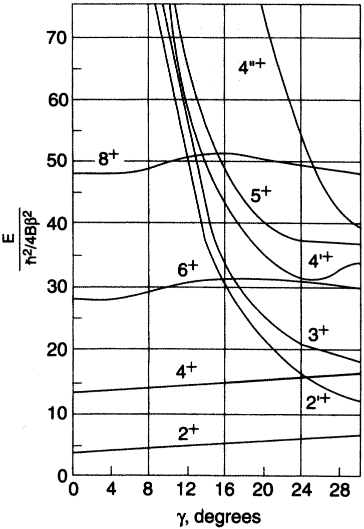
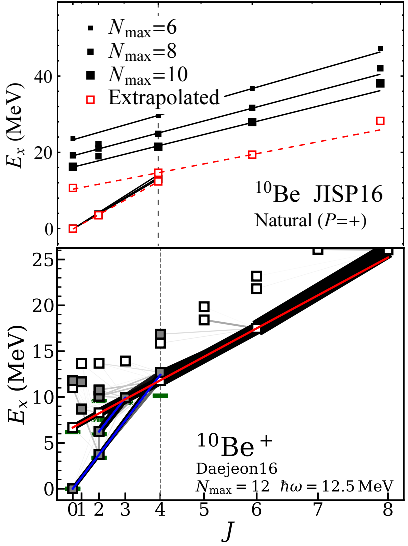
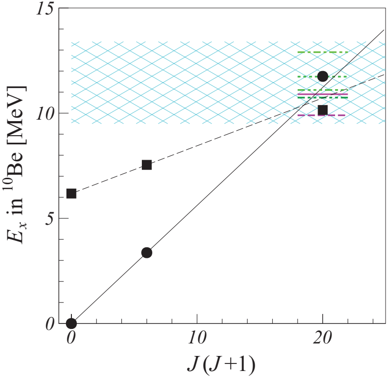


FIG. 6.24. Normal and anomalous levels of the triaxial rotor (Preston, 1975).

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

Convergence for “intruder” band ^{10}Be

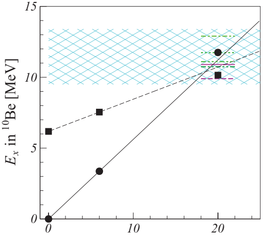




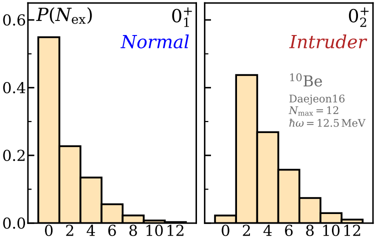
From D. Suzuki *et al.*, Phys. Rev. C **87**, 054301 (2013).

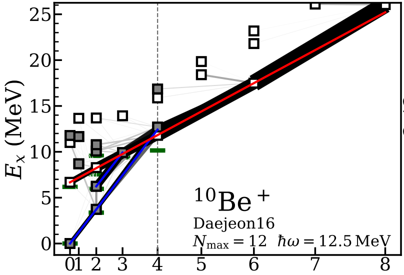
Extrapolation: Exponential in N_{max} (3-point); see P. Maris, J. P. Vary, and A. M. Shirokov, Phys. Rev. C **79**, 014308 (2009).

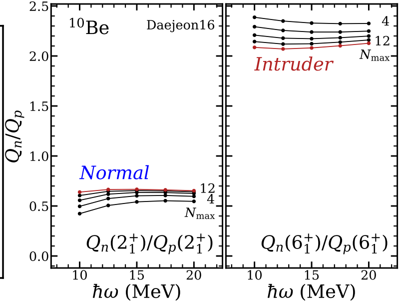
Structure of “intruder” band ^{10}Be



D. Suzuki (2013).





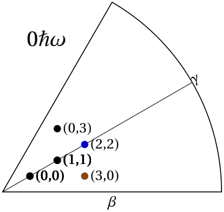


See also: M. A. Caprio, P. J. Fasano, A. E. McCoy, P. Maris, and J. P. Vary, Bulg. J. Phys. **46**, 455 (2019) (SDANCA19).

“Leading” U(3) irreps for ^{10}Be

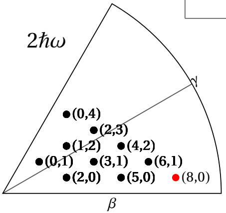
Intrinsic deformation for irrep (λ,μ)

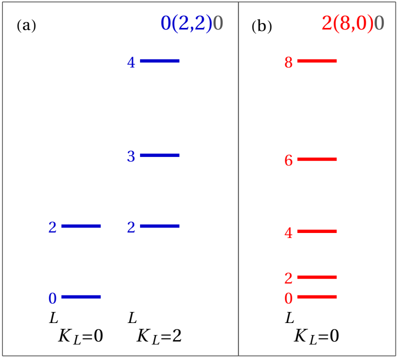
$$\beta \propto (Q\cdot Q)^{1/2}$$
$$\propto (\lambda^2+\lambda\mu+\mu^2+3\lambda+3\mu+3)^{1/2}$$
$$\gamma = \tan^{-1}\left(\frac{\sqrt{3}(\mu+3)}{2\lambda+\mu+3}\right)$$



Proton-neutron SU(3) structure

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





Elliott model

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

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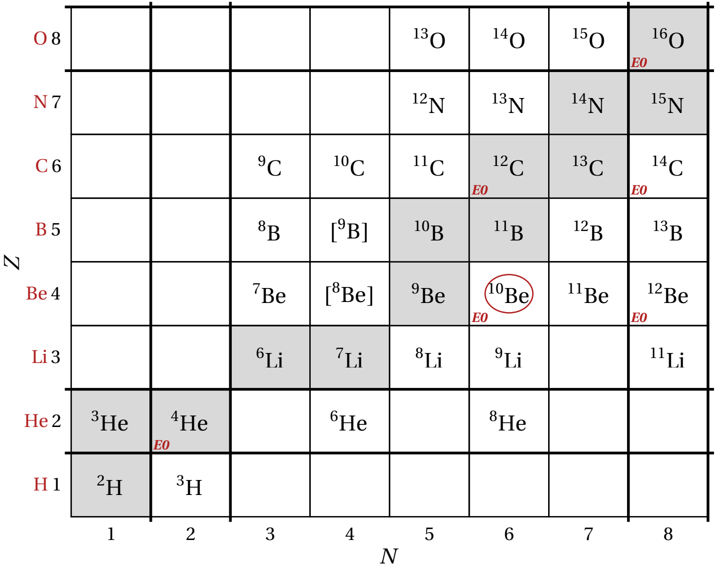
M. A. Caprio, A. E. McCoy, P. J. Fasano, and T. Dytrych, Bulg. J. Phys. **49**, 57 (2022) (SDANCA21).



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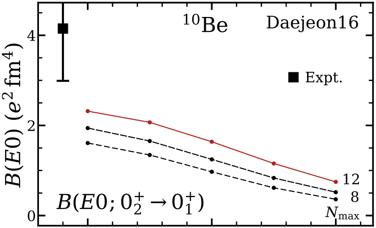
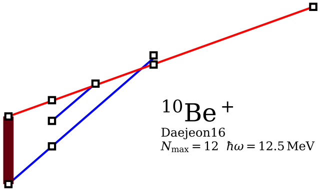
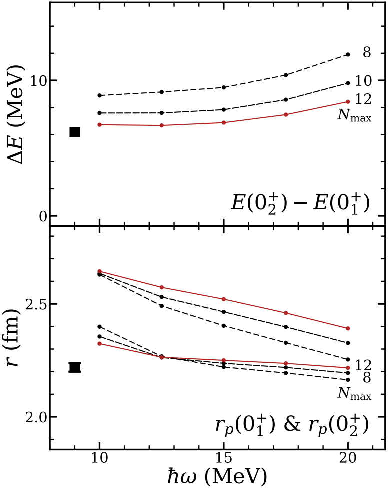
E0 = $E0$ measured ($0^+ \rightarrow 0^+$) [T. Kibédi, A. B. Garnsworthy, and J. L. Wood, PPNP **123**, 103930 (2022)]

Ab initio calculation of $E0$ transition in ^{10}Be

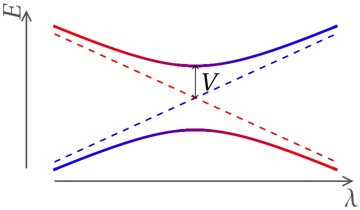
Daejeon16 interaction

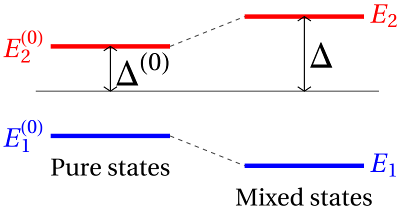






Two-state mixing





$$H = \begin{pmatrix} E_1^{(0)}(\lambda) & 0 \\ 0 & E_2^{(0)}(\lambda) \end{pmatrix} + \begin{pmatrix} 0 & V \\ V & 0 \end{pmatrix}$$

$$\begin{pmatrix} |\psi_1\rangle \\ |\psi_2\rangle \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} |\psi_1^{(0)}\rangle \\ |\psi_2^{(0)}\rangle \end{pmatrix}$$

Weak mixing (perturbative) limit… $V/\Delta^{(0)} \ll 1$

$$\theta \approx -\frac{V}{2\Delta^{(0)}}$$

Strong mixing (full) solution…

$$\tan 2\theta = -\frac{V}{\Delta^{(0)}}$$

Level repulsion…

$$\Delta^2 = (\Delta^{(0)})^2 + V^2$$

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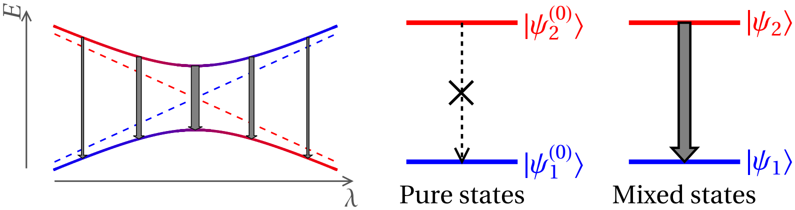
E.g., R. F. Casten, *Nuclear Structure from a Simple Perspective* (2000). K. Heyde and J. L. Wood, *Quantum Mechanics for Nuclear Structure* (2020).

Deducing mixing from transition



Suppose transition between pure states vanishes...

$$\langle\psi_2^{(0)}|\mathcal{M}|\psi_1^{(0)}\rangle = 0$$

Then transition between mixed states comes from "mixed in" contribution from diagonal matrix elements...

$$\langle\psi_1|\mathcal{M}|\psi_2\rangle = \tfrac{1}{2}(\sin 2\theta)\Big[\langle\psi_2^{(0)}|\mathcal{M}|\psi_2^{(0)}\rangle - \langle\psi_1^{(0)}|\mathcal{M}|\psi_1^{(0)}\rangle\Big]$$

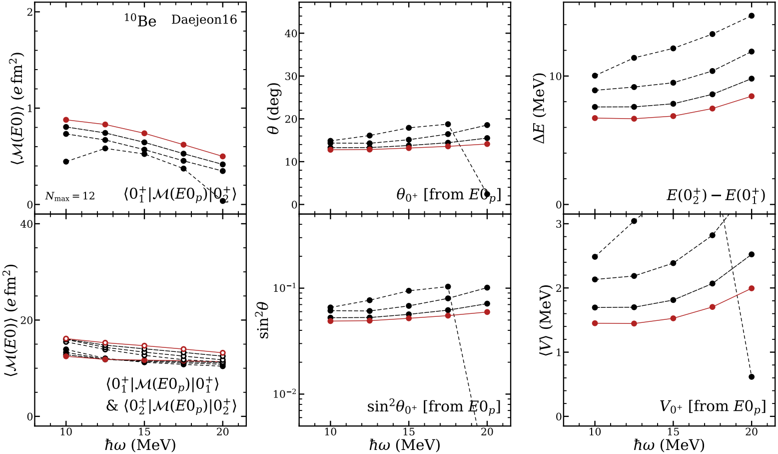
Invert to deduce mixing angle from "mixed" matrix elements...

$$\tan 2\theta = \frac{2\langle\psi_2|\mathcal{M}|\psi_1\rangle}{\langle\psi_2|\mathcal{M}|\psi_2\rangle - \langle\psi_1|\mathcal{M}|\psi_1\rangle}$$

Mixing analysis of *ab initio* calculations for ^{10}Be

Assume $\langle 0\hbar\omega | \mathcal{M}(E0) | 2\hbar\omega \rangle$ vanishes for "pure" (unmixed) 0^+ states.

Deduce mixing from matrix elements for NCCI calculated (mixed) states.



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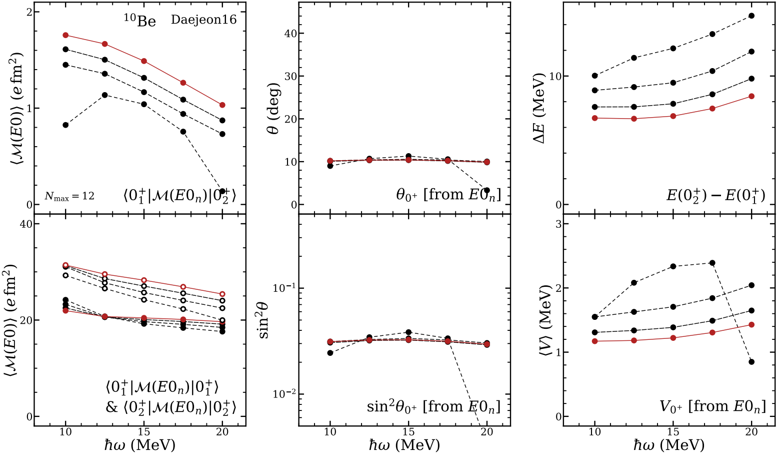
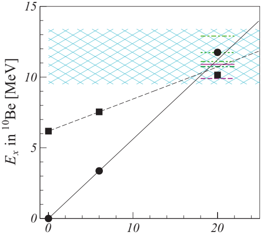
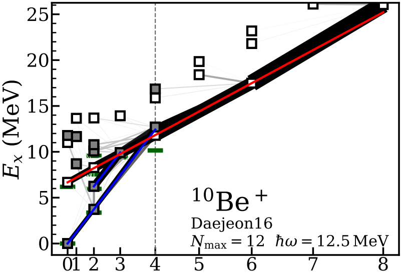
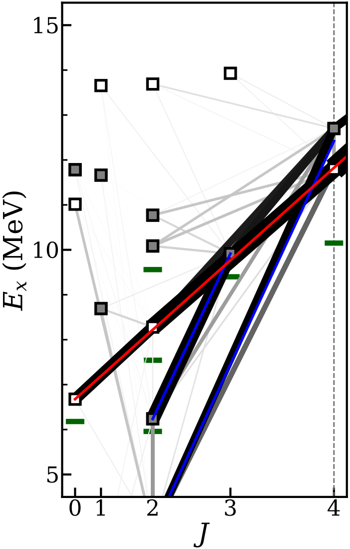


Crossing of 4^+ states in ^{10}Be (zoom)



D. Suzuki (2013).





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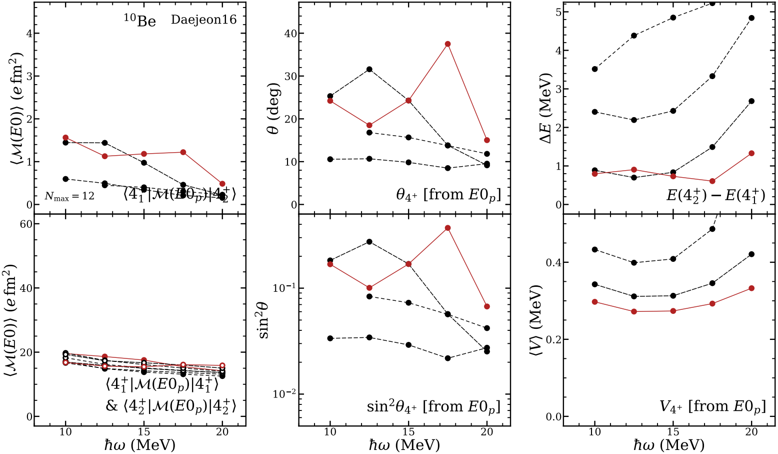

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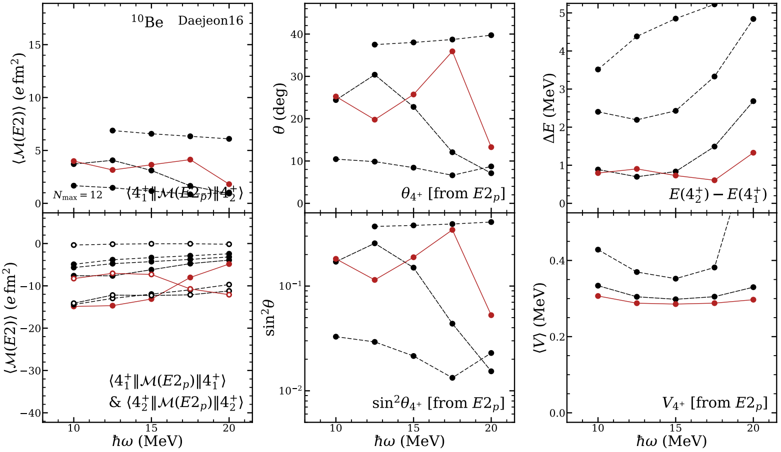
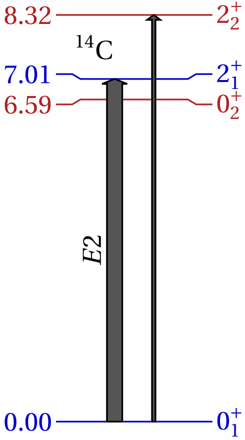
Mixing analysis of *ab initio* calculations for ^{10}Be

Assume $\langle 0\hbar\omega|\mathcal{M}(E2)|2\hbar\omega\rangle$ vanishes for "pure" (unmixed) 4^+ states.

Deduce mixing from matrix elements for NCCI calculated (mixed) states.



The $E2$ strength to the first 2^+ state(s) in ^{14}C?

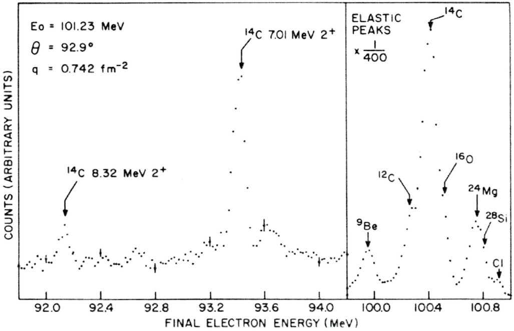


Electron Scattering from Low Lying 2^+ States in ^{14}C*

Hall Crannell, P.L. Hallowell, J.T. O'Brien,
J.M. Finn and F.J. Kline+
The Catholic University of America, Washington, D.C.

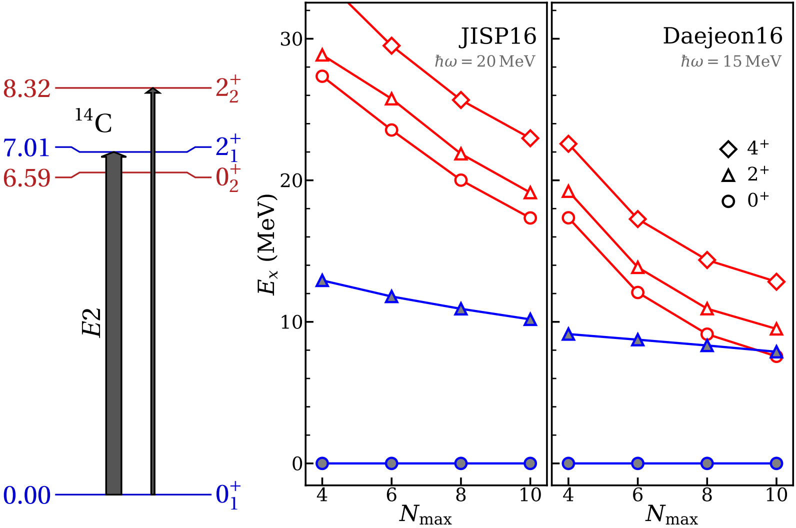
and

S. Penner, J.W. Lightbody, Jr., and S.P. Fivozinsky
National Bureau of Standards, Washington, D.C.



H. Crannell *et al.*, Proc. Int. Conf. Nucl. Struct. Studies Using Electron Scattering and Photoreaction, Sendai, Japan (1972).

Convergence of intruder state energies in ^{14}C



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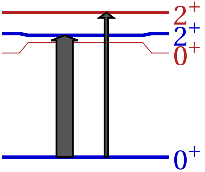
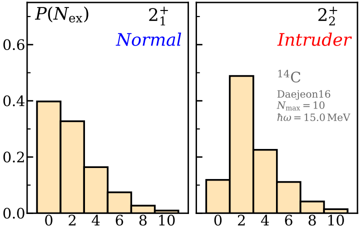
Low-lying intruder structure in ^{14}C

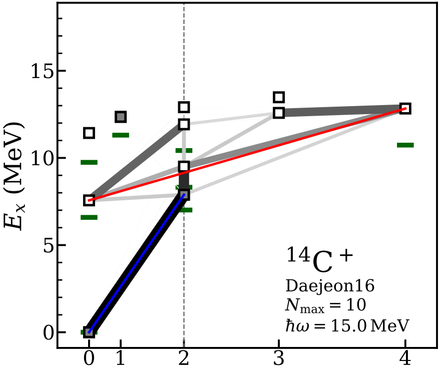
Coexisting 0^+-2^+ sequences: $0\hbar\omega$ and $2\hbar\omega$

Very different “moments of inertia” ⇒ 2^+ states approach and mix

Excited structure as triaxial rotor? *Elliott* SU(3)







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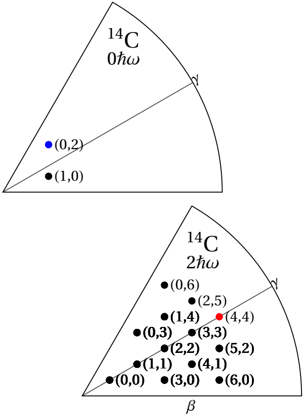
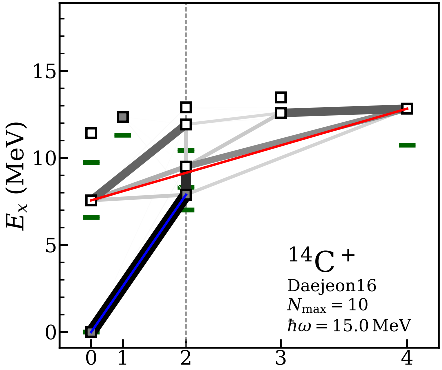
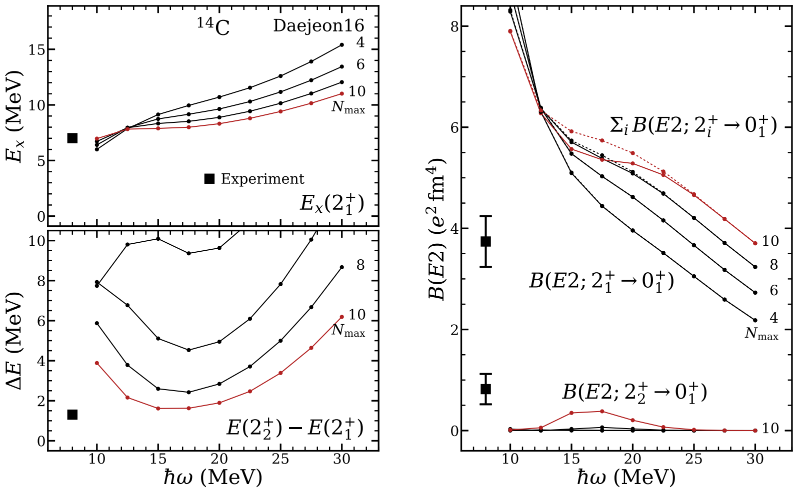




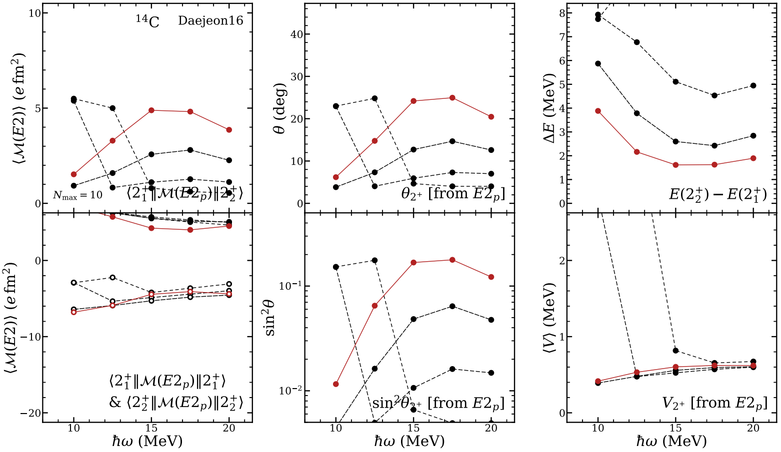
The $E2$ strength to the first 2^+ state(s) in ^{14}C?



Mixing analysis of *ab initio* calculations for ^{14}C

Assume $\langle 0\hbar\omega | \mathcal{M}(E2) | 2\hbar\omega \rangle$ vanishes for "pure" (unmixed) 2^+ states.

Deduce mixing from matrix elements for NCCI calculated (mixed) states.



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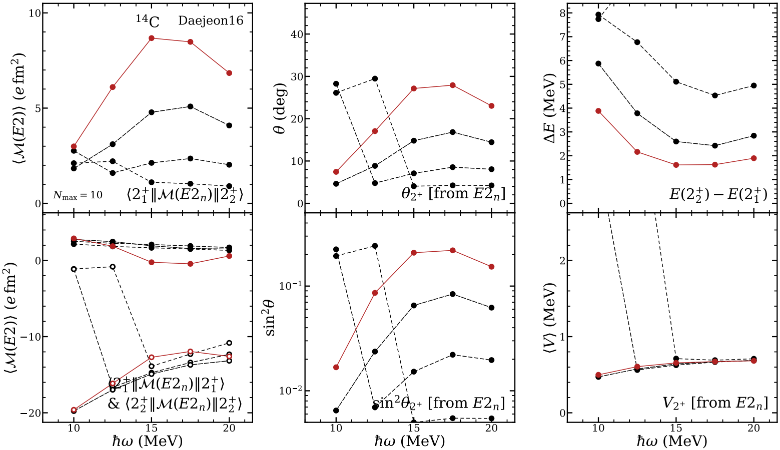
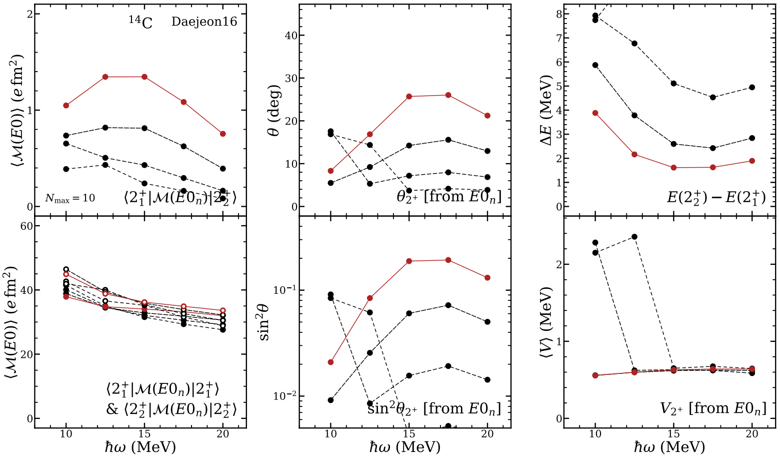


Mixing analysis of *ab initio* calculations for ^{14}C

Assume $\langle 0\hbar\omega | \mathcal{M}(E0) | 2\hbar\omega \rangle$ vanishes for "pure" (unmixed) 2^+ states.

Deduce mixing from matrix elements for NCCI calculated (mixed) states.



Notes on emergent mixing in ^{10}Be & ^{14}C

Three related but distinct questions...

Are *truncated ab initio* calculations well-described by mixing?

If so, how "constant" is the mixing matrix element?

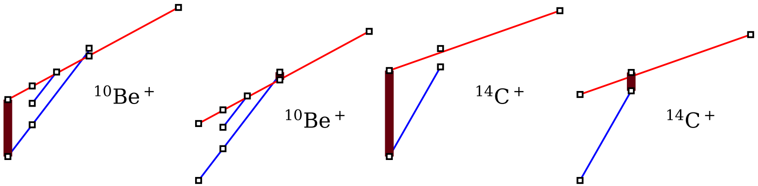
Is the solution to the *untruncated* problem well-described by mixing?

Predicted structure depends (at least in detail) on interaction

What is the actual structure (and mixing) in the *physical nucleus*?

For $0^+ \rightarrow 0^+$ ground-state transition (weak mixing)... Slowly converging "emergent" shape mixing matrix element ($\approx 1\,\mathrm{MeV}$).

For $J^+ \rightarrow J^+$ excited-state transition (strong mixing)... Robust convergence of "emergent" shape mixing matrix element ($\lesssim 0.5\,\mathrm{MeV}$).



Summary

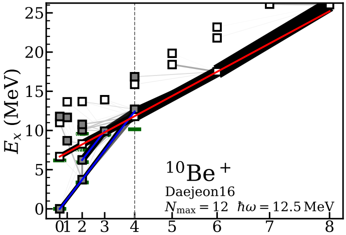
Different states in low-lying spectrum have different…

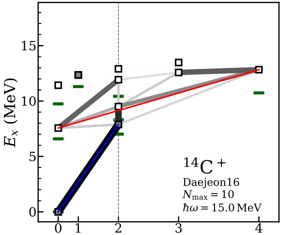
- Rotational moments of inertia *Energy spacing within band*
- Shell model character *Normal* $(0\hbar\omega)$ *vs.* *intruder* $(2\hbar\omega)$
- Shape/deformation & Elliott SU(3) symmetry

Intruders hard to converge, but tractable with soft interaction *Daejeon16*

Two-state mixing emerges in *ab initio* NCCI results…

- Can be transient (as energies cross) or persistent (at physical energies)
- *Mixing matrix element* extracted from normal-intruder transition
- $B(E0; 0^+ \rightarrow 0^+)$ depends on intruder radius *Slowly convergent*





Island of inversion at $N = 8$ *(ab initio)*

The intruder becomes the ground state…

- Parity inversion ^{11}Be
  J. Chen *et al.*, Phys. Rev. C **100**, 064314 (2019).
- Predominantly $2\hbar\omega$ (or strongly mixed) ground state ^{11}Li, ^{12}Be
  Anna E. McCoy *et al.*, *Intruder band mixing in an ab initio description of* ^{12}Be, `arXiv:2402.12606`.

	3	4	5	6	7	8
O 8			^{13}O (3/2−)	^{14}O 0+	^{15}O 1/2−	^{16}O 0+
N 7			^{12}N 1+	^{13}N 1/2−	^{14}N 1+	^{15}N 1/2−
C 6	^{9}C (3/2−)	^{10}C 0+	^{11}C 3/2−	^{12}C 0+	^{13}C 1/2−	^{14}C 0+
B 5	^{8}B 2+	[^{9}B] 3/2−	^{10}B 3+	^{11}B 3/2−	^{12}B 1+	^{13}B 3/2−
Be 4	^{7}Be 3/2−	[^{8}Be] 0+	^{9}Be 3/2−	^{10}Be 0+	^{11}Be 1/2+	^{12}Be 0+
Li 3	^{6}Li 1+	^{7}Li 3/2−	^{8}Li 2+	^{9}Li 3/2−		^{11}Li 3/2−