Intruder structure, shape coexistence, and configuration mixing from an *ab initio* perspective

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Progress in *Ab Initio* Nuclear Theory
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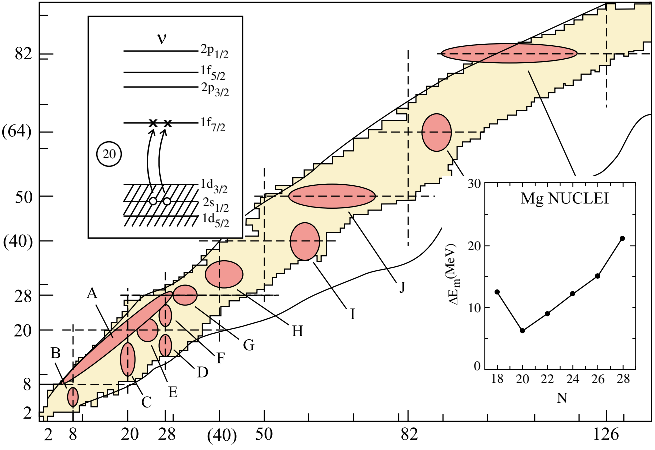
Intruder structure (and shape coexistence)

"[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).

In ab initio no-core configuration interaction (NCCI) calculations...

How do “normal” and “intruder” states converge? ^{9}Be, ^{10}Be

What do we find for intruder structure at $N = 8$? ^{11}Li, ^{14}C

Can we describe mixing of normal & intruder configurations?

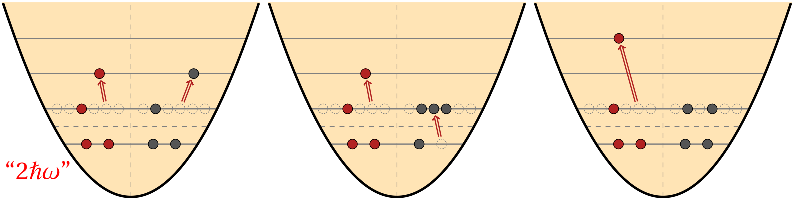
Postscript: Can we see the $4\hbar\omega$ intruder in ^{16}O?

	3	4	5	6	7	8
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−

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

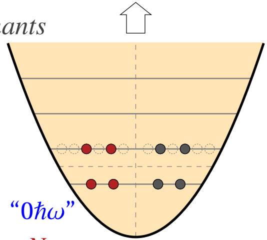
Organize basis by # oscillator excitations N_{ex}

relative to lowest Pauli-allowed filling

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

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).

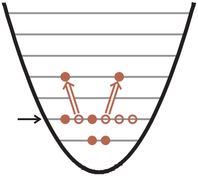
Convergence of NCCI calculations

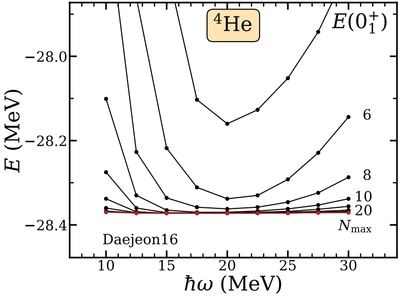
Results in finite space depend upon:

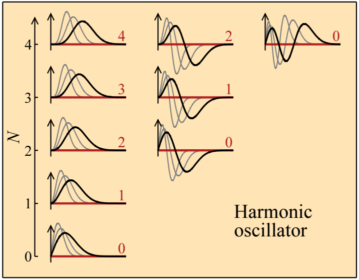
- Many-body truncation $N_{\max}$
- Oscillator length b (or $\hbar\omega$)

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

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







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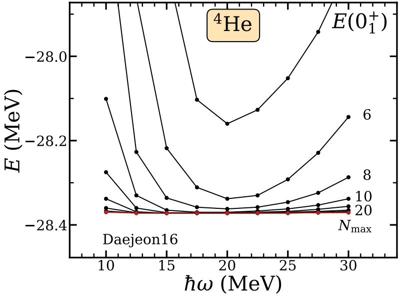
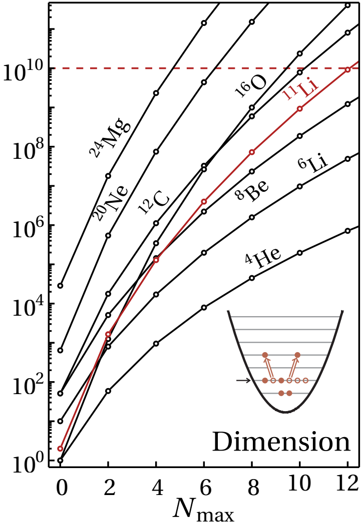
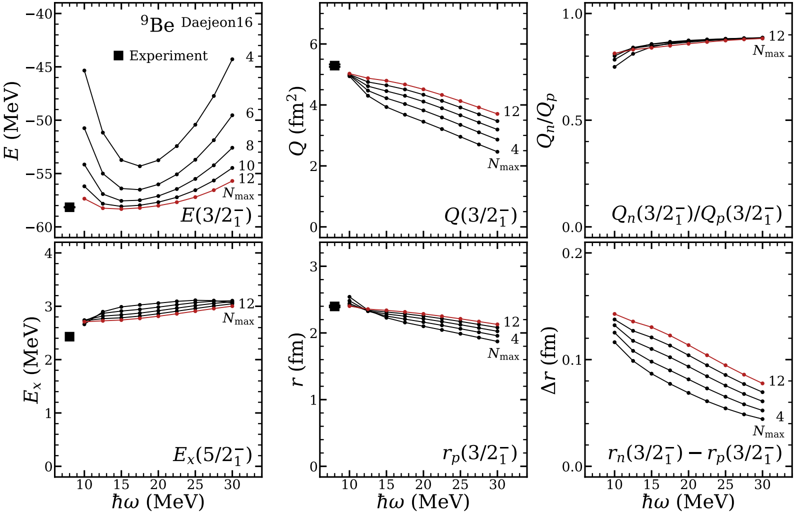


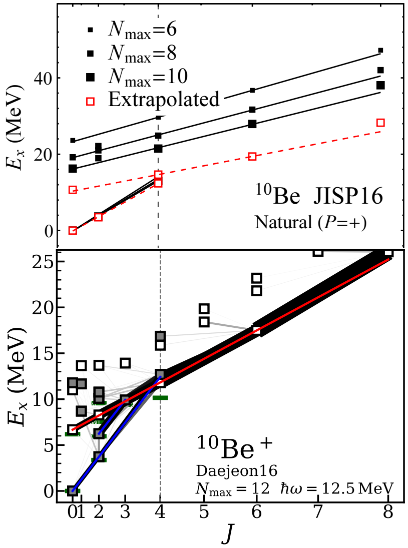


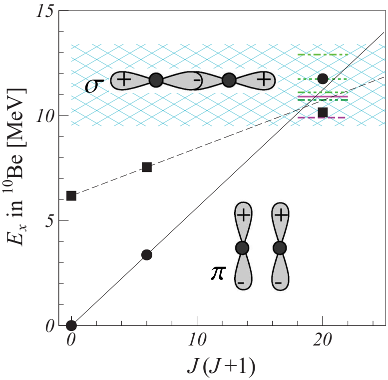
Convergence for “normal” states ^{9}Be



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

Convergence for "intruder" band ^{10}Be

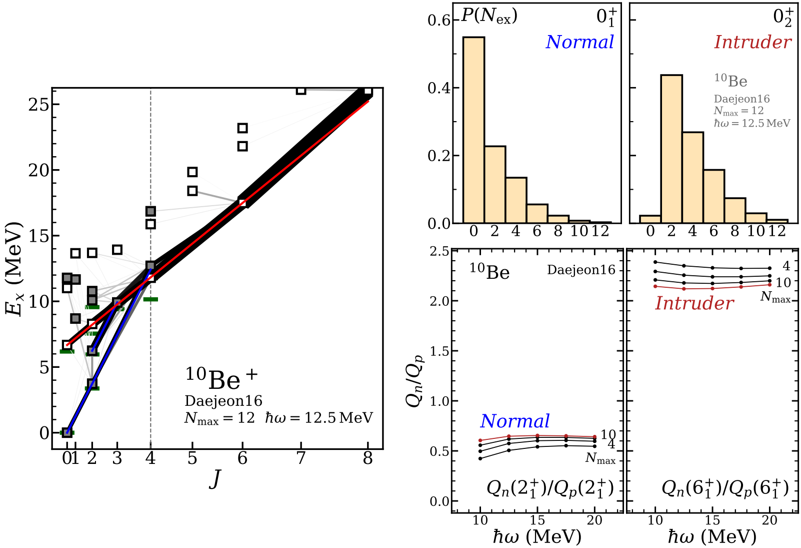




From D. Suzuki *et al.*, Phys. Rev. C **87**, 054301 (2013). Orbital schematics from Y. Kanada-En'yo, H. Horiuchi, and A. Doté, Phys. Rev. C **60**, 064304 (1999).

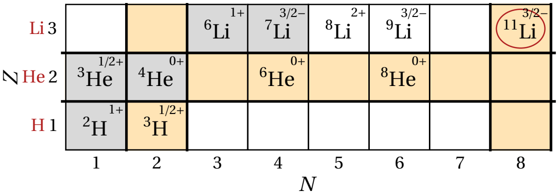
Extrapolation: Exponential in N_{max} (3-point); see P. Maris, J. P. Vary, and A. M. Shirokov, Phys. Rev. C **79**, 014308 (2009).

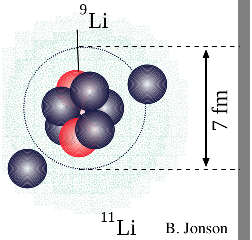
Structure of "intruder" band ^{10}Be



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

Structure of the ^{11}Li ground state?





Shell model: Doubly-magic plus one proton

Closed shell neutron

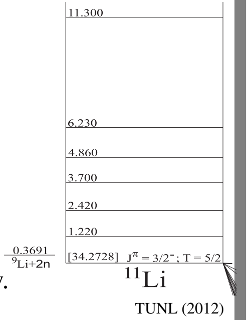
Interaction σ & p scattering: Enhanced matter radius

Neutron halo

Neutron knockout: Neutron $(0p_{3/2})^2$ and $(1s_{1/2})^2$ contribute about equally to ground state

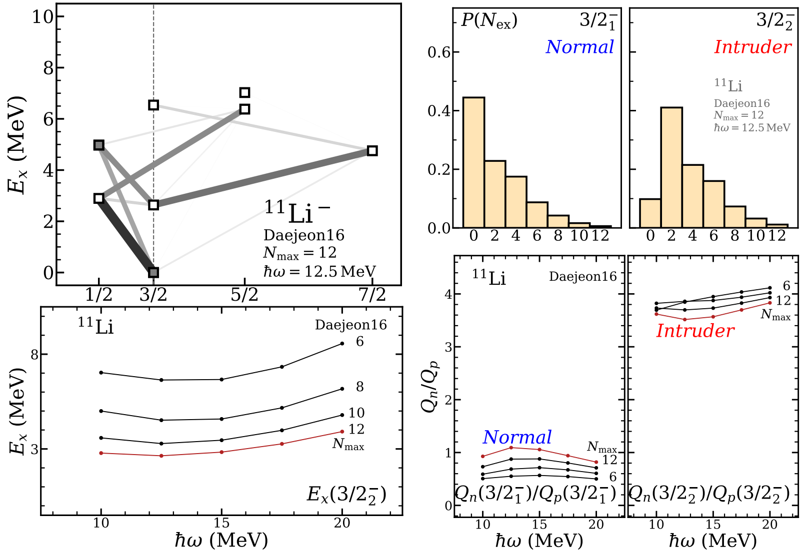
Intruder configurations

Excitation spectrum: Not particularly illuminating! No J^P assignments. Unbound, but relatively narrow.

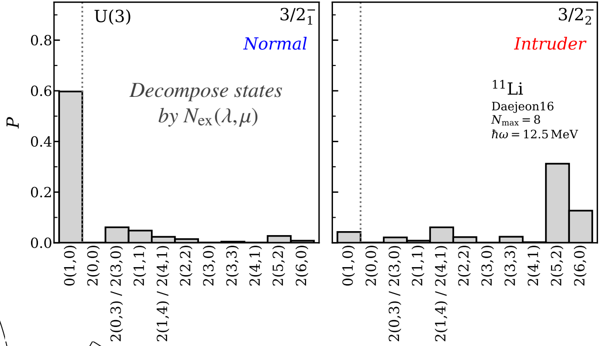


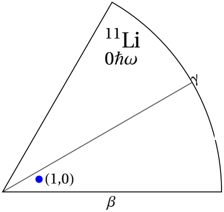
B. Jonson, Phys. Rep. **389**, 1 (2004).

Low-lying intruder structure in ^{11}Li



Elliott SU(3) symmetry for ^{11}Li

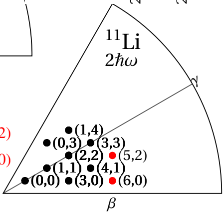




Proton-neutron structure

$\pi(1,0)\times\nu(4,2) \Rightarrow (5,2)$

$\pi(1,0)\times\nu(5,0) \Rightarrow (6,0)$



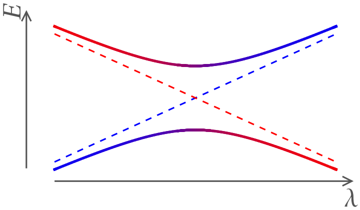
Intrinsic deformation for irrep (λ,μ)

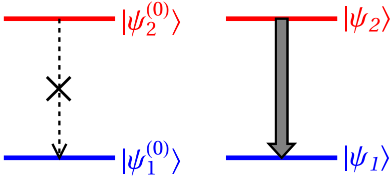
$$\beta \propto (Q\cdot Q)^{1/2}$$

$$\propto (\lambda^2+\lambda\mu+\mu^2+3\lambda+3\mu+3)^{1/2}$$

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

Transition as measure of intruder mixing





$$H = \begin{pmatrix} E_1(\lambda) & V \\ V & E_2(\lambda) \end{pmatrix} \qquad \begin{pmatrix} |\psi_1\rangle \\ |\psi_2\rangle \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} |\psi_1^{(0)}\rangle \\ |\psi_2^{(0)}\rangle \end{pmatrix}$$

Mixing depends on *energy difference* $E_2 - E_1$ and *mixing matrix element* V.

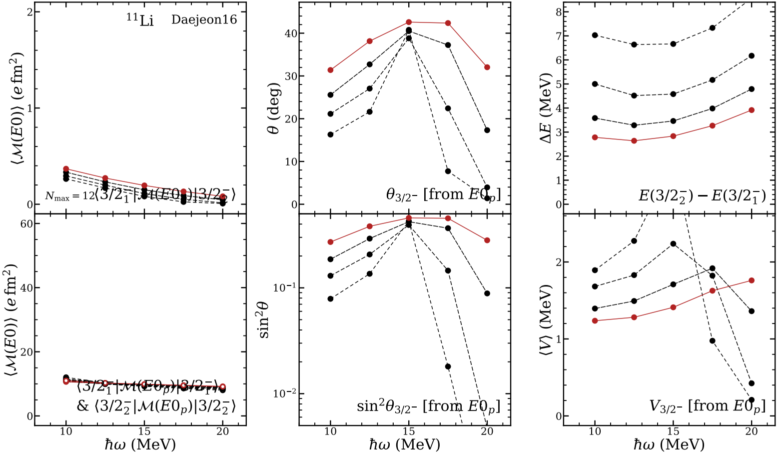
If transition operator $\mathcal{M}$ does not connect "pure" (unmixed) states, transition matrix element for "mixed" states measures: (1) their *mixing* and (2) the difference in diagonal matrix elements, *i.e.*, moments $M_2 - M_1$:

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

Mixing analysis of *ab initio* calculations for ^{11}Li

Assume $\langle 0\hbar\omega|\mathcal{M}(E0)|2\hbar\omega\rangle$ vanishes for "pure" (unmixed) $3/2^-$ states.

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



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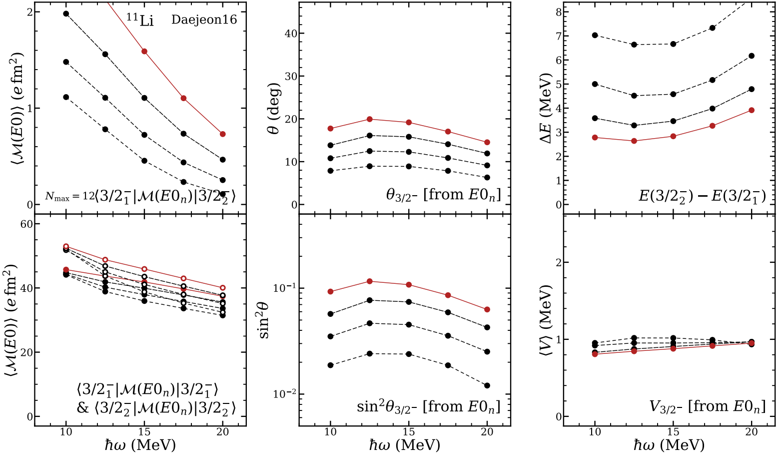

Mixing analysis of *ab initio* calculations for ^{11}Li

Assume $\langle 0\hbar\omega | \mathcal{M}(E2) | 2\hbar\omega \rangle$ vanishes for "pure" (unmixed) $3/2^-$ states.

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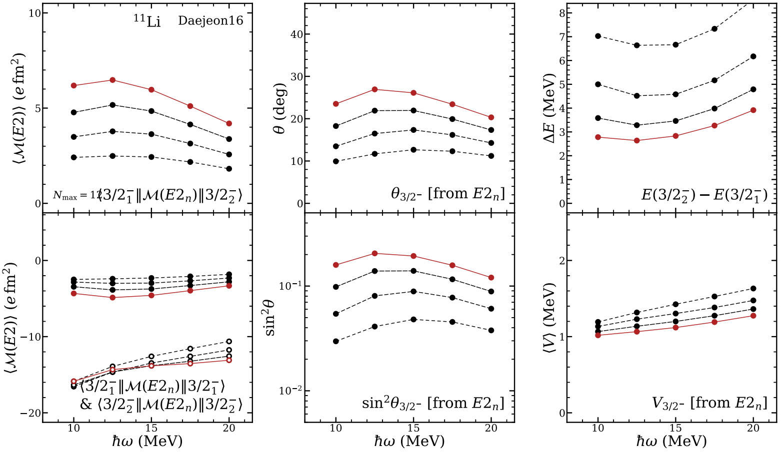
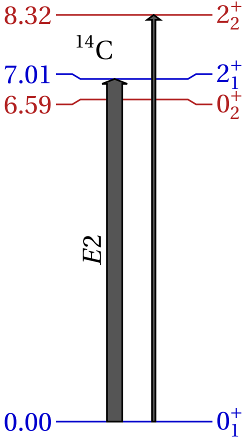


The $E2$ strength to the first 2^+ state(s) in ^{14}C?

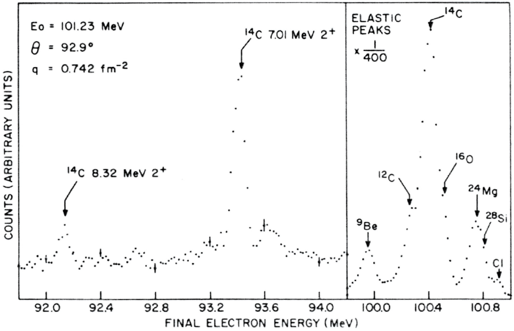


Electron Scattering from Low Lying 2^+ States in ^{14}C*

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).

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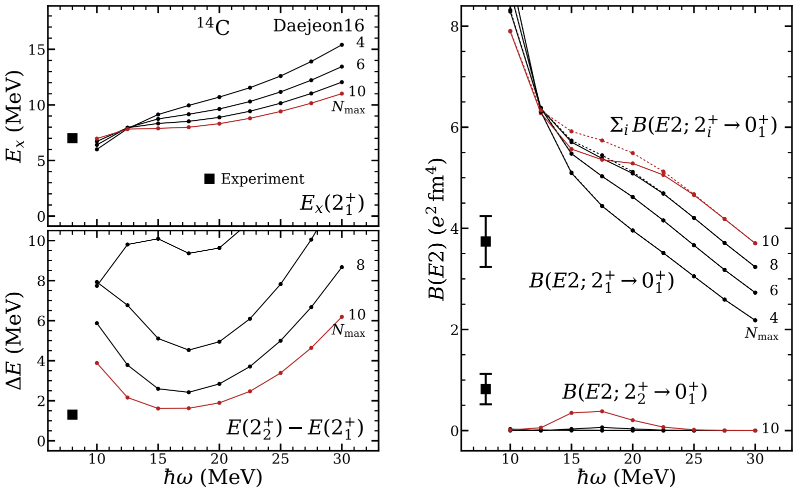
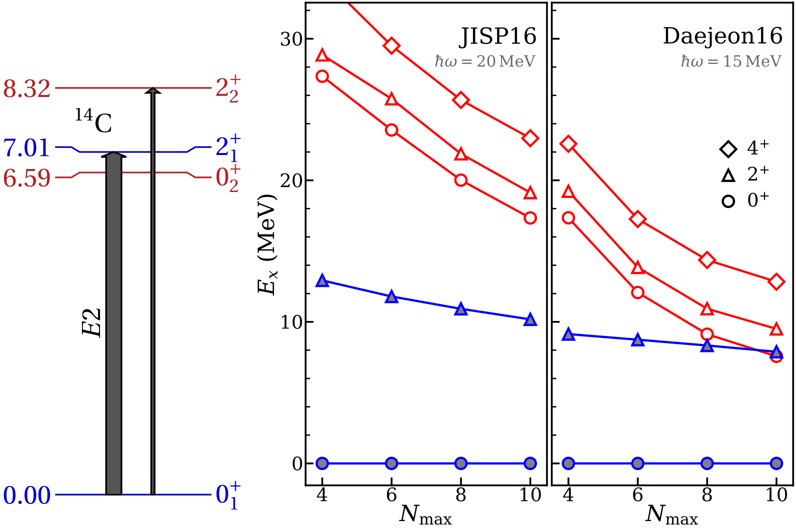


Convergence of intruder state energies in ^{14}C

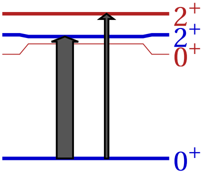


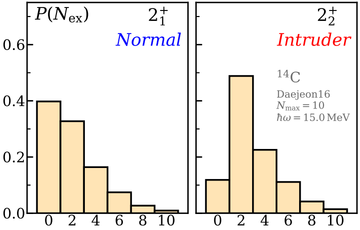
Low-lying intruder structure in ^{14}C

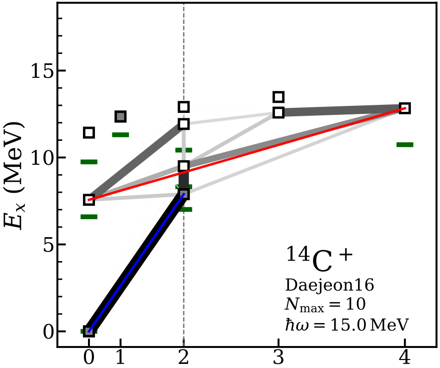
Coexisting 0^+-2^+ sequences: $0\hbar\omega$ and $2\hbar\omega$

Very different “moments of inertia” $\Rightarrow$ 2^+ states approach and mix

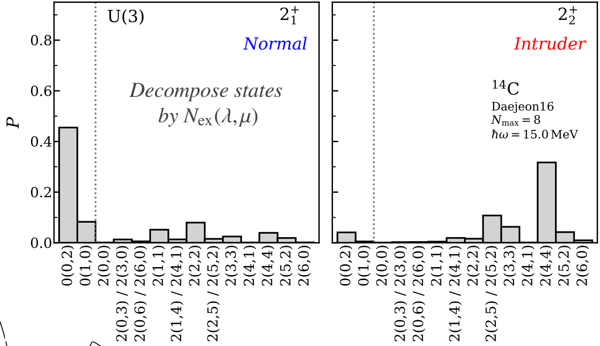
Excited structure as triaxial rotor? *Elliott* SU(3)

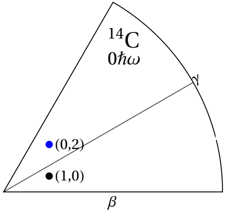


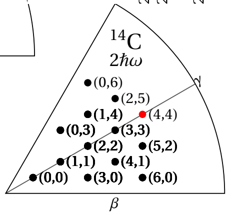




Elliott SU(3) symmetry for ^{14}C







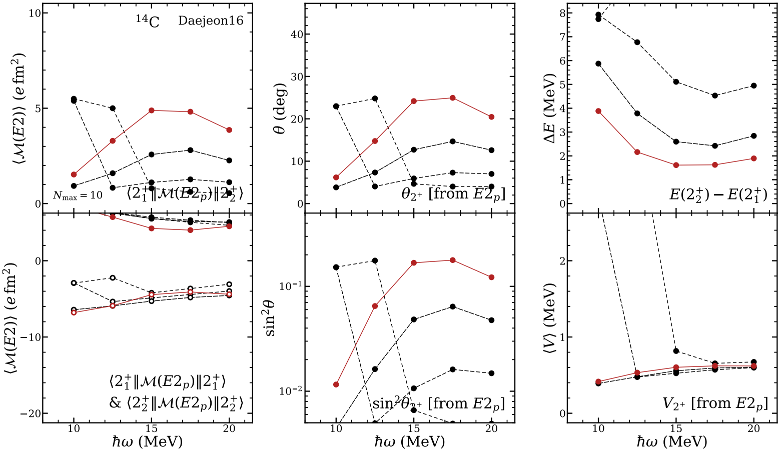
Proton-neutron triaxiality

$$\underbrace{\pi(0,2)}_{\text{oblate}}\times\underbrace{\nu(4,2)}_{\text{prolate}} \Rightarrow (4,4)$$

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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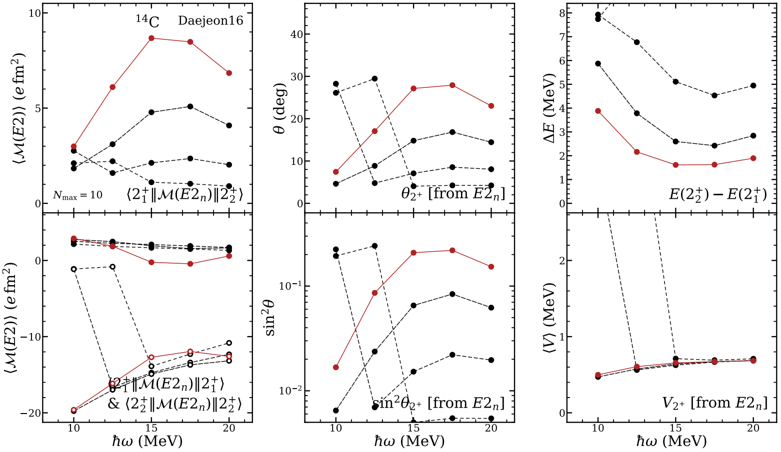

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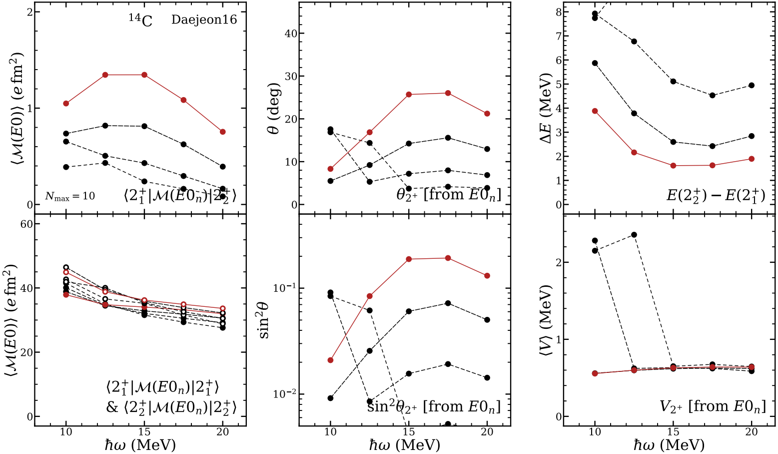


M. A. Caprio, University of Notre Dame

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

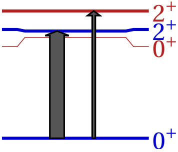
Two-state mixing estimate

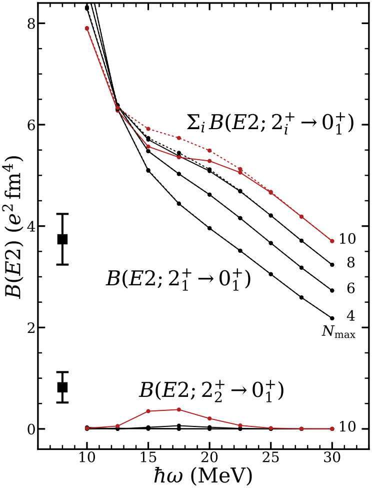
$V \approx 0.6\,\mathrm{MeV}$ *Ab initio*

$$\Delta \equiv \tfrac{1}{2}[E(2_2^+) - E(2_1^+)]$$
$$= \tfrac{1}{2}[(8.32\,\mathrm{MeV}) - (7.01\,\mathrm{MeV})]$$
$$= 0.65\,\mathrm{MeV}$$ *Experiment*

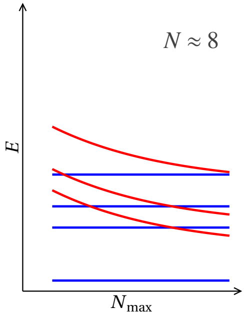
$$\sin 2\theta = -\frac{V}{\Delta} \Rightarrow |\theta| \approx 34^\circ$$ *Delicate!*

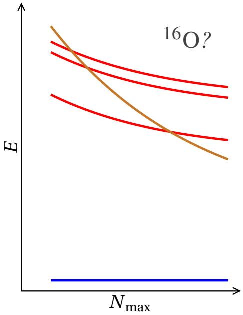
$$\frac{B(E2;0_1^+ \rightarrow 2_2^+)}{B(E2;0_1^+ \rightarrow 2_1^+)} = \frac{\sin^2\theta}{\cos^2\theta} \approx \boxed{0.44}$$

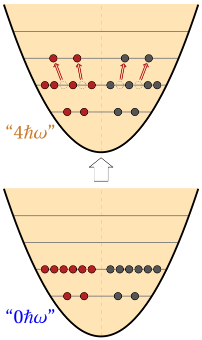


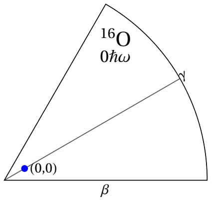


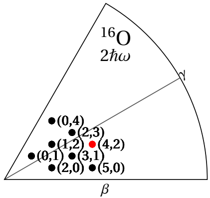
Convergence of normal, intruder, and “super-intruder” states?

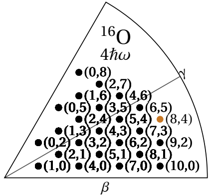




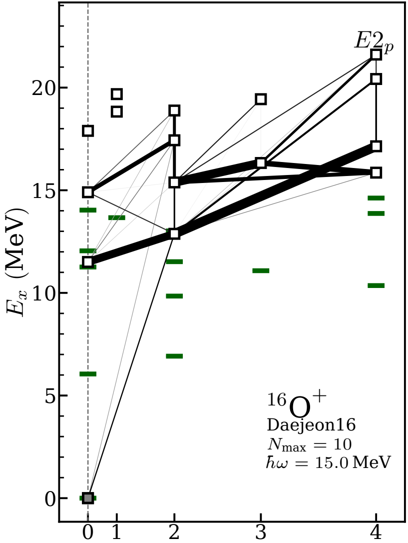


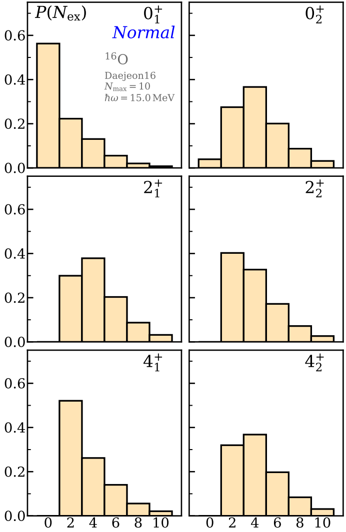






Low-lying (super-)intruder structure in ^{16}O?





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* ($2\hbar\omega$)
- Proton/neutron asymmetric deformation Q_n/Q_p
- Elliott SU(3) symmetry (≈"shape")

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

Mixing in *ab initio* results... *Emergent two-state mixing?*

- Strong mixing as same-J states approach *Within a few* MeV
- Mixing can be transient as energies cross ^{10}Be 4^+_1 & 4^+_2
- Mixing can be physical ^{11}Li *ground state* / ^{14}C 2^+_1 & 2^+_2
- Transition matrix element provides handle on mixing angle θ
- Calculated "energy denominator" may be unconverged or inexact
- *But...* Can robustly extract emergent mixing matrix element V

  $\Rightarrow$ *Estimate expected mixing at "physical" energy difference*

Beware! Ignore imminent mixing with an intruder at your own risk!

For $N = Z$... Elusive $4\hbar\omega$ intruder states within reach? ^{16}O 0^+_2