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

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Nuclear Theory in the Supercomputing Era
Busan, Republic of Korea
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intrude verb

in·trude in-ˈtrüd

intruded; intruding

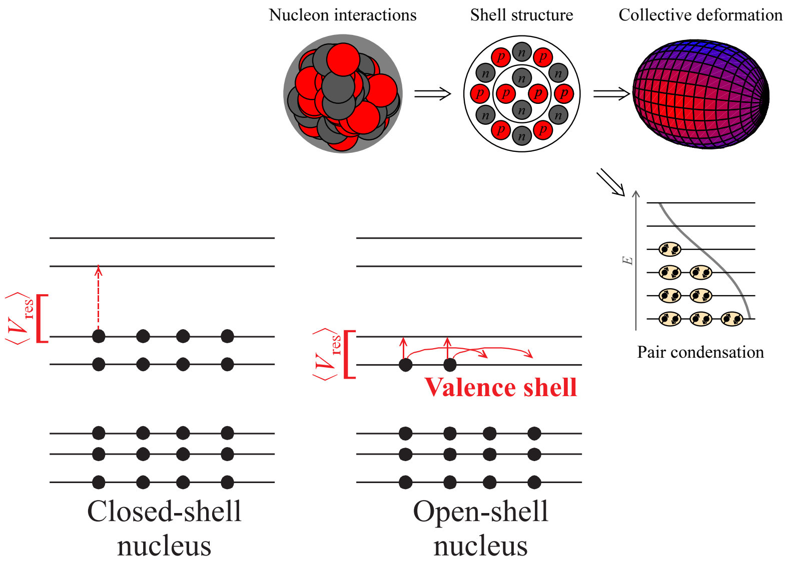
Synonyms of *intrude* >

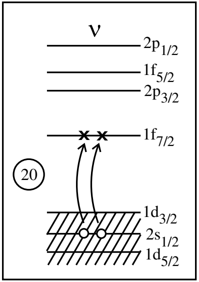
intransitive verb

1 **:** to thrust oneself in without invitation, permission, or welcome

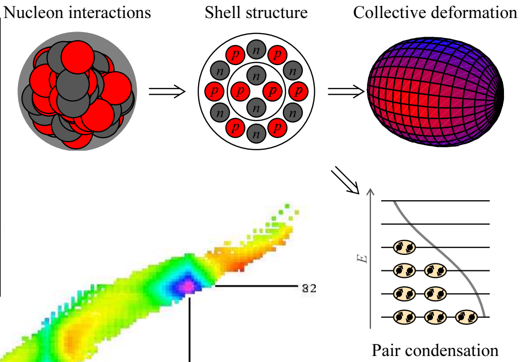
Merriam-Webster Est. 1828

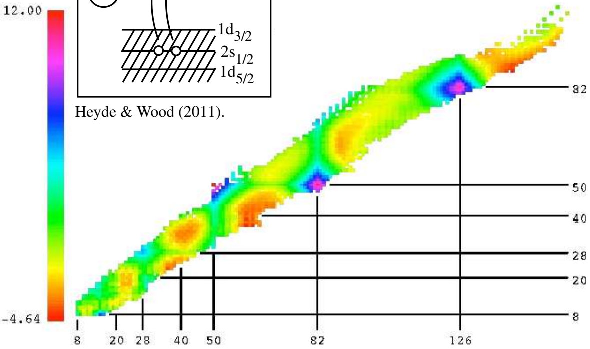
https://www.merriam-webster.com/dictionary/intrude


Nucleon interactions
Shell structure
Collective deformation
Pair condensation
E
⟨V_res⟩
Valence shell
⟨V_res⟩
Closed-shell nucleus
Open-shell nucleus



Heyde & Wood (2011).

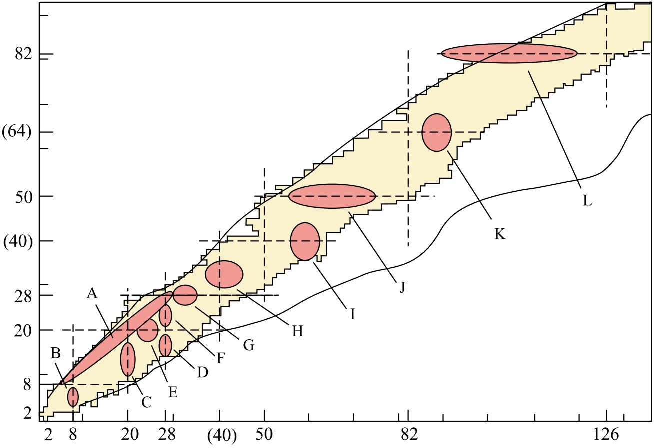




P. Van Isacker, AIP Conf. Proc. No. 819 (2006), p. 57.

Regions of 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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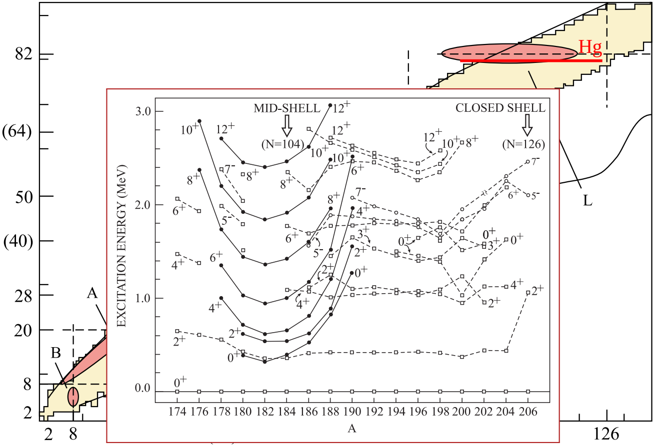

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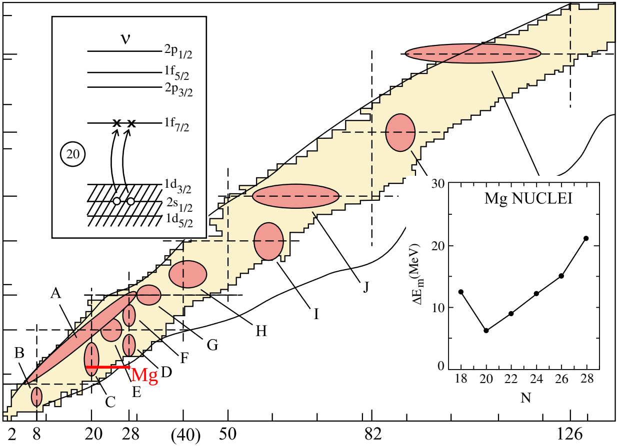

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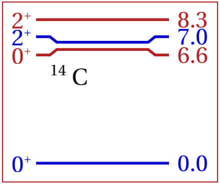
An intruder state at $N = 8$?



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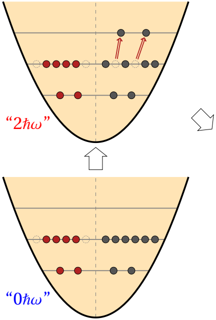
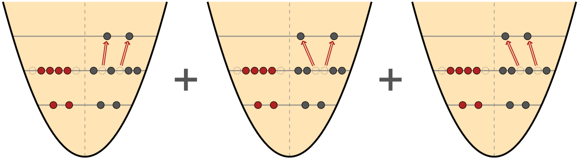
B 5	^{8}B 2+	[^{9}B] 3/2−	^{10}B 3+	^{11}B 3/2−	^{12}B 1+	^{13}B 3/2−
Be 4	^{7}Be 3/2−	[^{8}Be] 0+	^{9}Be 3/2−	^{10}Be 0+	^{11}Be 1/2+	^{12}Be 0+
Li 3	^{6}Li 1+	^{7}Li 3/2−	^{8}Li 2+	^{9}Li 3/2−		^{11}Li 3/2−





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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 $N = 8$? ^{14}C→^{12}Be

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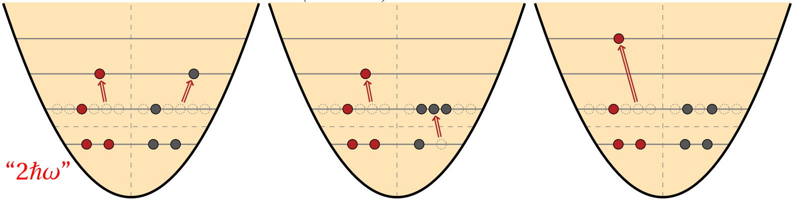
Many-body problem in an oscillator basis

No-core configuration interaction (NCCI) approach

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



Antisymmetrized product basis *Slater determinants*

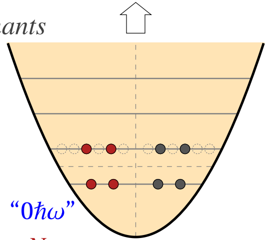
Distribute nucleons over oscillator shells

Organize basis by # oscillator excitations N_{ex}

relative to lowest Pauli-allowed filling

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

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



Convergence towards exact result with increasing $N_{\text{max}}\ldots$

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

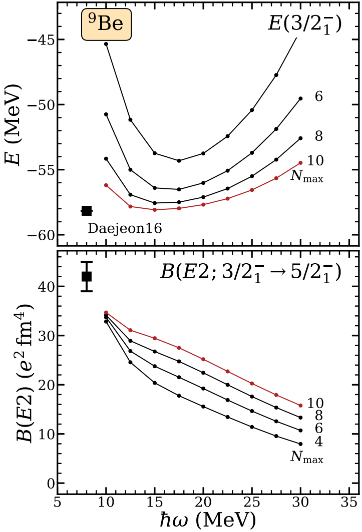
Convergence challenge for NCCI calculations

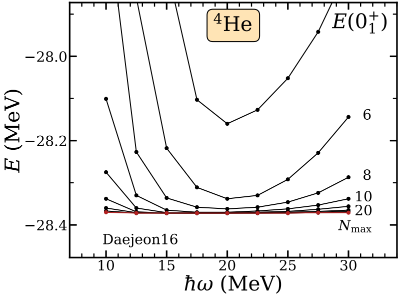
Results in finite space depend upon:

- Many-body truncation $N_{\max}$
- Oscillator scale parameter $\hbar\omega$

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

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





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Separation of rotational degree of freedom

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

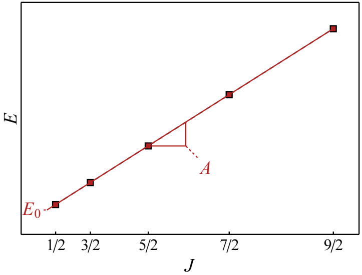
$|\phi_K\rangle$ *Intrinsic structure* *($K \equiv$ a.m. projection on symmetry axis)*

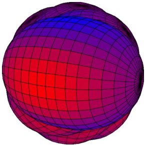
$\mathcal{D}^J_{MK}(\vartheta)$ *Rotational motion in Euler angles ϑ*

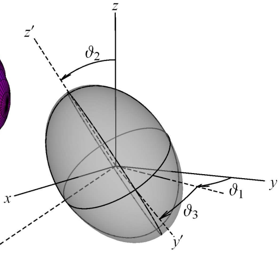
Rotational energy

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

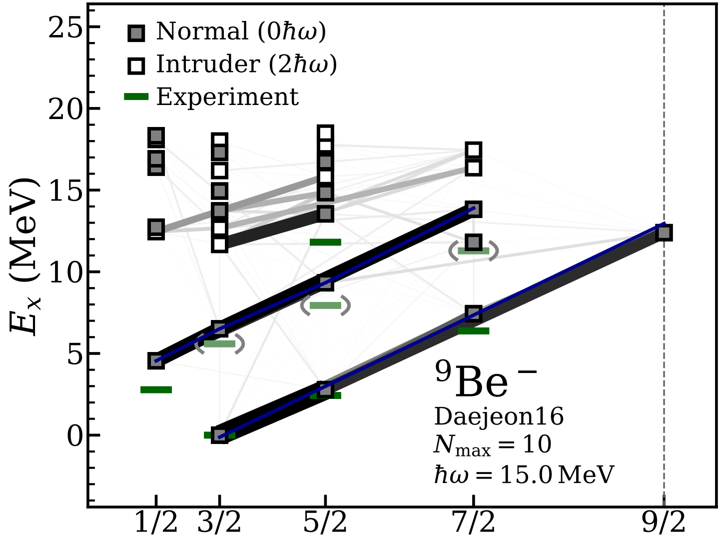
Takaharu OTSUKA talk







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



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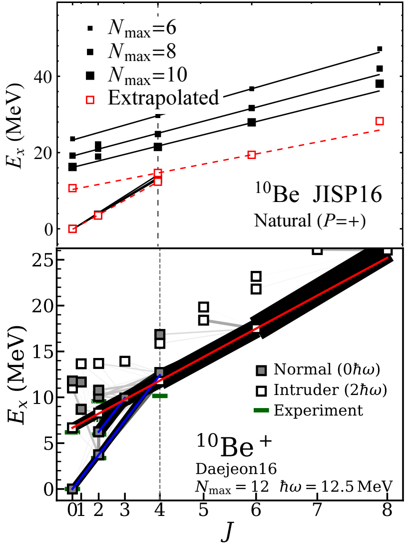
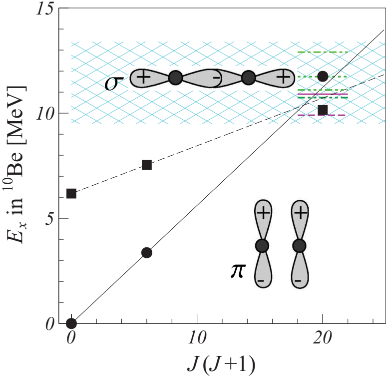
Calculations from: M. A. Caprio, P. J. Fasano, P. Maris, A. E. McCoy, J. P. Vary, Eur. Phys. J. A **56**, 120 (2020).

Convergence for “intruder” band ^{10}Be

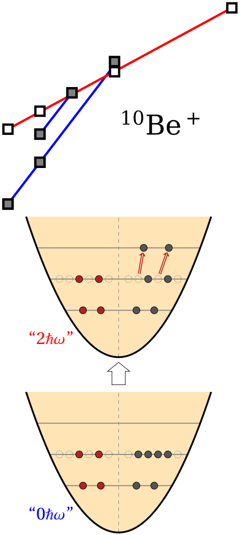


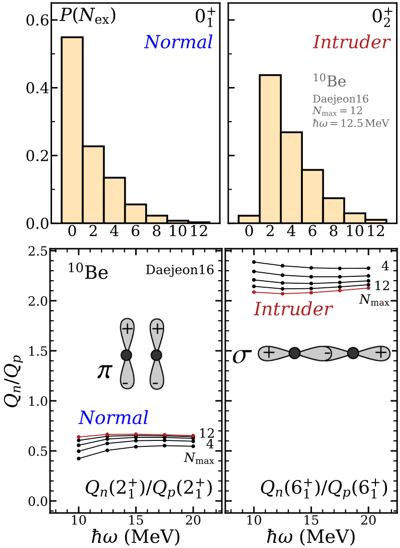


From D. Suzuki *et al.*, Phys. Rev. C **87**, 054301 (2013). Orbital schematics from Y. Kanada-En’yo, H. Horiuchi, and A. Doté, Phys. Rev. C **60**, 064304 (1999).

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 normal and intruder states in ^{10}Be





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See also: M. A. Caprio, P. J. Fasano, A. E. McCoy, P. Maris, and J. P. Vary, Bulg. J. Phys. **46**, 455 (2019) (SDANCA19).
M. A. Caprio, A. E. McCoy, P. J. Fasano, and T. Dytrych, Bulg. J. Phys. **49**, 57 (2022) (SDANCA21).

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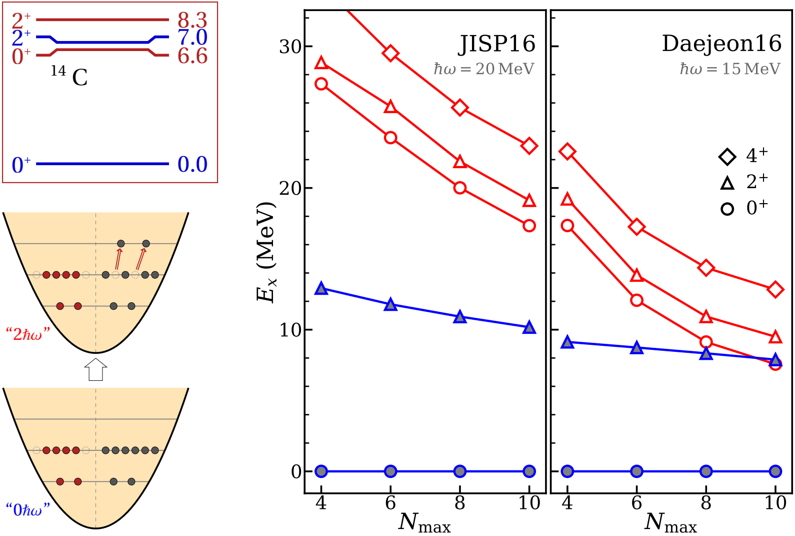
**With a brief tutorial on two-level mixing...*

Convergence of intruder state energies in ^{14}C



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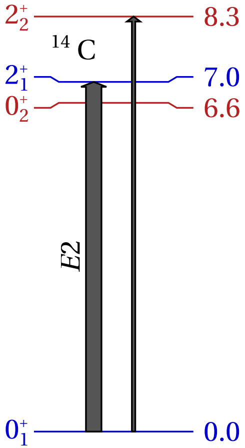
The $E2$ strength to the first 2^+ state(s) in ^{14}C?

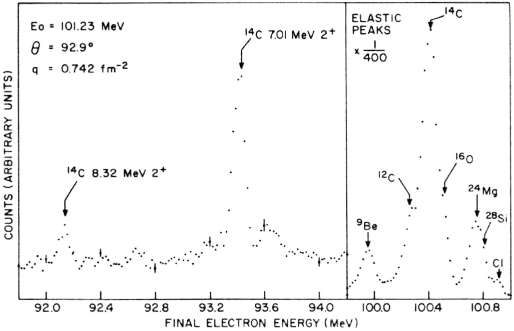


Electron Scattering from Low Lying 2^+ States in ^{14}C*

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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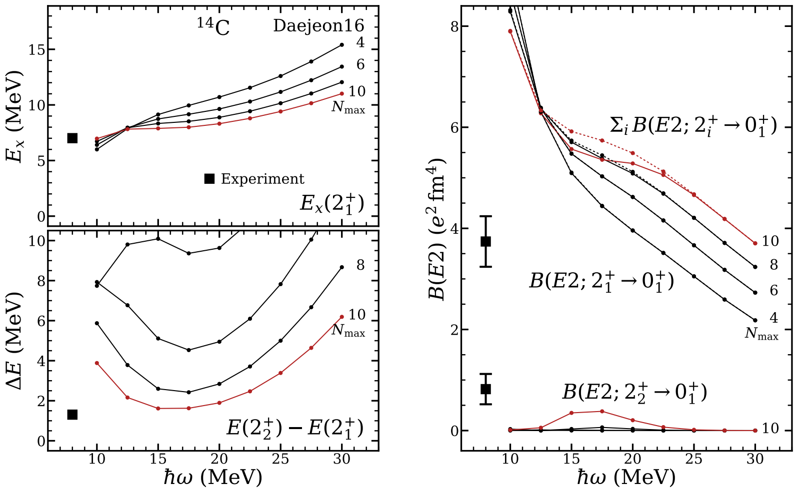
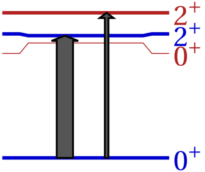


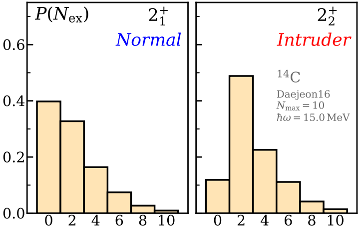
Low-lying intruder structure in ^{14}C

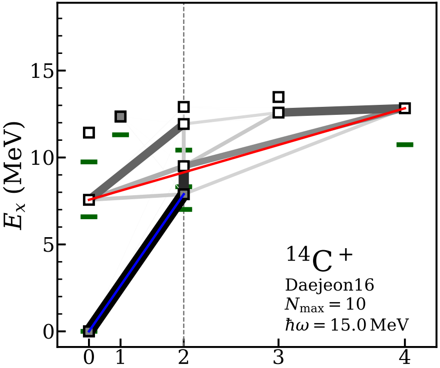
Coexisting 0^+-2^+ sequences: $0\hbar\omega$ and $2\hbar\omega$

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

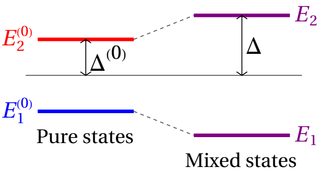
Excited structure as triaxial rotor? *Elliott* SU(3)

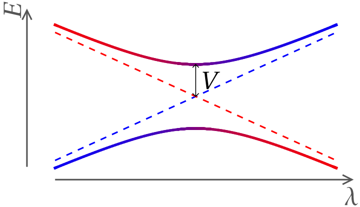






Two-state mixing





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

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

Mixing depends on relative size of:

- Mixing matrix element V
- Energy denominator $E_2^{(0)} - E_1^{(0)} \equiv 2\Delta^{(0)}$

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

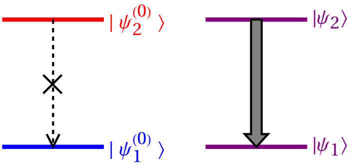
$$\Delta^2 = (\Delta^{(0)})^2 + V^2$$

Questions...

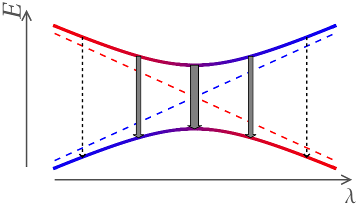
- Our calculated normal and intruder states are “mixing”.
- Can we tell *how mixed* they are (extract a mixing angle θ)?
- The answer will change as energy separation converges.
- But can we extract a *consistent mixing matrix element* V?

E.g., R. F. Casten, *Nuclear Structure from a Simple Perspective* (2000).

Transition as measure of mixing



Pure states   Mixed states



Suppose transition between pure states vanishes…   *e.g., E*0 *or E*2

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

Contributions from diagonal matrix elements (*i.e.*, moments) get "mixed in"…

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

From "mixed" observables, we can deduce mixing angle …

A. E. McCoy, M. A. Caprio, P. Maris, P. J. Fasano, Phys. Lett. B **856**, 138870 (2024).

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

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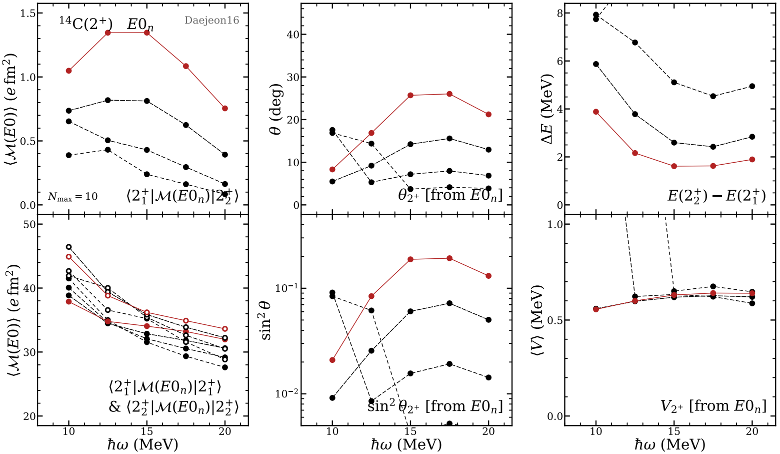
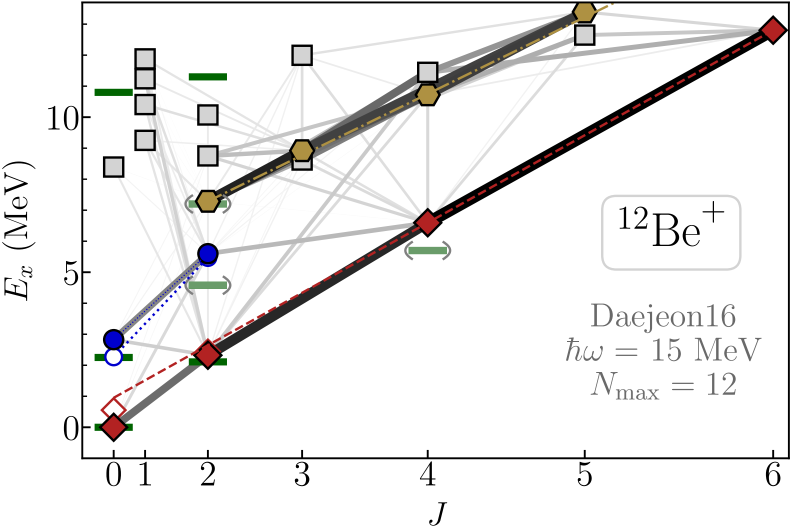
Mixing analysis of *ab initio* calculations for ^{14}C

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.



Intruder ground state and mixing in ^{12}Be



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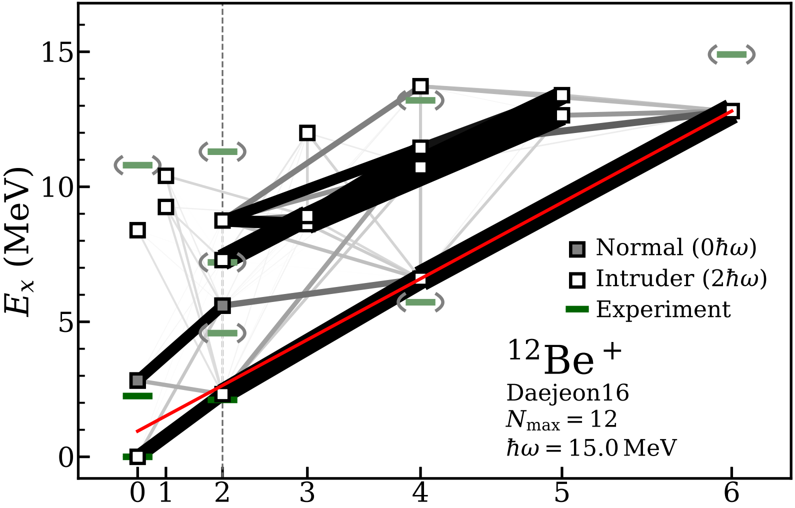

Calculations from: A. E. McCoy, M. A. Caprio, P. Maris, P. J. Fasano, Phys. Lett. B **856**, 138870 (2024).

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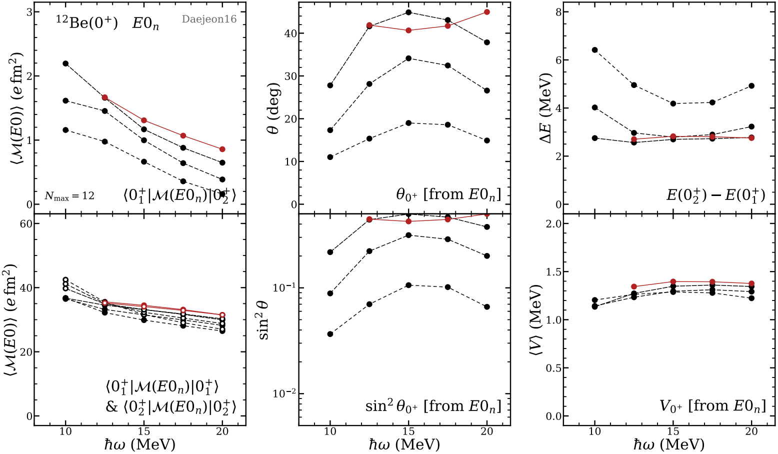

Summary

Different states in low-lying spectrum have...

- Different shell model character   *Normal* *(0ħω) vs. intruder (2ħω)*
- Different shape/deformation & Elliott SU(3) symmetry

Convergence is more challenging for intruders

But calculation of intruders is still tractable (with "soft" interaction)

Two-state mixing emerges in *ab initio* results...

- Amount of mixing is highly sensitive to convergence of energies
  A. E. McCoy *et al.*, Phys. Lett. B **856**, 138870 (2024).
- But we can extract a robust "mixing matrix element"