Meaningful comparison of $E2$ observables and radii with FRIB experiment

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Theoretical Justifications and Motivations for Early High-Profile FRIB Experiments
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Outline

- Convergence in *ab initio* no-core calculations

  The defining challenge for meaningful prediction & comparison

- Rotation and relative $E2$ strengths

  Emergent collective structure and correlated observables

- Calibration of $E2$ observables to ground-state Q and r_p

  Correlations among calculated long-range observables

- Intruder states, shape coexistence, and mixing

  No meaningful comparison without accounting for mixing

- Mirror $E2$ observables and M_n/M_p

  More correlations among calculated long-range observables (isoscalar/isovector structure)

Many-body problem in an oscillator basis

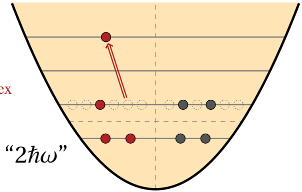
No-core configuration interaction (NCCI) approach

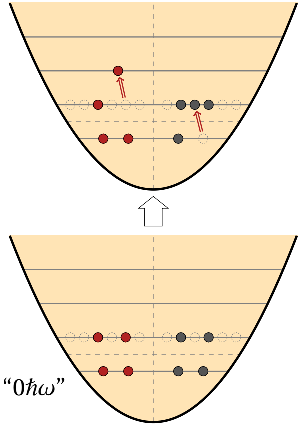
a.k.a. no-core shell model (NCSM)

$N_i = 2n_i + l_i$

$N_{\text{tot}} = \sum_i N_i = N_0 + N_{\text{ex}}$

$N_{\text{ex}} \leq N_{\text{max}}$





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

$N_{\text{ex}} = 0, 2, \ldots$ (“$0\hbar\omega$”, “$2\hbar\omega$”, …)

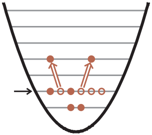
Basis must be truncated: $N_{\text{ex}} \leq N_{\text{max}}$

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:

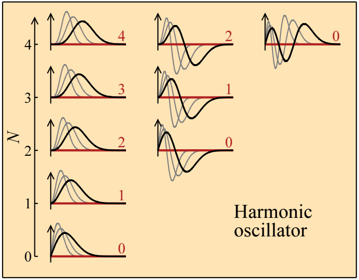


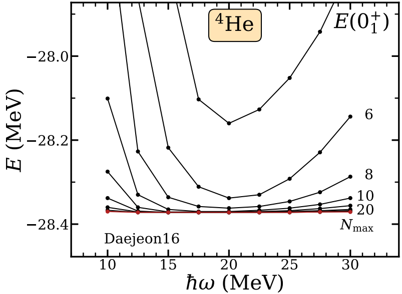
– Many-body truncation N_{max}

– Single-particle basis scale: oscillator length b (or $\hbar\omega$)

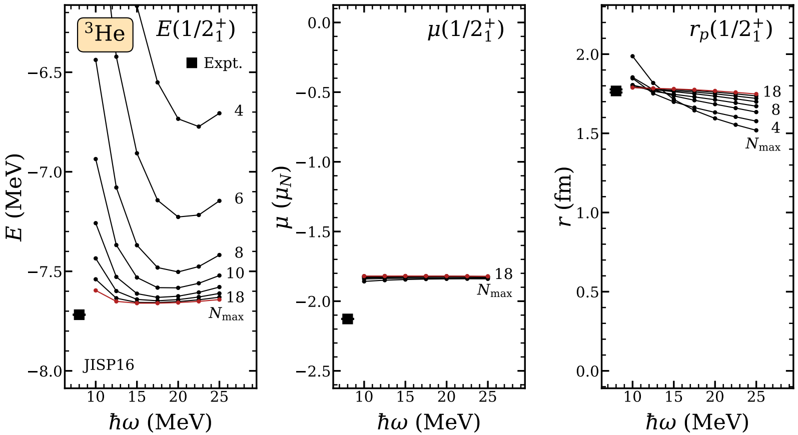
$$b = \frac{(\hbar c)}{[(m_N c^2)(\hbar\omega)]^{1/2}}$$

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

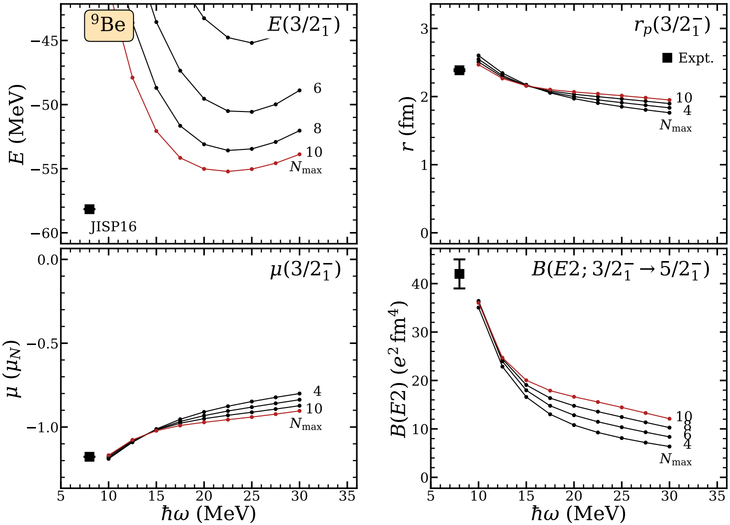




Convergence of NCCI calculations



Convergence of NCCI calculations



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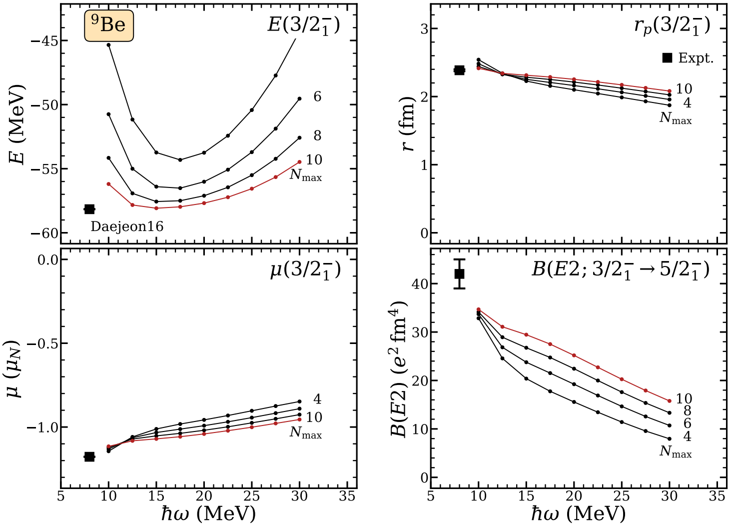
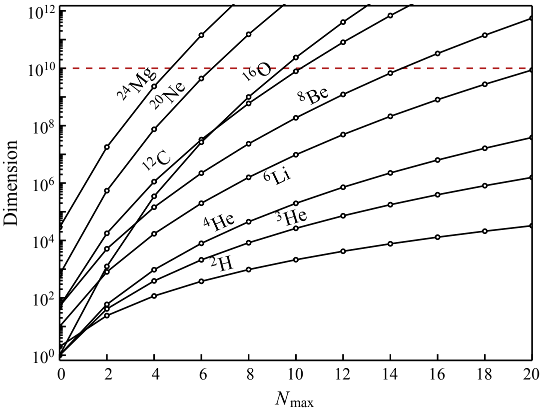


Dimension explosion for NCCI calculations



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

d = number of single-particle states

Z = number of protons

N = number of neutrons

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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)*

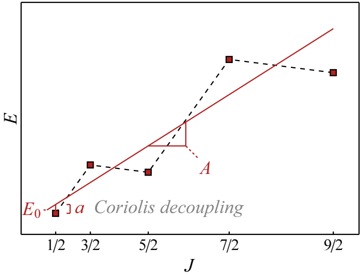
$\mathcal{D}^J_{MK}(\vartheta)$ *Rotational motion in Euler angles* ϑ

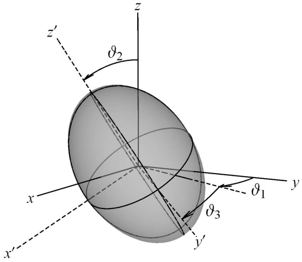
Rotational energy

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

Rotational relations (Alaga rules) on electromagnetic transitions

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





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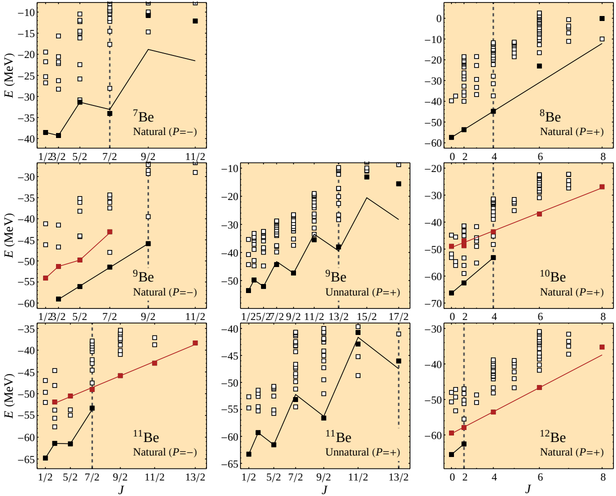
e.g., D. J. Rowe, *Nuclear Collective Motion: Models and Theory* (World Scientific, Singapore, 2010).

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						

N

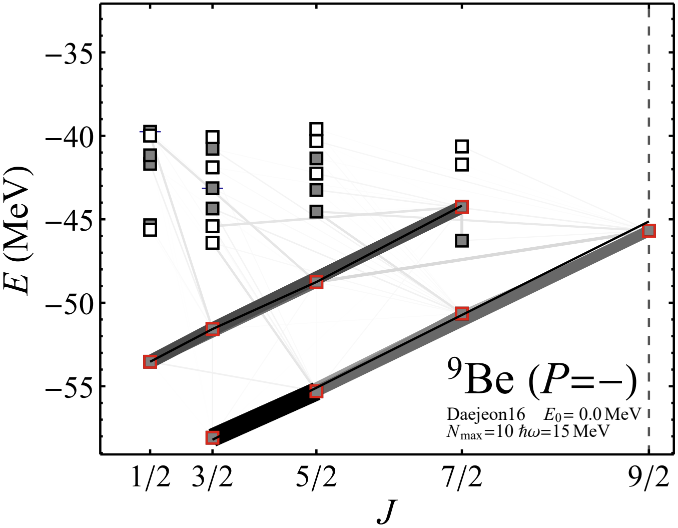
Rotational bands in $^{7\text{–}12}$Be from NCCI calculations



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

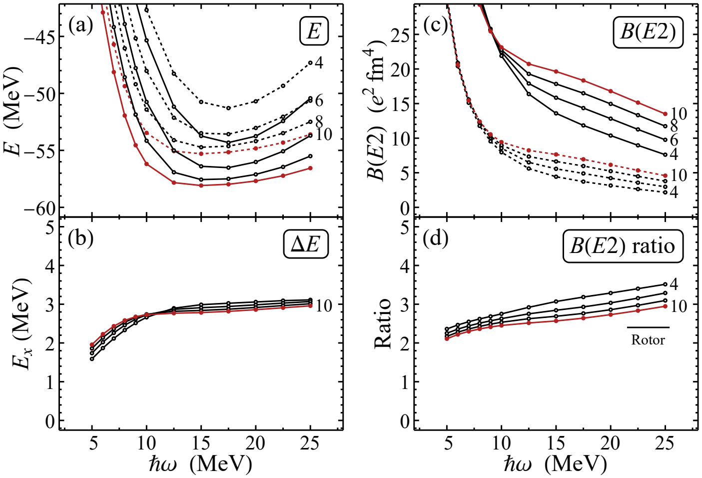
^{9}Be: NCCI calculated energies and $E2$ transitions



^{9}Be: Convergence of *relative* observables

^{9}Be $K = 3/2$ ground state band

$E(5/2^-_1) - E(3/2^-_1)$ & $B(E2; 5/2^- \rightarrow 3/2^-)/B(E2; 7/2^- \rightarrow 3/2^-)$



M. A. Caprio, P. J. Fasano, P. Maris, A. E. McCoy, J. P. Vary, Eur. Phys. J. A **56**, 120 (2020).
Daejeon16 interaction.

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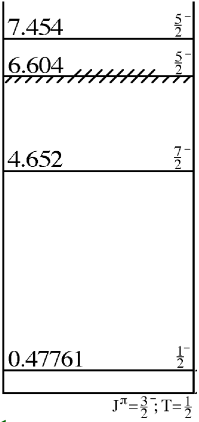
Ground-state transition in ^{7}Li



$1/2^- \rightarrow 3/2^-$ γ decay: $M1$

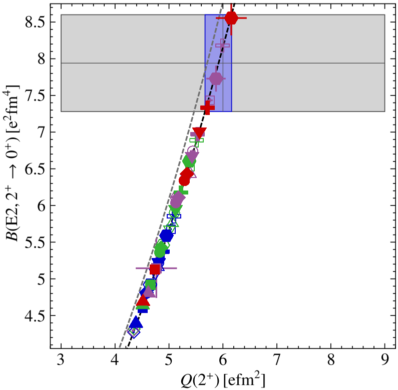
$3/2^- \rightarrow 1/2^-$ Coulomb excitation: $E2$

$B(E2; 3/2^- \rightarrow 1/2^-) = 8.3(5)\, e^2\mathrm{fm}^4$ *or* $\approx 10\,\mathrm{W.u.}$ Weller 1985

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

Sensitivities and correlations of nuclear structure observables emerging from chiral interactions

A. Calci and R. Roth, Phys. Rev. C **94**, 014322 (2016).



"... We find extremely robust correlations for $E2$ observables and illustrate how these correlations can be used to predict one observable based on an experimental datum for the second observable. In this way we circumvent convergence issues and arrive at far more accurate results than any direct *ab initio* calculation. A prime example for this approach is the quadrupole moment of the first 2^+ state in ^{12}C ..."

IT-NCSM, $\hbar\omega = 16\,\text{MeV}$, $N_{max} \leq 8$. EM/N2LO$_{opt}$/EGM interactions.

Dimensionless ratio of $E2$ observables

Compare…

$$B(E2;J_i \to J_f) \propto \left|\langle J_f \| \sum_{i\in p} r_i^2 Y_2(\hat{\mathbf{r}}_i) \| J_i\rangle\right|^2 \quad \textit{E2 transition strength}$$

…with…

$$eQ(J) \propto \langle JJ| \sum_{i\in p} r_i^2 Y_{20}(\hat{\mathbf{r}}_i) |JJ\rangle \quad \textit{E2 moment}$$

$$\propto \langle J \| \sum_{i\in p} r_i^2 Y_2(\hat{\mathbf{r}}_i) \| J\rangle \qquad \textit{…as reduced matrix element}$$

Dimensionless ratio *of like powers of E2 matrix elements*

$$\frac{B(E2)}{(eQ)^2} \propto \left|\frac{\langle\cdots\| \sum_{i\in p} r_i^2 Y_2(\hat{\mathbf{r}}_i) \|\cdots\rangle}{\langle\cdots\| \sum_{i\in p} r_i^2 Y_2(\hat{\mathbf{r}}_i) \|\cdots\rangle}\right|^2$$

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

N

Q = Q(g.s.) measured [N. J. Stone, ADNDT **111**, 1 (2016)]

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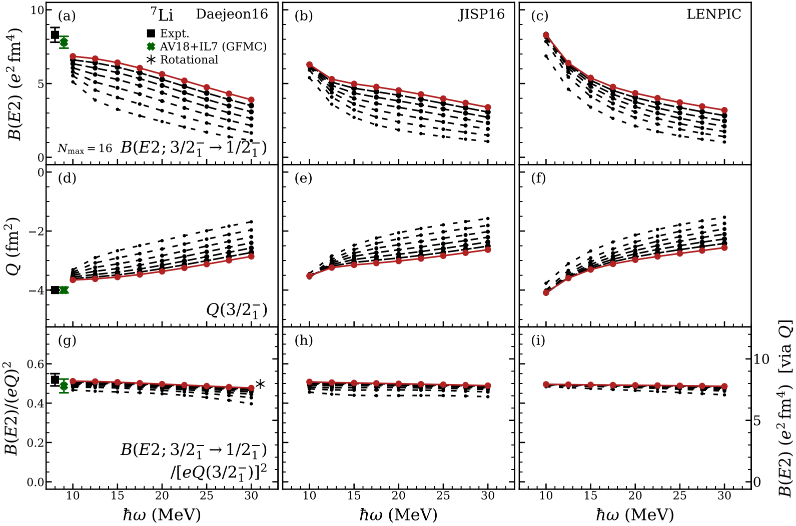
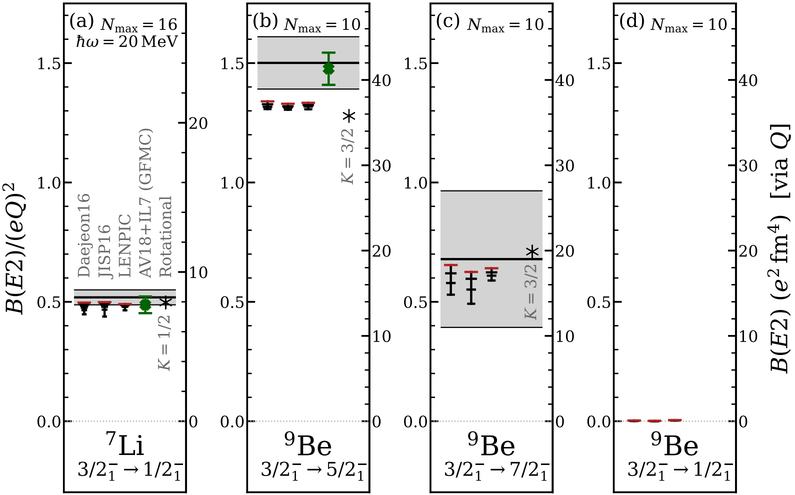
Ground-state transition in ^{7}Li relative to Q



M. A. Caprio and P. J. Fasano, Phys. Rev. C **106**, 034320 (2022).

GFMC: S. Pastore, S. C. Pieper, R. Schiavilla, and R. B. Wiringa, Phys. Rev. C **87**, 035503 (2013).

$E2$ strengths relative to Q in ^{7}Li and ^{9}Be



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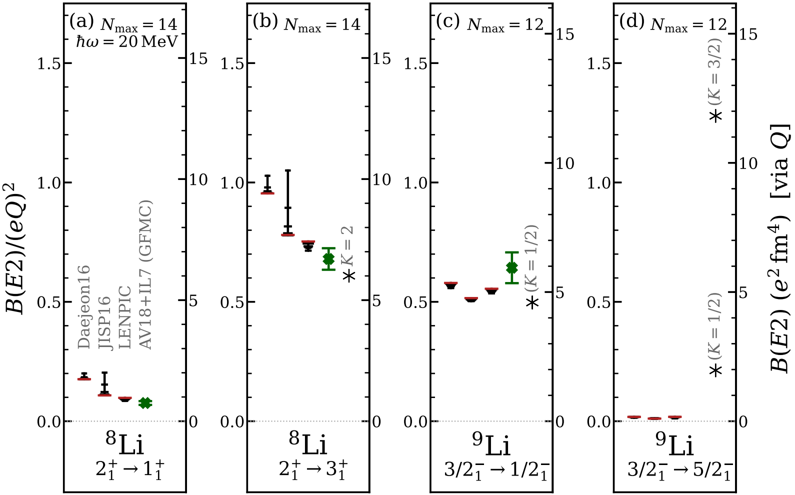
$E2$ strengths relative to Q in ^{8}Li and ^{9}Li



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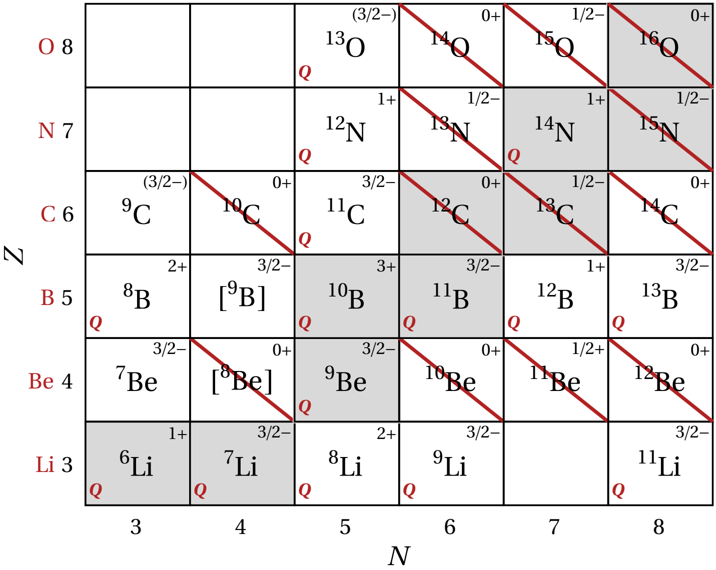

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Dimensionless ratio of $E2$ and radius observables

Compare...

$eQ(J) \propto \langle JJ | \sum_{i\in p} r_i^2 Y_{20}(\hat{\mathbf{r}}_i) | JJ \rangle$ *E2 moment*

...with...

$M(J) \propto \langle JJ | \sum_{i\in p} r_i^2 | JJ \rangle$ *E0 moment*

Dimensionless ratio *Of like powers of matrix elements*

$$\frac{B(E2)}{(e^2 r_p^4)} \propto \left| \frac{\langle \cdots \| \sum_{i\in p} r_i^2 Y_2(\hat{\mathbf{r}}_i) \| \cdots \rangle}{\langle \cdots \| \sum_{i\in p} r_i^2 \| \cdots \rangle} \right|^2 \qquad \frac{Q}{r_p^2} \propto \frac{\langle \cdots \| \sum_{i\in p} r_i^2 Y_2(\hat{\mathbf{r}}_i) \| \cdots \rangle}{\langle \cdots \| \sum_{i\in p} r_i^2 \| \cdots \rangle}$$

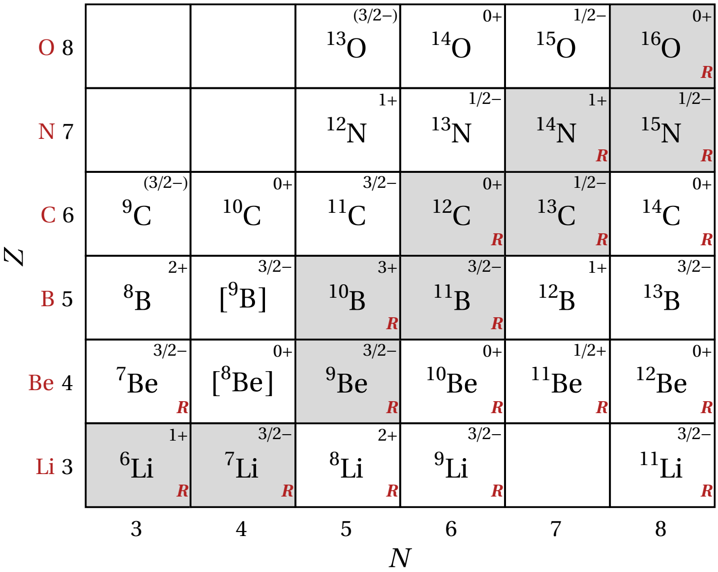
Radius (r.m.s.) of proton density

$$r_p = \left\langle \frac{1}{Z} \sum_{i\in p} r_i^2 \right\rangle^{1/2}$$

Measured charge radius includes hadronic effects (finite size of nucleon)

$$r_p^2 = r_c^2 - R_p^2 - (N/Z) R_n^2$$

e.g., L.-B. Wang *et al.*, Phys. Rev. Lett. **93**, 142501 (2004).



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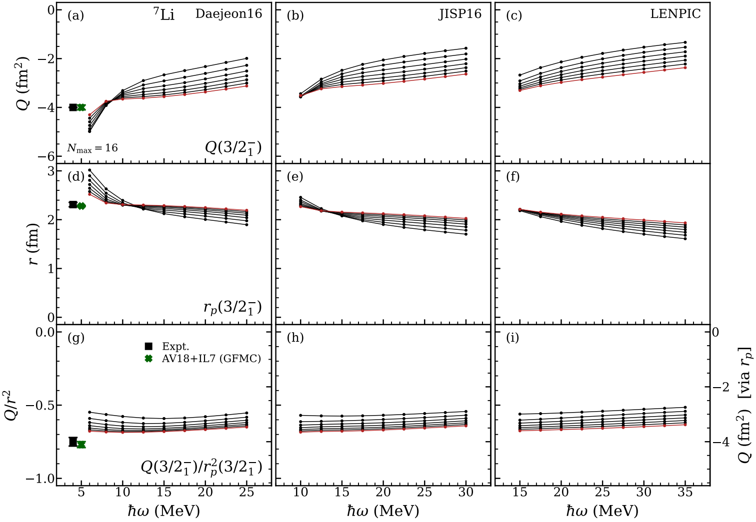
R = r_c(g.s.) measured [I. Angeli and K. P. Marinova, ADNDT **99**, 69 (2013); J. H. Kelley *et al.*, NPA **968**, 71 (2017)]

^{7}Li: $E2$ moment correlation with radius



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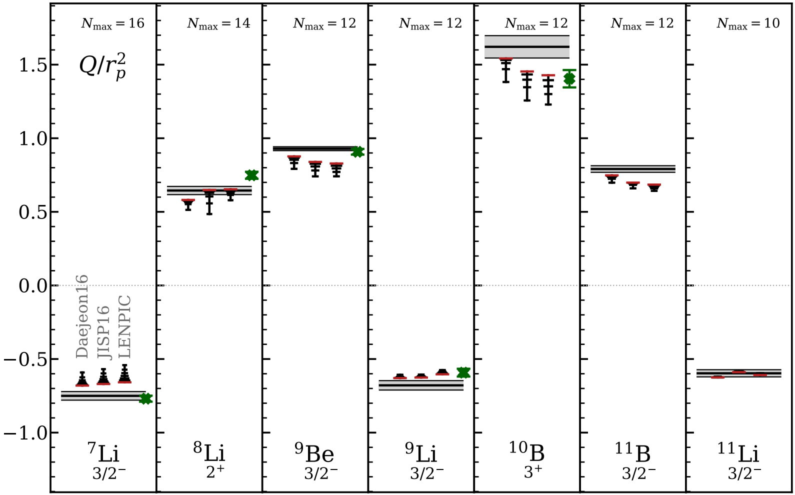
GFMC: S. Pastore, S. C. Pieper, R. Schiavilla, and R. B. Wiringa, Phys. Rev. C **87**, 035503 (2013).

Relation between Q and r_p for ground state (Q/r_p^2)



M. A. Caprio, P. J. Fasano, and P. Maris, Phys. Rev. C **105**, L061302 (2022).

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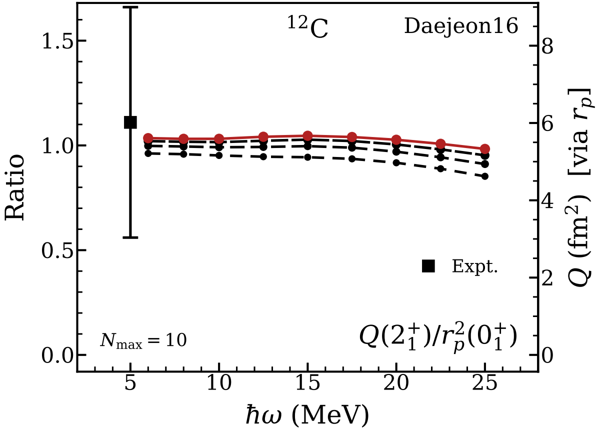
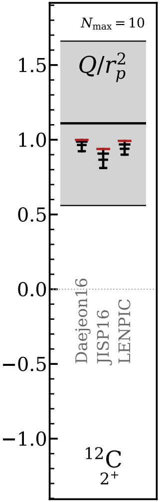
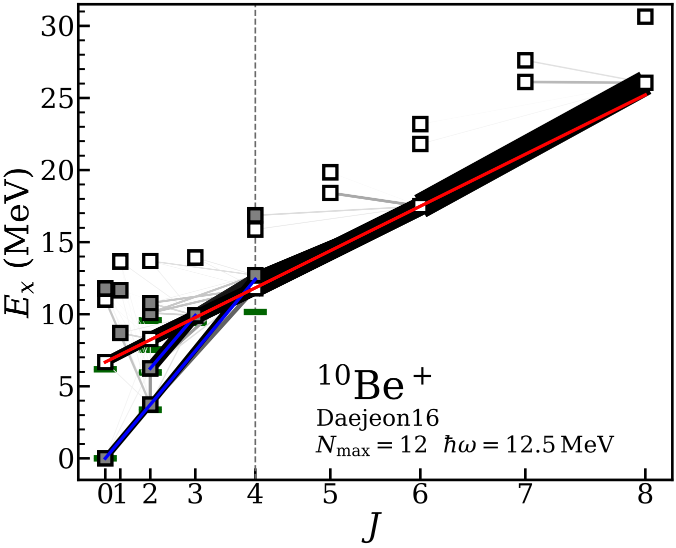
Excited-state quadrupole moment from radius in ^{12}C



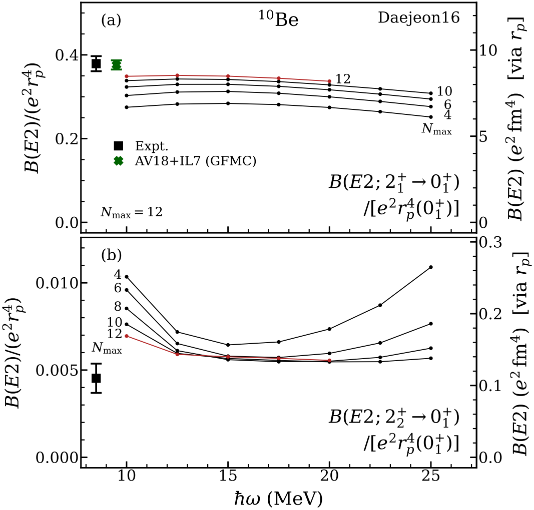


$Q(2_1^+) = +6(3)\,\mathrm{fm}^2$ Vermeer 1983 (Stone 2016)

Convergence of bands in ^{10}Be with Daejeon16



^{10}Be: $E2$ strengths by calibration to radius



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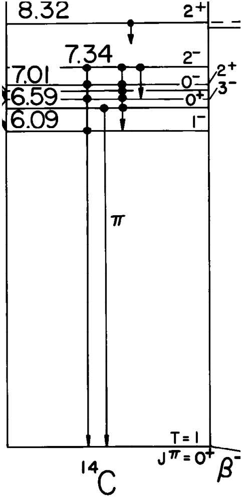
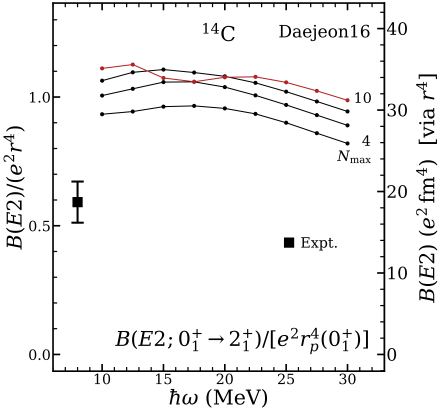
The $E2$ strength to the first 2^+ in ^{14}C?





Who ordered that?

Level scheme from TUNL evaluation [F. Azjenberg-Selove, Nucl. Phys. A **523**, 1 (1991)].

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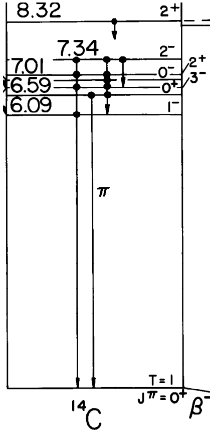
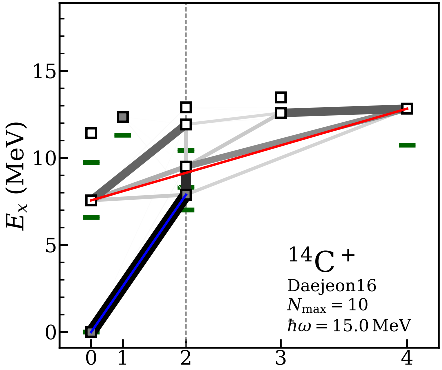
Ab initio structure of ^{14}C

Coexisting $0^+/2^+$ sequences — $0\hbar\omega$ and $2\hbar\omega$

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

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





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Level scheme from TUNL evaluation [F. Azjenberg-Selove, Nucl. Phys. A **523**, 1 (1991)].

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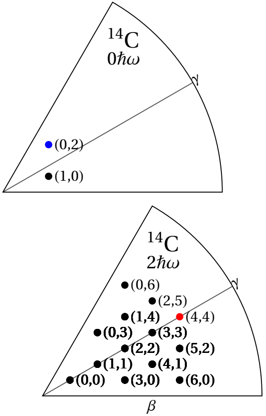
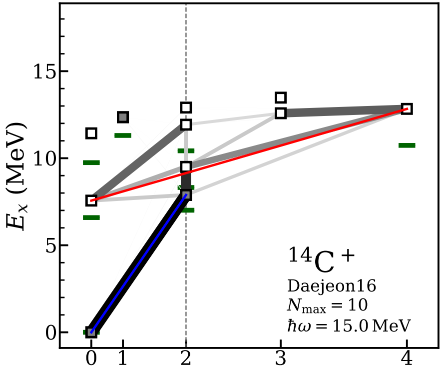
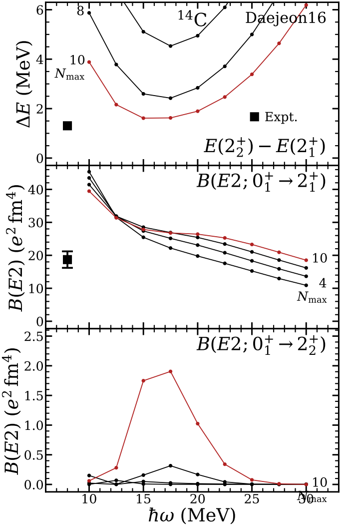
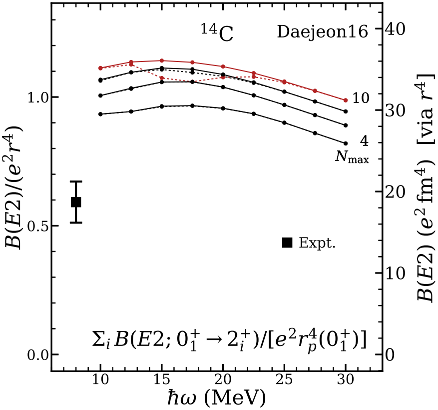




The $E2$ strength to the first 2^+ in ^{14}C?



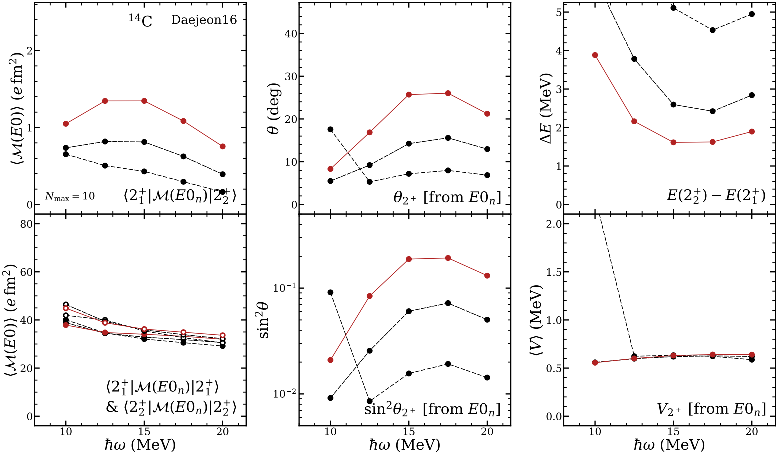


Predict summed strength

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

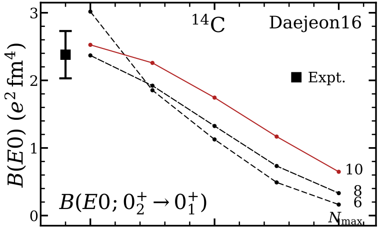
Assume $\langle 2^+_{0\hbar\omega}|\mathcal{M}(E0)|2^+_{2\hbar\omega}\rangle$ *vanishes for "pure" (unmixed) states*

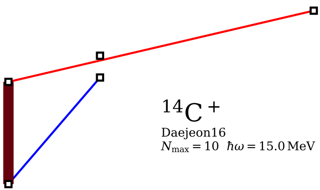
From $E0$ *matrix elements for "calculated" (mixed) states, deduce mixing*

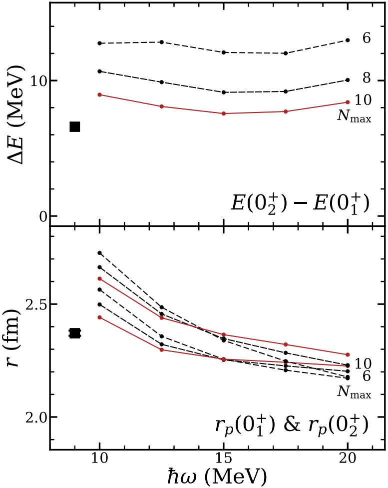


Ab initio calculation of $E0$ transition in ^{14}C

Daejeon16 interaction







Z \ N	1	2	3	4	5	6	7	8
O 8					^{13}O	^{14}O	^{15}O	^{16}O *E0*
N 7					^{12}N	^{13}N	^{14}N	^{15}N
C 6			^{9}C	^{10}C	^{11}C	^{12}C *E0*	^{13}C	^{14}C *E0*
B 5			^{8}B	[^{9}B]	^{10}B	^{11}B	^{12}B	^{13}B
Be 4			^{7}Be	[^{8}Be]	^{9}Be	^{10}Be *E0*	^{11}Be	^{12}Be *E0*
Li 3			^{6}Li	^{7}Li	^{8}Li	^{9}Li		^{11}Li
He 2	^{3}He	^{4}He *E0*		^{6}He		^{8}He		
H 1	^{2}H	^{3}H						

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

Outline

- Convergence in *ab initio* no-core calculations

  The defining challenge for meaningful prediction & comparison

- Rotation and relative $E2$ strengths

  Emergent collective structure and correlated observables

- Calibration of $E2$ observables to ground-state Q and r_p

  Correlations among calculated long-range observables

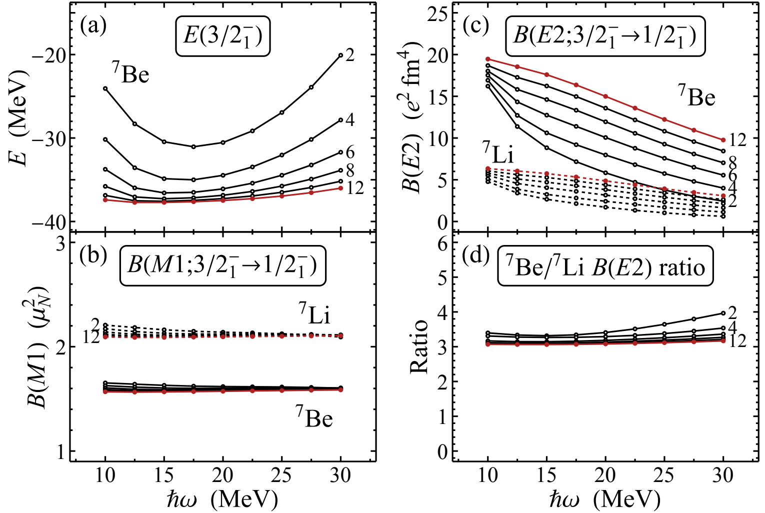
- Intruder states, shape coexistence, and mixing

  No meaningful comparison without accounting for mixing

- Mirror $E2$ observables and M_n/M_p

  More correlations among calculated long-range observables (isoscalar/isovector structure)

Convergence of $E2$ strengths and mirror ratio ($A = 7$)



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S. L. Henderson *et al.*, Phys. Rev. C **99**, 064320 (2019); Daejeon16 interaction; $N_{max} \le 12$

Ab initio predictions for M_n/M_p