Correlated observables and dimensionless ratios

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Progress in *Ab Initio* Nuclear Theory
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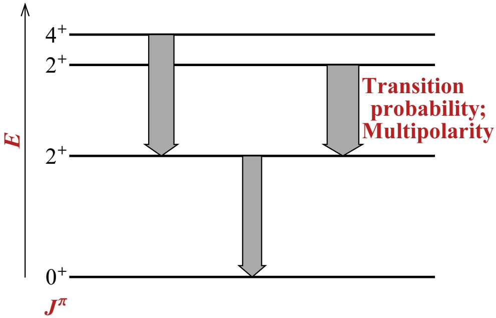
UNIVERSITY OF NOTRE DAME

Collaborators: Patrick J. Fasano (ND) & Pieter Maris (ISU)



Obtain detailed information on physical structure and excitation phenomena from spectroscopic properties

- Level energies and quantum numbers
- Electromagnetic transition probabilities and multipolarities

Fermi's golden rule $T_{i \to f} \propto \left| \langle \Psi_f \,|\, \hat{T} \,|\, \Psi_i \rangle \right|^2$

Electromagnetic probes (e-scattering), α decay, β decay, nucleon transfer reactions, . . .

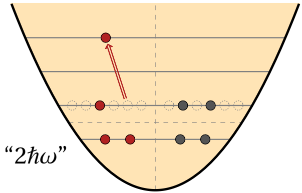
Outline

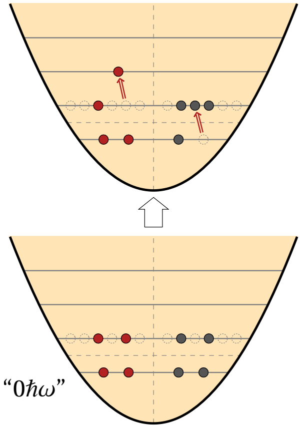
- No-core configuration interaction calculations
- Rotation and relative $E2$ strengths
- Calibration of $E2$ strengths to Q
- Calibration of $E2$ strengths to r_p

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

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

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

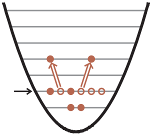
Convergence towards exact result with increasing $N_{\text{max}}\ldots$

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

Convergence of NCCI calculations

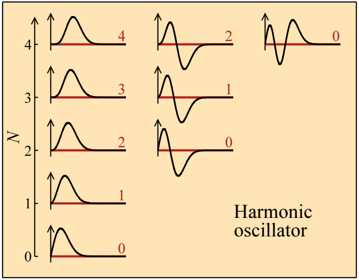
Results for calculation in finite space depend upon:

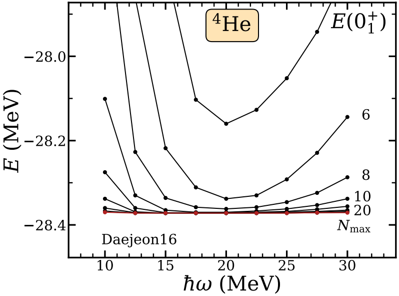
- Many-body truncation N_{max}
- Single-particle basis scale: oscillator length b (or $\hbar\omega$)



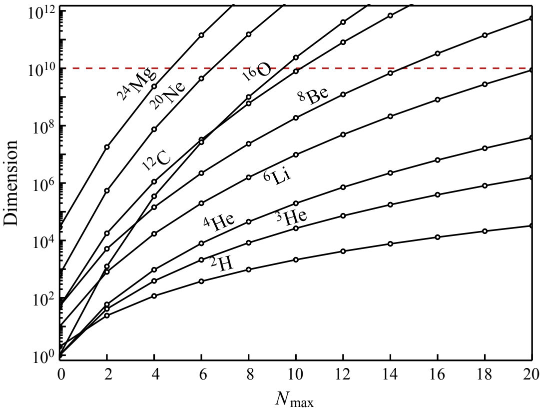
$$b = \frac{(\hbar c)}{[(m_N c^2)(\hbar\omega)]^{1/2}}$$

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





Dimension explosion for NCCI calculations



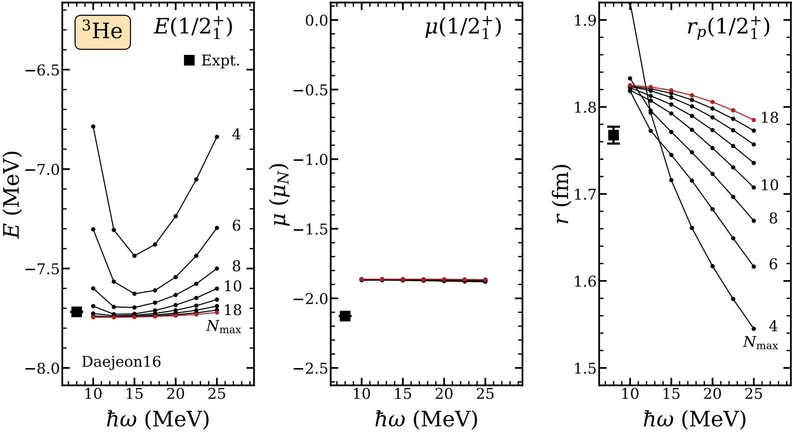
$$\text{Dimension} \propto \binom{d}{Z}\binom{d}{N}$$

d = number of single-particle states

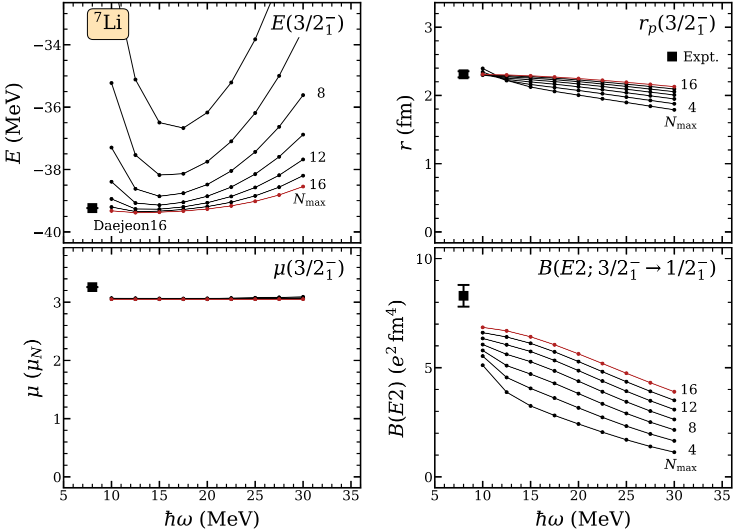
Z = number of protons

N = number of neutrons

Convergence of NCCI calculations



Convergence of NCCI calculations



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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)*

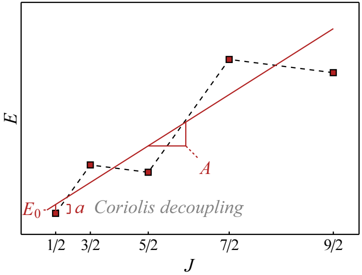
$\mathcal{D}^J_{MK}(\vartheta)$ *Rotational motion in Euler angles ϑ*

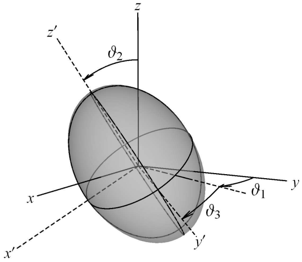
Rotational energy

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

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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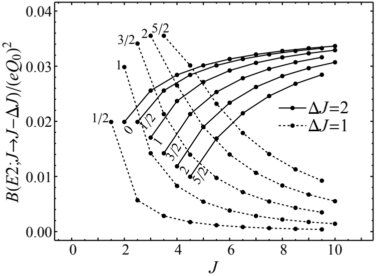
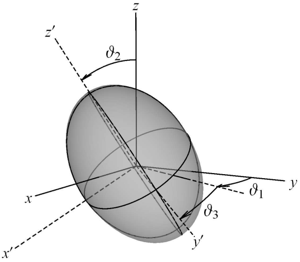
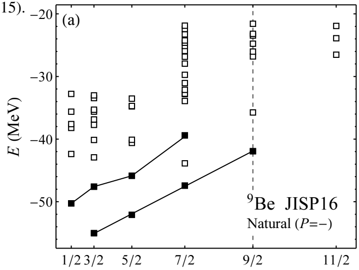




Rotational features emerge in *ab initio* calculations

P. Maris, M. A. Caprio, and J. P. Vary, Phys. Rev. C **91**, 014310 (2015).
C. W. Johnson, Phys. Rev. C **91**, 034313 (2015).
M. A. Caprio, P. J. Fasano, P. Maris, A. E. McCoy, J. P. Vary, Eur. Phys. J. A **56**, 120 (2020).



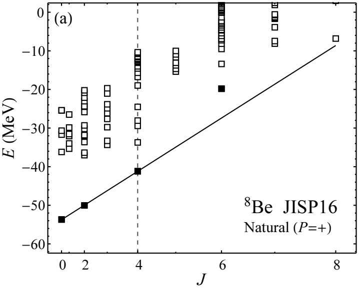
Valence shell structure? SU(3)

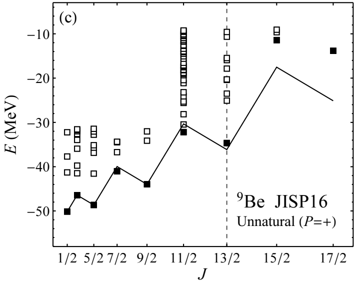
T. Dytrych *et al.*, Phys. Rev. Lett. **111**, 252501 (2013).

Multishell dynamics? $Sp(3,\mathbb{R})$

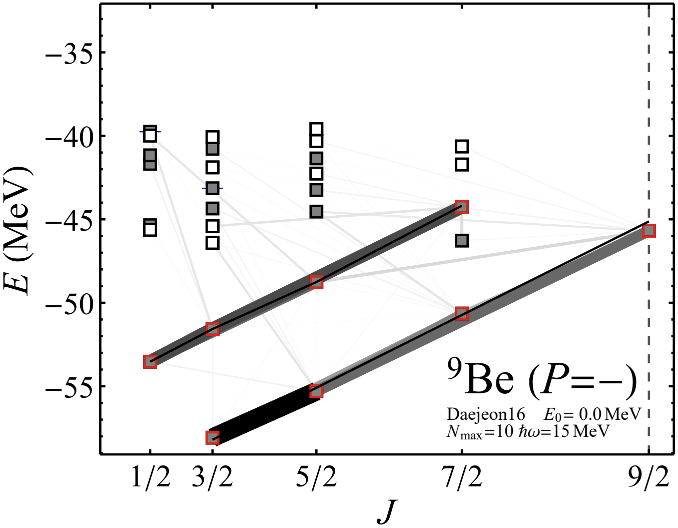
A. E. McCoy *et al.*, Phys. Rev. Lett. **125**, 102505 (2020).

Cluster rotation?





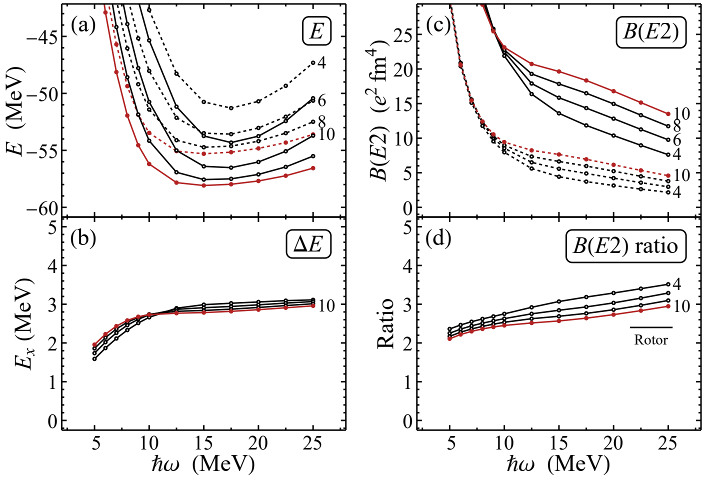
^{9}Be: NCCI calculated energies and $E2$ transitions



^{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, University of Notre Dame

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

Outline

- No-core configuration interaction calculations
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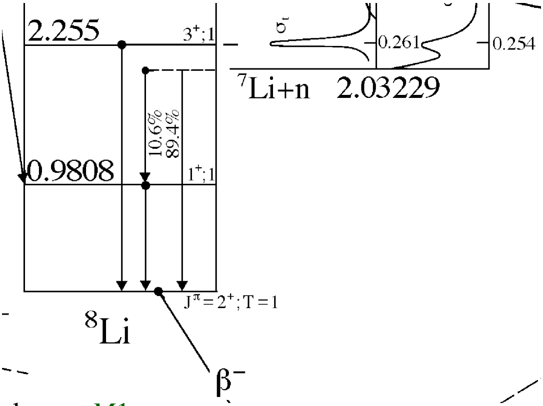
Enhanced (?) ground-state transition in ^{8}Li



$1^+ \rightarrow 2^+$ γ decay: $M1$

$2^+ \rightarrow 1^+$ Coulomb excitation: $E2$

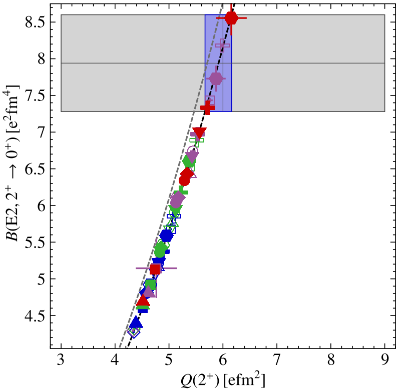
$B(E2; 2^+ \rightarrow 1^+) = 55(15)\, e^2\mathrm{fm}^4$ *or* $\approx 58\,\mathrm{W.u.}$ Brown 1991

Ab initio Green's function Monte Carlo (GFMC) predicts $\approx 0.8\, e^2\mathrm{fm}^4$ Pastore 2013

Figure from D. R. Tilley *et al.*, Nucl. Phys. A **745**, 155 (2004).

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, $\hbar\omega = 16\,\mathrm{MeV}$, $N_{\mathrm{max}} \leq 8$. EM/N2LO$_{\mathrm{opt}}$/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			(3/2−) ^{13}O **Q**	0+ ^{14}O	1/2− ^{15}O	0+ ^{16}O
N 7			1+ ^{12}N **Q**	1/2− ^{13}N	1+ ^{14}N **Q**	1/2− ^{15}N
C 6	(3/2−) ^{9}C	0+ ^{10}C	3/2− ^{11}C **Q**	0+ ^{12}C	1/2− ^{13}C	0+ ^{14}C
B 5	2+ ^{8}B **Q**	3/2− [^{9}B]	3+ ^{10}B **Q**	3/2− ^{11}B **Q**	1+ ^{12}B **Q**	3/2− ^{13}B **Q**
Be 4	3/2− ^{7}Be	0+ [^{8}Be]	3/2− ^{9}Be **Q**	0+ ^{10}Be	1/2+ ^{11}Be	0+ ^{12}Be
Li 3	1+ ^{6}Li **Q**	3/2− ^{7}Li **Q**	2+ ^{8}Li **Q**	3/2− ^{9}Li **Q**		3/2− ^{11}Li **Q**

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

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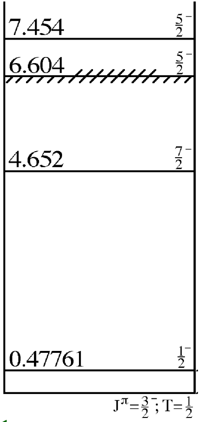
Ground-state transition in ^{7}Li



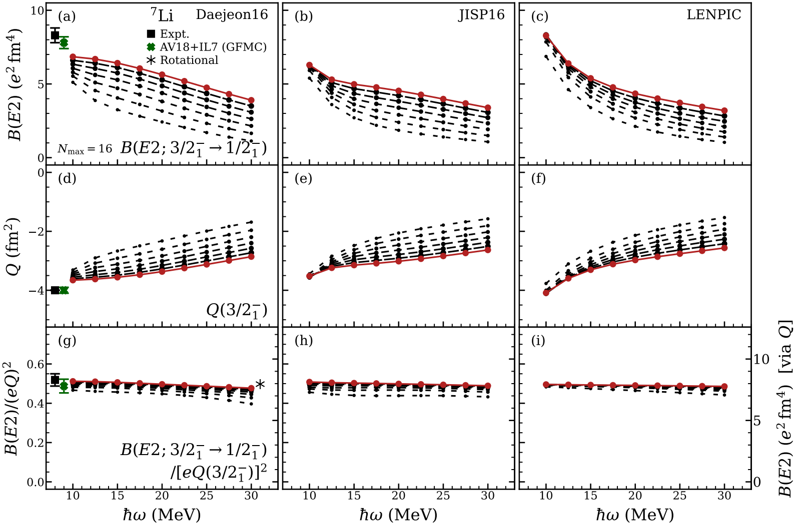
$1/2^- \rightarrow 3/2^-$ γ decay: $M1$

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

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

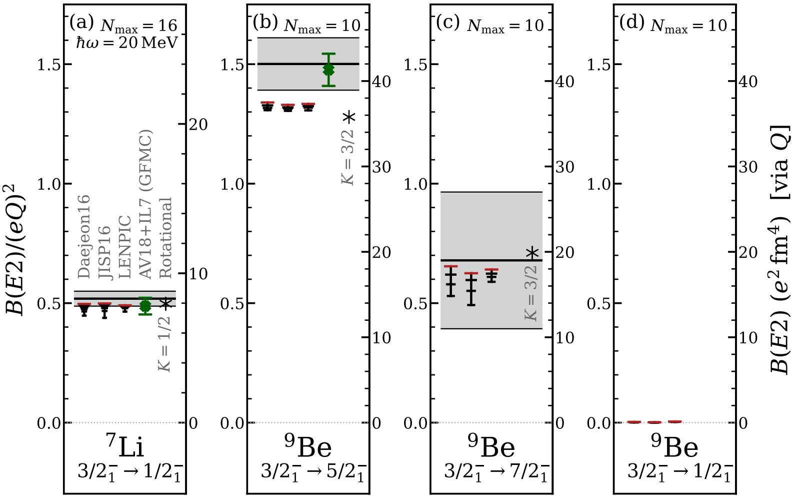
Figure from D. R. Tilley *et al.*, Nucl. Phys. A **708**, 3 (2002).

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



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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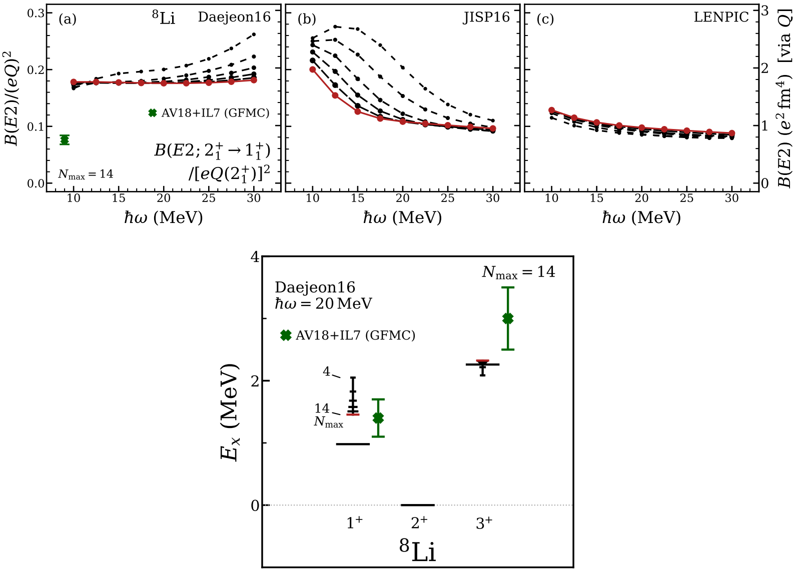

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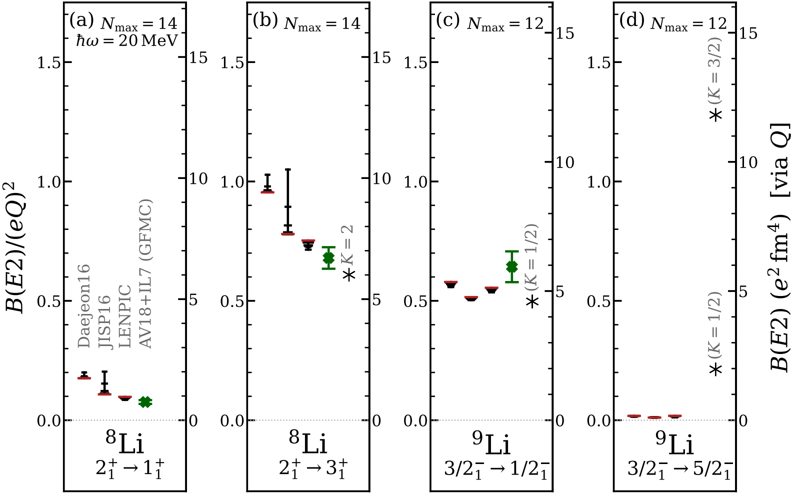
$E2$ strengths relative to Q in ^{8}Li and ^{9}Li



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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**

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

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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)

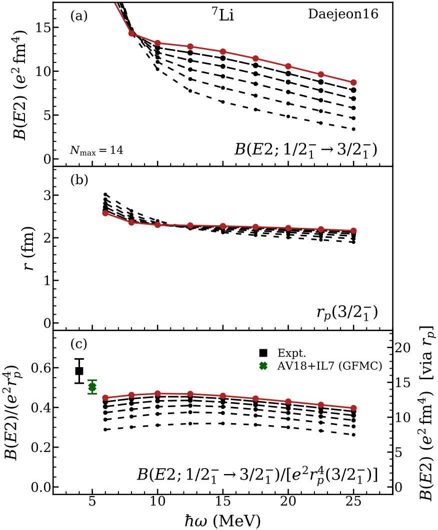
$$r_p^2 = r_c^2 - R_p^2 - (N/Z)R_n^2$$

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

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

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: $E2$ strength by calibration to radius

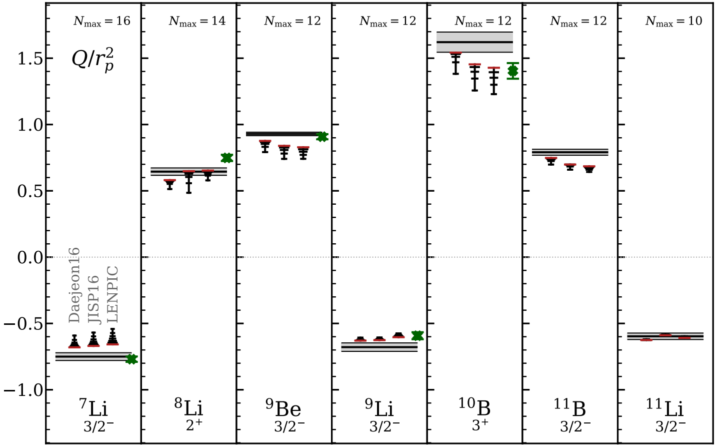


GFMC: S. Pastore, S. C. Pieper, R. Schiavilla, and R. B. Wiringa, Phys. Rev. C **87**, 035503 (2013).

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

Ab initio prediction of relation between precisely measured observables

Comparison: Normalization for calibration to Q *vs.* calibration to r_p



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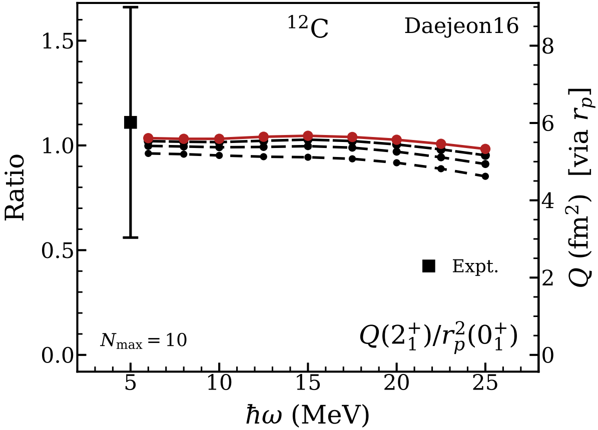
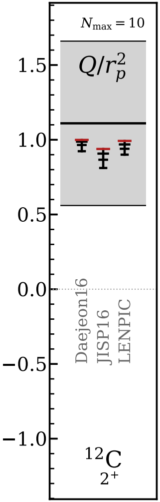
Excited-state quadrupole moment from radius in ^{12}C





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

Summary

Prediction of $E2$ observables hampered by poor convergence in NCCI

But… "Truncation error" correlated between $E2$ observables

Calibrate to one, predict another A. Calci and R. Roth, Phys. Rev. C **94**, 014322 (2016).

Robust *ab initio* prediction of dimensionless ratio $B(E2)/(eQ)^2$

Predict E2 observables by calibration to quadrupole moment

Robust *ab initio* prediction of $B(E2)/(e^2 r_p^4)$ or Q/r_p^2

Predict E2 observables by calibration to charge radius

M. A. Caprio, P. J. Fasano, and P. Maris, Phys. Rev. C **105**, L061302 (2022).
M. A. Caprio and P. J. Fasano, Phys. Rev. C **106**, 034320 (2022).