Seize the moment (or radius): What to do when your (long-range) observables don't converge?

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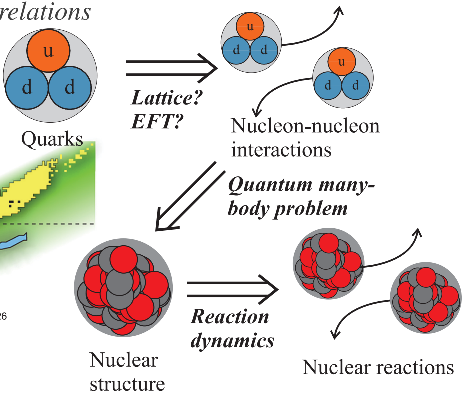
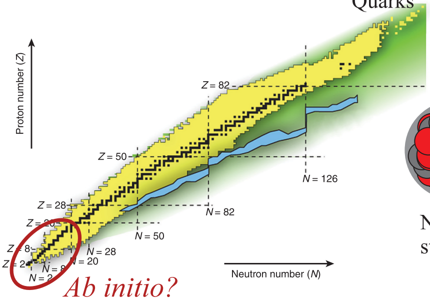
Goal of *ab initio* nuclear structure

First-principles understanding of nature *Nuclei from QCD*

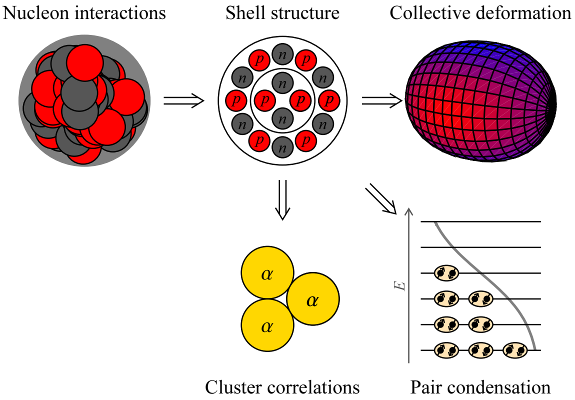
Can we understand the origin of "simple patterns in complex nuclei"?

i.e., emergent collective correlations





Adapted from B. Schwarzschild, Physics Today 63(8), 16 (2010).



Many-particle Schrödinger equation

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

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

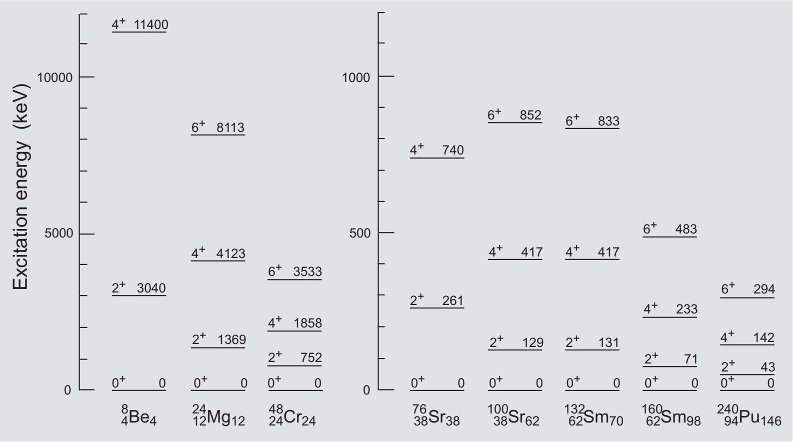
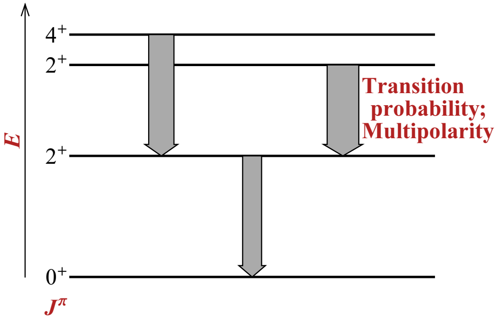


Figure from D. J. Rowe and J. L. Wood, *Fundamentals of Nuclear Models: Foundational Models* (World Scientific, Singapore, 2010).



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 $T_{i\rightarrow f} \propto |\langle \Psi_f | \hat{T} | \Psi_i \rangle|^2$

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

Solution of Schrödinger equation in a basis

One particle in *one* dimension

Hamiltonian

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

Eigenproblem

$$\hat{H}\psi(x) = E\psi(x)$$

Expand wave function in basis (unknown coefficients a_k)

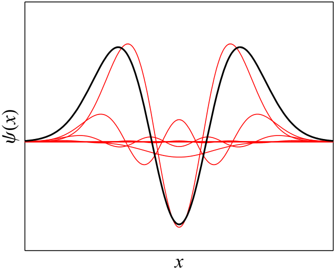
$$\psi(x) = \sum_{k=1}^{\infty} a_k \varphi_k(x)$$

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

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

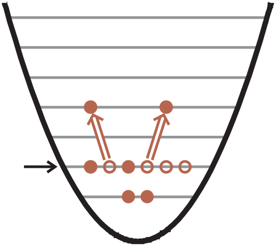


No-core configuration interaction (NCCI) approach

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

– Begin with orthonormal single-particle basis: 3-dim harmonic oscillator
– Construct many-body basis from product states (Slater determinants)
– Basis state described by distribution of nucleons over oscillator shells
– Basis must be truncated: N_{max} truncation by oscillator excitations
– Results depend on truncation N_{max} — and oscillator length (or $\hbar\omega$)

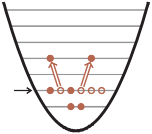
Convergence towards exact result with increasing N_{max}



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:

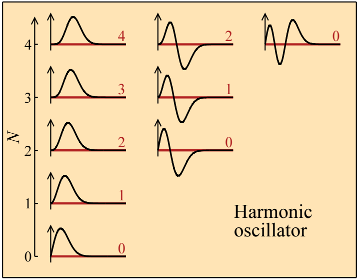


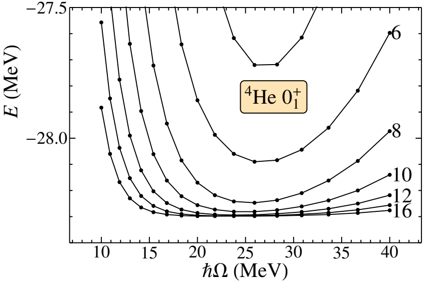
– Many-body truncation $N_{\max}$

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

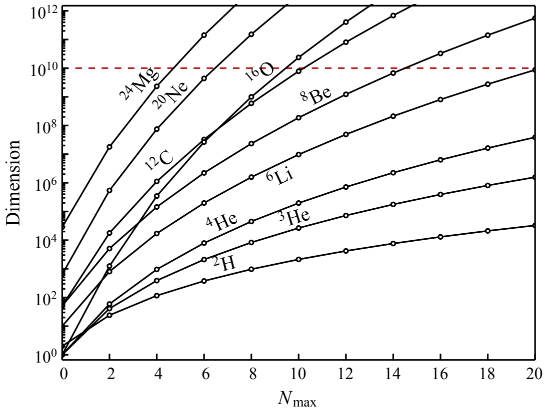
$$b = \frac{(\hbar c)}{[(m_N c^2)(\hbar\omega)]^{1/2}}$$

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





Dimension explosion for NCCI calculations



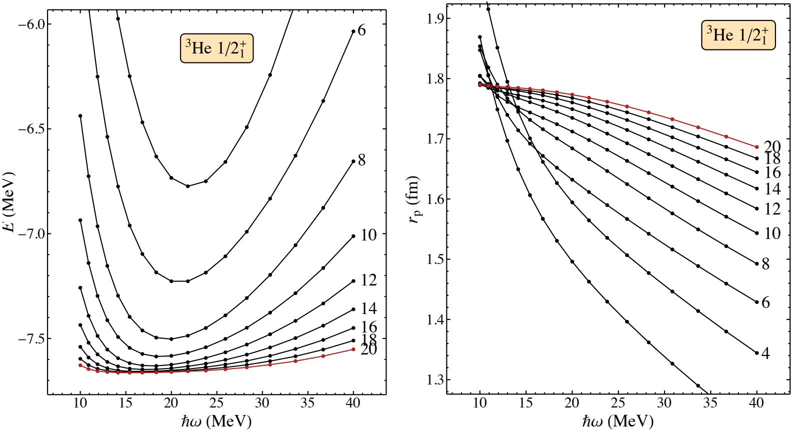
$$\text{Dimension} \propto \binom{d}{Z}\binom{d}{N}$$

d = number of single-particle states

Z = number of protons

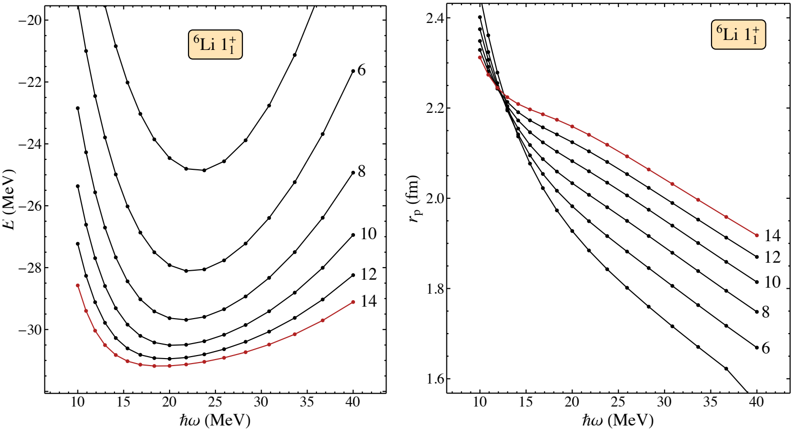
N = number of neutrons

Convergence of NCCI calculations



JISP16 + Coulomb interaction

Convergence of NCCI calculations



JISP16 + Coulomb interaction

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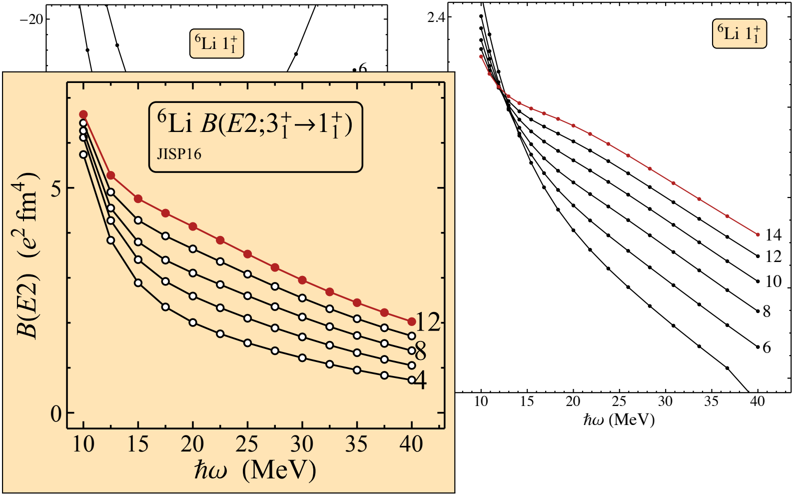
Convergence of NCCI calculations



JISP16 + Coulomb interaction

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)*

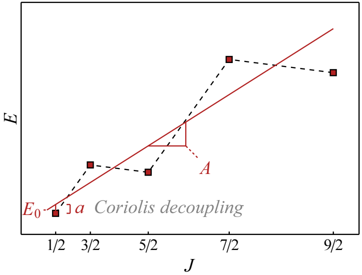
$\mathcal{D}^J_{MK}(\vartheta)$ *Rotational motion in Euler angles ϑ*

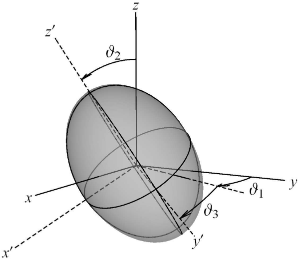
Rotational energy

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

Rotational relations (Alaga rules) on electromagnetic transitions

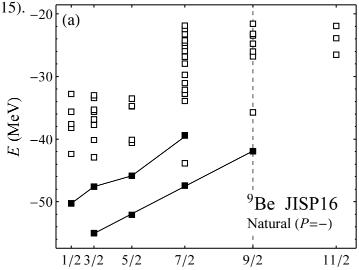
$$B(E2; J_i \rightarrow J_f) \propto (J_i K 2 0 | J_f K)^2 (eQ_0)^2 \qquad eQ_0 \propto \langle \phi_K | Q_{2,0} | \phi_K \rangle$$





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).



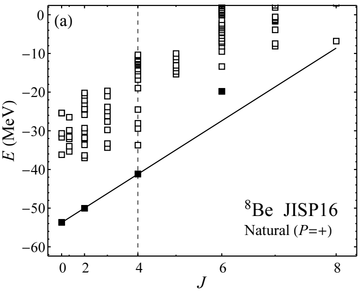
Valence shell structure? SU(3)

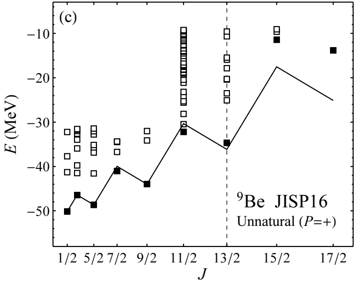
T. Dytrych *et al.*, Phys. Rev. Lett. **111**, 252501 (2013).

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

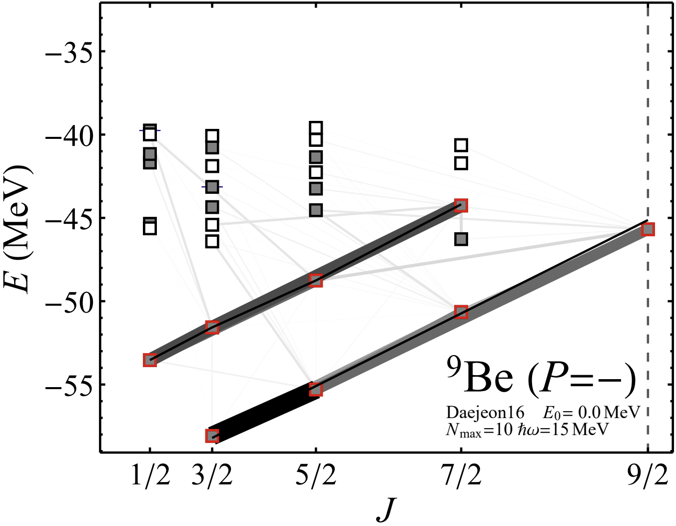
A. E. McCoy *et al.*, Phys. Rev. Lett. **125**, 102505 (2020).

Cluster rotation?





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



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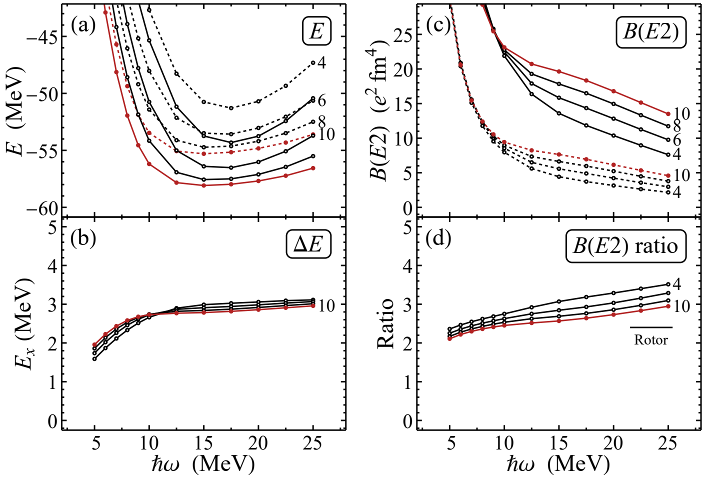
^{9}Be: Convergence of *relative* observables

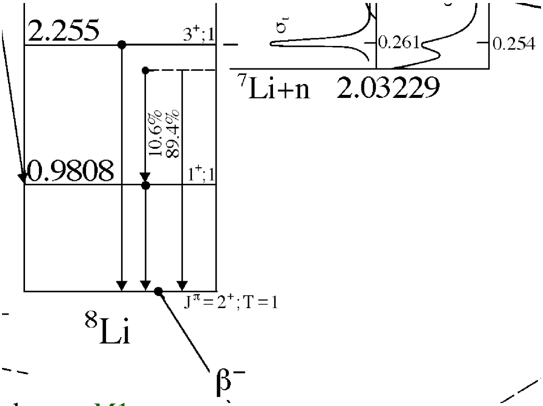
^{9}Be $K = 3/2$ ground state band

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



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

Enhanced (?) ground-state transition in ^{8}Li



$1^+ \rightarrow 2^+$ γ decay: $M1$

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

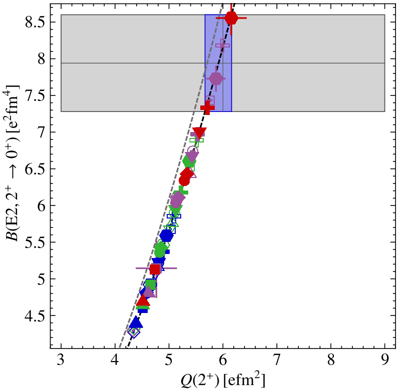
$B(E2; 2^+ \rightarrow 1^+) = 55(15)\, e^2\text{fm}^4$ *or* $\approx 58\,\text{W.u.}$ Brown 1991

Ab initio Green's function Monte Carlo (GFMC) predicts $\approx 0.8\, e^2\text{fm}^4$ 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, $\hbar\omega = 16\,\mathrm{MeV}$, $N_{max} \leq 8$. EM/N2LO$_{opt}$/EGM interactions.

Dimensionless ratio of $E2$ observables

Compare...

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

...with...

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

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

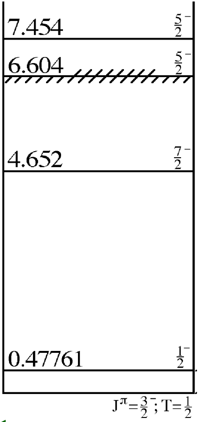
Dimensionless ratio *of like powers of E2 matrix elements*

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

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**

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

Ground-state transition in ^{7}Li

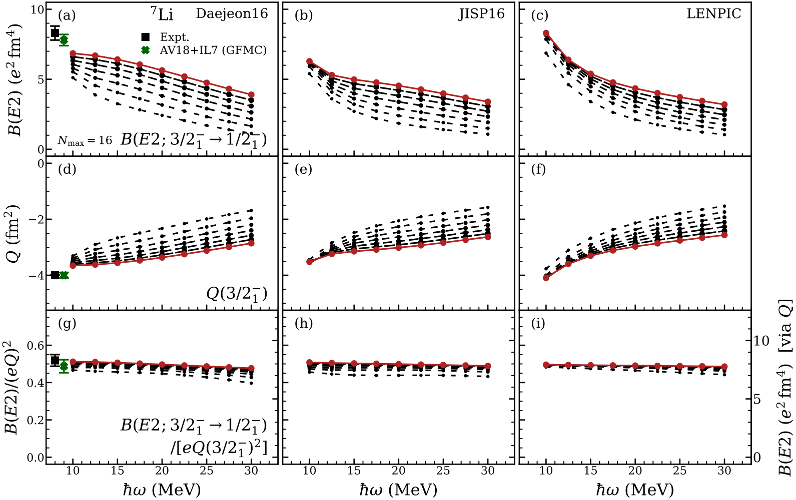


$1/2^- \rightarrow 3/2^-$ γ decay: $M1$

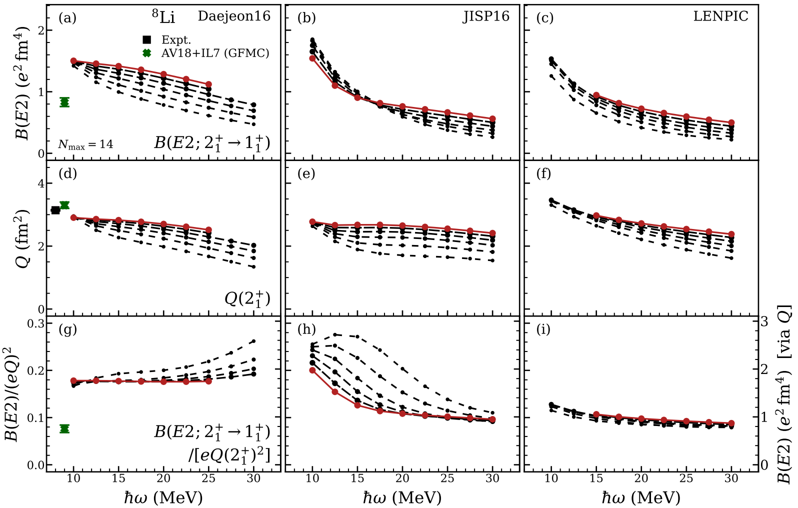
$3/2^- \rightarrow 1/2^-$ Coulomb excitation: $E2$

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

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



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



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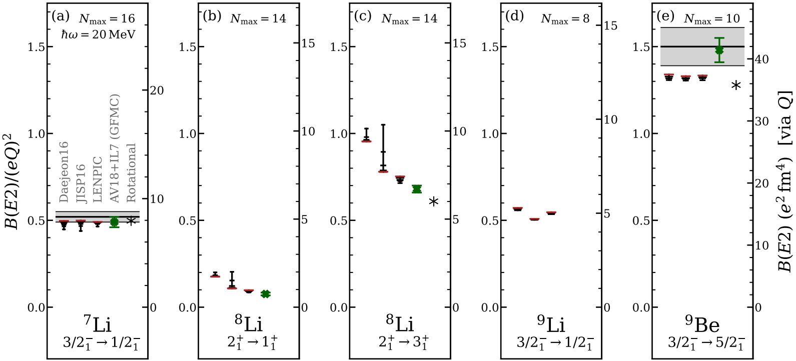
GFMC: S. Pastore, S. C. Pieper, R. Schiavilla, and R. B. Wiringa, Phys. Rev. C **87**, 035503 (2013).

^{8}Li and neighbors: $E2$ strength by calibration to Q



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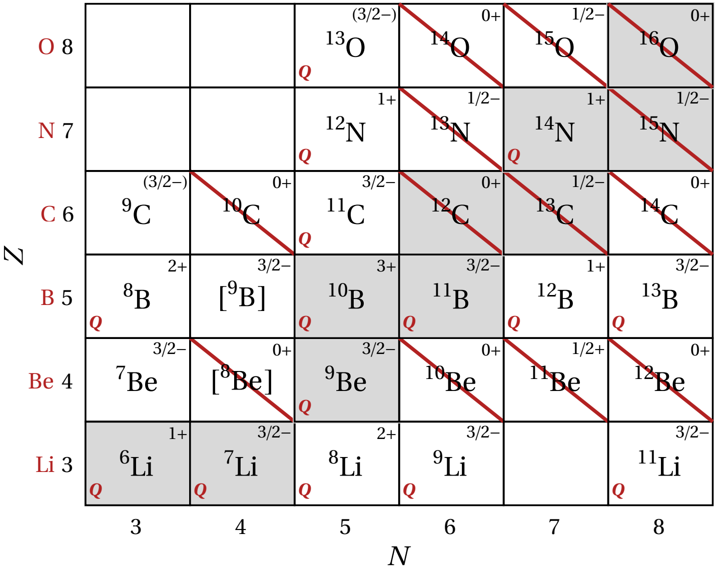

Q = Q(g.s.) measured [N. J. Stone, ADNDT **111**, 1 (2016)]

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Dimensionless ratio of $E2$ and radius observables

Compare…

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

…with…

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

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

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

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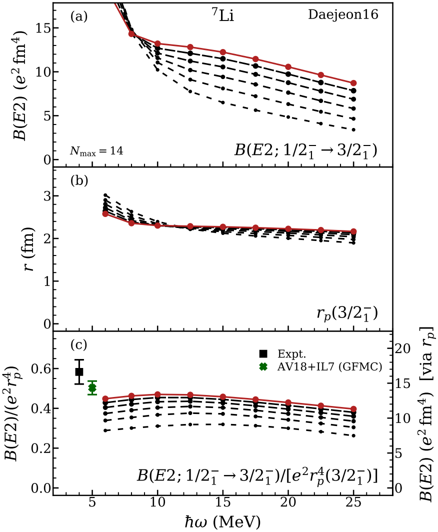
R = r_c(g.s.) measured [I. Angeli and K. P. Marinova, ADNDT **99**, 69 (2013); J. H. Kelley *et al.*, NPA **968**, 71 (2017)]

^{7}Li: $E2$ strength by calibration to radius



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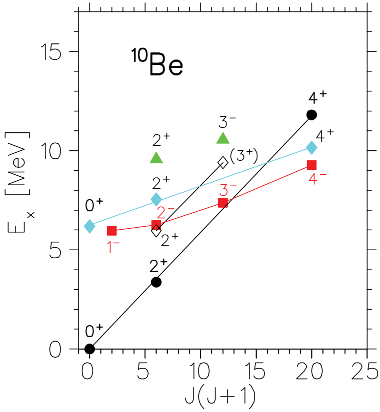
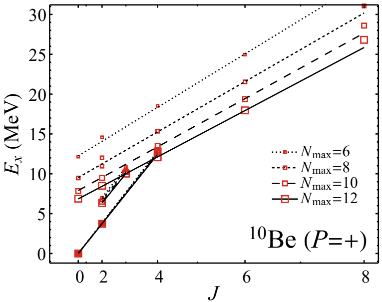
GFMC: S. Pastore, S. C. Pieper, R. Schiavilla, and R. B. Wiringa, Phys. Rev. C **87**, 035503 (2013).

Experimental and calculated bands in ^{10}Be

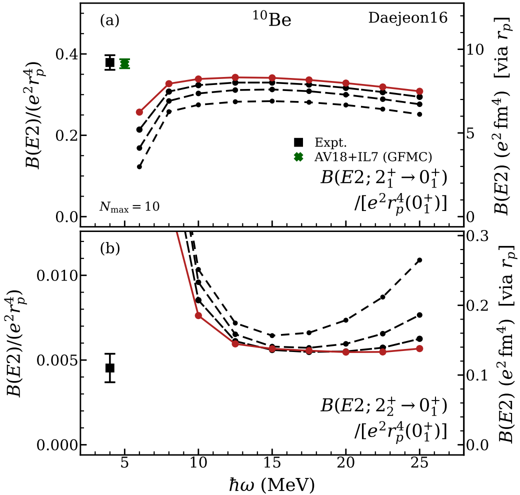


H. G. Bohlen *et al.*, Phys. Rev. C **75**, 054604 (2007).



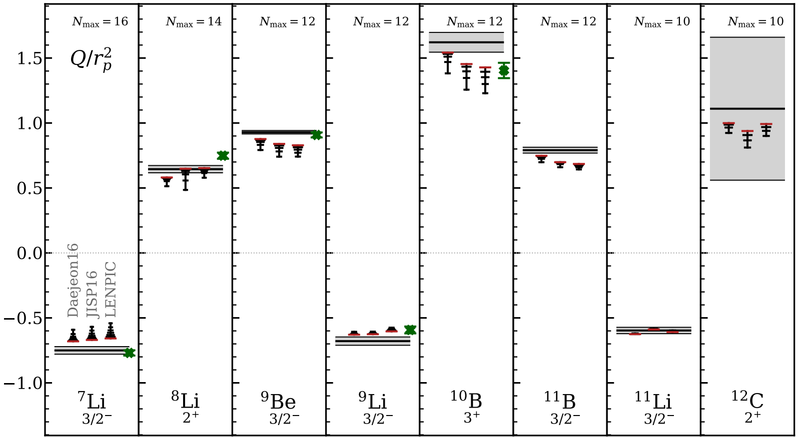
M. A. Caprio, P. J. Fasano, A. E. McCoy, P. Maris, J. P. Vary, Bulg. J. Phys. **46**, 455 (2019) (SDANCA19).

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



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

Ground state Q by calibration to radius



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

Summary

Ab initio prediction of $E2$ observables hampered by sensitivity to large-distance tails of wave function *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 $B(E2)/(eQ)^2$

Prediction of E2 observables by calibration to quadrupole moment

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

Prediction of E2 observables by calibration to charge radius