Shape coexistence and shape invariants

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Progress in *Ab Initio* Techniques in Nuclear Physics
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Rotational structure from *ab initio* nuclear theory?

Ab initio theory should be able to describe nuclei

Light nuclei display rotational band structure

∴ *Ab initio* theory should be able to predict rotational bands

But... Convergence challenges in calculation of relevant observables

– Qualitative emergence of rotational “features”?

Rotational energies, rotational transition patterns

– Robust quantititative prediction of rotational observables?

Rotational energy parameters, intrinsic E2 matrix elements

– Physical nature of rotation in light nuclei — What can we learn?

M. A. Caprio, P. J. Fasano, P. Maris, A. E. McCoy, J. P. Vary, EPJA Topical Issue, `arXiv:1912.00083`.
M. A. Caprio, P. J. Fasano, A. E. McCoy, P. Maris, J. P. Vary, Bulg. J. Phys. (SDANCA19), `arXiv:1912.06082`.

Rapid convergence with Daejeon16 interaction

A. M. Shirokov and I. J. Shin and Y. Kim and M. Sosonkina and P. Maris and J. P. Vary, Phys. Lett. B **761**, 87 (2016).

Shape coexistence and quadrupole shape invariants ^{10}Be & ^{10}C

Separation of rotational degree of freedom

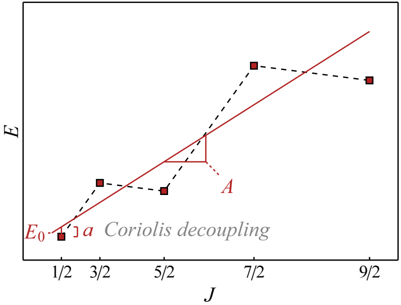
Intrinsic state $|\phi_K\rangle$ & rotation in Euler angles ϑ $\qquad (J = K, K+1, \ldots)$

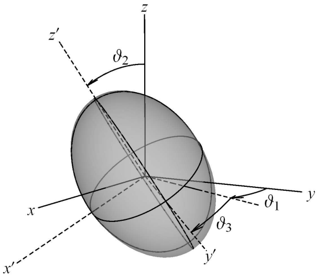
$$|\psi_{JKM}\rangle \propto \int d\vartheta \Big[\mathcal{D}^J_{MK}(\vartheta)|\phi_K;\vartheta\rangle + (-)^{J+K}\mathcal{D}^J_{M-K}(\vartheta)|\phi_{\bar{K}};\vartheta\rangle \Big]$$

Rotational energy

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

Rotational relations on electromagnetic transitions ($E2$, $M1$, ...)





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).

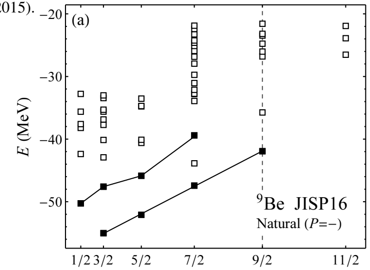
Valence shell structure?

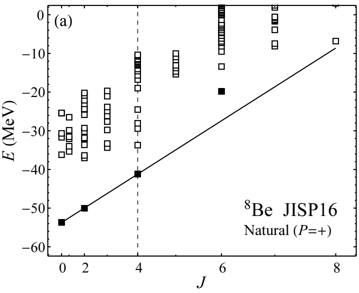
Multishell dynamics?

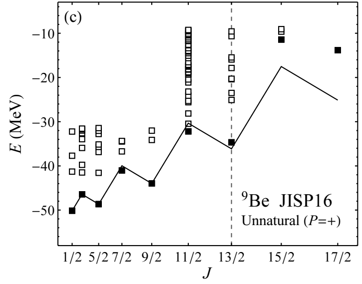
Elliott SU(3), Sp(3, $\mathbb{R}$)*?*

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

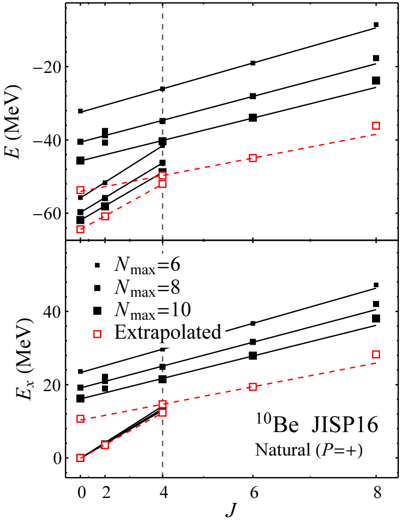
Cluster rotation?

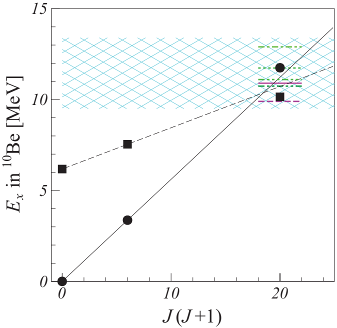






Yrast and excited bands in ^{10}Be

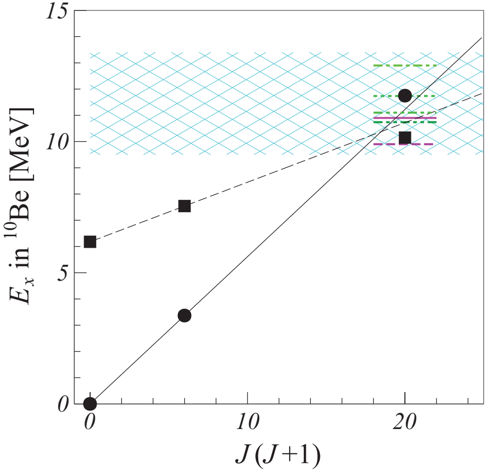


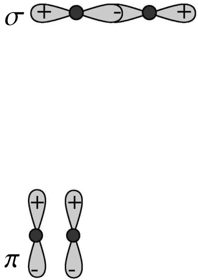


From D. Suzuki *et al.*, Phys. Rev. C **87**, 054301 (2013).

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

Yrast and excited bands in ^{10}Be

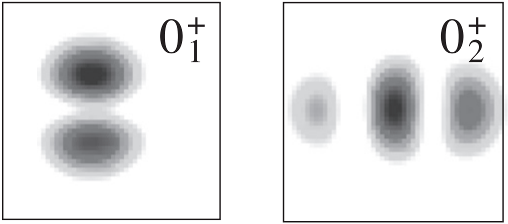


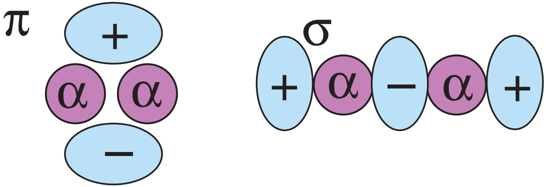


From D. Suzuki *et al.*, Phys. Rev. C **87**, 054301 (2013). Orbital schematics from Y. Kanada-En'yo, H. Horiuchi, and A. Doté, Phys. Rev. C **60**, 064304 (1999).

Yrast and excited bands of ^{10}Be from AMD

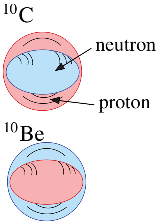
Antisymmetrized molecular dynamics (AMD)



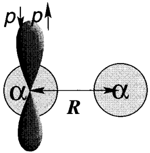


Y. Kanada-En'yo, M. Kimura, and A. Ono, Prog. Theor. Exp. Phys. **2012**, 01A202 (2012).

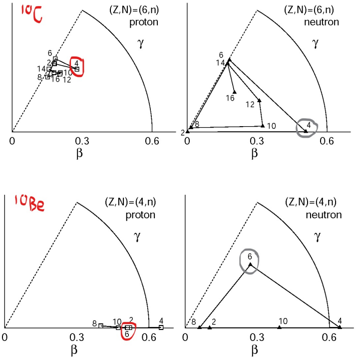
Proton-neutron triaxiality in $^{10}_{4}\mathrm{Be}_6$ & $^{10}_{6}\mathrm{C}_4$?



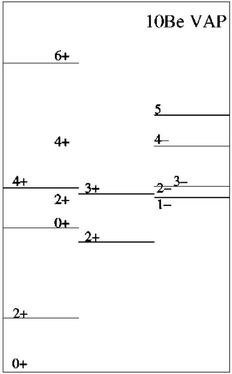
Y. Kanada-En'yo, M. Kimura, and A. Ono, Prog. Theor. Exp. Phys. **2012**, 01A202 (2012).



Y. Kanada-En'yo and H. Horiuchi, Phys. Rev. C **55**, 2860 (1997).



Y. Kanada-En'yo and H. Horiuchi, Prog. Theor. Phys. Suppl. **142**, 205 (2001).



Y. Kanada-En'yo, H. Horiuchi, and A. Doté, Phys. Rev. C **60**, 064304 (1999).

Triaxial $\mathrm{SU}^*_{\pi\nu}(3)$ structure in the IBM-2

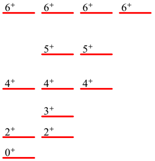
A. E. L. Dieperink and R. Bijker, Phys. Lett. B **116**, 77 (1982).

A proton fluid with prolate deformation and a neutron fluid with oblate deformation, coupled with symmetry axes orthogonal to each other, yield a composite shape with overall triaxial deformation.

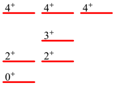
Energies follow usual $\mathrm{SU}(3)$ relation

$$E(\lambda,\mu,L) = aC_2(\lambda,\mu) + bL(L+1),$$

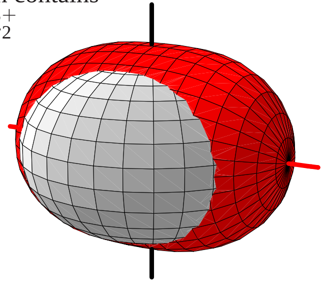
but representations present are different from those for $\mathrm{SU}_{\pi\nu}(3)$ axial rotor. Even the ground state representation contains multiple degenerate K bands ($\Rightarrow 2^+_1$ and 2^+_2 degenerate).



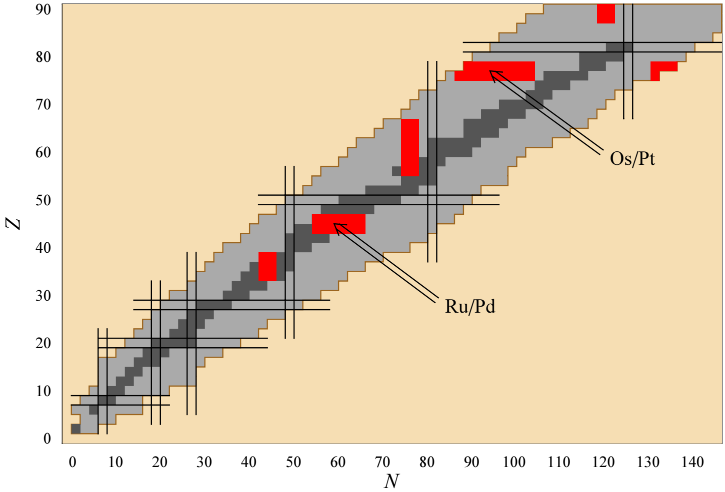
$(\lambda, \mu) = (2N_\pi, 2N_\nu)$



$(\lambda, \mu) = (2N_\pi + 2, 2N_\nu - 4)$

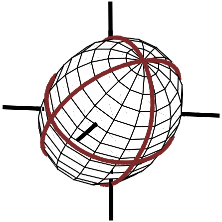


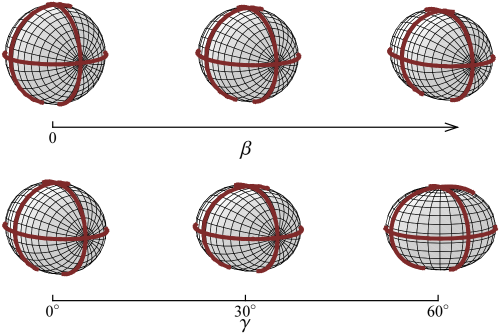
Prospective regions for $SU^*_{\pi\nu}(3)$ triaxial structure



Nuclear quadrupole deformation

$$R(\theta,\varphi) = R_0\left[1 + \sum_M \alpha_{2M} Y_{2M}(\theta,\varphi) + \cdots\right]$$





β – Overall deformation

γ – Prolate/triaxial/oblate

θ_1, θ_2, θ_3 – Euler angles

$$\alpha_{2M} = \beta\cos\gamma\,\mathscr{D}^{(2)}_{0,M}(\Omega) + \frac{1}{\sqrt{2}}\beta\sin\gamma\left[\mathscr{D}^{(2)}_{2,M}(\Omega) + \mathscr{D}^{(2)}_{-2,M}(\Omega)\right]$$

$$\Omega \equiv (\theta_1,\theta_2,\theta_3)$$

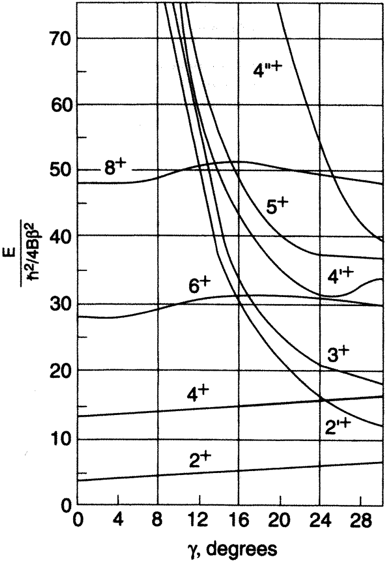


FIG. 6.24. Normal and anomalous levels of the triaxial rotor (Preston, 1975).

R. F. Casten, *Nuclear Structure from a Simple Perspective*, 2ed. (Oxford, 2000).

No-core configuration interaction (NCCI) approach

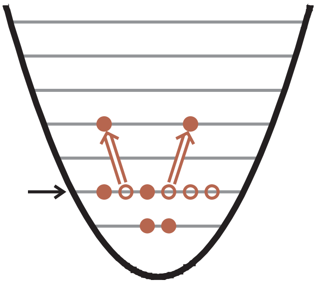
P. Navratil, J. P. Vary, and B. R. Barrett, Phys. Rev. Lett. **84**, 5728 (2000).

– 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}

Convergence towards exact result with increasing N_{max}

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

$N_{\text{ex}} \leq N_{\text{max}}$ $\qquad N = 2n + l$

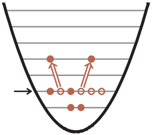


Convergence of NCCI calculations

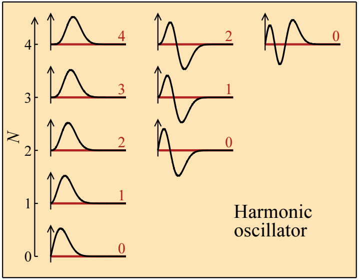
Results for calculation in finite space depend upon:

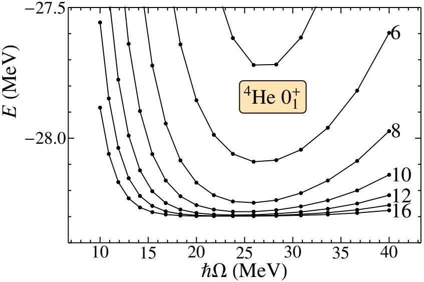
- Many-body truncation N_{max}
- Single-particle basis scale: oscillator length b (or $\hbar\omega$)

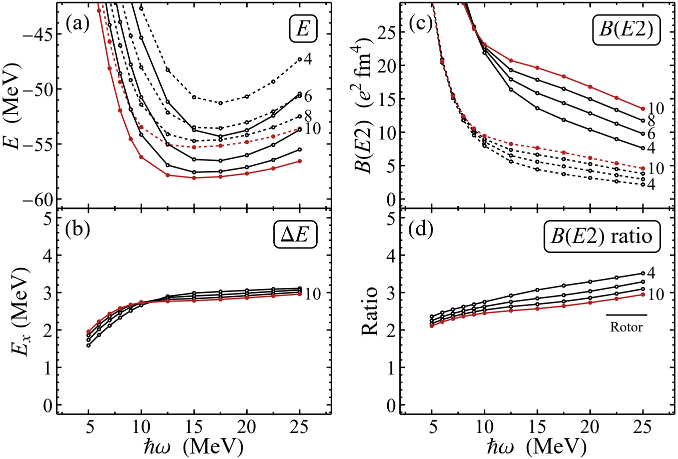
$$b = \frac{(\hbar c)}{[(m_N c^2)(\hbar\omega)]^{1/2}}$$



Convergence of calculated results (with respect to basis truncation) is signaled by independence of these parameters







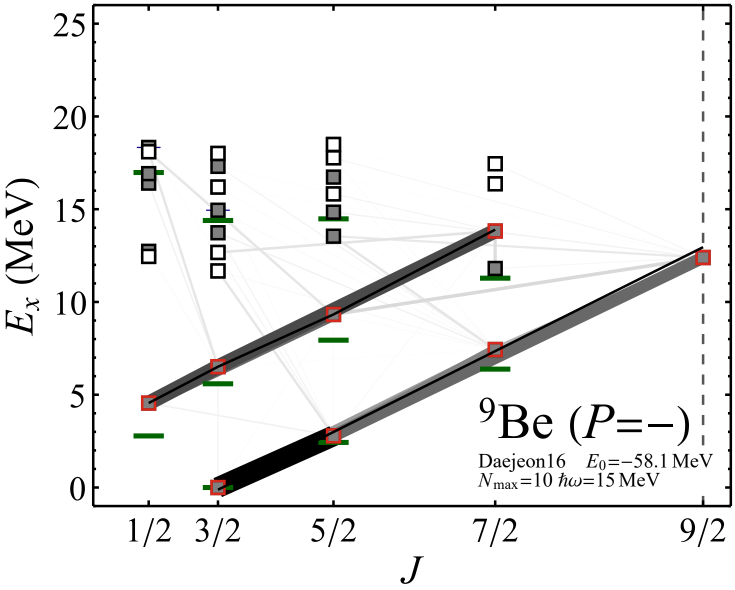
(a) $E(3/2^-_1)$ & $E(5/2^-_1)$

$\Rightarrow$ (b) $E(5/2^-_1) - E(3/2^-_1)$

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

$\Rightarrow$ (d) $B(E2; 5/2^- \rightarrow 3/2^-)/B(E2; 7/2^- \rightarrow 3/2^-)$

^{9}Be, Daejeon16 + Coulomb; `arXiv:1912.00083`.



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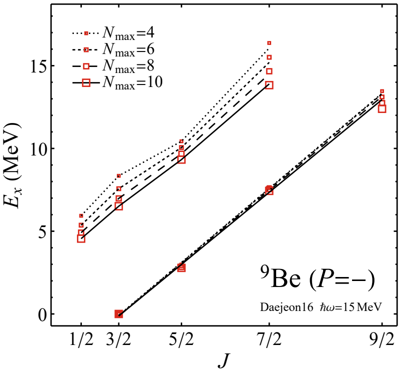
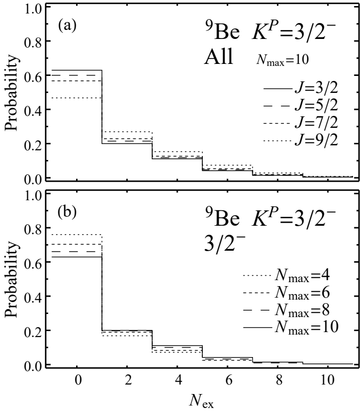
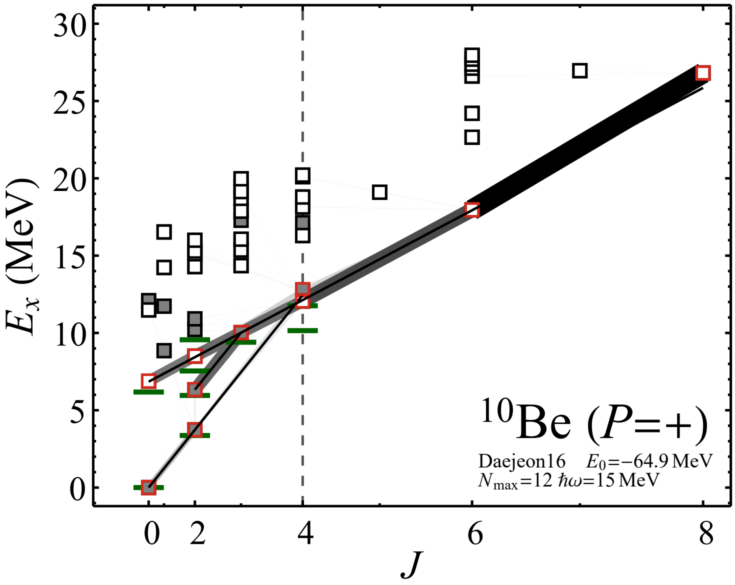
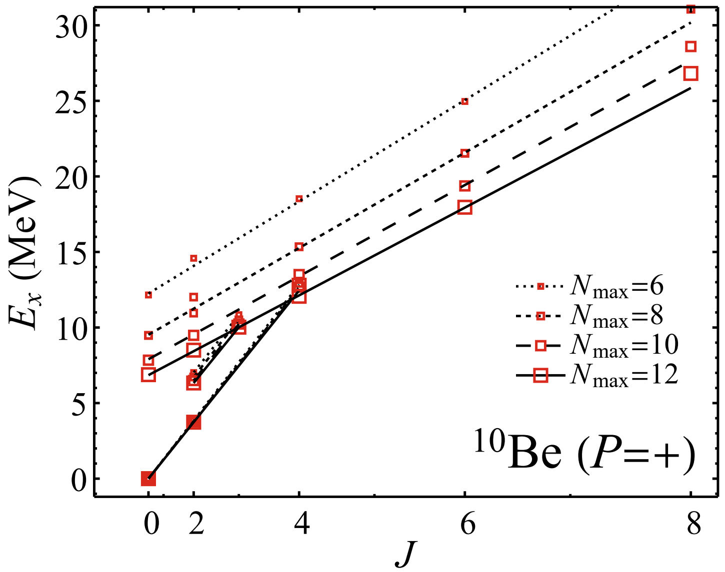




M. A. Caprio, P. J. Fasano, P. Maris, A. E. McCoy, J. P. Vary, EPJA Topical Issue, `arXiv:1912.00083`.


30
25
20
15
10
5
0
E_x (MeV)
0 2 4 6 8
J
^{10}Be (P=+)
Daejeon16 E_0=−64.9 MeV
$N_{\max}$=12 $\hbar\omega$=15 MeV



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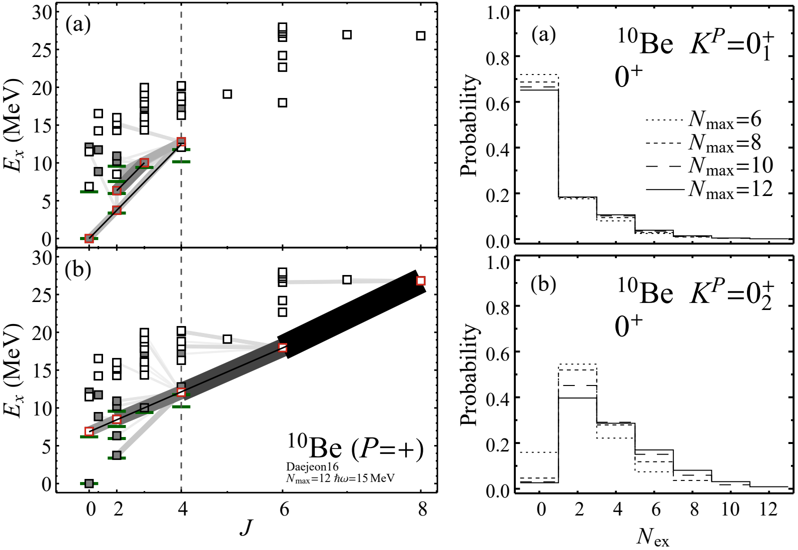
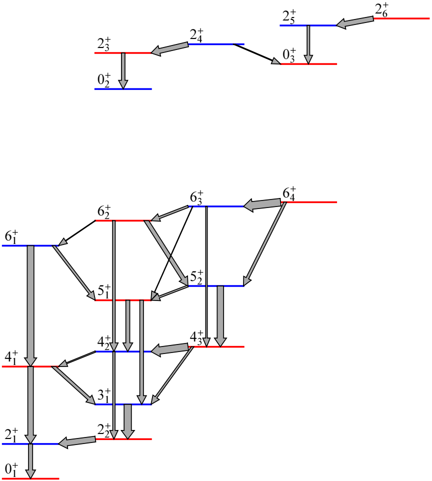


M. A. Caprio, P. J. Fasano, A. E. McCoy, P. Maris, J. P. Vary, Bulg. J. Phys. (SDANCA19), arXiv:1912.06082.

The $\mathrm{SU}^*_{\pi\nu}(3)$ dynamical symmetry: Levels and quadrupole transitions



$\mathrm{SU}^*_{\pi\nu}(3)$ perturbed with Majorana operator for degeneracy breaking.
$(N_\pi, N_\nu) = (5,5)$

Quadrupole shape invariants (Q-invariants)

Quadrupole tensor in rotational intrinsic frame

$$Q_{2\mu} = \sum_i r_i^2 Y_{2\mu}(\hat{\mathbf{r}}_i)$$

$$\langle Q_{2,0}\rangle = q\cos\gamma \qquad \langle Q_{2,\pm1}\rangle = 0 \qquad \langle Q_{2,\pm2}\rangle = \frac{1}{\sqrt{2}}q\sin\gamma$$

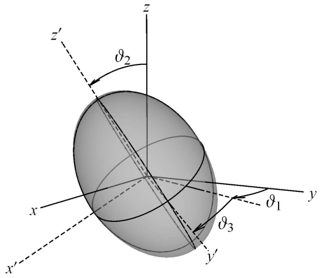
$$\langle Q_2\cdot Q_2\rangle = q^2 \qquad = \sqrt{5}\langle (Q_2\times Q_2)_{00}\rangle$$

Rotational invariant operators

$$Q^{(2)} \equiv (Q\times Q)_{00} \qquad = \sqrt{\tfrac{1}{5}}\bar{q}^2$$

$$Q^{(3)} \equiv (Q\times Q\times Q)_{00} \qquad = -\sqrt{\tfrac{2}{35}}\bar{q}^3\,\overline{\cos 3\gamma}$$

K. Kumar, Phys. Rev. Lett. **28**, 249 (1972).
D. Cline, Annu. Rev. Nucl. Part. Sci. **36**, 683 (1986).
A. Poves, F. Nowacki, Y. Alhassid, `arXiv:1906.07542`.



Relation to Bohr deformation*

$$\alpha_{2\mu} \approx \left(\frac{4\pi}{3AR^2}\right)Q_{2\mu} \quad \Rightarrow \quad \beta \approx \left(\frac{4\pi}{3AR^2}\right)q$$

* To within factors of Ze/A, $(16\pi/5)^{1/2}$, *etc. Caveat emptor!*

Quadrupole shape invariants and fluctuations

Rotational invariant operators

$$Q^{(2)} \equiv (Q \times Q)_{00} = \sqrt{\tfrac{1}{5}}\,\bar{q}^2$$

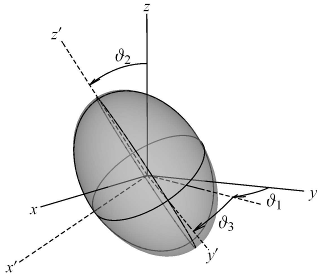
$$Q^{(3)} \equiv (Q \times Q \times Q)_{00} = -\sqrt{\tfrac{2}{35}}\,\bar{q}^3\,\overline{\cos 3\gamma}$$

Variances of Q-invariants

$$\sigma^2(Q^{(2)}) = \langle Q^{(2)} Q^{(2)} \rangle - \langle Q^{(2)} \rangle^2$$

$$\sigma^2(Q^{(3)}) = \langle Q^{(3)} Q^{(3)} \rangle - \langle Q^{(3)} \rangle^2$$

Fluctuations in shape distribution



$$\frac{\sigma(q)}{\bar{q}} = \frac{1}{2}\frac{\sigma(Q^{(2)})}{\langle Q^{(2)} \rangle}$$

$$\frac{\sigma^2(\cos 3\gamma)}{(\overline{\cos 3\gamma})^2} = \frac{\sigma^2(Q^{(3)})}{\langle Q^{(3)} \rangle^2} + \frac{9}{4}\frac{\sigma^2(Q^{(2)})}{\langle Q^{(2)} \rangle^2} - 3\,\frac{\langle Q^{(2)} Q^{(3)} \rangle - \langle Q^{(3)} \rangle \langle Q^{(2)} \rangle}{\langle Q^{(3)} \rangle \langle Q^{(2)} \rangle}$$

A. Poves, F. Nowacki, Y. Alhassid, `arXiv:1906.07542`.

Evaluation of Q-invariants

Q-invariants and the center-of-mass degree of freedom

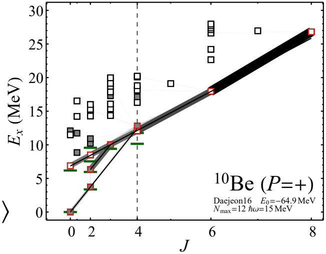
$$Q^{(2)} \equiv (Q\times Q)_{00} \qquad \Rightarrow (Q'\times Q')_{00}$$

$$Q^{(3)} \equiv (Q\times Q\times Q)_{00} \qquad \Rightarrow (Q'\times Q'\times Q')_{00}$$

$$Q_2 = Q_2' + Q_2^{\text{c.m.}}$$

$$Q_{2\mu} = \sum_i r_i^2 Y_{2\mu}(\hat{\mathbf{r}}_i) = \sqrt{\tfrac{15}{8\pi}}\sum_i (\mathbf{r}_i\times\mathbf{r}_i)_{2\mu}$$

$$\Rightarrow Q'_{2\mu} = \sqrt{\tfrac{15}{8\pi}}\sum_i [(\mathbf{r}_i-\mathbf{R})\times(\mathbf{r}_i-\mathbf{R})]_{2\mu}$$



Resolution of identity

over center-of-mass 0*s states*

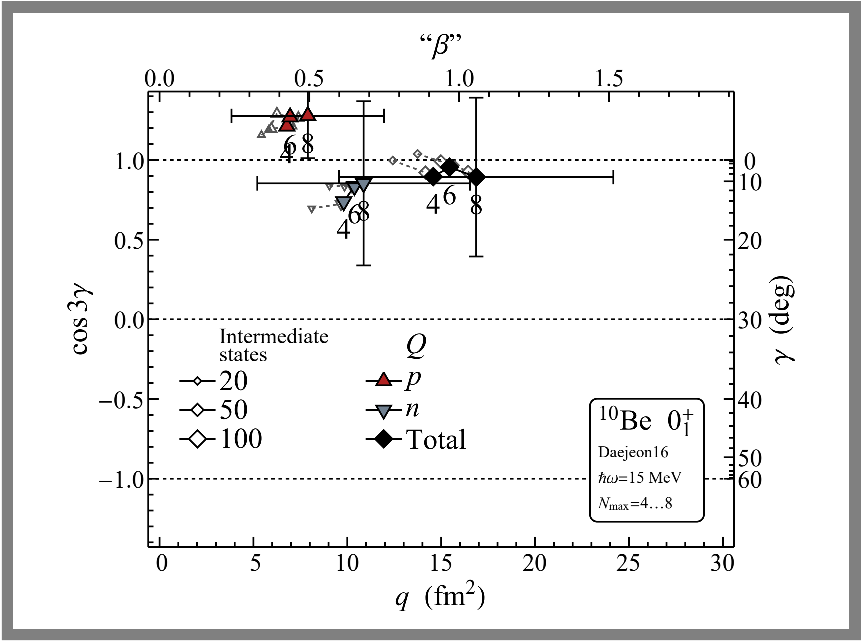
$$\langle a|Q^{(2)}|a\rangle \propto \sum_r \begin{Bmatrix} 2 & 2 & 0 \\ a & a & r \end{Bmatrix} \langle a\|Q_2\|r\rangle\langle r\|Q_2\|a\rangle$$

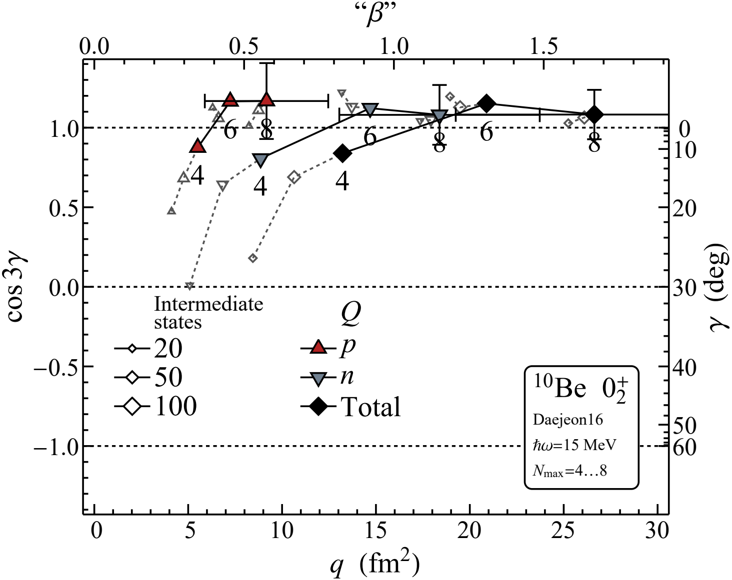
$$\langle a|Q^{(3)}|a\rangle \propto \sum_{rs} \begin{Bmatrix} 2 & 2 & 2 \\ s & a & r \end{Bmatrix}\begin{Bmatrix} 2 & 2 & 0 \\ a & a & s \end{Bmatrix} \langle a\|Q_2\|r\rangle\langle r\|Q_2\|s\rangle\langle s\|Q_2\|a\rangle$$

Need *lots* of intermediate states MFDn wave function postprocessor (P. Maris & P. J. Fasano)

$$\langle 0|Q^{(2)}|0\rangle \qquad 0\rightarrow 2\rightarrow 0$$

$$\langle 0|Q^{(3)}|0\rangle \qquad 0\rightarrow 2\rightarrow 2\rightarrow 0$$


"β"
0.0
0.5
1.0
1.5
cos 3γ
γ (deg)
q (fm²)
Intermediate states
20
50
100
Q
p
n
Total
¹⁰Be 0⁺₁
Daejeon16
ħω=15 MeV
Nmax=4…8


"β"
0.0
0.5
1.0
1.5
cos 3γ
γ (deg)
q (fm²)
Intermediate states
20
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Q
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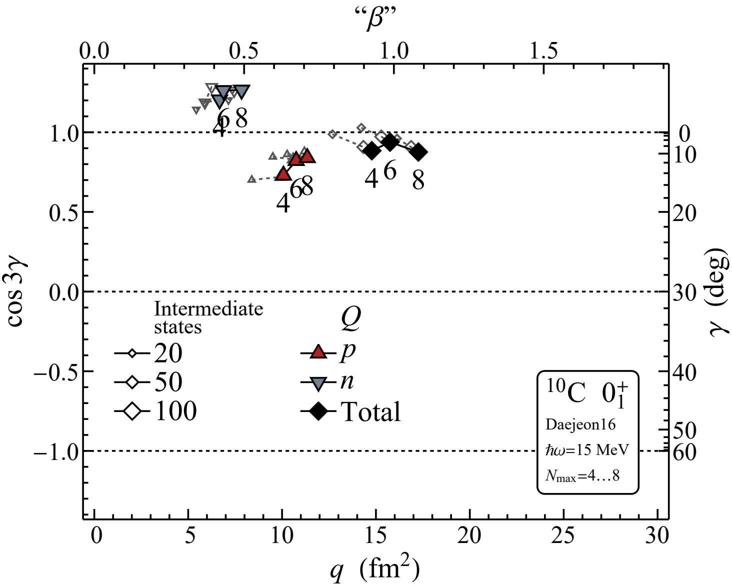
Total
¹⁰Be 0₂⁺
Daejeon16
ħω=15 MeV
N_max=4…8


"β"
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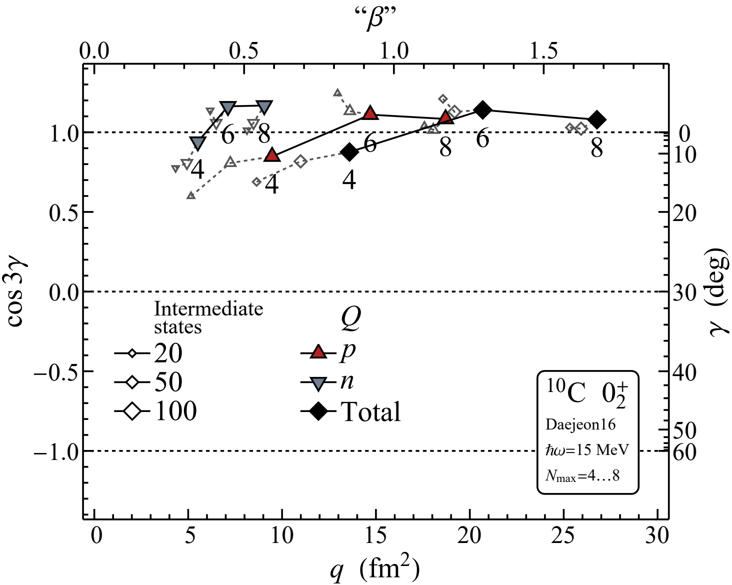
1.5
1.0
0.5
0.0
−0.5
−1.0
cos 3γ
0
10
20
30
40
50
60
γ (deg)
4
6
8
4
6
8
4
6
8
Intermediate states
20
50
100
Q
p
n
Total
^{10}C 0_1^+
Daejeon16
ℏω=15 MeV
$N_{\max}$=4…8
0
5
10
15
20
25
30
q (fm^2)


"β"
0.0
0.5
1.0
1.5
cos 3γ
γ (deg)
q (fm²)
Intermediate states
20
50
100
Q
p
n
Total
¹⁰C 0₂⁺
Daejeon16
ℏω=15 MeV
N_max=4…8