

Shape coexistence in medium-mass nuclei

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Deformation and shape coexistence

Deformation is everywhere:

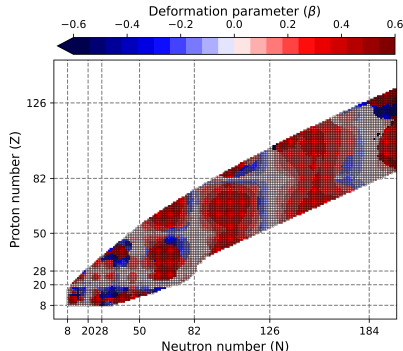
- ▶ Magical nuclei are spherical
- ▶ Deformation is enhanced mid-shell

Quadrupole deformation:

- ▶ Most important shape
- ▶ Prolate: elongated sphere
- ▶ Oblate: flattened sphere

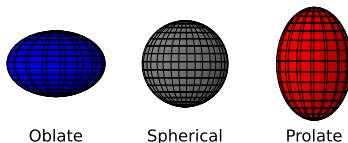
Shape coexistence:

- ▶ Different shapes coexist within the **same nucleus** at different energies
- ▶ Present in most nuclei



P. Möller, et al. Atom. Data Nucl. Data Tabl.

109-110 (2016)



Intrinsic vs laboratory frame

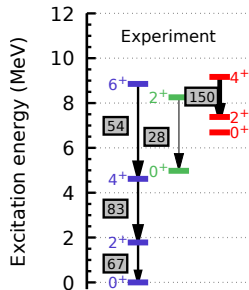
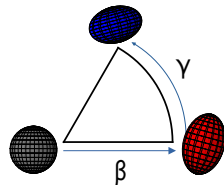
Deformation is characterized in the **intrinsic frame**: (β, γ)

However, measurements are done in **lab frame**: $(B(E2), Q_s)$

Relation between lab and intrinsic frame:

$$Q_s(J) = \frac{3K^2 - J(J+1)}{(J+1)(2J+3)} Q_{0,s},$$

$$B(E2, J_i \rightarrow J_f) = \frac{5Q_{0,t}^2}{16\pi} \langle J_i K 2 0 | J_f K \rangle$$



► If $Q_{0,s} \simeq Q_{0,t}$: well deformed rotor

1. For even-even nuclei ($J=0$) $\rightarrow Q_s = 0$

2. Triaxial shapes diminish Q_s

3. $B(E2)$: scattered across out-band states

\rightarrow Perfect axial rotor assumption!

Shape invariants $\langle Q^n \rangle$: model independent measure of deformation

Shape invariants: Intermediate-state expansion

Couple Q_2 (tensor) to obtain a scalar:

- ▶ $\langle Q^2 \rangle = \langle [Q_2 \times Q_2]_0 \rangle \rightarrow \beta$
- ▶ $\langle Q^3 \rangle = \langle [[Q_2 \times Q_2]_2 \times Q_2]_0 \rangle \rightarrow \gamma$
- ▶ All $\langle Q^n \rangle$ up to $\langle Q^6 \rangle$ are needed for fluctuations of (β, γ)

K. Kumar, Phys. Rev. Lett. 28, 249 (1972)

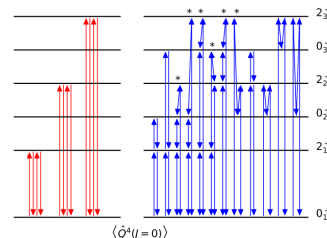
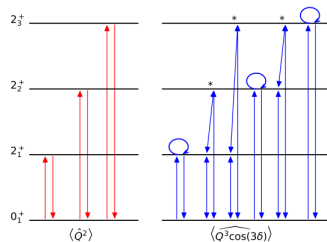
D. Cline, Nuclear Structure 313–326 (1985)

Intermediate-state expansion:

- ▶ Expansion in terms of $M_{if} = \langle i || Q || f \rangle \leftarrow Q_s \text{ or } B(E2)$
- ▶ Needs **all the nuclear states!**
- ▶ Harder convergence for higher $\langle Q^n \rangle$

$$\langle Q^2 \rangle_i \sim \sum_t M_{it} M_{ti}$$

$$\langle Q^3 \rangle_i \sim \sum_{u,t} M_{iu} M_{ut} M_{ti}$$



Henderson, J. Phys Rev C 102, 054306 (2020)

Shape invariants: Sum rule method

1). Apply the \hat{Q}_{20} operator to a state:

$$\hat{Q}_{20}|0^+\rangle = \text{SR1}(2^+)^{1/2}|\overline{2^+(1)}\rangle$$

$$\rightarrow \langle Q^2 \rangle = 5\text{SR1}(2^+)$$

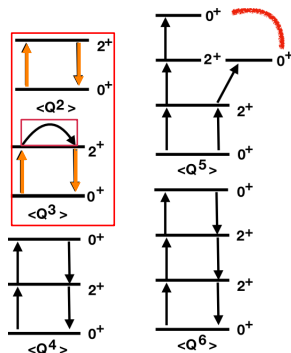
- $|\overline{2^+(1)}\rangle$ not an eigenstate but contains the whole quadrupole strength

2). Evaluate $\langle\langle Q \rangle\rangle = \langle 2^+(1)|Q|2^+(1)\rangle/\sqrt{5}$

$$\rightarrow \langle Q^3 \rangle = \langle Q^2 \rangle \langle\langle Q \rangle\rangle$$

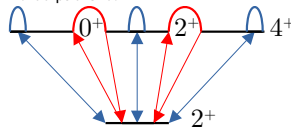
3). Apply \hat{Q}_{20} a second and third time to obtain $\langle Q^4 \rangle$, $\langle Q^5 \rangle$, and $\langle Q^6 \rangle$

- **Exact** calculation (up to numeric)
- Computationally cheap
- Currently only for $J = 0$
- **New!:** extension for any J up to $\langle Q^4 \rangle$



Poves, A., Nowacki, F. & Alhassid, Y.
Phys. Rev. C 101, 054307 (2020)

To be published:



Shell model valence space

Schrödinger equation

$$\mathcal{H}|\Psi\rangle = E|\Psi\rangle$$

► Interacting shell model:

$$\mathcal{H}_{\text{eff}} = \mathcal{H}_0 + \mathcal{H}_{\text{res}}$$

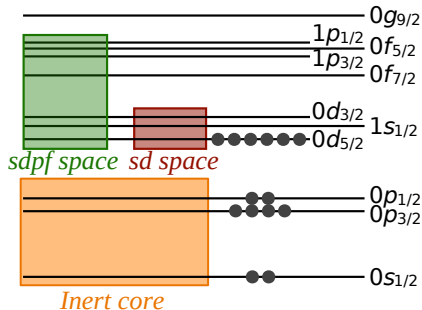
\mathcal{H}_{res} : valence space

► Slater determinant basis $\{\Phi_i\}$

► Phenomenological interactions:

USDB and SDPF-NR

Caurier E., et al. Rev. Mod. Phys. **77**, 427 (2005)



Valence space: $Z_v = N_v = 6$ (^{28}Si)

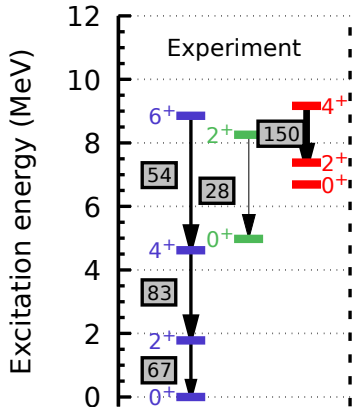
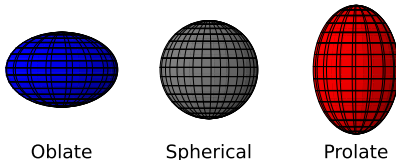
Inert core: ^{16}O nucleus

Motivation for ^{28}Si

► Coexistence of different collective structures:

1. 0_1^+ (0.0 MeV): **Oblate**
bandhead of a rotational band
2. 0_2^+ (5.0 MeV): **Vibration** of the ground state
3. 0_3^+ (6.7 MeV): **Prolate**
bandhead of a rotational band
4. **Superdeformed** rotational band? ($E \gtrsim 10$ MeV)

Taniguchi, Y., et al. Phys. Rev. C **80**, 044316 (2009)



- $E \sim J(J+1)$; $J = 0^+, 2^+, 4^+ \dots$
- Strong $B(E2)$ strengths

Shell model calculation of ^{28}Si

USDB: fails in $B(E2)$ transitions of **prolate band**

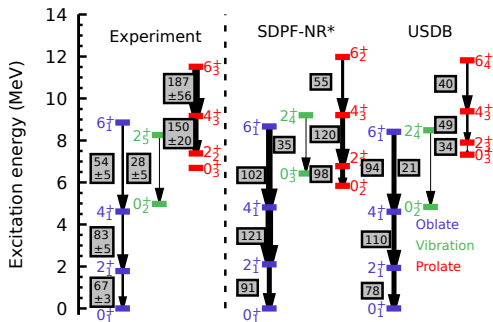
SDPF-NR[†]: Adjusted SDPF-NR[†] interaction to reproduce ^{28}Si shell gap

Additional deformation from pf -shell particles:

- ▶ Slight gain for **oblate** and **vibration**
- ▶ Significant gain in **prolate** deformation
- ▶ 1 particle in pf -shell (38% of *sdpf* 2p-2h)

[†]S. Nummela Phys. Rev. C **63**,

044316 (2001)



Experiment vs Theory (SDPF-NR*):

$$B(E2, 2_{\text{obl}}^+ \rightarrow 0_{\text{obl}}^+) = 67 \pm 3 \text{ vs } 91 \text{ e}^2\text{fm}^4$$

$$B(E2, 2_{\text{vib}}^+ \rightarrow 0_{\text{vib}}^+) = 28 \pm 5 \text{ vs } 35 \text{ e}^2\text{fm}^4$$

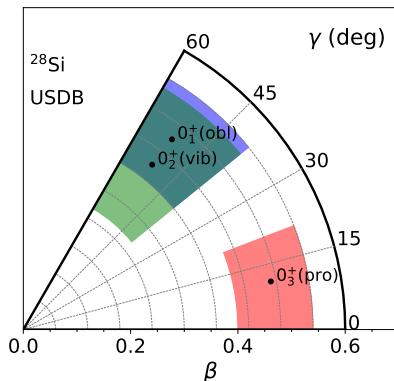
$$B(E2, 4_{\text{pro}}^+ \rightarrow 2_{\text{pro}}^+) = 150 \pm 20 \text{ vs } 120 \text{ e}^2\text{fm}^4$$

D. Frycz, et al. Phys. Rev. C **110**, 054326 (2024)

Shape invariants for ^{28}Si

^{28}Si shape coexistence (USDB):

- ▶ **Oblate**: $\beta = 0.45 \pm 0.09$
 $\gamma = 53$ (39 – 60)
- ▶ **Vibration**: $\beta = 0.39 \pm 0.13$
 $\gamma = 53$ (39 – 60)
- ▶ **Prolate**: $\beta = 0.47 \pm 0.07$
 $\gamma = 11$ (0 – 21)
- Shapes are γ **and** β **soft**
- **Vibration** is **similar** in deformation to **oblate GS**
- Prolate shape has similar deformation as GS



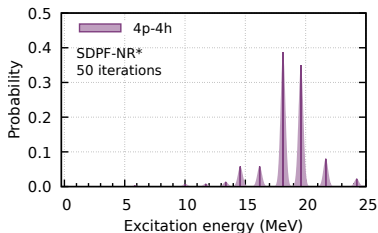
Superdeformation

Superdeformed (SD) band predicted with:

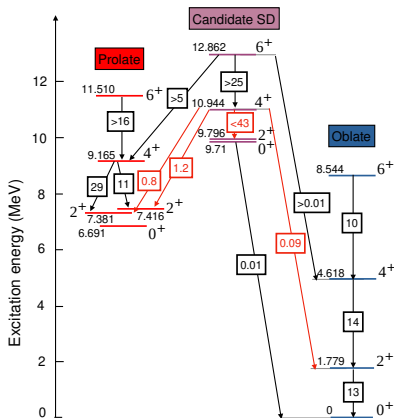
- Deformation: $\beta_{theo} \approx 1$
- **4p-4h** into *pf* shell
- ~ 13 MeV bandhead

Taniguchi, Y., et al. Physical Review C, 2009. **80**, 044316

Our prediction lies at 18 MeV:



Frycz, et al. Phys. Rev. C **110**, 054326 (2024)



Experimental attempts

- $B(E2, 4^+ \rightarrow 2^+) \leq 217 \text{efm}^2$
- Not found: $\beta_{exp} \leq 0.6$

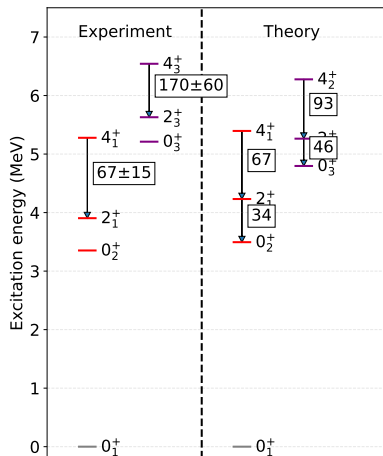
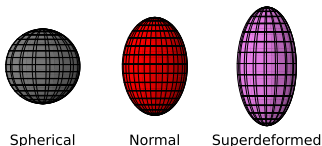
Morris, L. et al. Phys. Rev. C **104**, 054323 (2021)

Spectrum of ^{40}Ca

Doubly magical nucleus
($Z = N = 20$)

Shape coexistence in ^{40}Ca :

1. 0_1^+ (0.0 MeV):
Spherical 0p-0h
2. 0_2^+ (3.4 MeV):
Deformed 4p-4h
3. 0_3^+ (5.2 MeV):
Superdeformed 8p-8h



Accurate description of ^{40}Ca

E. Caurier, J. Menéndez, F. Nowacki, and A. Poves
Phys. Rev. C **75**, 054317 (2007)

Shape invariants for ^{40}Ca

^{40}Ca shape coexistence (SDPF):

► “Spherical”:

$$\beta = 0.07 \pm 0.14$$

$$\gamma = - (0 - 60)$$

Compatible with $\beta = 0$ but
reaches up to $\beta = 0.2$

► Normal deformed:

$$\beta = 0.47 \pm 0.09$$

$$\gamma = 17 (4 - 23)$$

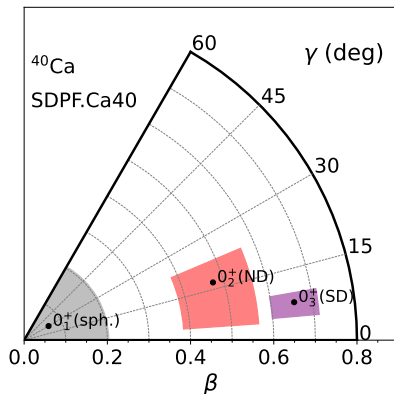
Considerable fluctuations

► Superdeformed:

$$\beta = 0.66 \pm 0.06$$

$$\gamma = 8 (5 - 10)$$

Lower fluctuations for SD

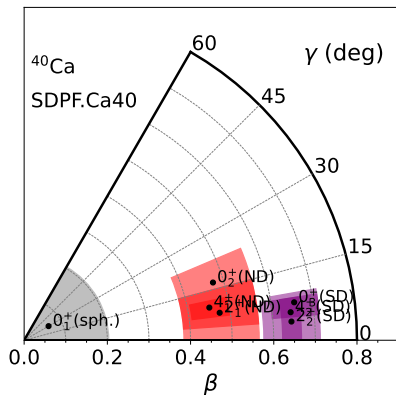


Band evolution in ^{40}Ca

Band evolution of (β, γ) :

^{40}Ca	$\beta \pm \Delta\beta$	γ ($\Delta\gamma$)
0^+_{sph}	0.07 ± 0.14	- (0-60)
0^+_{ND}	0.47 ± 0.09	17 (4-23)
2^+_{ND}	0.47 ± 0.09	8 (0-15)
4^+_{ND}	0.45 ± 0.05	10 (7-12)
0^+_{SD}	0.66 ± 0.06	8 (5-10)
2^+_{SD}	0.64 ± 0.07	4 (0-9)
4^+_{SD}	0.64 ± 0.02	6 (0-9)

- ▶ Band states overlap
- ▶ (β, γ) are consistent
- ▶ Robust method to identify states with the same intrinsic shape



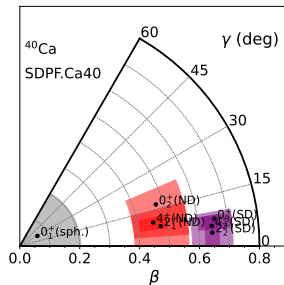
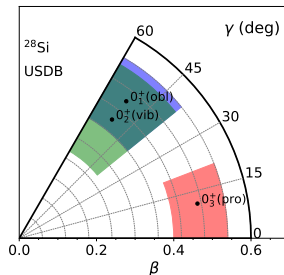
Conclusions

Conclusions:

- ▶ Shape coexistence is challenging to describe
- ▶ **Shape invariants provide a method to identify shapes**
- ▶ (β, γ) fluctuations are large
- ▶ **Extension of sum rule method for any J (up to $\langle Q^4 \rangle$)**
- ▶ **Deformation parameters are constant across the band**

Outlook:

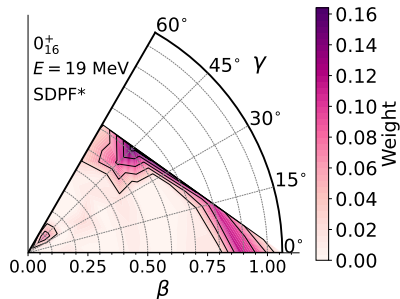
- ▶ Shape invariants for odd nuclei
- ▶ Study of $^{48\pm 1}\text{Cr}$
- ▶ Octupole shape invariants?



Full *sdpf* space calculation

- ▶ Full *sdpf* space
- ▶ Superdeformed state ($\beta \geq 0.6$)
- ▶ ~ 3 particles into the *pf* shell
- ▶ Energy: $E \approx 19$ MeV
- ▶ In agreement with the shell model calculation

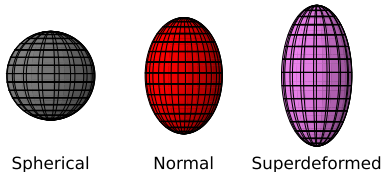
PGCM calculation in *sdpf* space
with SDPF-NR* interaction:



Fixed np - nh configurations

Analytical SU(3) models:

- sd -shell ($\beta \leq 0.5$)
- $sdpf$ space ($\beta \geq 0.5$)
SD for $\geq 4p$ - $4h$ ($\beta \approx 0.8$)

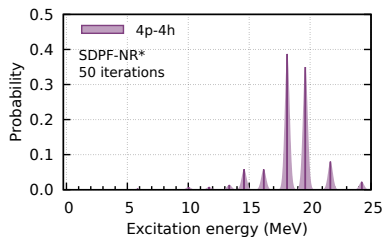
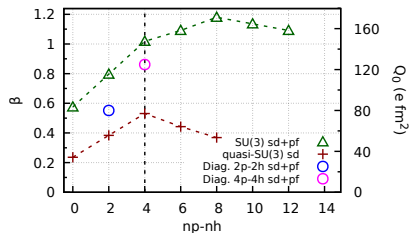


Lanczos strength function:

Decomposition of a fixed $4p$ - $4h$ configuration into the fully mixed states of the Hamiltonian:

$$|0_{np-nh}^+\rangle = \frac{1}{N} \sum_{\sigma} S(\sigma) |0_{\sigma}^+\rangle$$

Energies: $4p$ - $4h$ at 18-20 MeV



Exact diagonalization (ISM)

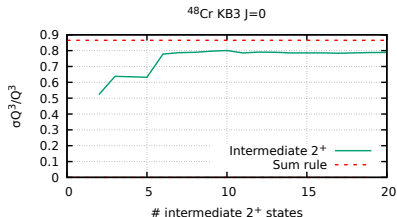
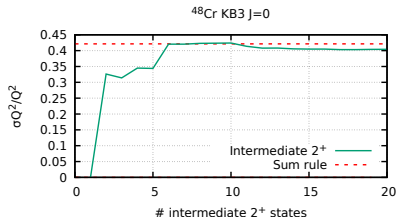
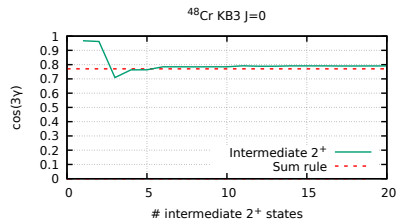
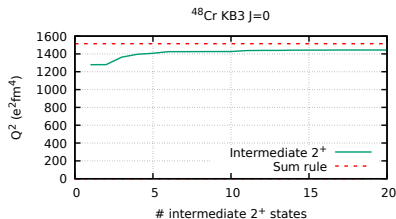
- **Most accurate solution** of $\mathcal{H}_{\text{eff}}|\Psi\rangle = E|\Psi\rangle$
- **Large set** of **simple Slater determinants**
 $|\Phi_i\rangle = c_{i1}^\dagger c_{i2}^\dagger \dots c_{iA}^\dagger |0\rangle$
- Best suited for **smaller valence spaces** (sd)
- Cannot explore a single **degree of freedom** ($Q_{\lambda\mu}$)

Beyond-mean-field (PGCM)

- **Approximate solution** to $\mathcal{H}_{\text{eff}}|\Psi\rangle = E|\Psi\rangle$
- **Smaller set** of more **complex wavefunctions** (HFB)
 $\beta_k^\dagger = \sum_l (U_{lk} c_l^\dagger + V_{lk} c_l)$
- Alternative for **large valence spaces** ($sdpf$)
- Exploration of relevant **degrees of freedom** ($Q_{\lambda\mu}$)

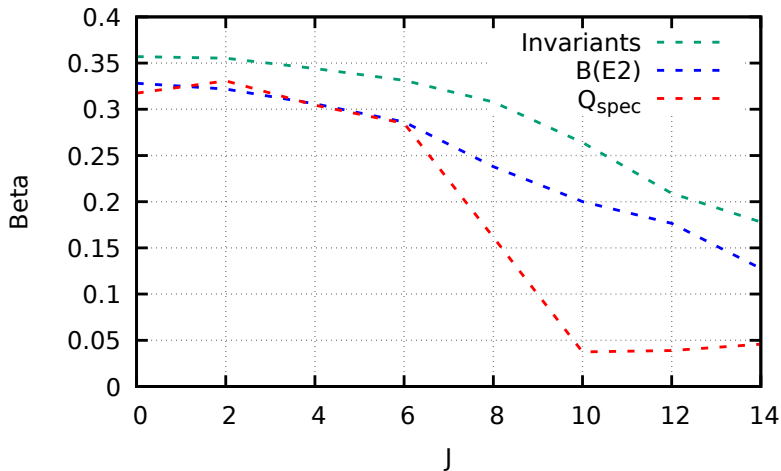
Convergence of $\langle Q^n \rangle$

A word of caution:

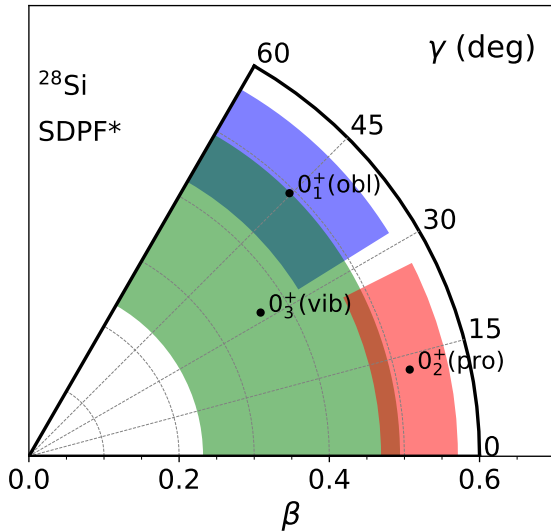


The convergence is worse for more complex nuclei and other J

Backbending ^{48}Cr



SDPF Si-28 invariants



Shape invariants