Shell-model study of ²⁸Si: Shape coexistence and superdeformation

Dorian Frycz

Universitat de Barcelona & Institut de Ciències del Cosmos

Collaborators: J. Menéndez, A. Rios,

B. Bally, T. R. Rodríguez & A. M. Romero



Institut de Ciències del Cosmos UNIVERSITAT DE BARCELONA







Shape coexistence in ²⁸Si

- Different shapes among states of the same nucleus within few MeV.
- Motivation for ²⁸Si (Z = N = 14):
 - Oblate ground state.
 - 2 Prolate structure (\sim 6 MeV).
 - Superdeformed structure? $(E \gtrsim 10 \text{ MeV})$

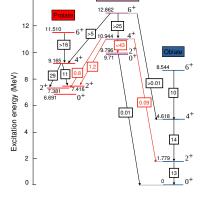
Taniguchi, Y., et al. Phys. Rev. C 80, 044316 (2009)



Oblate







Candidate SD

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

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

Interacting shell model

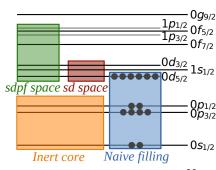
Schrödinger equation

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

- 28 Si: Z = N = 14 Slater determinant (spherical!)
- Interacting shell model: $\mathcal{H}_{\text{eff}} = \mathcal{H}_0 + \mathcal{H}_{\text{res}}$

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

- Slater determinant. basis $\{\Phi_i\}$
- Configuration mixing: $|\Psi_{\rm ISM}\rangle = \sum_i C_i |\Phi_i\rangle$



Valence space: $Z_v = N_v = 6$ (²⁸Si)

Inert core: 16O nucleus

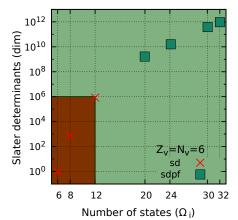
Exact diagonalization (ISM)

- **Diagonalization** of \mathcal{H}_{eff} : $\mathcal{H}_{\mathsf{eff}}|\Psi_{\mathsf{ISM}}\rangle = E|\Psi_{\mathsf{ISM}}\rangle$
- Slater determinants $|\Phi_i\rangle$:

$$\mathsf{dim} = \begin{pmatrix} \Omega_Z \\ Z_\nu \end{pmatrix} \begin{pmatrix} \Omega_N \\ N_\nu \end{pmatrix}$$

- ANTOINE: shell model code E. Caurier and F. Nowacki, Acta Phys. Pol. B 30, 705 (1999).
- Lanczos method

sd $(dim=10^6)$: easily computable $sdpf (dim=10^{12})$: beyond our capability



Variational method

Exact diagonalization

- Most accurate solution of $\mathcal{H}_{eff}|\Psi\rangle=E|\Psi\rangle$
- 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 $(Q_{\lambda\mu})$

Variational method

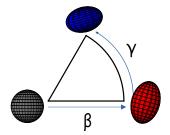
- Approximate solution to $\mathcal{H}_{\text{eff}}|\Psi\rangle=E|\Psi\rangle$
- Smaller set of more complex wavefunctions (HFB) $\beta_k^{\dagger} = \sum_l (U_{lk}c_l^{\dagger} + V_{lk}c_l)$ HFB:Hartree-Fock-Bogoliubov
- Alternative for large valence spaces (sdpf)
- Exploration of relevant degrees of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

Ground state (Mean field)

• Quadrupole-constrained HFB basis $|\phi(q)\rangle$:

$$\mathcal{H}_{\mathsf{eff}}' = \mathcal{H}_{\mathsf{eff}} - \lambda \sum_{\mu} {\mathsf{Q}_{\mathsf{2},\mu}}$$

• (β, γ) parameters:

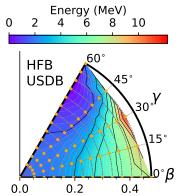


• TAURUS_{vap} code

B. Bally, et al. Eur. Phys. J. A 57, 69 (2021)

 $Z_{\rm v}=N_{\rm v}=6$ USDB interaction[†]

[†]W. A. Richter, et al. Phys. Rev. C **78**, 064302 (2008)



Oblate minimum ($\beta \approx -0.4$)

Ground state (Beyond mean field)

Mean field:

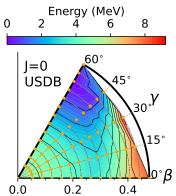
• Quadrupole-constrained HFB basis $|\phi(q)\rangle$: $\mathcal{H}'_{eff} = \mathcal{H}_{eff} - \lambda \sum_{\mu} Q_{2,\mu}$

Beyond mean field:

- Symmetry restoration $|\phi^{NZJ}\rangle = P^N P^Z P_{MK}^J |\phi\rangle$
- Configuration mixing of projected states (PGCM) $|\Psi_{\text{GCM}}\rangle = \sum_{q} f_{q} |\phi^{NZJ}(q)\rangle$ GCM: generator coordinate method
- TAURUS_{pav,mix} codes
 B. Bally, et al. Eur. Phys. J. A 60, 62 (2024)

 $Z_{\nu} = N_{\nu} = 6$ USDB interaction[†]

 † W. A. Richter, et al. Phys. Rev. C **78**, 064302 (2008)



Oblate minimum ($\beta \approx -0.4$)

Spectrum of ²⁸Si (USDB)

Oblate rotational band: well described, slightly more deformed

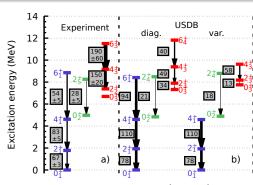
Vibrational band based on the ground state is also well described

Prolate rotational band has too weak B(E2)

D. Frycz, J. Menéndez, A. Rios, B. Bally,

T. R. Rodríguez and A. M. Romero,

[arXiv:2404.14506 [nucl-th]]



Experiment vs Theory (USDB):

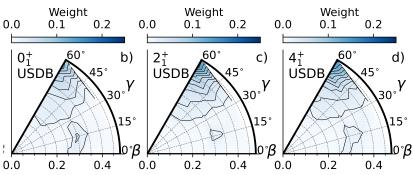
$$B(E2, 2_{\text{obl}}^+ \rightarrow 0_{\text{obl}}^+) = 67 \pm 3 \text{ vs } 78 \text{ e}^2 \text{fm}^4$$

$$B(E2, 2_{\text{vib}}^+ \rightarrow 0_{\text{vib}}^+) = 28 \pm 5 \text{ vs } 21 \text{ e}^2 \text{fm}^4$$

$$B(E2, 4_{\text{pro}}^+ \rightarrow 2_{\text{pro}}^+) = 150 \pm 20 \text{ vs } 50 \text{ } e^2 \text{fm}^4$$

Oblate rotational band (USDB)

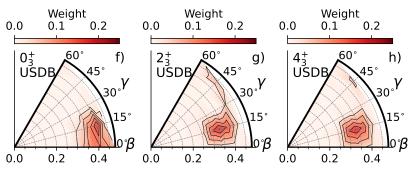
Collective wavefunctions: weight of each wf in the mixed state



- Shared intrinsic deformation ($\beta \approx -0.45$)
- Rotational band behaviour:
 - $E \sim J(J+1)$ and **strong** B(E2): 67 ± 3 vs $78 e^2$ fm⁴
- D. Frycz, J. Menéndez, A. Rios, B. Bally, T. R. Rodríguez and A. M. Romero, [arXiv:2404.14506 [nucl-th]]

Prolate rotational band (USDB)

Collective wavefunctions: weight of each w.f. in the mixed state

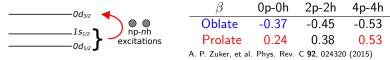


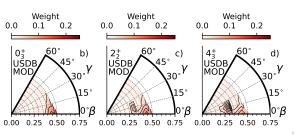
- Different deformation patterns
- Reduced deformation for J=2 and J=4 ($\beta\approx0.35$)
- Weak B(E2) transition strengths: 150 ± 20 vs $50 e^2$ fm⁴
- D. Frycz, J. Menéndez, A. Rios, B. Bally, T. R. Rodríguez and A. M. Romero, [arXiv:2404.14506 [nucl-th]]

Modification of the interaction

Energy competition in quasi-SU(3): $\mathcal{H} = \mathcal{H}_0 - \kappa \beta^2$

- Gains energy with deformation but looses with excitations
- Prolate band: excitations from $d_{5/2} + s_{1/2}$ to $d_{3/2}$



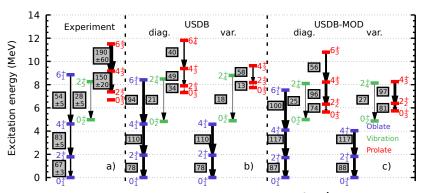


USDB-MOD

Single particle energy $d_{3/2}$ from:

5 MeV → 3.5 MeV

Spectrum of ²⁸Si (USDB-MOD)



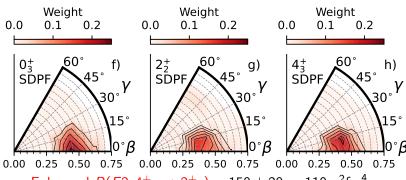
Stronger $B(E2, 4^+_{pro} \rightarrow 2^+_{pro}) = 150 \pm 20 \text{ vs } 96 \text{ } e^2\text{fm}^4$ Oblate and vibrational bands remain unperturbed (0p-0h)

D. Frycz, J. Menéndez, A. Rios, B. Bally, T. R. Rodríguez and A. M. Romero, [arXiv:2404.14506 [nucl-th]]



sdpf valence space

- The SDPF-NR[†] interaction (*sdpf* space) **naturally** reproduces the prolate rotational band. †S. Nummela Phys. Rev. C **63**, 044316 (2001)
- Enhanced collectivity from the pf shell
- **0.57 particles** in *pf* shell: 24% of *sdpf* 2p-2h contribution

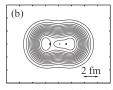


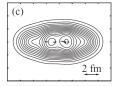
• Enhanced $B(E2, 4_{pro}^+ \rightarrow 2_{pro}^+) = 150 \pm 20 \text{ vs } 110 \text{ e}^2 \text{fm}^4$

Superdeformation

Superdeformed (SD) band predicted with:

- Deformation: $\beta \approx 1$
- 4p-4h into pf shell
- ullet ~ 13 MeV bandhead

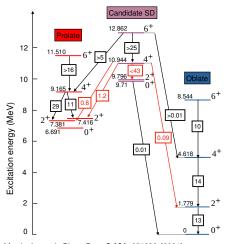




Taniguchi, Y., et al. Physical Review C, 2009. 80, 044316

Experimental attempts

- $B(E2, 4^+ \rightarrow 2^+) \le 217 \text{efm}^2$
- Not found: $\beta_{exp} \leq 0.6$ Morris, L. et al. Phys. Rev. C 104, 054323 (2021)



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

Fixed *n*p-*n*h configurations

Analytical SU(3) models:

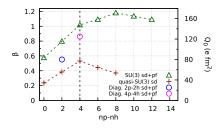
- sd-shell ($\beta \leq 0.5$)
- sdpf space $(\beta \ge 0.5)$ SD for $\ge 4p-4h$ $(\beta \approx 0.8)$

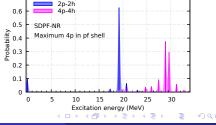
Lanczos strength function:

Decomposition of a fixed *np-nh* configuration into the fully mixed states of the Hamitonian:

$$|0^{+}_{n extsf{p-}n extsf{h}}
angle = rac{1}{N}\sum_{\sigma}S(\sigma)|0^{+}_{\sigma}
angle$$

Truncation: maximum of 4p-4h into pf shell (Dimension: $9 \cdot 10^9$) **Energies**: 2p-2h at 19 MeV and 4p-4h at **30** MeV!!!





Full sdpf space

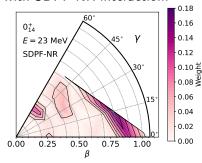
- Full sdpf space
- Superdeformed state $(\beta \approx 0.75)$
- \sim **3.7 particles** into the *pf* shell
- Energy: $E \approx 23 \text{ MeV}$
- Not compatible with SD state E ≤ 20 MeV



Normal

Superdeformed

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



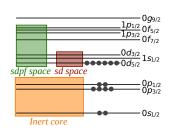
Conclusions

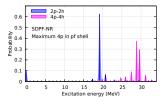
Shape coexistence of **structures** within the *sd* shell or *sdpf*

- Exact diagonalization and variational method (PGCM)
- USDB interaction describes oblate band
- USDB-MOD or SDPF-NR is needed for prolate band

Superdeformed structures **disfavoured** at low energies ($E \le 20 \text{ MeV}$)

Preprint: D. Frycz, J. Menéndez, A. Rios, B. Bally, T. R. Rodríguez and A. M. Romero, [arXiv:2404.14506 [nucl-th]]





Outlook

sdpf shell gap:

²⁸Si negative parity states

Ab initio interaction:

Valence space in-medium renormalization grop

Stroberg, S. Ragnar, et al. Ann. Rev. Nucl. Part. Sci. **69**, 307 (2019)

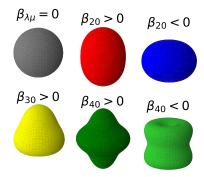
Shape coexistence and SD:

- N = Z: ³²S, ²⁴Mg...
- Neutron-rich: ^{30–42}Si
- E0 transitions

Multipole deformations:

•
$$\beta_4(^{28}Si) = 0.03 \pm 0.01$$

Y. K. Gupta et al., Phys. Lett. B 845, 138120 (2023)



SU(3) model

- Quadrupole interactions: realistic Hamiltonians
- Restriction to a major shell (Fermi surface)

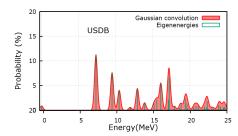
$$\frac{-1 d3/2 - (4)}{2s} = \frac{1 d5/2 - (6)}{1 d5/2}$$

- Energy **competition**: $\mathcal{H} = \mathcal{H}_0 \kappa Q_0^2$
 - Correlation energy decreases as Q_0^2
 - Single particle energy increases with promoted particles (from $d_{5/2}$ to $s_{1/2}$ or $d_{3/2}$)
- Intrinsic quadrupole moment Q_0 :
 - Spherical: $Q_0 = 0$
 - Prolate: $Q_0 > 0$
 - Oblate: $Q_0 < 0$

Elliott, J. P. Proc R Soc Lon Ser-A, 1958. 245, 128.

Modification of the interaction

- The prolate 4p-4h is lost in configuration mixing
- $|4p4h\rangle = \sum_{i} c_{i} |\Psi\rangle_{i,\text{full sd}} \rightarrow$
- USDB: prolate band only has 10% of $|4p4h\rangle$



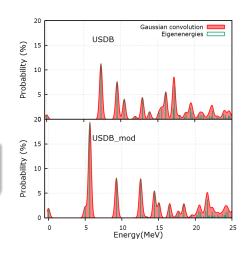
Modification of the interaction

- The prolate 4p-4h is lost in configuration mixing
- $|4p4h\rangle = \sum_{i} c_{i} |\Psi\rangle_{i,\text{full sd}} \rightarrow$
- USDB: prolate band only has 10% of $|4p4h\rangle$

Too high single-particle energies

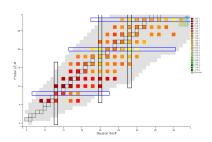
Gap between $d_{5/2}+s_{1/2}$ and $d_{3/2}$ 5 MeV ightarrow 3.6 MeV

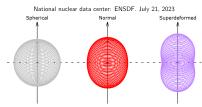
 4p-4h concentrated in 0₃⁺: now goes up to 20%



Objectives

- Why are some nuclei deformed?
 - Magic nuclei are spherical
 - Most nuclei are deformed
- What kind of deformation?
 - Quadrupole deformations
- Will they be prolate or oblate?
 - Axial symmetry
- Can different shapes coexist?
 - Spherical, prolate and oblate
- How much deformation?
 - Normal deformation (3:2 ratio)
 - Superdeformation (2:1 ratio)





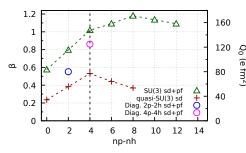
Fixed *np-nh* configurations

Analytical SU(3) models:

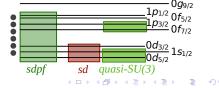
- sd-shell deformations: $\beta \le 0.5$; $Q_0 \le 80 \text{ efm}^2$ too low for SD!
- sdpf space deformations: $\beta \ge 0.5$; $Q_0 \ge 80 \text{ efm}^2$ SD for $\ge 4\text{p-4h}$

Numerical calculations:

 Shell model np-nh: Similar to quasi-SU(3) sdpf

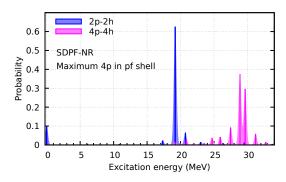


 β parameters for SU(3) schemes and nuclear shell model np-nh configurations



Lanczos strength functions

Decomposition of a fixed np-nh configuration into the fully mixed states of the Hamitonian: $|0_{np-nh}^+\rangle_{sdpf} = \frac{1}{N}\sum_{\sigma}S(\sigma)|0_{\sigma}^+\rangle_{sdpf}$ **Truncation**: maximum of 4 particles into *pf* shell (**dimensions!**)



Energies: 2p-2h at 19 MeV and 4p-4h at 30 MeV!!!

Lanczos algorithm

- ullet Initial state: |1
 angle
- Next step: $E_{12}|2\rangle = (H E_{11})|1\rangle$
- Then: $E_{23}|3\rangle = (H E_{22})|2\rangle E_{12}|1\rangle$
- Generalizing: $E_{NN+1}|N+1\rangle = (H-E_{NN})|N\rangle E_{N-1N}|N-1\rangle$

Where: $E_{NN} = \langle N|H|N\rangle$

$$\left(\begin{array}{ccc} E_{11} & E_{12} & 0 \\ E_{12} & E_{22} & E_{23} \\ 0 & E_{23} & E_{33} \end{array}\right),$$

Finally, diagonalize and check convergence

Projected generator coordinate method (PGCM)

Variational approach:

 Configuration mixing of Hartree-Fock-Bogoliubov (HFB) states:

$$|\Psi_{\mathsf{GCM}}\rangle = \sum_{q} f_{q} |\phi_{\mathsf{HFB}}(q)\rangle$$

B. Bally, et al. Eur. Phys. J. A $\mathbf{60}$, 62 (2024)

- Similar deformations for all interactions
- $2\nu\beta\beta$ matrix elements are larger for similar deformations

T. R. Rodríguez and G. Martínez-Pinedo

Phys. Rev. C 85, 044310 (2012)

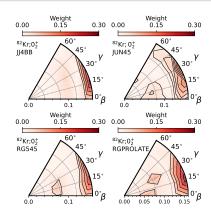


Figure: Contribution of each HFB wavefunction to fully mixed state for 82 Kr (0_2^+) with all interactions.