Nuclear structure studies using beyond-mean-field approaches

Tomás R. Rodríguez

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GSI-Darmstadt

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Acknowledgments

With the work of…

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Adrián Sánchez-Fernandez (U. York)

Vimal Vijayan (GSI)

J. Luis Egido / Marta Borrajo (UAM)

Kamila Sieja (Strasbourg)

Outline

1. Introduction

2. Projected Generator Coordinate Method

3. Multiple shape-coexistence in ^{80}Zr

4. Variational methods in valence spaces

5. Summary

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Nuclear many-body problem(s)

The nuclear many-body problem is…

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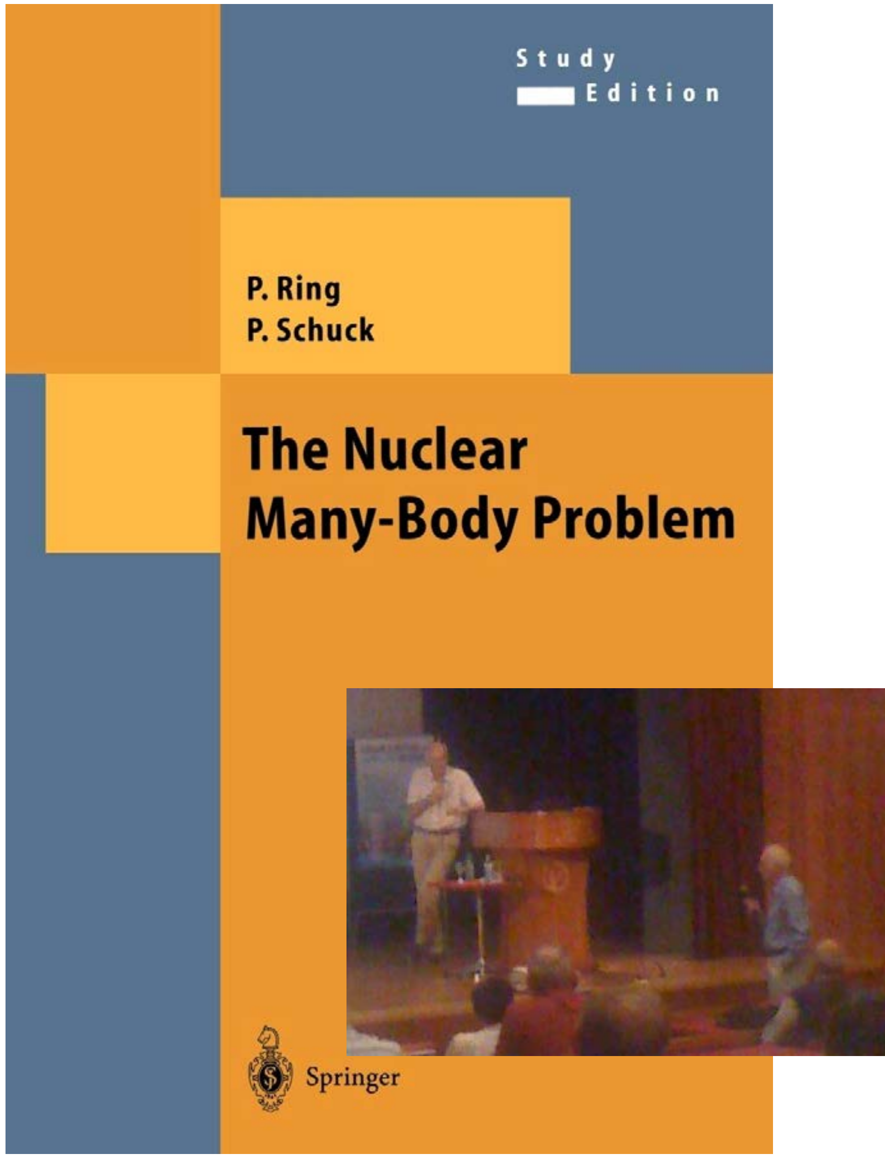

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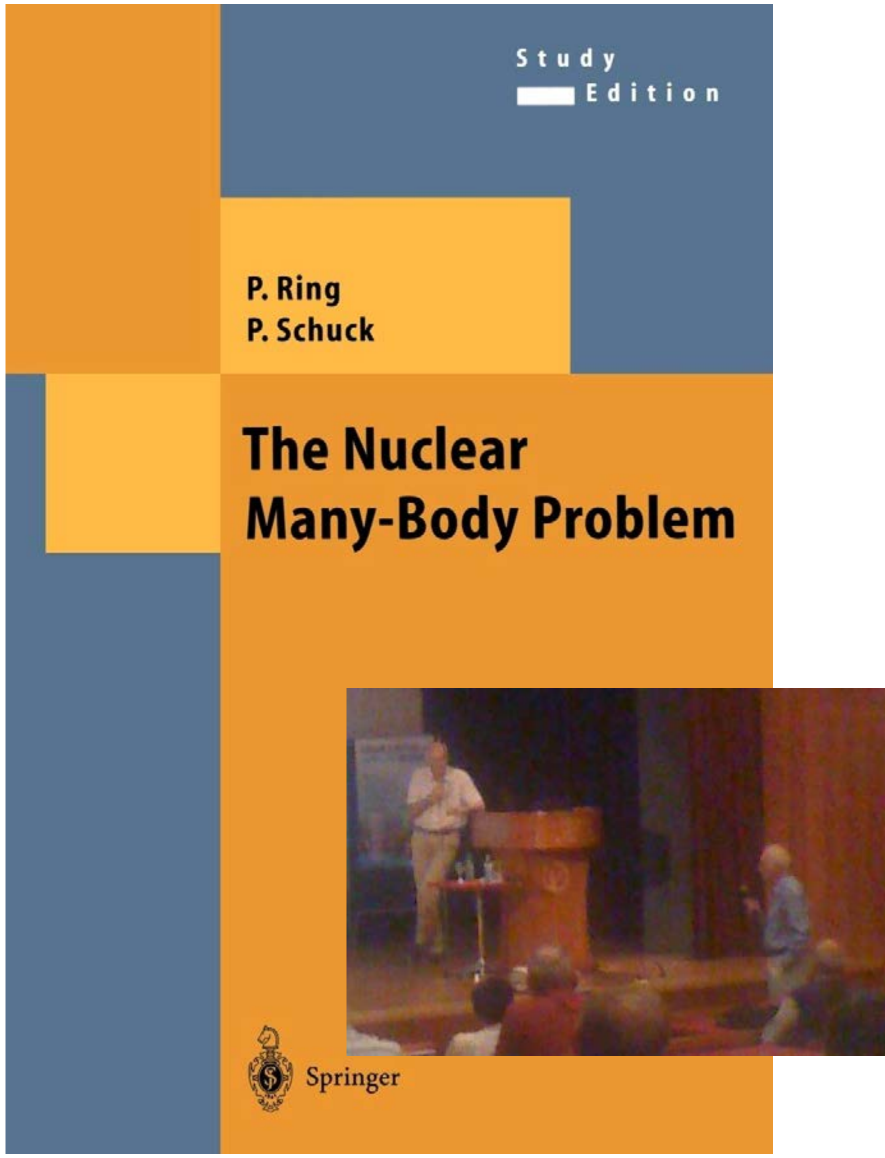

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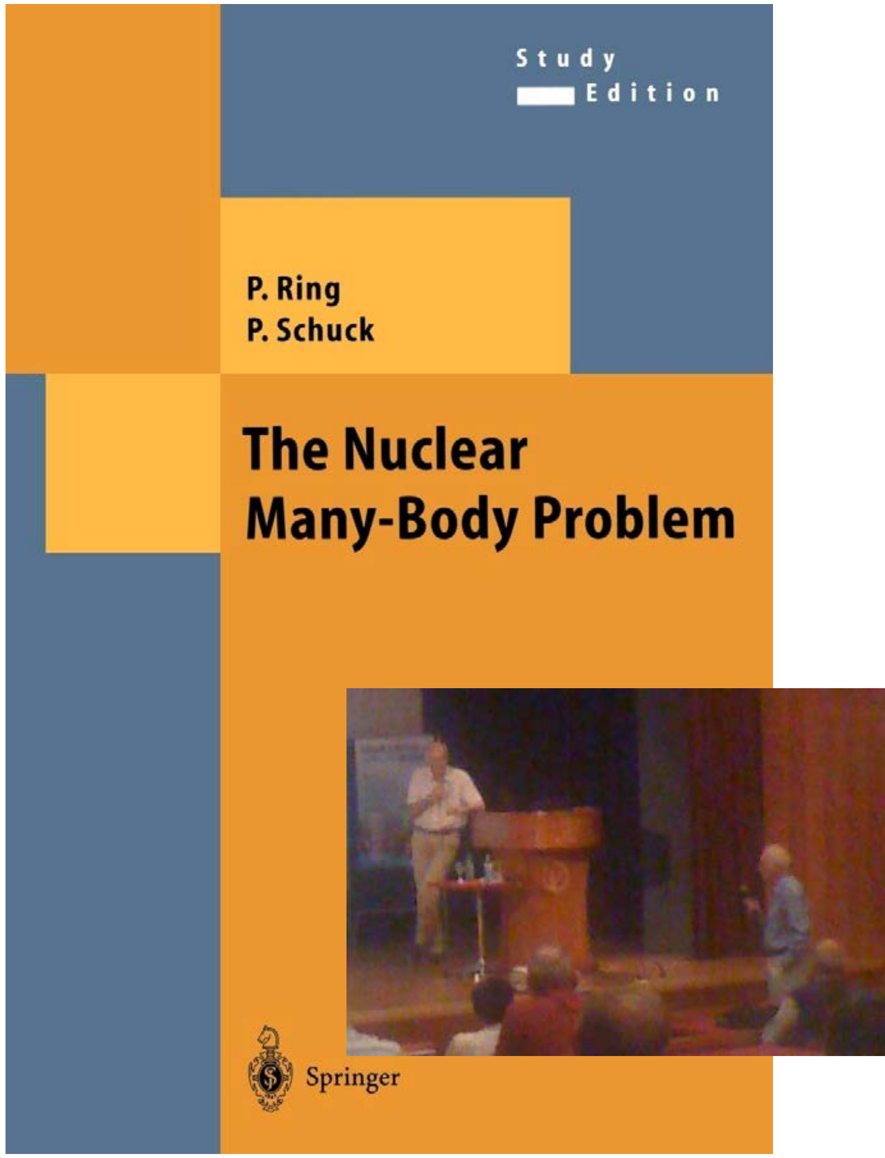
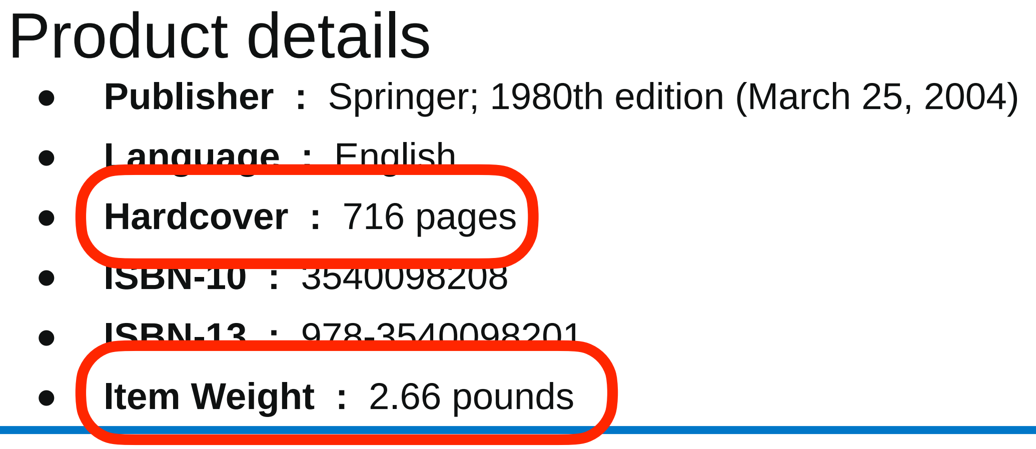


Study Edition

P. Ring
P. Schuck

The Nuclear Many-Body Problem

Springer



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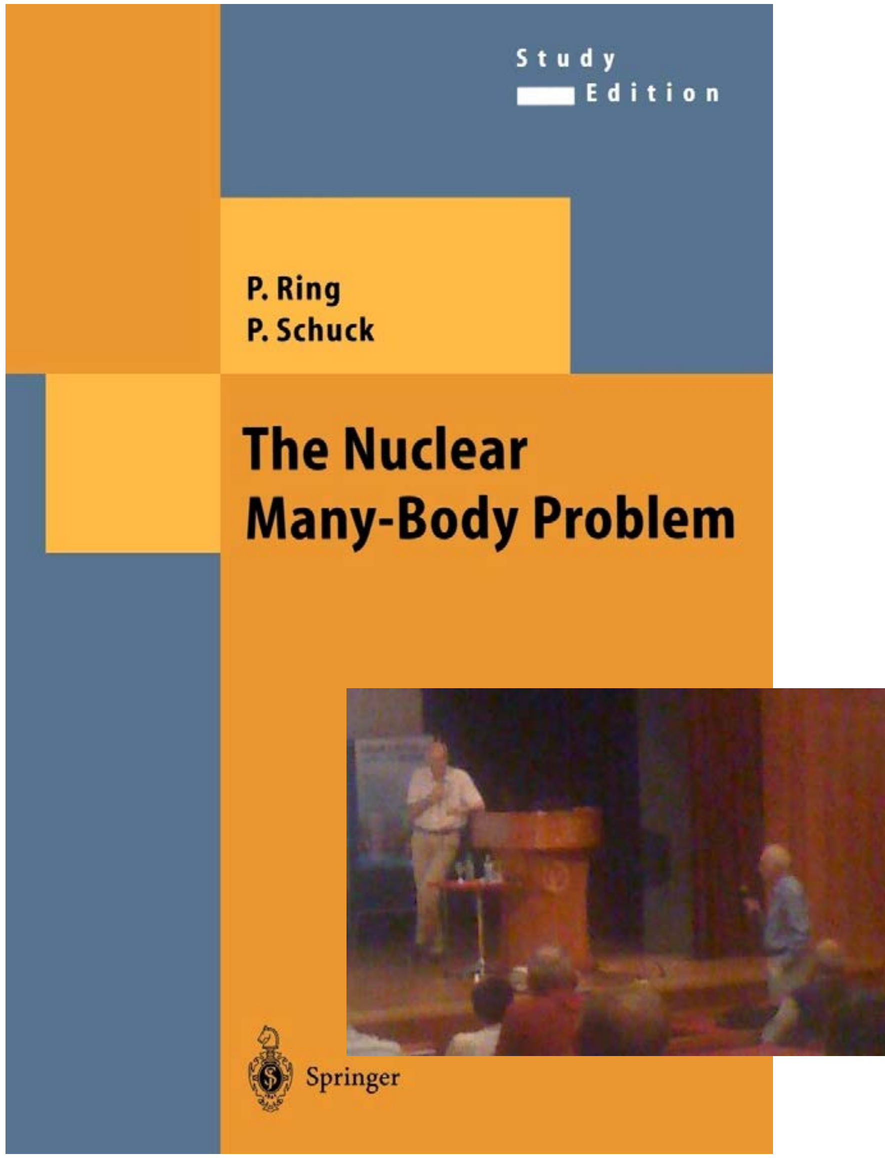
We rely on models!



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Amazing progress in ***ab initio*** **methods** in recent years

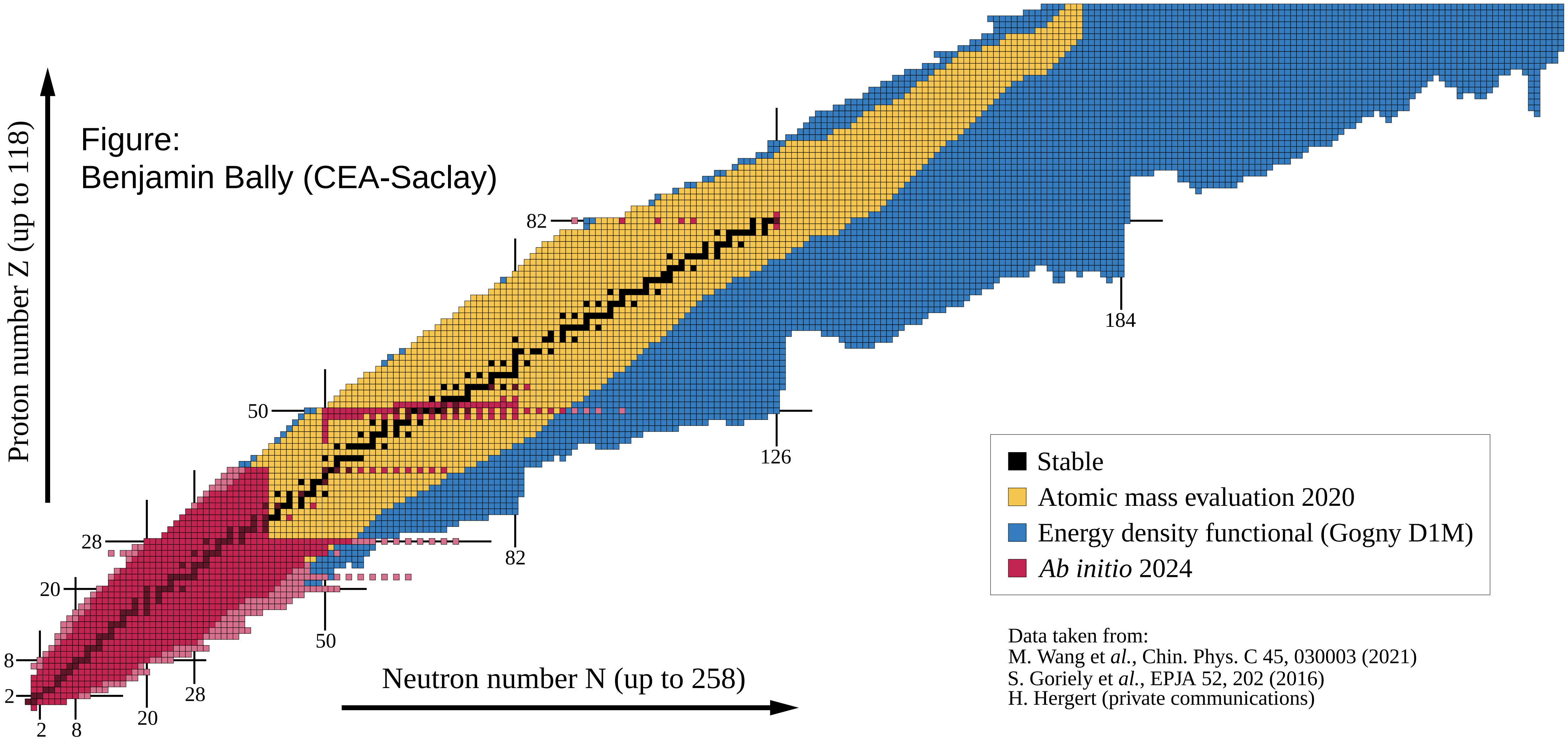

Figure:
Benjamin Bally (CEA-Saclay)

Data taken from:
M. Wang et *al.*, Chin. Phys. C 45, 030003 (2021)
S. Goriely et *al.*, EPJA 52, 202 (2016)
H. Hergert (private communications)

Nuclear many-body problem(s)

Amazing progress in ***ab initio* methods** in recent years

- Nuclear interactions based on χEFT (QCD-inspired) fitted (supposedly) to NN+NNN data.

- Systematically improvable.

- Systematic error assessment.

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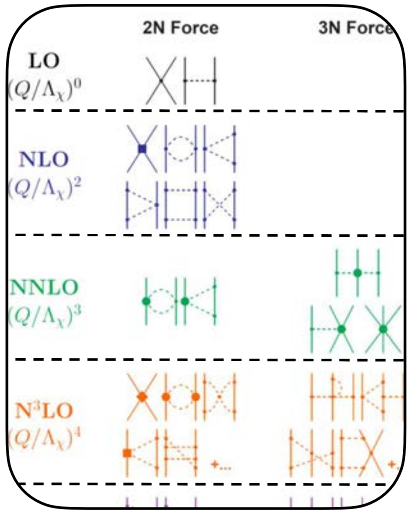

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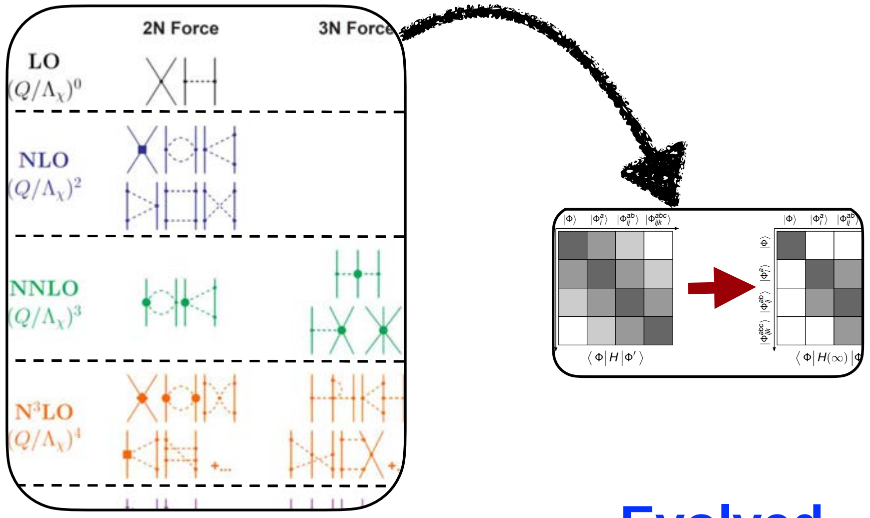

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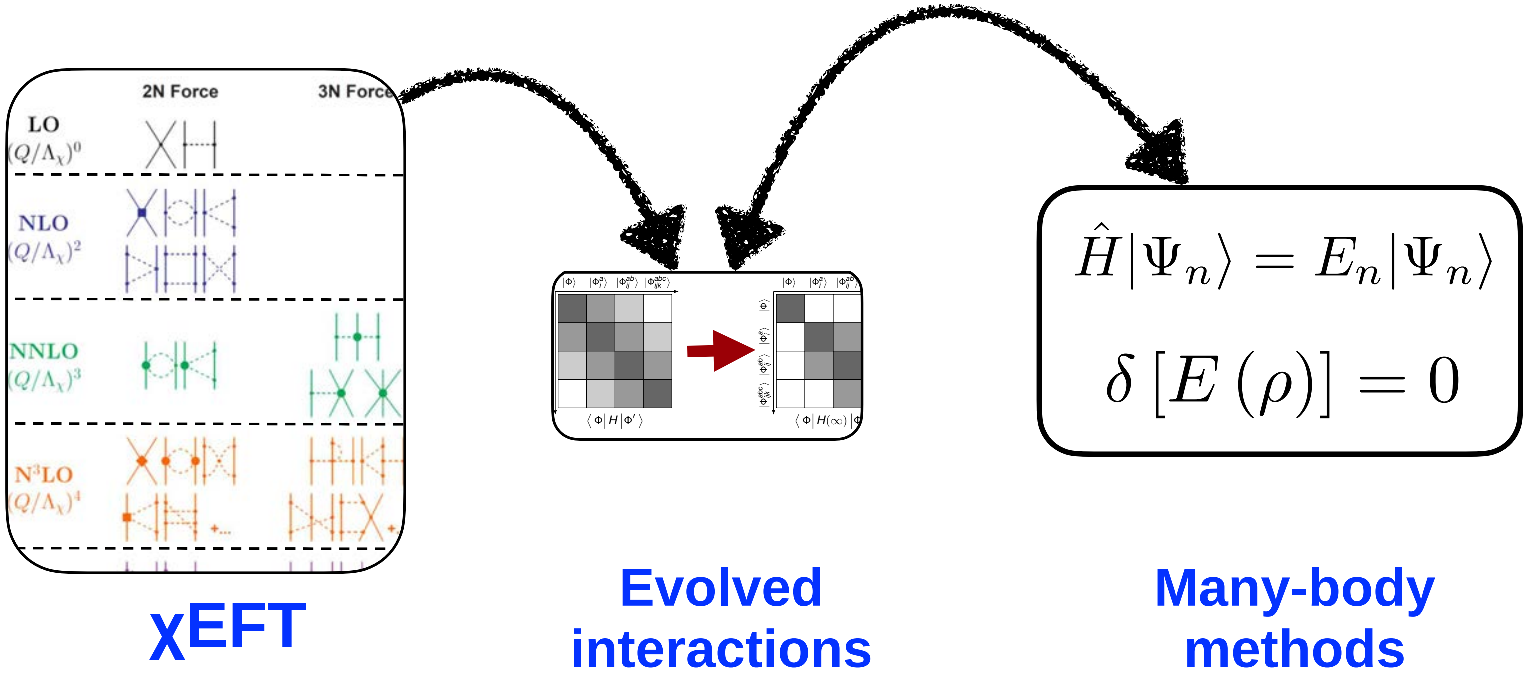

$$\hat{H}|\Psi_n\rangle = E_n|\Psi_n\rangle$$

$$\delta\left[E\left(\rho\right)\right] = 0$$

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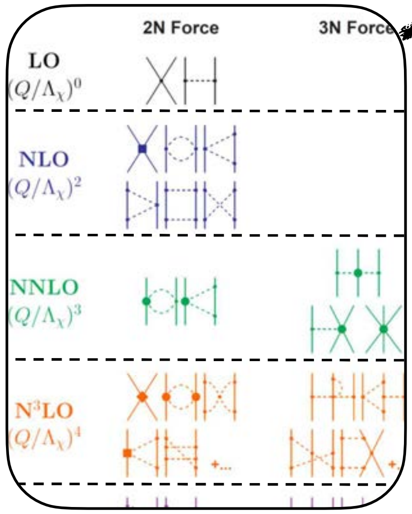

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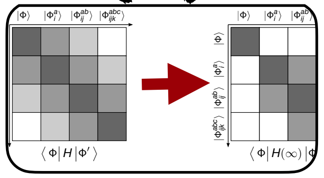

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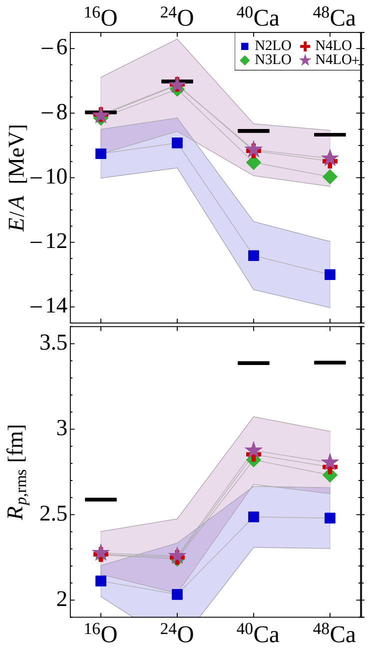
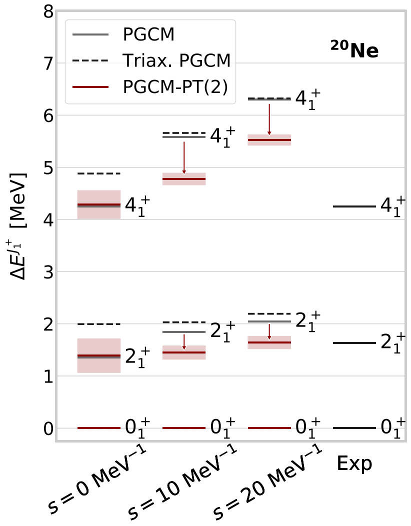


PRC 106, 064002 (2022)



EPJA 58, 63 (2022)

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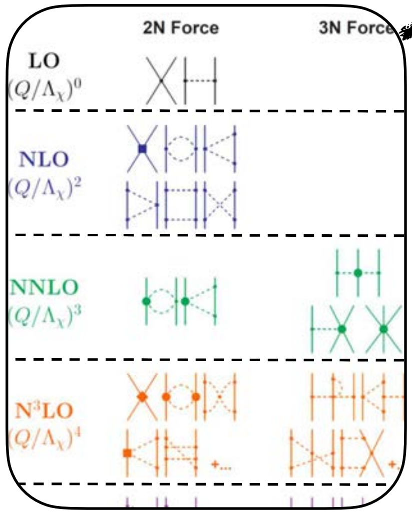

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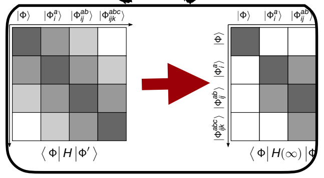

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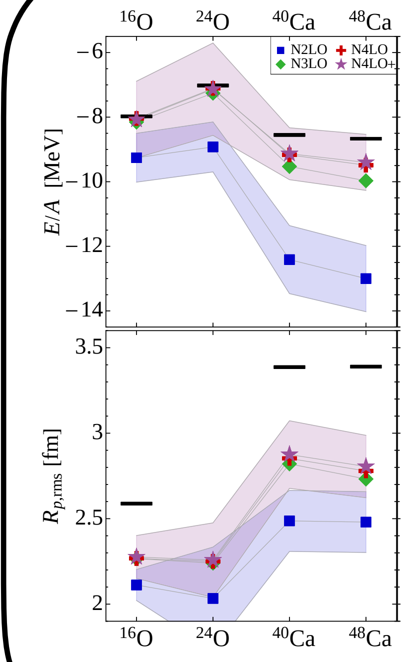

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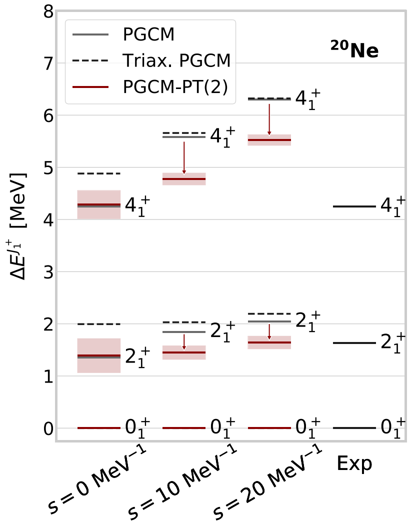

EPJA 58, 63 (2022)

Results

- Still large uncertainties.

- Plethora of nuclear interactions (including phenomenological adjustments).

- Similar or more limitations than the many-body methods that use phenomenological interactions.

Nuclear many-body problem(s)

Nuclear theory with **phenomenological interactions** is still in good shape

- Single-particle energies and interaction matrix elements with phenomenological adjustments.

- Parameters of the interaction fitted to experimental data.

- (Systematically) improvable.

- Large range of applicability and a wide catalog of observables and pseudo-observables.

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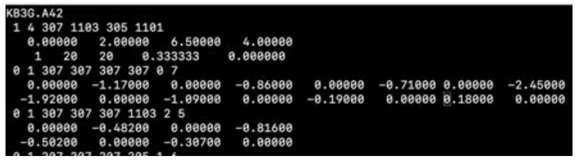

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  -1.92000   0.00000  -1.09000   0.00000  -0.19000   0.00000 0.18000   0.00000
 0 1 307 307 307 1103 2 5
   0.00000  -0.48200   0.00000  -0.81600
  -0.50200   0.00000  -0.30700   0.00000
```

$$v(1,2) = v_c(1,2) + v_{\mathrm{LS}}(1,2) + v_{\mathrm{DD}}(1,2) + v_{\mathrm{Coul}}(1,2)$$

$$v_c(1,2) = \sum_{i=1,2} \mathrm{e}^{-\frac{|\vec{r}_1-\vec{r}_2|^2}{\mu_i^2}} (W_i + B_i P_\sigma - H_i P_\tau - M_i P_\sigma P_\tau).$$

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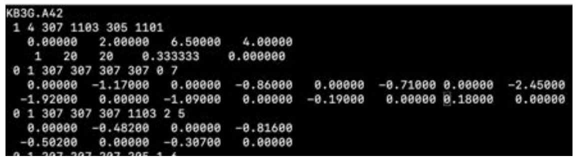

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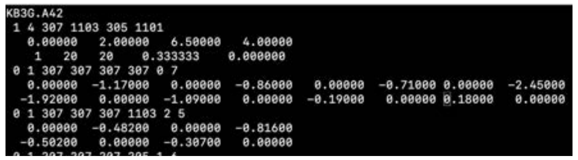

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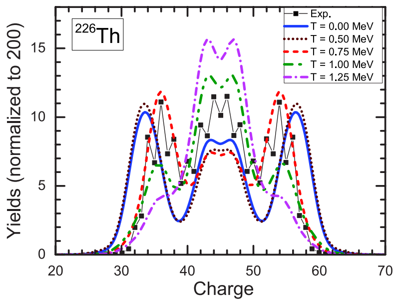
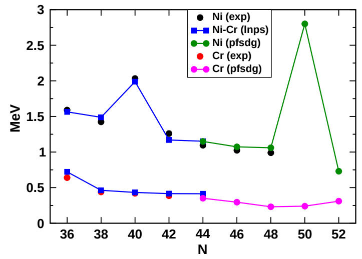
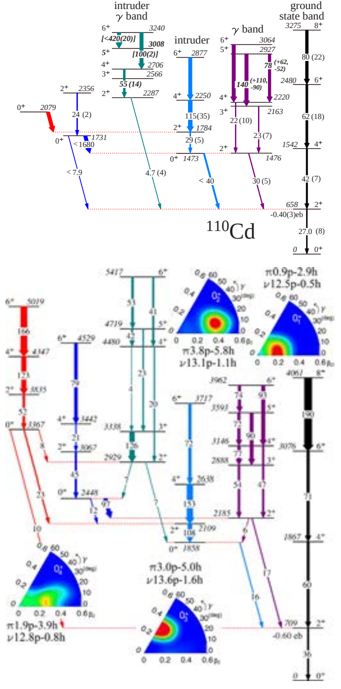


PRC 99, 014618 (2019)



PRL 117, 272501 (2016)



PRL 123, 142502 (2019)

Results

Nuclear many-body problem(s)

Let us assume that *we know* the nuclear interaction. Exact nuclear wave functions and energies cannot be obtained in general because of:

a) the exploding dimensionality of the many-body Hilbert space

b) the huge amount of two-, three- (eventually, *N*-) body matrix elements that are impossible to store

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Nuclear wave functions: Generator Coordinate Method (GCM) ansatz

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Intrinsic (HFB-like, Bogoliubov quasiparticle vacuum) state:

$$|\Phi(q)\rangle \rightarrow \beta_{b}(q)|\Phi(q)\rangle = 0 \;\; \forall \;\; b \qquad \beta_{b}^{\dagger}(q) = \sum_{a} U_{ab}(q) c_{a}^{\dagger} + V_{ab}(q) c_{a}$$

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variational!

We minimize the particle number projected energy functional

even-even

$$E'_{\mathrm{PNVAP}}\left[|\Phi(q)\rangle\right] = \frac{\langle\Phi(q)|\hat{H}P^{N}P^{Z}|\Phi(q)\rangle}{\langle\Phi(q)|P^{N}P^{Z}|\Phi(q)\rangle} - \langle\Phi(q)|\lambda_q\hat{Q}|\Phi(q)\rangle$$

M. Anguiano, J. L. Egido, and L. M. Robledo, Nucl. Phys. A 696, 467 (2001).

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$$E'_{\mathrm{PNVAP}}\left[|\Phi(q)\rangle\right] = \frac{\langle\Phi(q)|\hat{H}P^{N}P^{Z}|\Phi(q)\rangle}{\langle\Phi(q)|P^{N}P^{Z}|\Phi(q)\rangle} - \langle\Phi(q)|\lambda_q\hat{Q}|\Phi(q)\rangle$$

M. Anguiano, J. L. Egido, and L. M. Robledo, Nucl. Phys. A 696, 467 (2001).

Constraints $q \longrightarrow$ quadrupole deformations; octupole deformations; pairing content; intrinsic rotations

Theoretical framework

Nuclear wave functions: Generator Coordinate Method (GCM) ansatz

$$|\Psi_{\sigma}^{JMNZ\pi}\rangle = \sum_{qK} f_{\sigma;qK}^{JMNZ\pi} P^{J}_{MK} P^{N} P^{Z} P^{\pi} \boxed{|\Phi(q)\rangle}$$

$$\Gamma \equiv (JMNZ\pi)$$

“basis” states

Intrinsic (HFB-like, Bogoliubov quasiparticle vacuum) state:

$$|\Phi(q)\rangle \rightarrow \beta_b(q)|\Phi(q)\rangle = 0 \;\; \forall \;\; b \qquad \beta_b^{\dagger}(q) = \sum_a U_{ab}(q) c_a^{\dagger} + V_{ab}(q) c_a$$

variational!

We minimize the particle number projected energy functional

even-even

$$E'_{\mathrm{PNVAP}}\left[|\Phi(q)\rangle\right] = \frac{\langle\Phi(q)|\hat{H}P^{N}P^{Z}|\Phi(q)\rangle}{\langle\Phi(q)|P^{N}P^{Z}|\Phi(q)\rangle} - \langle\Phi(q)|\lambda_q \hat{Q}|\Phi(q)\rangle$$

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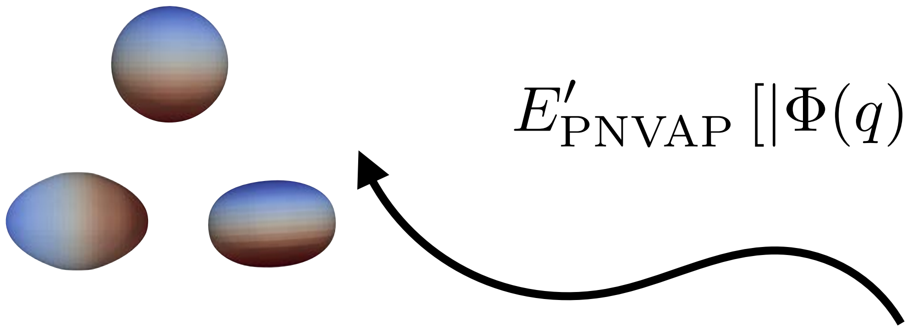

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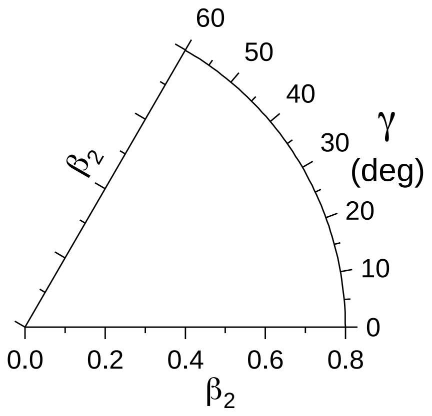

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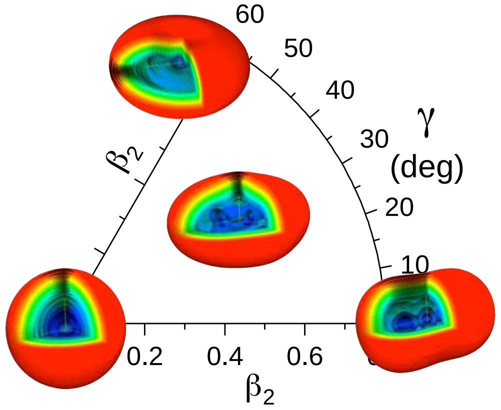

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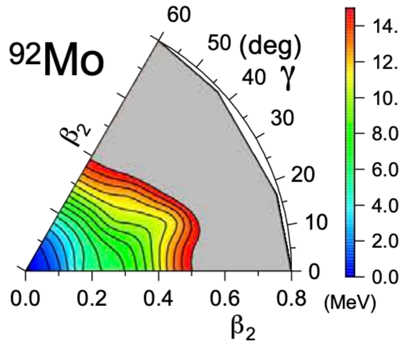
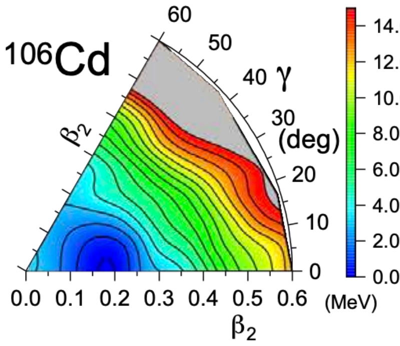
Intrinsic (HFB-like, Bogoliubov quasiparticle vacuum) state:

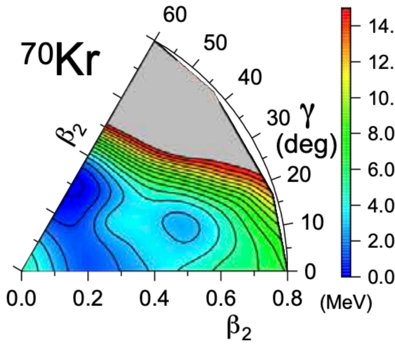
Spherical



Axial prolate



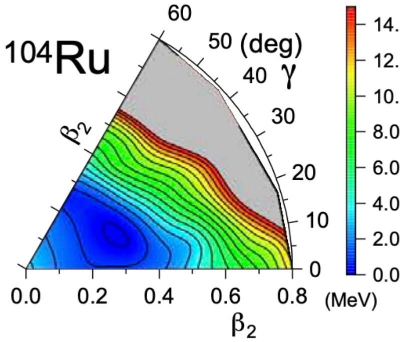
Axial oblate



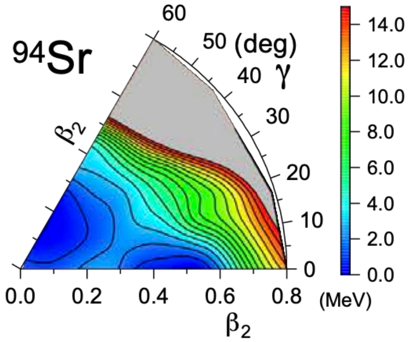
- First classification of the collective quadrupole behavior of the nucleus based on the **total energy surfaces** (**TESs**)

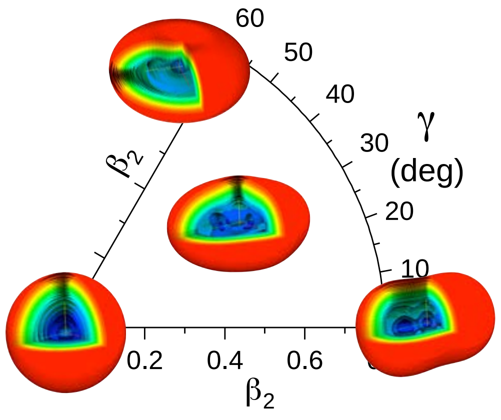
- Final theoretical interpretation of the spectrum is given by the analysis of the excitation energies, electromagnetic properties and the collective wave functions

Triaxial / γ-soft



Shape-coexistence





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"basis" states

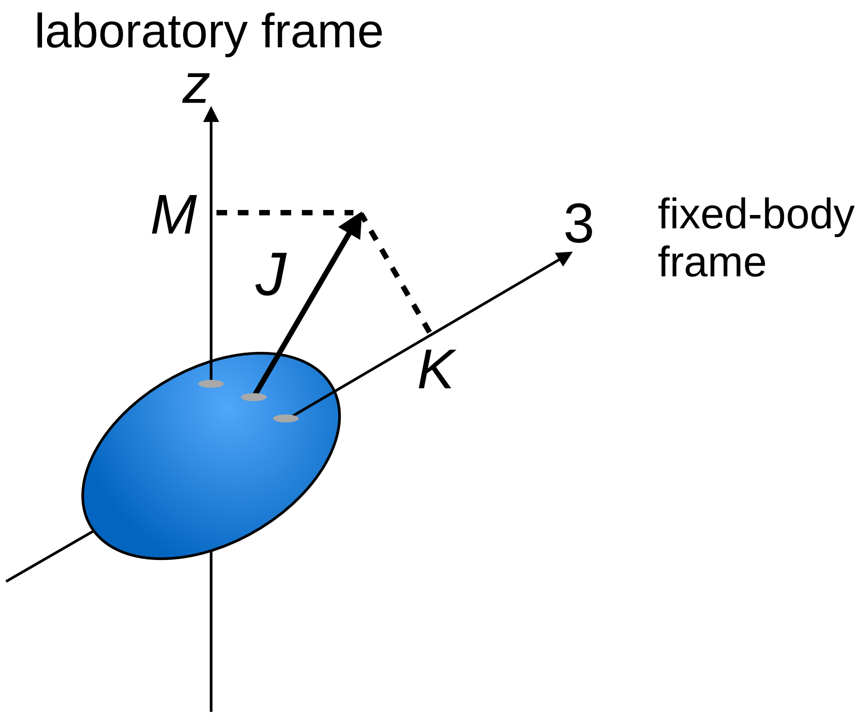
Symmetry restoration

P_{MK}^{J} $\longrightarrow$ angular momentum projector

P^{N} $\longrightarrow$ neutron number projector

P^{Z} $\longrightarrow$ proton number projector

P^{π} $\longrightarrow$ spatial parity projector



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$$\Gamma \equiv (JMNZ\pi)$$

coefficients of the linear combination

The coefficients are obtained by minimizing the expectation value of the Hamiltonian (energy) with those coefficients as the variational parameters:

$$\sum_{q'K'} \left(\mathcal{H}_{qK,q'K'}^{\Gamma} - E_{\sigma}^{\Gamma}\mathcal{N}_{qK,q'K'}^{\Gamma}\right) f_{\sigma;q'K'}^{\Gamma} = 0$$

Hill-Wheeler-Griffin (HWG) equation

$$\mathcal{H}_{qK,q'K'}^{\Gamma} = \langle\Phi(q)|\hat{H} P_{KK'}^{J} P^{N} P^{Z} P^{\pi}|\Phi(q')\rangle,$$
$$\mathcal{N}_{qK;q'K'}^{\Gamma} = \langle\Phi(q)|P_{KK'}^{J} P^{N} P^{Z} P^{\pi}|\Phi(q')\rangle$$

Hamiltonian and norm kernels

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Hamiltonian and norm kernels

movie reality

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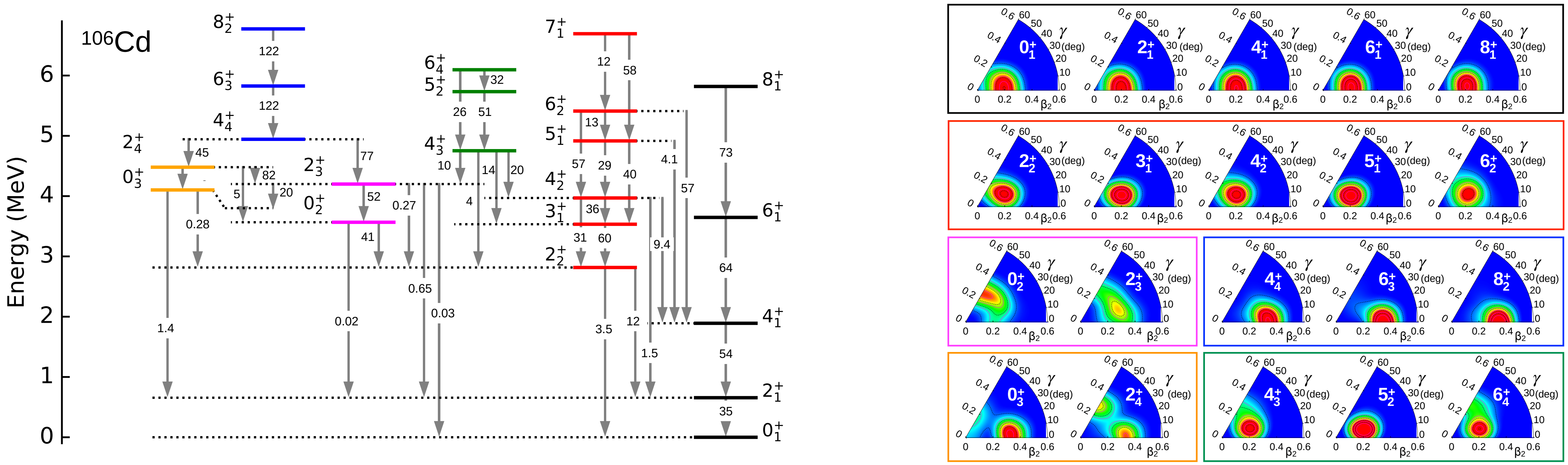


M. Siciliano et al., Physical Review C 104, 034320 (2021)

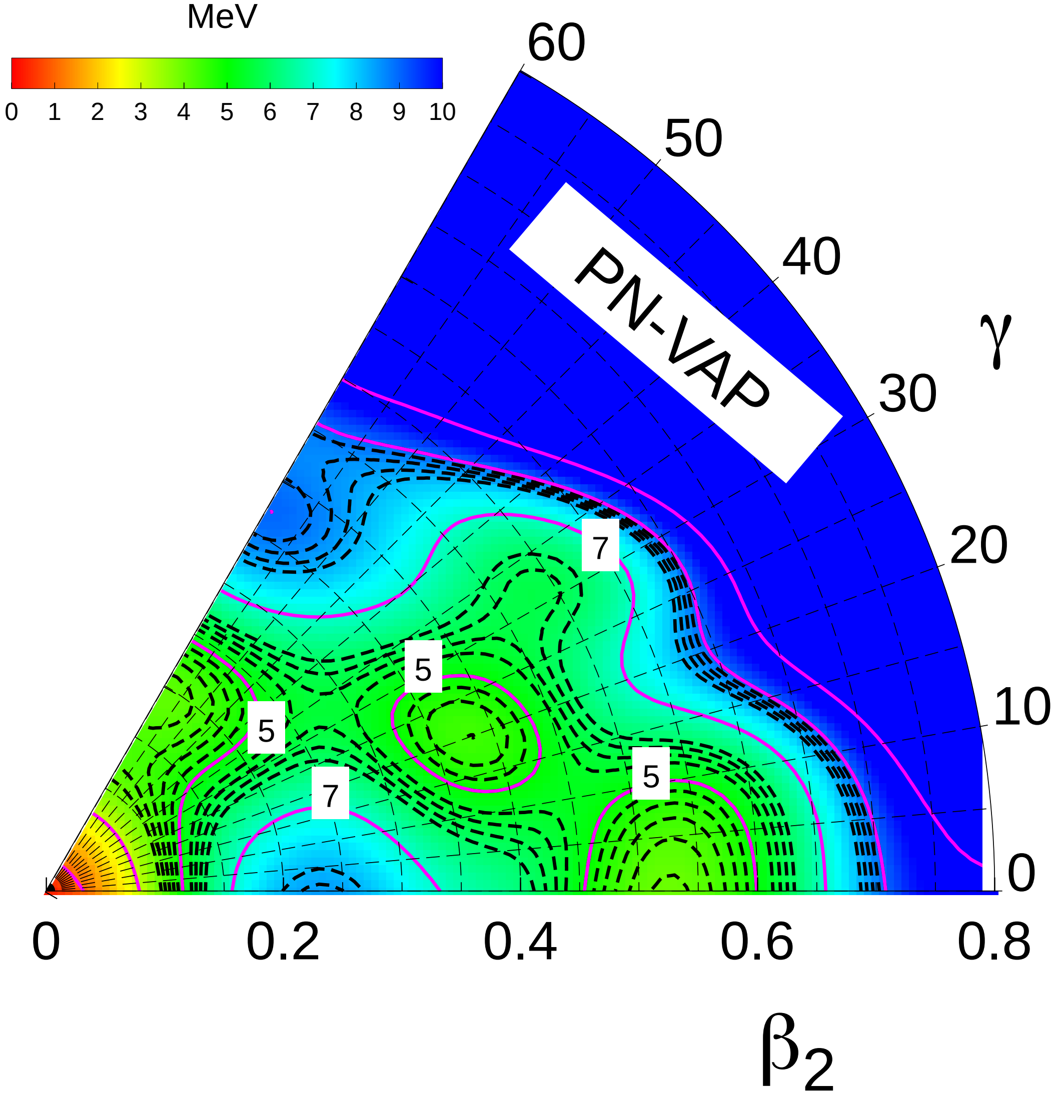
Outline

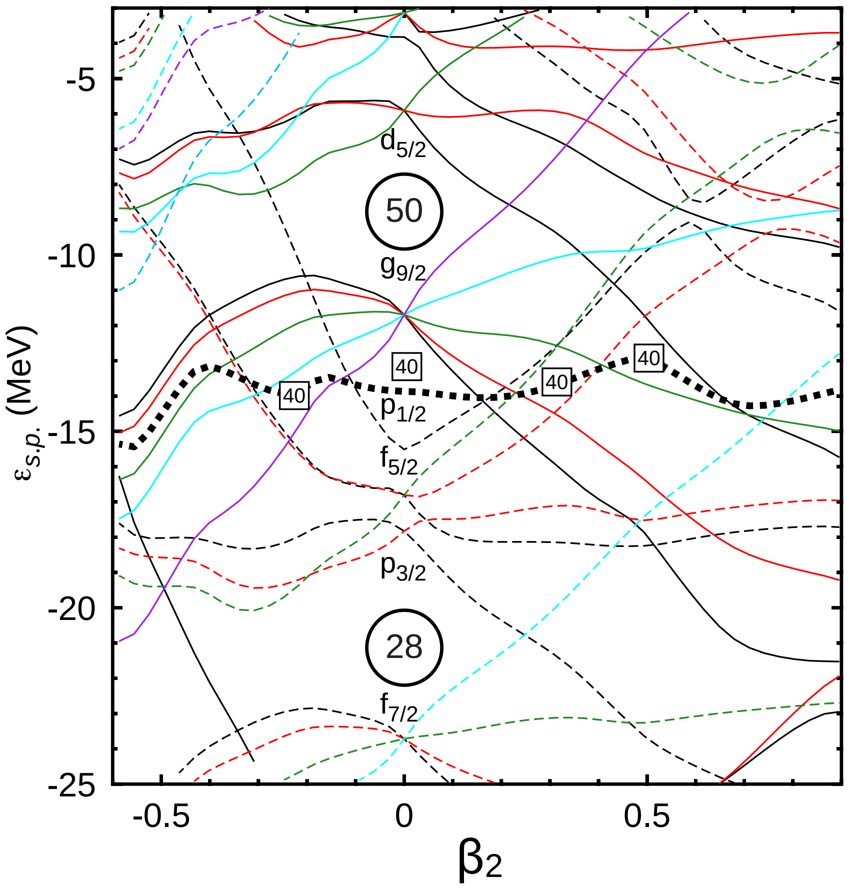
Multiple Shape Coexistence

$^{80}\mathrm{Zr}_{40}$

$$\delta E^{N,Z}\left[\bar{\Phi}(\beta,\gamma)\right]\Big|_{\bar{\Phi}=\Phi}=0$$

$$E^{N,Z}[\Phi]=\frac{\langle\Phi|\hat{H}_{2\mathrm{b}}\hat{P}^{N}\hat{P}^{Z}|\Phi\rangle}{\langle\Phi|\hat{P}^{N}\hat{P}^{Z}|\Phi\rangle}+\varepsilon^{N,Z}_{DD}(\Phi)-\lambda_{q_{20}}\langle\Phi|\hat{Q}_{20}|\Phi\rangle-\lambda_{q_{22}}\langle\Phi|\hat{Q}_{22}|\Phi\rangle$$



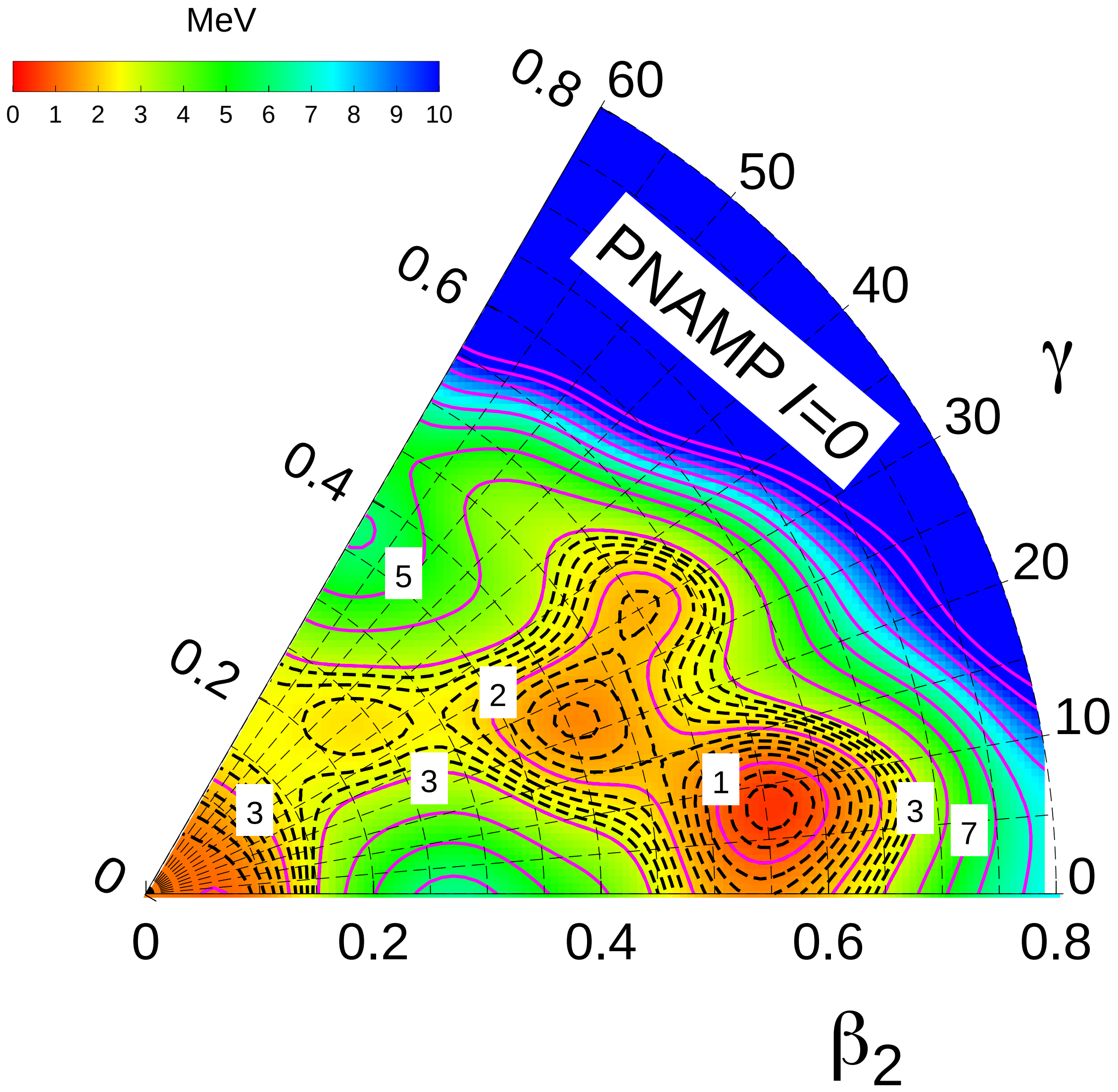


- Up to five minima in the potential energy surface.
- Absolute minimum corresponds to spherical configuration (*N*=40 spherical gap)
- Other minima related to the filling in and emptying of $g_{9/2}$, $p_{1/2}$, $f_{5/2}$ and $d_{5/2}$ orbits.

T. R. R., J. L. Egido, Phys. Lett. B 705, 255 (2011)

Multiple Shape Coexistence

$$|IMK;NZ;\beta\gamma\rangle = \frac{2I+1}{8\pi^2}\int \mathcal{D}^{I*}_{MK}(\Omega)\hat{R}(\Omega)\hat{P}^N\hat{P}^Z|\Phi(\beta,\gamma)\rangle d\Omega \qquad |IM;NZ;\beta\gamma\rangle = \sum_K g_K^{IM;NZ;\beta\gamma}|IMK;NZ;\beta\gamma\rangle$$



- Five minima are closer in energy whenever the rotational invariance is restored.
- Absolute minima corresponds to deformed configuration β_2~0.55
- Barriers between the minima are less than 1 MeV.

Mixing?

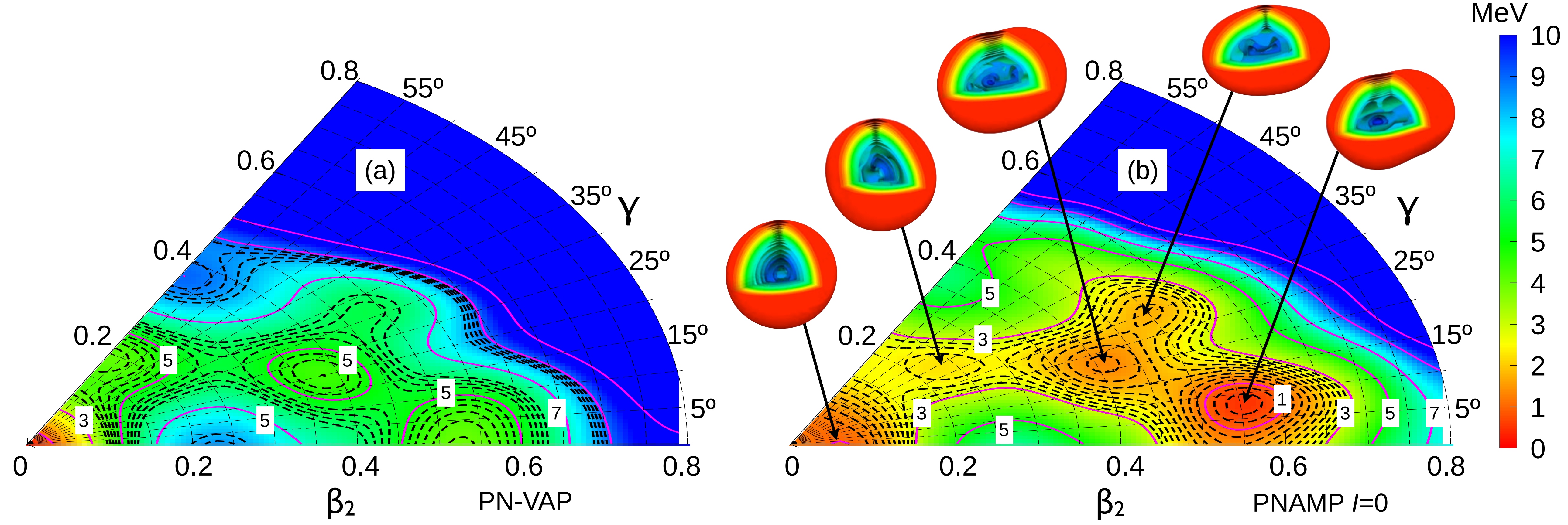
T. R. R., J. L. Egido, Phys. Lett. B 705, 255 (2011)

Multiple Shape Coexistence

$^{80}Zr_{40}$

Relevance of angular momentum projection

(Similar feature as in ^{32}Mg, see R. Rodriguez-Guzmán et al., Nucl. Phys. A 709, 201 (2002))



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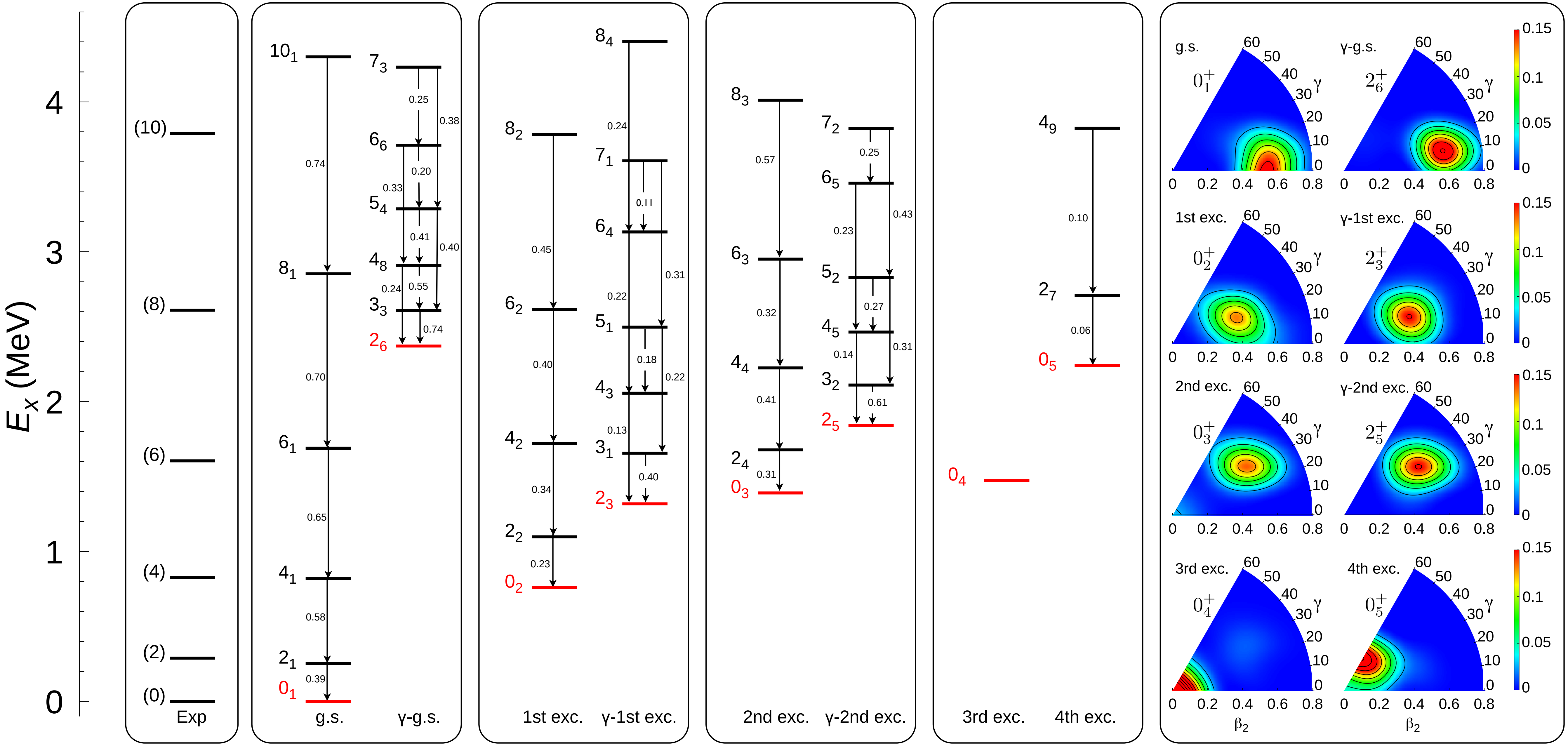

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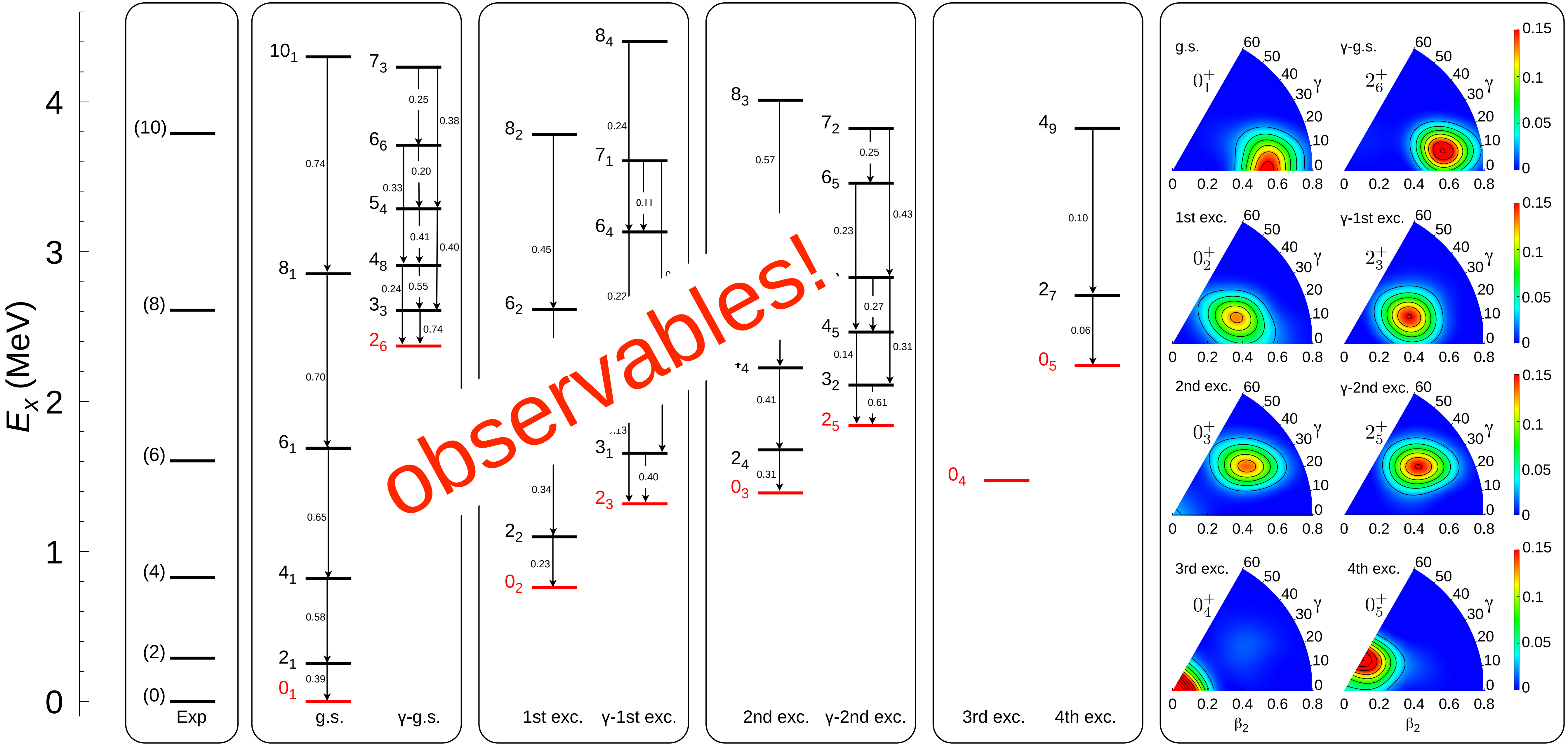

observables!

Multiple Shape Coexistence

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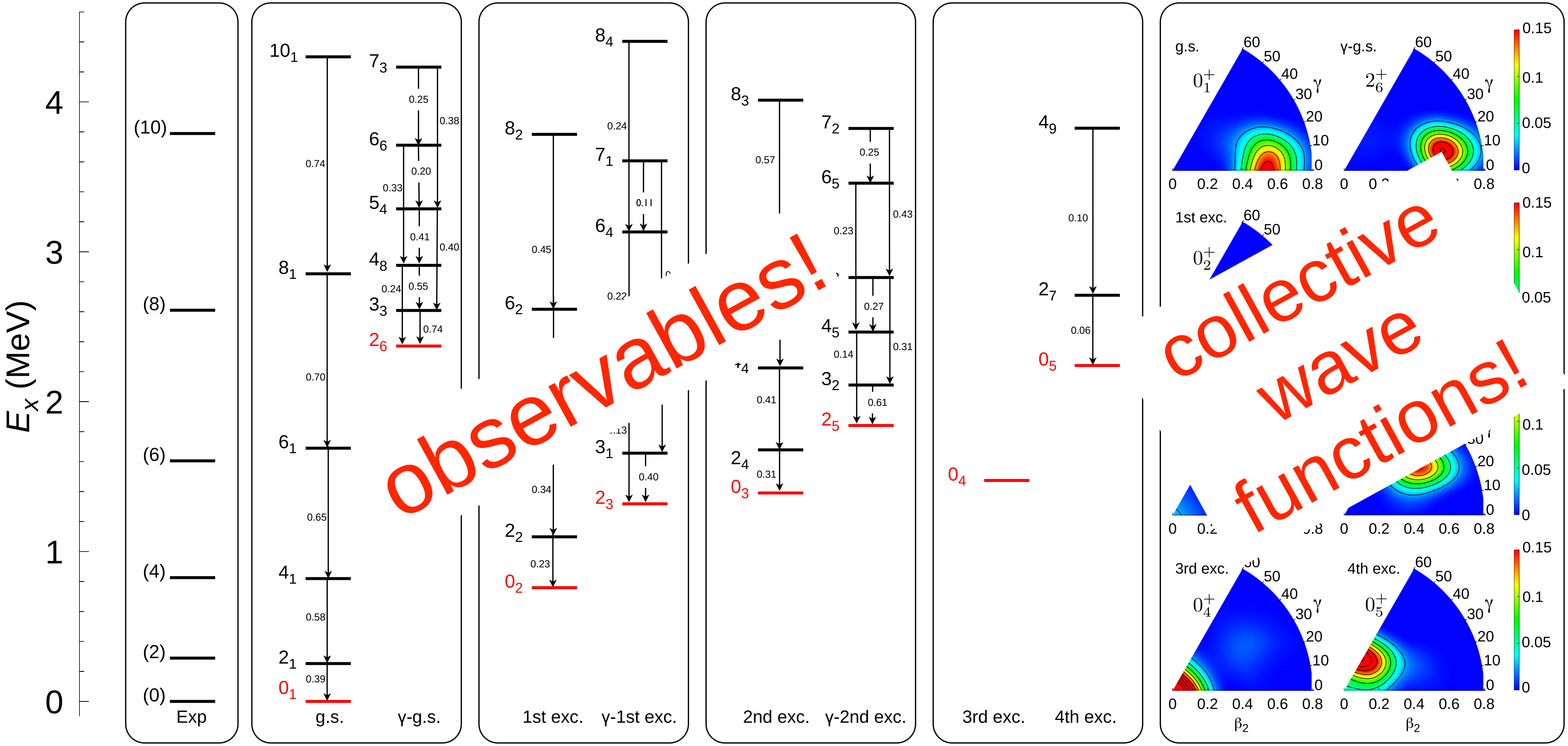

observables!

collective wave functions!

Outline

1. Introduction

2. Projected Generator Coordinate Method

3. Multiple shape-coexistence in ^{80}Zr

4. Variational methods in valence spaces

5. Summary

Variational methods in valence spaces

- Extend the range of applicability of shell model calculations
- Provide an interpretation of the SM states in terms of intrinsic collective shapes

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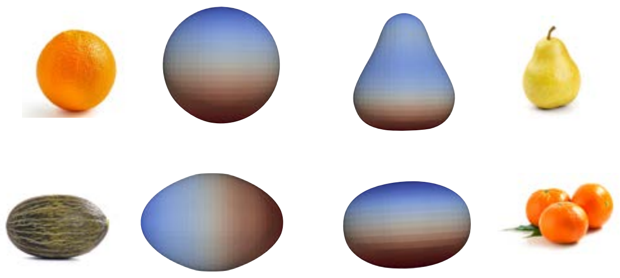

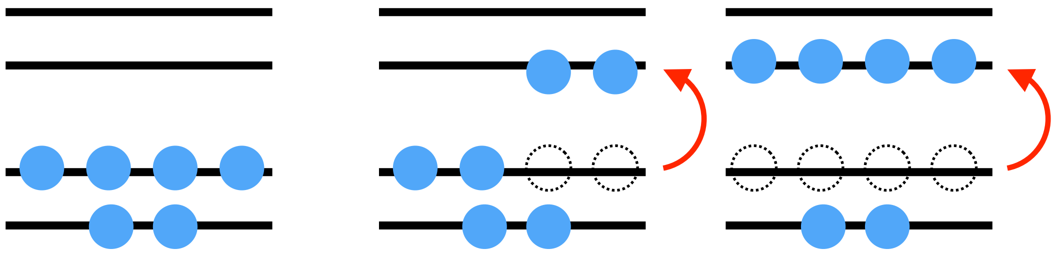

shapes / collective motion ↔ **shell structure / particle-hole excitations**

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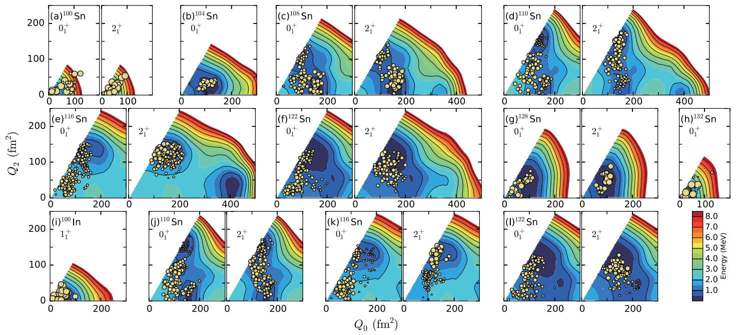
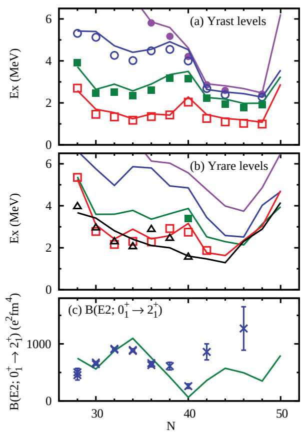
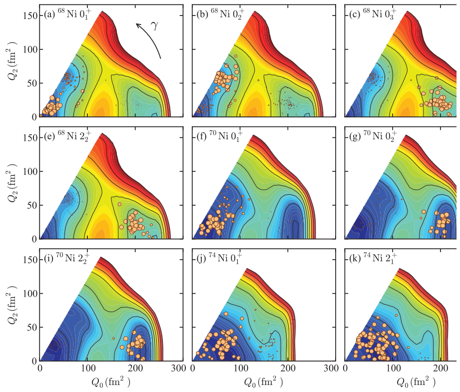
Monte Carlo Shell Model

MCSM







Y. Tsunoda et al., PRC 89, 031301(R) (2014), Y. Utsuno et al., PRL 114, 032501 (2015), …

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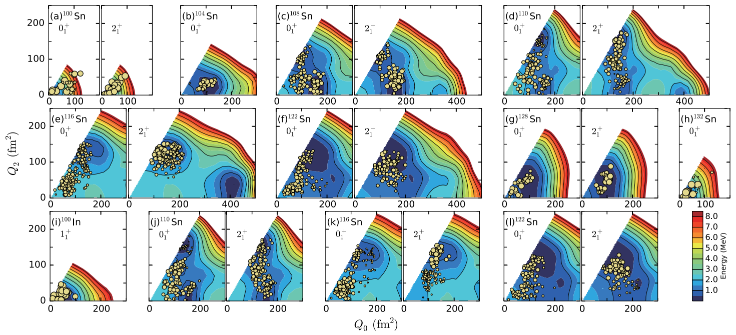

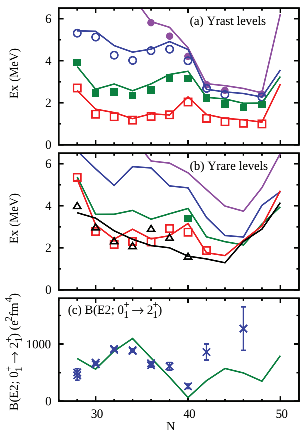

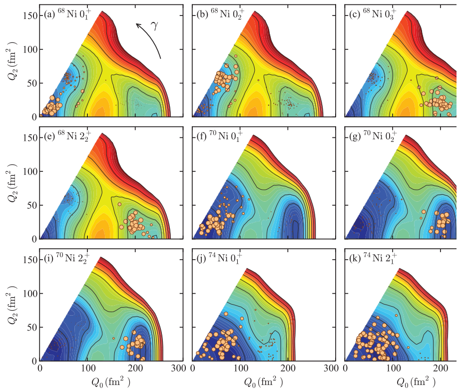

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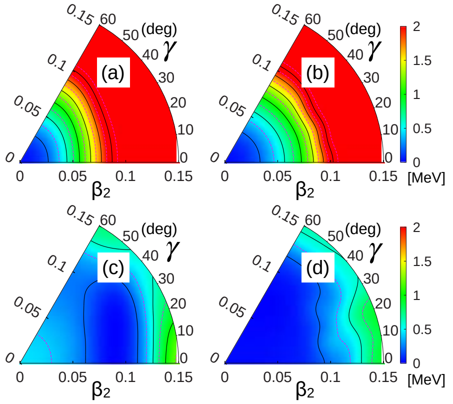
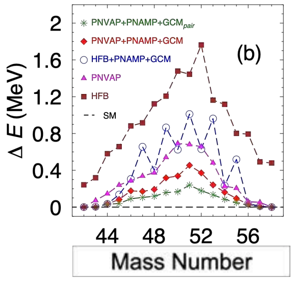
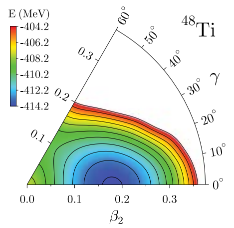
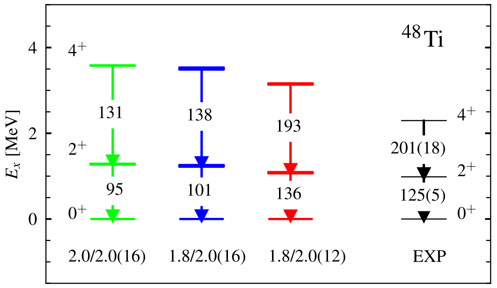
Projected Generator Coordinate Method

PGCM









C. F. Jiao et al, PRC 96, 054310, B. Bally et al., PRC 100, 044308 (2019), PRC 104, 054306 (2021), …

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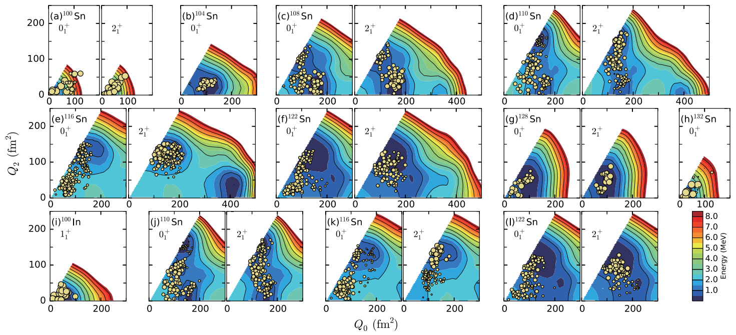

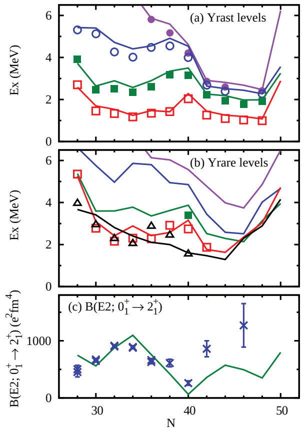

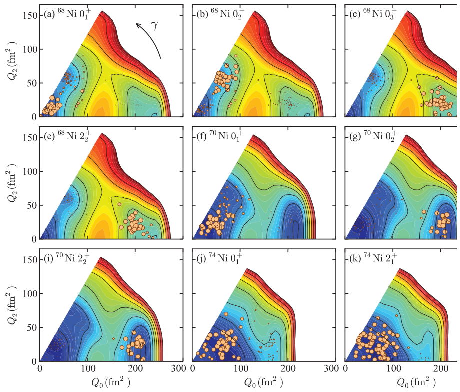

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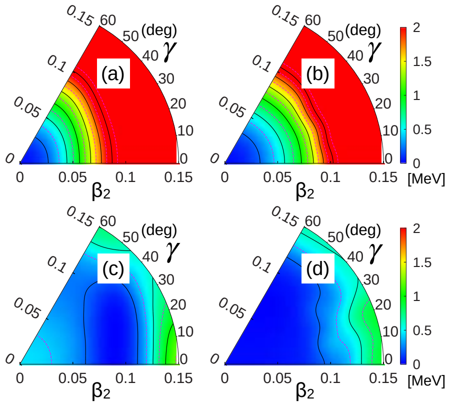
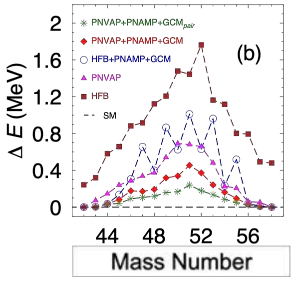
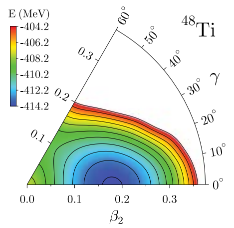
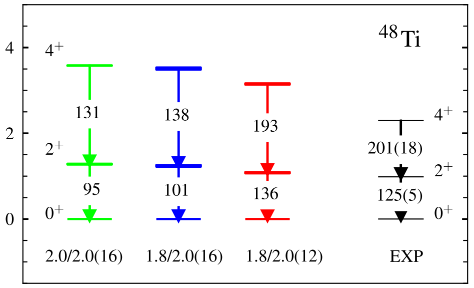




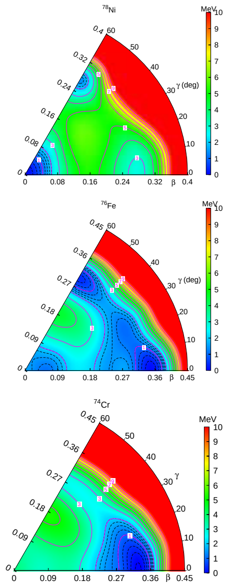


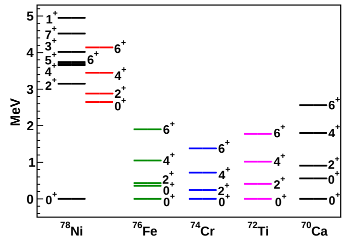


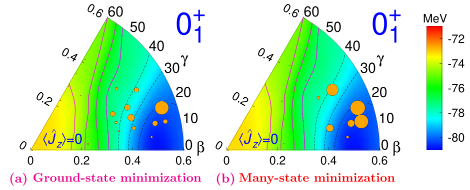
C. F. Jiao et al, PRC 96, 054310, B. Bally et al., PRC 100, 044308 (2019), PRC 104, 054306 (2021), …

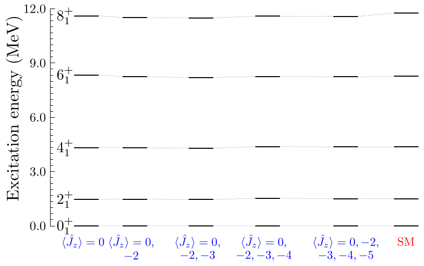
Discrete Non-orthogonal Shell Model

DNO-SM









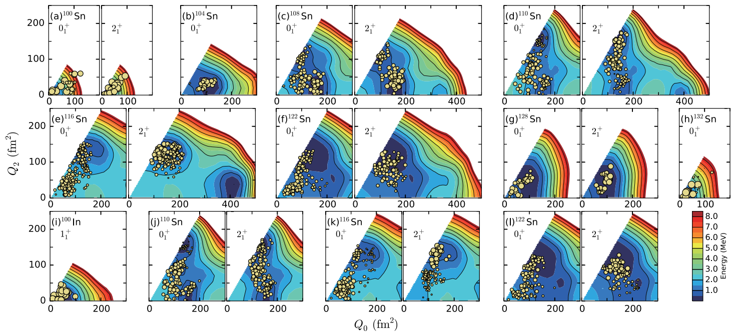
B. Bounthong, D. D. Dao and F. Nowacki, PRL 117, 272501 (2016), PRC 105 054314 (2022, …

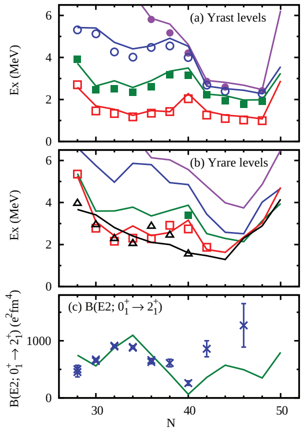
Variational methods in valence spaces

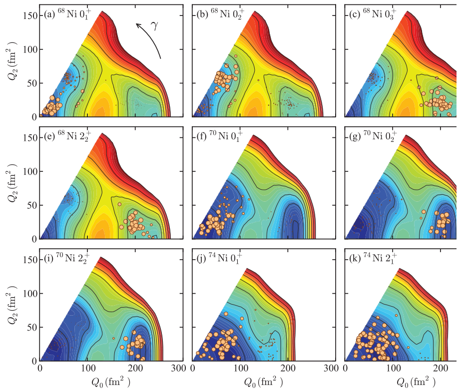
- Extend the range of applicability of shell model calculations

- Provide an interpretation of the SM states in terms of intrinsic collective shapes

Monte Carlo Shell Model
MCSM

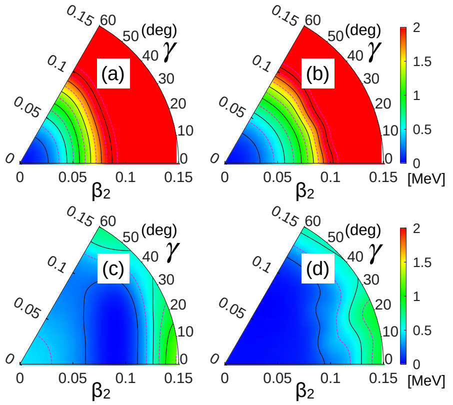


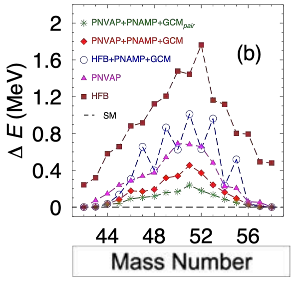


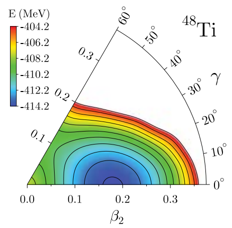


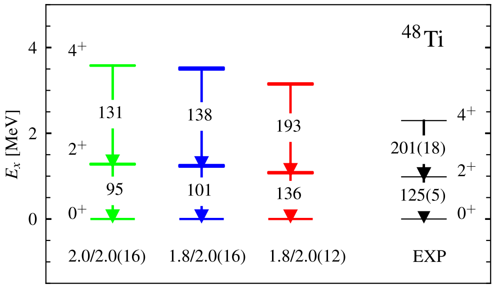
Y. Tsunoda et al., PRC 89, 031301(R) (2014), Y. Utsuno et al., PRL 114, 032501 (2015), …

Projected Generator Coordinate Method
PGCM



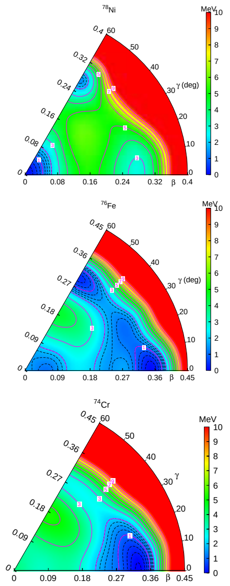


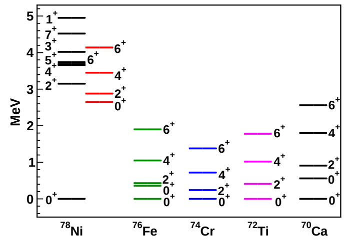


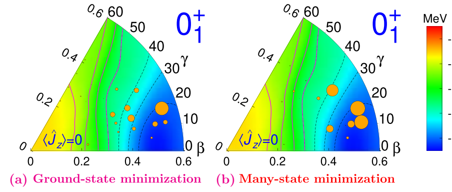


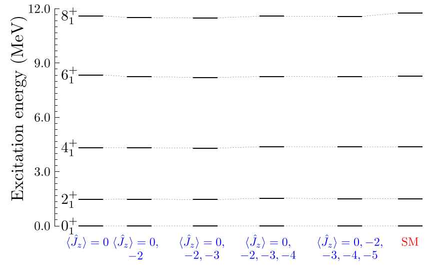
C. F. Jiao et al, PRC 96, 054310, B. Bally et al., PRC 100, 044308 (2019), PRC 104, 054306 (2021), …

Discrete Non-orthogonal Shell Model
DNO-SM









B. Bounthong, D. D. Dao and F. Nowacki, PRL 117, 272501 (2016), PRC 105 054314 (2022, …

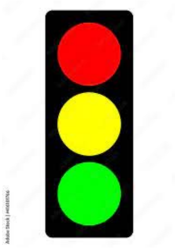
other approaches: VAMPIR, PSM, …

ISM with PGCM

Projected Generator Coordinate Method (EDF)

- *Kind of nuclei*

- even-even nuclei
- Multi-quasiparticle excitations are included
- even-odd/odd-even nuclei (blocking mandatory)
- odd-odd nuclei (blocking mandatory)



- *Observables and physical quantities*

- Bulk properties: masses, radii, nuclear densities.
- Excitation energies
- electromagnetic transition probabilities
- Beta-decay rates
- Double-beta decay matrix elements
- Electromagnetic responses
- Fission properties
- Reaction properties
- …

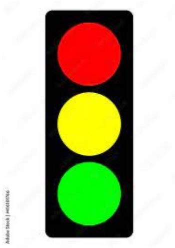
CATALOG OF
SERVICES

ISM with PGCM

Projected Generator Coordinate Method (Hamil)

- Kind of nuclei

- **even-even nuclei**
- **Multi-quasiparticle excitations are included**
- **even-odd/odd-even nuclei (blocking mandatory)**
- **odd-odd nuclei (blocking mandatory)**



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- **…**

CATALOG OF
SERVICES

TAURUS

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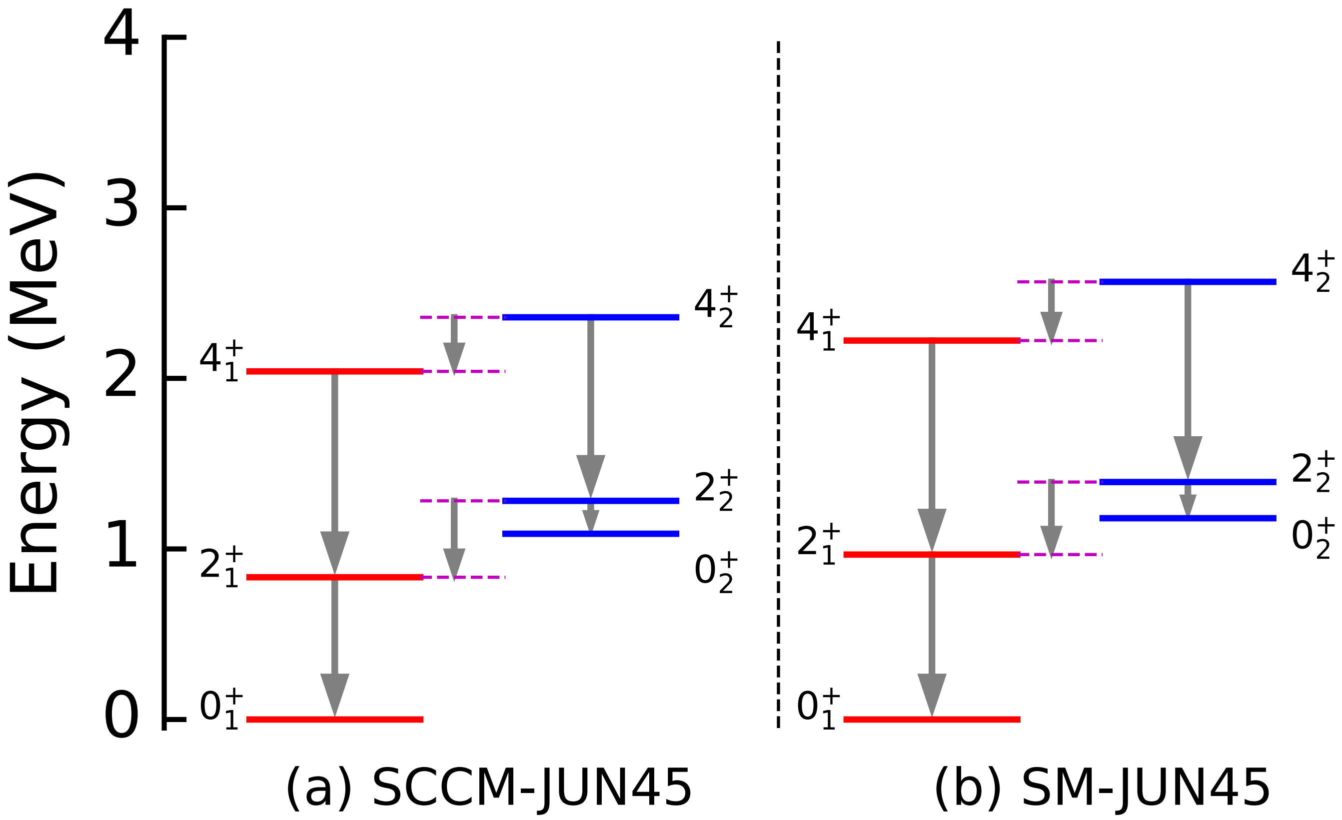
Theory for **A U**nified
desc**R**iption of n**U**clear
Structure

B. Bally, T.R.R.

Shape coexistence in ^{66}Se

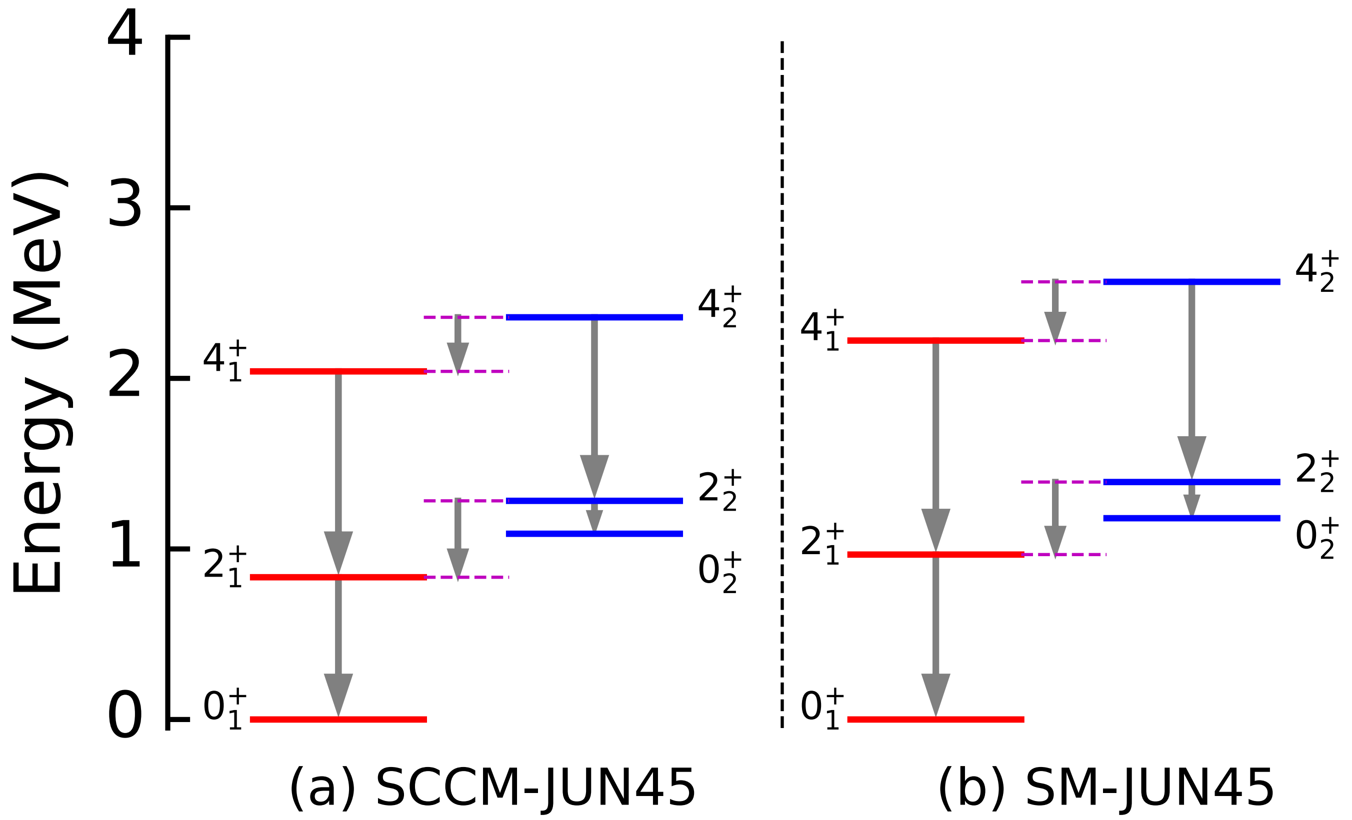


Shape coexistence in ^{66}Se:

We can interpret the exact SM results in terms of collective coordinates (deformations)

PLB 844, 138072 (2023)

Shape coexistence in ^{66}Se



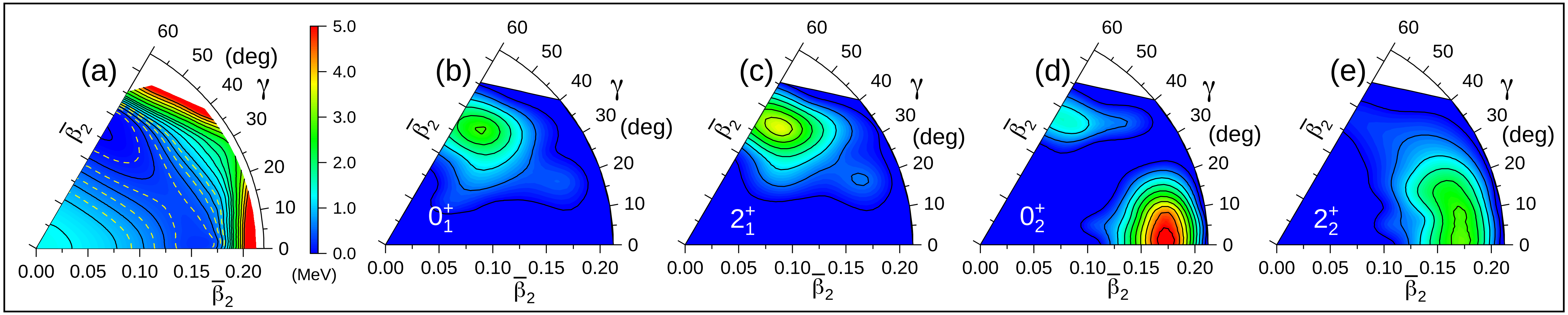
(a) SCCM-JUN45

(b) SM-JUN45

Shape coexistence in ^{66}Se:

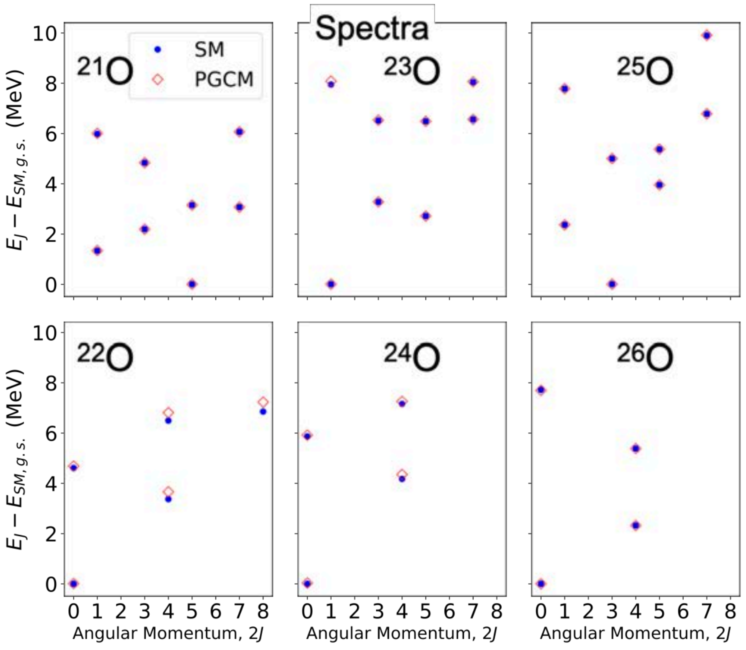
We can interpret the exact SM results in terms of collective coordinates (deformations)

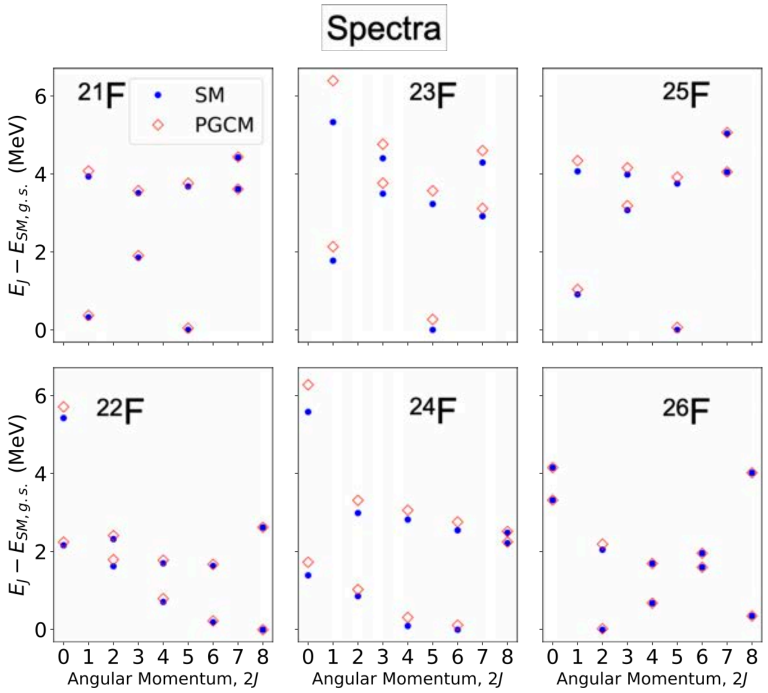
PLB 844, 138072 (2023)



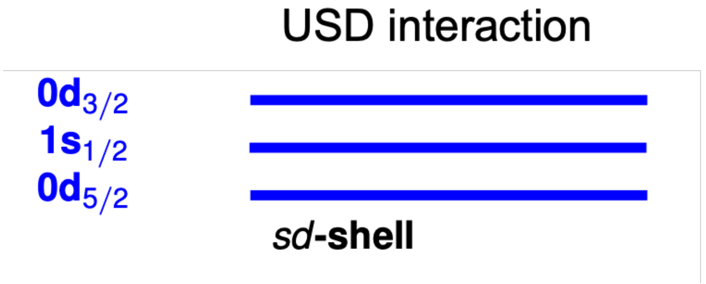
Beta-decay properties

Benchmark of the PGCM method against exact results.

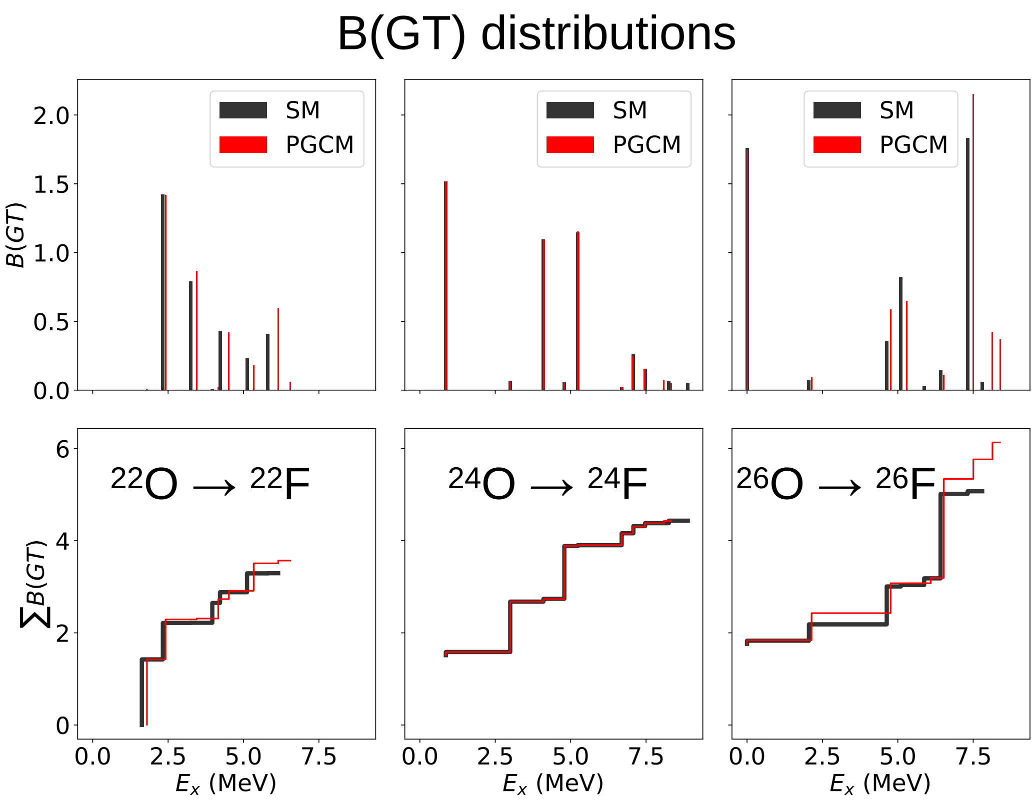




*B. H. Wildenthal, M. S. Curtis, B. A. Brown, PRC 28, 1343 (1983)



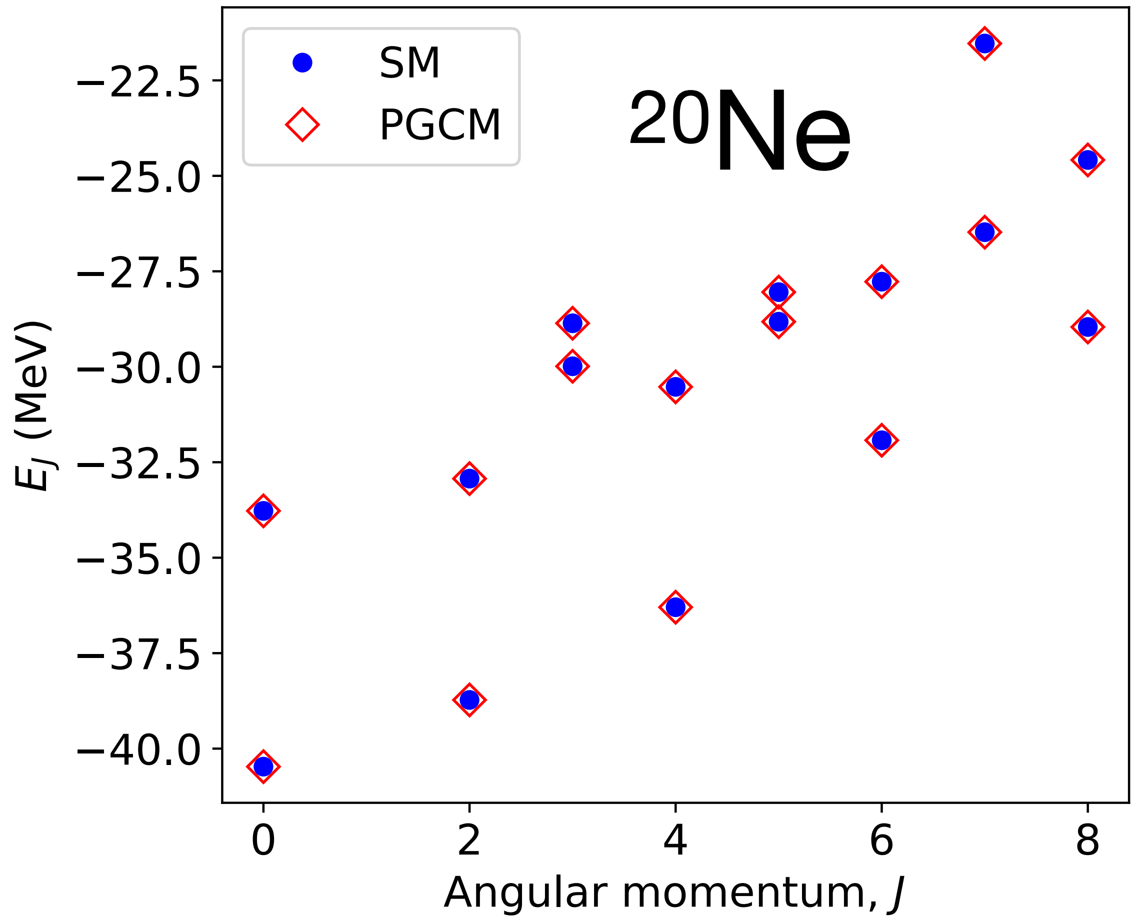
		B(GT)$_{SM*}$	**B(GT)$_{PGCM}$**	B.R.
^{21}O (5/2$^+$) → ^{21}F				
	(3/2$^+$)$_1$	**0.040**	**0.042**	34 %
	(5/2$^+$)$_2$	**0.151**	**0.151**	29 %
^{22}O (0$^+$) → ^{22}F				
	(1$^+$)$_2$	**1.423**	**1.417**	82 %
	(1$^+$)$_3$	**0.790**	**0.867**	15 %
^{23}O (1/2$^+$) → ^{23}F				
	(1/2$^+$)$_1$	**0.287**	**0.249**	55 %
	(3/2$^+$)$_1$	**0.267**	**0.250**	20 %
^{24}O (0$^+$) → ^{24}F				
	(1$^+$)$_1$	**1.515**	**1.517**	83 %
	(1$^+$)$_2$	**1.094**	**1.093**	10 %
^{25}O (3/2$^+$) → ^{25}F				
	(5/2$^+$)$_1$	**0.638**	**0.648**	75 %
^{26}O (0$^+$) → ^{26}F				
	(1$^+$)$_1$	**1.758**	**1.746**	83 %
	(1$^+$)$_4$	**0.822**	**0.648**	6 %

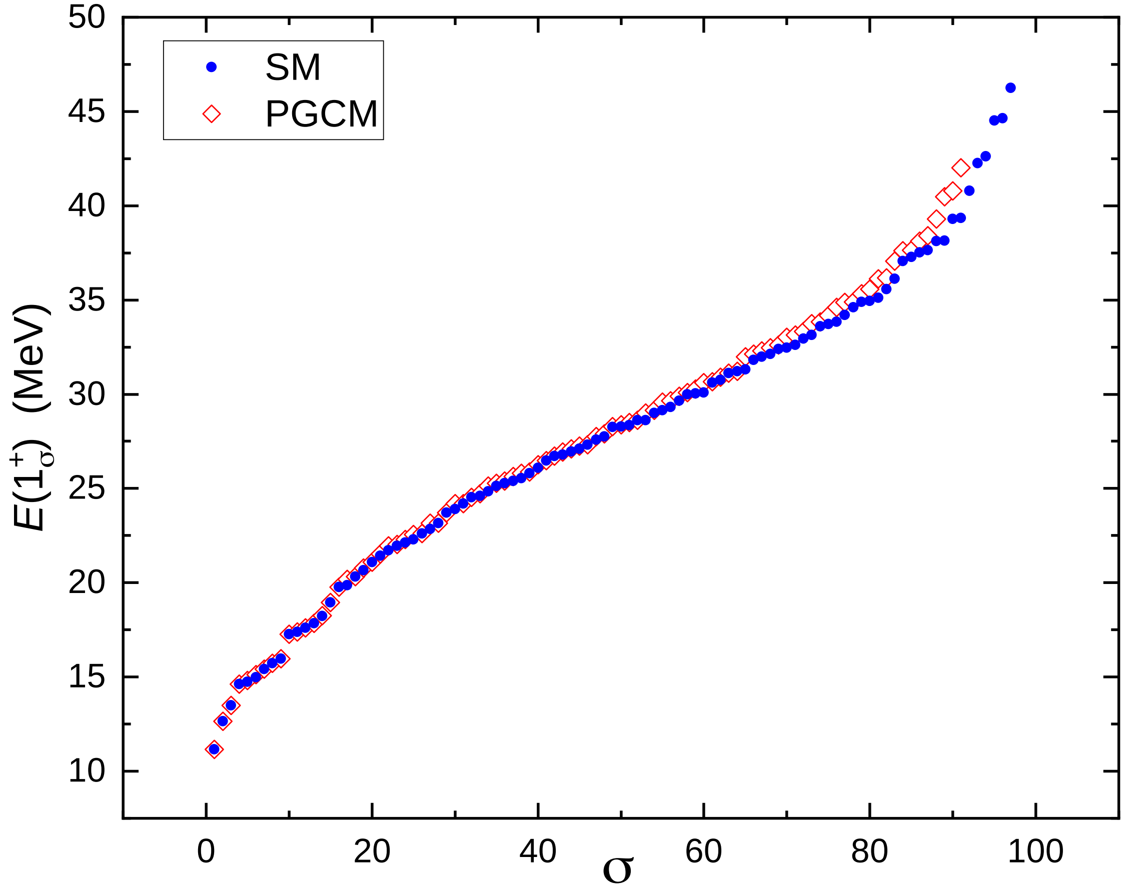


V. Vijayan et al., in preparation

B(M1) strength functions in e-e nuclei

Exploring cranking, pn-pairing (isoscalar and isovector)





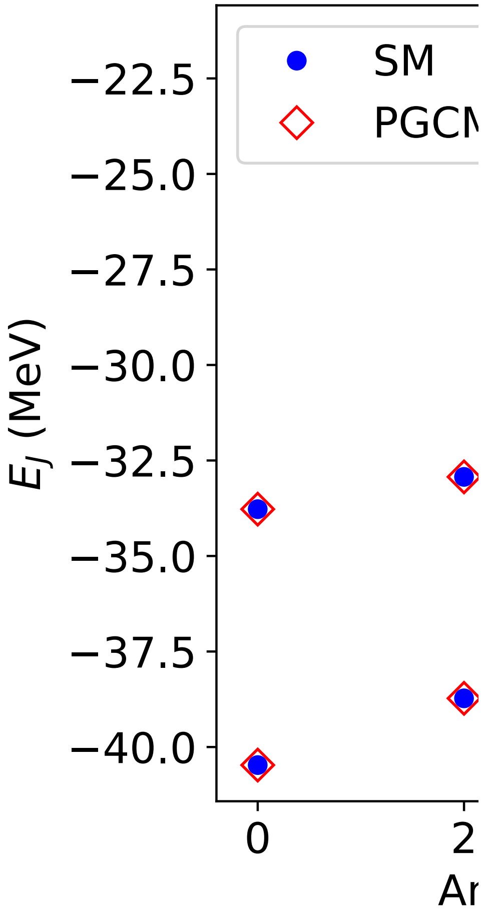
- exact ground state energy
- exact description of low-lying excited energies

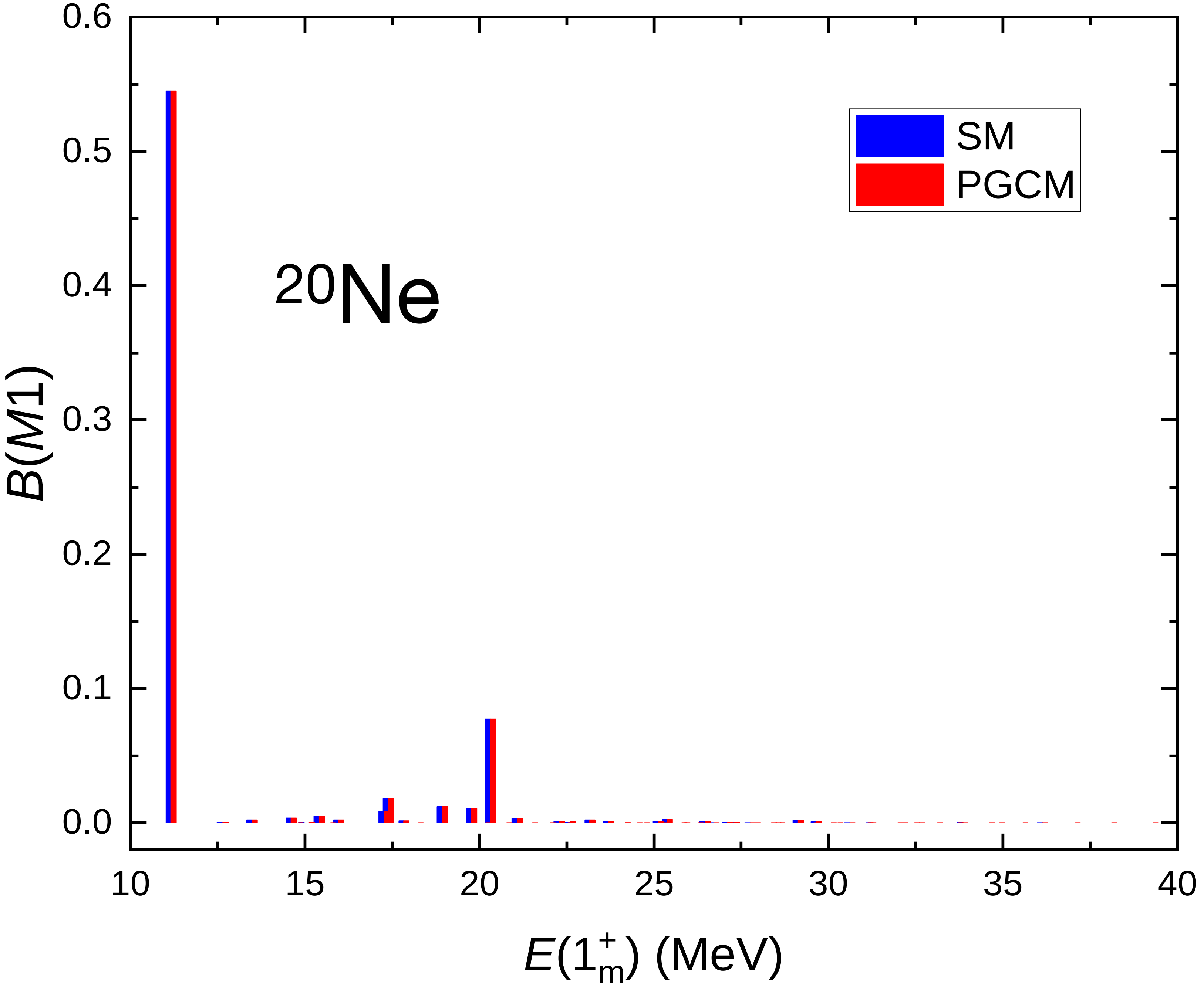
- Excellent description of the lowest excited 1^+ states

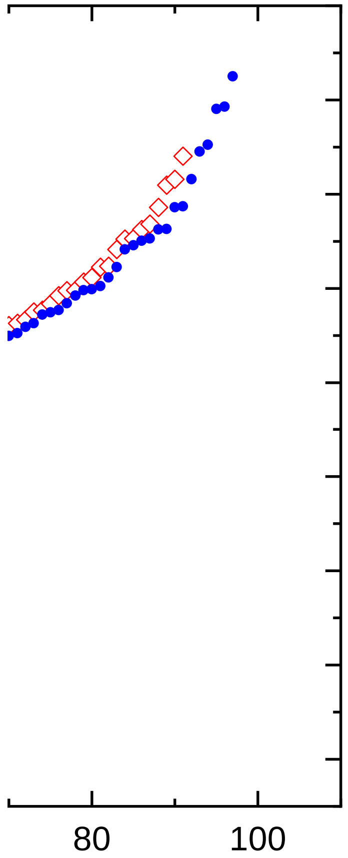
S. Bofos, J. Martínez-Larraz et al., in preparation

B(M1) strength functions in e-e nuclei

Exploring cranking, pn-pairing (isoscalar and isovector)







- exact grou of the lowest
- exact desc excited en

S. Bofos, J. Martínez-Larraz et al., in preparation

Outline

1. Introduction

2. Projected Generator Coordinate Method

3. Multiple shape-coexistence in ^{80}Zr

4. Variational methods in valence spaces

5. Summary

Summary

- PGCM methods provide a reliable description of nuclear structure observables.

- It is a very flexible method to approach exact solutions although the present implementation tends to favor correlations in the ground state (stretched spectra).

- Shape coexistence can be visible in the TES (several minima) and/or in the GCM calculation (bands with different collective wave functions).

- Multiple shape coexistence is predicted for ^{80}Zr.

- ISM states can be studied in terms of intrinsic shapes in the valence space.

- PGCM is able to compute beta-decay transition probabilities and B(M1) strength functions

Thank you!