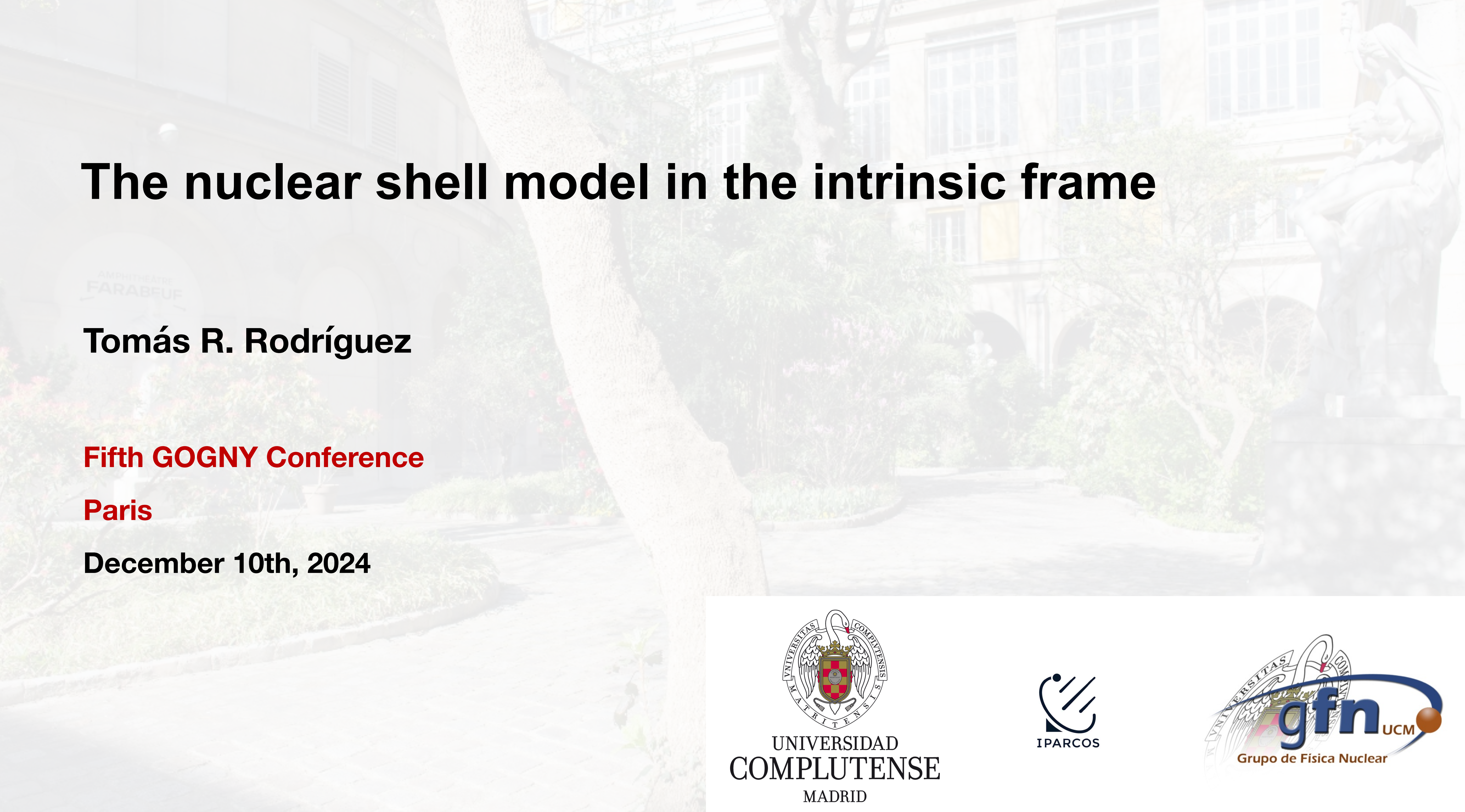

The nuclear shell model in the intrinsic frame

Tomás R. Rodríguez

Fifth GOGNY Conference

Paris

December 10th, 2024

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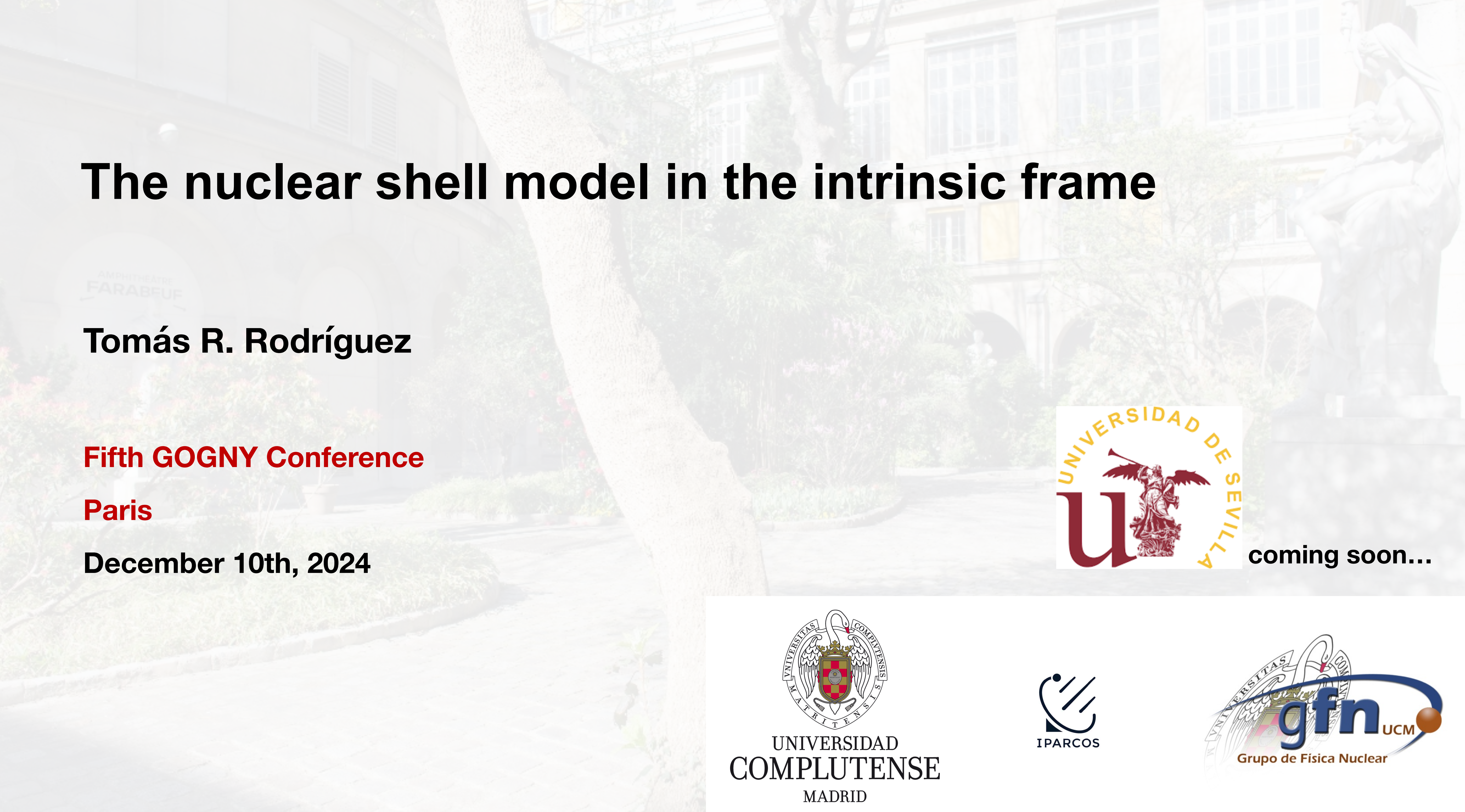
Grupo de Física Nuclear



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coming soon…

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Acknowledgments

Benjamin Bally (CEA-Saclay)

Adrián Sánchez-Fernández (ULB-Brussels)

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Vimal Vijayan (GSI-Darmstadt)

Kamila Sieja (Strasbourg)

Outline

1. Introduction

2. Projected Generator Coordinate Method (PGCM)

3. Benchmarking PGCM against shell model with TAURUS

4. Summary and Outlook

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Nuclear many-body problem(s)

Nuclear structure theory rationale

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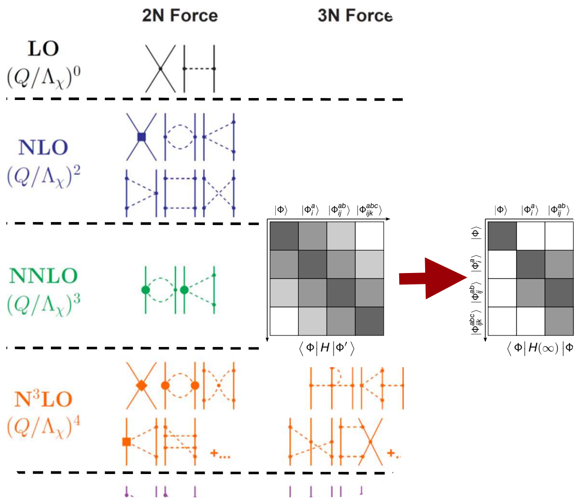

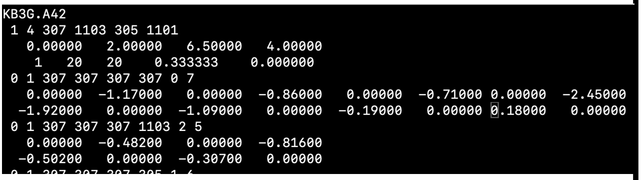

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  -1.92000   0.00000  -1.09000   0.00000  -0.19000   0.00000 0.18000   0.00000
 0 1 307 307 307 1103 2 5
   0.00000  -0.48200   0.00000  -0.81600
  -0.50200   0.00000  -0.30700   0.00000
 0 1 307 307 307 305 1 6
```

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

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

$$v_{\mathrm{LS}}(1,2) = \mathrm{i} W_{\mathrm{LS}} (\vec{\nabla}_{12} \delta(\vec{r}_1 - \vec{r}_2) \wedge \vec{\nabla}_{12})(\vec{\sigma}_1 + \vec{\sigma}_2)$$

$$v_{\mathrm{DD}}(1,2) = t_3 (1 + P_\sigma x_0) \delta(\vec{r}_1 - \vec{r}_2) \rho^\alpha ((\vec{r}_1 + \vec{r}_2)/2)$$

effective interactions

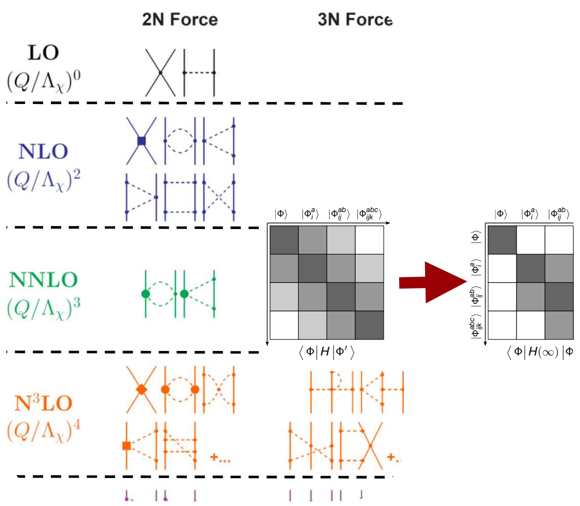
$$\hat{H}|\Psi_n\rangle = E_n|\Psi_n\rangle$$

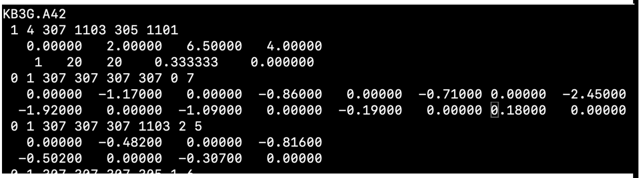
$$\delta\left[E\left(\rho\right)\right] = 0$$

Many-body methods

Nuclear many-body problem(s)

Nuclear structure theory rationale





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   0.00000   2.00000   6.50000   4.00000
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  -0.50200   0.00000  -0.30700   0.00000
 0 1 307 307 307 305 1 6
```

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

$$v_c(1,\,2) = \sum_{i=1,2} {\rm e}^{-\frac{|\vec{r}_1-\vec{r}_2|^2}{\mu_i^2}}(W_i + B_iP_\sigma - H_iP_\tau - M_iP_\sigma P_\tau).$$

$$v_{\rm LS}(1,\,2) = {\rm i}W_{\rm LS}(\vec{\nabla}_{12}\delta(\vec{r}_1-\vec{r}_2)\wedge\vec{\nabla}_{12})(\vec{\sigma}_1+\vec{\sigma}_2)$$

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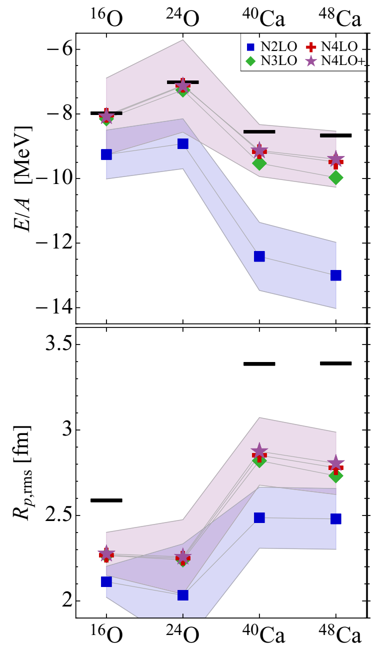
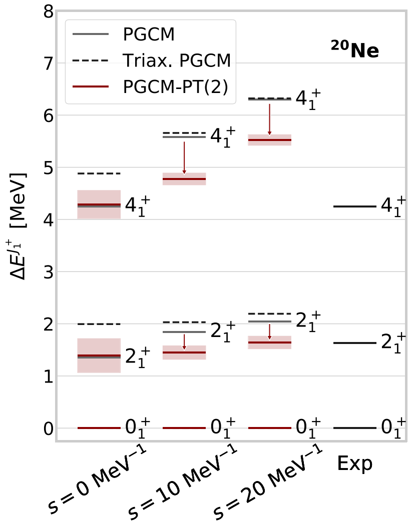


PRC 106, 064002 (2022)



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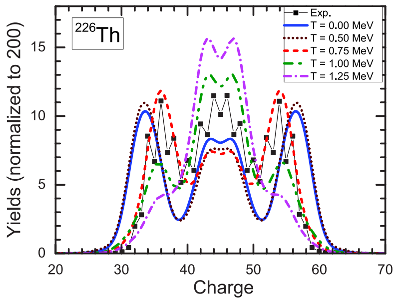

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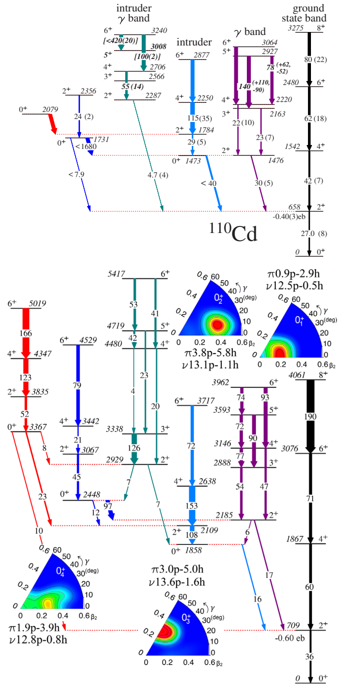
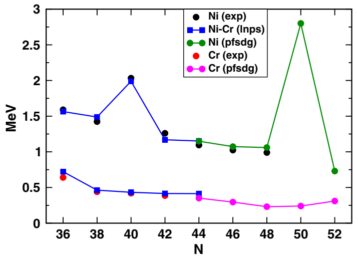


PRL 123, 142502 (2019)



PRL 117, 272501 (2016)

Results

Nuclear many-body problem(s)

Nuclear methods must provide a wide catalog of physical quantities that can be reliably compared with experimental data

Nuclear structure theory:

- Kind of nuclei

- even-even nuclei
- even-odd/odd-even nuclei
- odd-odd nuclei

- 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

Nuclear many-body problem(s)

Let us assume that ***we know*** the nuclear interaction.

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

??

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Solving the quantum many-body exactly is (in general) **impossible**

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Let us assume that ***we know*** the nuclear interaction.

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

??

Solving the quantum many-body exactly is (in general) **impossible**

Most widely used ***solutions*** to attack this problem:

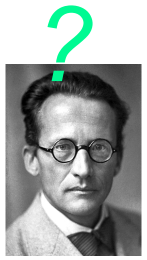
- **Valence-space or no-core (Shell Model) calculations**
- **Variational approximate methods** (mean-field and beyond-mean-field).
- **Expansion techniques** (e.g., many-body perturbation theory, Coupled-cluster)

Interacting Shell Model (in a nutshell)

Full diagonalization of an *adapted* Hamiltonian within a valence space

$$\hat{H}_{v.s.}|\Psi^{n}_{v.s.}\rangle = E_n\,|\Psi^{n}_{v.s.}\rangle$$

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



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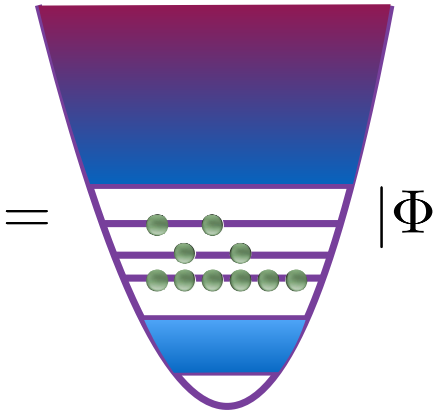
Full diagonalization of an *adapted* Hamiltonian within a valence space

$$\hat{H}_{v.s.}|\Psi^n_{v.s.}\rangle = E_n\,|\Psi^n_{v.s.}\rangle$$

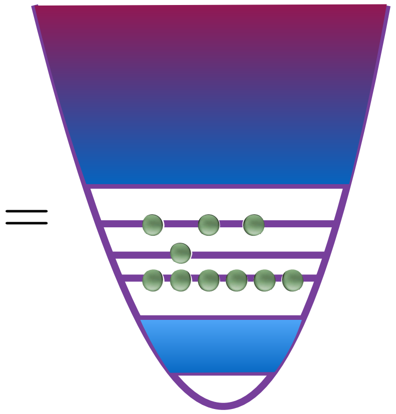
Nuclear wave functions are linear combinations of Slater determinants written in terms of occupations of spherical orbits

$$|\Psi^n_{v.s.}\rangle = \sum_{k\in\, v.s.} C^n_k|\Phi^k\rangle$$

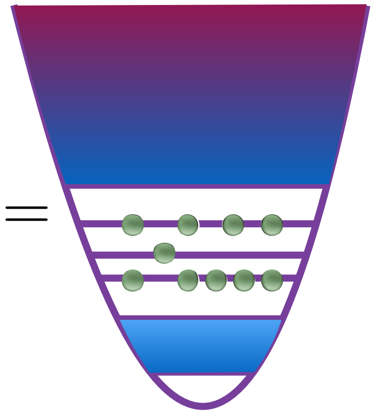
$|\Phi^1\rangle =$



$|\Phi^2\rangle =$

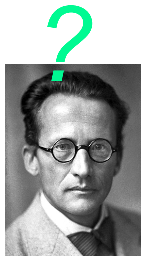


$|\Phi^3\rangle =$



...

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



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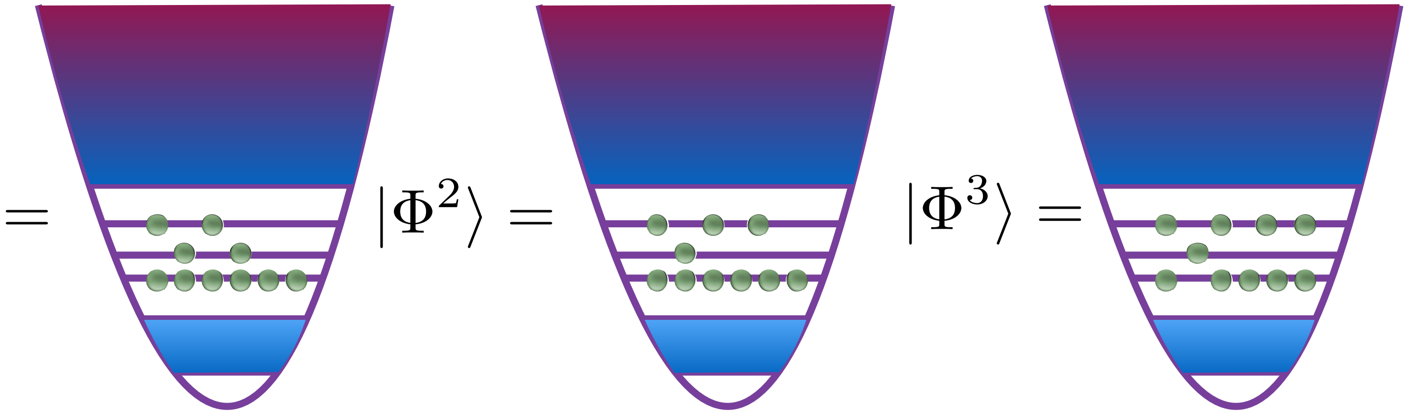
Wave functions are defined in the LABORATORY SYSTEM

⇒ SHAPES?!?!



$|\Phi^{1}\rangle =$ $|\Phi^{2}\rangle =$ $|\Phi^{3}\rangle =$ ...

$$\hat{H}|\Psi_{n}\rangle = E_{n}|\Psi_{n}\rangle$$

?

Interacting Shell Model (in a nutshell)

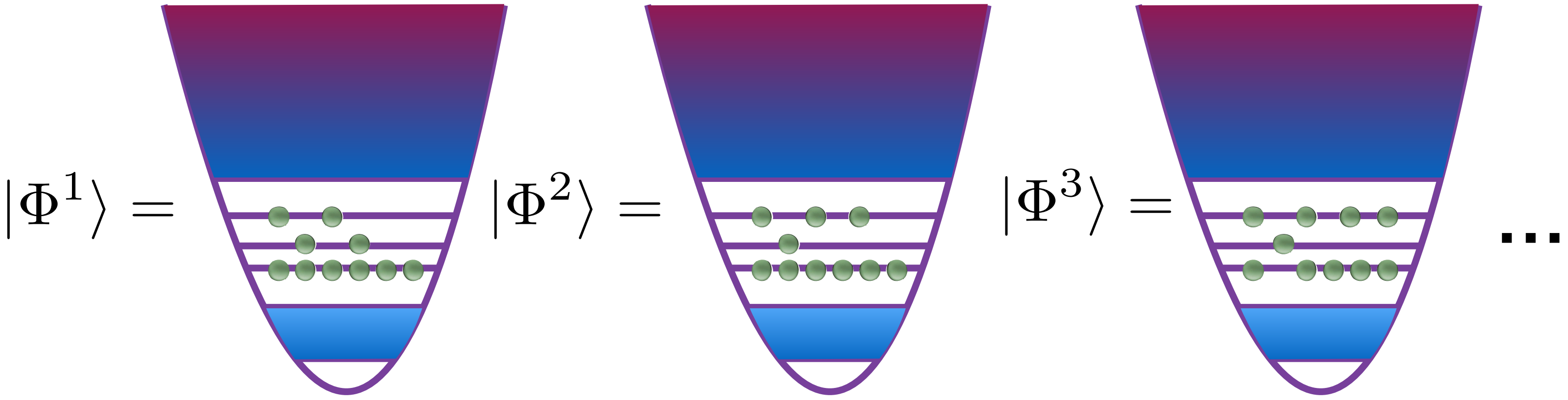
Full diagonalization of an *adapted* Hamiltonian within a valence space

$$\hat{H}_{v.s.}|\Psi^{n}_{v.s.}\rangle = E_{n}\,|\Psi^{n}_{v.s.}\rangle$$

Nuclear
occupat

d in
EM

Limited by the combinatorial increase of the number of configurations



$$|\Phi^{1}\rangle = \quad |\Phi^{2}\rangle = \quad |\Phi^{3}\rangle = \quad \ldots$$

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Variational methods in SM 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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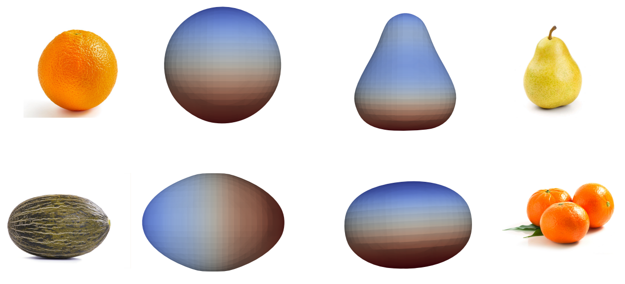

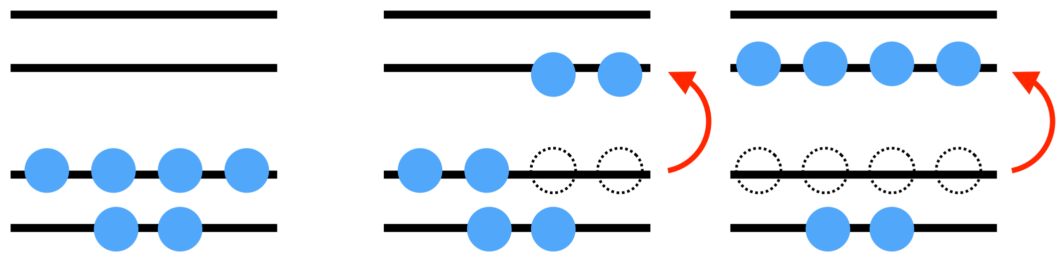

shapes / collective motion ⟷ shell structure / particle-hole excitations

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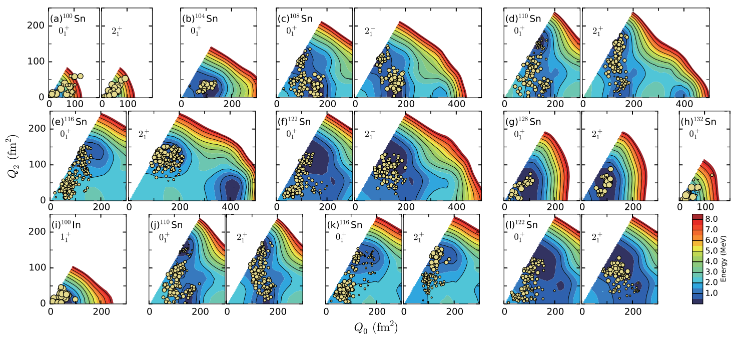
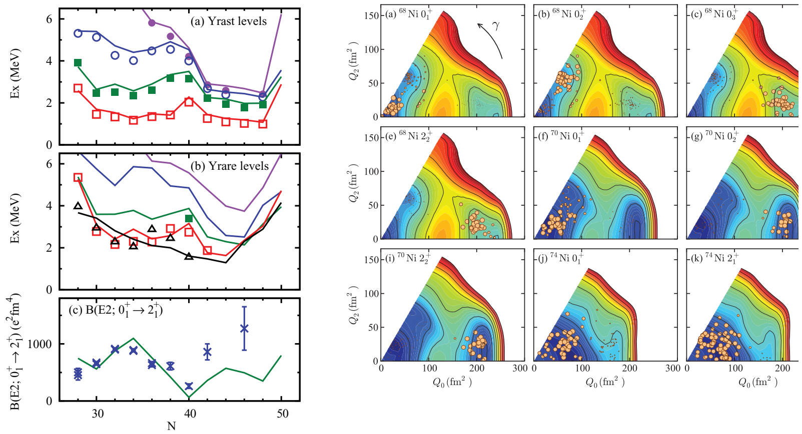
Monte Carlo Shell Model

MCSM





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

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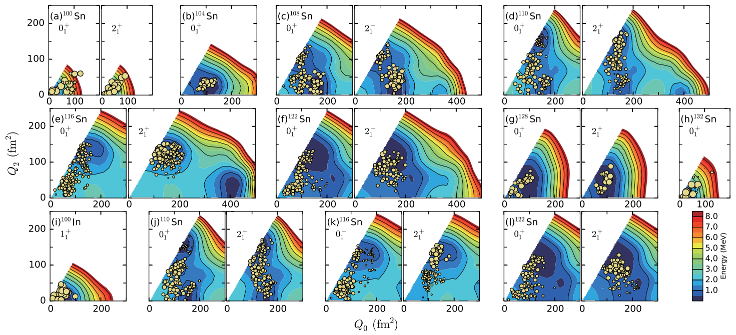

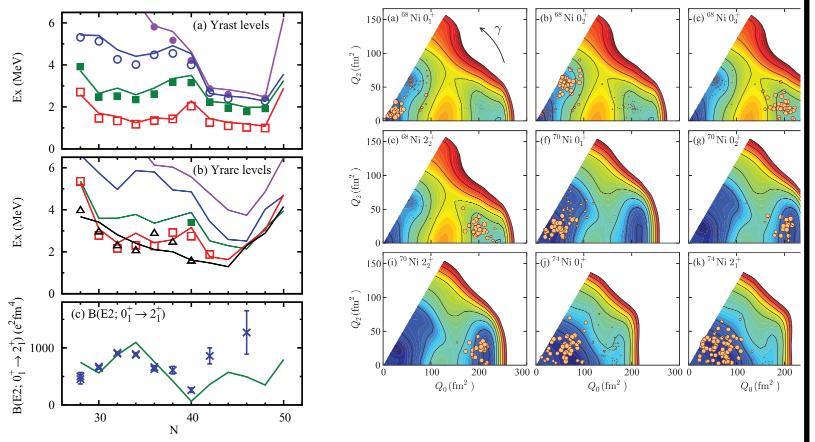

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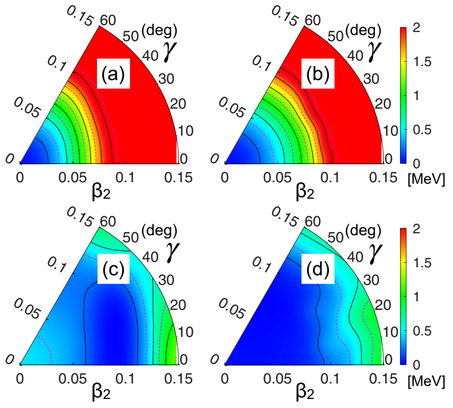
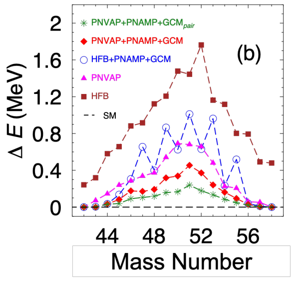
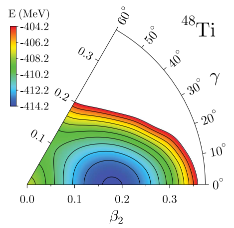
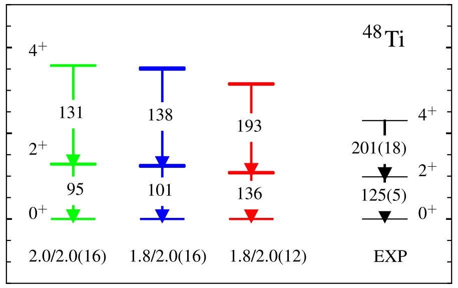
Projected Generator Coordinate Method
PGCM









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

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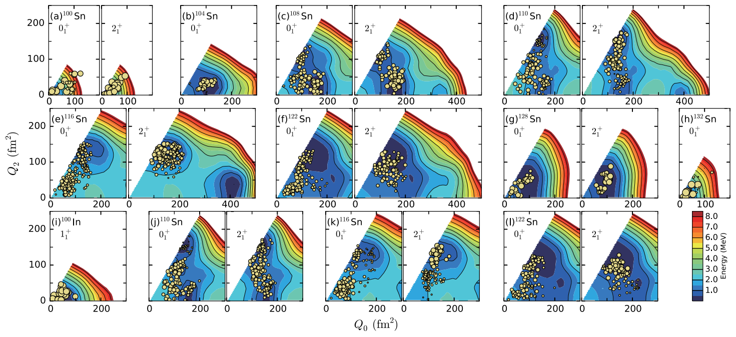

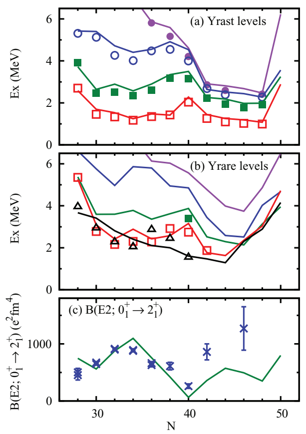

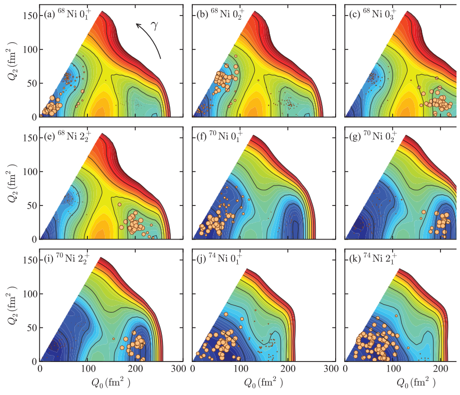

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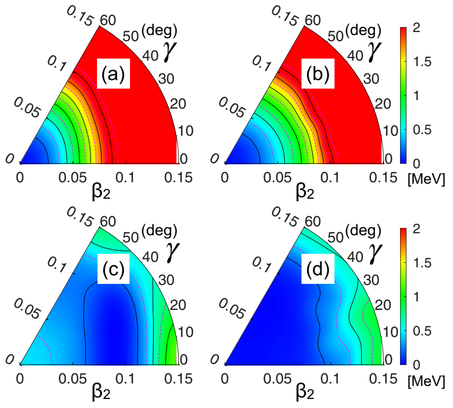

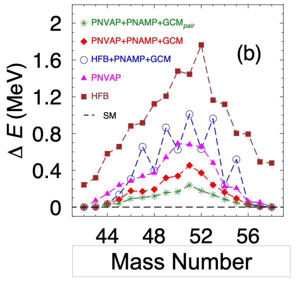

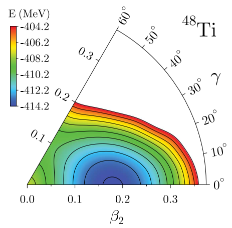

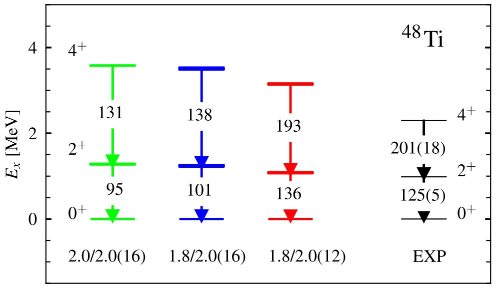

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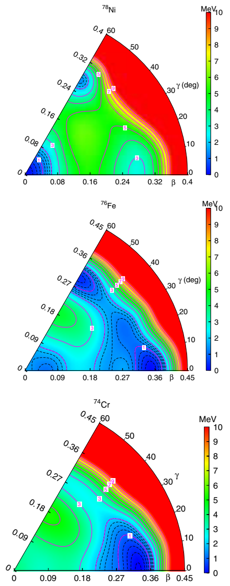
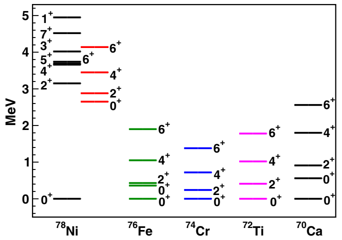
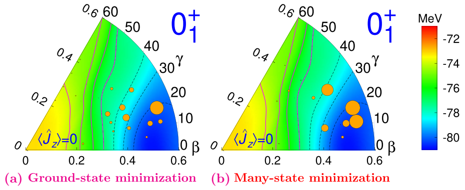
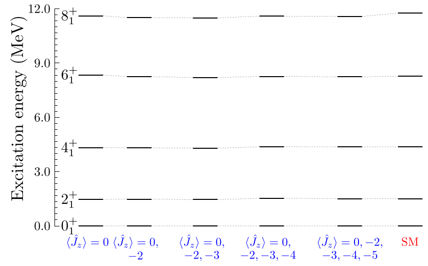
Discrete Non-orthogonal Shell Model

DNO-SM









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

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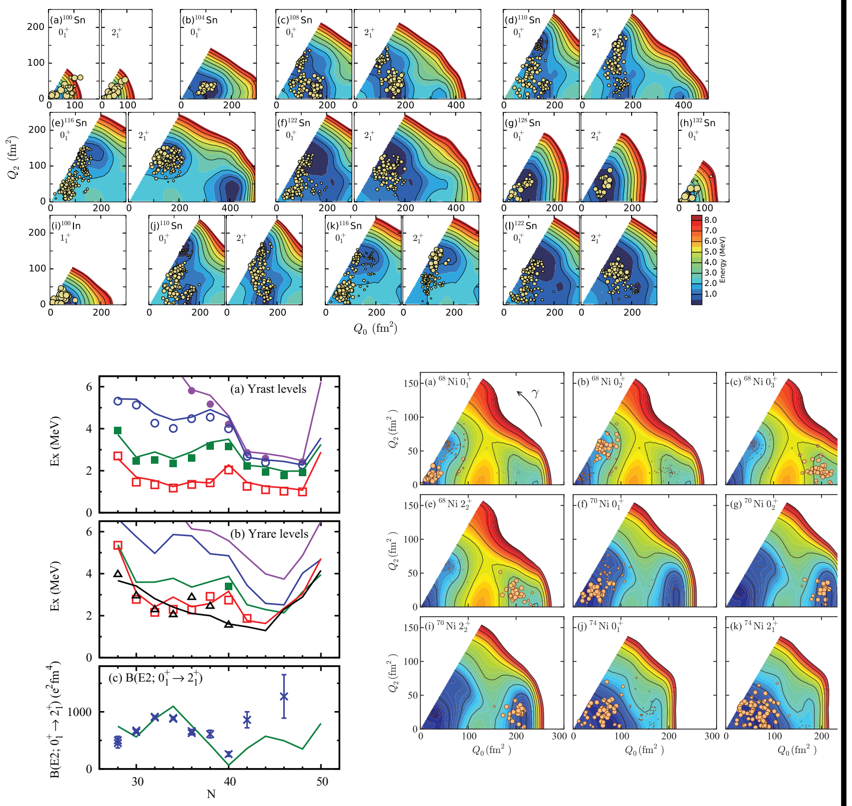

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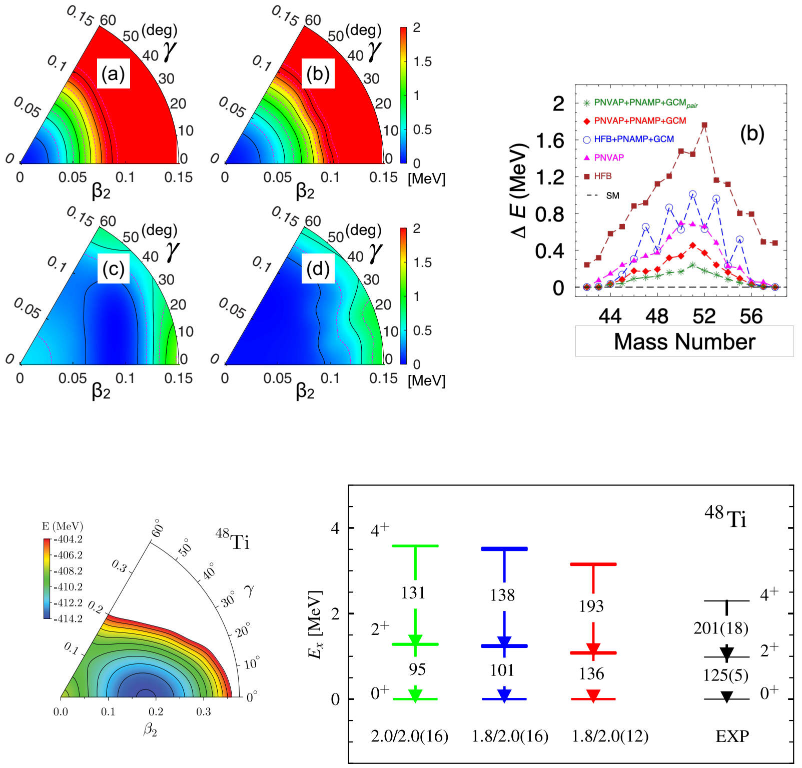

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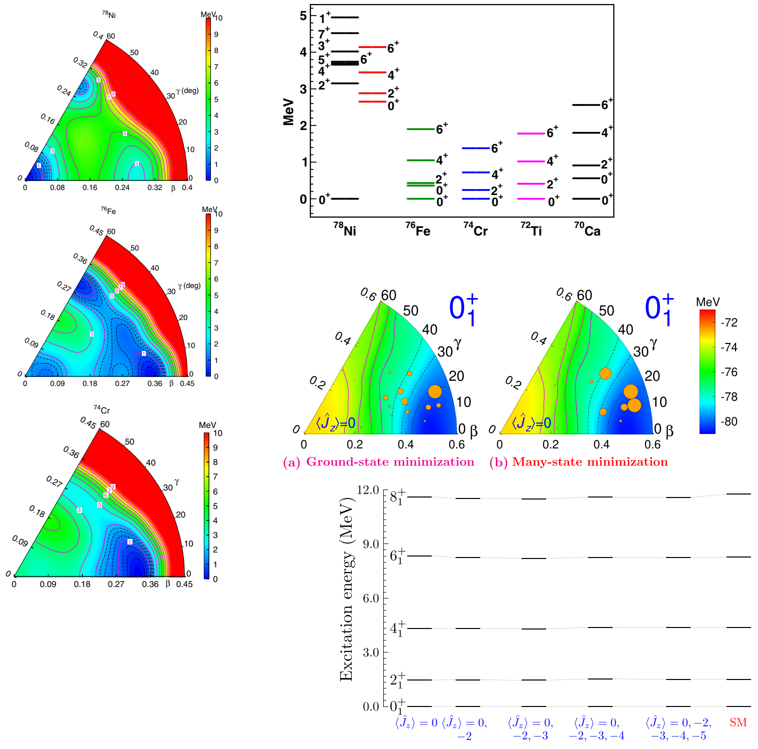

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other approaches: VAMPIR, PSM, …

Outline

Projected GCM

Nuclear wave functions: Generator Coordinate Method (GCM) ansatz

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

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

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linear combination

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linear combination

coefficients of the linear combination

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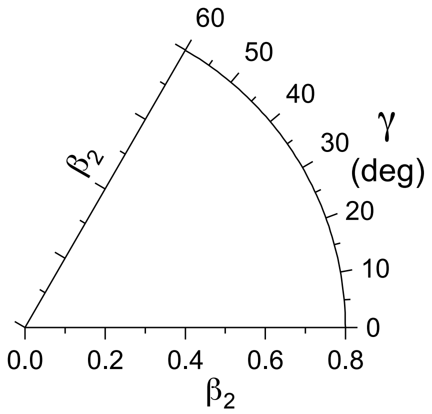

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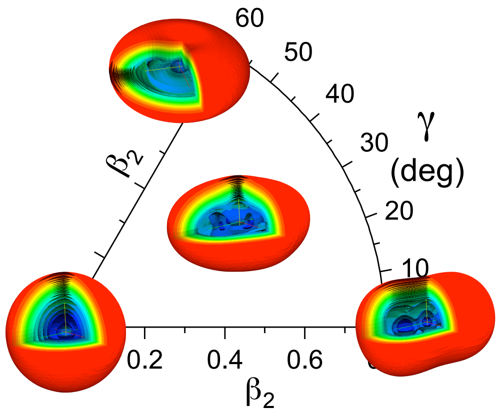

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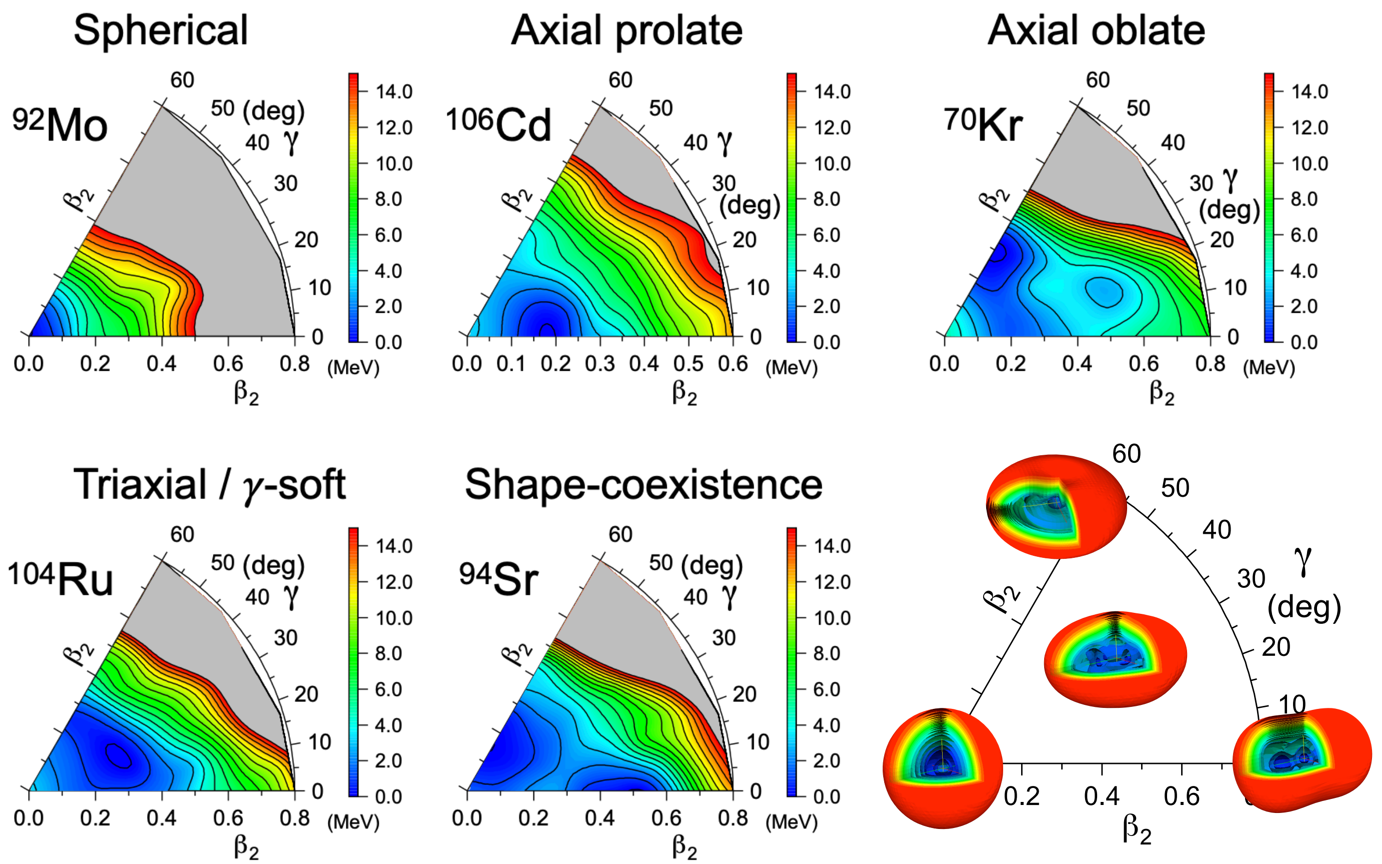
Spherical

Axial prolate

Axial oblate

Triaxial / γ-soft

Shape-coexistence

- **First classification** of the collective behavior of the nucleus based on the total energy surfaces (**TESs**) (our spherical-cow approach)

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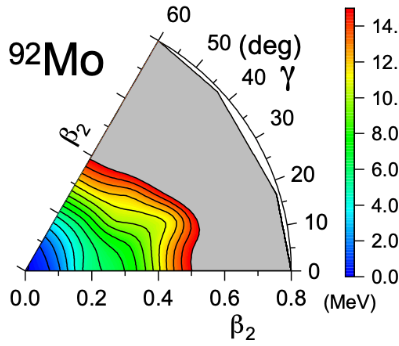
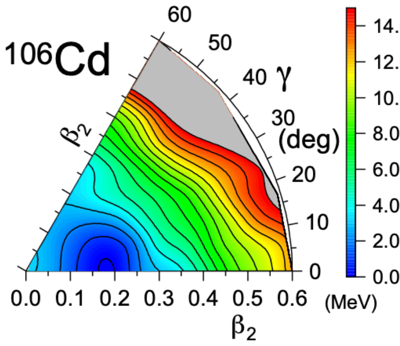


Axial prolate



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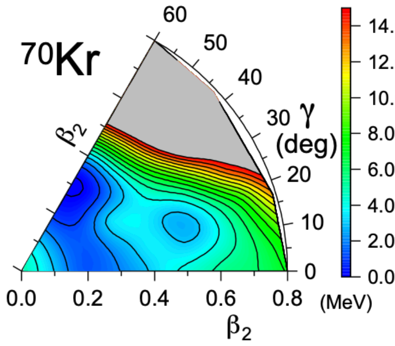

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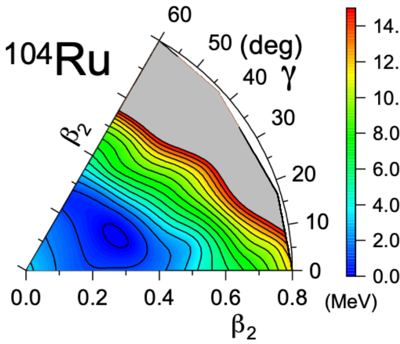

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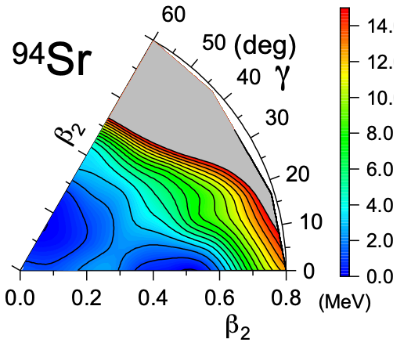

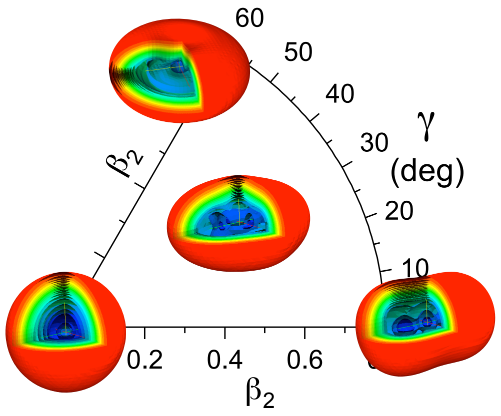

credits: M. Salgado

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"basis" states

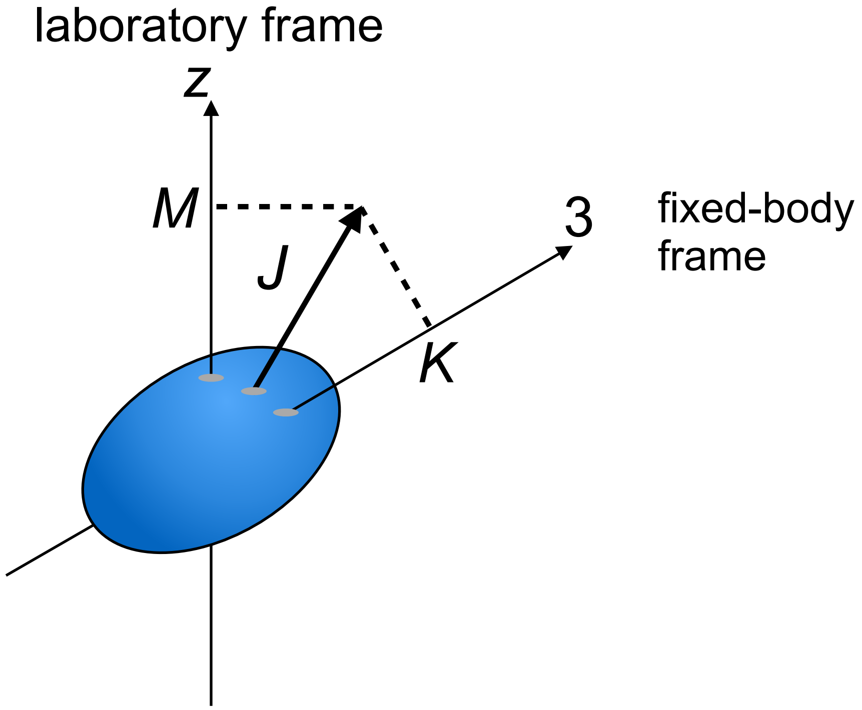
Symmetry restoration

P^J_{MK} → angular momentum projector

P^N → neutron number projector

P^Z → proton number projector

P^π → spatial parity projector



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Hill-Wheeler-Griffin (HWG) equation

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

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Outline

1. Introduction

2. Projected Generator Coordinate Method (PGCM)

3. Benchmarking PGCM against shell model with TAURUS

4. Summary and Outlook

ISM / PGCM

Comparison between Interacting Shell Model calculations and variational approaches

- Benchmark of the PGCM method against exact results.

- Same effective Hamiltonian defined in the same valence space

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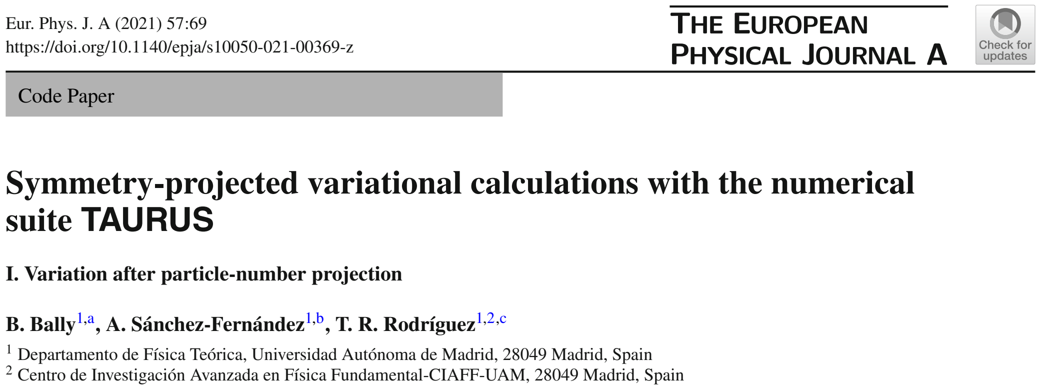
TAURUS

Theory for **A** **U**nified descrip**R**tion of n**U**clear **S**tructure



Eur. Phys. J. A (2021) 57:69
https://doi.org/10.1140/epja/s10050-021-00369-z

THE EUROPEAN PHYSICAL JOURNAL A

Code Paper

Symmetry-projected variational calculations with the numerical suite TAURUS

I. Variation after particle-number projection

B. Bally[1,a], **A. Sánchez-Fernández**[1,b], **T. R. Rodríguez**[1,2,c]

[1] Departamento de Física Teórica, Universidad Autónoma de Madrid, 28049 Madrid, Spain
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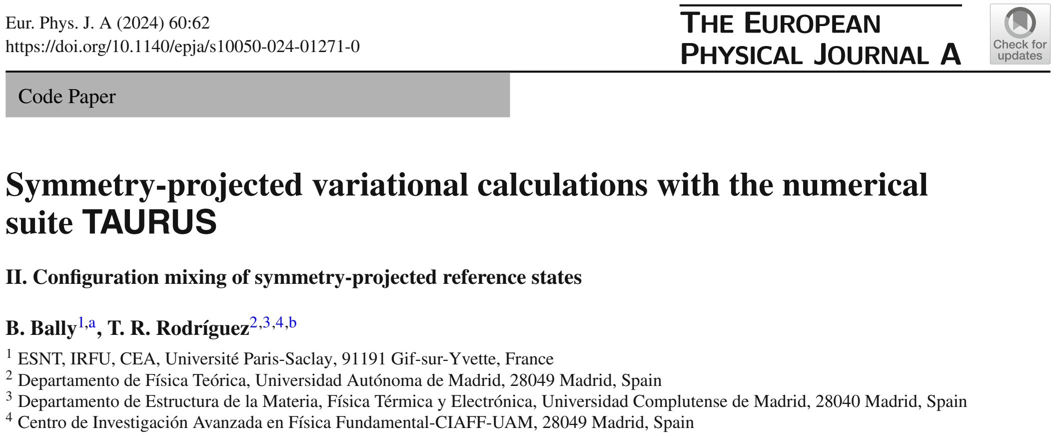

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THE EUROPEAN PHYSICAL JOURNAL A

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Symmetry-projected variational calculations with the numerical suite TAURUS

II. Configuration mixing of symmetry-projected reference states

B. Bally[1,a], **T. R. Rodríguez**[2,3,4,b]

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Marie Skłodowska-Curie Actions
TAURUS (ID:839847)

Comparison between Interacting Shell Model calculations and variational approaches

- Benchmark of the PGCM method against exact results.
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TAURUS

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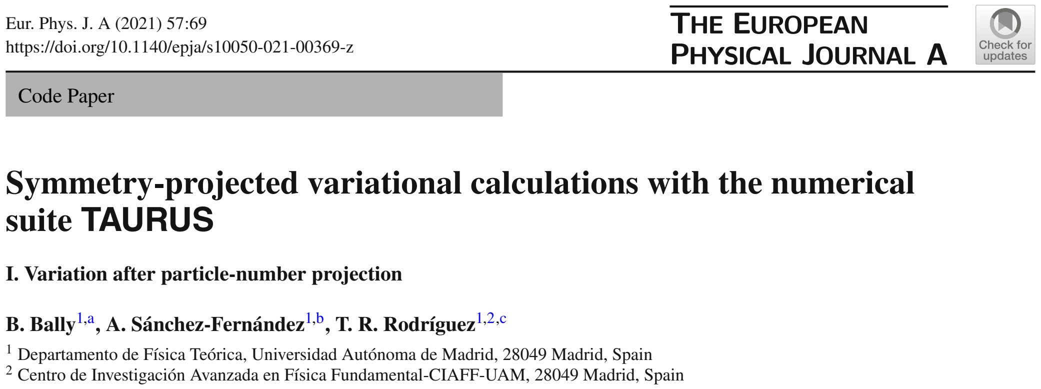

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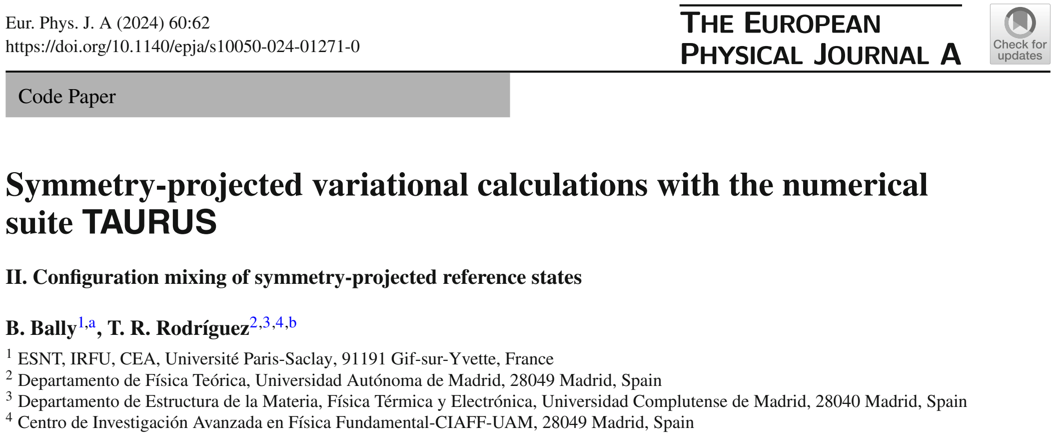

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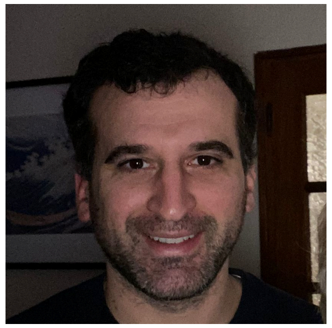

European Commission
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TAURUS (ID:839847)

ISM vs PGCM

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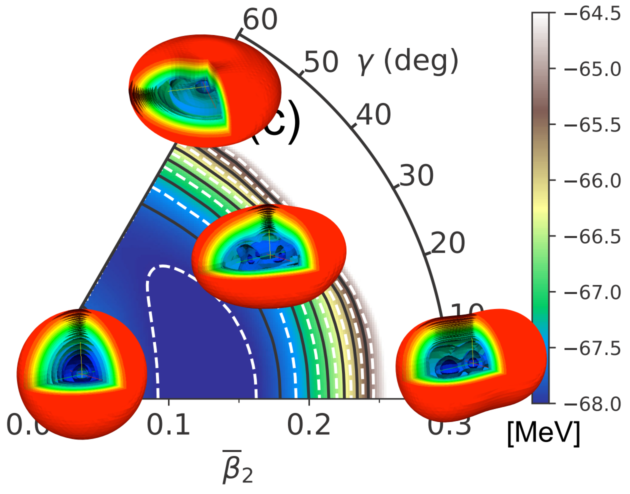

multipole deformations

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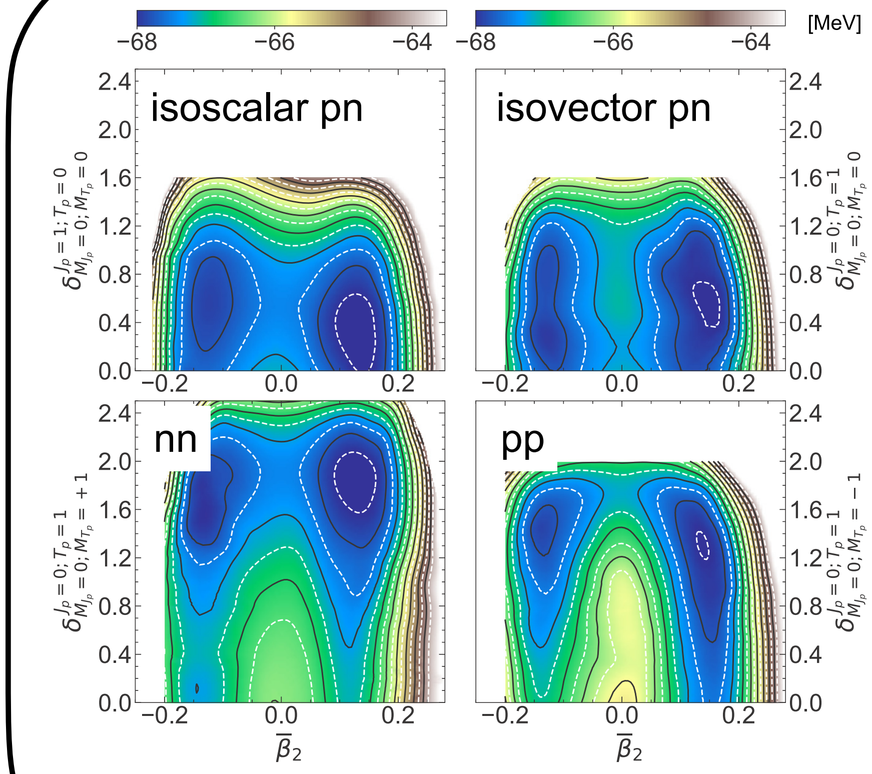
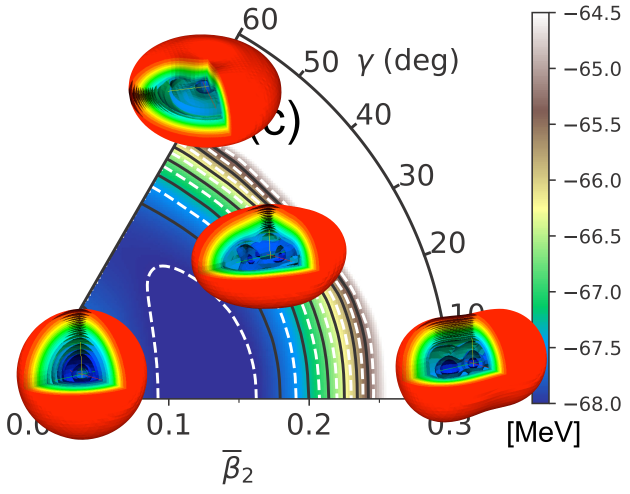


pairing fluctuations



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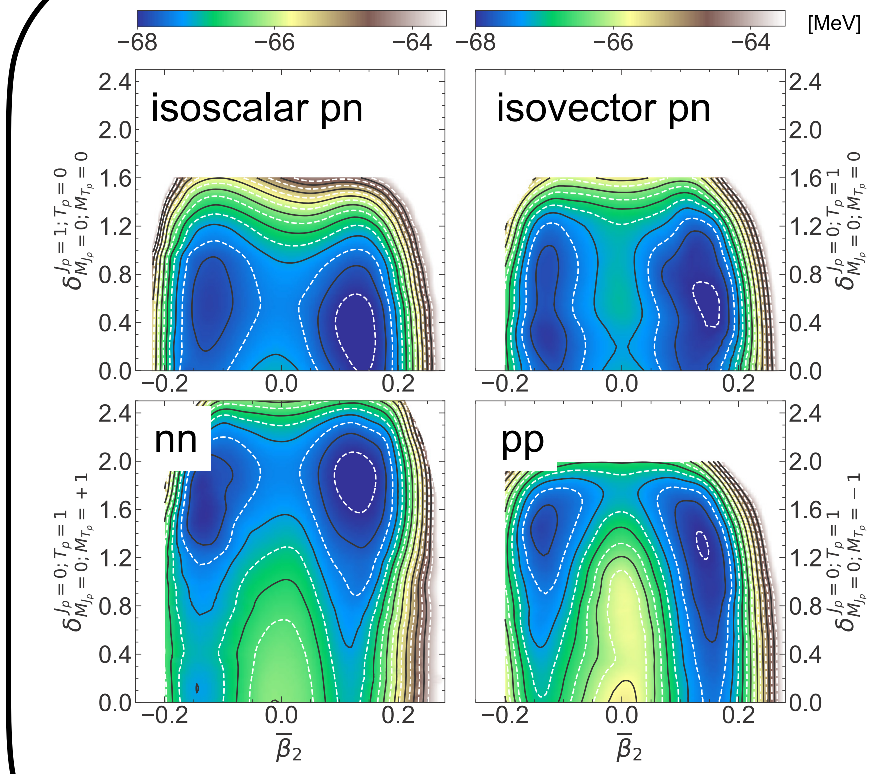

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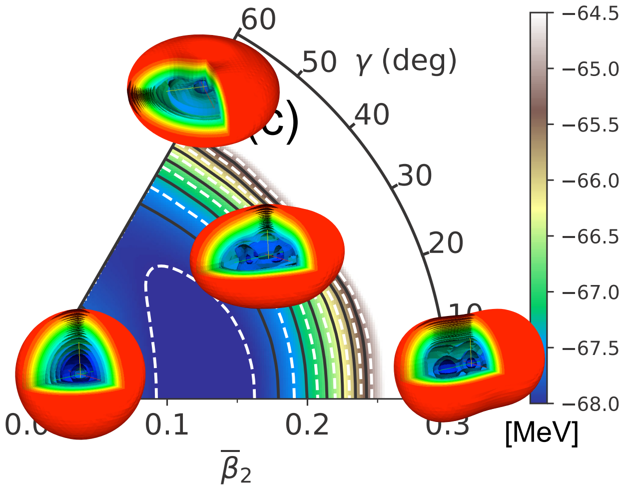
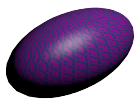


multipole deformations

J_{crank}=0



intrinsic rotations (cranking)

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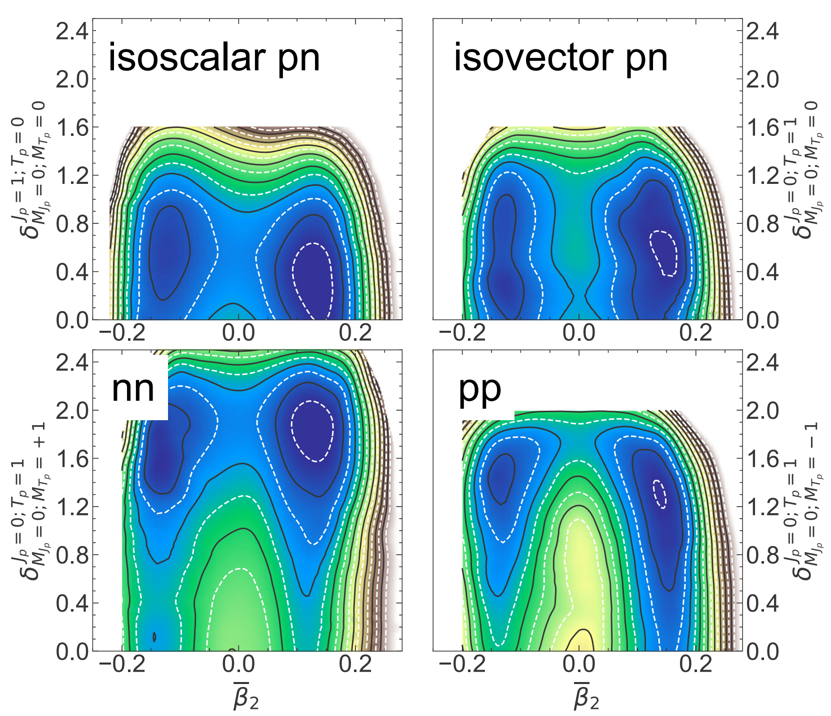

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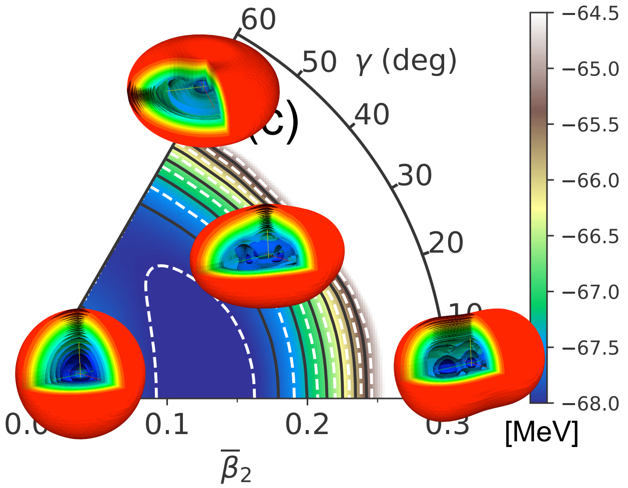

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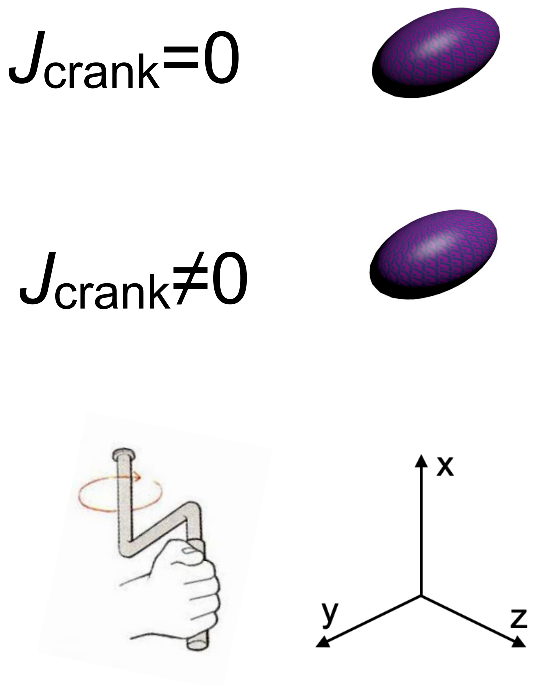

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intrinsic rotations (cranking)

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- Ground and excited state energies
- Gamow-Teller distributions
- Magnetic dipole responses

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USD interaction

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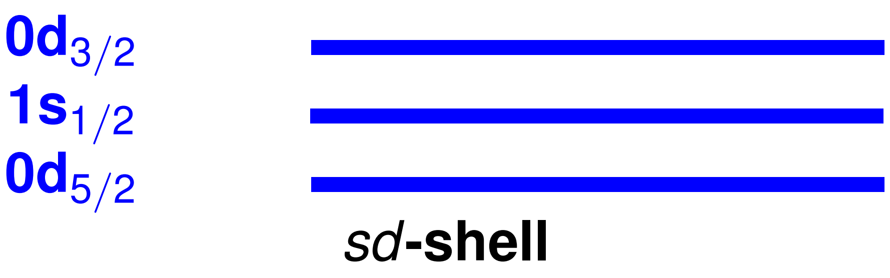

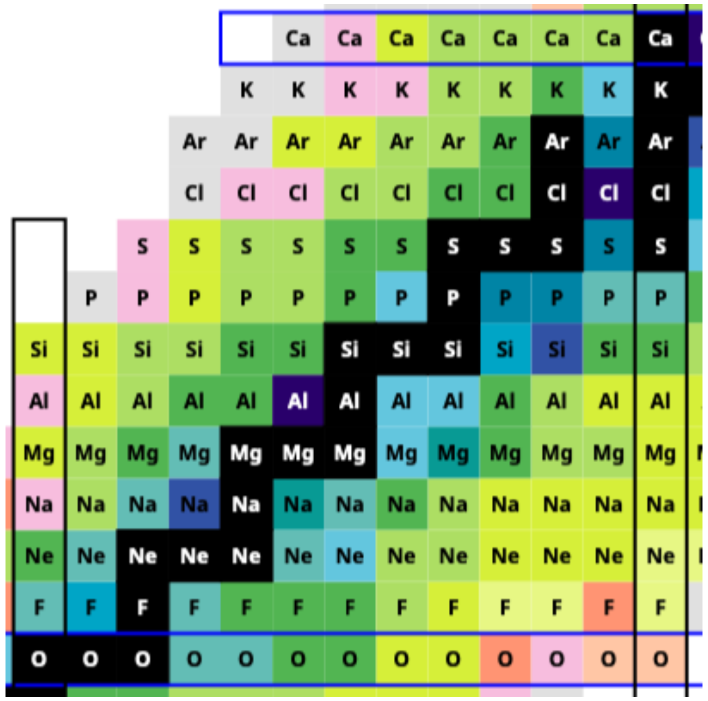

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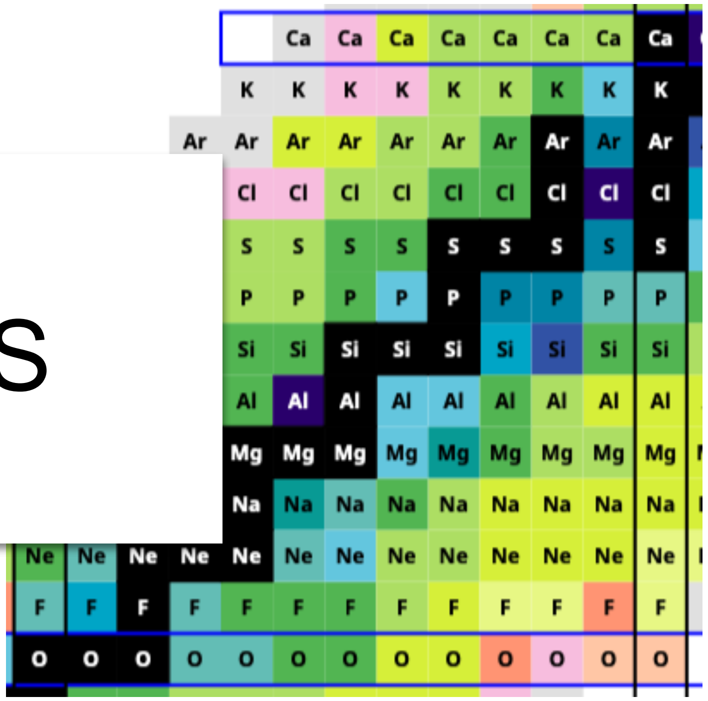
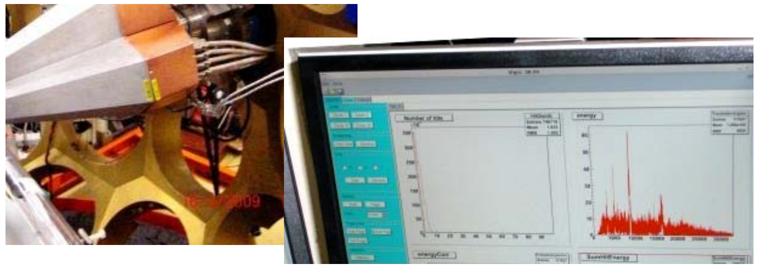
sd-**shell**





AGATA commissioning 2009

Commissioning TAURUS

Ground state energies e-e / e-o

Global performance of the PGCM method in the *sd*-shell

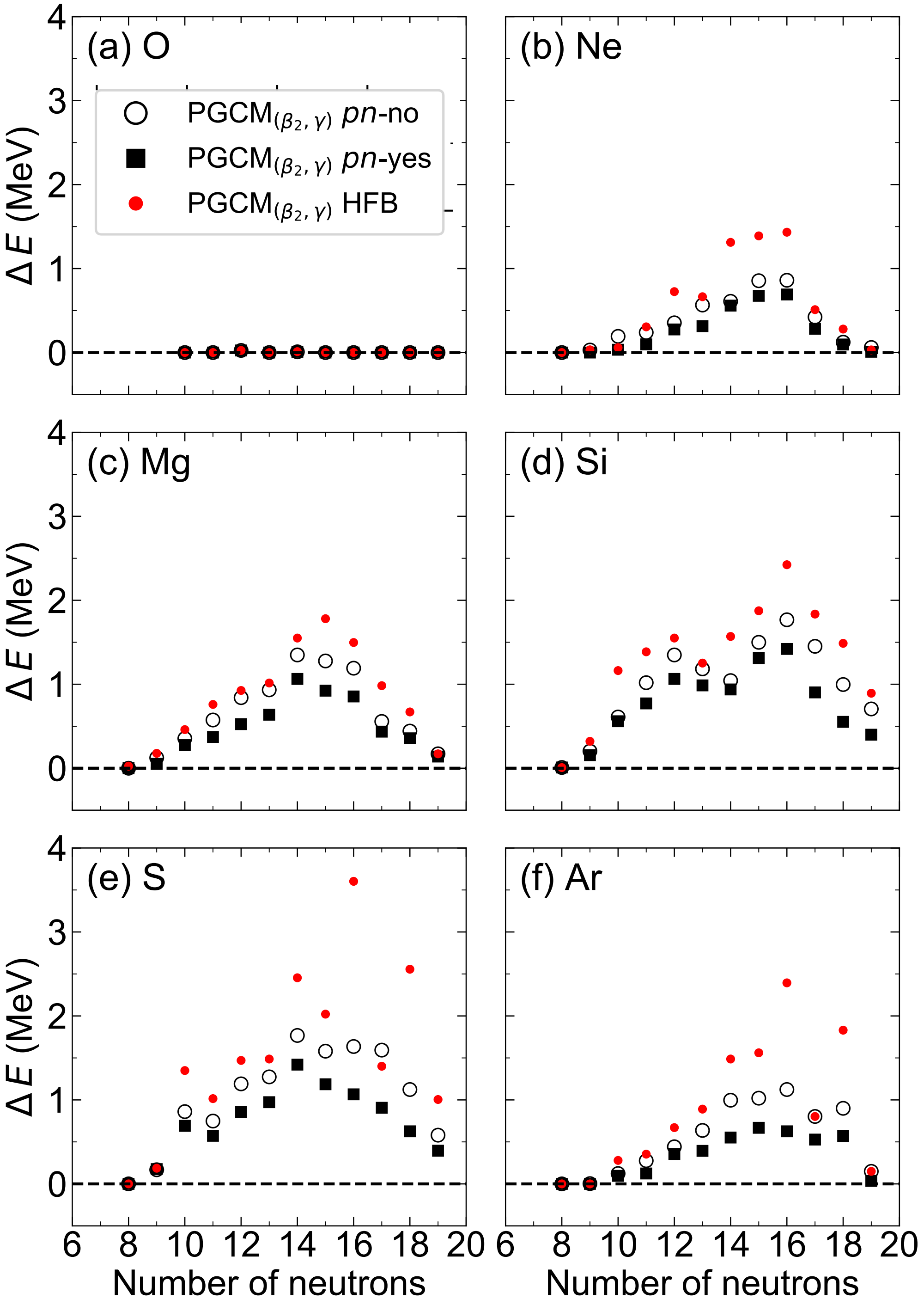
$$\Delta E = E_{\mathrm{PGCM}} - E_{\mathrm{SM}}$$

- We compare different choices of PGCM depending on the type of intrinsic wave function

- Best approach to the exact ground state energy is provided by the PNVAP minimization that allows proton-neutron mixing

- Largest difference are obtained in mid-shell nuclei

- Angular momentum of the g.s. of e-o systems is well-reproduced with PNVAP *pn*-mixing

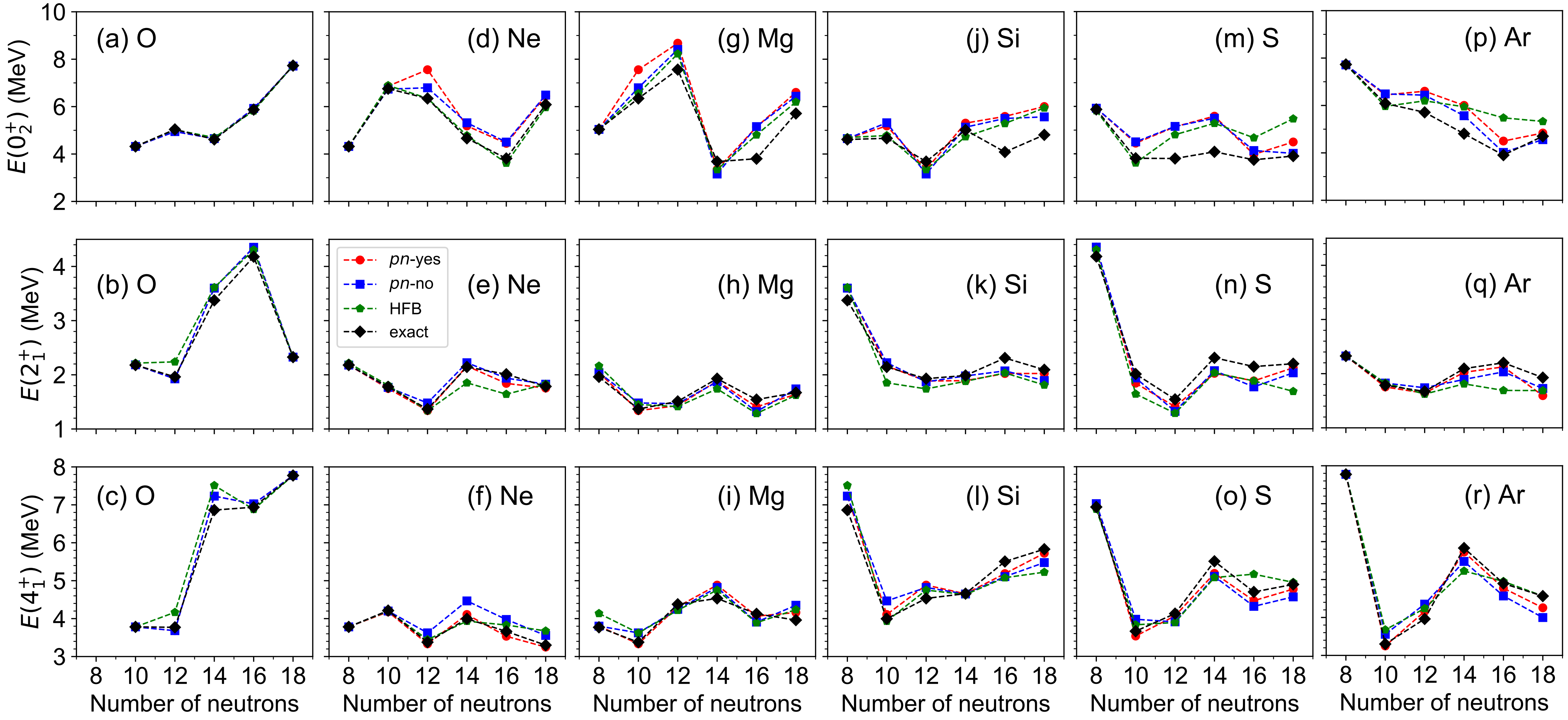


A. Sánchez, B. Bally, T. R. R., PRC 104, 054306 (2021)

Excited states e-e

Global performance of the PGCM method in the *sd*-shell

Excited states in **even-even** nuclei

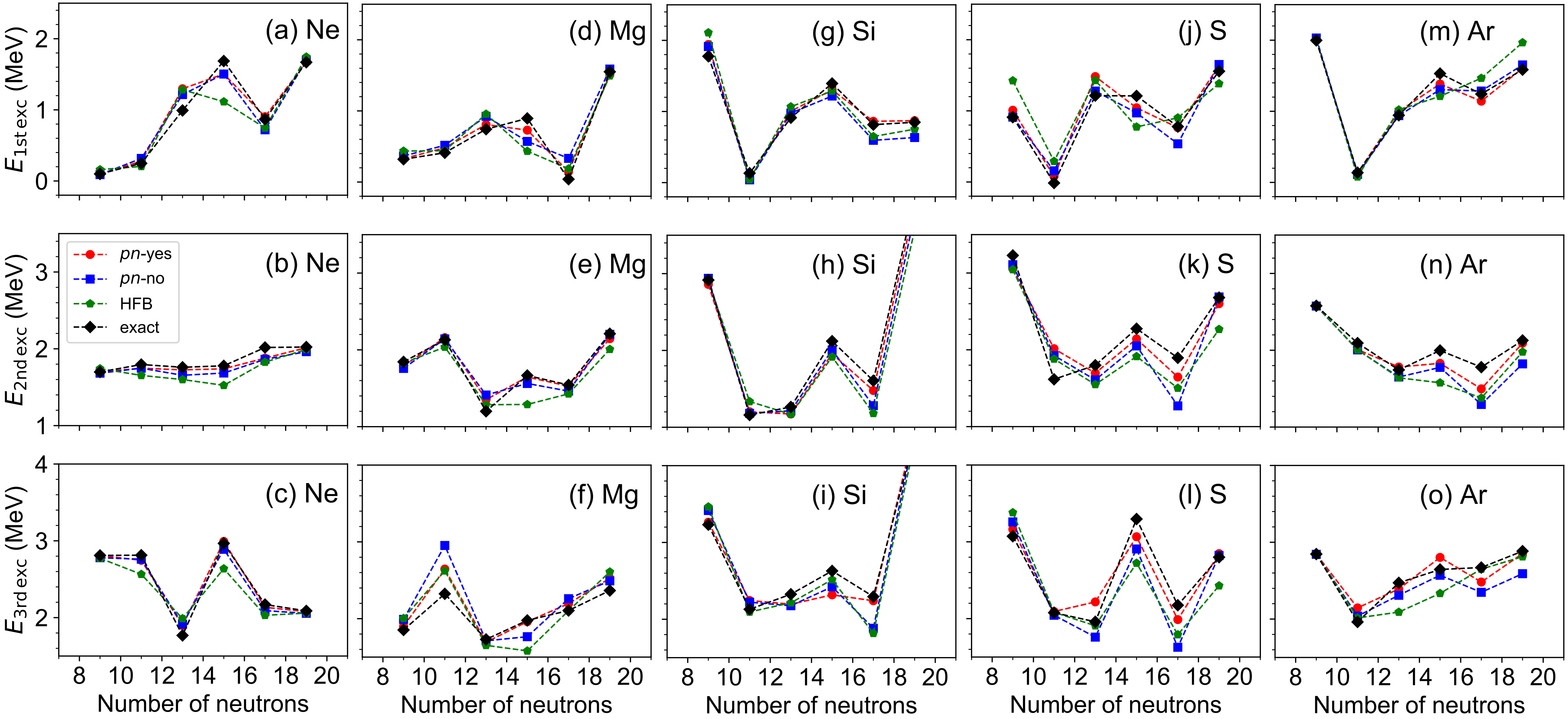


A. Sánchez, B. Bally, T. R. R., PRC 104, 054306 (2021)

Excited states e-o

Global performance of the PGCM method in the *sd*-shell

Excited states in **even-odd** nuclei



A. Sánchez, B. Bally, T. R. R., PRC 104, 054306 (2021)

Beta-decay properties

Transition matrix elements

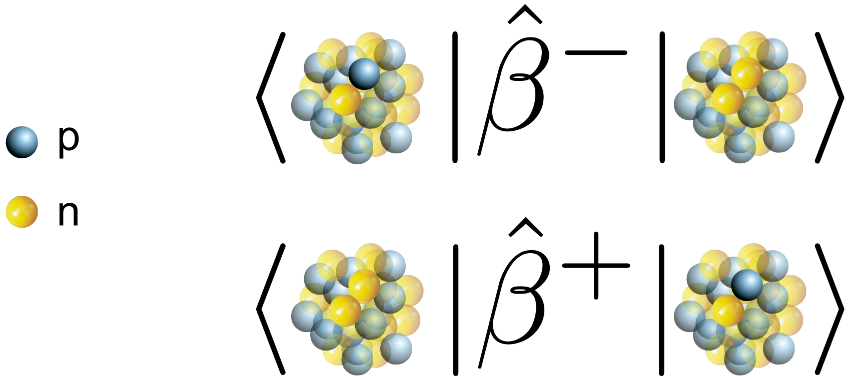
$|\Psi^{\Gamma_i}_{\sigma_i}\rangle \longrightarrow$ initial state

$|\Psi^{\Gamma_f}_{\sigma_f}\rangle \longrightarrow$ final state

$$\langle\Psi^{\Gamma_f}_{\sigma_f}|\hat{M}_{\lambda\mu}|\Psi^{\Gamma_i}_{\sigma_i}\rangle = \sum_{\substack{q_fK_f\\ q_iK_i}} f^{\Gamma_f *}_{\sigma_f;q_fK_f}\langle\Phi_f(q_f)|P^{J_f}_{K_fM_f}P^{N_f}P^{Z_f}P^{\pi_f}\hat{M}_{\lambda\mu}P^{\pi_i}P^{Z_i}P^{N_i}P^{J_i}_{M_iK_i}|\Phi_i(q_i)\rangle f^{\Gamma_i}_{\sigma_i;q_iK_i}$$

$\boldsymbol{t}_\pm, \boldsymbol{\sigma}\boldsymbol{t}_\pm$

$$B(GT^\pm) = \left(\frac{g_A}{g_V}\right)^2 \frac{1}{(2J_i+1)}\left|\langle f||\sum_k \boldsymbol{\sigma}^k\boldsymbol{t}^k_\pm||i\rangle\right|^2$$



Beta-decay properties

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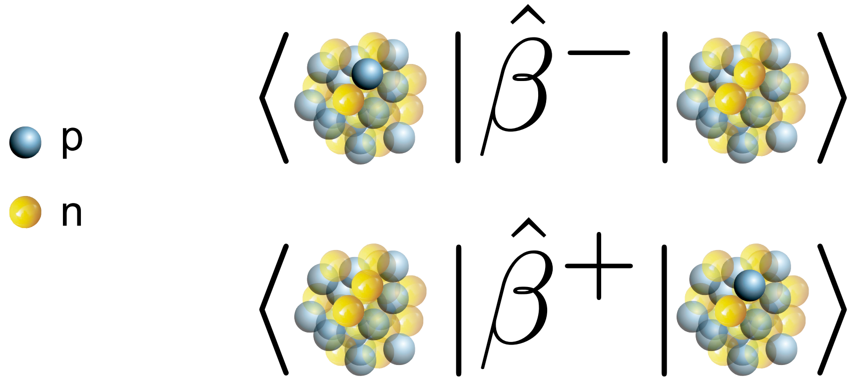
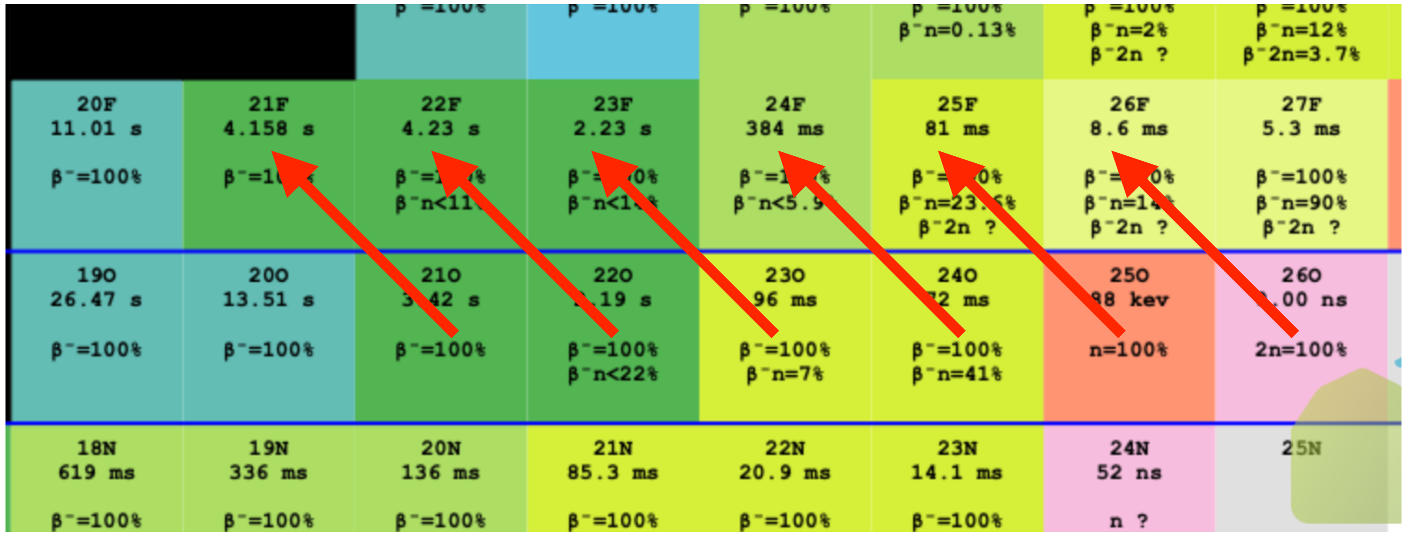


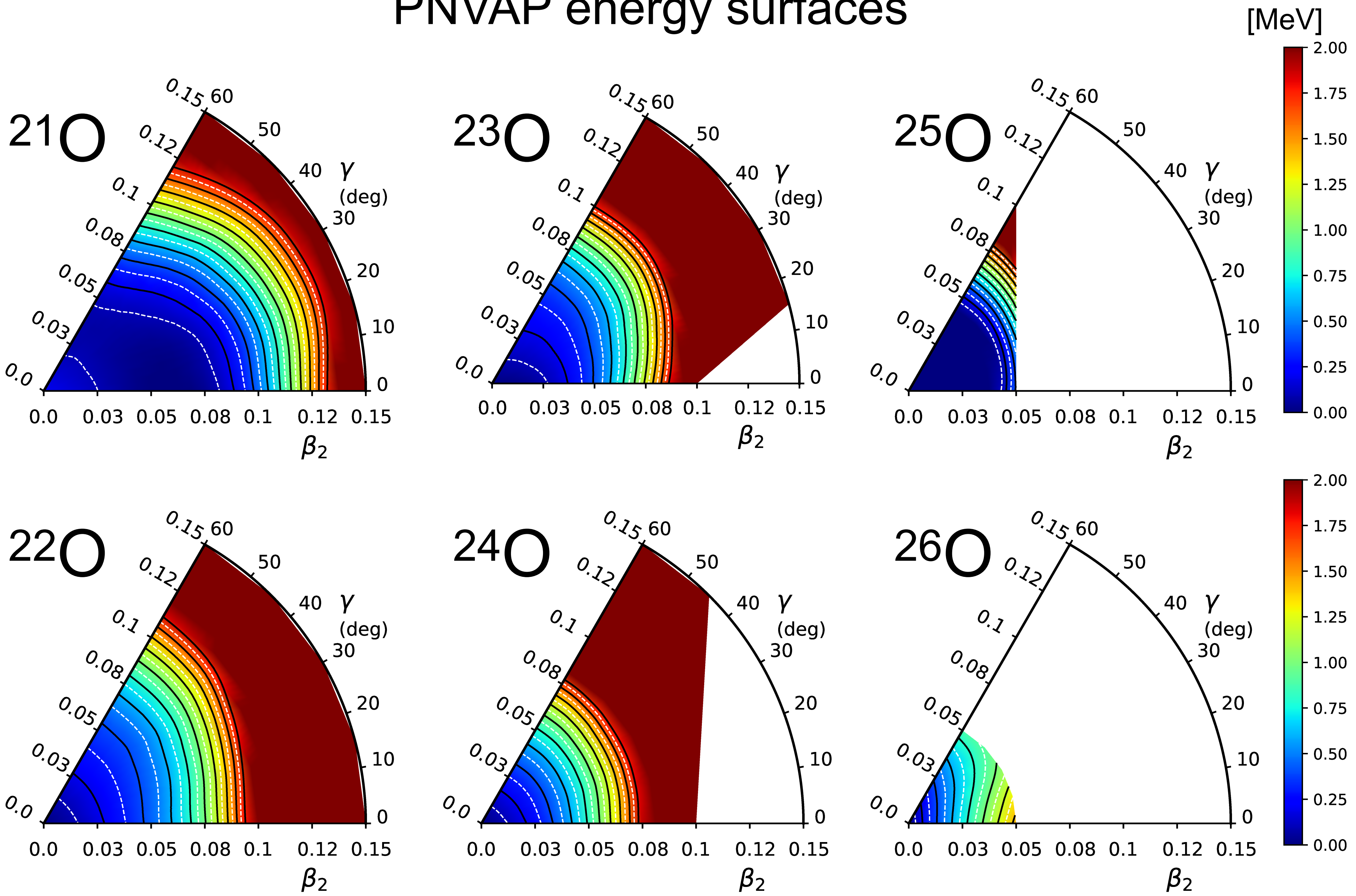


		β^-=100%	β^-=100%	β^-=100%	β^-=100% β^-n=0.13%	β^-=100% β^-n=2% β^-2n ?	β^-=100% β^-n=12% β^-2n=3.7%
20F 11.01 s β^-=100%	21F 4.158 s β^-=10	22F 4.23 s β^-=1 % β^-n<11	23F 2.23 s β^-= 0% β^-n<1	24F 384 ms β^-=1 % β^-n<5.9	25F 81 ms β^-= 0% β^-n=23. % β^-2n ?	26F 8.6 ms β^-= 0% β^-n=14 β^-2n ?	27F 5.3 ms β^-=100% β^-n=90% β^-2n ?
19O 26.47 s β^-=100%	20O 13.51 s β^-=100%	21O 3 42 s β^-=100%	22O .19 s β^-=100% β^-n<22%	23O 96 ms β^-=100% β^-n=7%	24O 2 ms β^-=100% β^-n=41%	25O 8 kev n=100%	26O .00 ns 2n=100%
18N 619 ms β^-=100%	19N 336 ms β^-=100%	20N 136 ms β^-=100%	21N 85.3 ms β^-=100%	22N 20.9 ms β^-=100%	23N 14.1 ms β^-=100%	24N 52 ns n ?	25N

Beta-decay properties

- Oxygen isotopes: no protons in the *sd*-shell, only neutrons contribute (no *pn* channel)

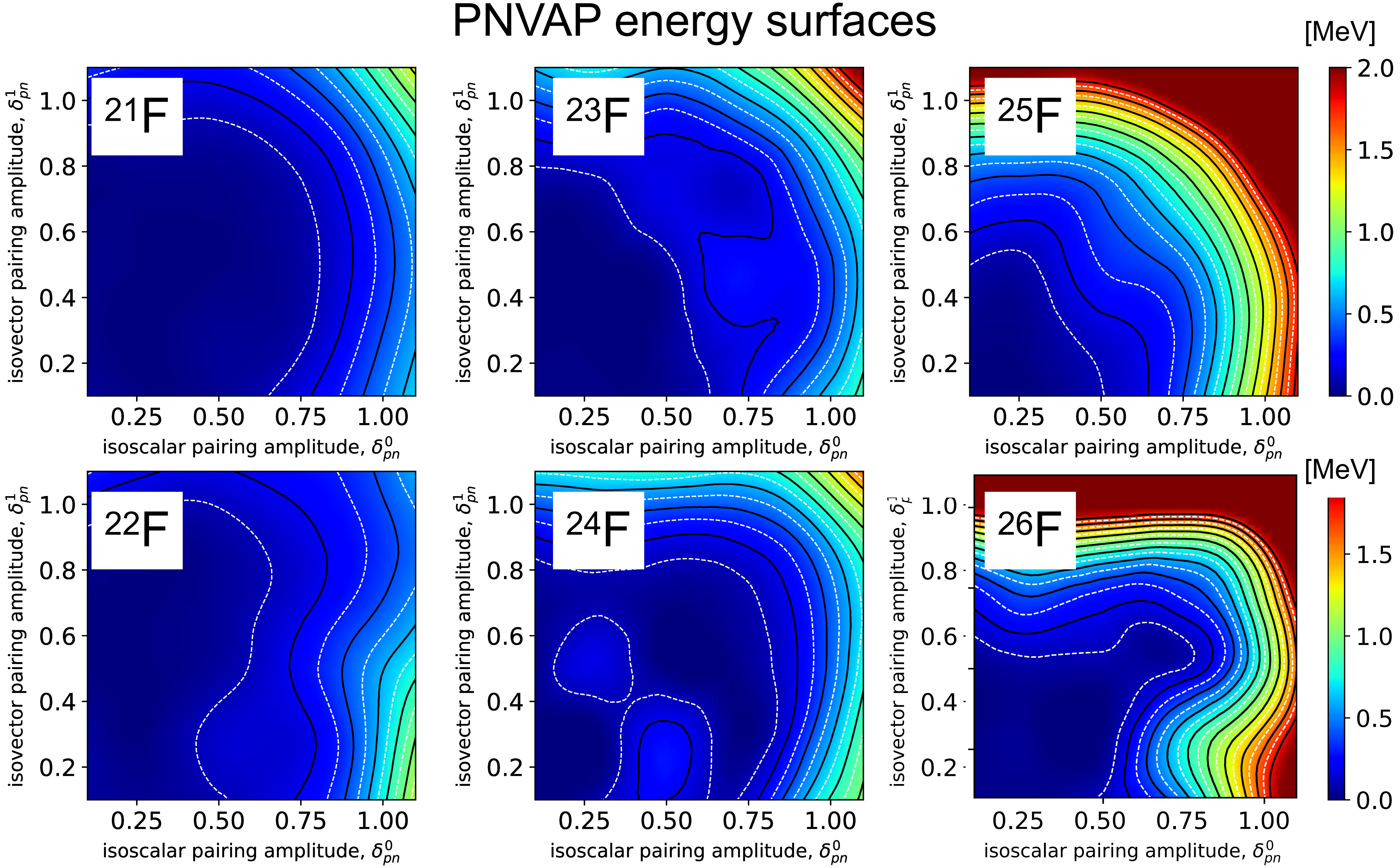
PNVAP energy surfaces



Beta-decay properties

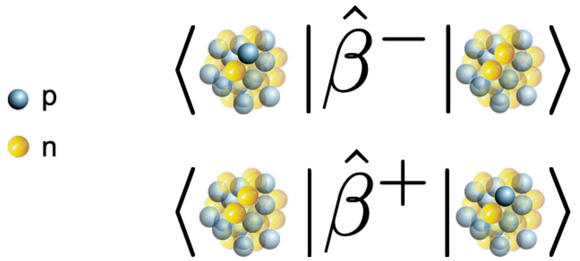
- Fluorine isotopes

PNVAP energy surfaces

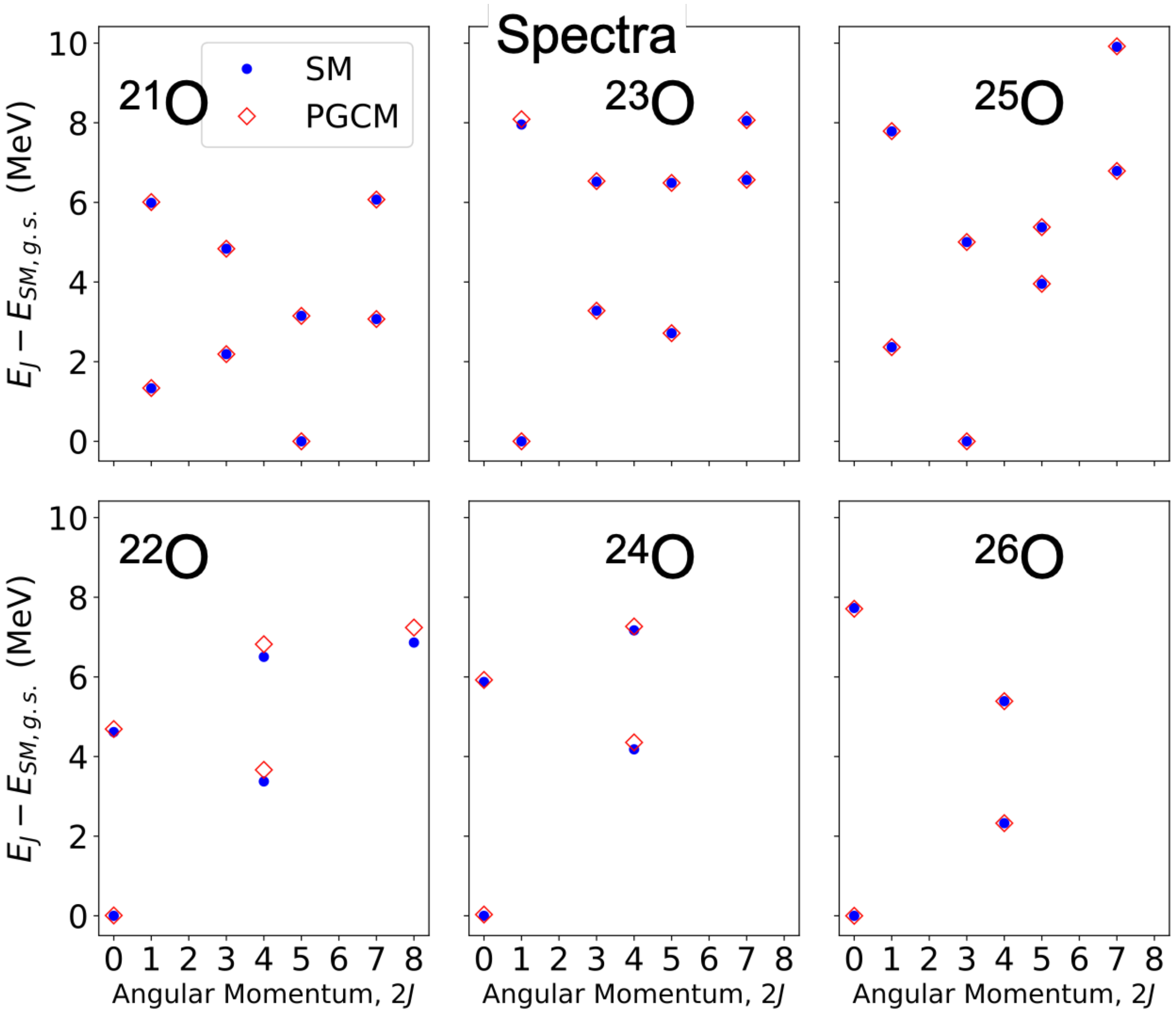


Beta-decay properties

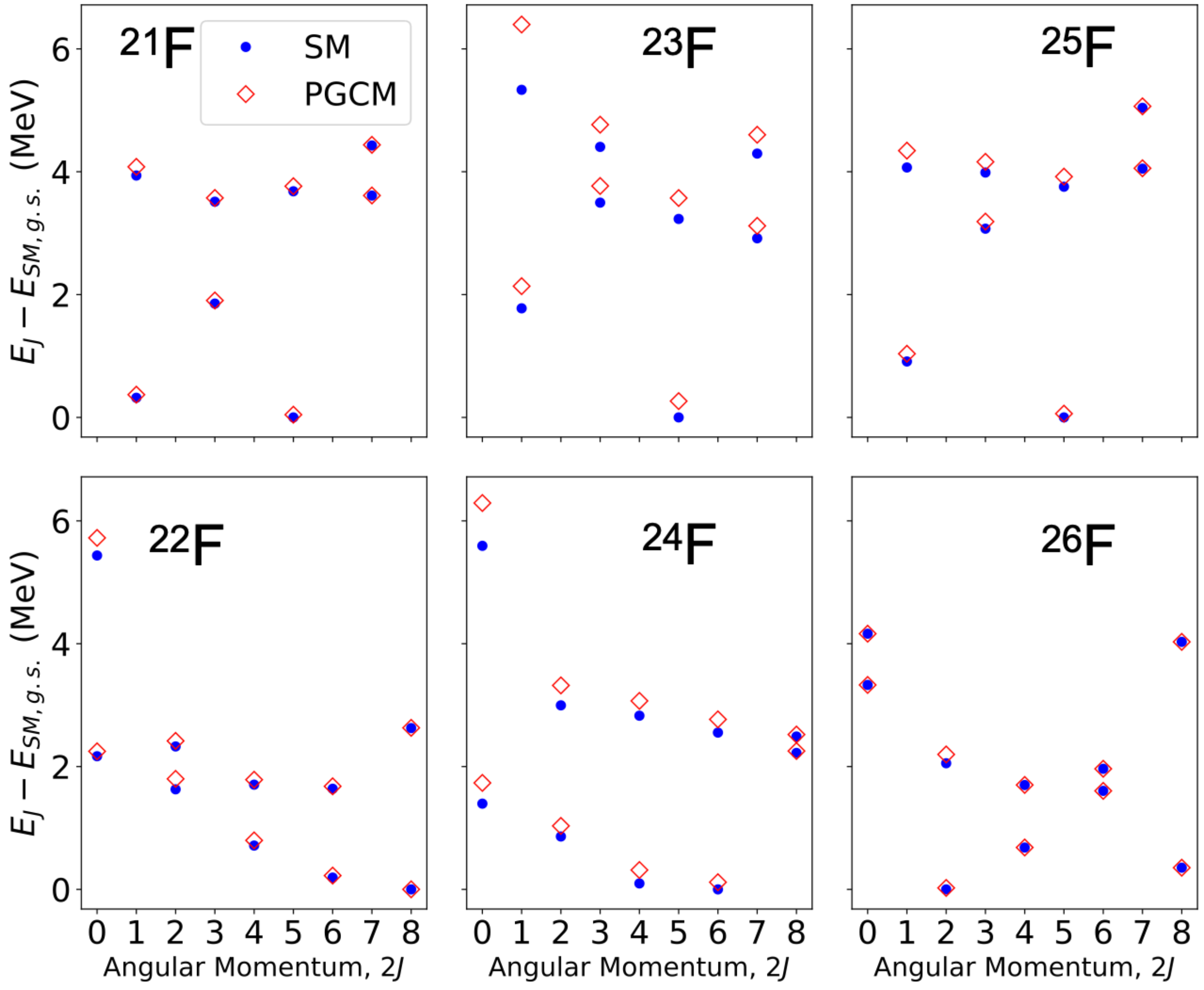
Benchmark of the PGCM method against exact results.



mother nuclei



daughter nuclei

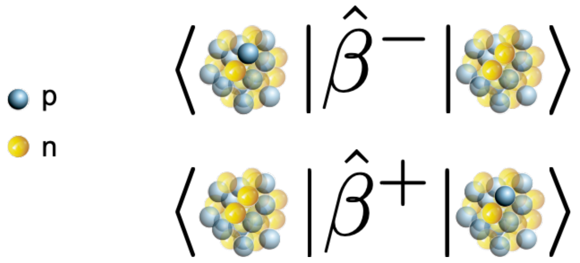


V. Vijayan et al., in preparation

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

V. Vijayan et al., in preparation

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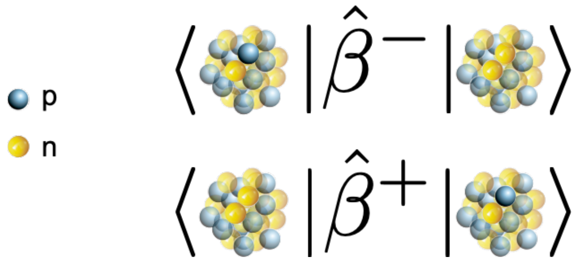

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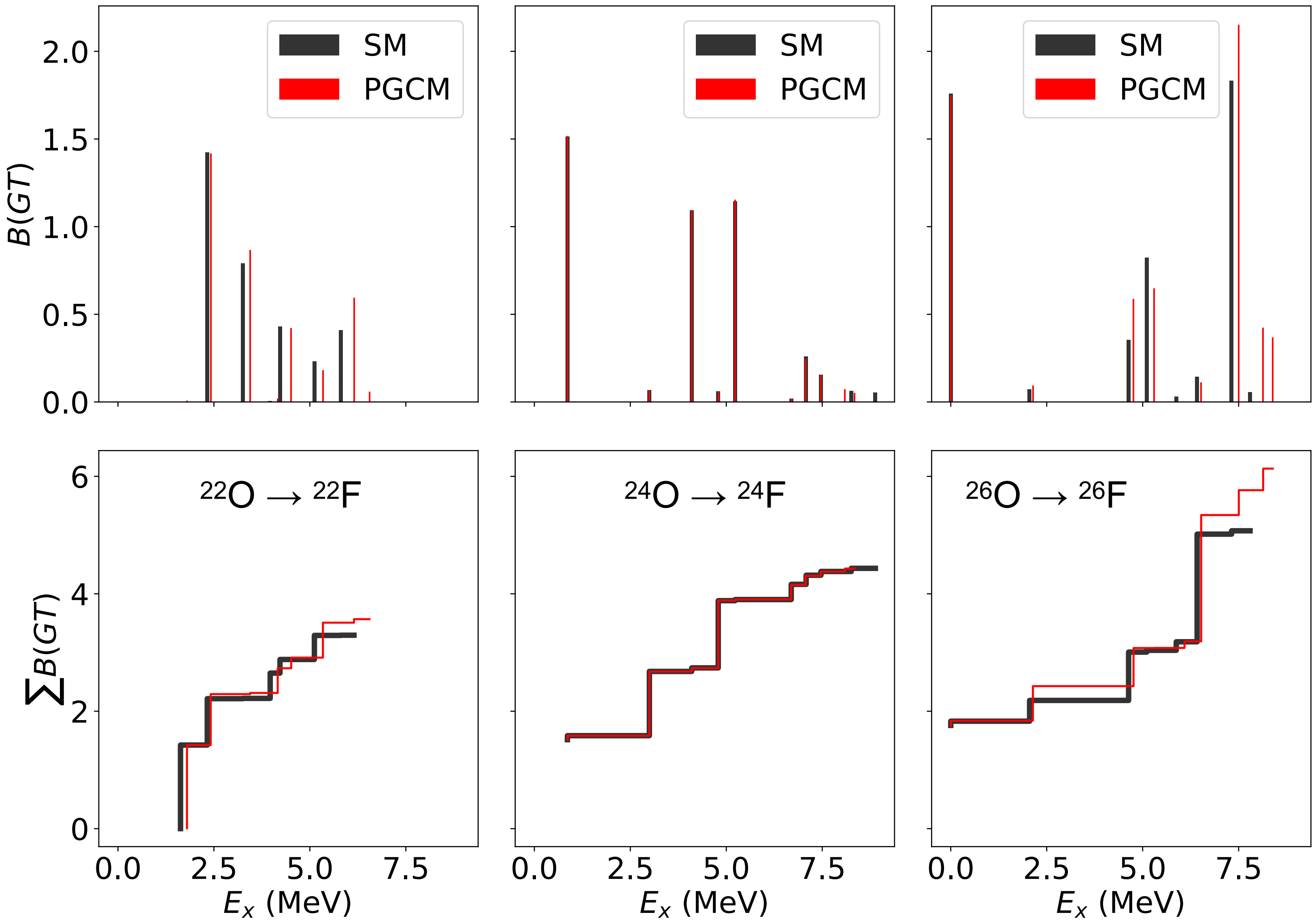
B(GT) distributions



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B(M1) strength functions in e-e nuclei

Magnetic transitions

$$B(M\lambda, J_i \to J_f f) = \frac{1}{2J_i+1} | \langle J_f || \hat{M}_{\lambda\mu} || J_i \rangle |^2$$

$$\hat{M}_{\lambda\mu} = \left(g_s \vec{s} + \frac{2}{\lambda+1} g_l \vec{l} \right) \vec{\nabla} r^{\lambda} Y_{\lambda\mu}$$

***B*(*M*1)**

$$|J_f\rangle = |0^+_1\rangle \qquad |J_i\rangle = |1^+_m\rangle$$

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B(M1)

$$\boxed{|J_f\rangle = |0_1^+\rangle}$$

ground state

$$\boxed{|J_i\rangle = |1_m^+\rangle}$$

set of excited states
(level densities)

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😥

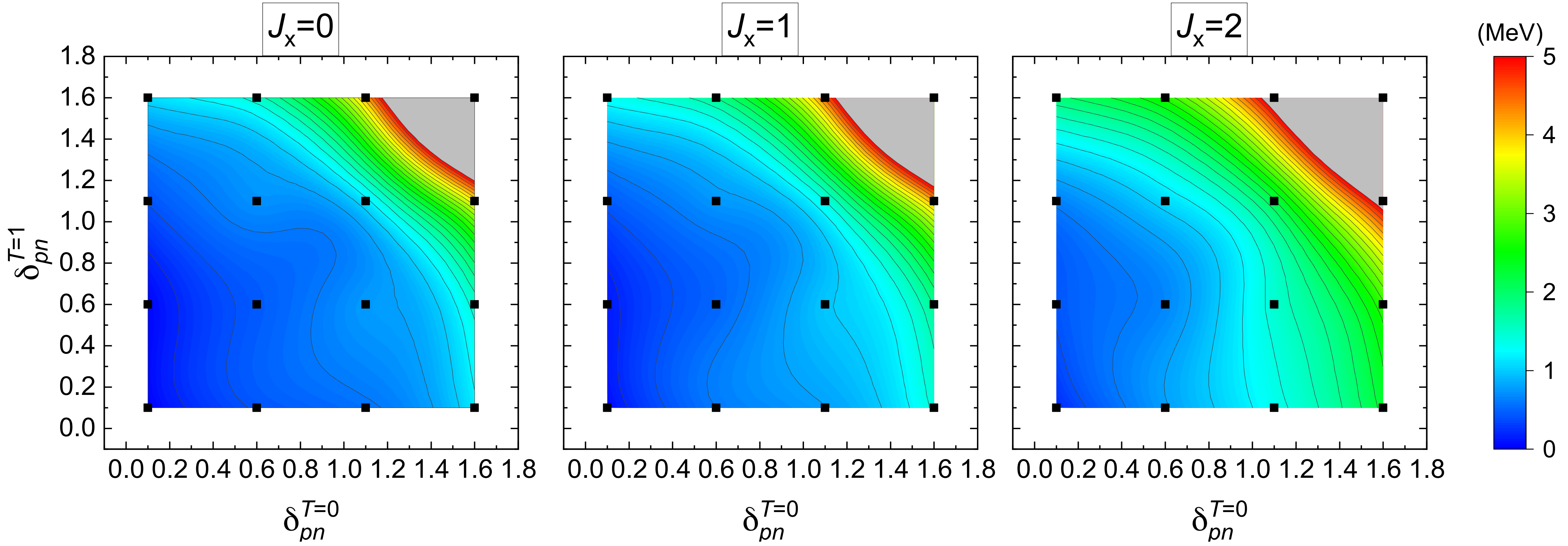
set of excited states
(level densities)

challenging!

B(M1) strength functions in e-e nuclei

Exploring cranking, pn-pairing (isoscalar and isovector) $\{|\Phi(j_x, \delta_{pn}^{T=0}, \delta_{pn}^{T=1})\rangle\}$

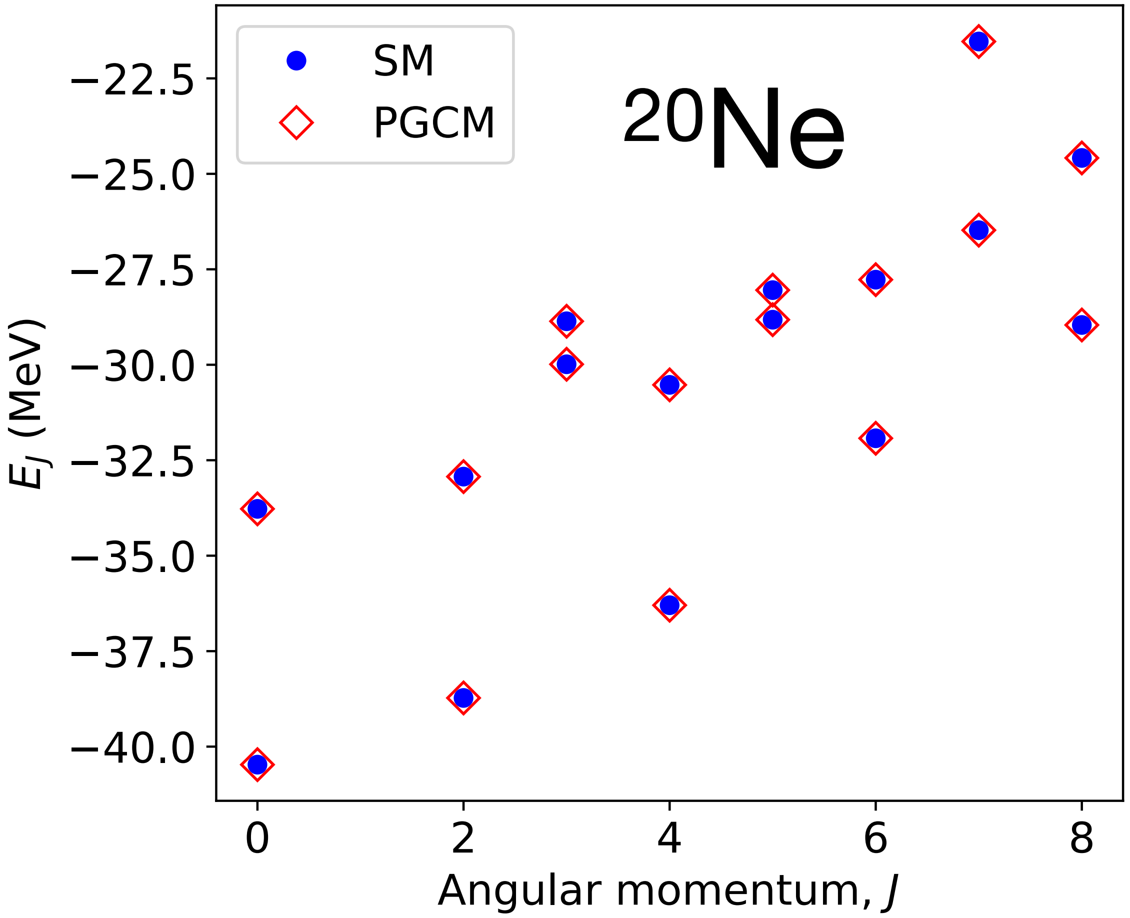
Particle-number-projected energy surfaces

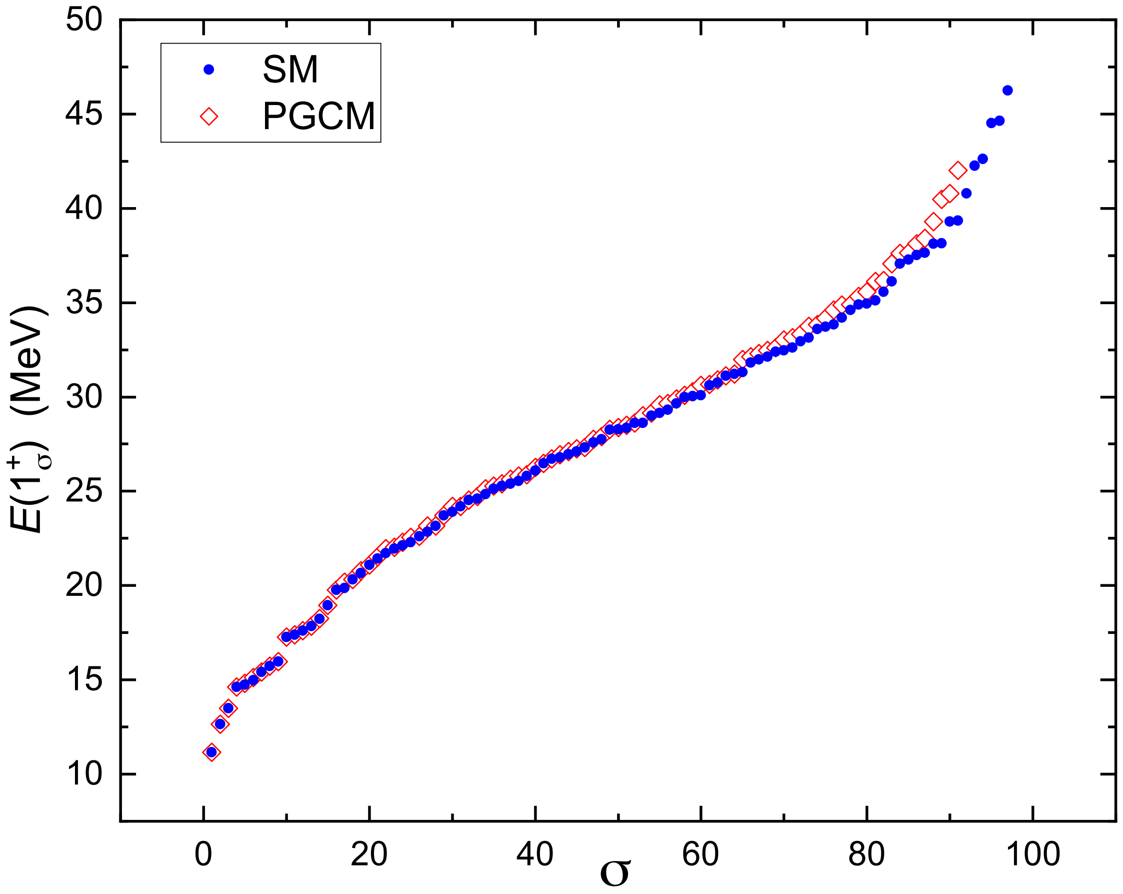


- Small pn-pairing configurations are favored in this case
- Pairing is less favored with increasing cranking

B(M1) strength functions in e-e nuclei

Exploring cranking, pn-pairing (isoscalar and isovector) $\{|\Phi(j_x, \delta_{pn}^{T=0}, \delta_{pn}^{T=1})\rangle\}$





- exact ground state energy

- exact description of low-lying excited energies

- Excellent description of the lowest excited 1^+ states

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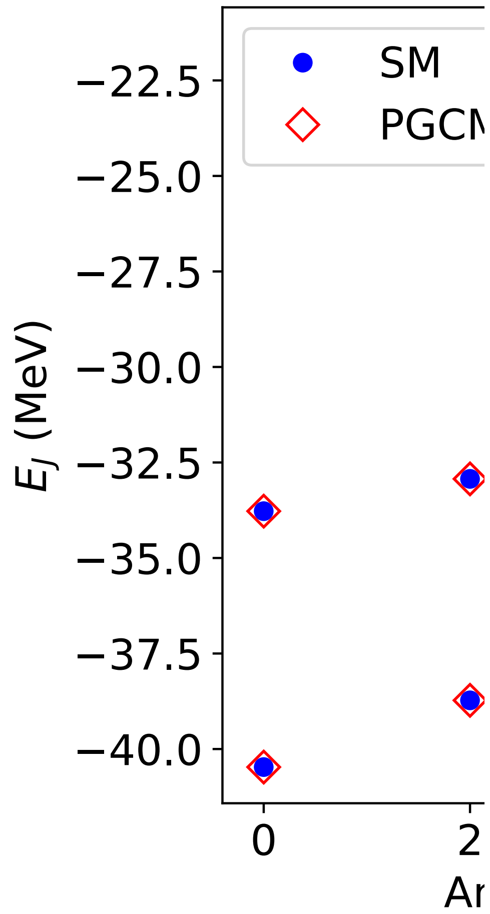
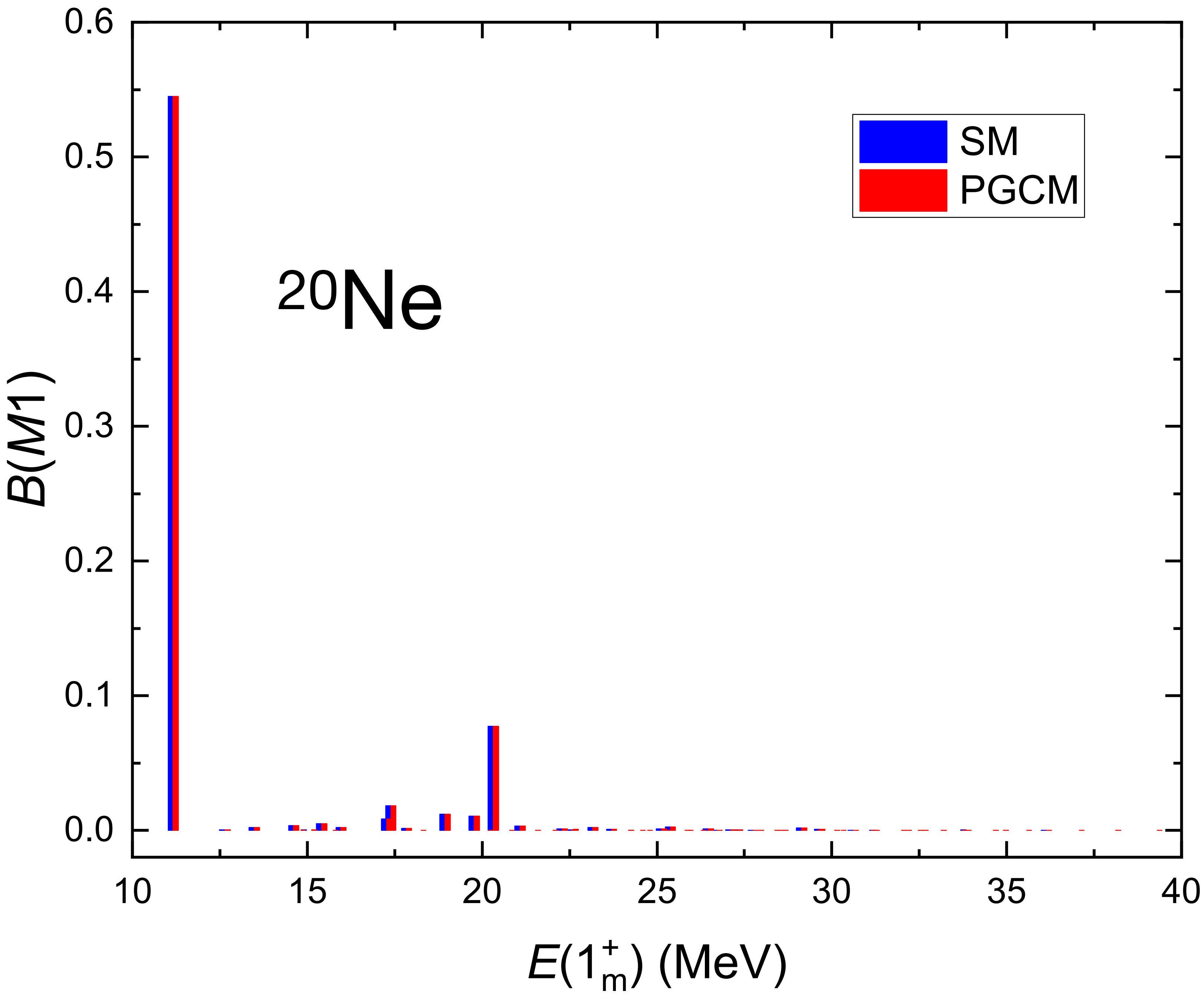
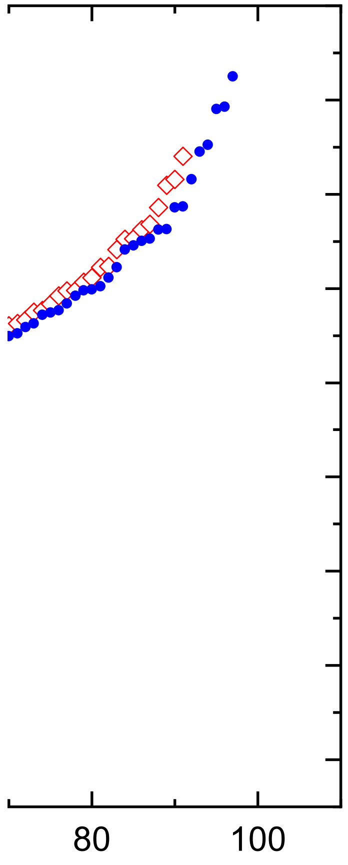
B(M1) strength functions in e-e nuclei

Exploring cranking, pn-pairing (isoscalar and isovector) $\{|\Phi(j_x, \delta_{pn}^{T=0}, \delta_{pn}^{T=1})\rangle\}$







- exact grou

- exact desc
  excited en

of the lowest

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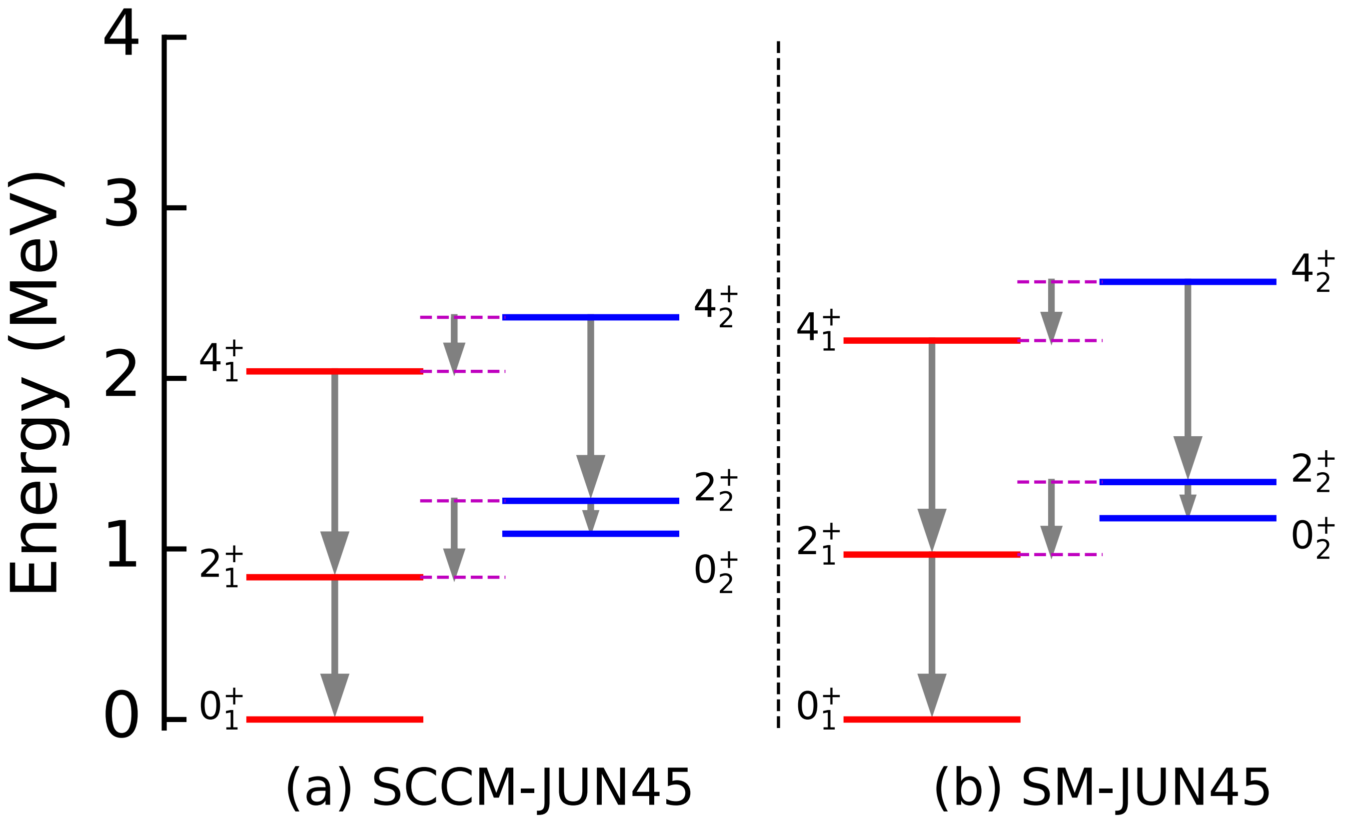
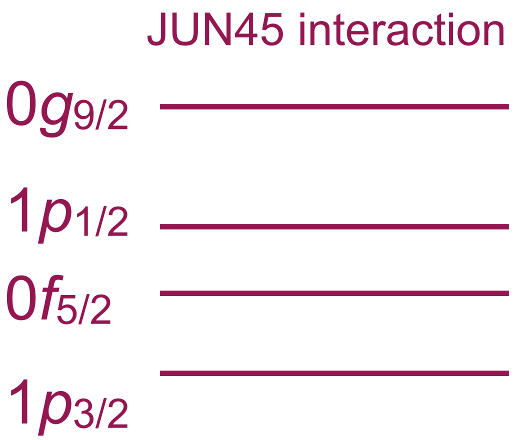
Shape coexistence in ^{66}Se



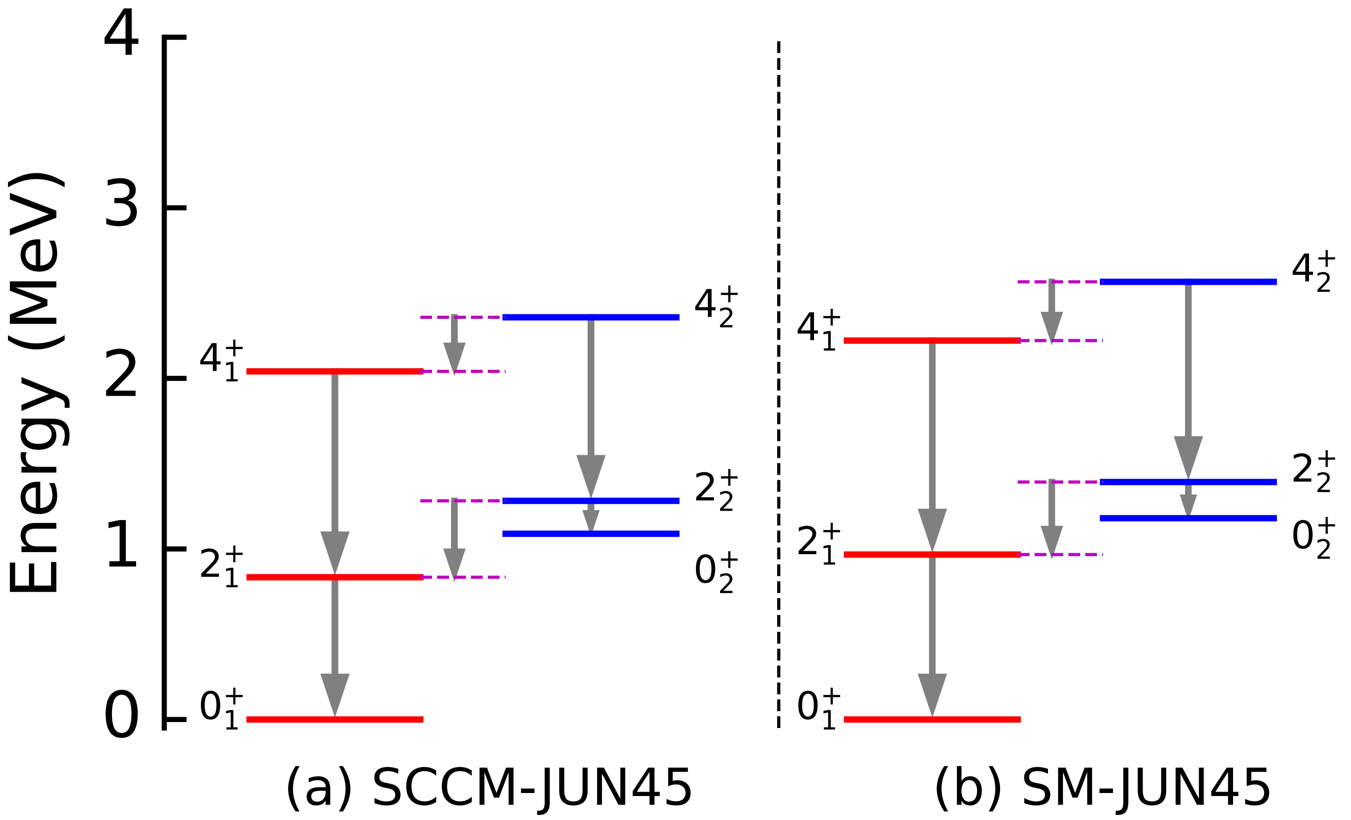
Shape coexistence in ^{66}Se:

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



Z. Elekes et al., PLB 844, 138072 (2023)

Shape coexistence in ^{66}Se



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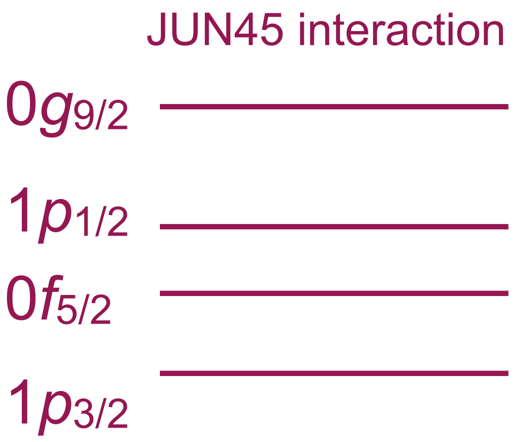

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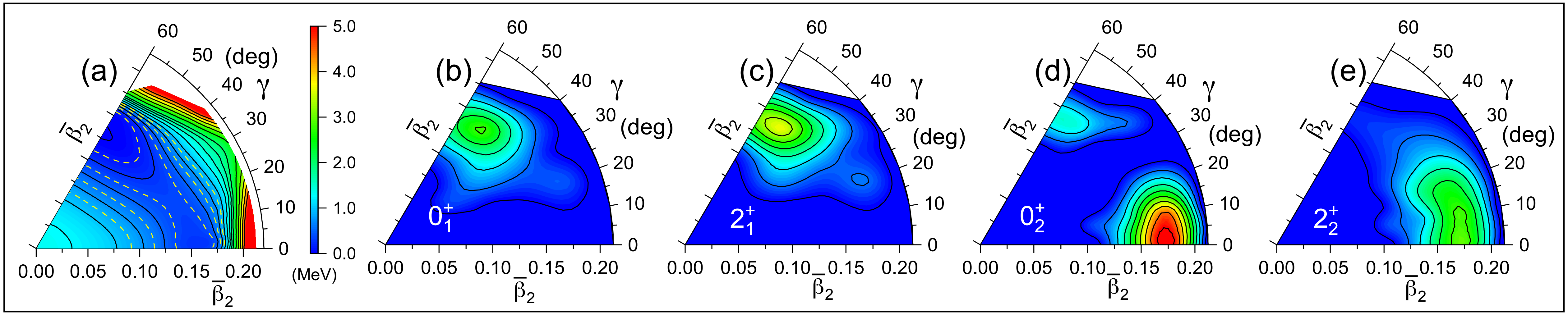

Outline

1. Introduction

2. Projected Generator Coordinate Method (PGCM)

3. Benchmarking PGCM against shell model with TAURUS

4. Summary and Outlook

Summary and Outlook

SUMMARY

- PGCM / ISM are complementary methods to provide a reliable description of nuclear structure observables.
- PGCM is a very flexible method to approach exact solutions.
- ISM states can be studied in terms of intrinsic shapes in the valence space.

OUTLOOK

- Extend the calculations to many-shell (no-core) PGCM with realistic interactions.
- Interpret ISM states in terms of collective variables (shapes)
- Include explicitly quasiparticle excitations into the PGCM wave functions (single-particle excitations).

Acknowledgments

Benjamin Bally (CEA-Saclay)

Adrián Sánchez-Fernández (U. York)

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Vimal Vijayan (GSI-Darmstadt)

Kamila Sieja (Strasbourg)

Thank you!