Multi-reference description of open-shell nuclei

SSNET 2024, Thursday 7th 2024

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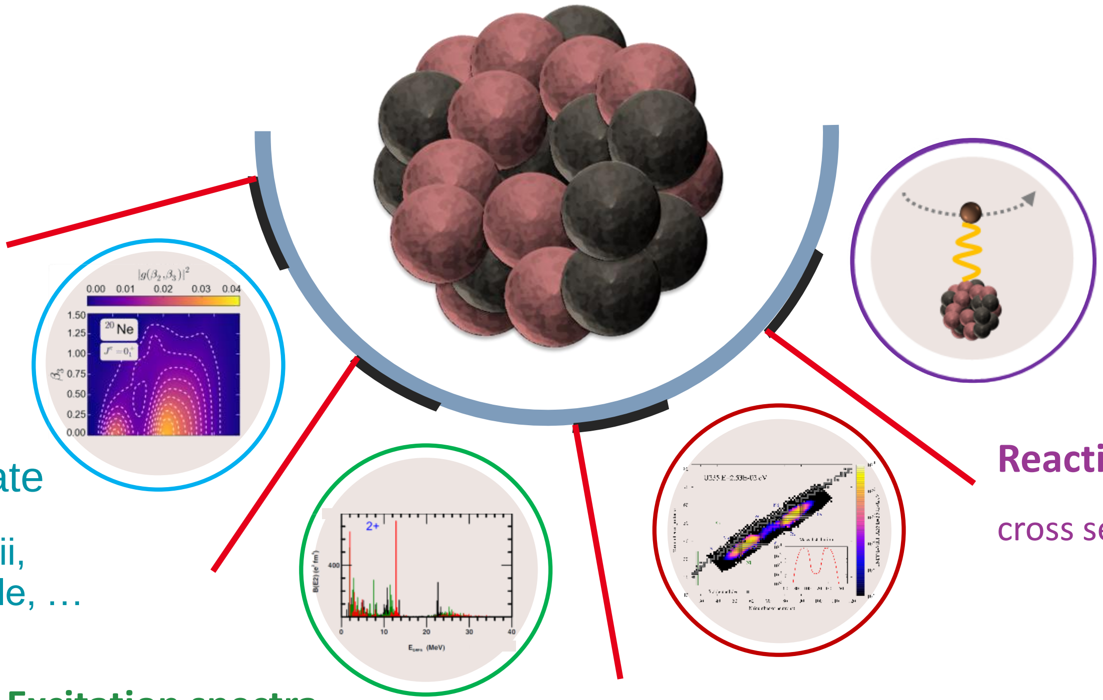
Microscopic models of nuclei

From nucleons to nuclei

Prediction of macroscopic properties from interacting nucleons

*Towards a **complete**, **coherent** and **systematically improvable** description of nuclei for nuclear data*



Ground-state

masses, radii, density profile, …

Excitation spectra

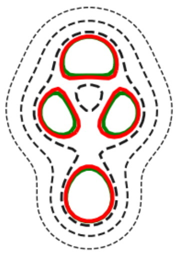
energies, transition probabilities, response function to electroweak probes, …

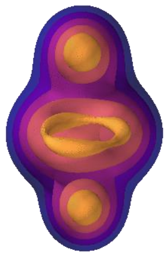
Decay modes

lifetime, yields, …

Reactions

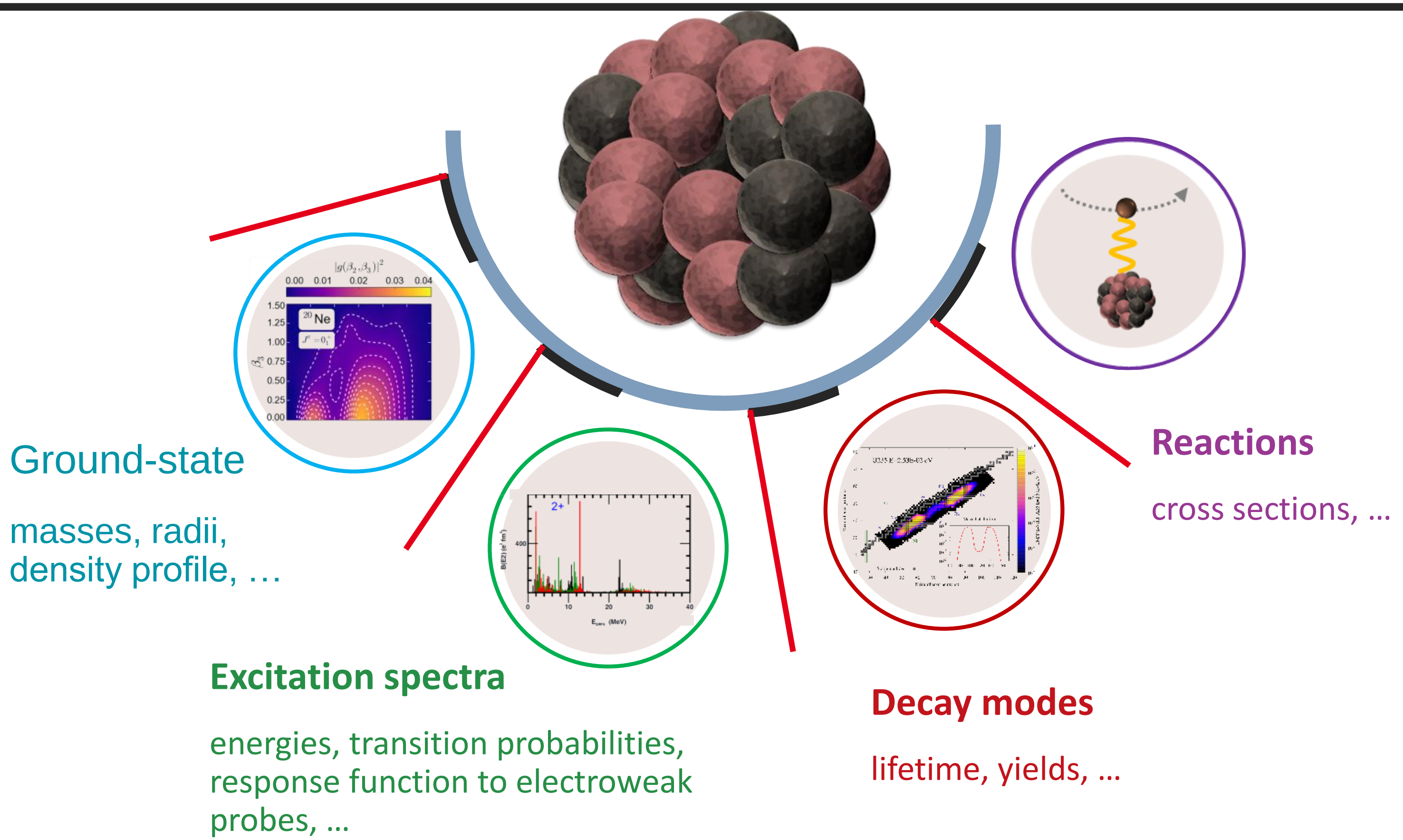
cross sections, …

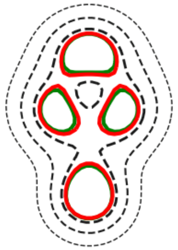


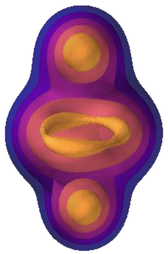


Microscopic models of nuclei

Presentation focused on particular *ab initio* method
Objective : **solve A-body Schrödinger equation** to given accuracy
Multi-reference Perturbation Theory (PGCM-PT)
How can **multi-reference expansion methods** help towards a complete picture?







Outline

1. **Expansion methods for open-shell nuclei**
   Progress of ab initio / in medias res methods
   Single and multi-reference expansion methods
   Circumventing the complexity of three body interactions

2. **Application: from low-lying spectroscopy to giant resonances**
   PGCM-PT(2) and scale decoupling
   Application of PGCM in realistic model space

3. **Conclusion**

1. Formalism

- Progress of ab initio / in medias res methods
- Single and multi-reference expansion methods
- Circumventing the complexity of three body interactions

Progress of *ab initio / in medias res* methods

Ab initio **methods**

1) A structure-less nucleons as degrees of freedom
2) Interaction mediated by pions and contact terms (e.g. Weinberg PC)
3) **Solve A-body Schrödinger equation to relevant accuracy***

** controlled and improvable way*

Steady progress in the last decades

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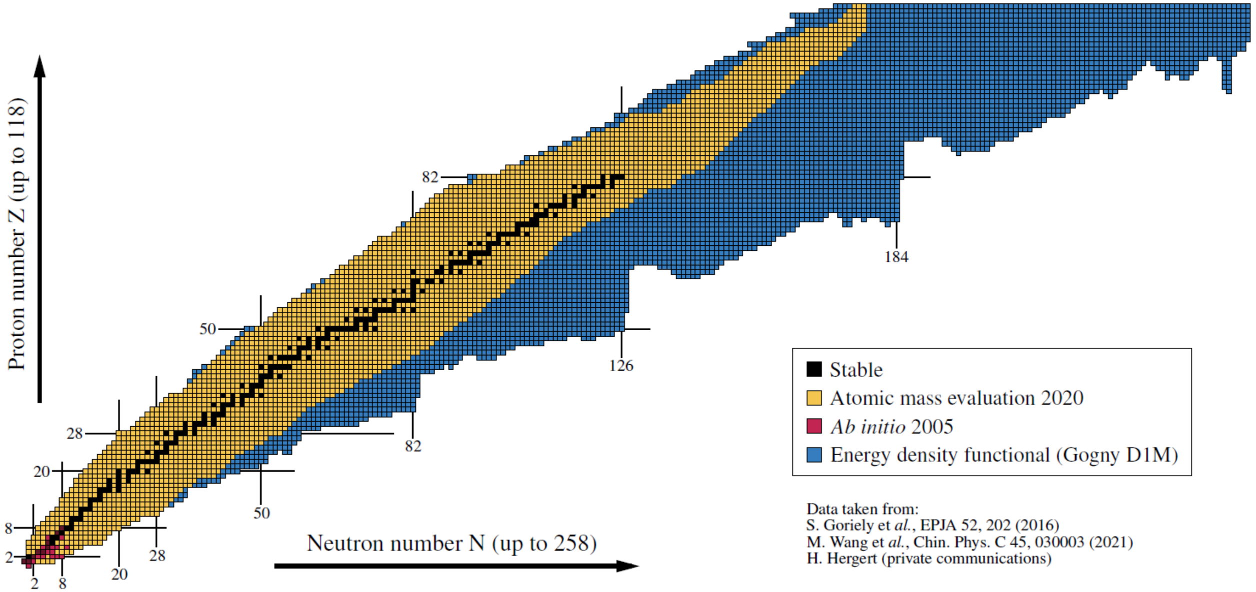

Courtesy of B. Bally

Steady progress in the last decades

Light nuclei		
Quasi-exact methods	**1990's**	Exponential scaling

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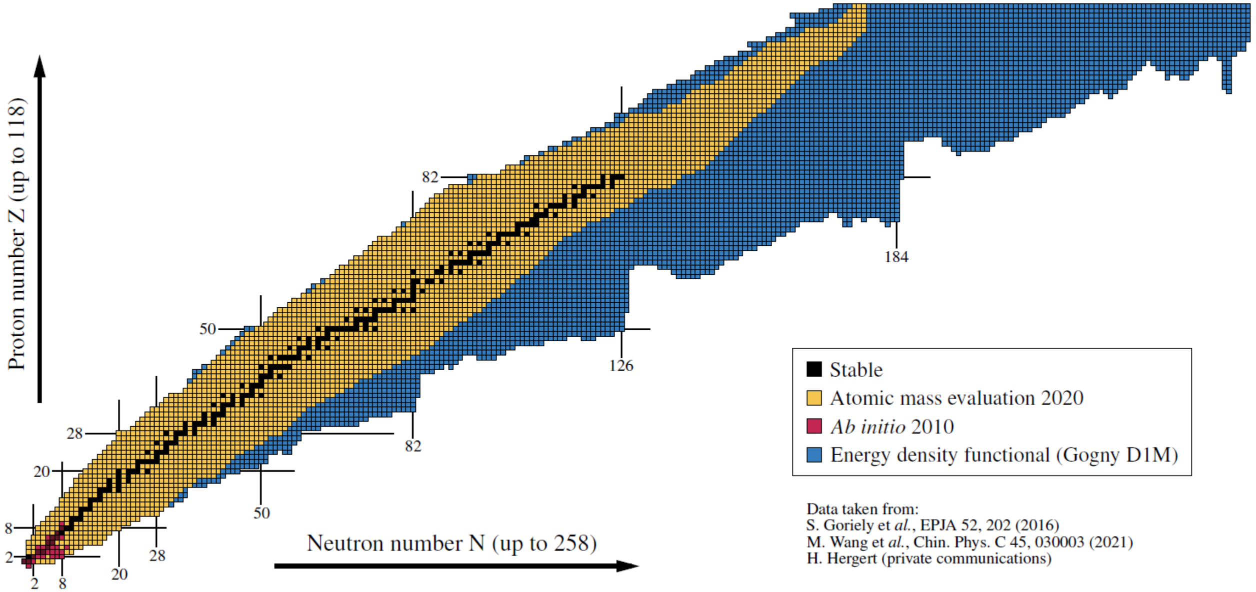

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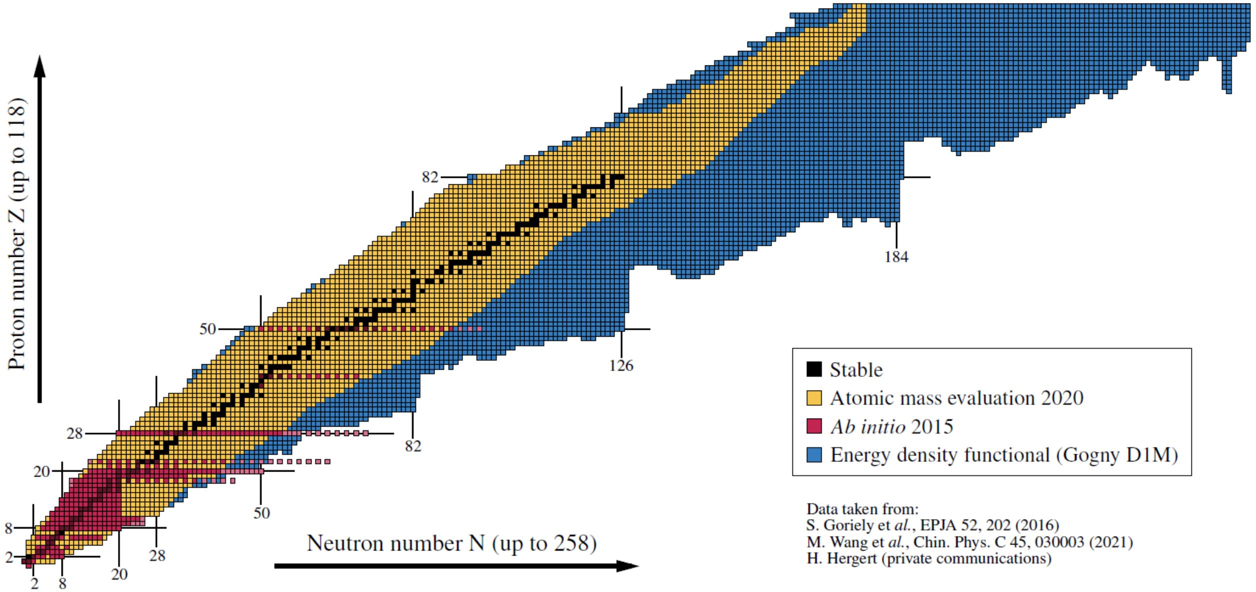

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Steady progress in the last decades

Nuclei	Methods	Decade	Scaling
Light nuclei	**Quasi-exact methods**	**1990's**	Exponential scaling
Closed shells	**Expansion methods Single-reference**	**2000's**	Polynomial scaling
Singly open-shells	**Symmetry-breaking Multi-reference**	**2010's**	Polynomial scaling

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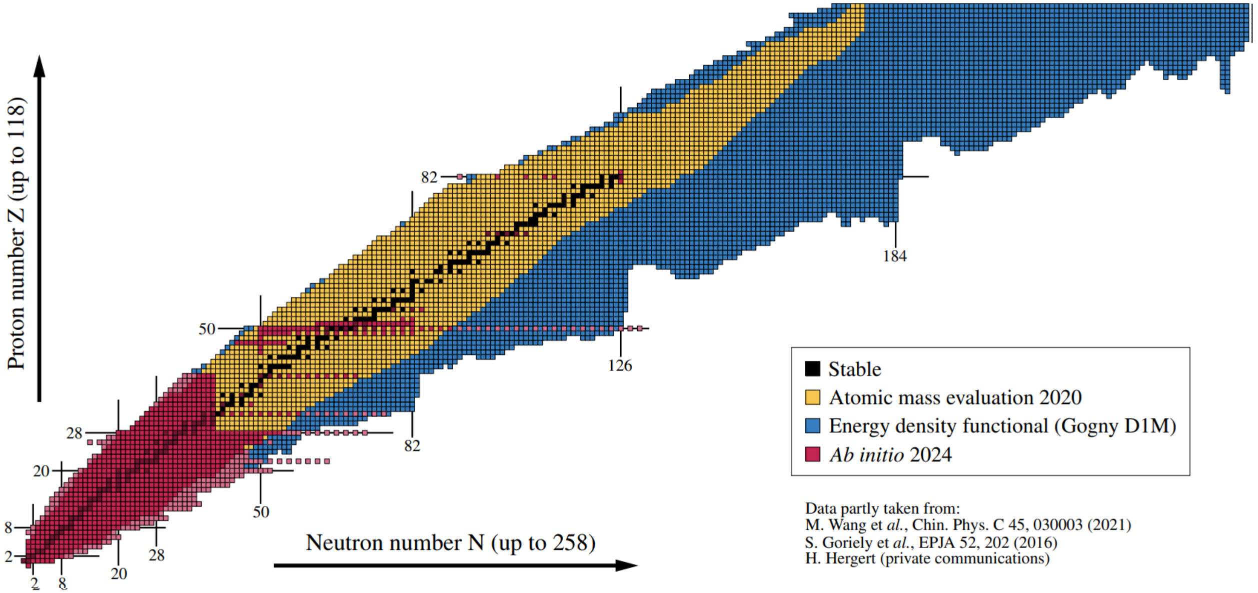

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Singly open-shells	**Symmetry-breaking Multi-reference**	**2010's**	Polynomial scaling
Doubly open-shells	**Valence space** **Symmetry-breaking Multi-reference**	**2020-?**	Mixed / Polynomial Scaling

Single and multi-reference expansion

$[H, R] = 0$

Expansion methods

Nucleon interaction
1-,2-,3-… body

$$H|\Psi^\sigma\rangle = E^\sigma|\Psi^\sigma\rangle$$

Correlated wave-function
A! parameters

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Partitioning

Unperturbed problem
« Easy »

$$H \equiv H_0 + H_1$$

Residual interaction
Treated approximatively

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Perturbation Theory
Coupled Cluster
IMSRG
Green's functions

$$\mathcal{W} \sim \sum_k H_1^k$$
$$\sim e^T = e^{\mathcal{T}_1 + \mathcal{T}_2 + \cdots}$$
$$\ldots$$

$$|\Psi\rangle \equiv \mathcal{W}|\Theta^{(0)}\rangle$$

Wave operator
Expressed as ***tensor network***

Expansion method
➔ Efficient for **short range**
➔ 2p2h, 3p3h, …

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at polynomial cost ?

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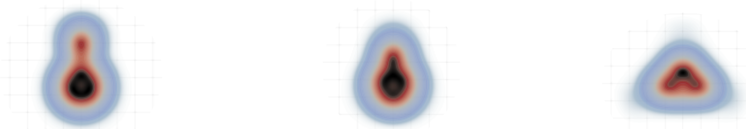
Projected Generator Coordinate Method

Frosini et al; Eur.Phys.J.A 58 (2022) 4, 62



$|\Phi(q_1)\rangle$ $|\Phi(q_2)\rangle$ $|\Phi(q_n)\rangle$

$P^{J^\pi NZ}|\Phi(q_1)\rangle$ $P^{J^\pi NZ}|\Phi(q_2)\rangle$ $P^{J^\pi NZ}|\Phi(q_n)\rangle$

Projection
Rotation

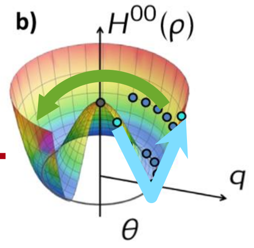
$$|\Psi^{J^\pi NZ}\rangle \equiv \int_q dq\, f^{J^\pi NZ}(q) P^{J^\pi NZ}|\Phi(q)\rangle$$

Shape mixing
Vibration

Variational HWG
Low dimensional

$$\sum_q H^\sigma_{pq} f^\sigma_\mu = \mathcal{E}^\sigma_\mu(q) \sum_q N^\sigma_{pq} f^\sigma_\mu(q)$$

Hamiltonian kernel *Norm kernel*



Symmetry breaking minimum

Shape oscillations / rotations accounting for mpmh effects

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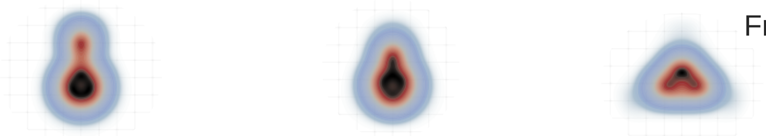

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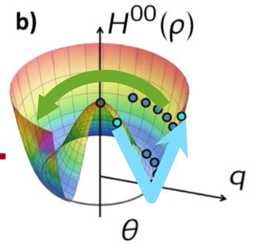

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Multi-reference (non orthogonal) perturbation theory

PGCM + perturbative 2p2h

Strong static / collective correlations captured by PGCM reference
Weak / dynamical correlations captured in perturbation
Versatile but **expansive symmetry conserving** expansion method
Different from PCC
- **project + partition + expand** / **partition + expand & project**

Circumventing the problem of three-body interaction

Ab initio Hamiltonian

$$H = T + V^{NN} + \mathbf{V^{NNN}} + \cdots$$

Similar to other interactions

Neglected for now

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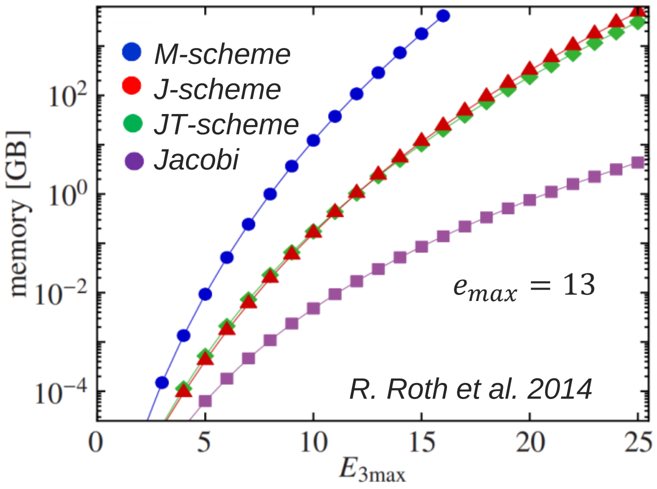

⊕

Essential for predictivity of the theory
True Hamiltonian (no spurisities BMF)

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Memory bottleneck ($O(N^6)$ vs $O(N^4)$)
Runtime bottleneck

Cost increase in deformed calculation
too large to be handled

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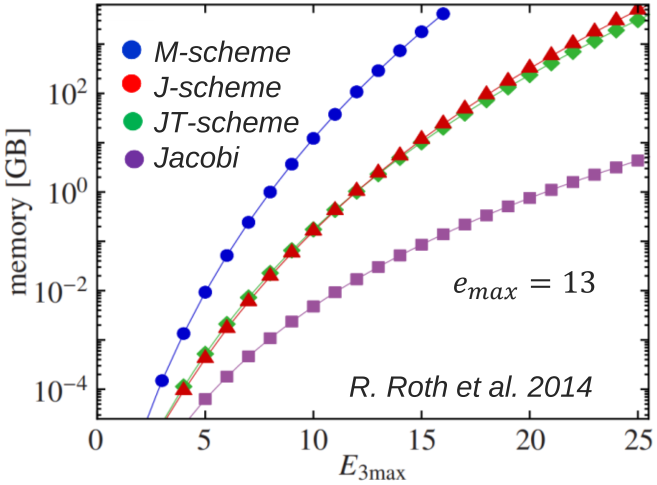

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In medium interactions

Frosini et al, Eur.Phys.J.A 57 (2021) 4, 151

1. Apply same contractions with arbitrary « **well chosen** » ρ
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3. Convert **back to single particle** basis

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Applications:
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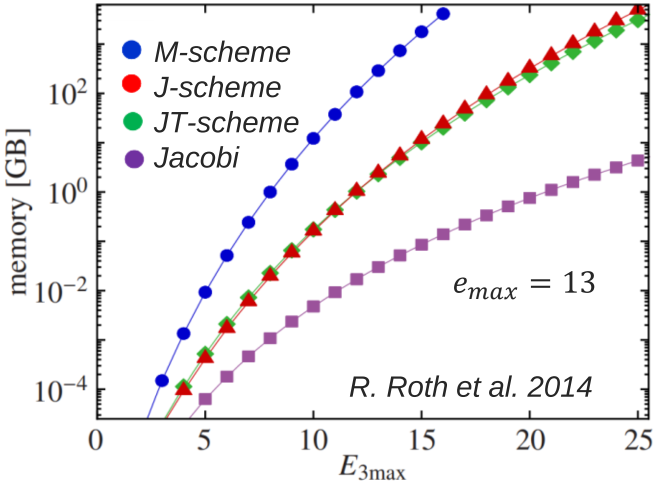

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Limitations of the method

Total Energy Curve in axial calculations at different basis size
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T. Miyagi Eur. Phys. J. A 59, 150 (2023)

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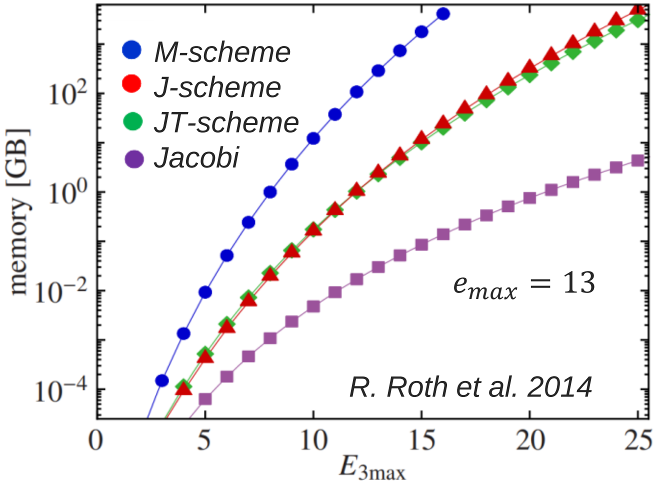

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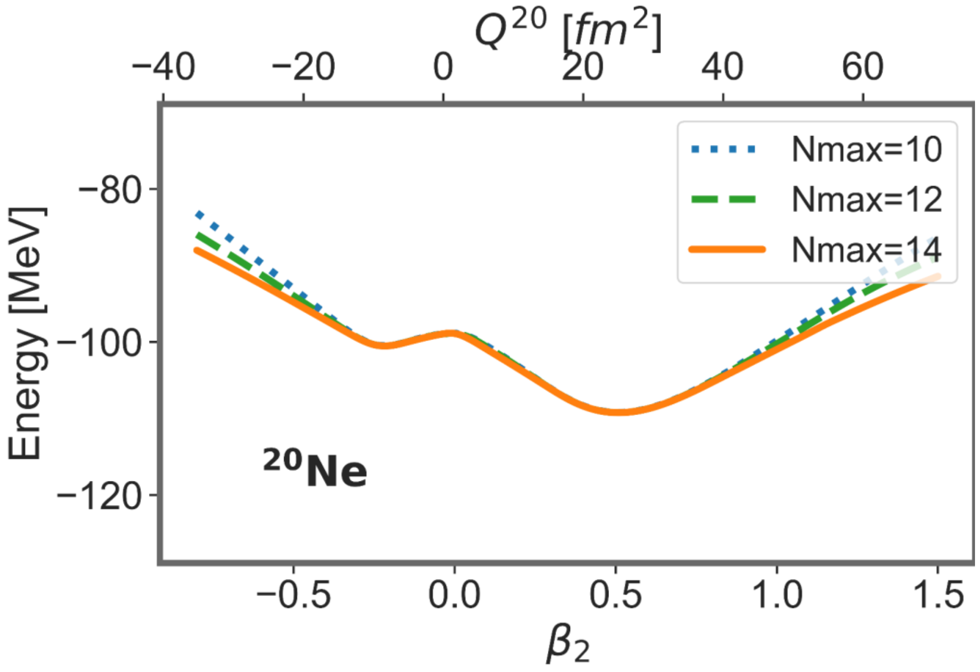

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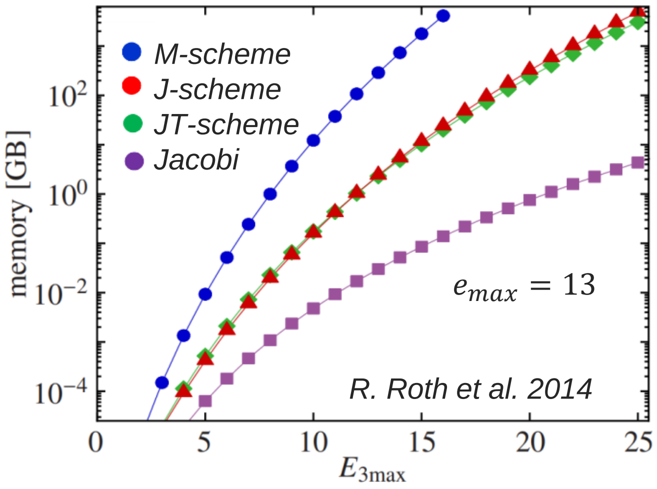

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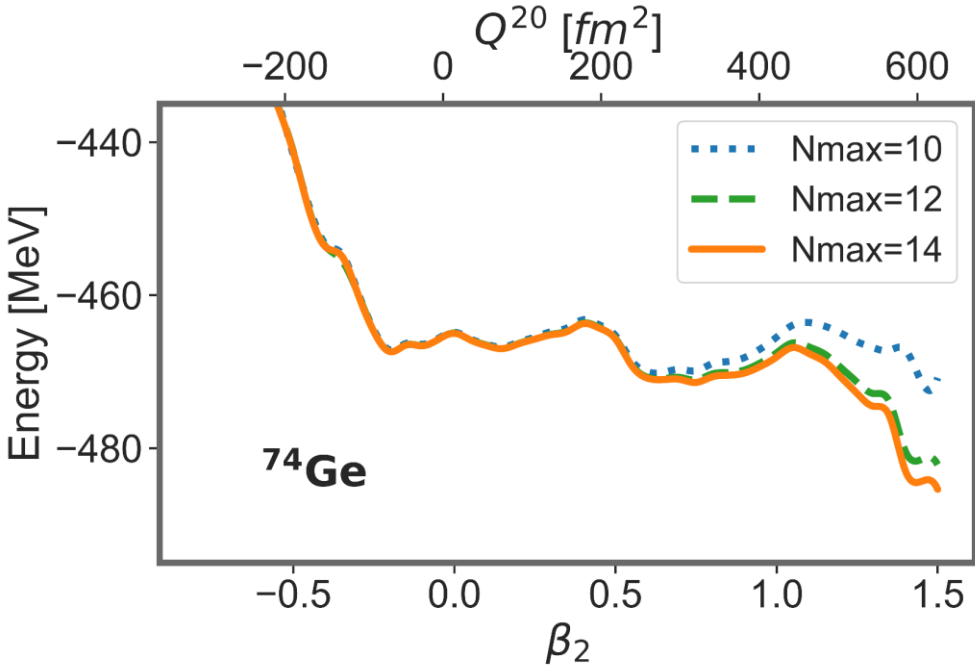

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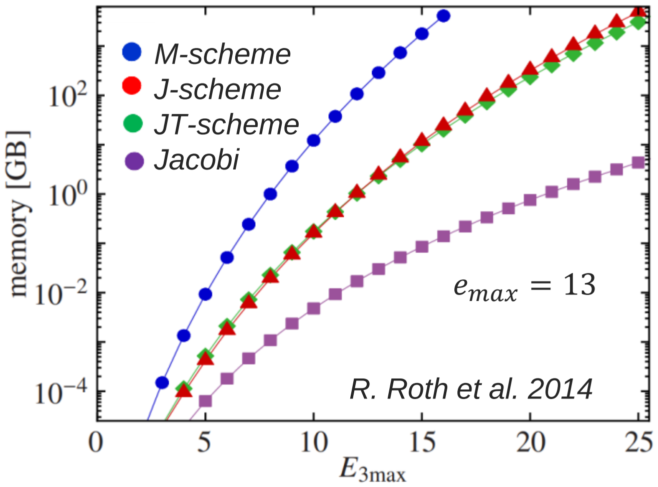

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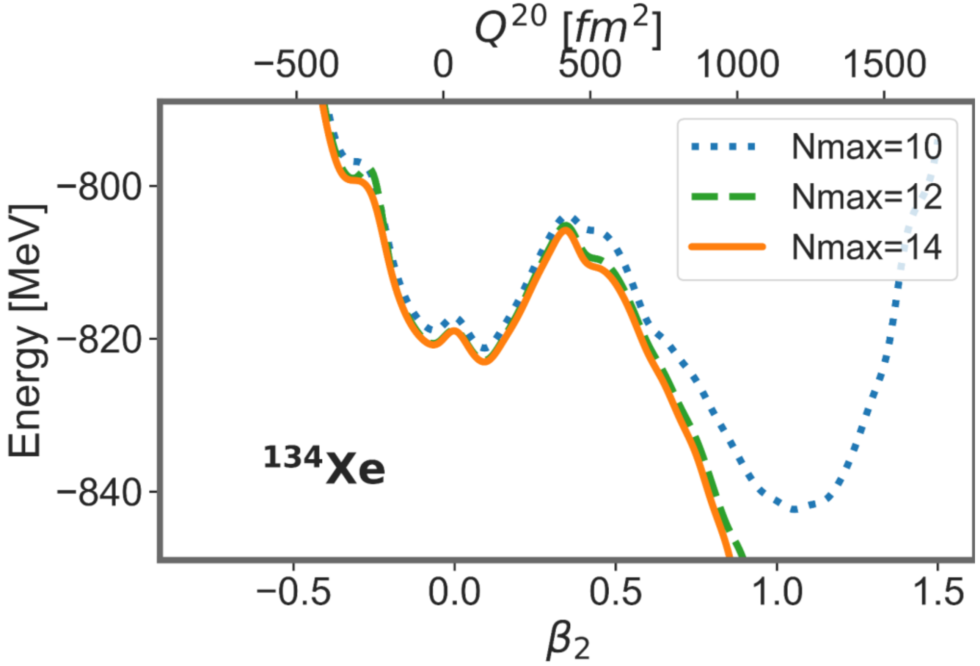

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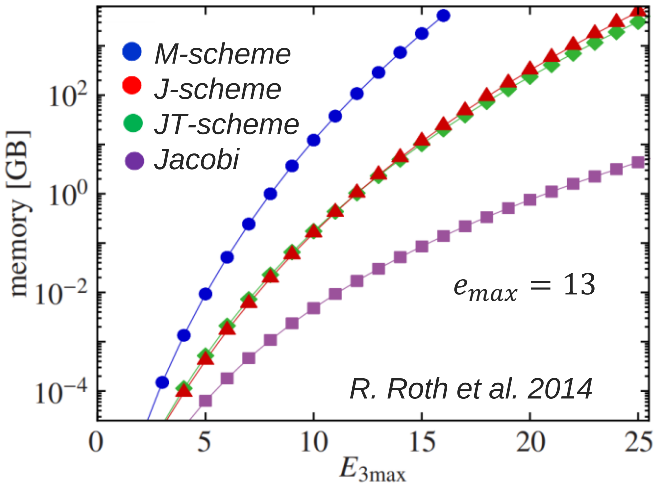

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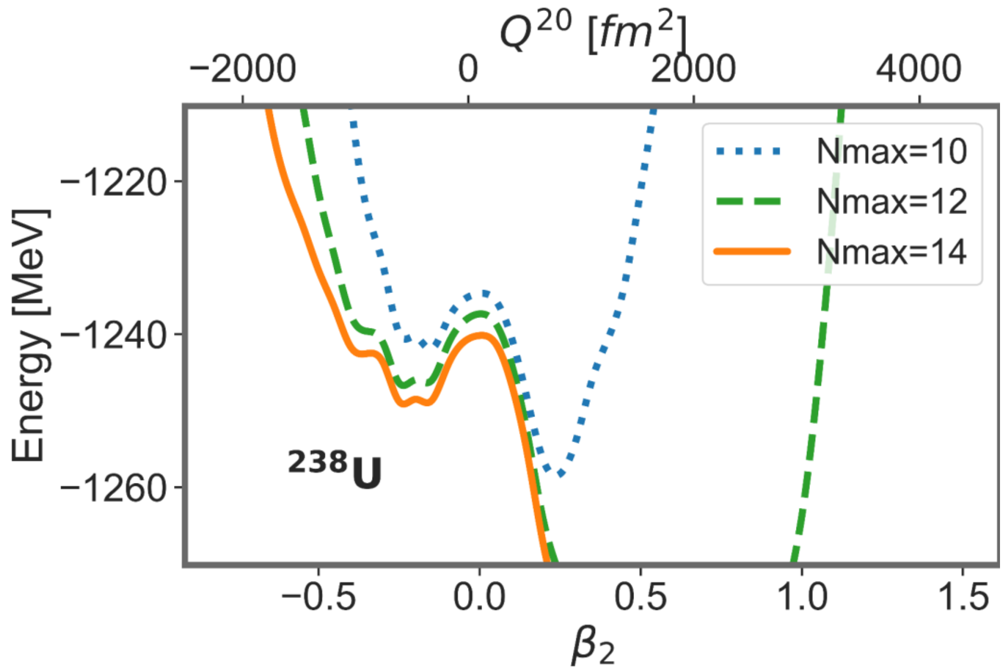

The exact origin is still under inverstigation…

- But no doubt approximation we perform on 3-body is responsible
- Already observed by Hergert, Bally, Yao… five years ago!
- Exact 3-body (very expensive) / MR-IMSRG…?

For now, from different tests (deformed), three mass ranges identified
3 – 80 (safe) / **80 – 150 (danger zone)** / **150 + not under control**

3. Application: from low-lying spectroscopy to giant resonances

- PGCM-PT(2) and scale decoupling
- Application of PGCM in realistic model space

PGCM-PT(2) and effective decoupling of scales

How well long vs. short range physics decouple?

Best way to understand it is to change the scale !
Applying MR-IMSRG evolution to shuffle correlations
Comparing bare PGCM and PGCM-PT(2)
Long (static) ⇔ Short (dynamical)

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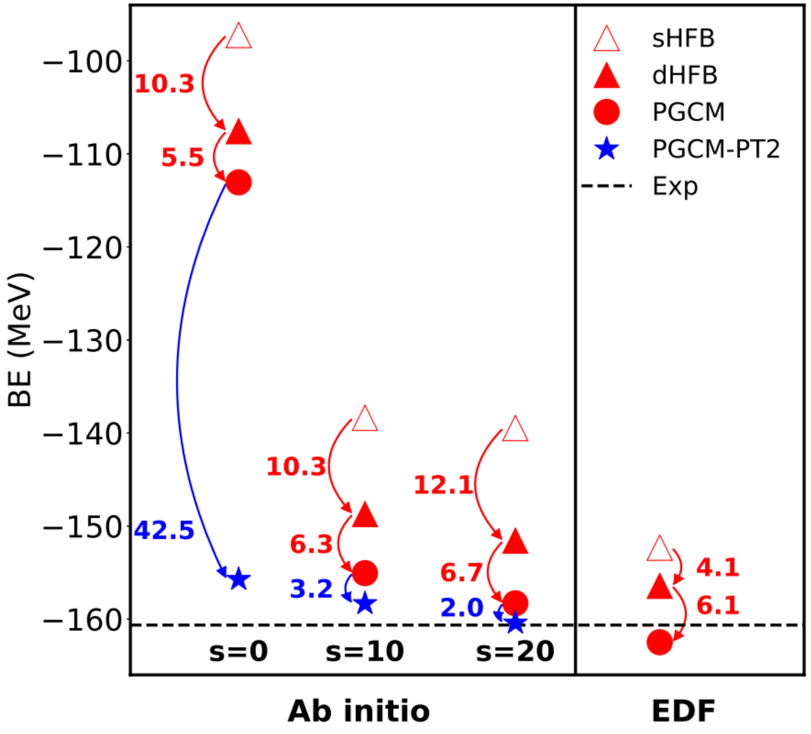

Reshuffling of correlations
- Much lower mean-field
- **Increase of static** correlations
- Link with EDF?

PGCM-PT(2) **dynamical correlations**
- Strong decrease due to reshuffling
- Not vanishing (approximate decoupling)
- Higher order effects (PGCM-PT(3))?

Ne20, EM 1.8/2.0 interaction

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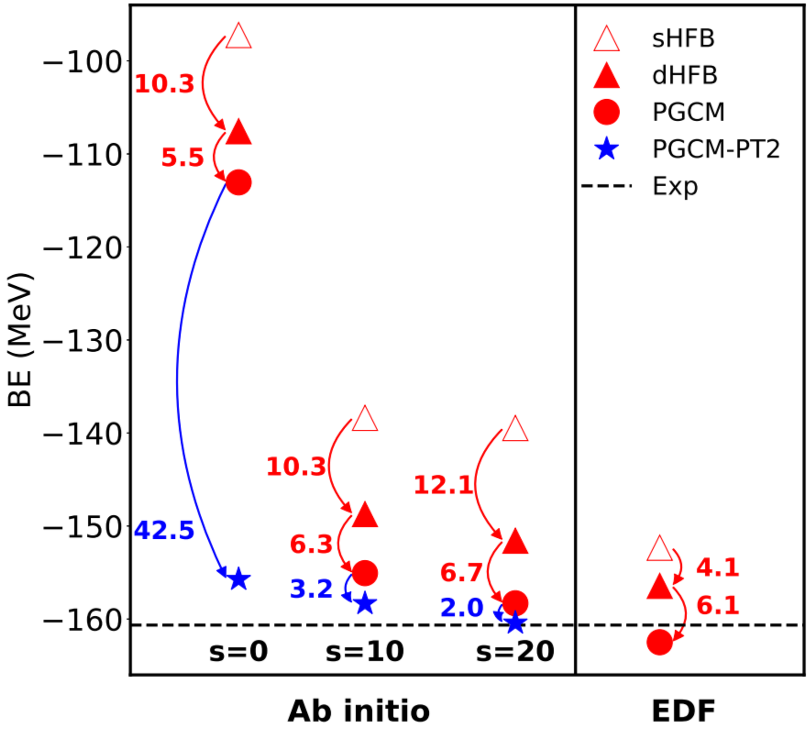

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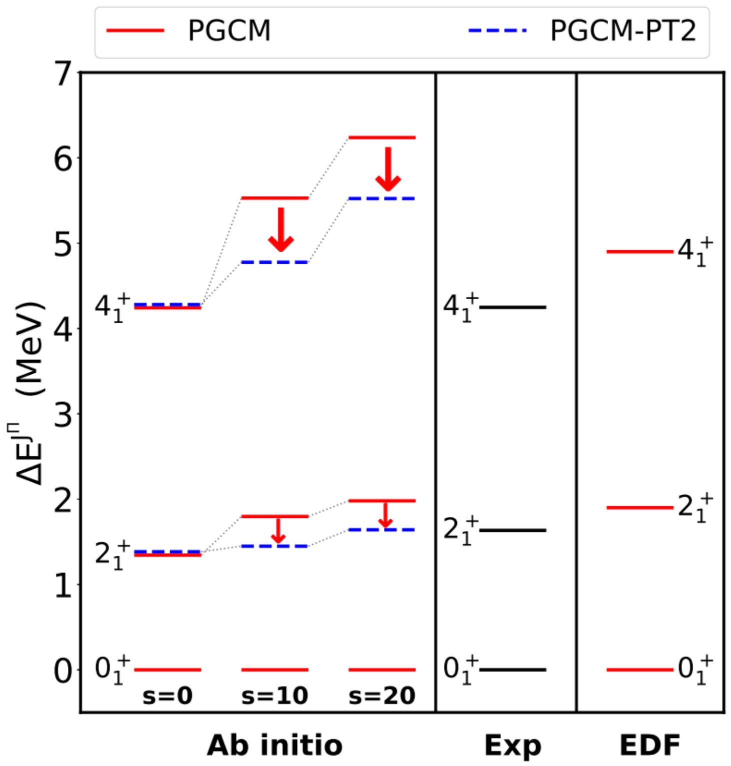
Effect on excited states
- Dilatation of rotational spectrum
- PGCM-PT(2) contracts back spectra



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Duguet et al Eur.Phys.J.A 59 (2023)
Frosini et al Eur.Phys.J.A 58 (2022)

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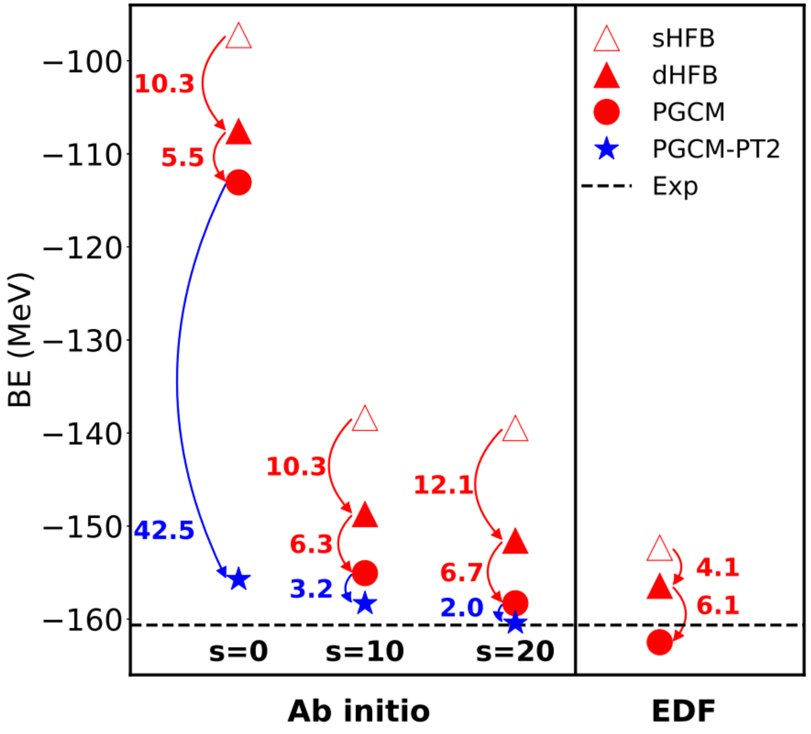
Conclusion
Good scale decoupling with vacuum interaction
PGCM reliable for low-lying rotational spectroscopy
independently confirmed by *Sun et al.*
effective confirmation with QRPA
What about vibrations? Until when can we go?
In the following, calculations at PGCM level…

Porro et al EPJA 60 (2024)
Gonzalez-Miret et al. (2025)



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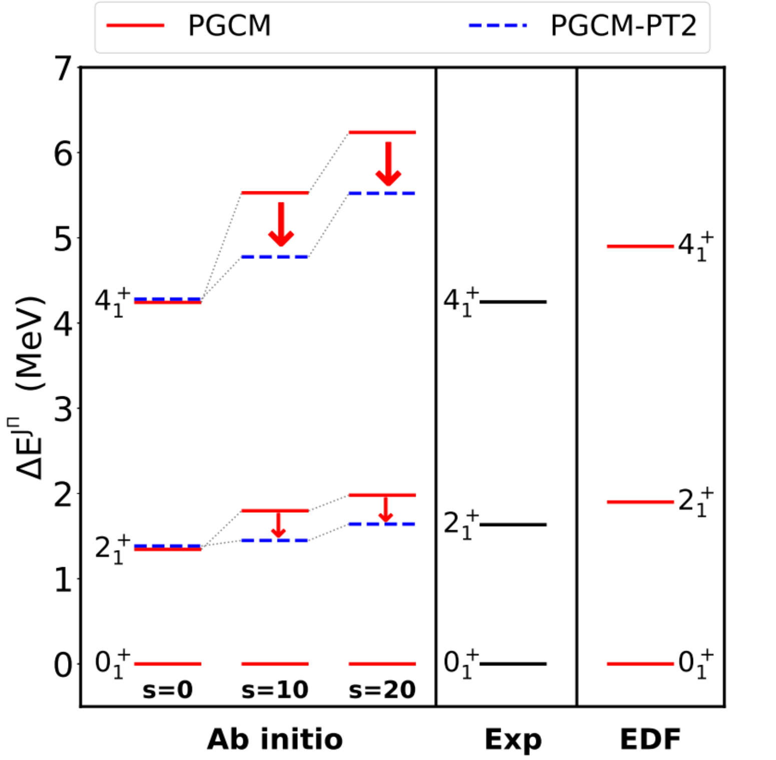

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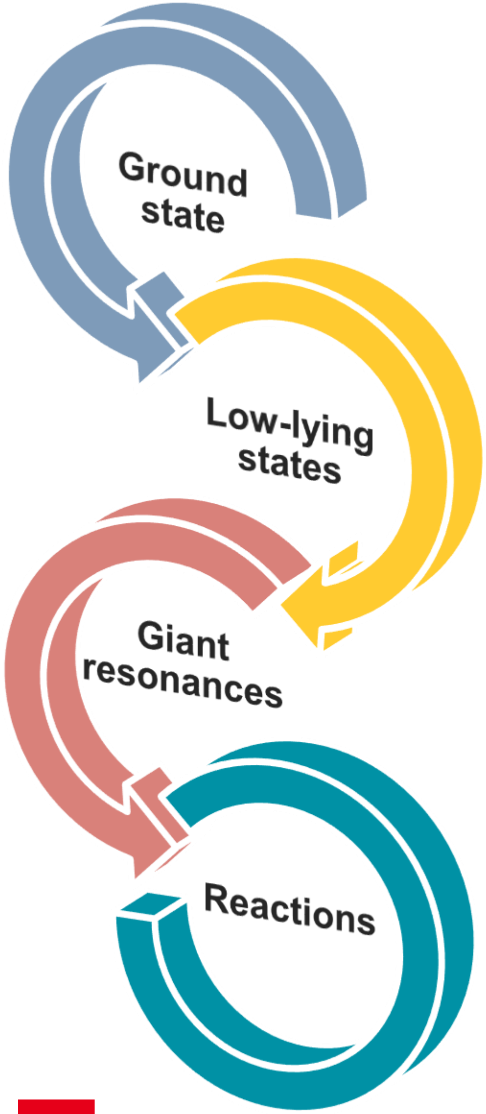
Applications of PGCM in realistic model spaces



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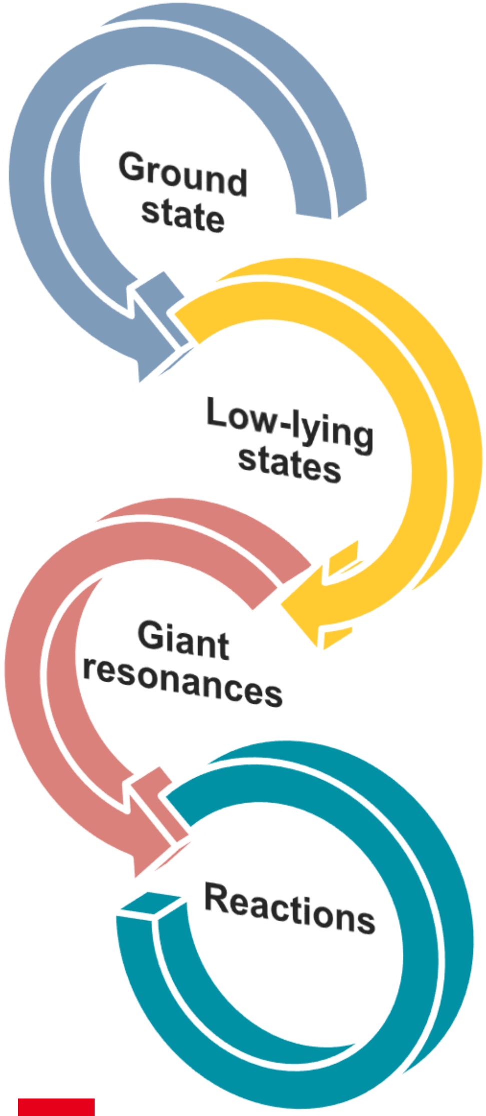
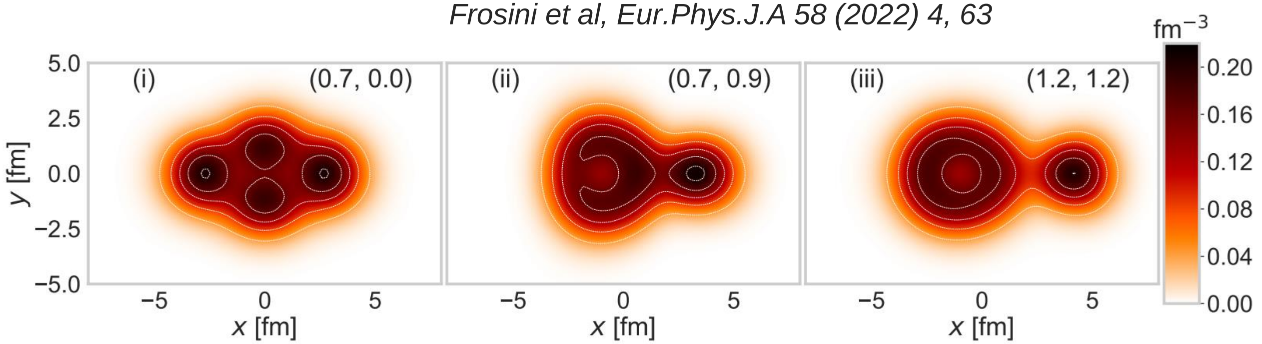
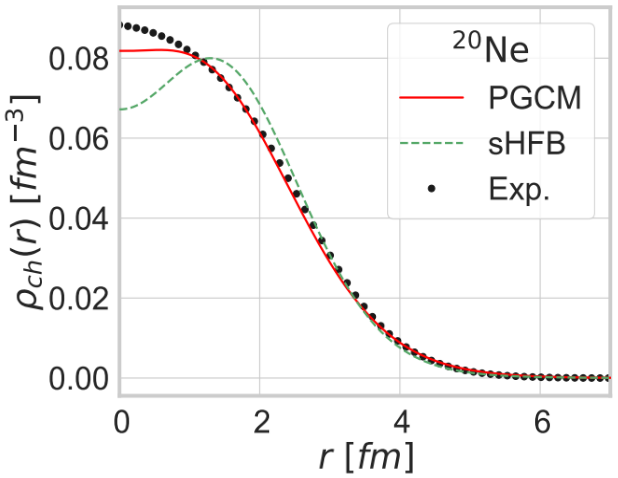


Shape mixing : deep insight on structure
Coherent superposition of clustered states
Improvement wrt spherical mean-field
Applications to heavy-ion collision

Frosini et al, Eur.Phys.J.A 58 (2022) 4, 63





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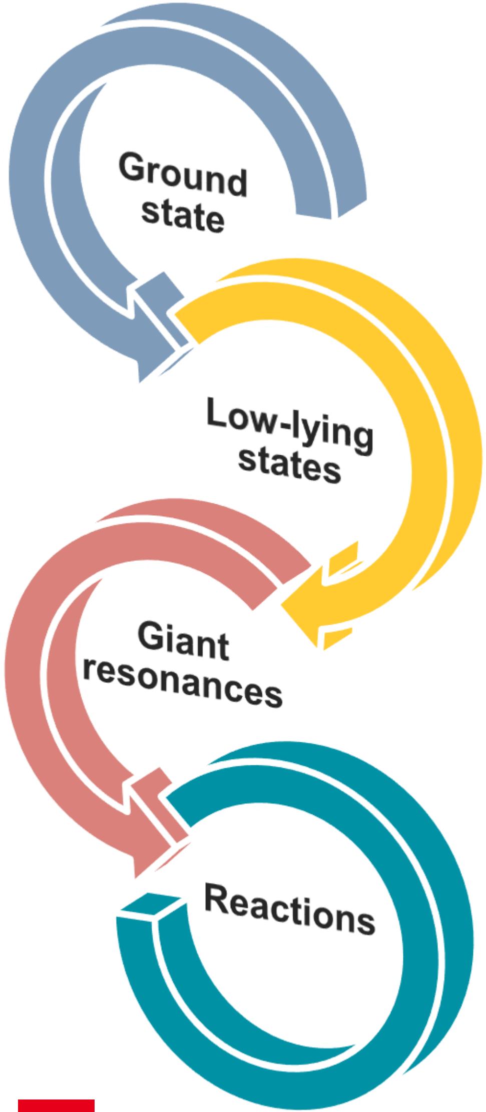

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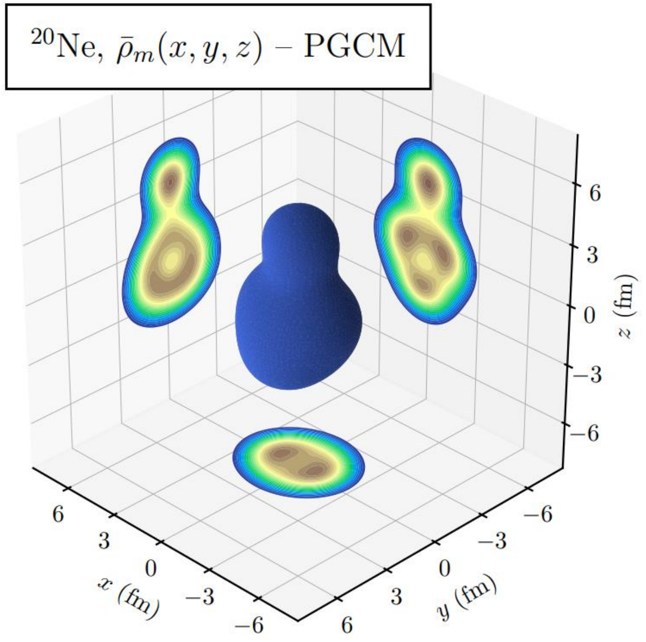

Giacolone, Bally et al. (2024) arxiv 2402.05995

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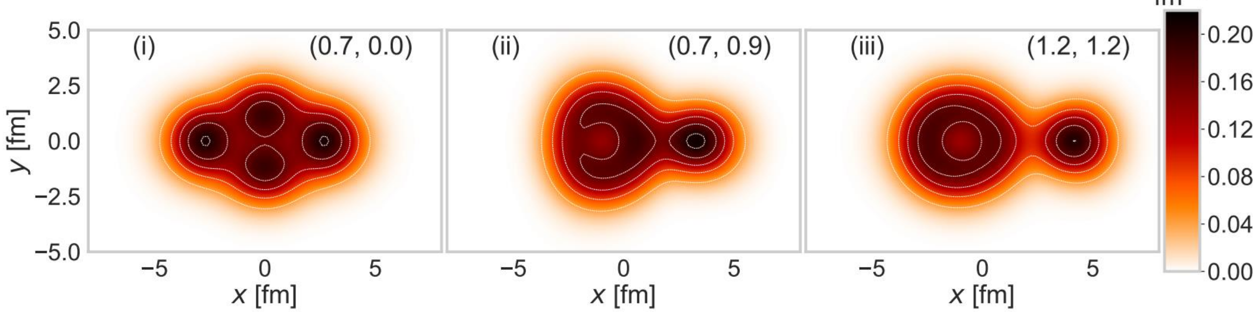

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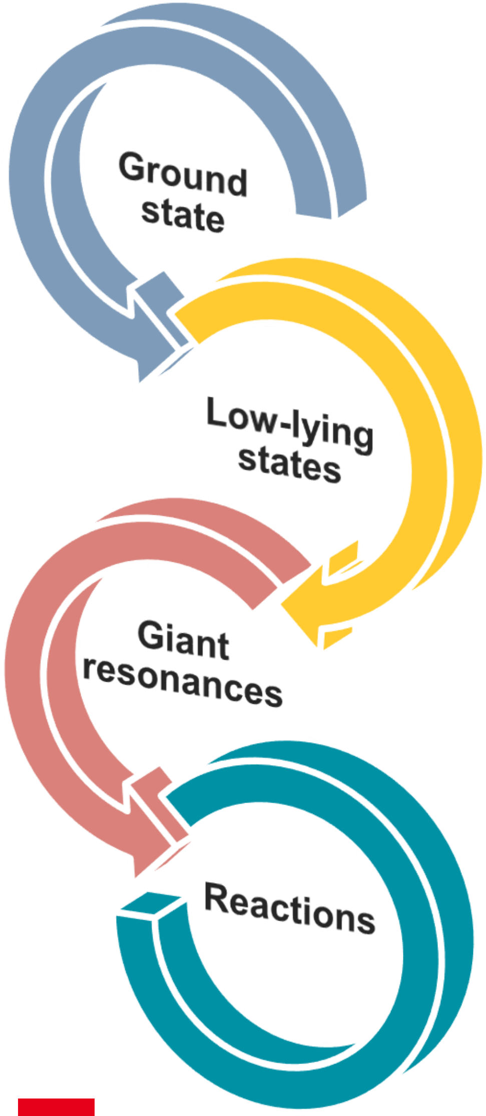

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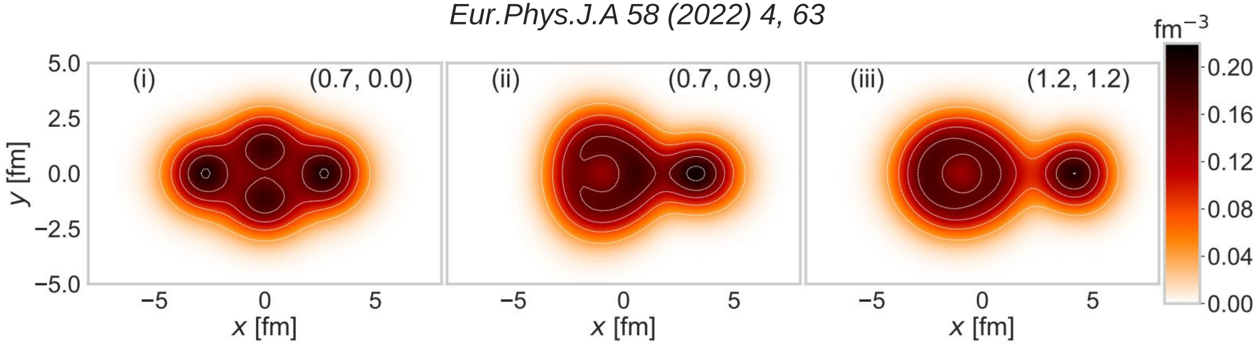

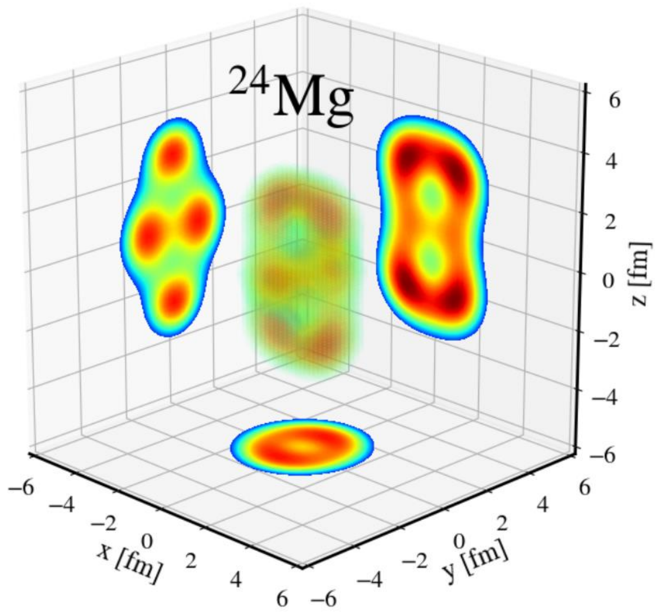

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Gonzalez-Miret (in preparation)

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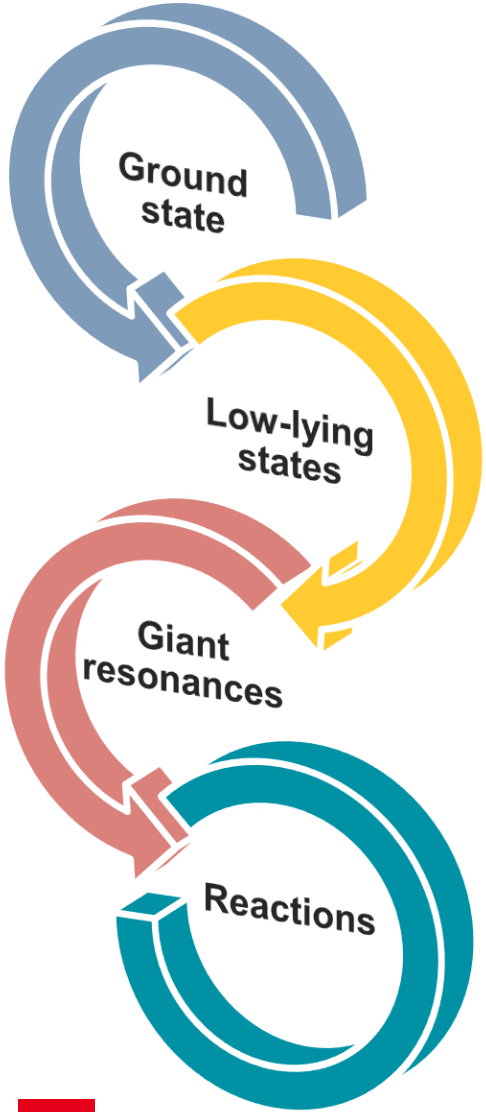

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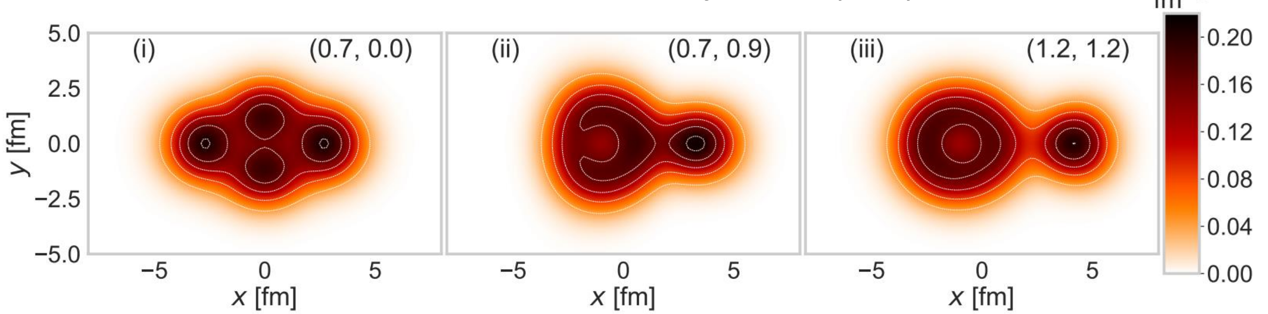

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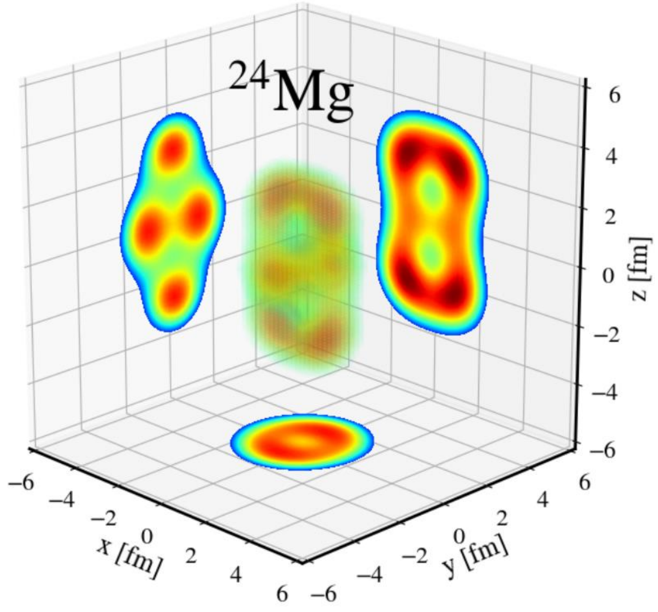

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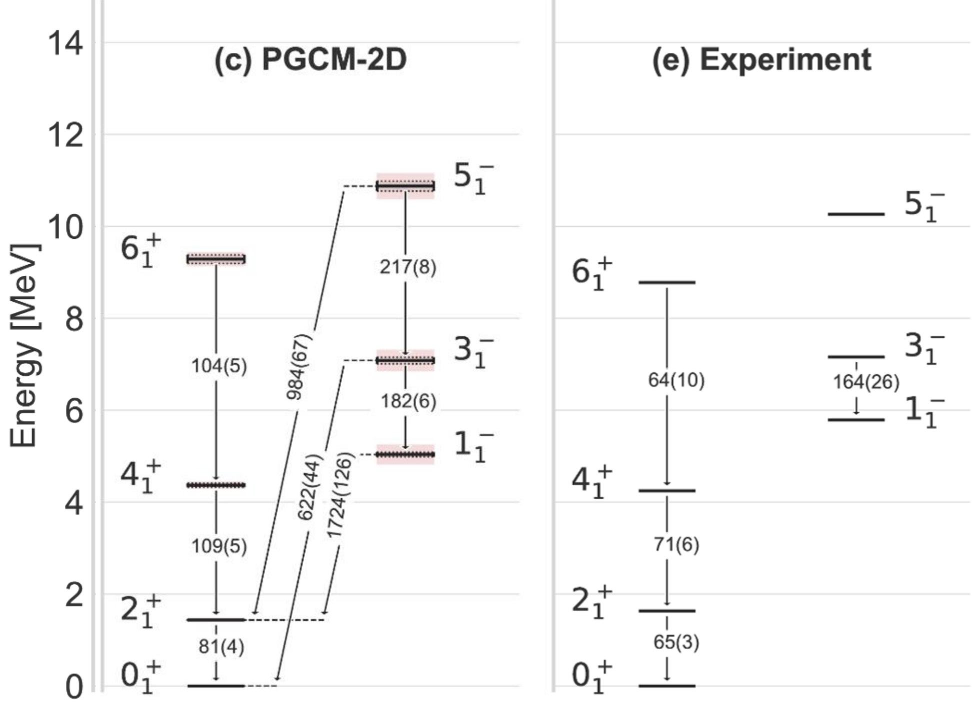

Rotational & vibrational states
Good agreement with experiment
Reproduction of B(E2), Q2, etc.

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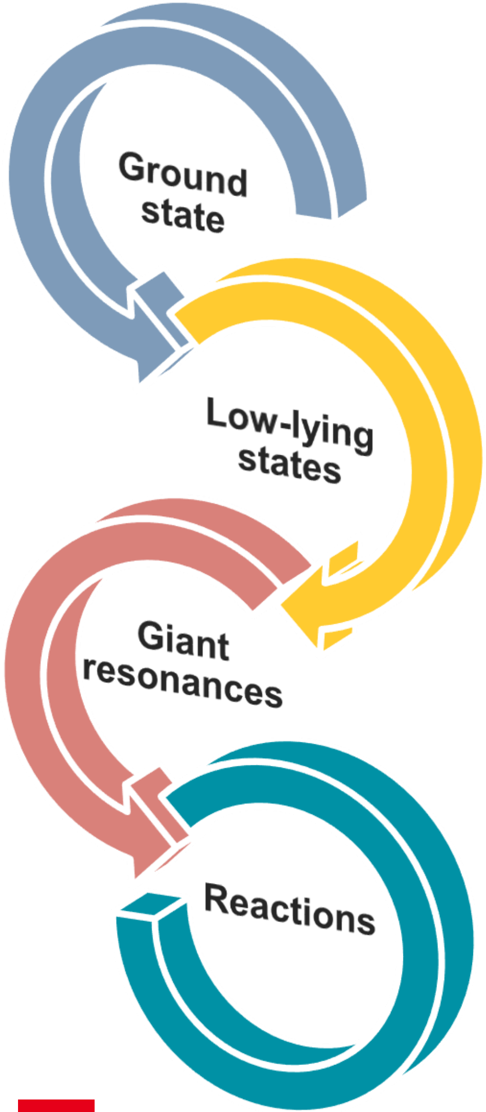
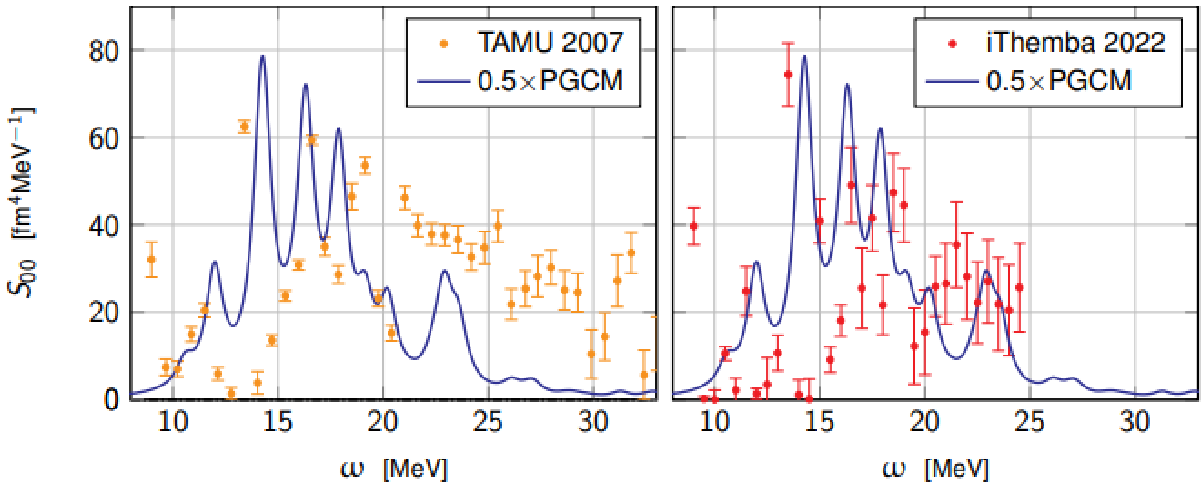


A. Porro et al. Eur.Phys.J.A 60 (2024)



Giant resonance description

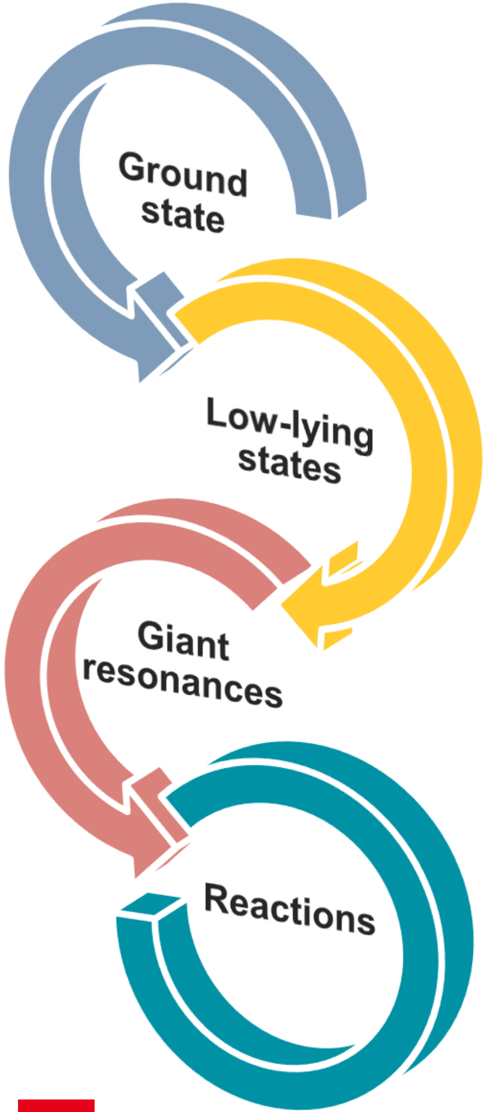
Monopole study in N=Z nuclei

PGCM : Good fractioning (wrt QRPA)

No *ad hoc* shift

When dynamical become important?

Applications of PGCM in realistic model spaces



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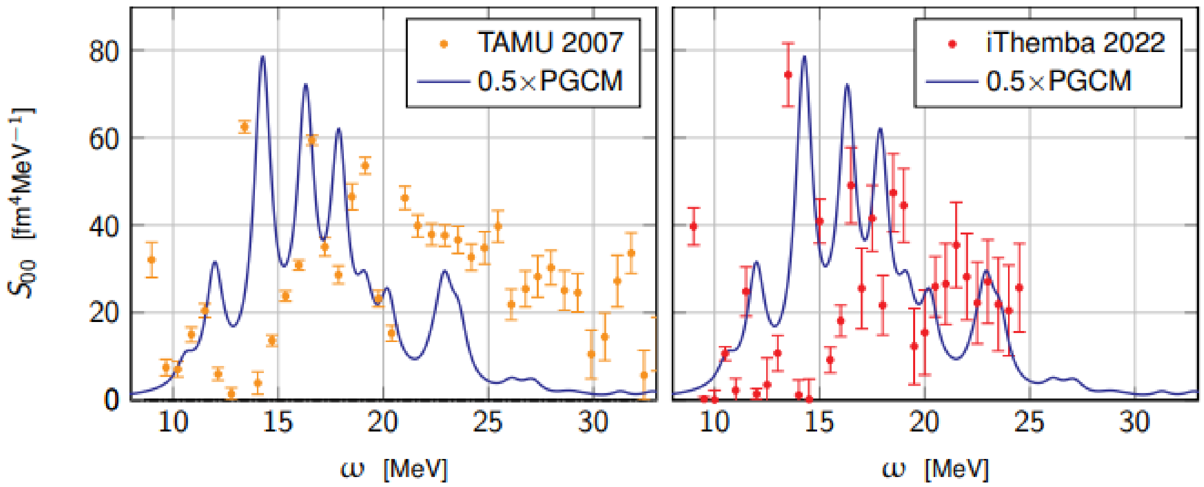

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Choice of GC? VS benchmarks

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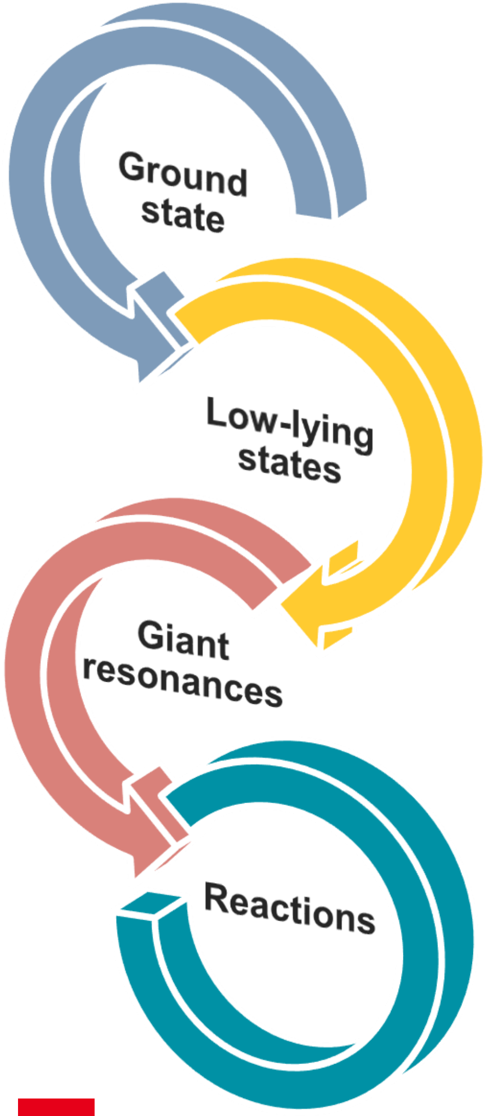

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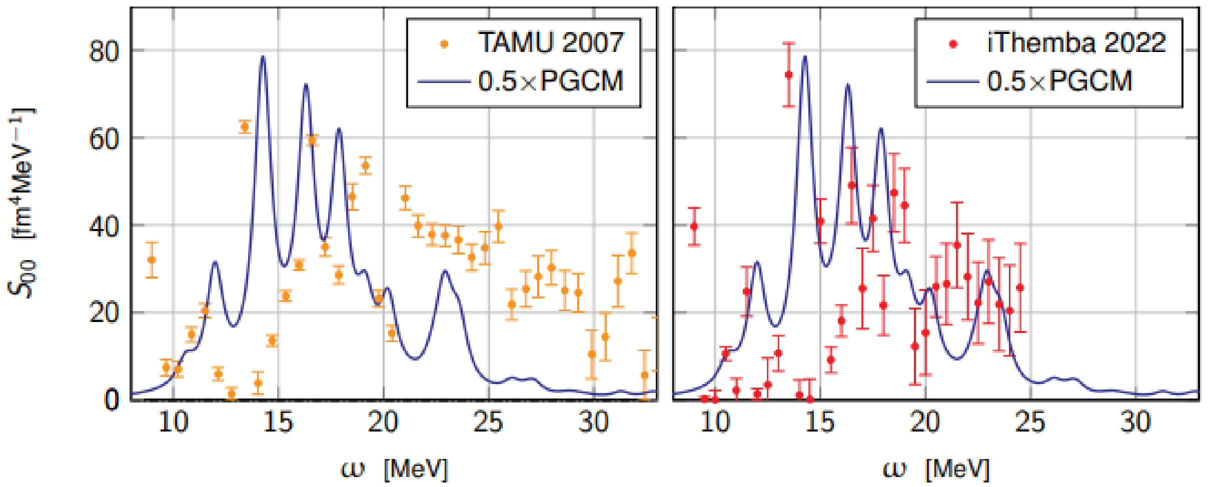

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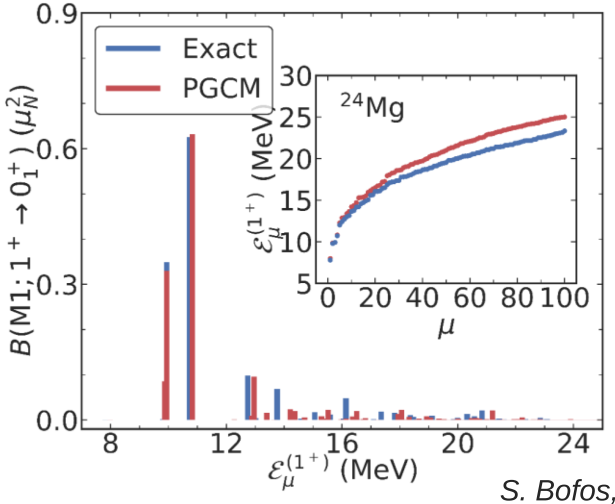
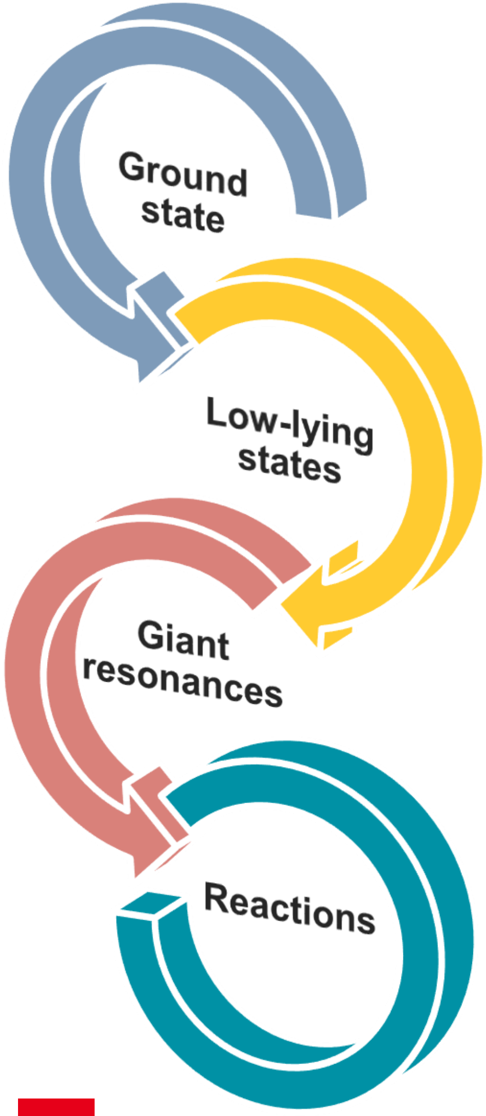


S. Bofos, J. Martinez et al. in preparation

Applications of PGCM in realistic model spaces



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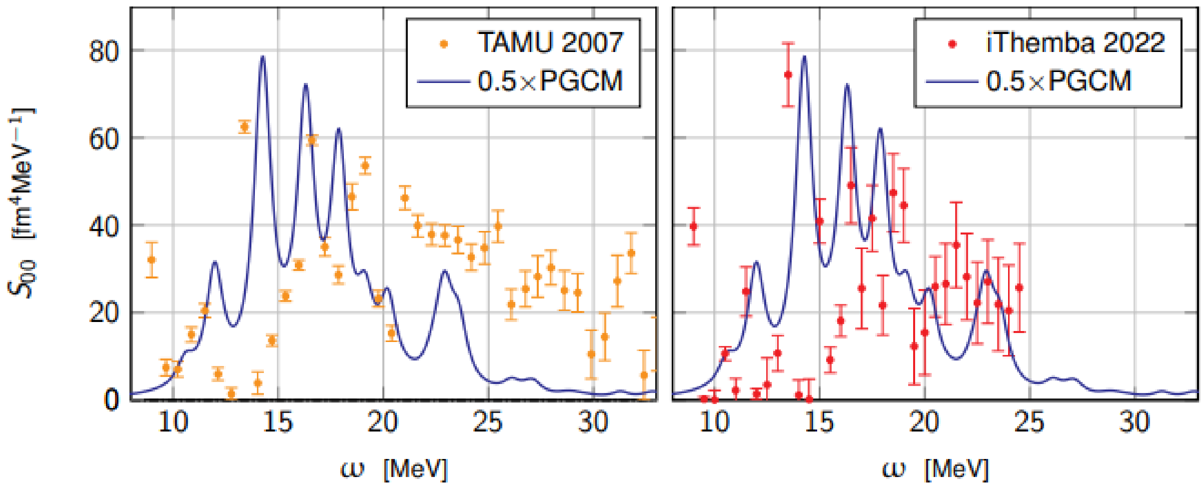

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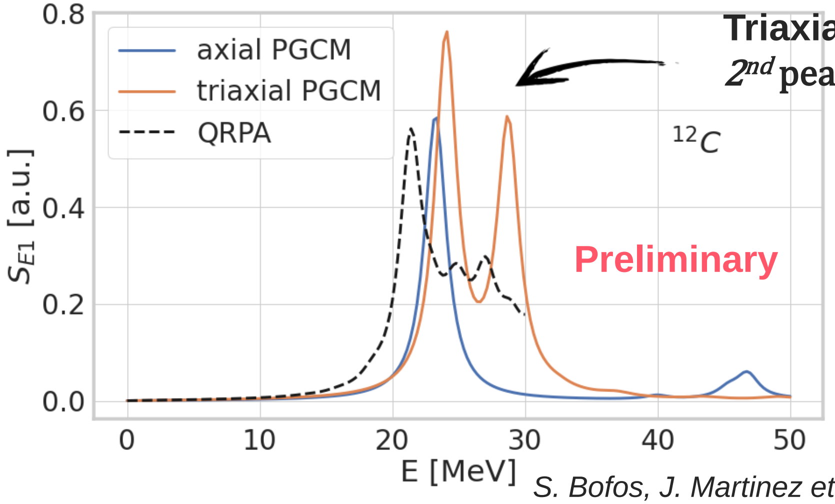

Triaxiality essential for 2^{nd} peak

S. Bofos, J. Martinez et al. in preparation

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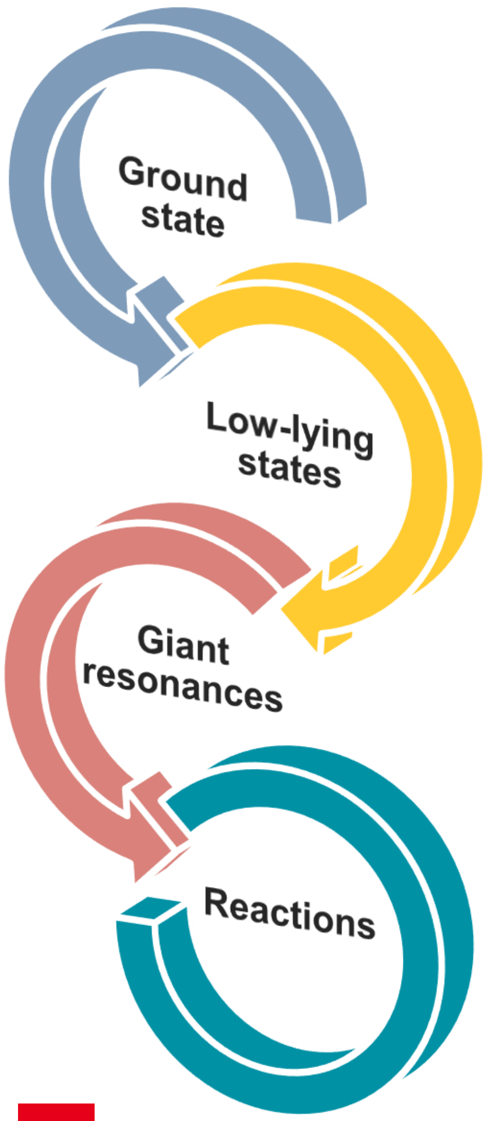

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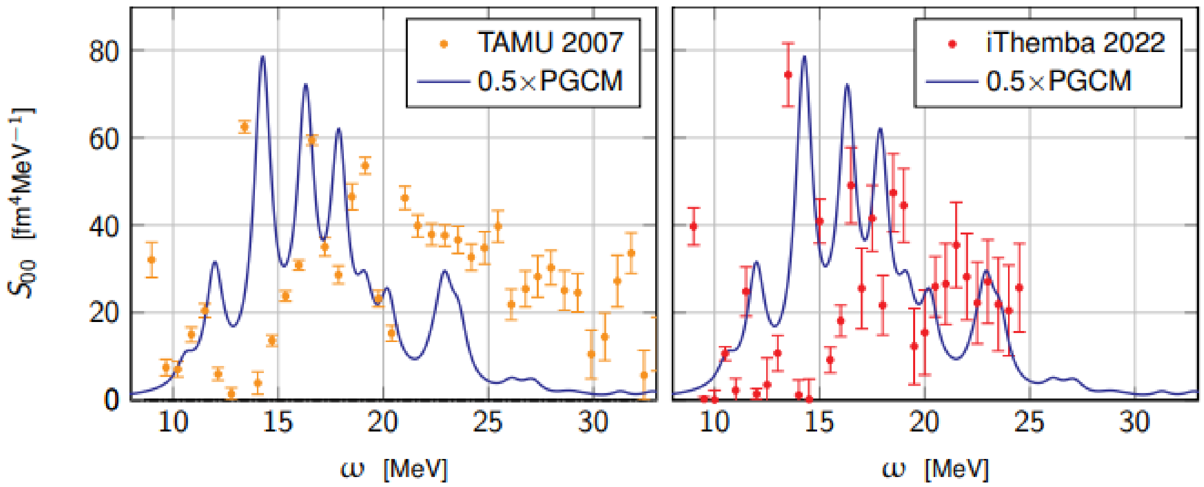

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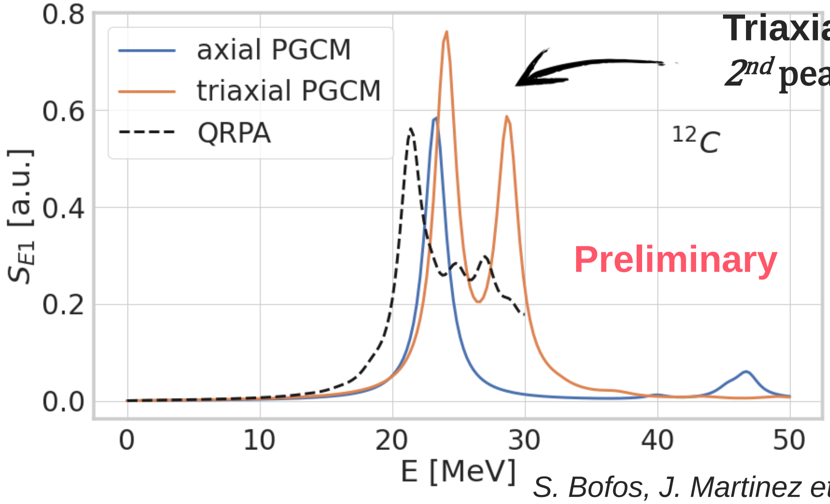

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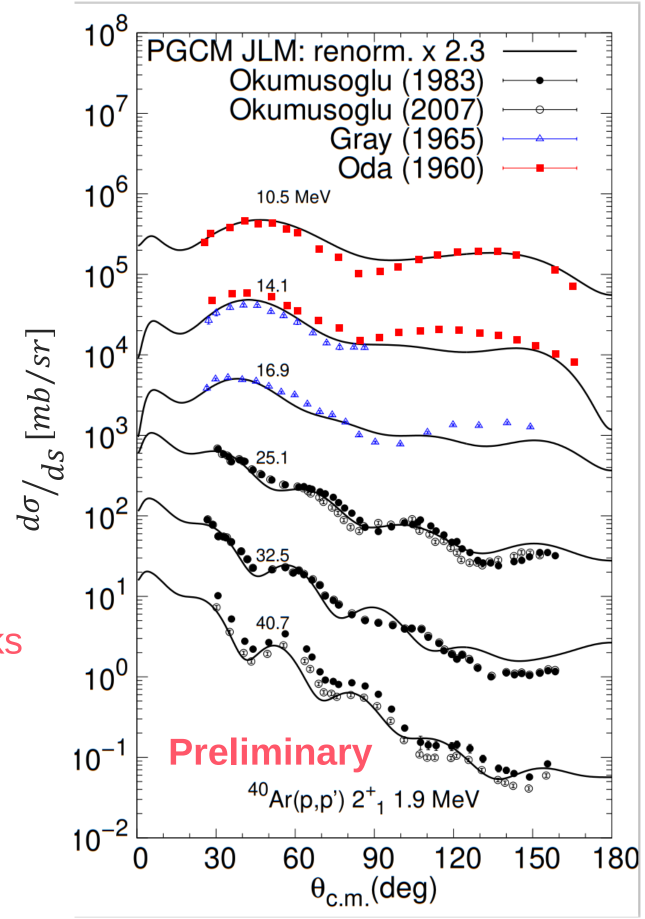
S. Bofos, J. Martinez et al. in preparation



Application to reactions
Transitions densities between excited states
Feeding reaction model with excited states
Very preliminary results

P. Da Costa, M. Dupuis et al. in preparation

4. Conclusion

Conclusion

Multi-reference methods are a powerful tool towards universal modelling of nuclei

Coherent account of vibrational & rotational physics (PGCM)
Short range dynamical correlations captured perturbatively (PGCM-PT)
Observation of *accidental* scale decoupling between static & dynamical

Many developments needed and ongoing to scale up

Better account of 3-body interaction
Limitations of the current method
Deformed heavy nuclei not reliable yet **(A>150)**
Large E^3_{max} did not solve the issue…

Optimizing MR-Perturbation Theory
Current implementation still very heavy
Many avenues exist to leverage the cost
Ongoing project being revived

Lowering the cost of PGCM
Restoring symmetries comes at a significant cost
Many nuclei / applications require triaxiality
Applying dimensionality reduction techniques?

S. Bofos (2025)

Thanks for your attention

Rémi Bernard
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Gianluca Stelini

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