PGCM calculations with chiral EFT interactions

Benjamin Bally

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Motivations

- Progress in *ab initio* description of atomic nuclei
  - Development of new methods but also revisiting old ones
  - Example: phenomenological shell model $\longrightarrow$ *ab initio* VS-IMSRG

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- Used with success in the context of Energy Density Functional (EDF)

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  → technical know-how

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  - ◇ Development of new methods but also revisiting old ones
  - ◇ Example: phenomenological shell model $\longrightarrow$ *ab initio* VS-IMSRG
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  $\rightarrow$ technical know-how
- Several advantages
  - ◇ Efficient at capturing static correlations (e.g. deformation)
  - ◇ Respects the symmetries of H
  - ◇ Access to excited states and various observables
  - ◇ Scales as n_{dim}^4 $\times$ large prefactor

PGCM: main principles

- Low-dimensional linear combination of symmetry-projected mean-field states

$$|\Psi_\epsilon^\sigma\rangle = \sum_{iK} f_{\epsilon,i}^{\sigma K} P^{\sigma K} |\Phi_i\rangle \quad \text{where} \quad \sigma \equiv Z, N, J, M, \pi$$

- Reference states $\{|\Phi_i\rangle\}$ → capture collective correlations
- Restore the symmetries through quantum-number projection $P^{\sigma K}$
- Variational principle

$$\delta \left(\frac{\langle \Psi_\epsilon^\sigma | H | \Psi_\epsilon^\sigma \rangle}{\langle \Psi_\epsilon^\sigma | \Psi_\epsilon^\sigma \rangle} \right) = 0 \Rightarrow f_{\epsilon,i}^{\sigma K}$$

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- Recent developments: combination with *ab initio* techniques
  - ◇ PGCM + PT → see Thomas' talk
  - ◇ PGCM + MR-IMSRG

  Yao, PRL 124, 232501 (2020); Zhou, arXiv.2410.23113 (2024)

Spectroscopy of ^{24}Mg

- Good benchmark
  - Experimental data available
  - Rotational bands (middle of sd shell)
  - MR-EDF calculations

    Bender, PRC 78, 024309 (2008) Yao, PRC 81, 044311 (2010); Rodríguez, PRC 81, 064323 (2010)

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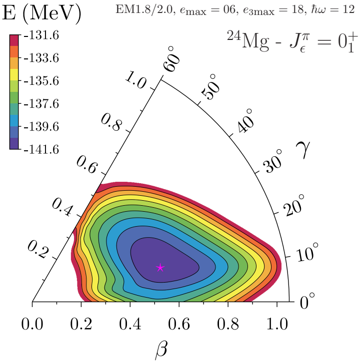
- Details of the calculation
  - Hamiltonian: EM1.8/2.0

    Hebeler, PRC 83, 031301 (2011)
  - Rank-reduction of 3N to an effective 2N

    Frosini, EPJA 57, 151 (2021)
  - $e_{\text{max}} = 6, 8$ (7, 9 HO shells), $e_{3\text{max}} = 18$, $\hbar\omega = 12$
  - Collective coordinates: β, γ (triaxial deformations)

- More information: Bally, EPJA 60, 62 (2024)

Spectroscopy of ^{24}Mg



- Triaxial minimum: $\beta \approx 0.54$, $\gamma \approx 15°$

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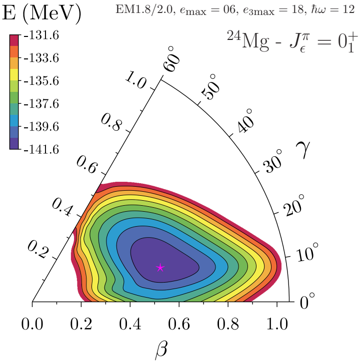

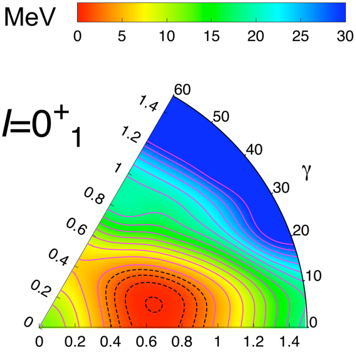

Gogny D1S

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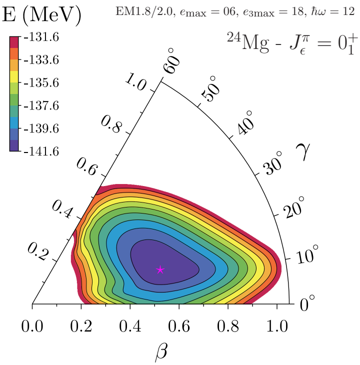

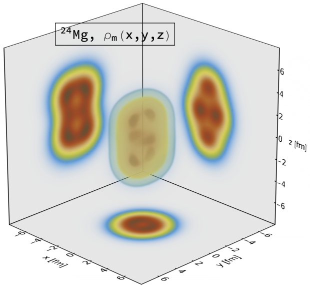

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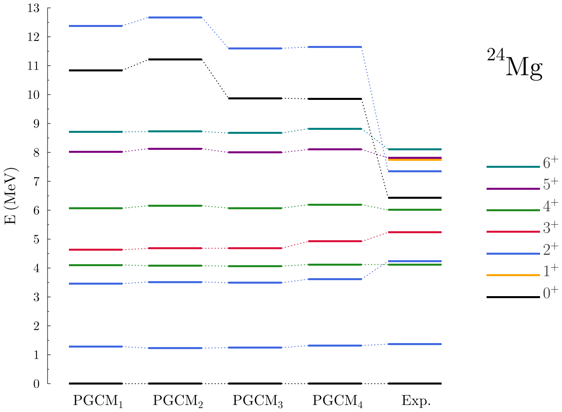
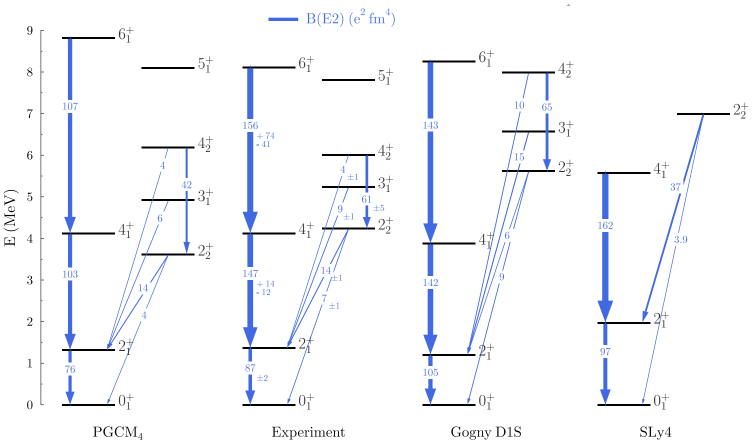


- PGCM$_1$: $e_{\text{max}} = 6$, $\Delta\beta = 0.05$, $E_{\text{thr}} = 5$ MeV
- PGCM$_2$: $e_{\text{max}} = 6$, $\Delta\beta = 0.10$, $E_{\text{thr}} = 5$ MeV
- PGCM$_3$: $e_{\text{max}} = 6$, $\Delta\beta = 0.10$, $E_{\text{thr}} = 10$ MeV
- PGCM$_4$: $e_{\text{max}} = 8$, $\Delta\beta = 0.10$, $E_{\text{thr}} = 10$ MeV



- Gogny D1S: Rodríguez, PRC 81, 064323 (2010)
- SLy4: Bender, PRC 78, 024309 (2008)
  (other states appear at energies > 9 MeV)

Spectroscopy of ^{24}Mg

- Magnetic dipole moment μ (μ_N)
- Electric quadrupole moment Q_s ($e$fm^2)

Quantity	PGCM	Experiment	Gogny D1S	SLy4
$\mu(2_1^+)$	$+1.04$	$+1.08(3)$		
$\mu(2_2^+)$	$+1.06$	$+1.3(4)$		
$\mu(4_1^+)$	$+2.06$	$+1.7(12)$		
$\mu(4_2^+)$	$+2.07$	$+2.1(16)$		

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$Q_s(2_1^+)$	-17.0	-29(3) or -16(6) or -18(2)	-20.8	-19.4

Spectroscopy of ^{20}O (preliminary)

- ^{20}O: Recent experimental results compared with *ab initio* calculations

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  - Hamiltonian: EM1.8/2.0
    Hebeler, PRC 83, 031301 (2011)
  - Rank-reduction of 3N to an effective 2N
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  - $e_{\text{max}} = 6$ (7 HO shells), $e_{3\text{max}} = 18$, $\hbar\omega = 12$
  - Collective coordinates: triaxial deformations (β, γ), cranking (ω)

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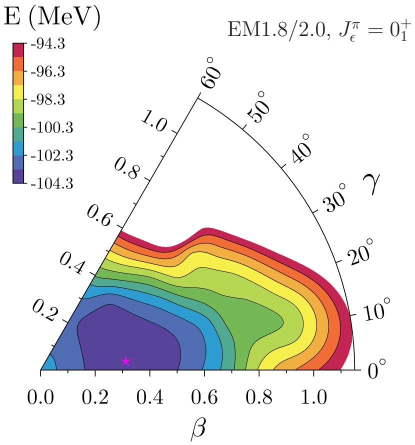

- Minimum only slightly triaxial: $\beta \approx 0.31$, $\gamma \approx 6^{\circ}$

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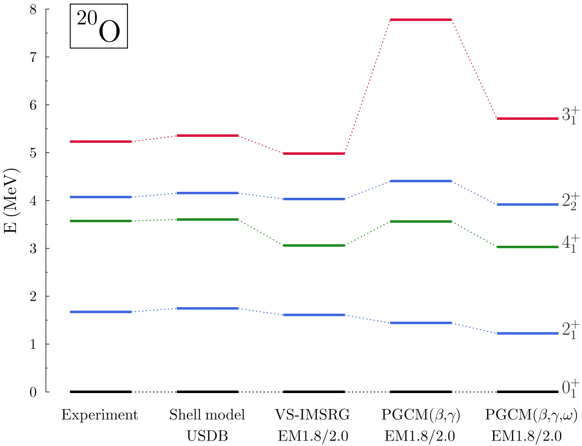

[Data partly taken from Zanon, PRL 131, 262501 (2023)]

- PGCM(β, γ, ω) consistent with VS-IMSRG calculations

Spectroscopy of ^{20}O (preliminary)

$B(E2)$ (e^2fm^4)	Experiment	Shell model USDB	VS-IMSRG EM1.8/2.0	PGCM(β,γ) EM1.8/2.0	PGCM(β,γ,ω) EM1.8/2.0
$2^+_1 \rightarrow 0^+_1$	5.9(2)	3.25	0.89	1.59	1.33
$2^+_2 \rightarrow 0^+_1$	1.3(2)	0.77	0.20	0.45	0.45
$3^+_1 \rightarrow 2^+_1$	0.32(7)	0.57	0.17	1.13	0.34

- Theory does not reproduce experimental data
- Still, PGCM a bit more collective than VS-IMSRG
- Cranking does not change much the transition probabilities except for 3^+_1

Conclusions

- Developments of PGCM with EFT-based interactions
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- Good descripton of ^{24}Mg and ^{20}O spectra

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  → useful tool to describe low-energy spectroscopy (as with EDF)

- Good descripton of ^{24}Mg and ^{20}O spectra

- To improve:
  - More systematic in the exploration of collective coordinates
  - Check more carefully the convergence
  - Computational cost
    → work in progress: PhD of S. Bofos (CEA Cadarache)

- New methods: PGCM-PT, IM-GCM
  → Include dynamical correlations

Collaborators

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