Introduction to the Projected Generator Coordinate Method

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TECHNISCHE UNIVERSITÄT DARMSTADT

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- Originally formulated to describe fission

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- Recently, used with chiral interactions obtained from EFT

PGCM in a nutshell

- Muli-reference variational method where one considers the ansatz

$$|\Theta^{\sigma M}_{\epsilon}\rangle = \sum_{qK} f^{\sigma M}_{\epsilon,qK} P^{\sigma}_{MK} |\Phi(q)\rangle \quad \text{where} \quad \sigma \equiv Z, N, J, \pi$$

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  - $\{|\Phi(q)\rangle\}$ ≡ set of (symmetry-breaking) reference states that explores collective degrees of freedom
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- Important aspects

  - $\{|\Phi(q)\rangle\}$ ≡ set of (symmetry-breaking) reference states that explores collective degrees of freedom
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  - P_{MK}^{σ} ≡ projection operator that restores the symmetries
    → good quantum numbers Z, N, J, π

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  - ◇ P^{σ}_{MK} ≡ projection operator that restores the symmetries
    → good quantum numbers Z, N, J, π
  - ◇ $f^{\sigma M}_{\epsilon,qK}$ ≡ weights determined variationally

$$\frac{\delta}{\delta f^{\sigma M *}_{\epsilon,qK}} \left(\frac{\langle \Theta^{\sigma M}_{\epsilon} | H | \Theta^{\sigma M}_{\epsilon} \rangle}{\langle \Theta^{\sigma M}_{\epsilon} | \Theta^{\sigma M}_{\epsilon} \rangle} \right) = 0 \quad \Leftrightarrow \quad Hf = eNf$$

Remark: $\langle \Phi(q_1) | \Phi(q_2) \rangle \neq 0$

PGCM in a nutshell (technical supplement I)

- $|\Phi(q)\rangle \equiv$ Bogoliubov quasi-particle states

$$|\Phi(q)\rangle = \prod_i \beta_i(q)|0\rangle$$

$$\begin{pmatrix} \beta(q) \\ \beta^\dagger(q) \end{pmatrix} = \begin{pmatrix} U^\dagger(q) & V^\dagger(q) \\ V^T(q) & U^T(q) \end{pmatrix} \begin{pmatrix} a \\ a^\dagger \end{pmatrix} \equiv \mathcal{W}^\dagger(q) \begin{pmatrix} a \\ a^\dagger \end{pmatrix}$$

$$\mathcal{W}(q)\mathcal{W}^\dagger(q) = \mathcal{W}^\dagger(q)\mathcal{W}(q) = 1$$

- Includes pairing correlations but breaks particle-number conservation

PGCM in a nutshell (technical supplement II)

- Projection operator $P^{\sigma}_{MK} \equiv P^{Z} P^{N} P^{J}_{MK} P^{\pi}$

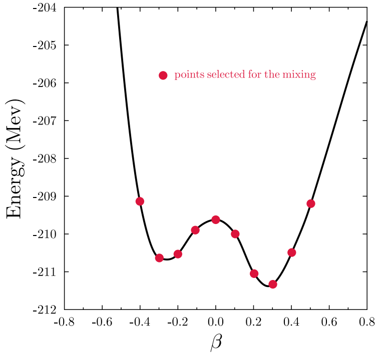
$$
\begin{aligned}
P^{Z} &= \frac{1}{2\pi} \int_0^{2\pi} d\phi_Z \, e^{i\phi_Z (\mathrm{Z} - Z)} \\
P^{N} &= \frac{1}{2\pi} \int_0^{2\pi} d\phi_N \, e^{i\phi_N (\mathrm{N} - N)} \\
P^{J}_{MK} &= \frac{2J+1}{16\pi^2} \int_0^{2\pi} d\alpha \int_0^{\pi} d\beta \, \sin(\beta) \int_0^{4\pi} d\gamma \, D^{J*}_{MK}(\alpha,\beta,\gamma) \, R(\alpha,\beta,\gamma) \\
P^{\pi} &= \frac{1}{2}(1 + \pi \Pi)
\end{aligned}
$$

- Full projection requires: $\mathrm{diag}(\langle \Phi(q) | H P^{\sigma}_{MK} | \Phi(q) \rangle) \rightarrow$ variational

PGCM: schematic illustration

Constrained Hartree-Fock-Bogoliubov calculations

$\delta\left(\langle\Phi(q)|H-\lambda Q|\Phi(q)\rangle\right) = 0$ with $\langle\Phi(q)|Q|\Phi(q)\rangle = q$



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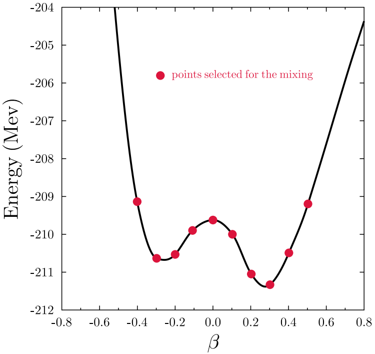
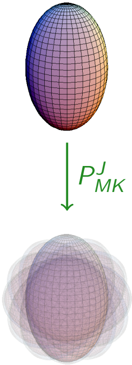


Restoration of rotational invariance



Courtesy of M. Aytekin

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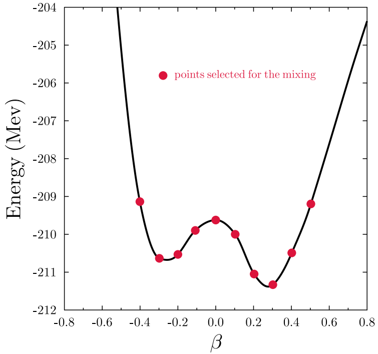

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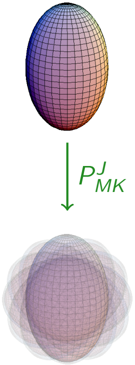

Courtesy of M. Aytekin

$\Rightarrow$ **Optimal superposition of deformed states rotated in all possible ways**

PGCM: scaling

- Evaluation of matrix elements: $\langle \Phi(q_1) | O R(\Omega) | \Phi(q_2) \rangle \rightarrow \sim n_{\text{basis}}^4$ (two-body O)

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- N_{set}: number of reference states
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- N_{set}: number of reference states
- N_{angles}: number of angles in discretization of P^{σ}_{MK}

$$\text{scaling} \propto \frac{N_{\text{set}}(N_{\text{set}}+1)}{2} N_{\text{angles}} n_{\text{basis}}^4$$

Numerical suite TAURUS

- Main features

  Bally *et al.*, EPJA 57, 69 (2021) ; Bally *et al.*, EPJA 60, 62 (2024)

  - Spherical Harmonic Oscillator basis (m-scheme)
  - Real general Bogoliubov reference states
  - Variation after particle-number projection
  - Projection after variation: Z, N, J, M, π
  - Configuration mixing of projected states

- GitHub: `https://github.com/project-taurus`

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TAURUS
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Spectroscopy of ^{24}Mg

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

    Bender *et al.*, PRC 78, 024309 (2008) ; Yao *et al.*, PRC 81, 044311 (2010) ; Rodríguez *et al.*, PRC 81, 064323 (2010)

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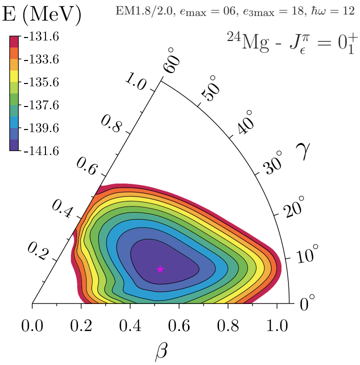
- Details of the calculation
  - Hamiltonian: EM1.8/2.0

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

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

- More information: Bally *et al.*, EPJA 60, 62 (2024)

Spectroscopy of ^{24}Mg



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

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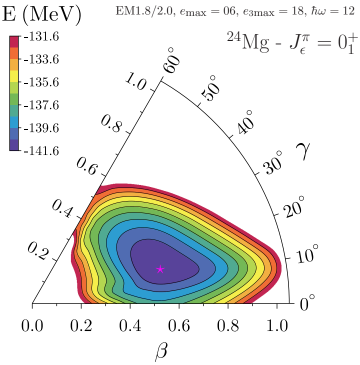

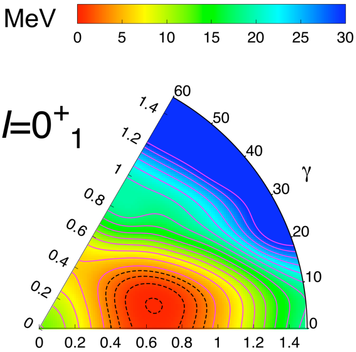

Gogny D1S

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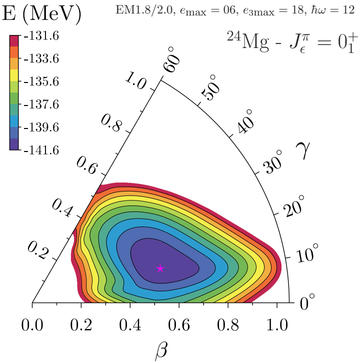

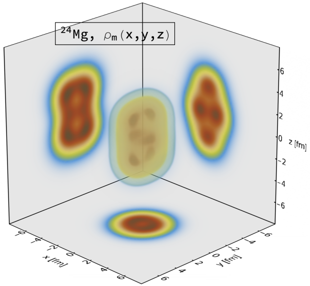

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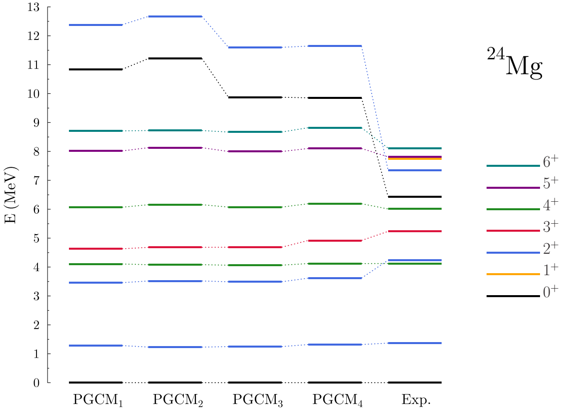
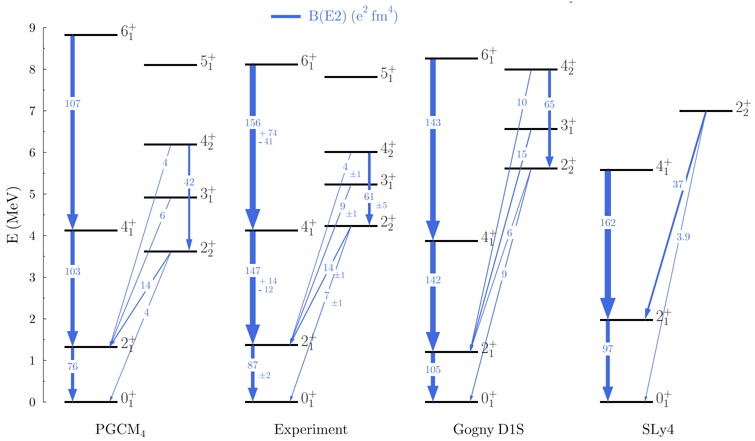


- PGCM$_1$: $e_{max} = 6$, $\Delta\beta = 0.05$, $E_{thr} = 5$ MeV
- PGCM$_2$: $e_{max} = 6$, $\Delta\beta = 0.10$, $E_{thr} = 5$ MeV
- PGCM$_3$: $e_{max} = 6$, $\Delta\beta = 0.10$, $E_{thr} = 10$ MeV
- PGCM$_4$: $e_{max} = 8$, $\Delta\beta = 0.10$, $E_{thr} = 10$ MeV

Spectroscopy of ^{24}Mg



- Gogny D1S: Rodríguez *et al.*, PRC 81, 064323 (2010)
- SLy4: Bender *et al.*, 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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$\mu(4_2^+)$	$+2.07$	$+2.1(16)$		
$Q_s(2_1^+)$	-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

  Zanon *et al.*, PRL 131, 262501 (2023)

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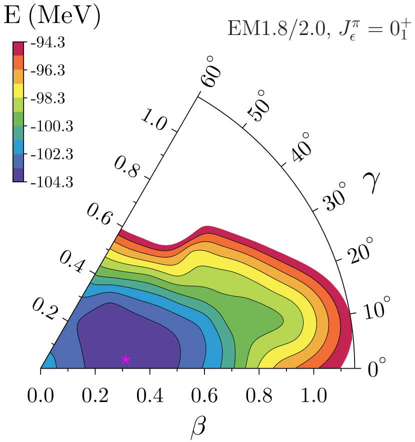
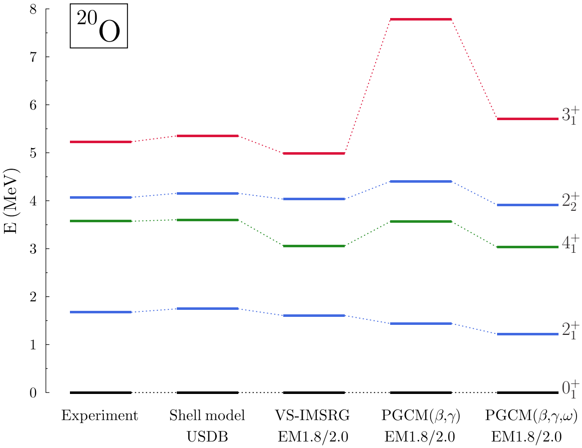
- Details of the calculation
  - Hamiltonian: EM1.8/2.0
  - Rank-reduction of 3N to an effective 2N
  - $e_{\max} = 6$ (7 HO shells), $e_{3\max} = 18$, $\hbar\omega = 12$
  - Collective coordinates: triaxial deformations (β, γ), cranking $(\langle J_x \rangle$ or $\omega)$

Spectroscopy of ^{20}O (preliminary)



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

Spectroscopy of ^{20}O (preliminary)



[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
$2_1^+ \to 0_1^+$	5.9(2)	3.25	0.89	1.59	1.33
$2_2^+ \to 0_1^+$	1.3(2)	0.77	0.20	0.45	0.45
$3_1^+ \to 2_1^+$	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^+

PGCM: advantages and drawbacks

- Many advantages:
  - Efficient at capturing static correlations (e.g. deformation)
  - Respects the symmetries of H
  - Access to excited states and various observables
  - Gentle scaling with A (mean field)

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- Many advantages:
  - Efficient at capturing static correlations (e.g. deformation)
  - Respects the symmetries of H
  - Access to excited states and various observables
  - Gentle scaling with A (mean field)

- But some limitations:
  - Inefficient at capturing dynamic correlations (few p-h excitations)
  - Computational cost grows rapidly with number of coordinates/reference states considered
  - Choice of collective coordinates requires some empirical knowledge

Extension: In-Medium PGCM

- Combine PGCM with IMSRG $\Rightarrow$ **see Heiko's talk**

  Yao *et al.*, PRC 98, 054311 (2018) ; Yao *et al.*, PRL 124, 232501 (2020)

  - PGCM $\rightarrow$ includes static/collective correlations (many p-h excitations)
  - IMSRG $\rightarrow$ includes dynamic correlations (a few p-h excitations)

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- Workflow

$$H(0) \xrightarrow{\text{PGCM}} |\Theta_{\epsilon}^{\sigma M}(0)\rangle \xrightarrow{\text{IMSRG}} H(s) = U(s)H(0)U^{\dagger}(s) \xrightarrow{\text{PGCM}} |\Theta_{\epsilon}^{\sigma M}(s)\rangle$$

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- Remark: first PGCM may be replaced by an ensemble of PHFB states:

$$\rho \equiv \sum_q c_q |P^\sigma \Phi(q)\rangle\langle P^\sigma \Phi(q)|$$

In-Medium PGCM: application to the $0\nu2\beta$ decay

- $^{76}\text{Ge} \rightarrow {}^{76}\text{Se} + 2e^{-}$

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- $^{76}\mathrm{Ge} \rightarrow {}^{76}\mathrm{Se} + 2e^-$
- Evaluate matrix element: $\langle 0_1^+(^{76}\mathrm{Se})|M_{0\nu}|0_1^+(^{76}\mathrm{Ge})\rangle$ $\Rightarrow$ **see Lotta's talk**

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- Evaluate matrix element: $\langle 0^+_1(^{76}\mathrm{Se}) | M_{0\nu} | 0^+_1(^{76}\mathrm{Ge}) \rangle$ $\Rightarrow$ **see Lotta's talk**
- Ensemble: $\rho \equiv \sum_{q,A} c_{q,A} | P^\sigma \Phi(q,A) \rangle \langle P^\sigma \Phi(q,A) |$

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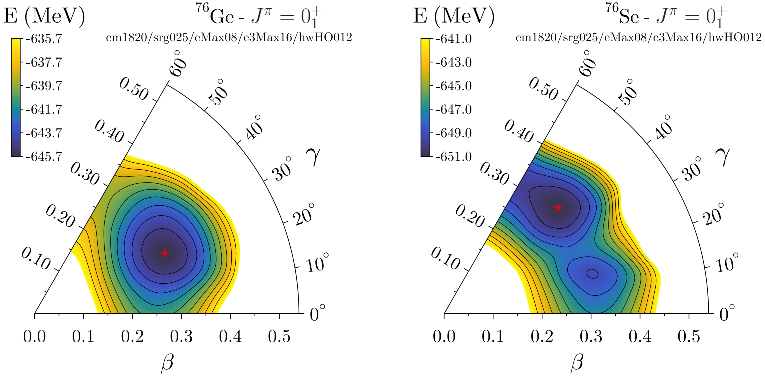

Belley *et al.*, PRL 132, 182502 (2024)

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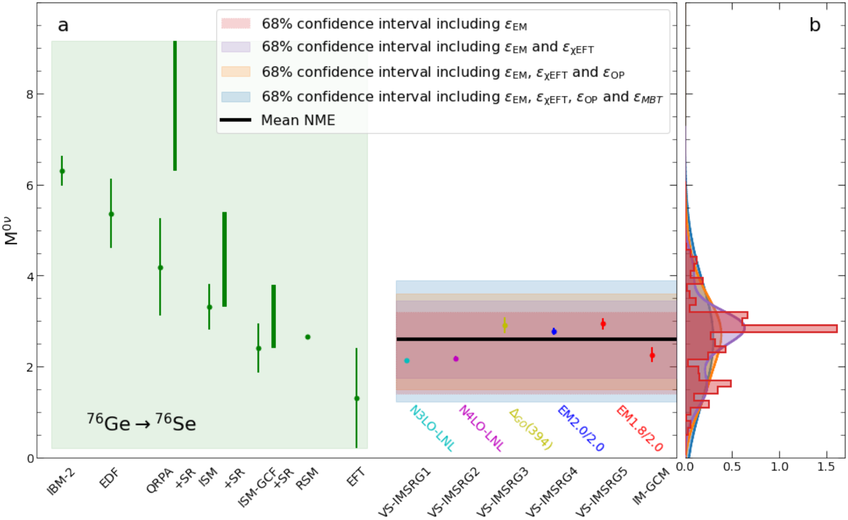

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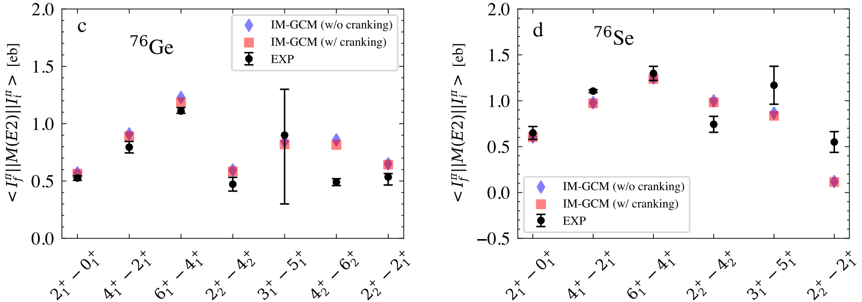
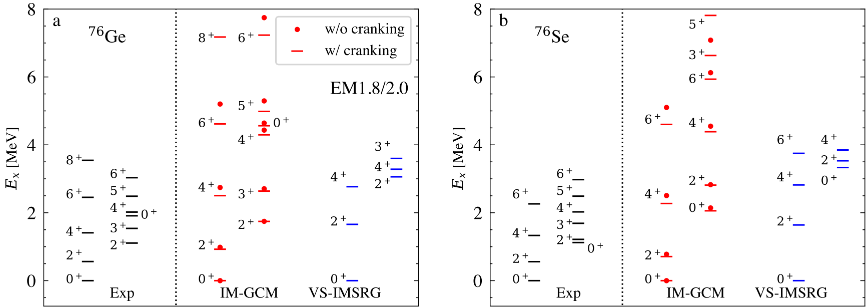
ELM transition probabilities for ^{76}Ge/Se





a
76Ge
b
76Se
w/o cranking
w/ cranking
EM1.8/2.0
Exp
IM-GCM
VS-IMSRG
E_x [MeV]

Extension: PGCM - Perturbation Theory

- Schrödinger equation

$$H(s)|\Psi_\epsilon^{\sigma M}(s)\rangle = E_\epsilon^{\sigma}|\Psi_\epsilon^{\sigma M}(s)\rangle$$

Extension: PGCM - Perturbation Theory

- Schrödinger equation

$$H(s)|\Psi_\epsilon^{\sigma M}(s)\rangle = E_\epsilon^\sigma |\Psi_\epsilon^{\sigma M}(s)\rangle$$

- Partition of the Hamiltonian

$$H(s) = H_0(s) + H_1(s)$$

such that

$$H_0(s)|\Theta_\epsilon^{\sigma M}(s)\rangle = E_\epsilon^{\sigma(0)}(s)|\Theta_\epsilon^{\sigma M}(s)\rangle$$

Extension: PGCM - Perturbation Theory

- Schrödinger equation

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$$|\Psi^{\sigma M}_{\epsilon}(s)\rangle = \Omega^{\mathrm{PT}}_{[\sigma,\epsilon,H_1(s)]}|\Theta^{\sigma M}_{\epsilon}(s)\rangle$$

- Multi-reference and symmetry-conserving expansion

- Scaling of PGCM-PT(2): $\mathrm{O}(n^8_{\mathrm{basis}})$

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- Scaling of PGCM-PT(2): $\text{O}(n_{\text{basis}}^8)$
- Details can be found in:

Frosini *et al.*, EPJA 50, 62, 182502 (2022)

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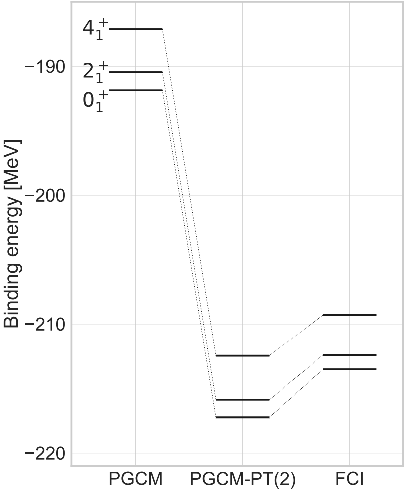
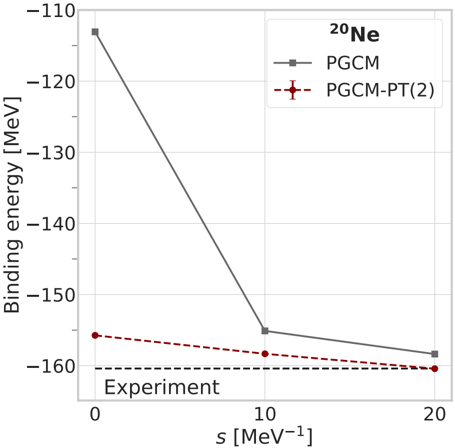
^{20}Ne: effects of PT(2) for $H(0)$



(e_{max} = 4, Hüther N3LO, axial deformations β_{20})

Frosini *et al.*, EPJA 50, 64, 182502 (2022)

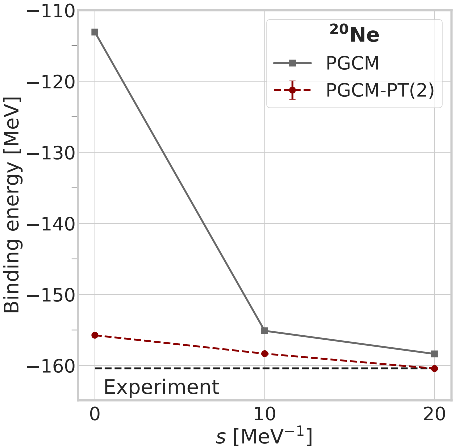
^{20}Ne: effects of PT(2) for $H(s)$

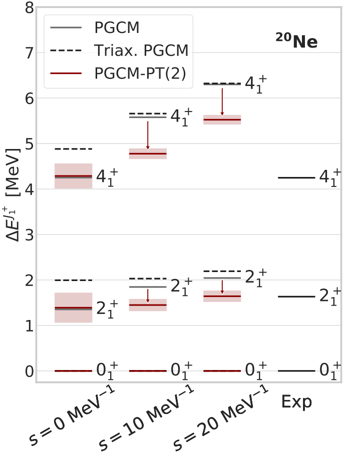


($e_{max} = 6$, EM1.8/2.0, axial deformations β_{20})

Frosini *et al.*, EPJA 50, 64, 182502 (2022)

^{20}Ne: effects of PT(2) for $H(s)$





($e_{\text{max}} = 6$, EM1.8/2.0, axial deformations β_{20})

Frosini *et al.*, EPJA 50, 64, 182502 (2022)

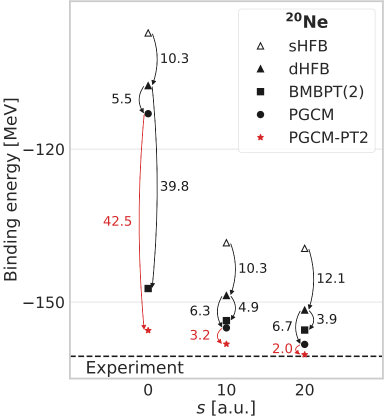
Conclusions

- PGCM is a powerful method
  - Variational
  - Multi-reference
  - Symmetry conserving
  - Capture collective correlations

- Already useful to describe relative properties

- Extensions to include dynamic correlations
  $\Rightarrow$ MR-IMSRG + PGCM + PT

- Optimal way to distribute correlations?



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