Low-lying spectroscopy of even-even nuclei via multi-reference perturbation theory based on PGCM state

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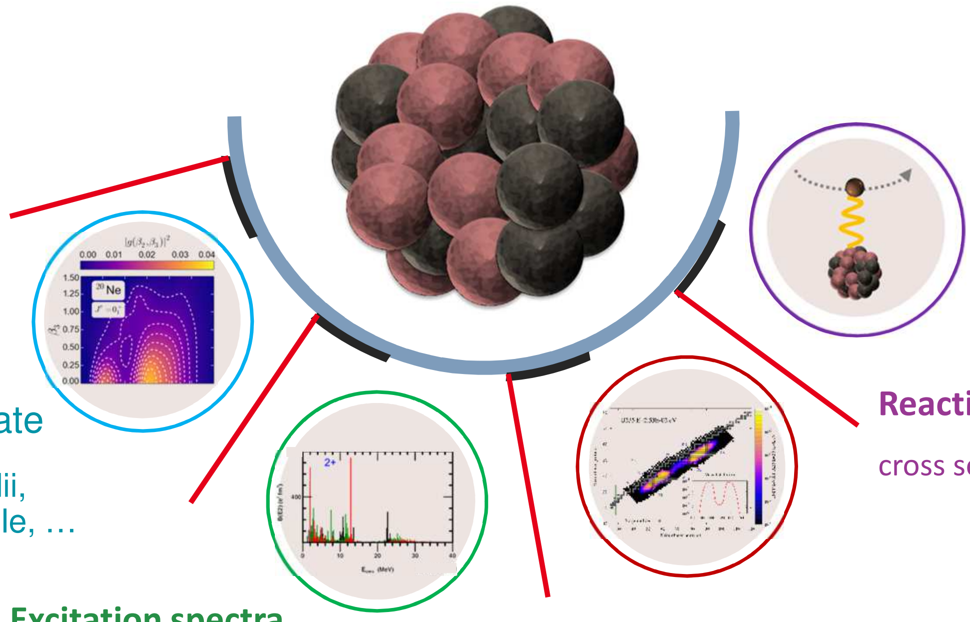
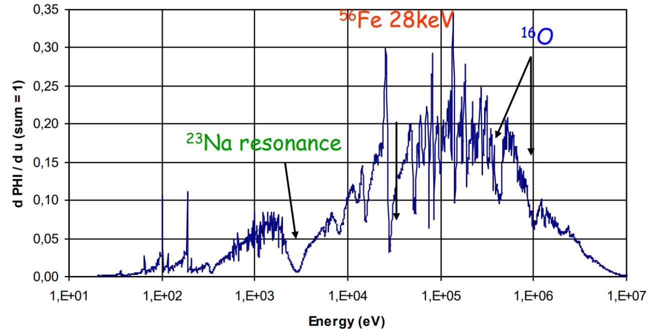
Microscopic models of nuclei for nuclear data

Presentation focused on particular *Ab Initio* method for both short and long range correlations
Objective : **solve A-body Schrödinger equation** to given accuracy
Projected Generator Coordinate Method Perturbation Theory
Focus on **formalism** and **first implementation**

RÉACTEUR NUMÉRIQUE





Ground-state

masses, radii,
density profile, …

Excitation spectra

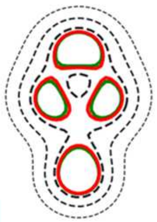
energies, transition probabilities,
response function to electroweak
probes, …

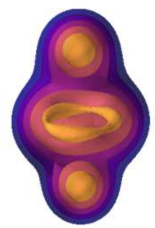
Decay modes

lifetime, yields, …

Reactions

cross sections, …



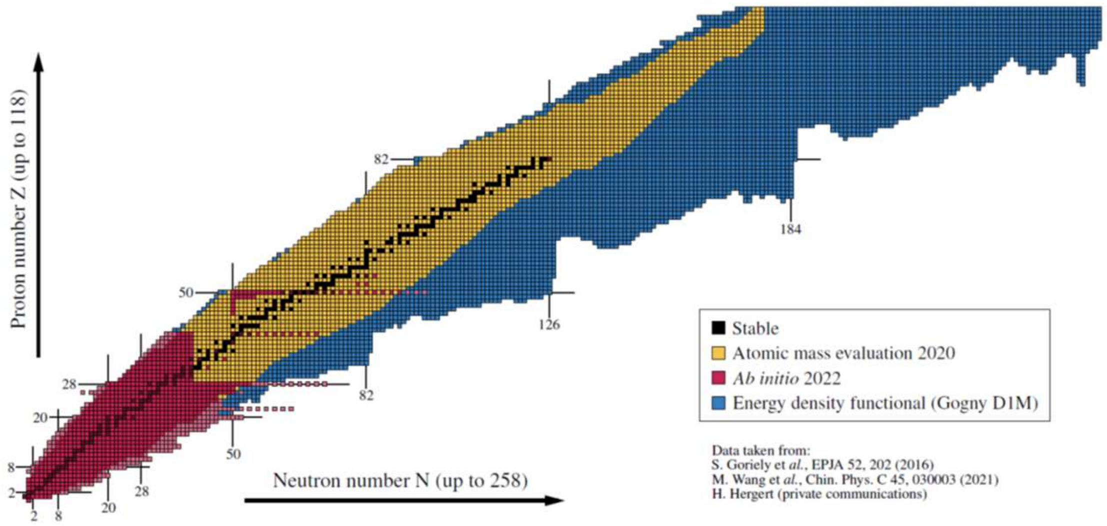


Progress of ab initio / in medias res methods

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*



Courtesy of B. Bally

Steady progress in the last decades

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
Doubly open-shells **Valence space** **Symmetry-breaking** **Multi-reference**	**2020-?**	Mixed / Polynomial Scaling

Outline

1. **Formalism**
   - Progress of ab initio / in medias res methods
   - Single and multi-reference expansion methods
   - Projected Generator Coordinate Method + Perturbation Theory
2. **Numerical aspects of PGCM-PT**
   - Circumventing the complexity of three body interactions
   - Calculation of matrix elements
3. **Application with IM-SRG evolved interaction**
   - Evolved interactions and parallel with EDF
   - Ground state energy calculations in closed shell nuclei
   - Spectroscopy in doubly open-shell Neon20
4. **Conclusion**

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1. Formalism

Single and Multi-Reference expansion methods

$[H, R] = 0$

Schrödinger equation

Nucleon interaction
1-,2-,3-… body

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

Correlated wave-function
A! parameters

Partitioning

$|\Phi^{(0)}\rangle$ reference state eigenstate of H_0

$\mathcal{P} \equiv |\Phi^{(0)}\rangle\langle\Phi^{(0)}|$

$\mathcal{Q} \equiv 1 - \mathcal{P}$

Unperturbed problem
« Easy »

$$H \equiv H_0 + H_1$$

Residual interaction
Treated approximatively

Formal RS
Perturbation Theory

$$|\Phi^{(1)}\rangle \equiv -\mathcal{Q}\left(H_0 - E^{(0)}\right)^{-1}\mathcal{Q}H_1|\Theta^{(0)}\rangle$$
$$|\Phi^{(2)}\rangle \equiv -\mathcal{Q}\left(H_0 - E^{(0)}\right)^{-1}\mathcal{Q}\overline{H_1}|\Theta^{(1)}\rangle$$
$$|\Phi^{(k)}\rangle \equiv \cdots$$

$$|\Psi\rangle \equiv \sum_k |\Theta^{(k)}\rangle$$

$$E^{(0)} = \langle\Theta^{(0)}|H_0|\Theta^{(0)}\rangle$$
$$E^{(1)} = \langle\Theta^{(0)}|H_1|\Theta^{(0)}\rangle$$
$$E^{(2)} = \langle\Theta^{(0)}|H_1|\Theta^{(1)}\rangle$$
$$E^{(k)} = \cdots$$

Systematic expansion
Open questions
- **Choice of reference state**
- **Choice of partitioning**

Optimal strategy ?

Single reference symmetry conserving PT in closed shells

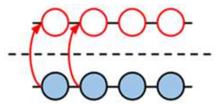
Spherical Hartree Fock $o(N^4)$

$$|\Theta^{(0)}\rangle = |sHF\rangle$$

$$E^{(2)} = -\sum_{I}^{S,D} \frac{|\langle\Phi|H_1|\Phi^I\rangle|^2}{E^I - E^{(0)}} = -\sum \frac{\left|H_{ab}^{ij}\right|^2}{E^a + E^b - E^i - E^j}$$

Canonical Partitioning

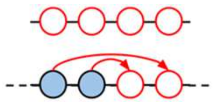
$$H_0 \equiv E^{(0)}|\Phi^{(0)}\rangle\langle\Phi^{(0)}| + \sum_{I}^{S,D,\cdots} E^I|\Phi^I\rangle\langle\Phi^I|$$



Strictly positive diagonal H_0

Single reference symmetry breaking PT in open shells

Degenerate unperturbed state
No expansion possible



Single and Multi-Reference expansion methods

$[H,R]=0$

Schrödinger equation

Nucleon interaction
1-,2-,3-… body

$$\underline{H}\,|\Psi^\sigma\rangle = E^\sigma \underline{|\Psi^\sigma\rangle}$$

Correlated wave-function
A! parameters

Partitioning

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$\mathcal{Q} \equiv 1-\mathcal{P}$

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« Easy »

$$\underline{H \equiv H_0} + \underline{H_1}$$

Residual interaction
Treated approximatively

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Perturbation Theory

$|\Phi^{(1)}\rangle \equiv -\mathcal{Q}\left(H-E^{(0)}\right)^{-1}\mathcal{Q}H_1|\Theta^{(0)}\rangle$

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$$|\Psi\rangle \equiv \sum_k |\Theta^{(k)}\rangle$$

$E^{(0)} = \langle\Theta^{(0)}|H_0|\Theta^{(0)}\rangle$

$E^{(1)} = \langle\Theta^{(0)}|H_1|\Theta^{(0)}\rangle$

$E^{(2)} = \langle\Theta^{(0)}|H_1|\Theta^{(1)}\rangle$

$E^{(k)} = \cdots$

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Canonical Partitioning

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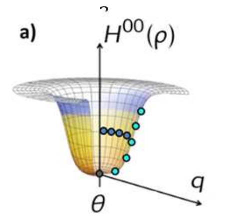
Strictly positive diagonal H_0



Symmetry conserving minimum

Single reference symmetry breaking PT in open shells

order par.
$\rho = qe^{i\theta}$

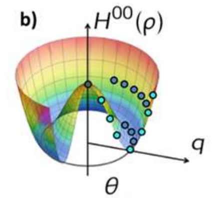
Symmetry breaking HF Bogoliubov $\boldsymbol{O(N^4)}$

$$|\Theta^{(0)}\rangle = |dHFB\rangle$$

Canonical SB Partitioning

$$[H_0,R] \neq 0, \qquad [H_1,R] \neq 0$$

SB expansion
Quasi-particle denominators
Contamination to all orders
- ***Restoration of symmetries?***



Symmetry breaking minimum

Multi reference symmetry conserving PT in open shels

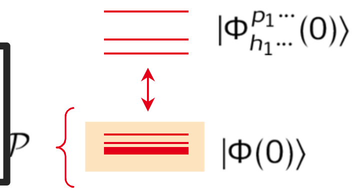
Symmetry conserving multi-reference state

$$|\Theta^{(0)}\rangle = \sum_i |\Phi_i\rangle$$

Non canonical SB Partitioning

$$[H_0,R] = 0, \qquad [H_1,R] = 0$$

Choice Ref State?
Choice of basis?
Non diagonal $\boldsymbol{H_0}$



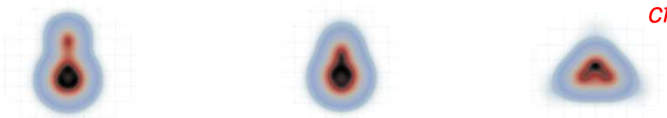
See A. Tichai's presentation

PGCM + Perturbation Theory

Projected Generator Coordinate Method

Frosini et al. (2022)
Porro et al. (2024)

cf A. Porro's presentation



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

Constrained mean-field
Symmetry breaking

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

Projection
Rotation

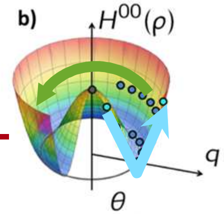
$$|\Psi^{J^\pi NZ}\rangle \equiv \int_q dq\, \boxed{f^{J^\pi NZ}(q)} P^{J^\pi NZ}|\Phi(q)\rangle$$

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

State-specific Partitioning

$$\mathcal{P}^\sigma_\mu \equiv \sum_K |\Theta^{\sigma K}_\mu\rangle\langle\Theta^{\sigma K}_\mu|$$

$$\mathcal{Q}^\sigma_\mu \equiv 1 - \mathcal{P}^\sigma_\mu$$

Baranger Hamiltonian

$$H_0 \equiv \mathcal{P}^\sigma_\mu F_{[|\Theta\rangle]} \mathcal{P}^\sigma_\mu + \mathcal{Q}^\sigma_\mu F_{[|\Theta\rangle]} \mathcal{Q}^\sigma_\mu$$

$$[H_0, R] = 0$$

Basis of $\mathcal{Q}$?

PGCM-PT(2) equation

Analytic inversion not possible in principle

$$|\Phi^{(1)}\rangle = -\mathcal{Q}\left(H_0 - E^{(0)}\right)^{-1} \mathcal{Q} H_1 |\Theta^{(0)}\rangle$$

Need for convenient representation of $\mathcal{Q}$ space

Projected excited HFB $|\Omega^I(q)\rangle \equiv \mathcal{Q}P^\sigma|\Phi^I(q)\rangle$

$$|\Phi^{(1)}\rangle \equiv \sum_q \sum_I^{S,D,\cdots} a^I(q)|\Omega^I(q)\rangle$$

Non orthonormal basis

Approximation: Truncation to singles and doubles

Matrix approximation of $H_0 - E^{(0)}$

$$\sum_{\mathbf{q}} \sum_{\mathbf{J}}^{\mathbf{SD}} \mathbf{M_{IpJq} a^J(q)} = -\mathbf{h^I_1(p)}$$

Vector representation of $H_1 \mathcal{Q}|\Theta\rangle$

$$M_{IpJq} \equiv \langle\Omega^{I(p)}|H_0 - E^{(0)}|\Omega^{J(q)}\rangle$$

$$h^I_1(p) \equiv \langle\Omega^{I(p)}|H_1|\Omega^{(0)}\rangle$$

Remarks at this stage

Strong static / collective correlations captured by PGCM reference
Weak / dynamical correlations captured in perturbation
Versatile but **expansive symmetry conserving** expansion method
- $\boldsymbol{O}(\boldsymbol{N^4})$ PGCM with large prefactor
- $\boldsymbol{O}(\boldsymbol{N^8})$ PT denominator matrix construction and inversion
- Applicable to ***all*** **systems**

Multiple **redundant copies** of Hilbert space → need special care
Following discussion on numerical aspects

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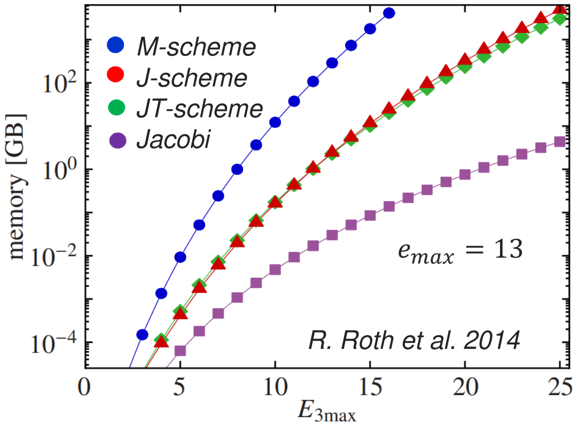
2. Numerical aspects

Circumventing the problem of three-body interaction

Ab initio Hamiltonian

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

Similar to other interactions — *Neglected for now*



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

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

Cost increase in deformed calculation
too large to be handled

Several solutions envisioned
- Compression via tensor factorisation
  - Pioneering works *Tichai et al. (2019)*
  - Factorized interaction in momentum space *Tichai et al. (2023)*
  - Challenge of symmetry broken beyond mean-field *Frosini et. al (2024)*
- *In medium* interactions
  - Rank reduction methods to remove higher rank terms
  - Effective nucleus-dependent two-body interaction *Frosini et. al (2021)*

NO2B Approximation beyond mean-field

Beyond mean-field, calculations almost never include exact three-body

$$:H:_{\rho^\Phi} \equiv H^{NO2B}[\rho^\Phi] = T\cdot\rho^\Phi + \frac{1}{2!}V^{NN}\cdot\rho^\Phi\rho^\Phi + \frac{1}{3!}V^{NNN}\cdot\rho^\Phi\rho^\Phi\rho^\Phi$$
$$+\, T + V^{NN}\cdot\rho^\Phi + V^{NNN}\cdot\rho^\Phi\cdot\rho^\Phi$$
$$+V^{NN} + V^{NNN}\cdot\rho$$
$$+\cancel{V^{NNN}}$$

Only convoluted « effective » three body treated beyond MF
- Source of problems in deformed calculations

Generalization to arbitrary densities

1. Apply same contractions with arbitrary « **well chosen** » ρ
2. **Discard pure three-body** terms
3. Convert **back to single particle** basis

$$\overline{E_0} \equiv \frac{1}{3!}V^{NNN}\cdot\rho\cdot\rho\cdot\rho$$
$$\bar{T} \equiv T - \frac{1}{2!}V^{NNN}\cdot\rho\cdot\rho$$
$$\bar{V} \equiv V + V^{NNN}\cdot\rho$$

ρ chosen to be symmetry conserving
Applications:
- Small error with reasonable ρ
- Very close to standard NO2B
- **True Hamiltonian** (e.g. for PGCM)

Easily generalisible to higher rank
Warning : may degrade for states very far from ρ

Construction of linear system

Constructing the linear system

$$\sum_{q}\sum_{J}^{SD} \mathbf{M_{IpJq} a^J(q) = -h_1^I(p)}$$

$h_1^I(p) \equiv \langle \Omega^{I(p)} | H_1 | \Omega^{(0)} \rangle = \langle \Phi^I(p) | P^\sigma H_1 | \Omega^{(0)} \rangle$ *(2-body)*

$N_{IpJq} \equiv \langle \Omega^{I(p)} | \Omega^{J(q)} \rangle = \langle \Phi^I(p) | P^\sigma | \Phi^J(q) \rangle$ *(0-body)*

$M_{IpJq} \equiv \langle \Omega^{I(p)} \big| H_0 - E^{(0)} \big| \Omega^{J(q)} \rangle = \langle \Phi^I(p) \big| \left(H_0 - E^{(0)}\right) P^\sigma \big| \Phi^J(q) \rangle$ *(1-body)*

Naive implementation

Construct each $|\Phi^I\rangle$ by permutations on U, V columns
Cost of each matrix element $O(N^3)$
Total cost $O\left(n_{gcm}^2 \cdot n_{proj} \cdot N^3 \cdot N^8\right)$ **Impractical**

Slater Condon rules in quantum chemistry
Burton et al. (2022)

Using Thouless theorem

$$\begin{aligned}\langle \Phi(p) | B^I O R(\theta) B^J | \Phi^J(q) \rangle &= \langle \Phi(p) \big| B^I O B_\theta^J \big| \Phi^J(q;\theta) \rangle \\ &= \langle \Phi(p) \big| B^I O B_\theta^J e^Z | \Phi(p) \rangle \langle \Phi(p) \big| \Phi^J(q;\theta) \rangle \\ &= \langle \Phi(p) \big| B^{I,Z} O^Z B_\theta^{J,Z} | \Phi(p) \rangle \langle \Phi(p) \big| \Phi^J(q;\theta) \rangle\end{aligned}$$

Total cost $O\left(n_{gcm}^2 \cdot n_{proj} \cdot N^5 + n_{gcm}^2 \cdot n_{proj} \cdot N^8\right)$ **(less) Impractical**
NB : huge prefactor (1000) to account for antisymmetry

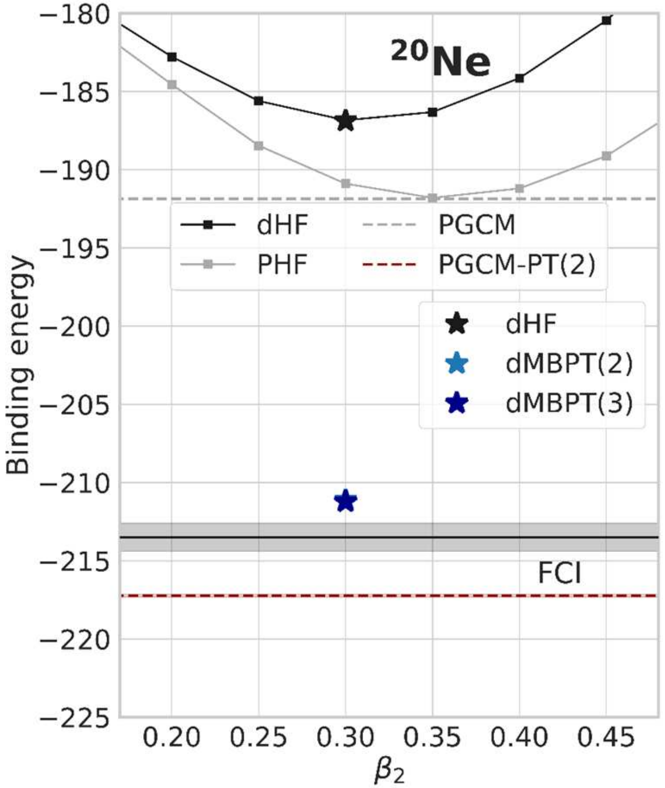
Large linear system

Antisymmetry : only to be solved for *strictly increasing* I, J
Axial + parity symmetry: I and J with good parity and K=0
Very large linear system ~ $\mathbf{500000}$ **configurations** in Neon20, 7 shells

How can we solve such a large system?

Validating PGCM-PT against FCI

Numerical setting
- ▶ $\mathbf{e_{max} = 4}$, $\hbar\omega$ = 20 MeV
- ▶ N^{3}LO **NN interaction** [Hüther et al 2020]
- ▶ λ_{srg} = 1.88 fm^{-1}



Ground state energy

Static correlations from J^2 breaking
- 13 MeV

Static correlations via PGCM
- 5 MeV from projection
- 10% underbound

Dynamical correlations via PGCM-PT(2)
- 1,7% error, slightly overshooting FCI

Deformed SR MBPT(2,3)
- Underbound
- Missing projection

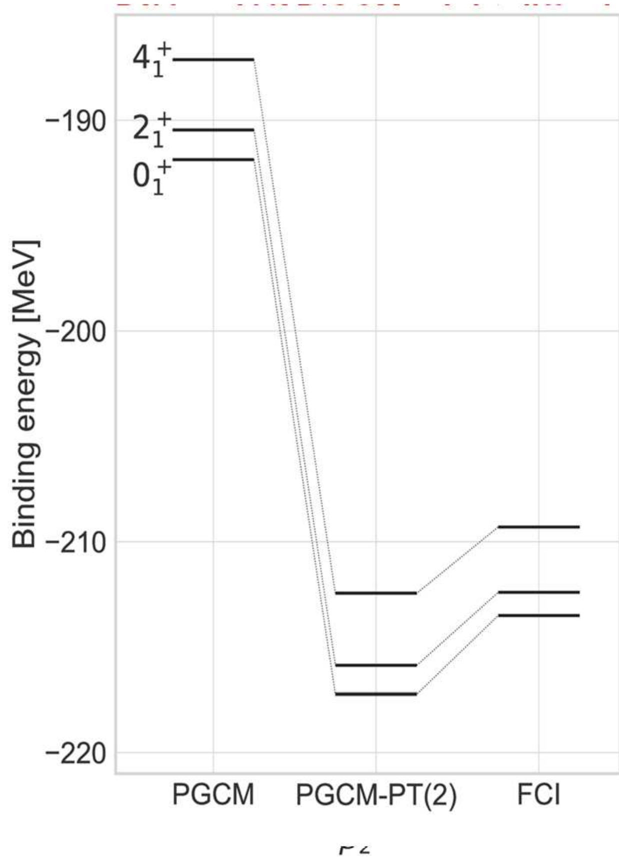
Spectroscopy of $2^+, 4^+$ states

PHFB strongly dependent on deformation
- **Not well converged**

PHFB-PT(2) flattens the curve
- **Empirical sign of convergence**
- Validation of theory

PGCM-PT(2) on top of PGCM
- Large **25MeV cancellations**
- Validation of numerics

Need physics **beyond 2p2h** / axial symmetry



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   Evolved interactions and parallel with EDF

   Ground state energy calculations in closed shell nuclei

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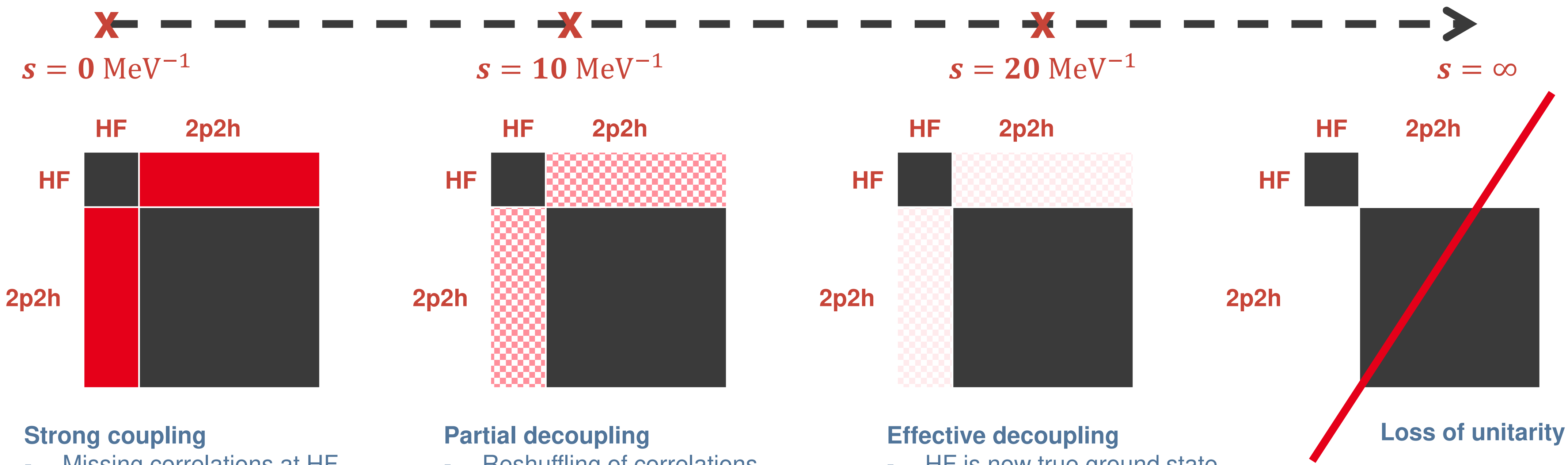
3. Application with IMSRG evolved interactions

IM-SRG evolved interactions and // with EDF

Hergert et al. (2016)

Unitary evolution of Hamiltonian



Strong coupling
- Missing correlations at HF

Partial decoupling
- Reshuffling of correlations

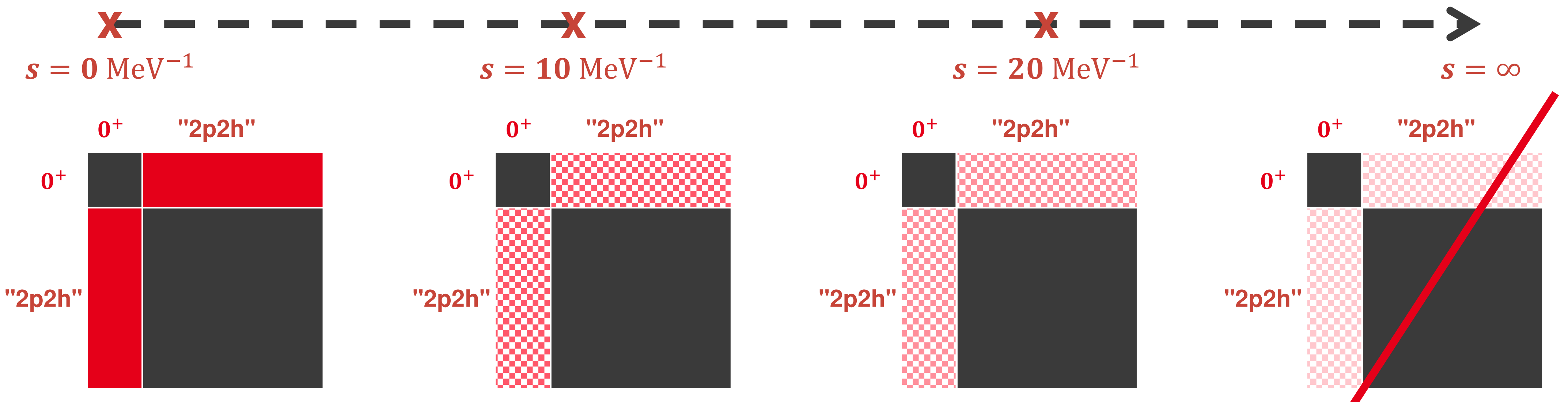
Effective decoupling
- HF is now true ground state

Loss of unitarity

Standard Single Reference IMSRG

IM-SRG evolved interactions and // with EDF

Unitary evolution of Hamiltonian



Strong coupling
- Missing dynamical correlations

Partial decoupling
- Reshuffling of correlations

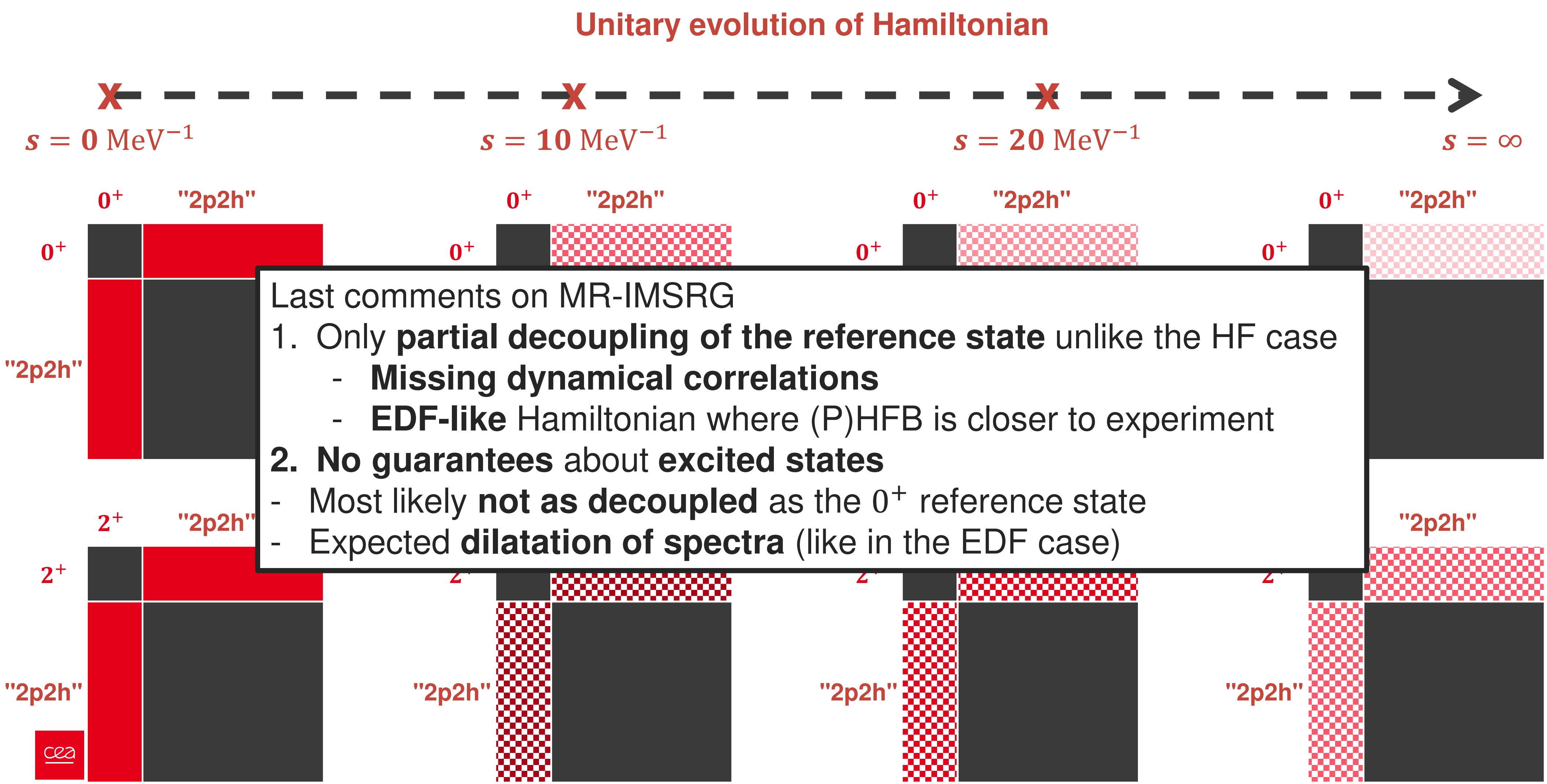
Partial decoupling
- PGCM nevel fully decoupled
- Dynamical correlations still missing
- Cranking and / or **PGCM-PT**

Loss of unitarity

Multi Reference IMSRG for open-shells
Replace HF by 0^+ PGCM

What happens to excited states?

IM-SRG evolved interactions and // with EDF



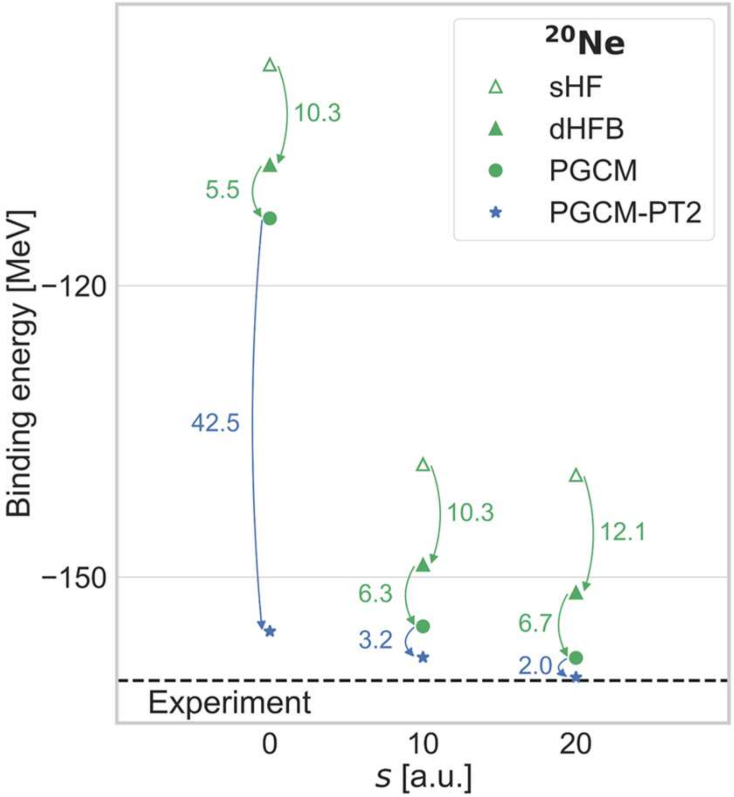
Last comments on MR-IMSRG

1. Only **partial decoupling of the reference state** unlike the HF case
    - **Missing dynamical correlations**
    - **EDF-like** Hamiltonian where (P)HFB is closer to experiment
2. **No guarantees** about **excited states**

- Most likely **not as decoupled** as the 0^+ reference state
- Expected **dilatation of spectra** (like in the EDF case)

PGCM-PT(2) with evolved interactions

Numerical setting
- ▶ $\mathbf{e_{max}} = \mathbf{6}$, $h\omega = 20$ MeV
- ▶ EM 1,8/2,0 interaction
- ▶ $\lambda_{srg} = 1.88$ fm-1

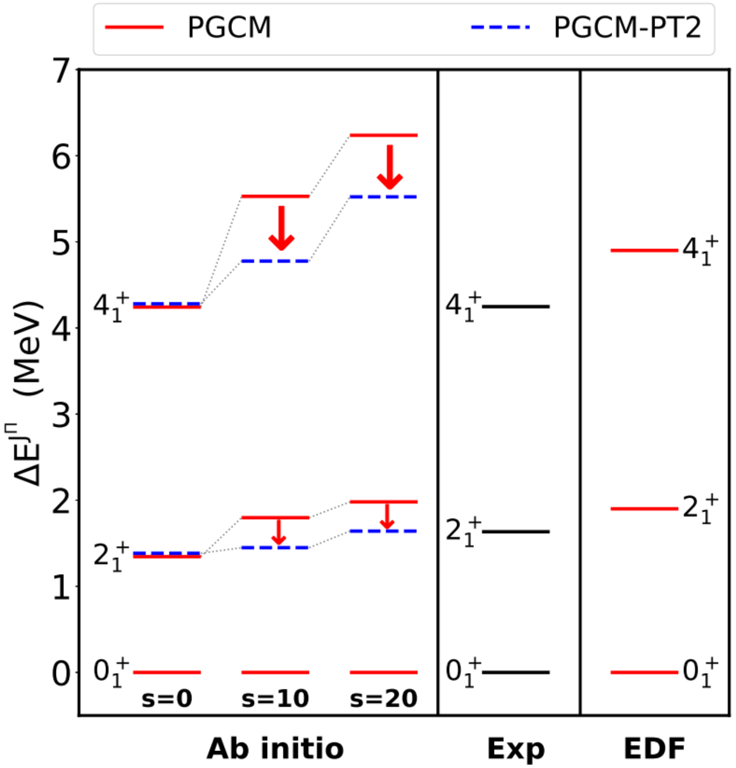


Reshuffling of correlations
- Much lower mean-field
- **Increase of static** correlations

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

Effect on excited states
- Dilatation of rotational spectrum
- Similar to EDF case
- Difficult to capture with PGCM*

Correction in perturbation
- PGCM-PT(2) contracts back spectra
- Still not scale independent
  - Higher order?
  - Richer PGCM?
  - What would PCC observe?



Duguet et al (2023)

* shown recently to be possible with cranking

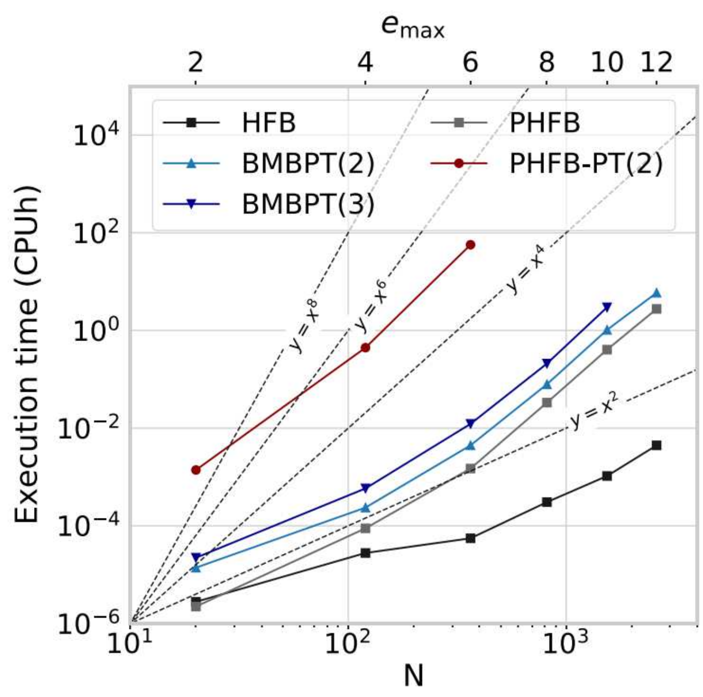
4. Conclusion

Conclusion

Envisioned improvements for PGCM-PT(2)
Today : first calculations
- Need to extend to larger bases
- Need to break more symmetries

Main limitation comes from $O(n_{gcm}^2 n_{proj} N^8)$ complexity
Possible ways out
- **Modified partitioning** (recover diagonal H_0 and $O(N^5)$)
- **Natural basis** (reduce N)
- **Tensor factorization** (data compression)
- **Improve PGCM** to reduce n_{gcm}

Extensions to be formalized
- Generic observables (transitions)
- Non yrast states



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Connection with EDF

Calculations with evolved interactions close to EDF

- 3-body captured via *in medium* interaction
- Correlations reshuffled from dynamical to static
- Dilatation of spectra (special case of g.s.)

Raising several questions:

- Dynamical correlations in EDF?
- Bypassing MR-IMSRG?
- Better interplay EDF / *ab initio*?

Duguet et al (2023)

Thanks for your attention

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