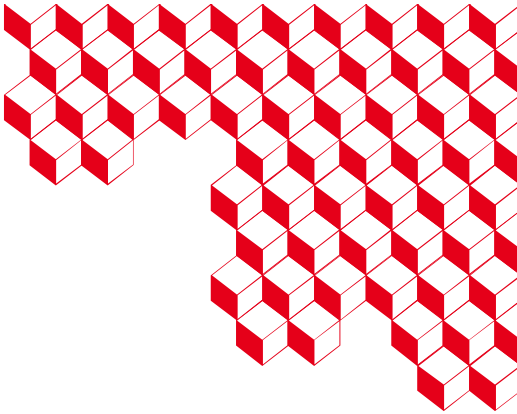


Ab Initio Projected Generator Coordinate Method + Perturbation Theory

ESNT Workshop, Tuesday 21st 2023

Mikael Frosini, DES/IRESNE/SPRC/LEPh

Microscopic models of nuclei

Energy Density Functional

Phenomenological *interaction*
– Inspired by DFT
– Adjusted in nuclei

Reasonable numerical cost
Large domain c
From **structure**

Not systematica
– Limited error
Tailored for me
- **Difficulties for spectroscopy**

From nucleons to nuclei
Prediction of macroscopic properties from interacting nucleons

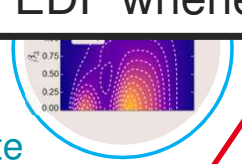
Ab Initio methods

Derived consistently with QCD
- Adjusted on **small systems**
- S**ystematic expansion**

Higher computational cost
count of 3-body
ed mass range

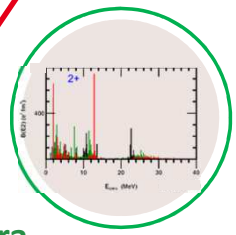
y improvable
imation »
ion
- ***No spuriosity***

Presentation focused on particular *Ab Initio* method
Objective : **solve A-body Schrödinger equation** to given accuracy
Projected Generator Coordinate Method Perturbation Theory
Focus on **formalism** and **first implementation**
Parallels with EDF whenever possible



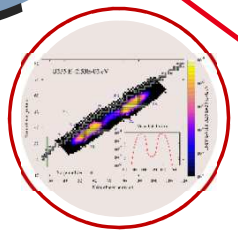
Ground-state

masses, radii,
density profile, …



Excitation spectra

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

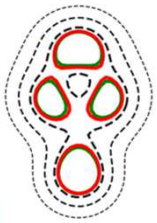


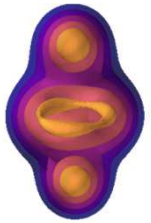
Decay modes

lifetime, yields, …

Reactions

cross sections, …



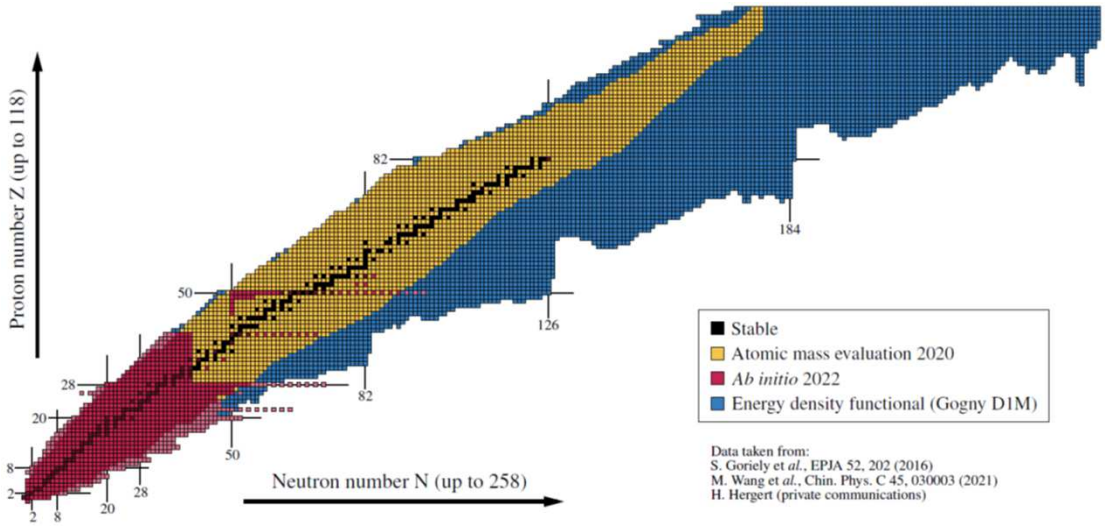


Progress of *ab initio / in medias res* methods

***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	**1990's**	Exponential scaling
Quasi-exact methods		
Closed shells	**2000's**	Polynomial scaling
Expansion methods **Single-reference**		
Singly open-shells	**2010's**	Polynomial scaling
Symmetry-breaking **Multi-reference**		
Doubly open-shells	**2020-?**	Mixed / Polynomial Scaling
Valence space **Symmetry-breaking** **Multi-reference**		

A word on PAN@CEA collaboration

+ Sophie Péru
+ David Régnier
+ Noël Dubray
+ Gilles Noguère

Thomas Duguet
Vittorio Somà
Benjamin Bally
Andrea Porro (TU Darmstadt)
Alberto Scalesi

Fundamental research

Jean-Paul Ebran
Philippe Da Costa
Lars Zurek
Luis Gonzales-Miret
Antoine Roux

Evaluated Data

PAN@CEA

Mikael Frosini
Alessandro Pastore
Pierre Tamagno
Clémentine Azam
Damien Blondeau-Patissier
Stavros Bofos

Nuclear Applications

(VAP)-HFB (no symmetry)
FAM-QRPA
BMBPT
PGCM (+ PT)
GSCGF

cea iresne

Chiral *ab initio*
Valence space interactions
Gogny D1S / D1M
Skyrme
Gogny 3b (Da Costa)

Several methods, Several interactions, One tool

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
   - Resolution of the linear system
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

Schrödinger equation

$[H, R] = 0$

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

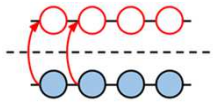
Spherical Hartree Fock $\mathbf{o}(N^4)$

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

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

Canonical Partitioning

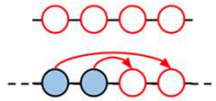
$$H_0 \equiv E^{(0)}|\Phi^{(0)}\rangle\langle\Phi^{(0)}| + \sum_I^{S,D,\cdots} E^I|\Phi^I\rangle\langle\Phi^I|$$



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

Schrödinger equation

$[H, R] = 0$

Nucleon interaction 1-,2-,3-… body — *Correlated wave-function A! parameters*

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

Partitioning

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$$|\Phi^{(k)}\rangle \equiv \cdots$$

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

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

Systematic expansion
Open questions
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$$|\Theta^{(0)}\rangle = |sHF\rangle$$

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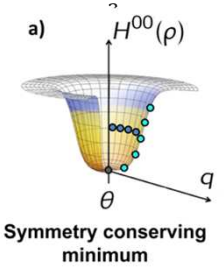
Canonical Partitioning

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

Strictly positive diagonal H_0

$|\Phi^{(0)}\rangle$ refe



Symmetry conserving minimum

Single reference symmetry breaking PT in open shells

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

Symmetry breaking HF Bogoliubov $O(N^4)$

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

Canonical SB Partitioning

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

$\equiv |\Phi($

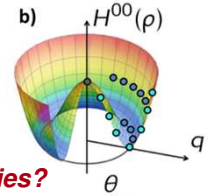
$\equiv 1 -$

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

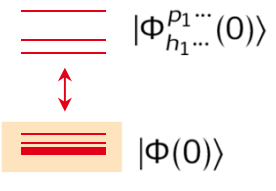
$$|\Theta^{(0)}\rangle = \sum_i |\Phi_i\rangle$$

Non canonical SB Partitioning

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

Choice Ref State?
Choice of basis?
Non diagonal H_0

$\mathcal{P}$

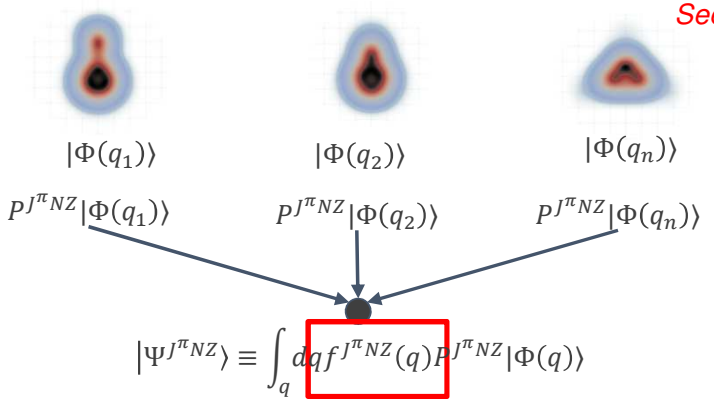


PGCM + Perturbation Theory

Projected Generator Coordinate Method

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

See A. Roux presentation



Constrained mean-field
Symmetry breaking

Projection
Rotation

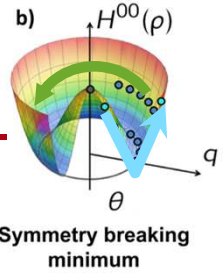
$$|\Psi^{J^\pi NZ}\rangle \equiv \int_q dq f^{J^\pi NZ}(q) P^{J^\pi NZ}|\Phi(q)\rangle$$

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*



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 $H_0 - E^{(0)}$

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

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

- $\boldsymbol{O(N^4)}$ PGCM with large prefactor
- $\boldsymbol{O(N^8)}$ 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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4. **Conclusion**

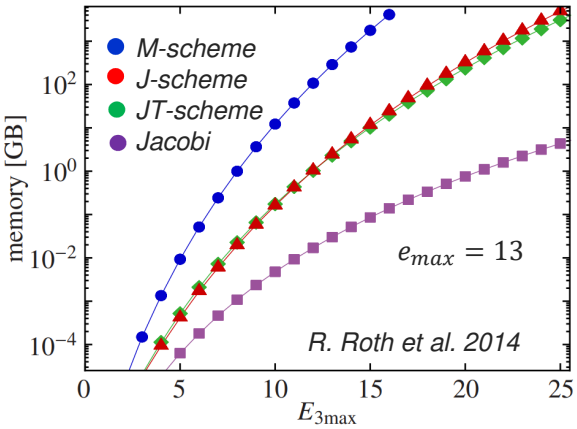
2. Numerical aspects

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
- *In medium* interactions

NO2B Approximation beyond mean-field

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

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

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)

Connection with EDF?

Could this idea be adapted to Gogny-like interactions?
- At least in PGCM, freeze density-dependant term once and for al

Probably needed trick for 3-body Gogny (cf. Philippe Dacosta's presentation)

$\boldsymbol{\rho^3 \rightarrow \rho^2\rho_0}$ …… $\boldsymbol{\rho^\alpha \rightarrow \rho^2\rho_0^{\alpha-2}}$?

Conversely, could ρ be obtained from EDF calculation for *ab Initio* applications

Construction of linear system

Constructing the linear system

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

$$h_1^I(p) \equiv \langle \Omega^{I(p)}|H_1|\Omega^{(0)}\rangle = \langle \Phi^I(p)|P^\sigma H_1|\Omega^{(0)}\rangle \quad \textit{(2-body)}$$
$$N_{IpJq} \equiv \langle \Omega^{I(p)}|\Omega^{J(q)}\rangle = \langle \Phi^I(p)|P^\sigma|\Phi^J(q)\rangle \quad \textit{(0-body)}$$
$$M_{IpJq} \equiv \langle \Omega^{I(p)}\big|H_0 - E^{(0)}\big|\Omega^{J(q)}\rangle = \langle \Phi^I(p)\big|\big(H_0 - E^{(0)}\big)P^\sigma\big|\Phi^J(q)\rangle \quad \textit{(3-body)}$$

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 ~ **500000 configurations** in Neon20, 7 shells

How can we solve such a large system?

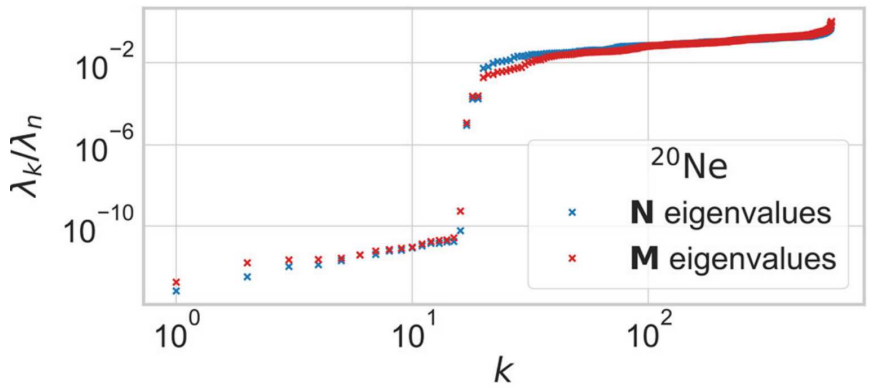
Solution of linear system $Ma = -h_1$

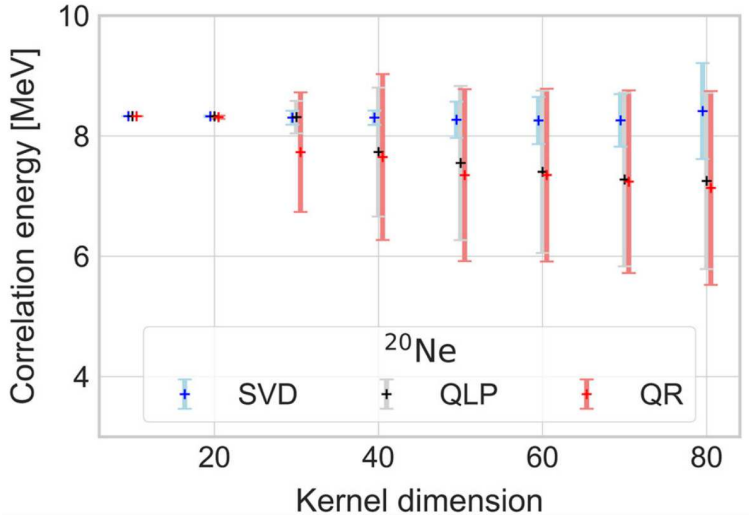
Direct methods for the solution of the symmetric linear system

Direct solutions of the system rely on various matrix decompositions
Ideally, one would like to use **symmetric eigendecomposition** $M = \mathbf{V}^{\mathbf{T}}\mathbf{\Sigma}\mathbf{V}$
- **Easy separation between range and kernel**
- Costly in large dimensions

An alternative could be rank revealing **QR** $M = QR$
- Cheaper but less precise

Intermediate : **rank-revealing QLP** $M = QLP$ $\quad L = \begin{pmatrix} \bar{L} & 0 \\ 0 & 0 \end{pmatrix}$





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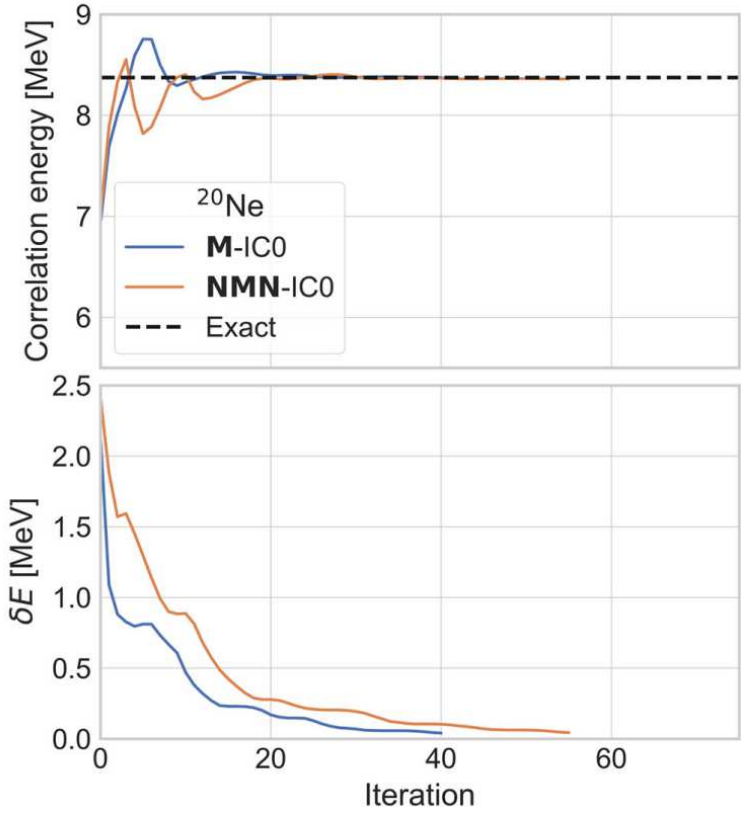
Switching to indirect methods in « realistic » space

Solving the system in Krylov space $\{X, MX, M^2X, \cdots\}$
MINRES-QLP [Choi11]
- Improvement of MINRES to for better handling of matrix kernel
- Only requires **matrix-vector product**
- **Strongly depends on problem preconditionning**

Very large linear system
High redundancies **Intruder state problem**
- Non orthogonal projected excitations
- Non orthogonal HFB states
- Negative M eigenvalues



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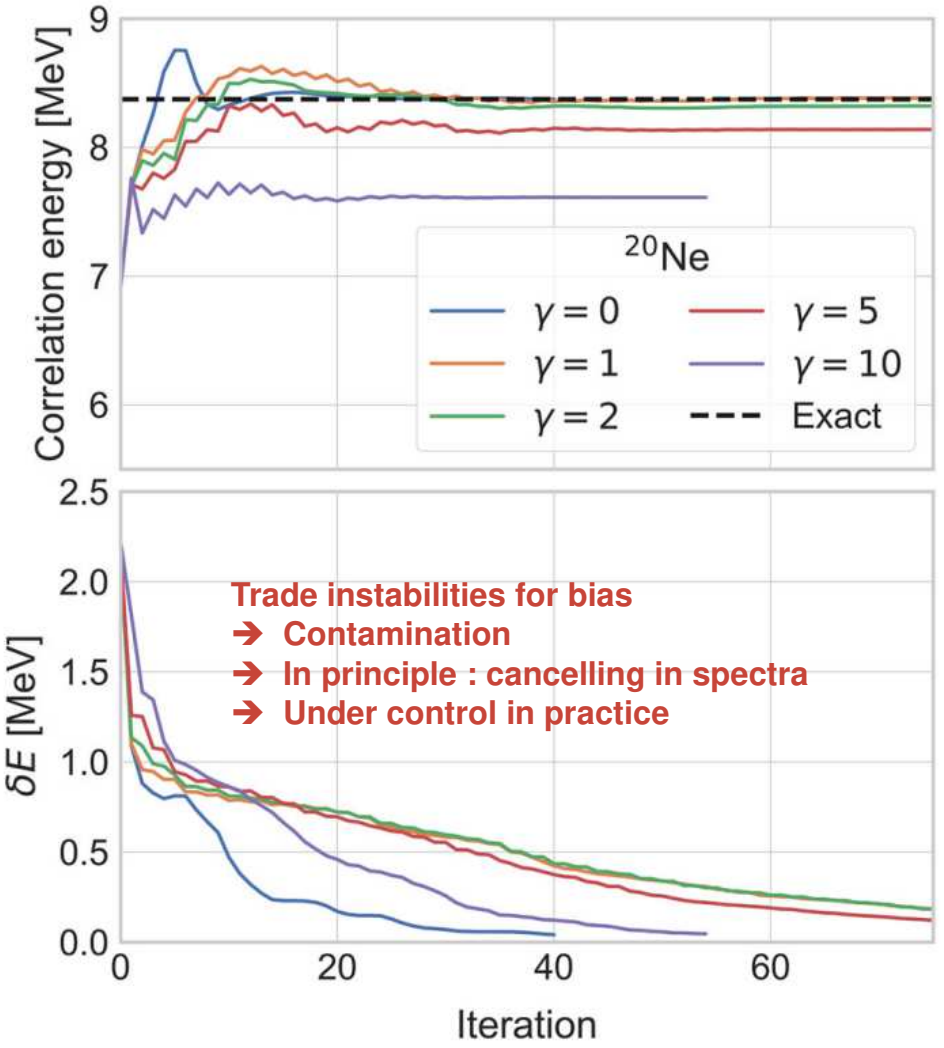
- Only requires **matrix-vector product**
- **Strongly depends on problem preconditionning**

Very large linear system
High redundancies
- Non orthogonal projected excitations
- Non orthogonal HFB states
- Negative H_0 eigenvalues

Intruder state problem

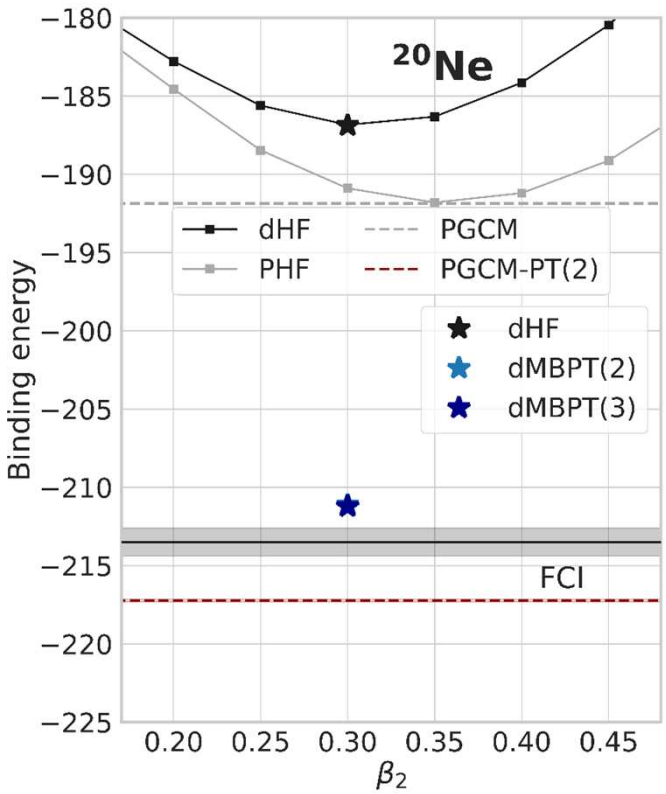
$$(M + i\gamma N)a = -h_1$$
$$\Leftrightarrow$$
$$\begin{pmatrix} M & -\gamma N \\ -\gamma N & -M \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} -h_1 \\ 0 \end{pmatrix}$$

Complex shift method



Validating PGCM-PT against FCI

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



Ground state energy

Static correlations from J^2 breaking
- 13 MeV

Static correlationc 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

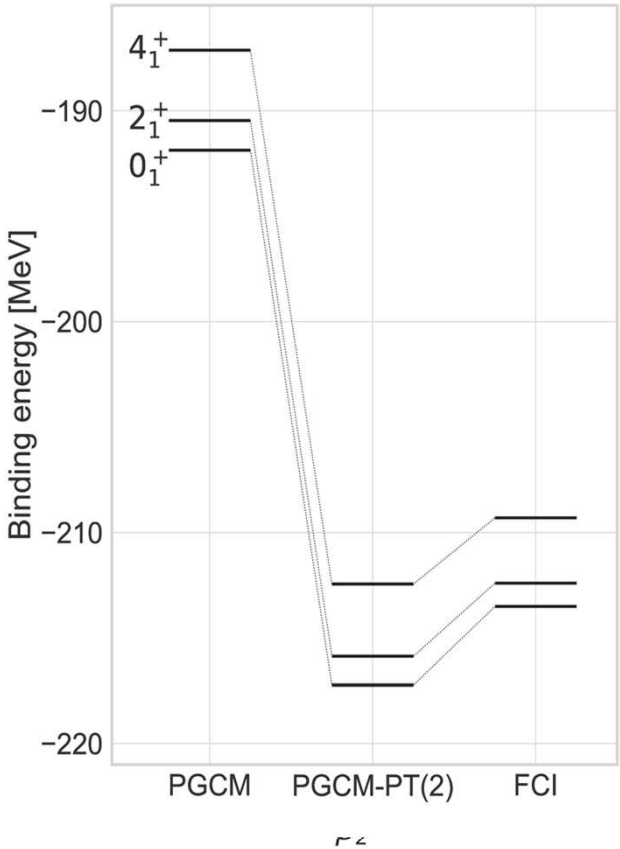
Spectroscopy of $2^+, 4^+$ states

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

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

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

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



Outline

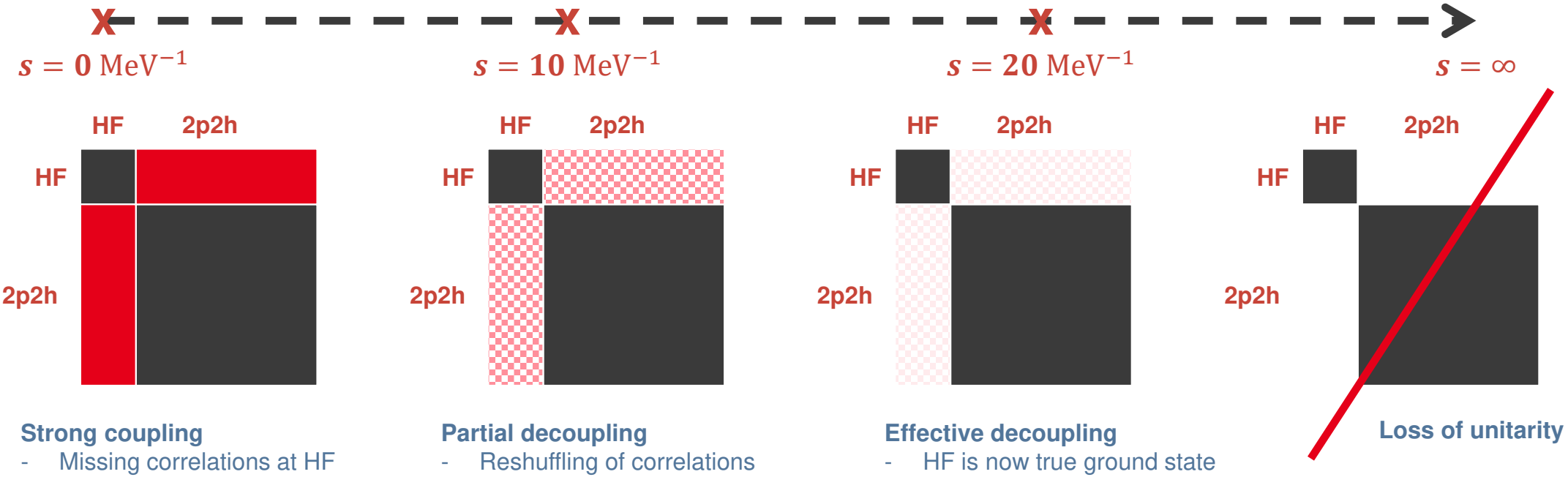
1. **Formalism**
   - Progress of ab initio / in medias res methods
   - Single and multi-reference expansion methods
   - Projected Generator Coordinate Method + Perturbation Theory
2. **Numerical aspects of PGCM-PT**
   - Circumventing the complexity of three body interactions
   - Calculation of matrix elements
   - Resolution of the linear system
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**

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

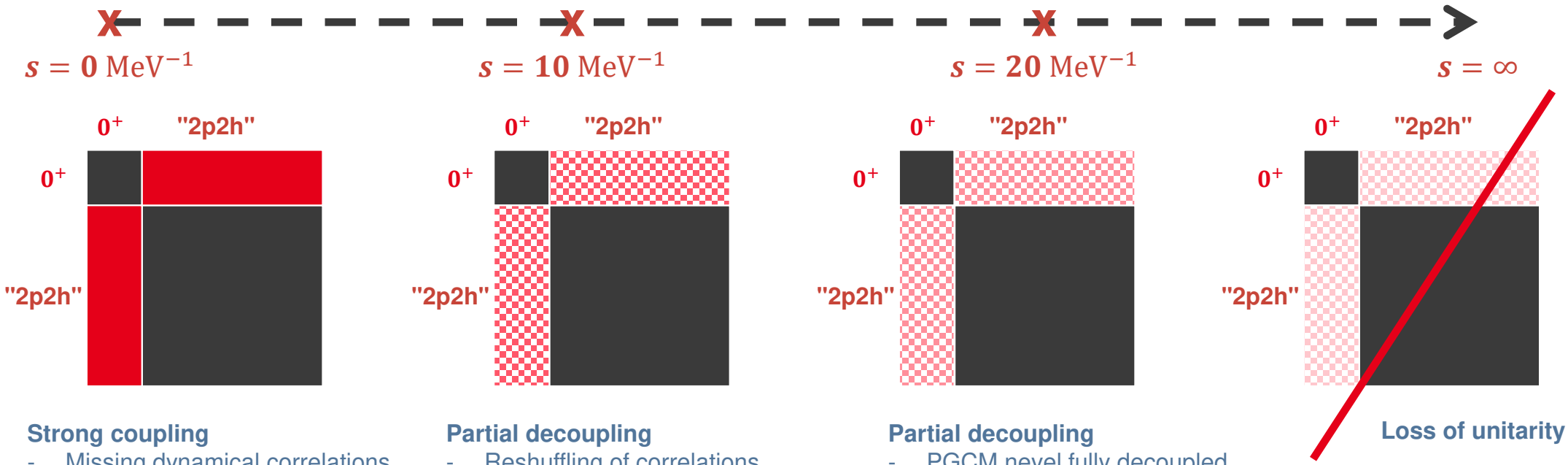
Effective decoupling
- HF is now true ground state

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
- Crancking and / or **PGCM-PT**

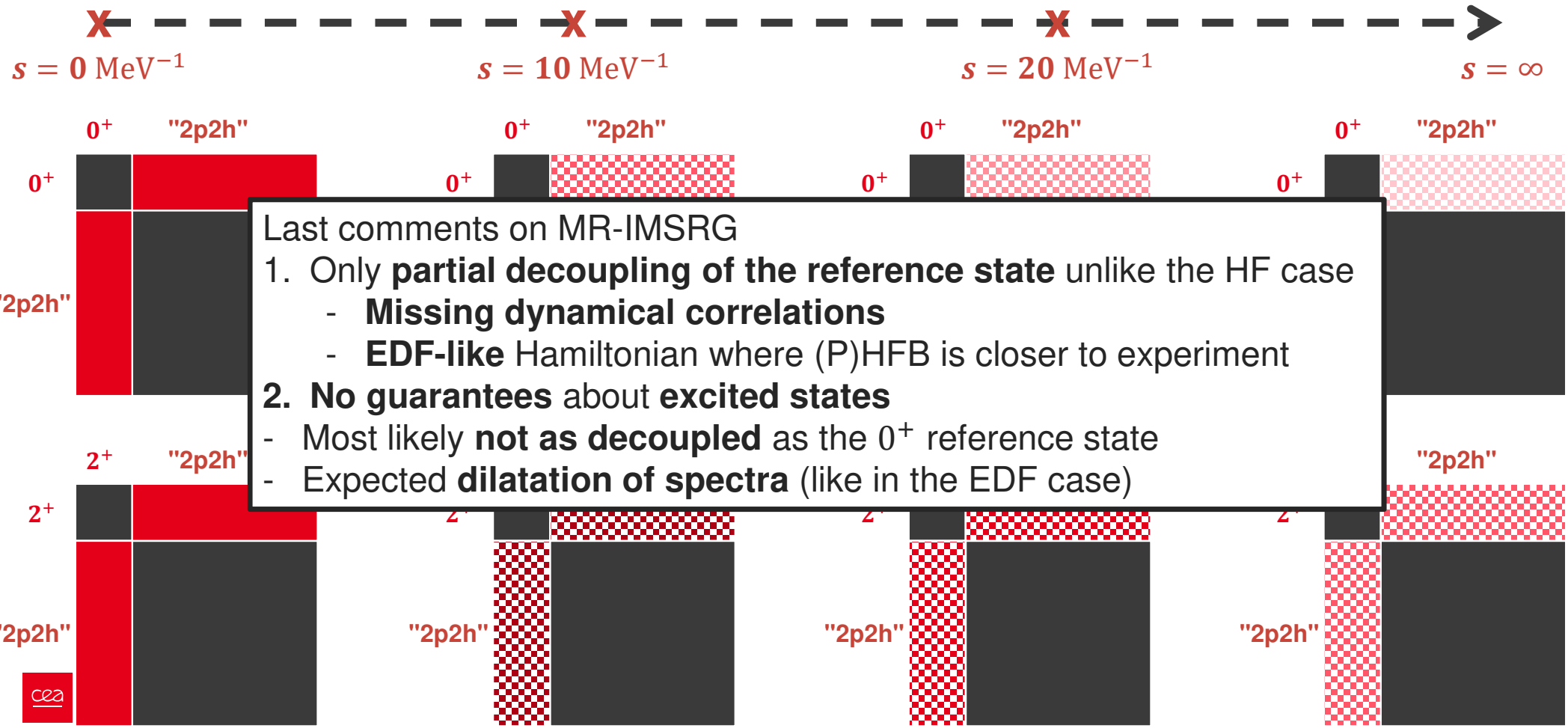
Loss of unitarity

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

What happens to excited states?

IM-SRG evolved interactions and // with EDF

Unitary evolution of Hamiltonian



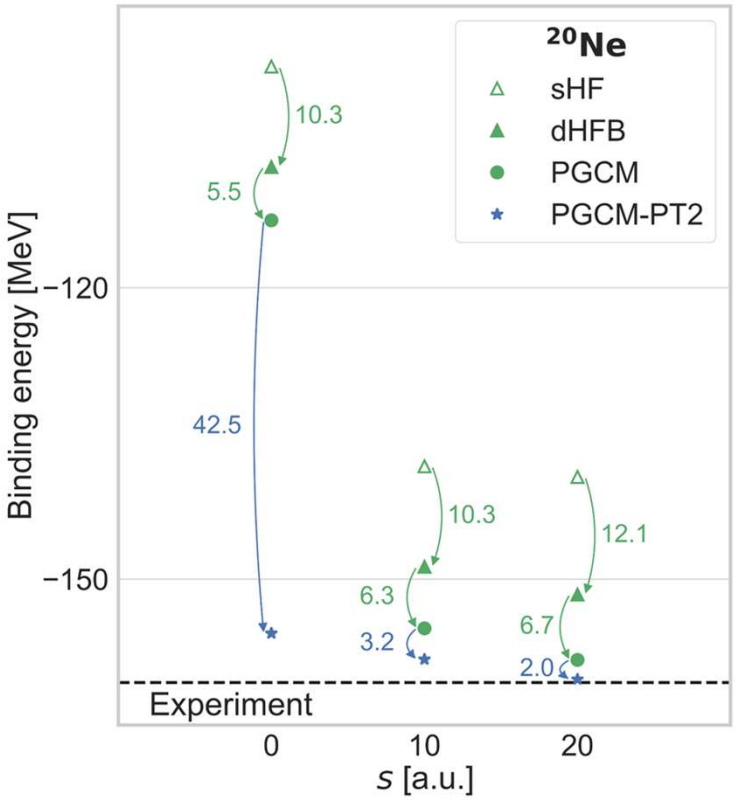
Last comments on MR-IMSRG

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

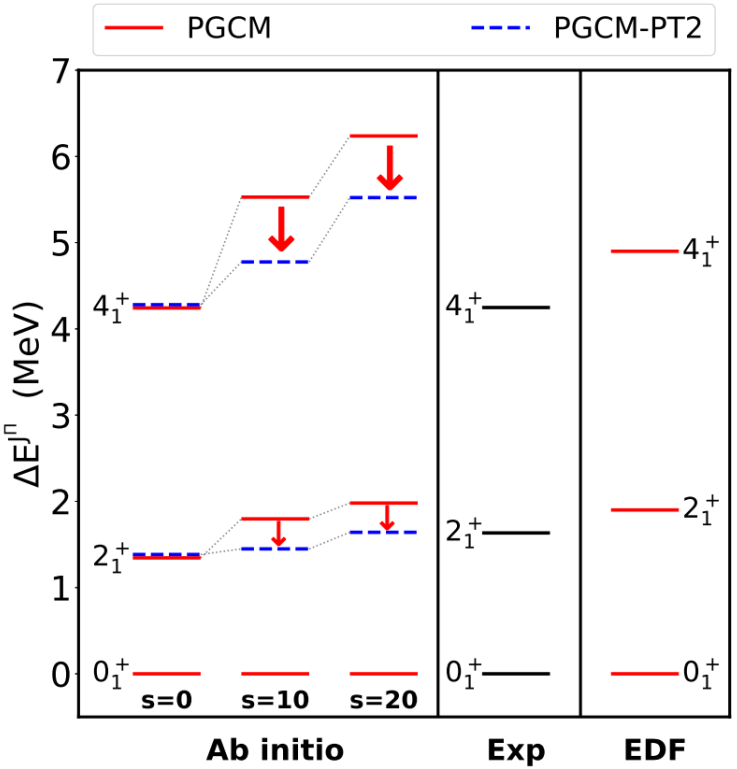


Reshuffling of correlations
- Much lower mean-field
- **Increase of static** correlations

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 inependent
  - Higher order?
  - Richer PGCM?



Duguet et al (2023)

* shown recently to be possible with cranking

4. Conclusion

Conclusion

Envisioned improvements for PGCM-PT(2)

Today : semi-realistic calculations

- Need to extend to larger bases
- Need to break more symmetries

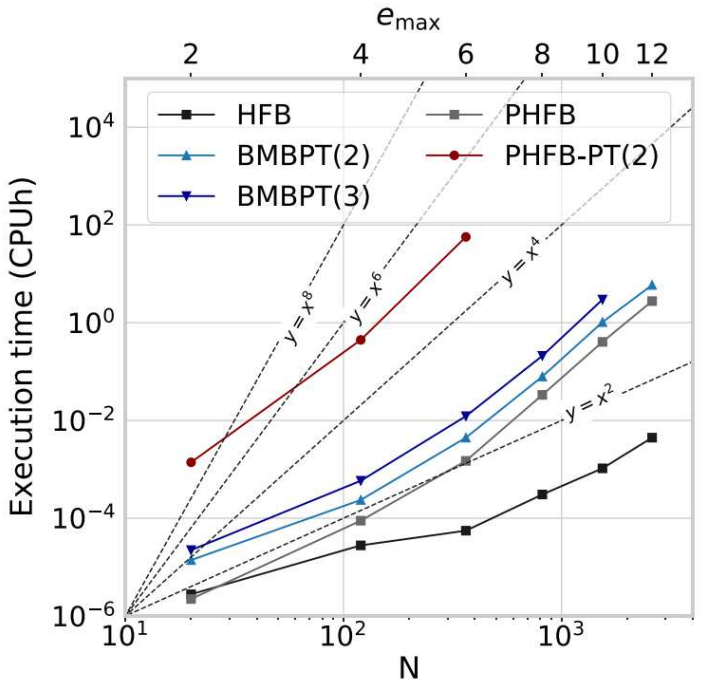
Main limitation comes from $O(n_{gcm}^2 n_{proj} N^8)$ complexity

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



Conclusion

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Extensions to be formalized
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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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