Ab initio description of doubly open-shell nuclei via a novel multi-reference perturbation theory

Vittorio Somà
CEA & Université Paris-Saclay, France

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Outline

- **Introduction**
- **PGCM-PT formalism** [1]
- **PGCM results** [2]
- **PGCM-PT(2) results** [3]
- **Outlook**

PGCM = Projected Generator Coordinate Method

[1] M. Frosini, T. Duguet, J.-P. Ebran, V. Somà,
arXiv:2110.15737

[2] M. Frosini, T. Duguet, J.-P. Ebran, B. Bally, T. Mongelli, T.R. Rodríguez, R. Roth, V. Somà,
arXiv:2111.00797

[3] M. Frosini, T. Duguet, J.-P. Ebran, B. Bally, H. Hergert, T.R. Rodríguez, R. Roth, J.M. Yao, V. Somà,
arXiv:2111.01461

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- **Introduction**
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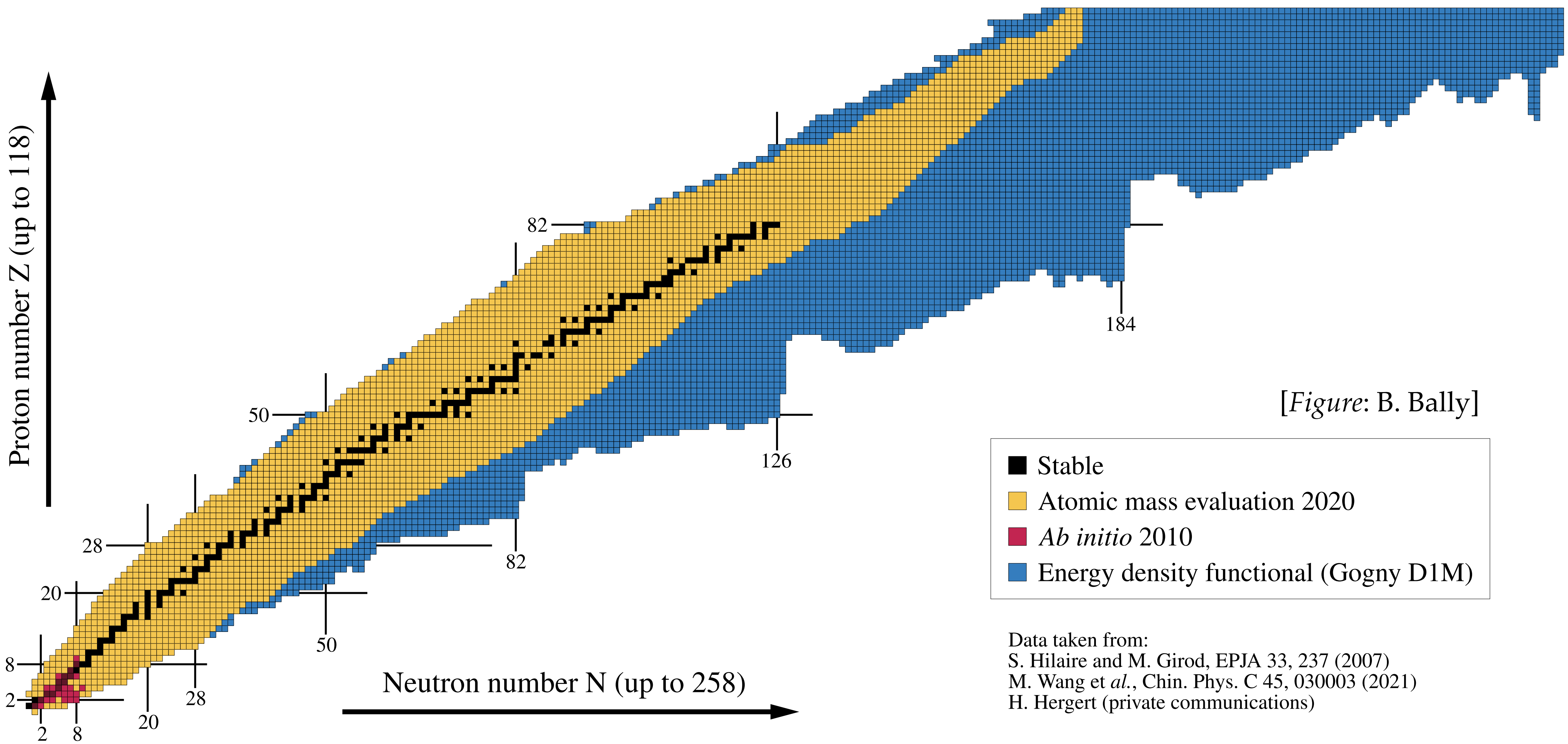
Ab initio nuclear chart

Energy density functional (EDF)

Hamiltonian (phenomenologically) incorporates in-medium correlations ➡ Simpler wave function allows gentle scaling with system size

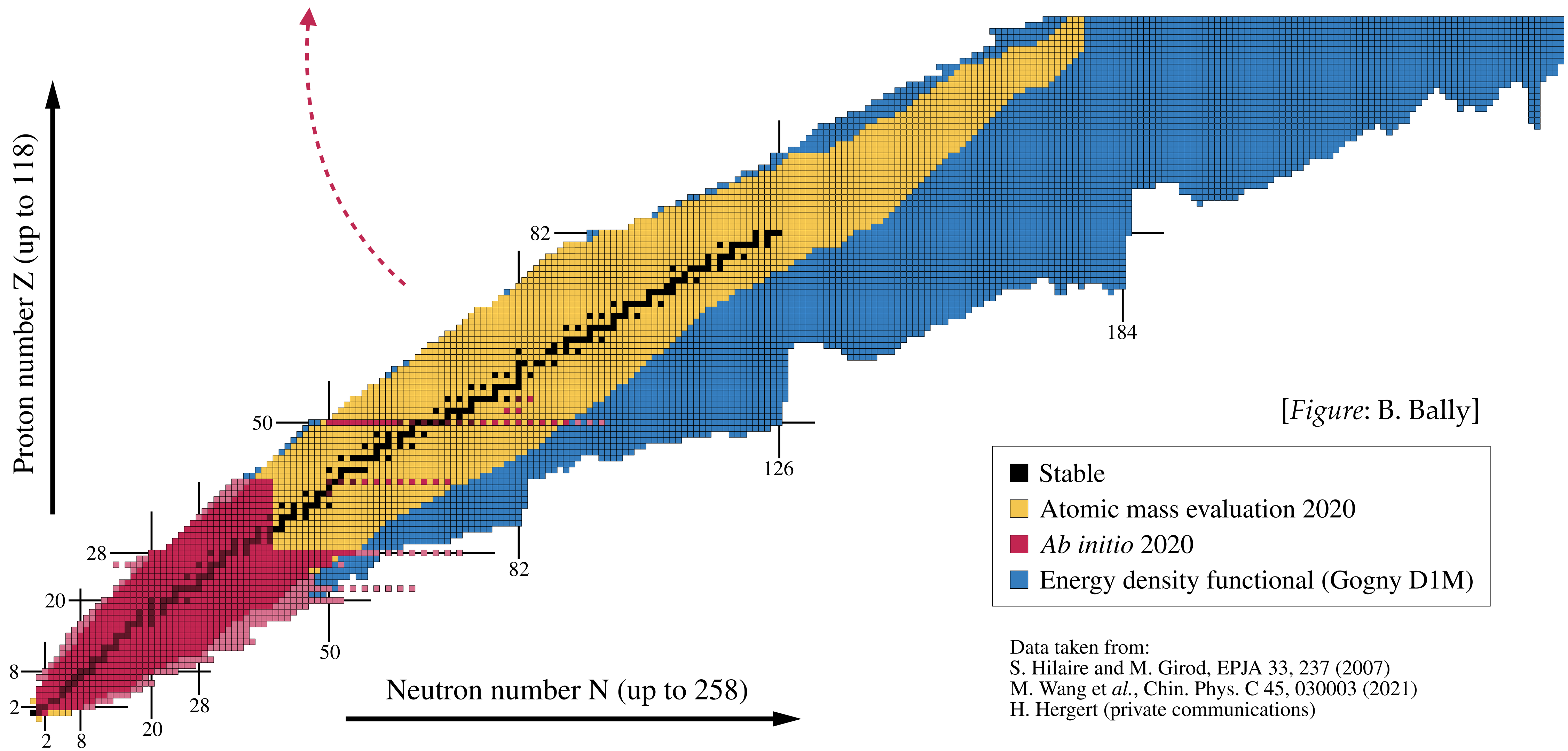


Ab initio

Hamiltonian describes “bare” NN & NNN interactions ➡ (Approximate) solution must be systematically improvable and approach the exact solution

Ab initio nuclear chart

- **Further progress hindered by**
  - Storage cost of Hamiltonian matrix elements (method-independent)
  - Runtime & memory costs of many-body calculations (method-dependent)



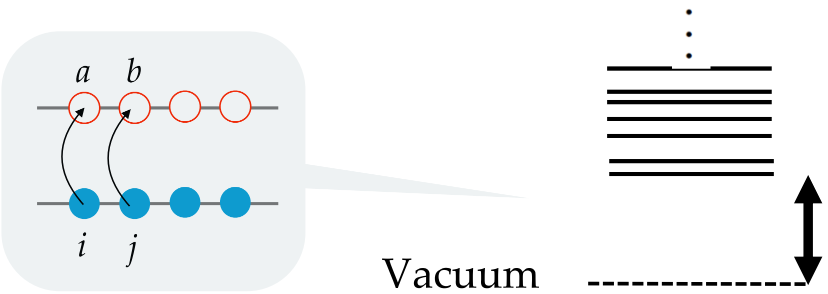
- **CI methods**
  - Full space diagonalisation
  - → **Exponential scaling**

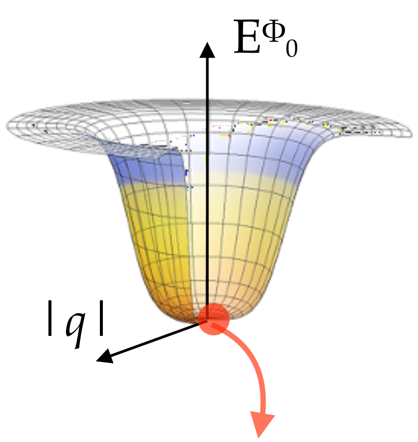
- **Hybrid methods**
  - Valence space diag.
  - → **Mixed scaling**

- **Expansion methods**
  - Partition, expand & truncate
  - → **Polynomial scaling**

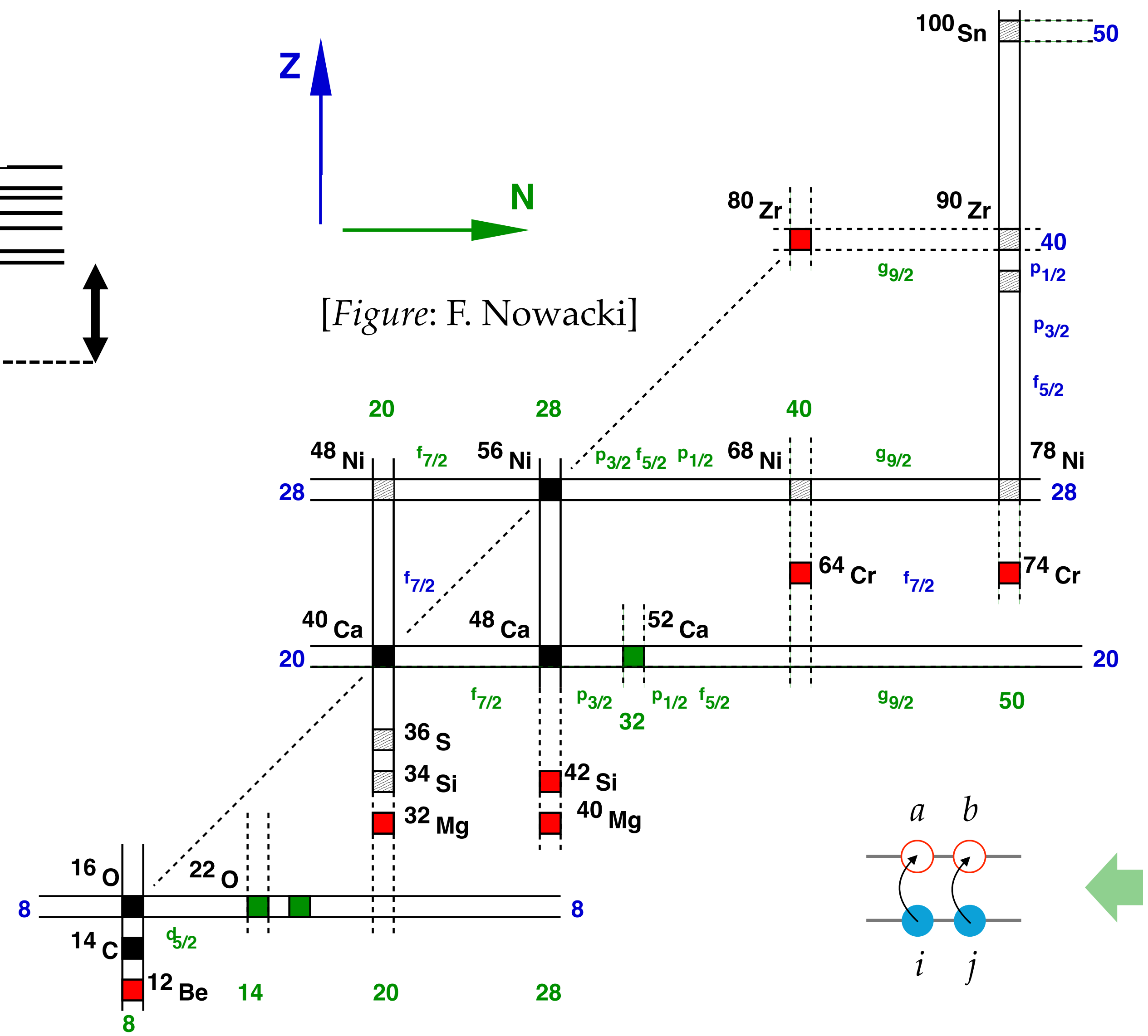
Closed- vs open-shell nuclei

Closed-shell



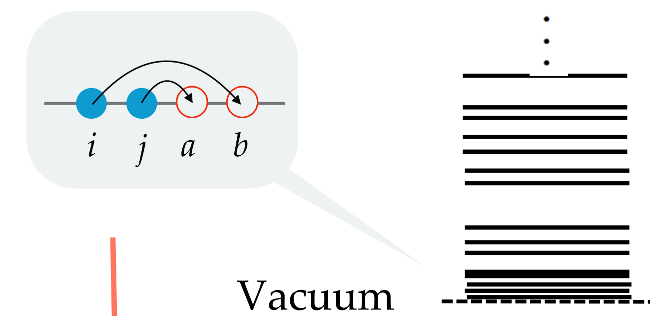


Symmetry-conserving minimum



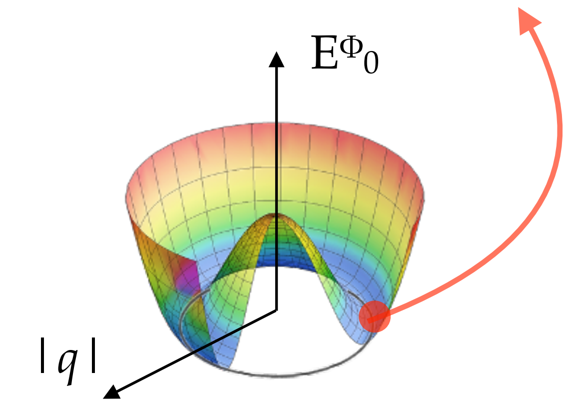
[*Figure*: F. Nowacki]

Open-shell



Breakdown of ph expansion

Symmetry-breaking minimum



Singly open-shell nuclei
➪ Sufficient to **break U(1)**

Doubly open-shell nuclei
➪ Necessary to **break SU(2)**

Symmetries must be eventually **restored**

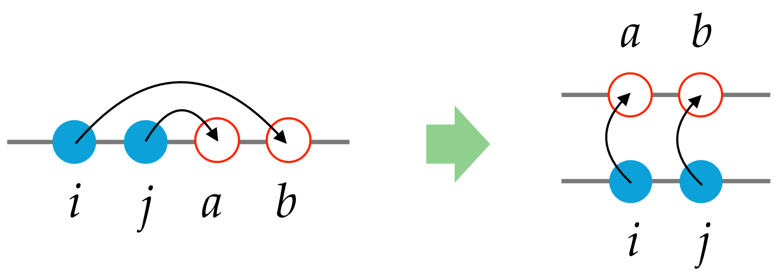
Symmetry breaking

Physical symmetry	*Group*	*Correlations*	
Rotational inv.	SU(2)	Deformation	⟶ d (deformed)
Particle-number inv.	$U(1)_N \times U(1)_Z$	Pairing	⟶ B (Bogolyubov)

Single- vs multi-reference strategy

Single-reference strategy

Gap reopened via **symmetry breaking**

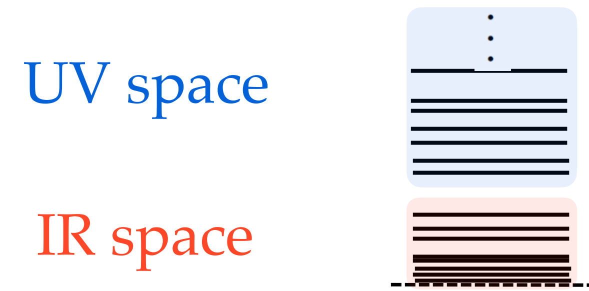


✓ ph expansion: simpler formalism

✗ Symmetries must be restored

Multi-reference strategy

Gap reopened via **pre-treatment of IR physics**



✓ Symmetries can be preserved

✗ ph expansion: complicated formalism

○ **U(1)**-breaking

→ Gorkov SCGF, BMBPT, BCC

○ **SU(2)**-breaking

→ Deformed CC

○ Symmetry restoration

→ Theory developed (excpet GF) [Duguet 2015]

→ Implementation: work in progress

○ IR physics via diagonalisation

→ Multi-configuration PT

→ *Diagonalisation step impacts scalability*

○ **This work: IR physics via PGCM**

→ Exploits symmetry breaking + restoration

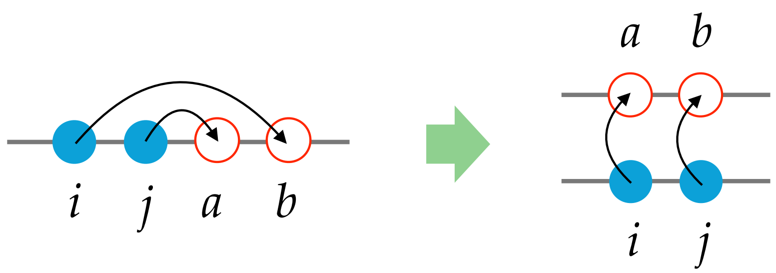
→ ***Symmetry-conserving & low dimensional***

→ PGCM-PT

Single- vs multi-reference strategy

Single-reference strategy

Gap reopened via **symmetry breaking**



✓ ph expansion: simpler formalism

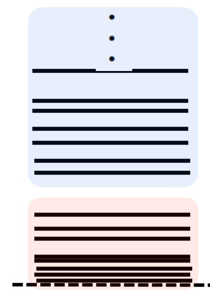
✗ Symmetries must be restored

Multi-reference strategy

Gap reopened via **pre-treatment of IR physics**

UV space

IR space



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Partition, then expand & project

○ **This work: IR physics via PGCM**

→ Exploits symmetry breaking + restoration

→ *Symmetry-conserving & low dimensional*

→ PGCM-PT

Partition & project, then expand

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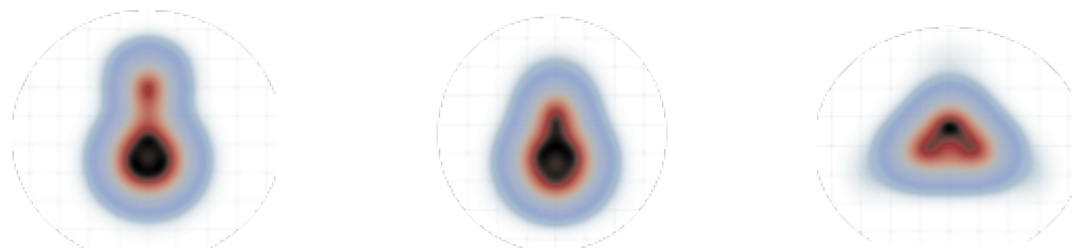
Unperturbed state

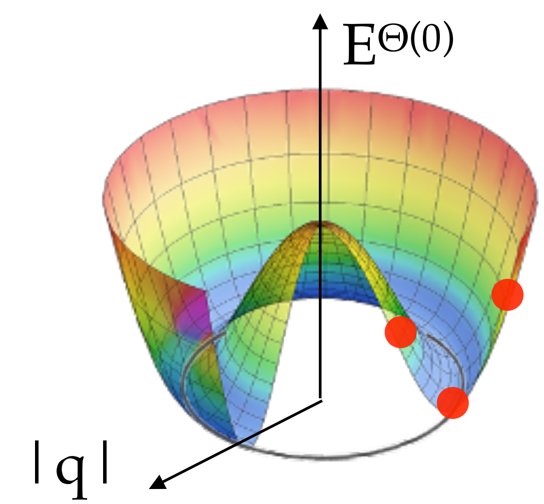
⊙ **Construction of the unperturbed state via projected generator coordinate method (PGCM)**

○ Low-dimensional linear combination of *non-orthogonal* Bogolyubov product states (← EDF)

Deformed vacua



$|\Phi(q_1)\rangle$ $|\Phi(q_2)\rangle$ $|\Phi(q_3)\rangle$



Projection

$\tilde{\sigma} \equiv (J^{\Pi}, N, Z)$

$P^{\tilde{\sigma}}|\Phi(q_1)\rangle$ $P^{\tilde{\sigma}}|\Phi(q_2)\rangle$ $P^{\tilde{\sigma}}|\Phi(q_3)\rangle$ → *Rotational modes*

Shape mixing

$$|\Theta^{\tilde{\sigma}}_{\mu}\rangle = \sum_q f^{\tilde{\sigma}}_{\mu}(q)\, P^{\tilde{\sigma}}\, |\Phi(q)\rangle$$

→ *Vibrational modes*

Variational principle → **Hill-Wheeler-Griffin eq.** $\sum_q H^{\tilde{\sigma}}_{qp} f^{\tilde{\sigma}}_{\mu}(q) = \epsilon^{\tilde{\sigma}}_{\mu} \sum_q N^{\tilde{\sigma}}_{qp} f^{\tilde{\sigma}}_{\mu}(q)$

➪ NOCI eigenvalue problem expressed in a set of non-orthogonal projected HFB states

Perturbative expansion

- **Formal perturbation theory**
  - Introduce partitioning $H = H_0 + H_1$
  - Expand exact wave function and energy as $|\Psi\rangle \equiv \sum_{k=0}^{\infty} |\Theta^{(k)}\rangle$ and $E \equiv \sum_{k=0}^{\infty} E^{(k)}$
  - Perturbative corrections can be identified by partitioning the Hilbert space via the projectors

$$\textit{Model space} \longleftarrow \mathcal{P} \equiv |\Theta^{(0)}\rangle\langle\Theta^{(0)}| \qquad \mathcal{Q} \equiv 1 - \mathcal{P} \longrightarrow \textit{External space}$$

  - Second-order energy correction reads

$$E^{(2)} = \langle\Theta^{(0)}|H_1\mathcal{Q}|\Theta^{(1)}\rangle \qquad \text{where} \qquad |\Theta^{(1)}\rangle = -\mathcal{Q}\left(H_0 - E^{(0)}\right)^{-1}\mathcal{Q}H_1|\Theta^{(0)}\rangle$$

➡ If eigenstates of H_0 are known, one can invert and obtain algebraic expressions

$$H_0 = E^{(0)}|\Phi^{(0)}\rangle\langle\Phi^{(0)}| + \sum_{I}^{S,D,\dots} E^I|\Phi^I\rangle\langle\Phi^I| \longrightarrow E^{(2)} = -\sum_{I}^{S,D} \frac{\left|\langle\Phi^{(0)}|H_1|\Phi^I\rangle\right|^2}{E^I - E^{(0)}}$$

➡ Non-orthogonal PT (present case): only one eigenstate of H_0 is known

→ No well-defined Hilbert-space partitioning, projector Q cannot be explicitly constructed

→ Rigorous PT formalised only recently: NOCI-PT [Burton & Thom 2020]

Perturbative expansion

⦿ Non-orthogonal perturbation theory

○ Construct reference Hamiltonian H_0

Baranger 1-body Hamiltonian

→ Introduce **state-specific** partitioning $H_0 \equiv \mathcal{P}_\mu^{\tilde{\sigma}} F_{[|\Theta\rangle]} \mathcal{P}_\mu^{\tilde{\sigma}} + \mathcal{Q}_\mu^{\tilde{\sigma}} F_{[|\Theta\rangle]} \mathcal{Q}_\mu^{\tilde{\sigma}}$

One-body operator $F(\rho(\Theta))$ such that Møller-Plesset partitioning is recovered in the single-determinant limit

○ Construct first-order wave function

→ Build all possible excitations on top of each Bogolyubov state entering $|\Theta^{(0)}\rangle$, then

$$|\Theta^{(1)}\rangle = \sum_q \sum_I a^I(q)|\Omega^I(q)\rangle \qquad \text{where} \qquad |\Omega^I(q)\rangle \equiv \mathcal{Q}P_{00}^{\tilde{\sigma}}|\Phi^I(q)\rangle$$

Excited Bogolyubov vacua, where $I \in$ S,D,T,. . .

○ Compute second-order energy as a function of $H_1 = H - H_0$ and $|\Theta^{(1)}\rangle$

→ Only $|\Phi^I(q)\rangle$ with $I \in$ S,D contribute → Approximate $|\Theta^{(1)}\rangle = \sum_q \sum_{I\in S,D} a^I(q)|\Omega^I(q)\rangle$

➡ Master equation $\sum_q \sum_{J\in S,D} M_{IpJq}\, a^J(q) = -h_1^I(p)$ where $\mathbf{M} \equiv \mathbf{H}_0 - E^{(0)}\mathbf{1}$

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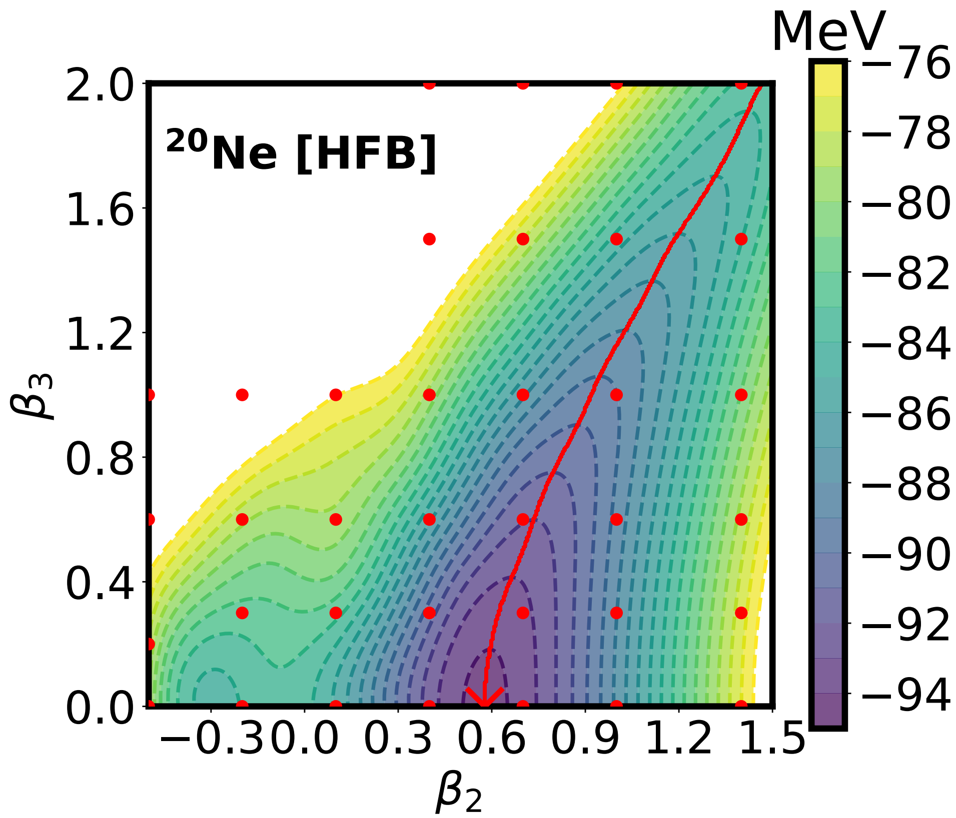
^{20}Ne

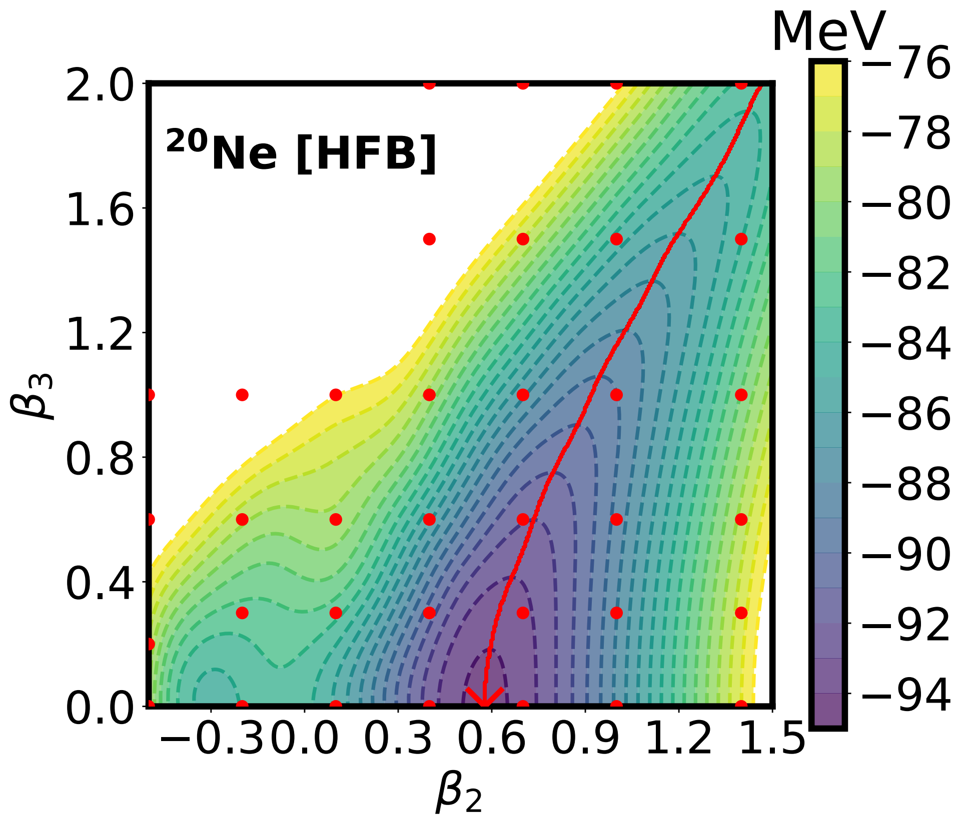
1. Constrained HFB



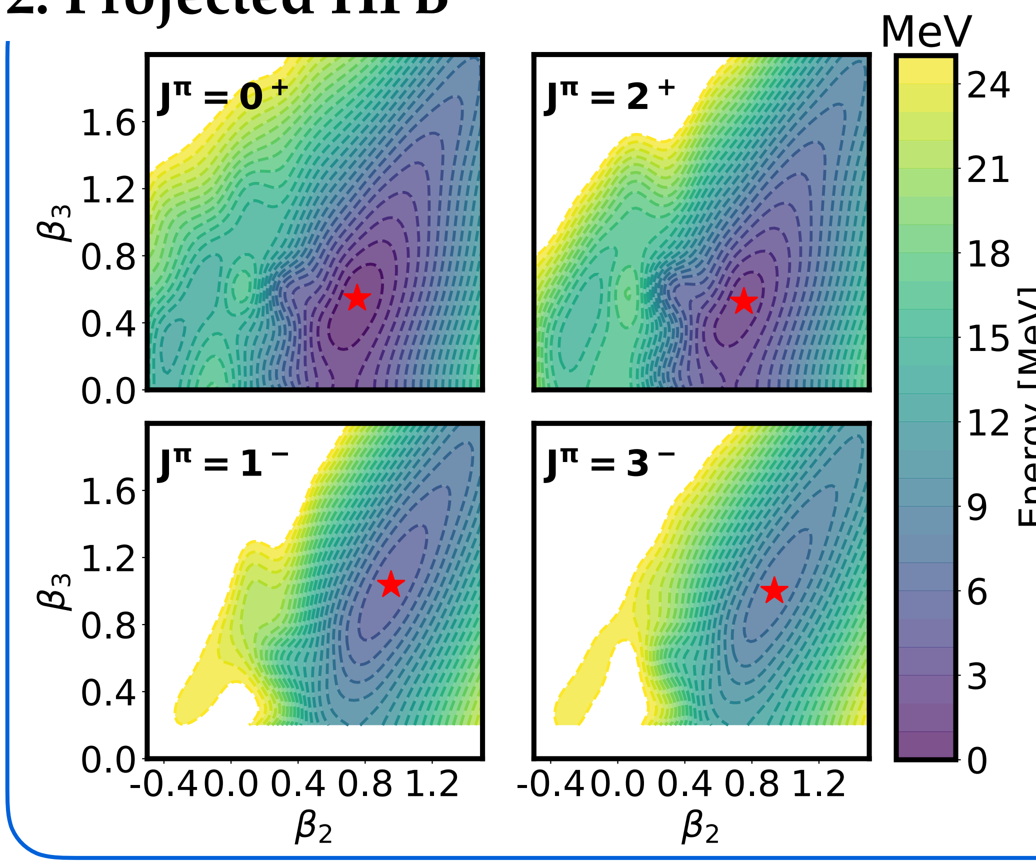
- **Constrained HFB calculations**
  - Maps total energy surface (TES)
  - Minimum at strongly deformed configuration
  - TES soft along the octupole direction

^{20}Ne

1. Constrained HFB



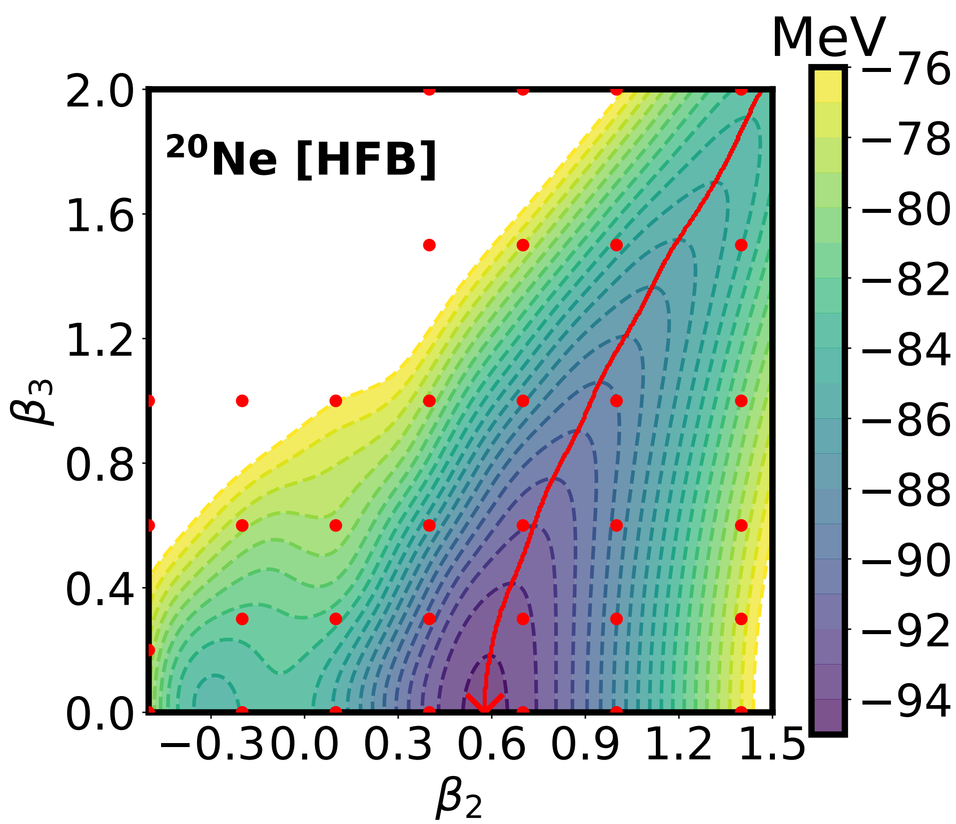
2. Projected HFB



- **Projected HFB calculations**
  - Projections favour deformed configurations
  - Negative parity states accessed
  - Provide input for computing PGCM state

^{20}Ne

1. Constrained HFB



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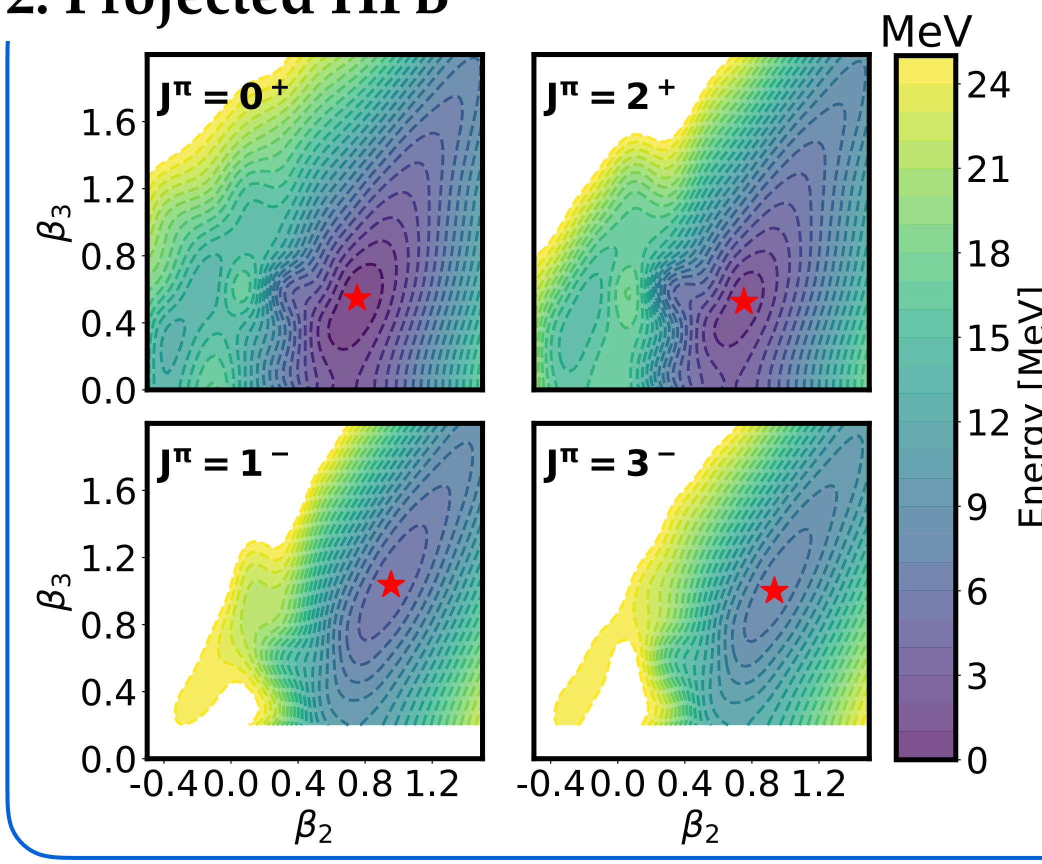
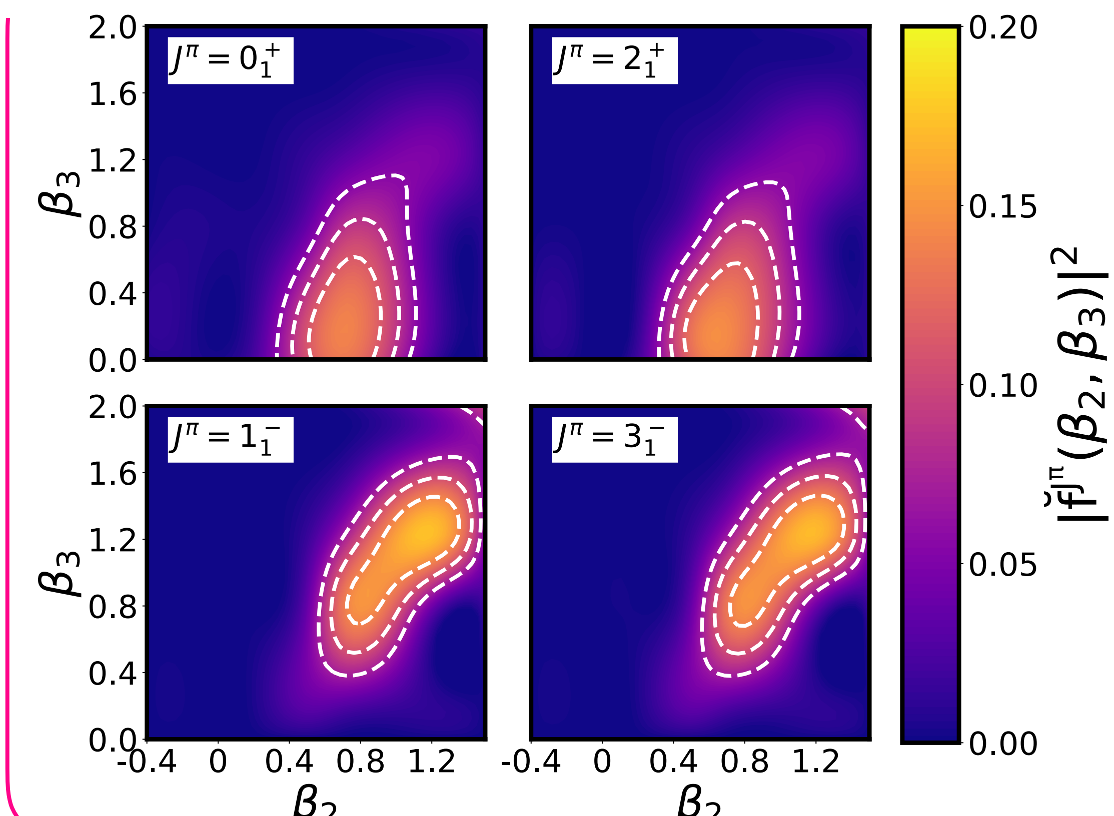
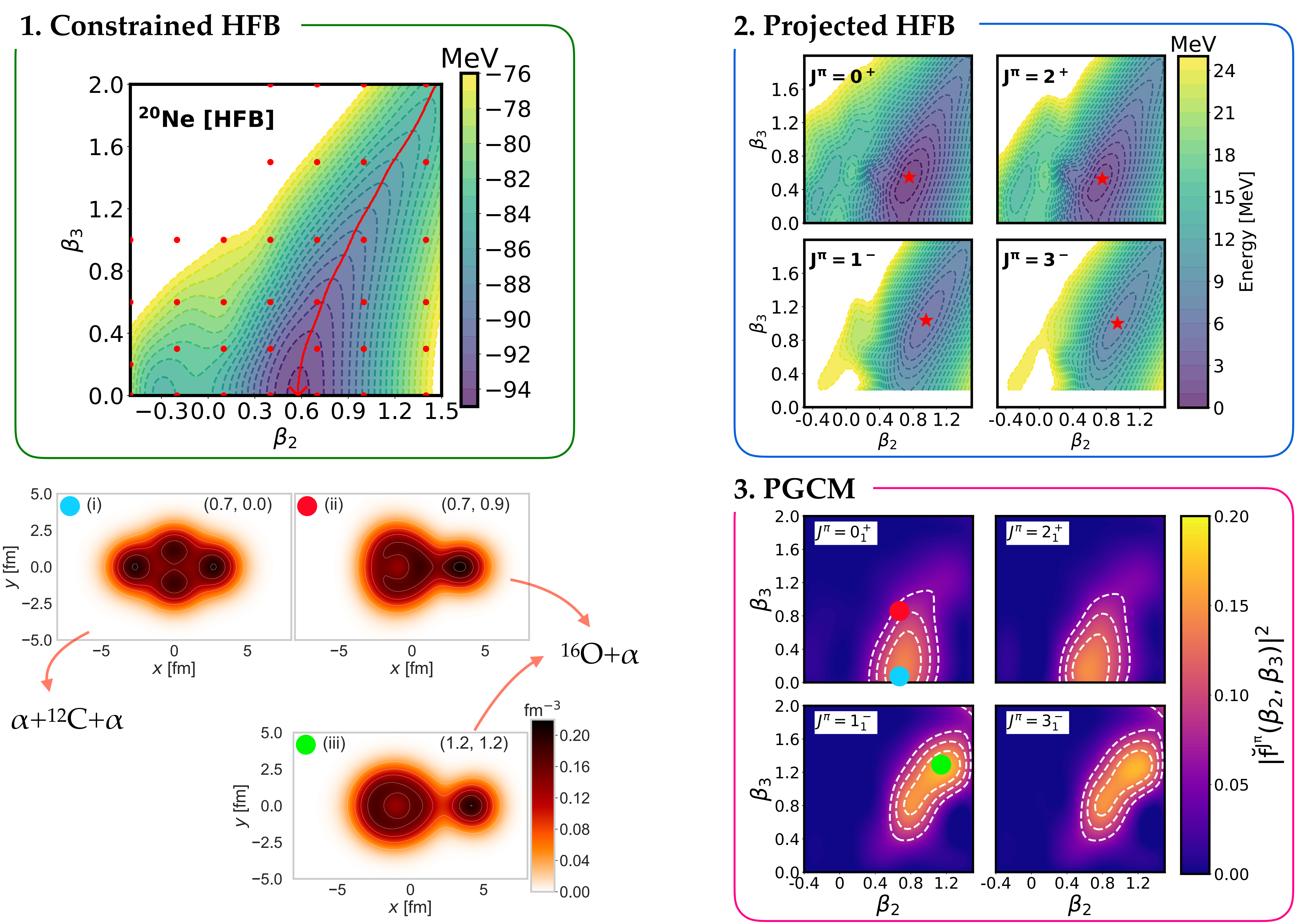


3. PGCM



- **PGCM mixing**
  - Collective w.f. → admixture of PHFB states
  - Significant shape fluctuations
  - Negative parities mix more deformations

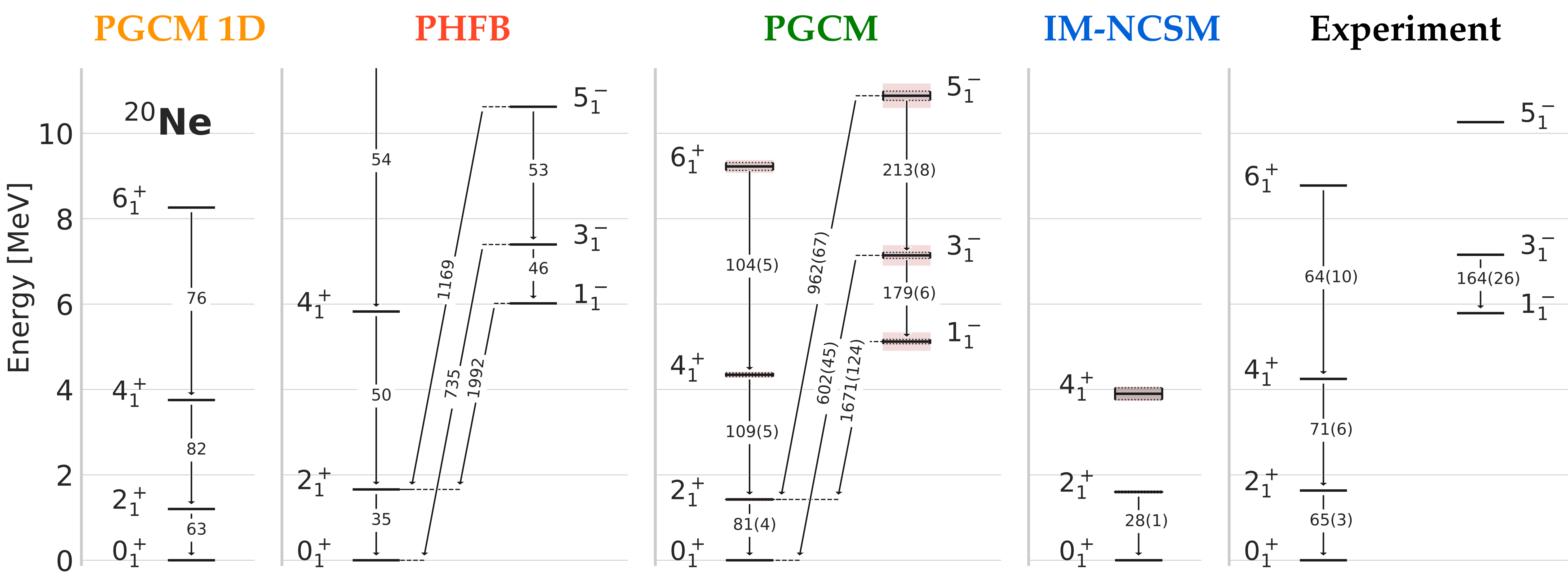
^{20}Ne



1. Constrained HFB
MeV
20Ne [HFB]
β3
β2
2. Projected HFB
MeV
Jπ = 0+
Jπ = 2+
Jπ = 1−
Jπ = 3−
Energy [MeV]
3. PGCM
Jπ = 0+1
Jπ = 2+1
Jπ = 1−1
Jπ = 3−1
|f̆Jπ(β2, β3)|2
(i)
(0.7, 0.0)
(ii)
(0.7, 0.9)
(iii)
(1.2, 1.2)
y [fm]
x [fm]
fm−3
16O+α
α+12C+α

^{20}Ne

- **PGCM excitation spectrum**
  - Reference: in-medium no-core shell model (IM-NCSM) [Mongelli & Roth]



→ Good agreement with experiment and (quasi-)exact IM-NCSM

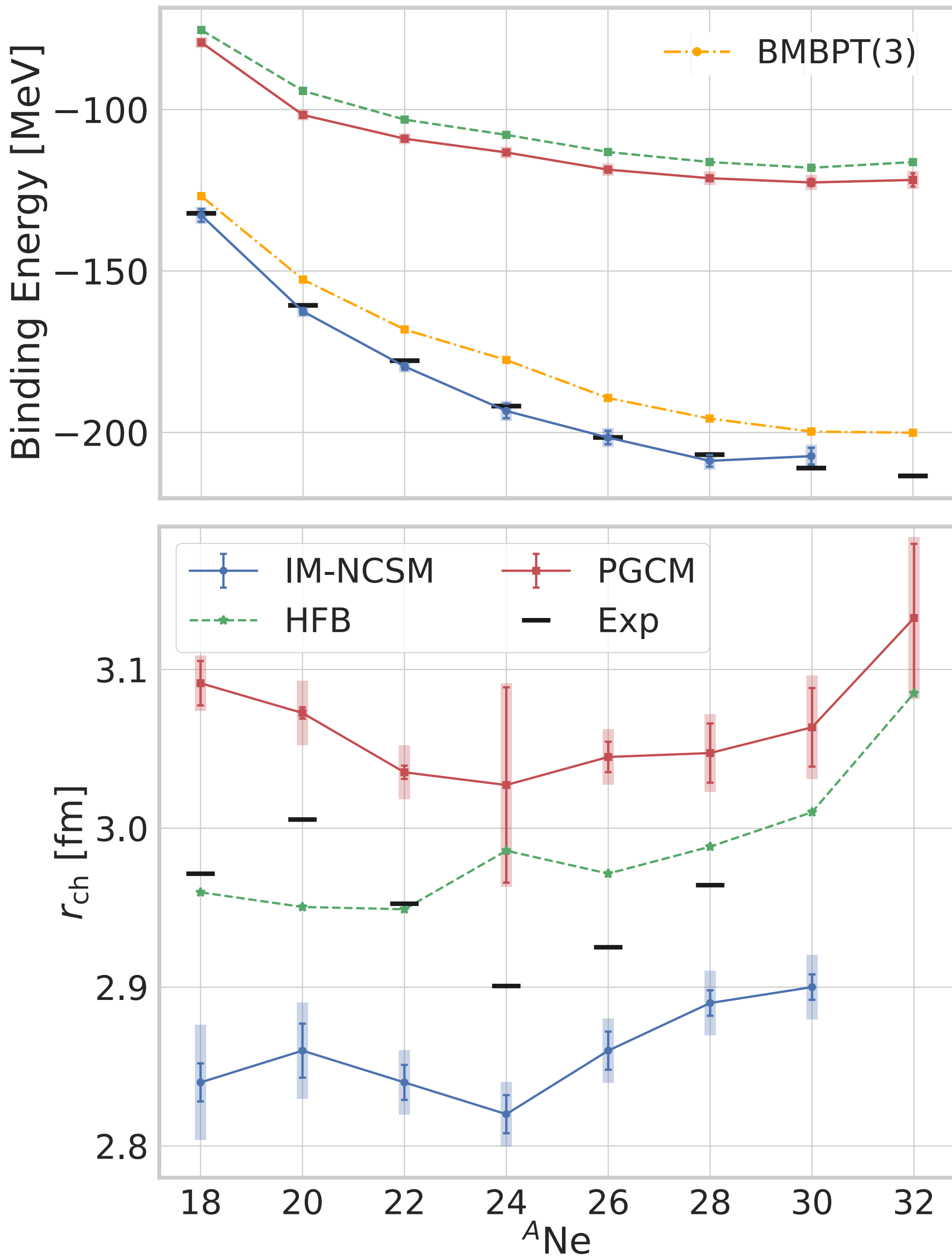
→ Essential **static correlations** captured by PGCM

→ Exaggerated collectivity [B(E2) systematically larger than experiment]

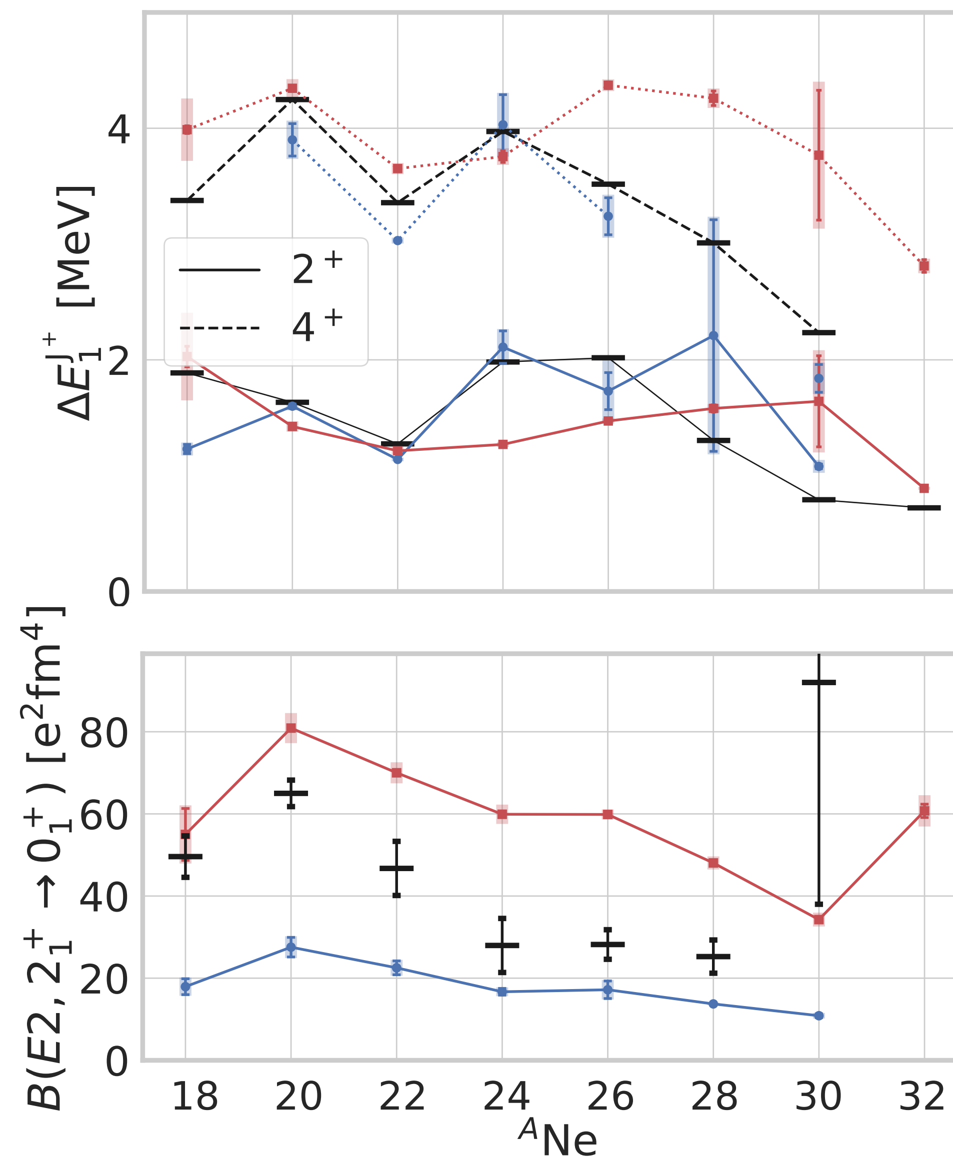
→ Restricting PGCM to 1D or PHFB **deteriorates spectrum**

Neon chain

G.s. properties



Excited states



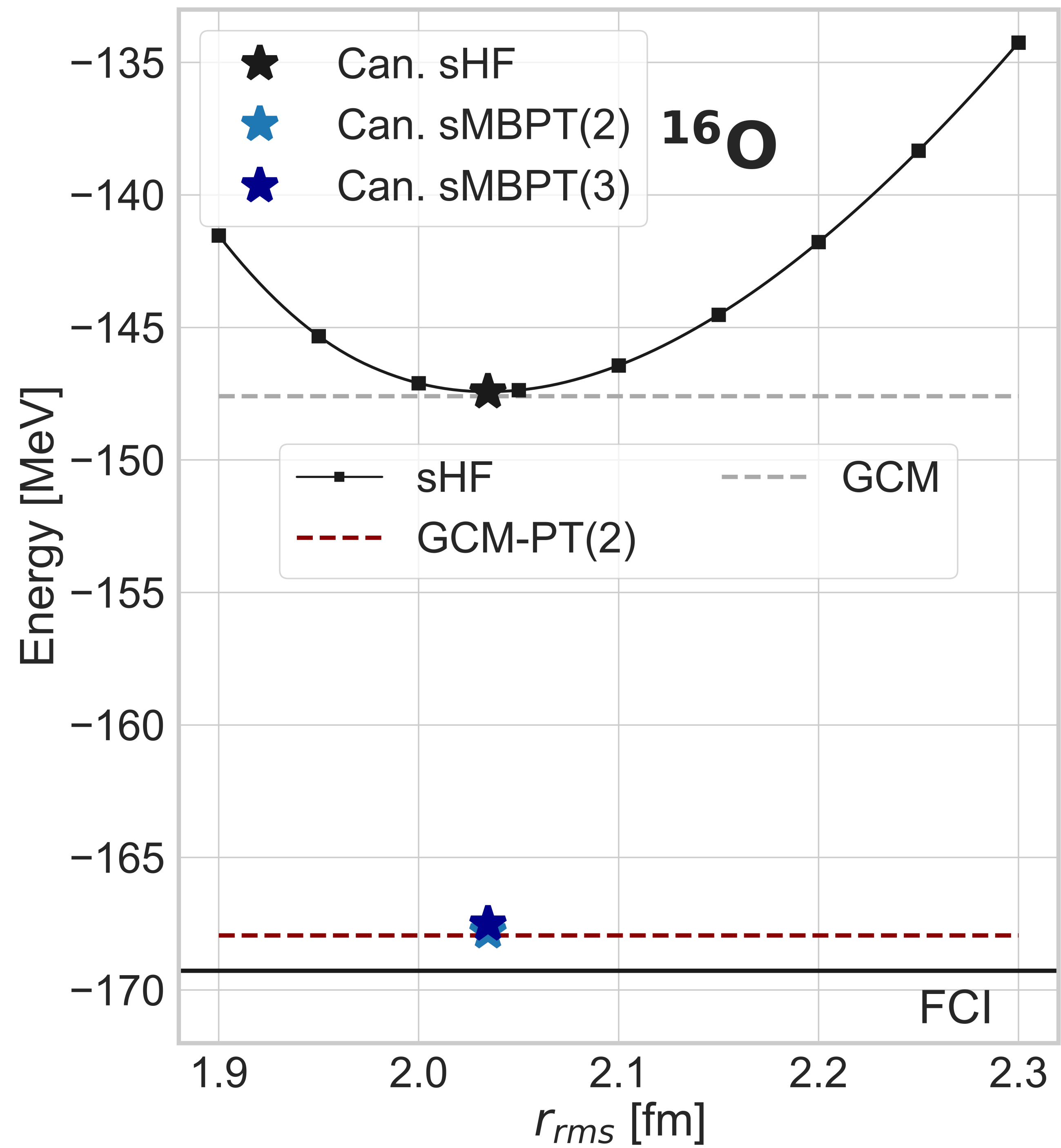
- ○ Dynamical correlations essential for B.E.
- ○ PT+projection provide good indication
- ○ Radii: trend corrected by PGCM

- ○ Good description until ^{24}Ne
- ○ ^{30}Ne off the trend
- ○ Heavier isotopes too collective in PGCM

Outline

PGCM-PT(2) validation

- **First proof-of-principle calculation in a small model space (e_{max}=4)**
  - NN interaction only
  - Compare to exact Full CI reference [R. Roth]
- **Doubly closed-shell ^{16}O**
  - Radius as collective coordinate
  - GCM yields small effect in closed-shells
  - GCM-PT(2) gets close to FCI
  - MBPT(2,3) consistent at canonical point



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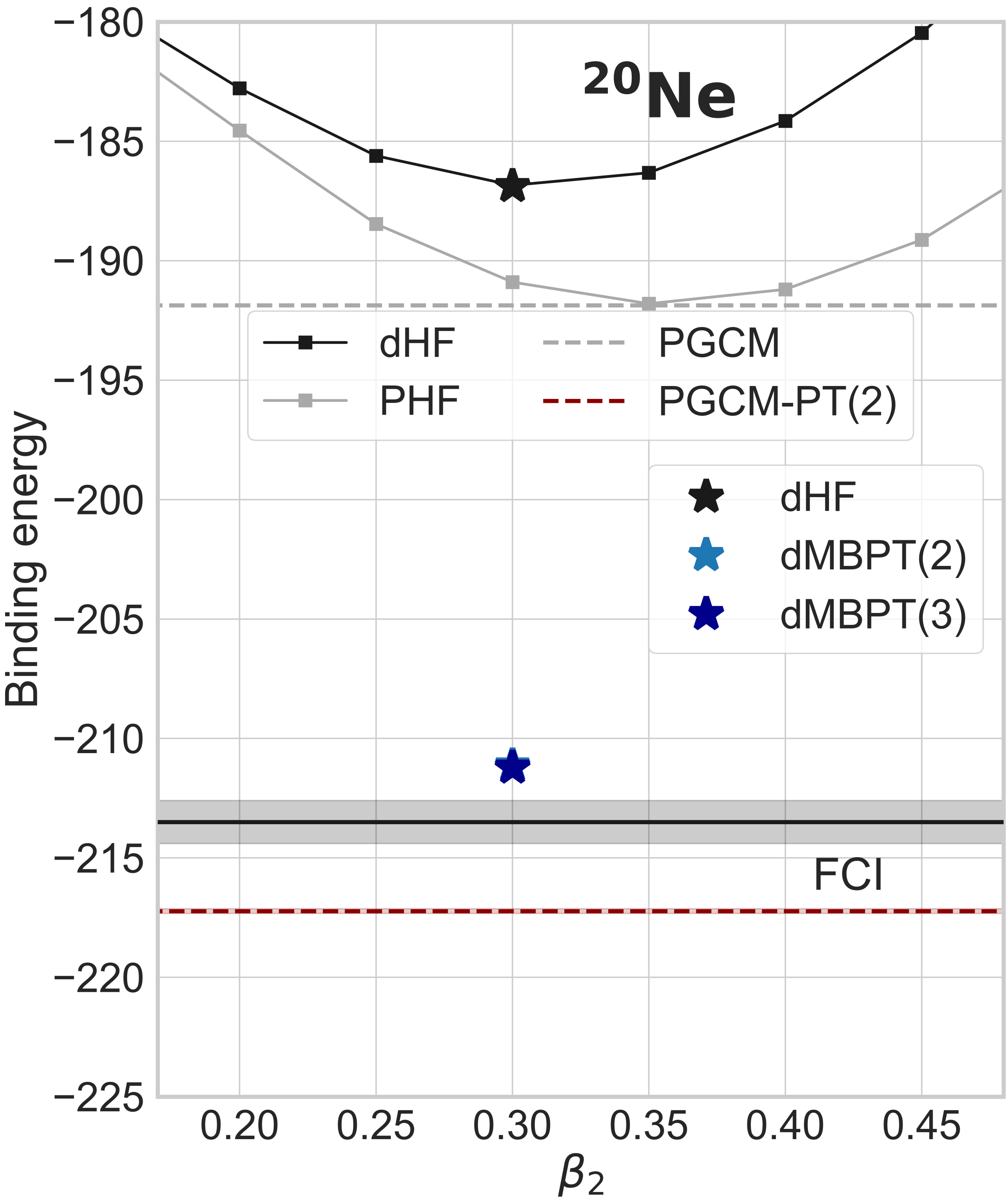
- **Doubly open-shell ^{20}Ne**
  - Quadrupole def. as collective coordinate
  - Projection brings 5 MeV binding
  - PGCM-PT(2) brings in dyn. correlations
  - dMBPT(2,3) underbinds → projection needed



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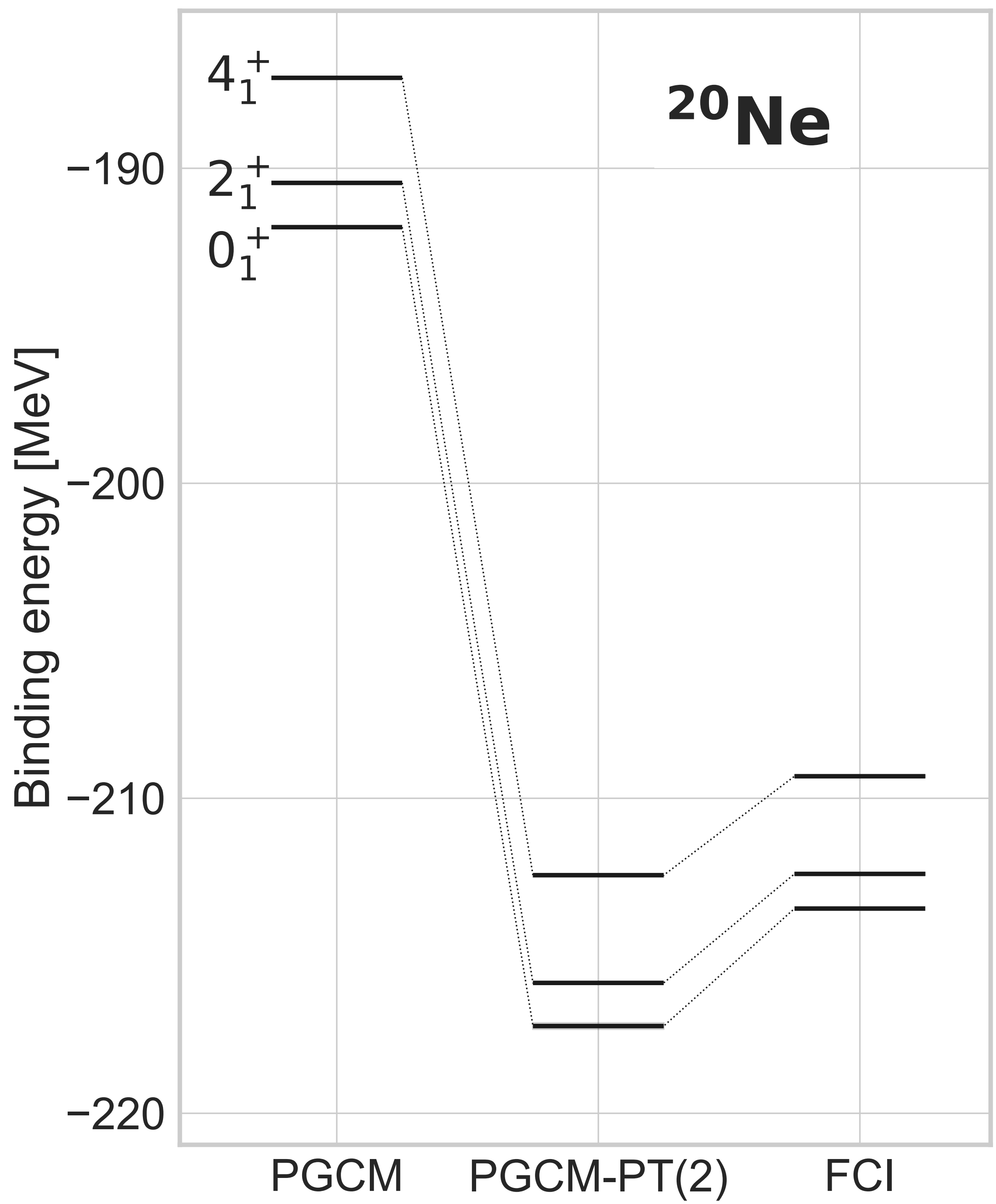
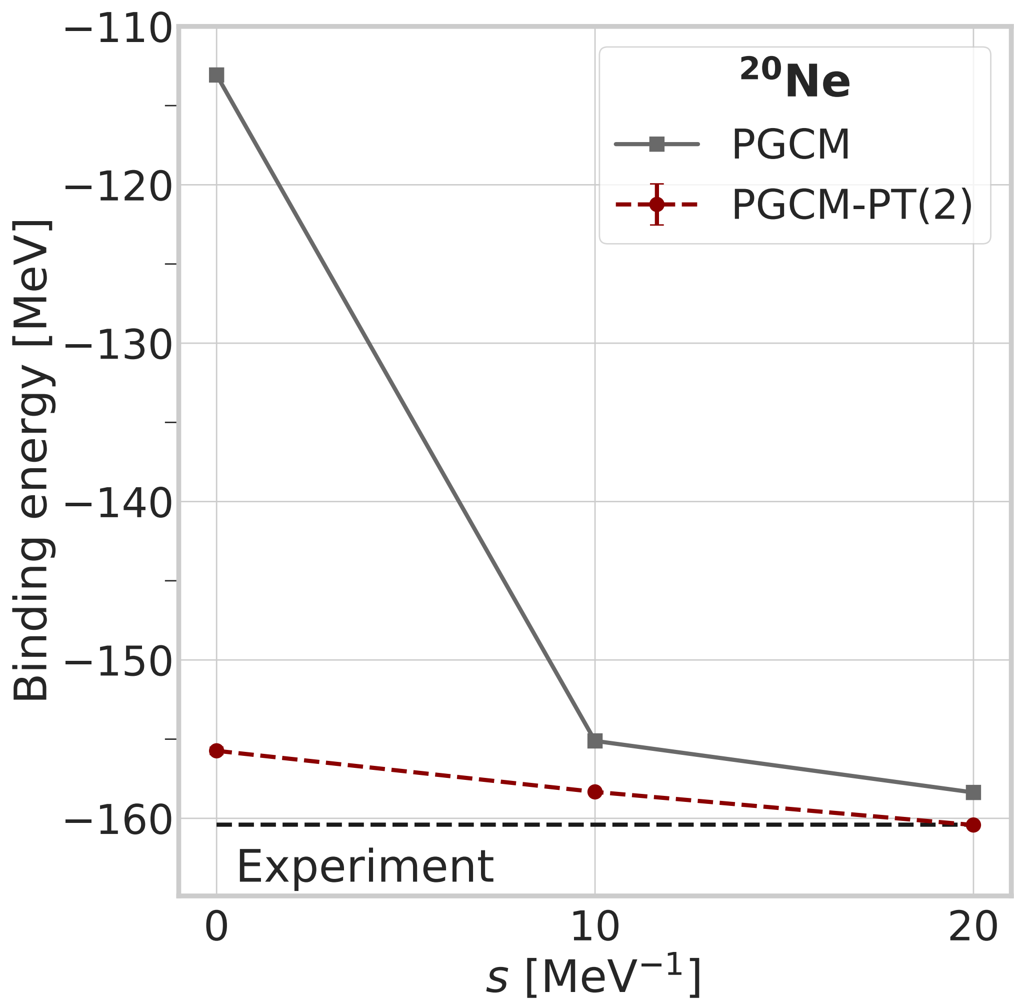
  - PGCM-PT(2) preserves quality of exc. spectra

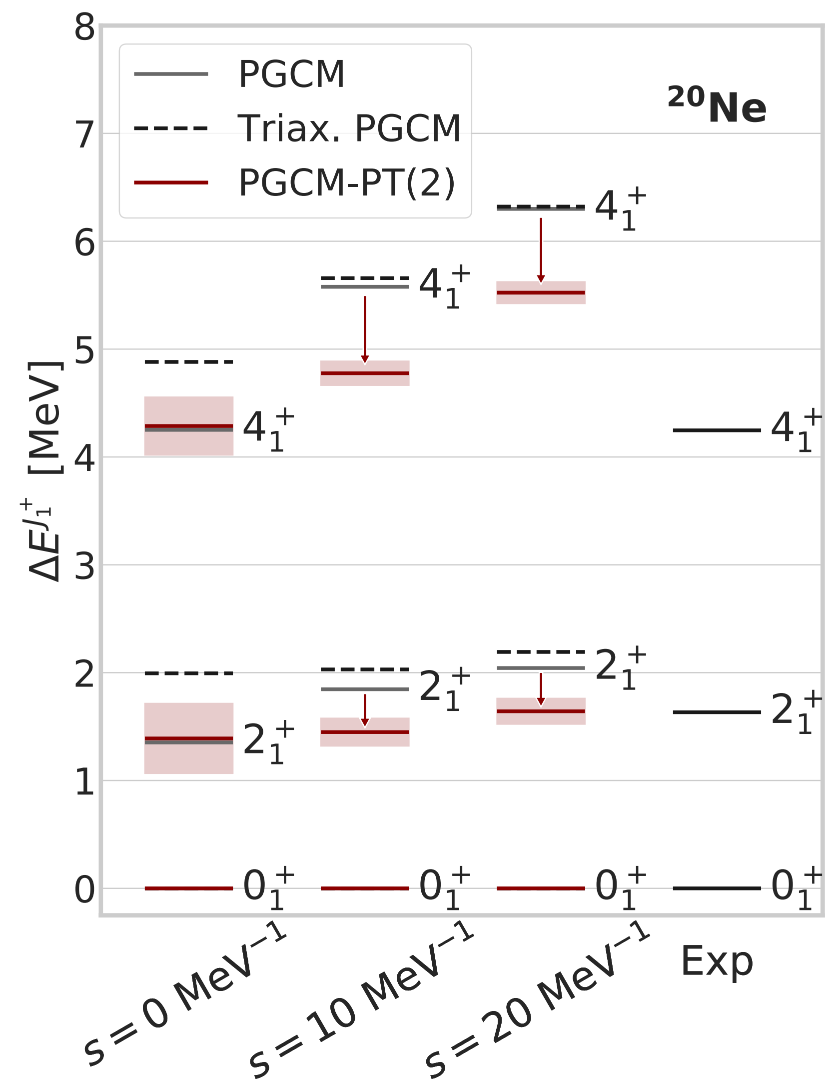


Combining PGCM-PT(2) with MR-IMSGR

⦿ **Multi-reference IMSRG:** nucleus-dependent transformation of H $\quad H(s) = U^\dagger(s) H U(s)$

- ○ Decouples $|\Theta^{(0)}\rangle$ from Q space as $s \to \infty$ → Dynamical correlations recast into H(s)
- ○ PGCM+MR-IMSRG recently explored by Yao et al. → Promising results; impact of PT?





→ Problem becomes more perturbative

→ PT(2) correction systematically decreases

→ PT(2) corrects for dilatation of spectrum

→ Triaxial GCM not enough

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Towards the ab initio description of complex nuclei

⦿ Three complementary levers to tackle complex mid-mass/heavy nuclei via expansion methods

1. Pre-processing of the Hamiltonian

→ Flow must resum bulk of dynamical correlations without inducing a large break of unitarity

2. Choice of reference state

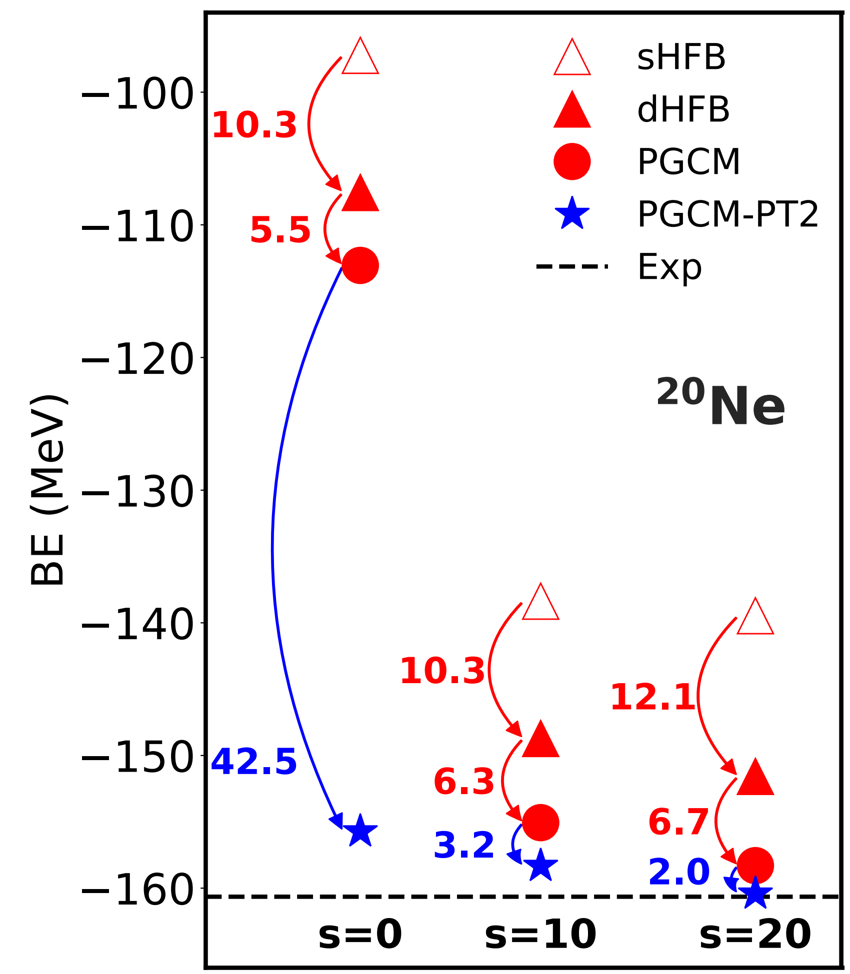
→ Rich enough to capture non-perturbative static correlations, but low dimensionality

3. Systematic expansion of the many-body Schrödinger equation

→ Low-order truncation with gentle scaling

⬇

Optimal balance between the three must be found



⦿ **Novel multi-reference perturbation theory**

○ PGCM accounts for collective/IR correlations

○ UV physics provided by well-defined non-orthogonal PT

○ Can be combined with pre-processing of H