Ab initio PGCM and applications to light nuclei

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INT PROGRAM INT-23-1A
Intersection of nuclear structure and high-energy nuclear collisions

❶ Context

Theoretical description of nuclear systems

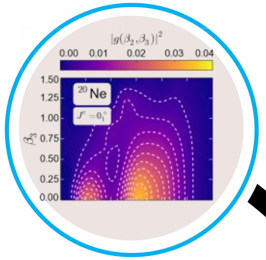
❷ PGCM

How to best account for nucleons correlations

❸ Application

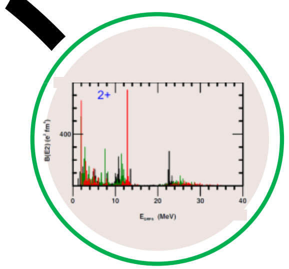
Context : General goal of nuclear structure theory

- Starting from the hadronic level of organization (nucleons + interactions), what novel structures emerge and how they evolve with E_{ex}, N, Z, …



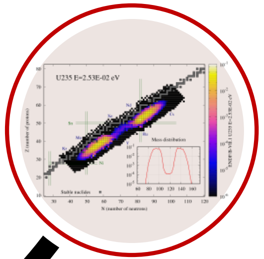
Ground-state

masses, radii, density profile, …



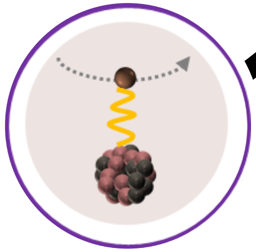
Excitation spectra

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



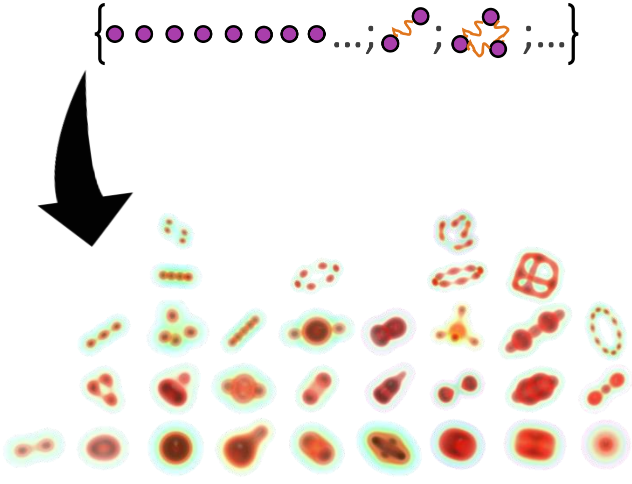
Decay modes

lifetime, yields, …



Reactions

cross sections, …



Intrinsic densities

Atomic nucleus

=

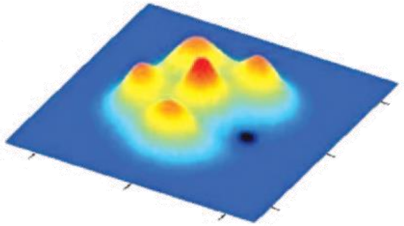
A mesoscopic, self-bound system of strongly correlated spin-1/2 and isospin-1/2 composite fermions in strong and electroweak interaction.

Emergent SSBs

Context : General goal of nuclear structure theory

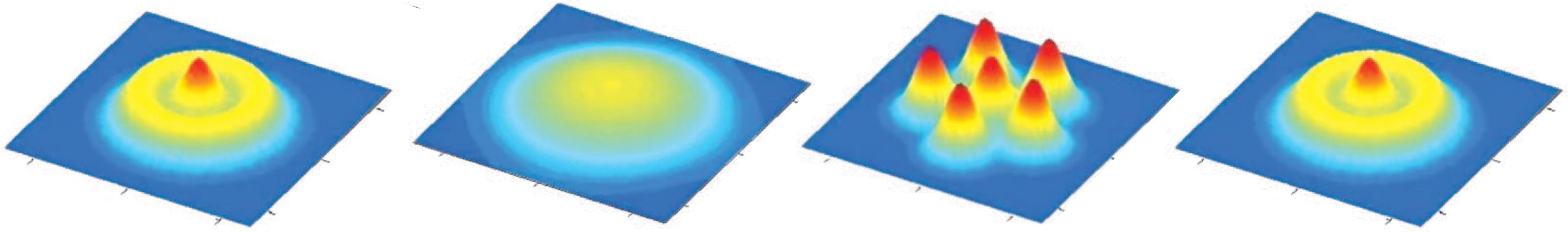
- Emergent SSBs : SSBs obscured by non-negligible fluctuations of order parameters but still leave traces

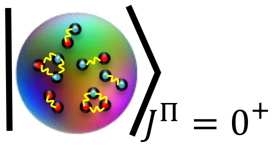
2-point correlation function



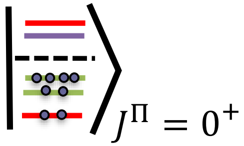
Revealing back long-range order

Density profile

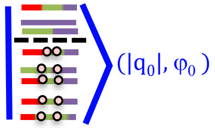




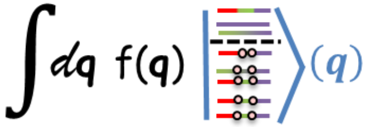
Exact WF



Approx :
Symmetry-preserving HF WF



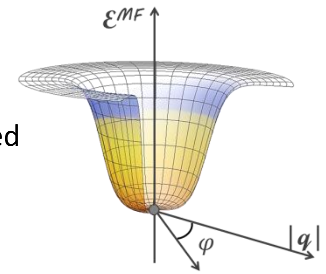
Approx :
Symmetry-broken HFB WF



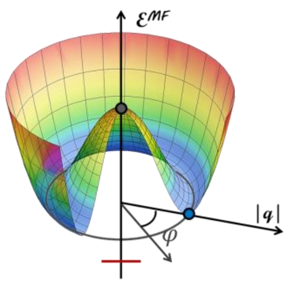
Approx :
PGCM WF

Spectroscopy

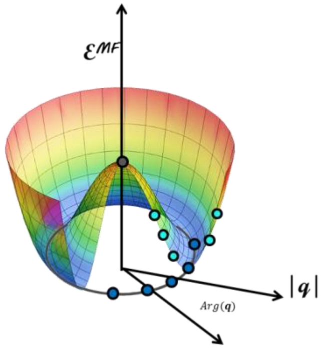
Selection rules satisfied
Symmetries of the Hamiltonian realized in the ground and excited states
BUT ALSO
Long-range order/collectivity



Closed-shell system



Open-shell system

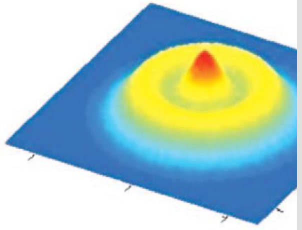


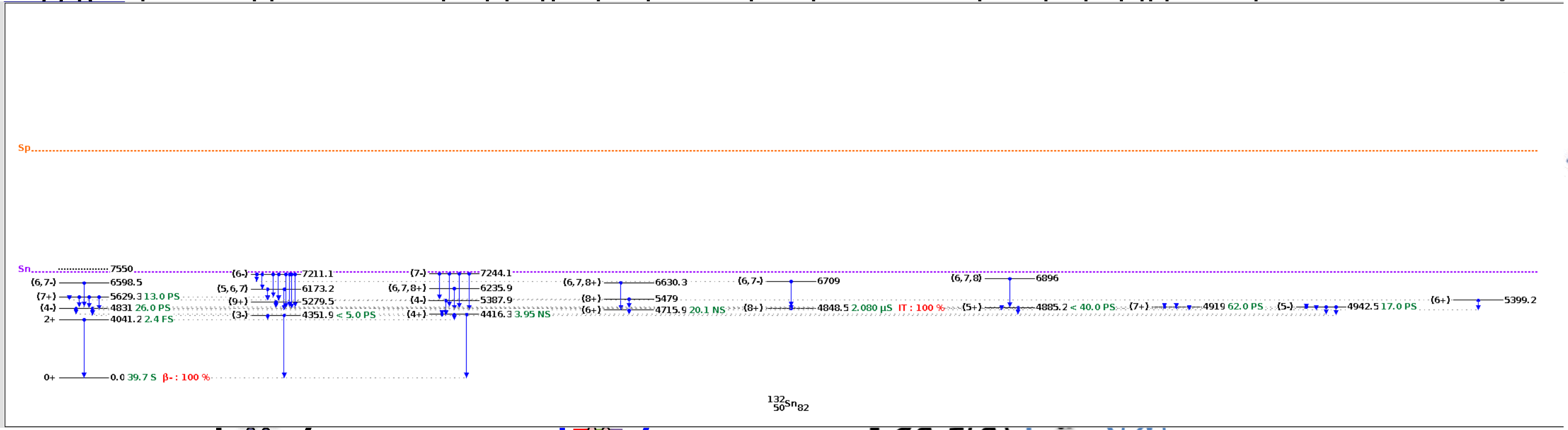
Yannouleas & Landman, 2017

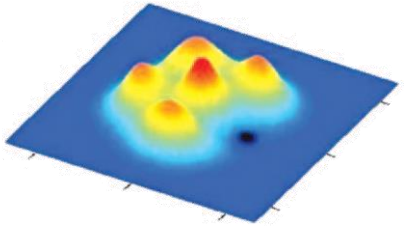
1 Context : General goal of nuclear structure theory

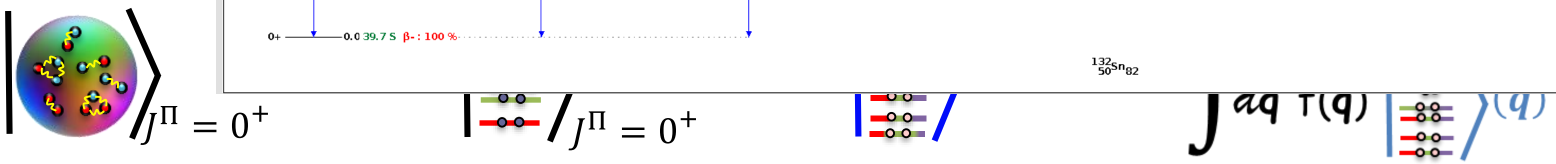
- Emergent SSB

2-point correlation function









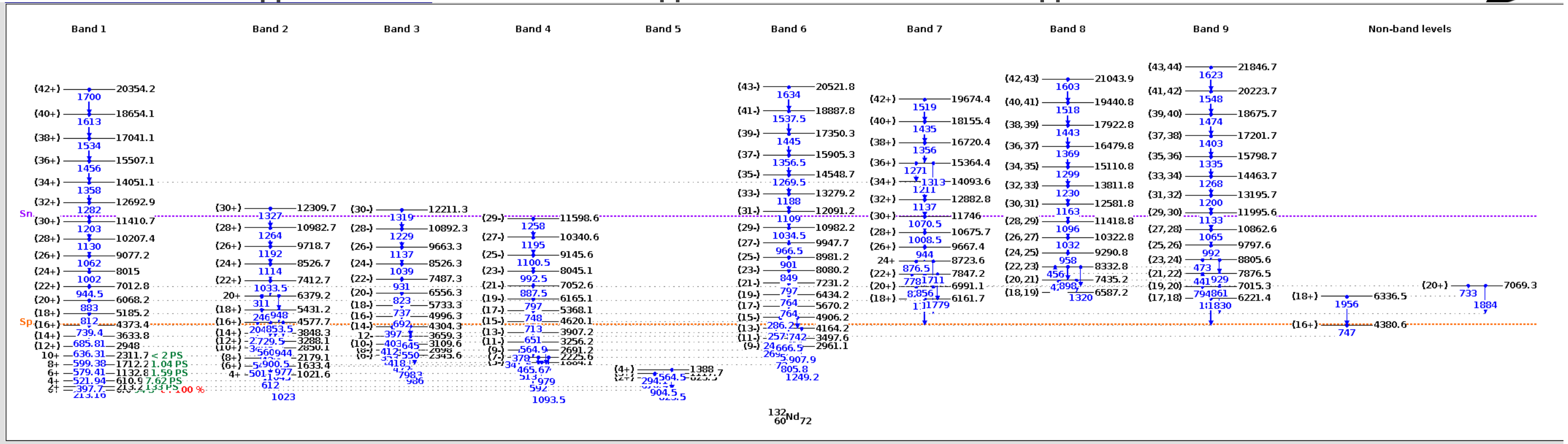
Exact WF

Approx :

Approx :

Approx :

Spectroscopy

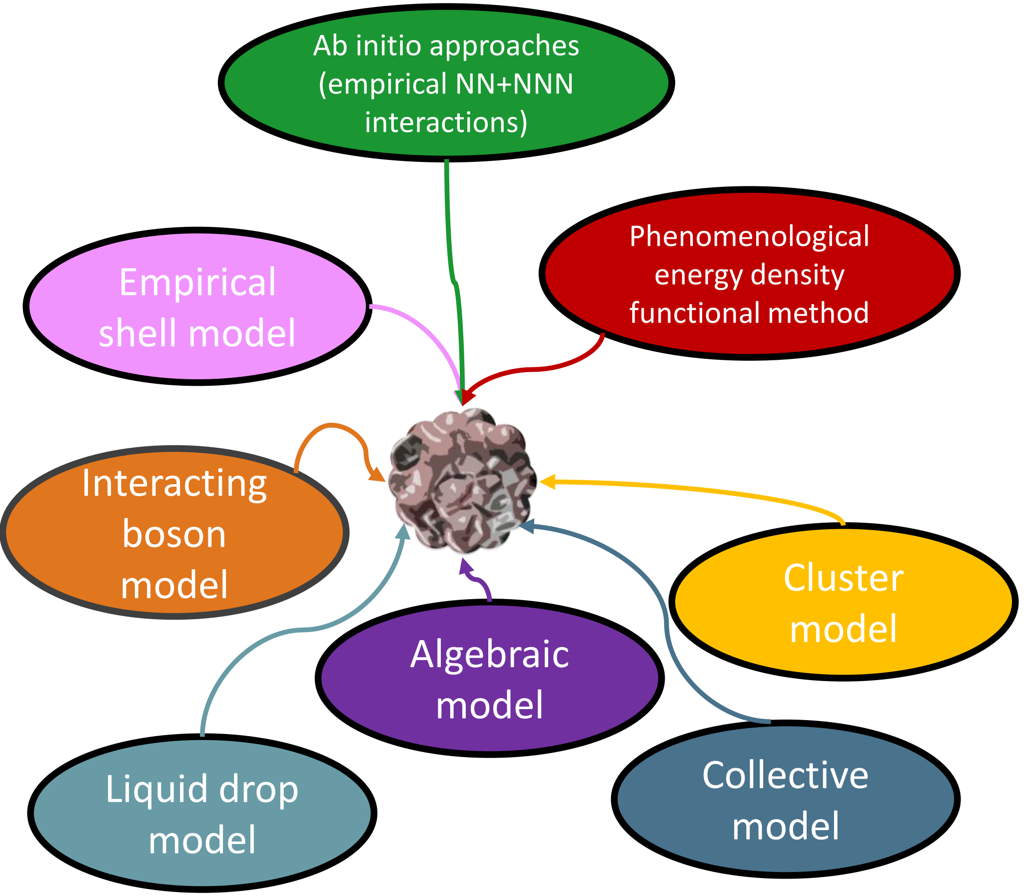


Selection rules satisfie
Symmetries of the Han
realized in the ground
states
BUT ALSO
Long-range order/colle

Yannouleas & Landman, 20

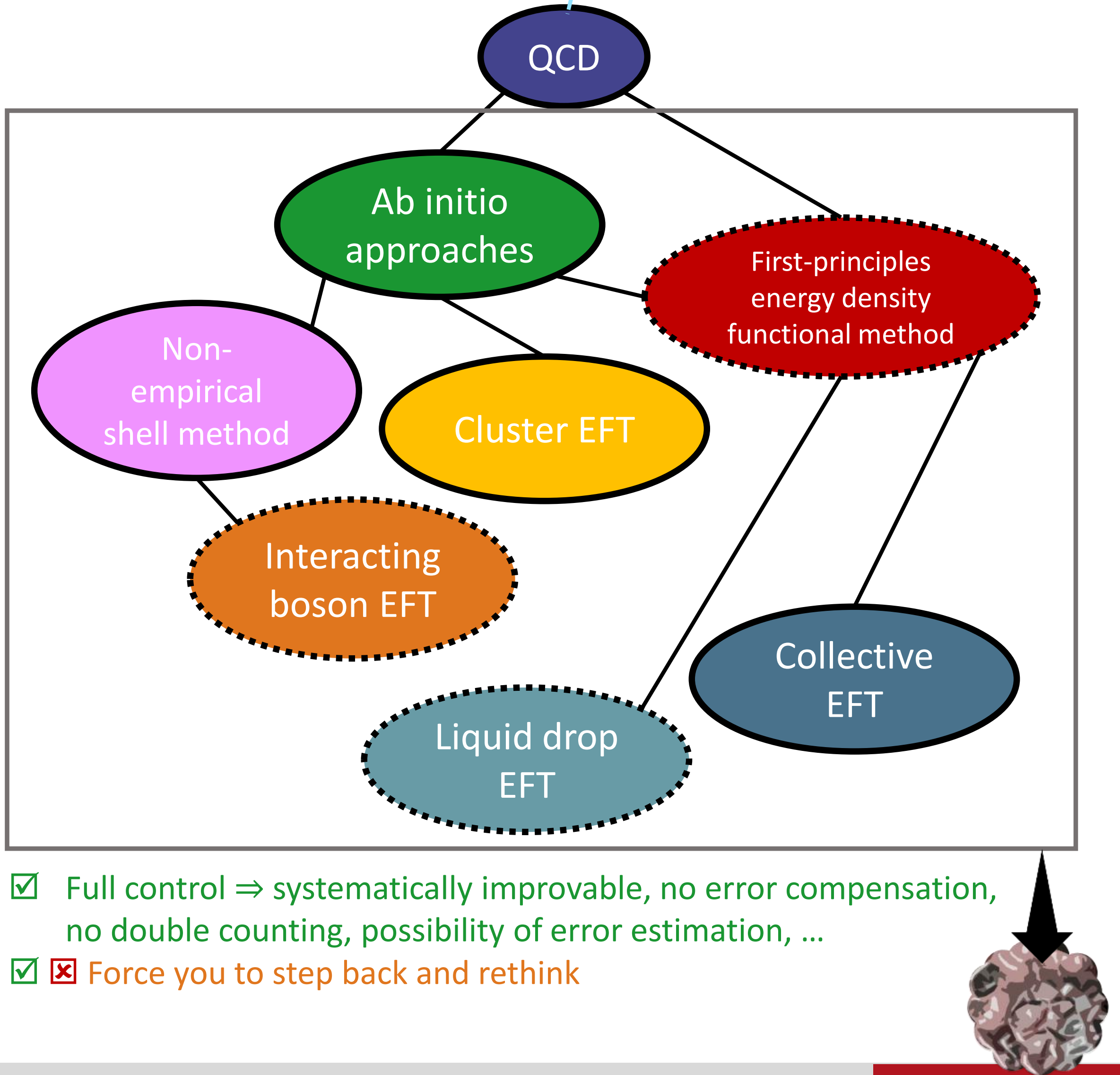
◉ Achieve a { *accurate* / *predictive* / *computationally affordable* } description ?

Era of models



☑ Gives insight about relevant scales/dofs
☑ Ready to be used
☒ Lack of control
⇒ double counting issues, error compensation, no error assessment

Era of effective (field) theories



☑ Full control ⇒ systematically improvable, no error compensation, no double counting, possibility of error estimation, …
☑ ☒ Force you to step back and rethink

1 Context : Nuclear structure from a microscopic viewpoint

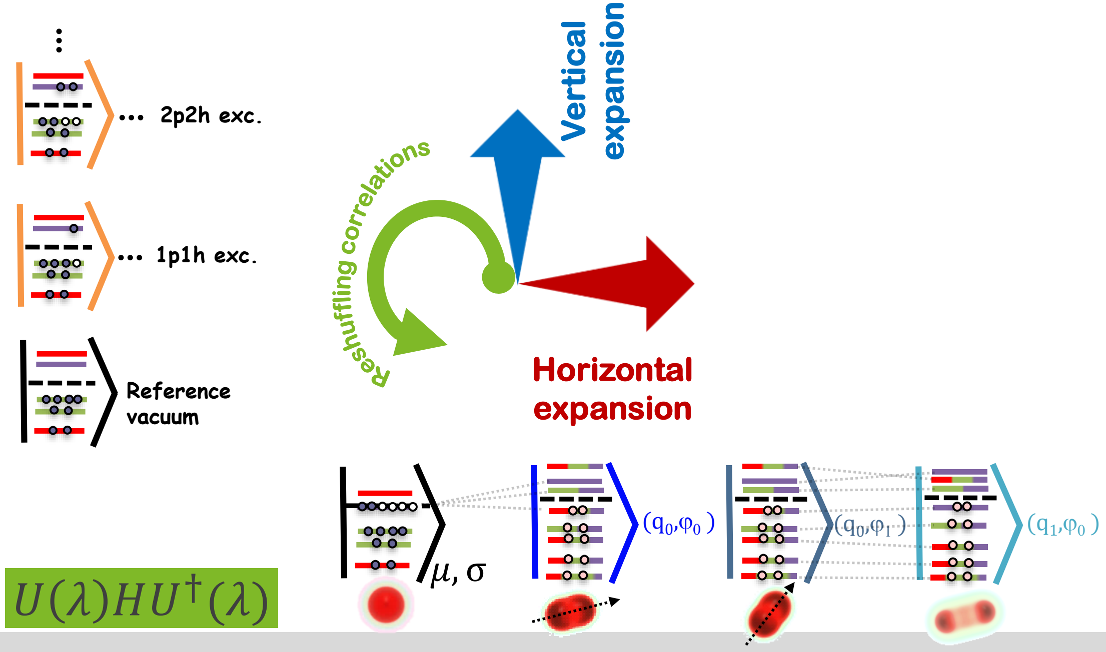
1) Nucleus: *A* interacting, structure-less nucleons
2) Structure & dynamic encoded in Hamiltonian, Functional, …
3) Solve *A*-nucleon Schrödinger/Dirac equation to desired accuracy

$$H(\ldots)|\Psi_{\mu,\sigma}\rangle = E_{\mu\tilde{\sigma}}|\Psi_{\mu,\sigma}\rangle$$

Strongly correlated WF

$$|\Psi_{gs}\rangle = \sum_{i_1<\cdots<i_A}^{L} C_{i_1\cdots i_A}|\phi_{i_1}\cdots\phi_{i_A}\rangle \equiv \sum_{I}^{N_{FCI}} C_I|\Phi_I\rangle$$

Rationale for grasping nucleon correlations

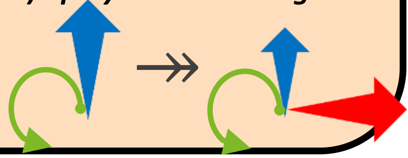


$U(\lambda)HU^{\dagger}(\lambda)$

Ab initio

- ◉ **Systematically improvable free-space Hamiltonian in χEFT**
- ◉ **Solving Schrödinger equation**
  - ◈ Pre-processing H
  - ◈ Refined many-body schemes with controlled uncertainties
    - ⇢ *CI (full space diag.) : exponential scaling*
    - ⇢ *Hybrids (valence space diag.) : mixed scaling*
    - ⇢ ***Expansion methods (partition, expand and truncate) : polynomial scaling***

⊗ *How to challenge ab initio frontiers*

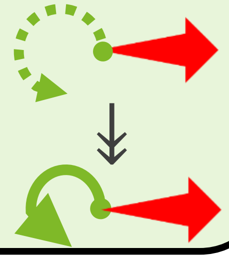


EDF

- ◉ **Effective pseudo-Hamiltonian**

Free-space interactions ; $|\Psi_{\mu,\sigma}\rangle$ *Complicated WF* ↠ *Effective in-medium interactions* ; $|\Theta_{\mu\sigma}\rangle$ Simplified auxiliary WF

- ◉ **Various levels of realization**
  - ⇢ *Hartree-Fock-Bogoliubov (HFB)*
  - ⇢ *Projected Generator Coordinate Method (PGCM)*
  - ⇢ *Quasiparticule Random Phase Approximation (QRPA)*



⊗ *How to improve current EDFs*

⊗ *How to turn EDF in EFT ?*

❶ Context

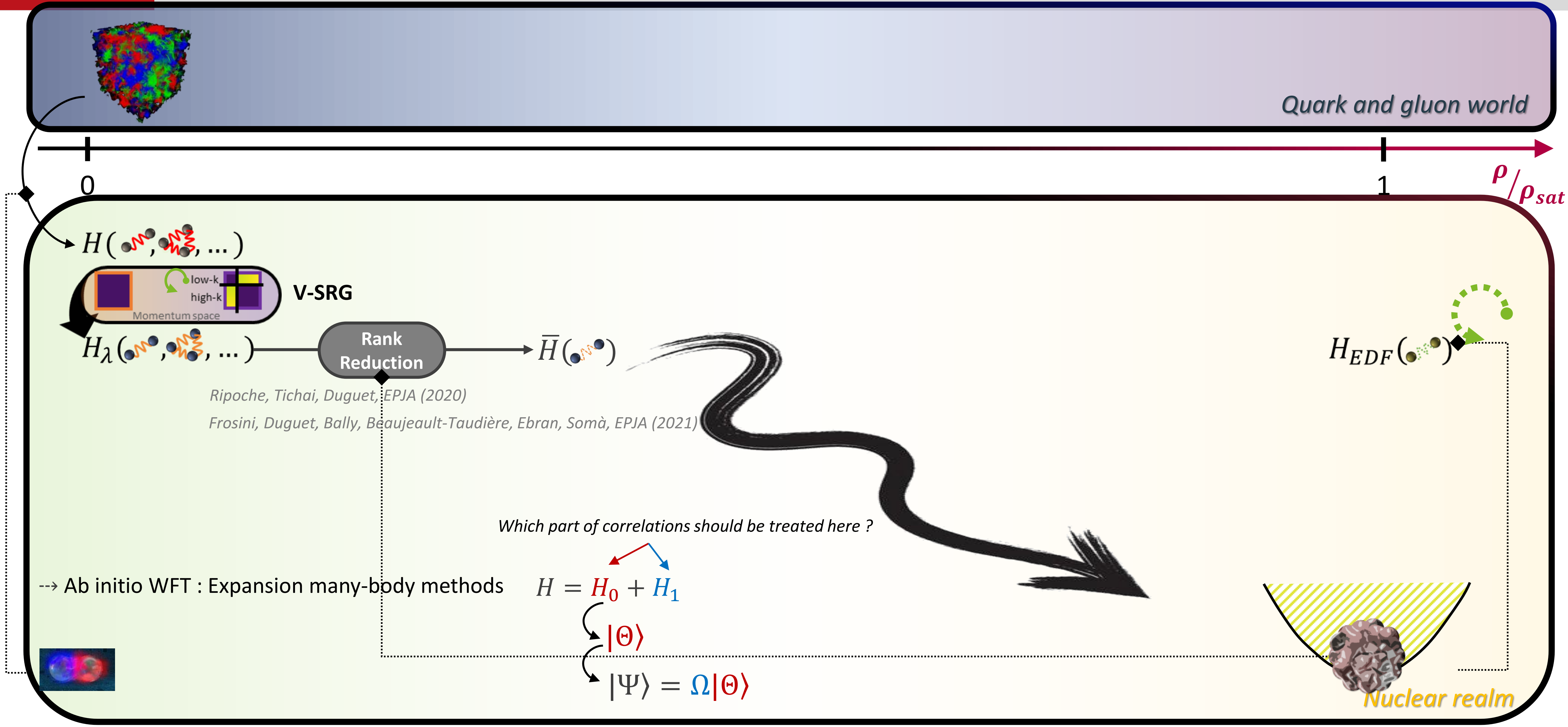
Theoretical description of nuclear systems

❷ PGCM

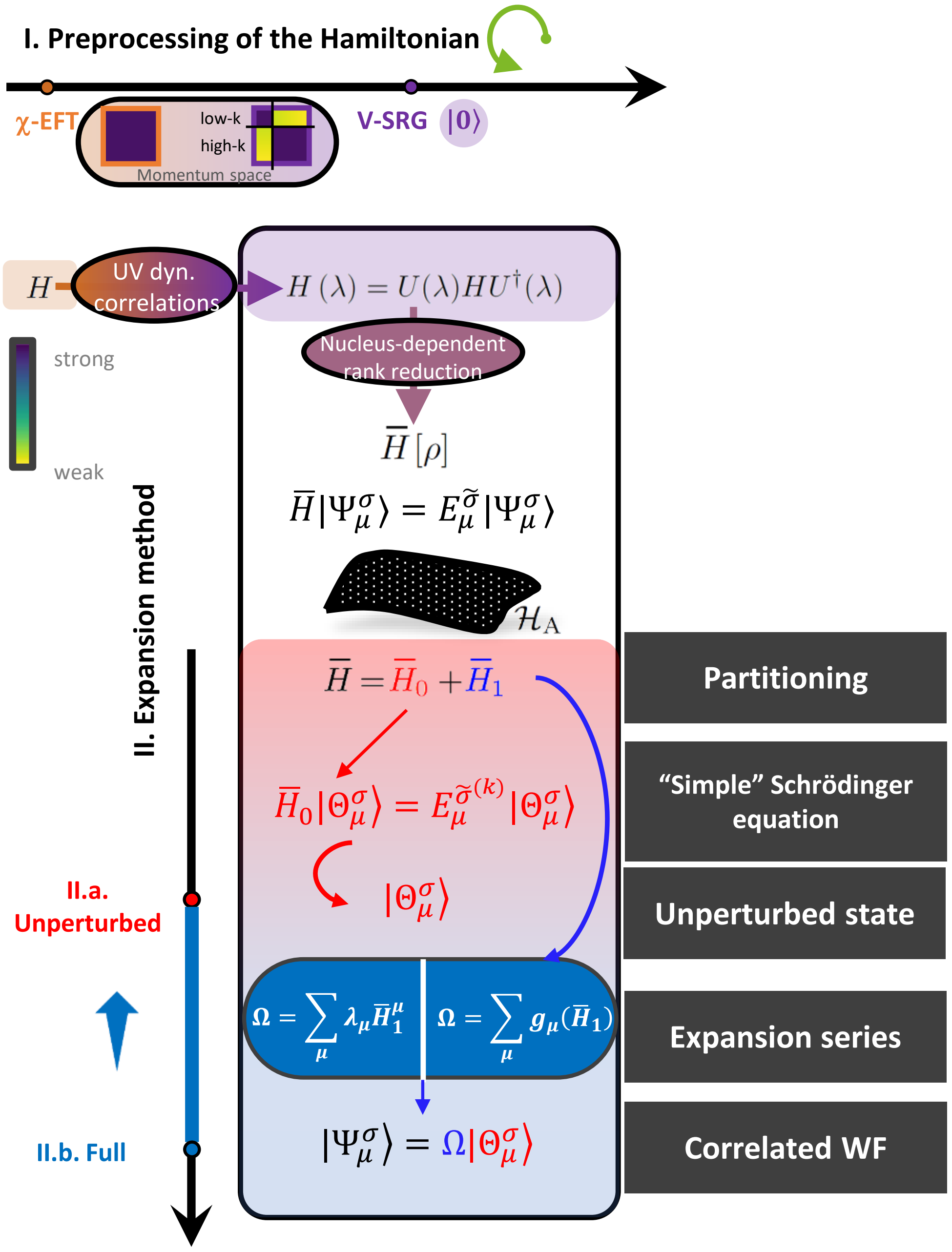
How to best account for nucleons correlations

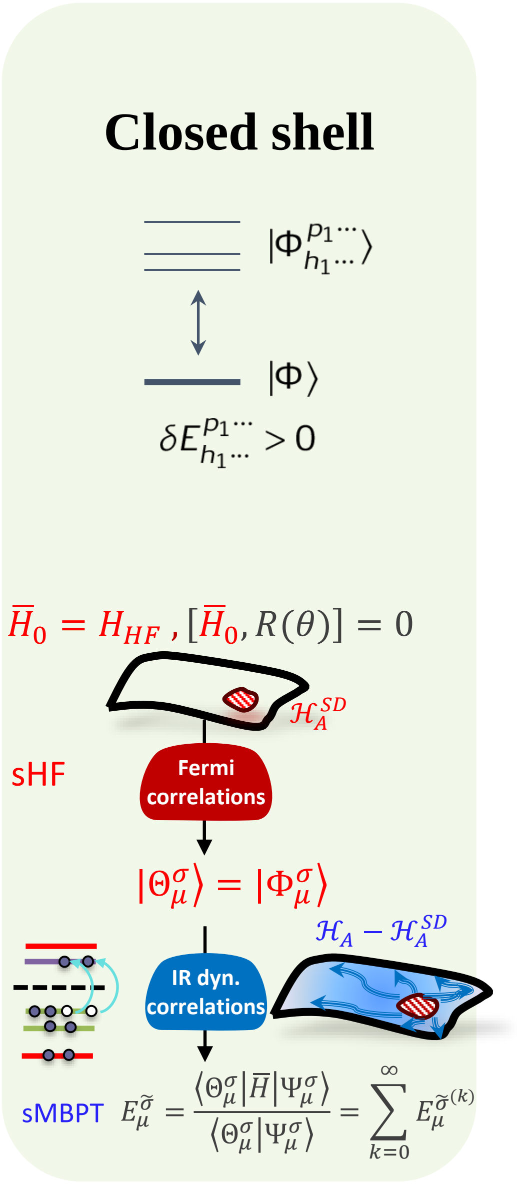
❸ Application

② Expansion Method



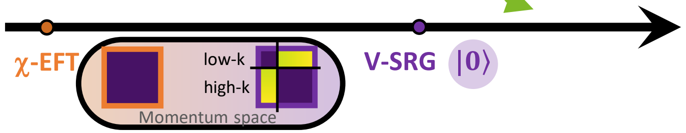
2 Simple expansion scheme



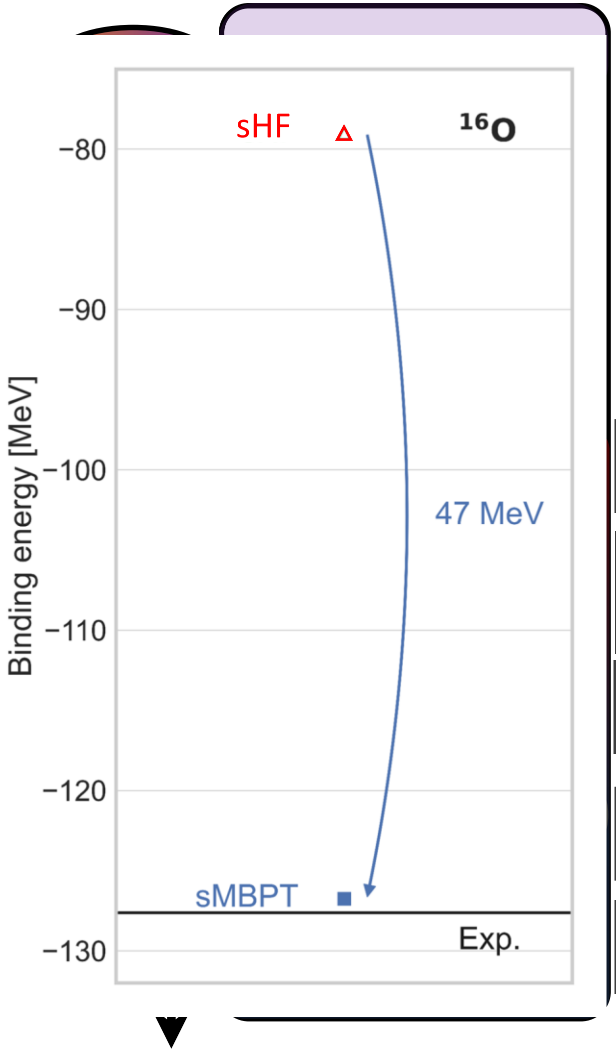


Tichai, Langhammer, Binder, Roth PLB(2016)

I. Preprocessing of the Hamiltonian



② Simple expansion scheme



Partitioning

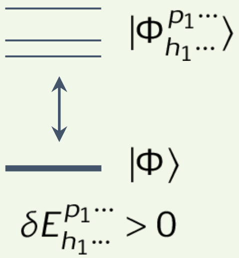
"Simple" Schrödinger equation

Unperturbed state

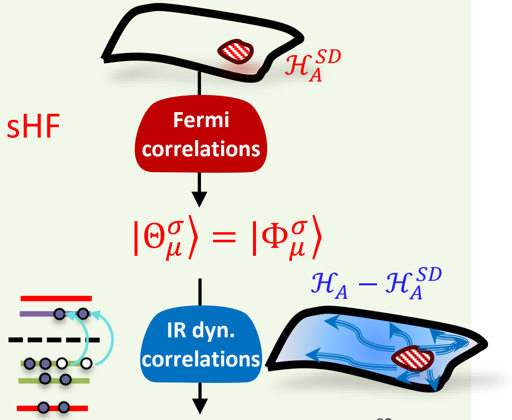
Expansion series

Correlated WF

Closed shell

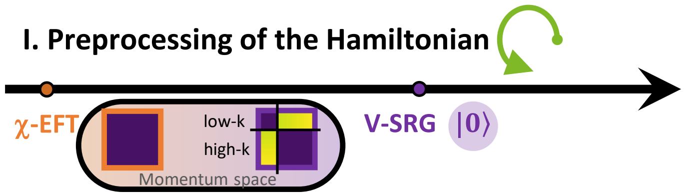


$\overline{H}_0 = H_{HF}\ , [\overline{H}_0, R(\theta)] = 0$

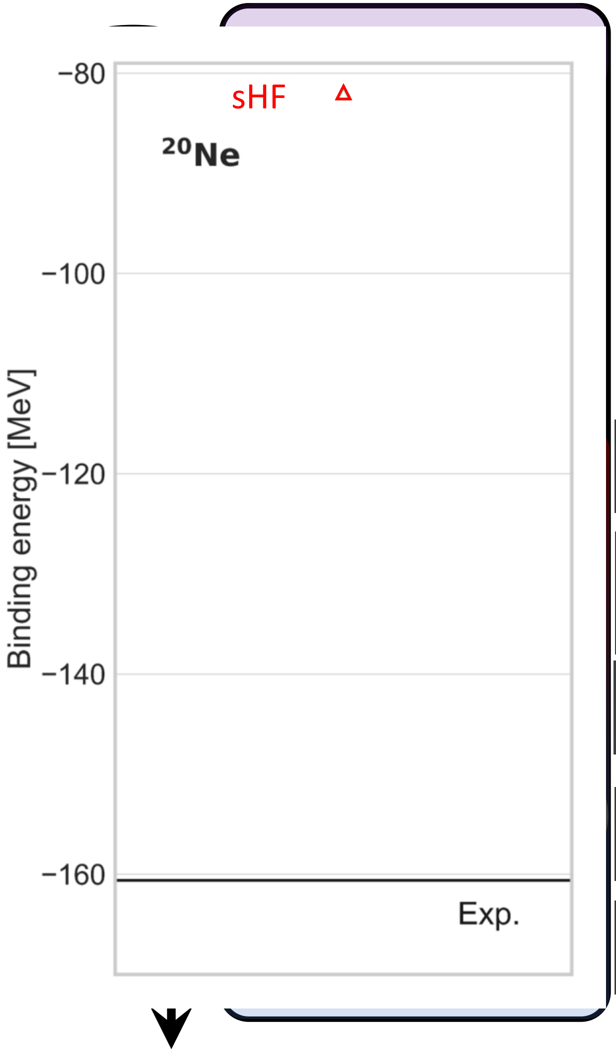


sMBPT $E^{\tilde{\sigma}}_{\mu} = \frac{\langle \Theta^\sigma_\mu | \overline{H} | \Psi^\sigma_\mu \rangle}{\langle \Theta^\sigma_\mu | \Psi^\sigma_\mu \rangle} = \sum_{k=0}^{\infty} E^{\tilde{\sigma}(k)}_{\mu}$

I. Preprocessing of the Hamiltonian



② Simple expansion scheme



Partitioning

"Simple" Schrödinger equation

Unperturbed state

Expansion series

Correlated WF

Closed shell

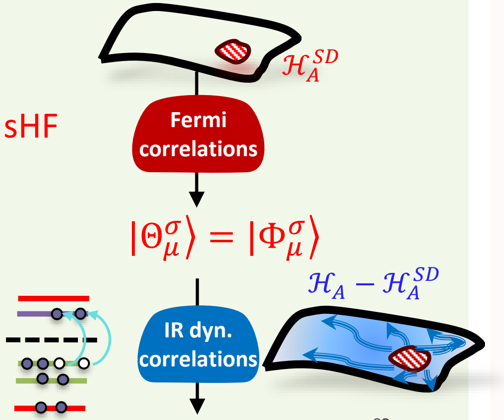
$|\Phi^{p_1\cdots}_{h_1\cdots}\rangle$

$|\Phi\rangle$

$\delta E^{p_1\cdots}_{h_1\cdots} > 0$

$\bar{H}_0 = H_{HF}\ , [\bar{H}_0, R(\theta)] = 0$

sHF



$|\Theta^\sigma_\mu\rangle = |\Phi^\sigma_\mu\rangle$

sMBPT $E^{\tilde{\sigma}}_\mu = \frac{\langle\Theta^\sigma_\mu|\bar{H}|\Psi^\sigma_\mu\rangle}{\langle\Theta^\sigma_\mu|\Psi^\sigma_\mu\rangle} = \sum_{k=0}^{\infty} E^{\tilde{\sigma}(k)}_\mu$

Open shell

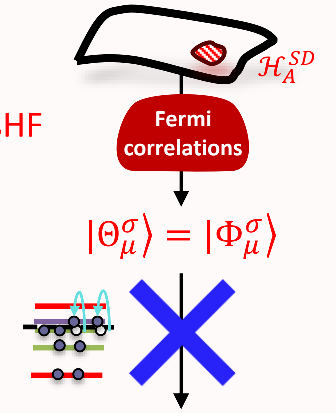
$|\Phi^{p_1\cdots}_{h_1\cdots}\rangle$

$|\Phi\rangle$

$\delta E^{p_1\cdots}_{h_1\cdots} \sim 0$

$\bar{H}_0 = H_{HF}\ , [\bar{H}_0, R(\theta)] = 0$

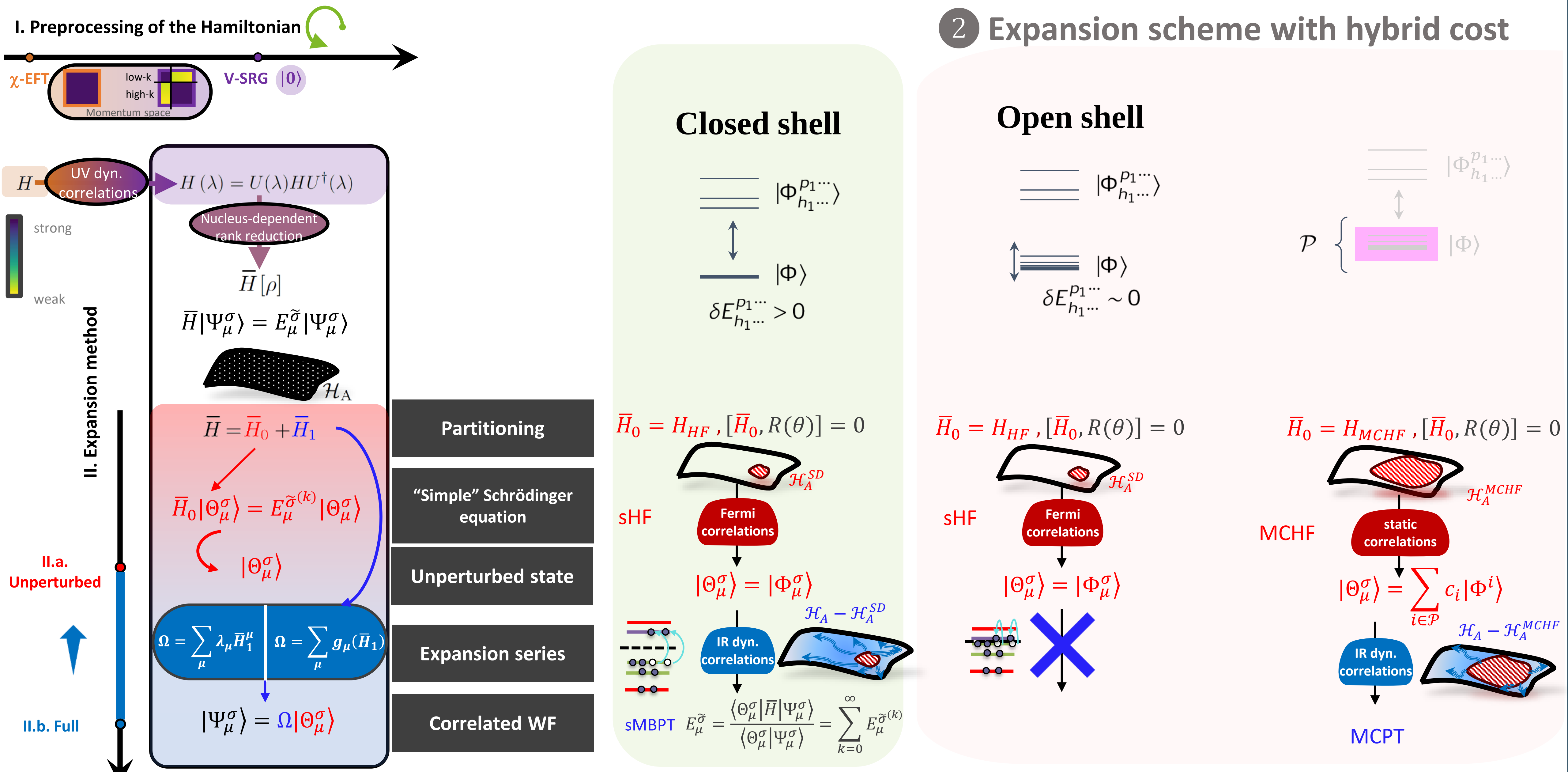
sHF



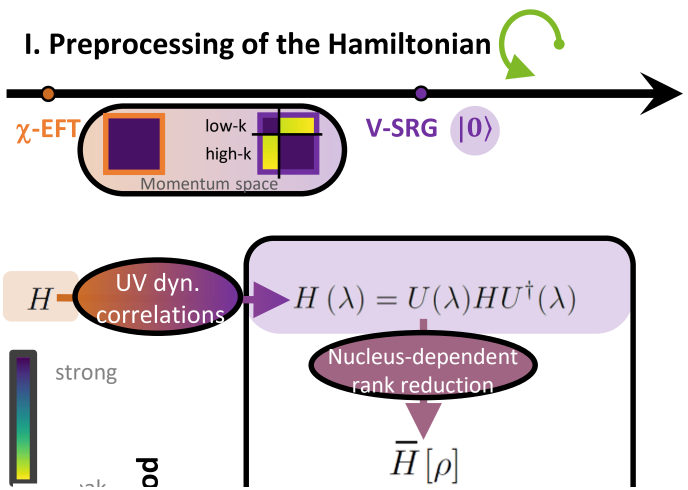
$|\Theta^\sigma_\mu\rangle = |\Phi^\sigma_\mu\rangle$

Need to include static correlations from the 0th order !

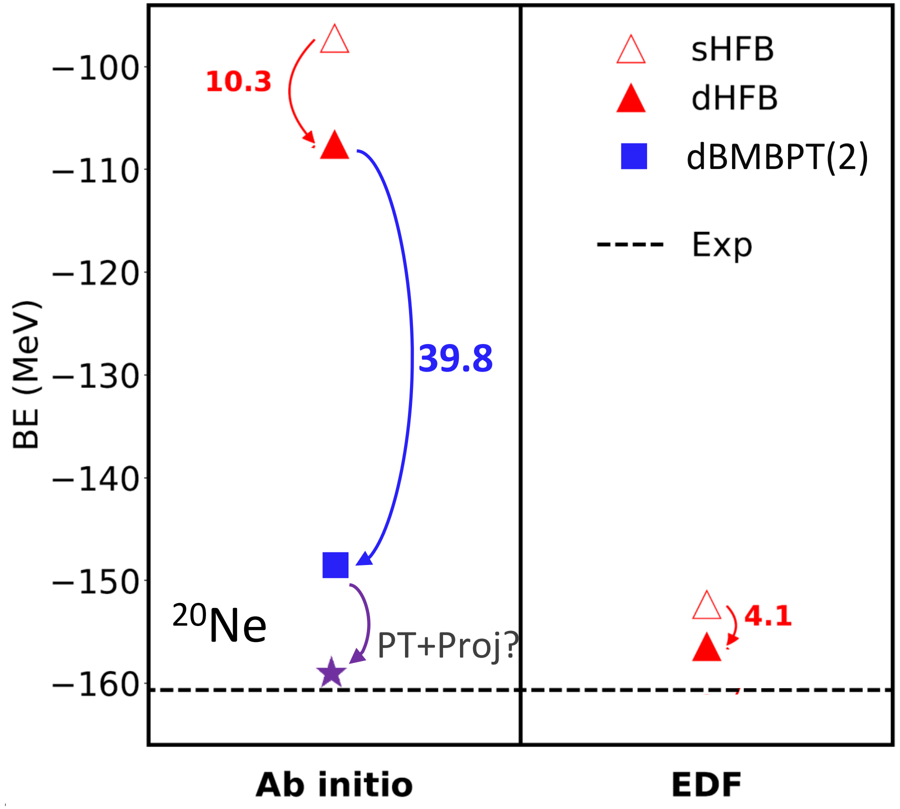
② Expansion scheme with hybrid cost

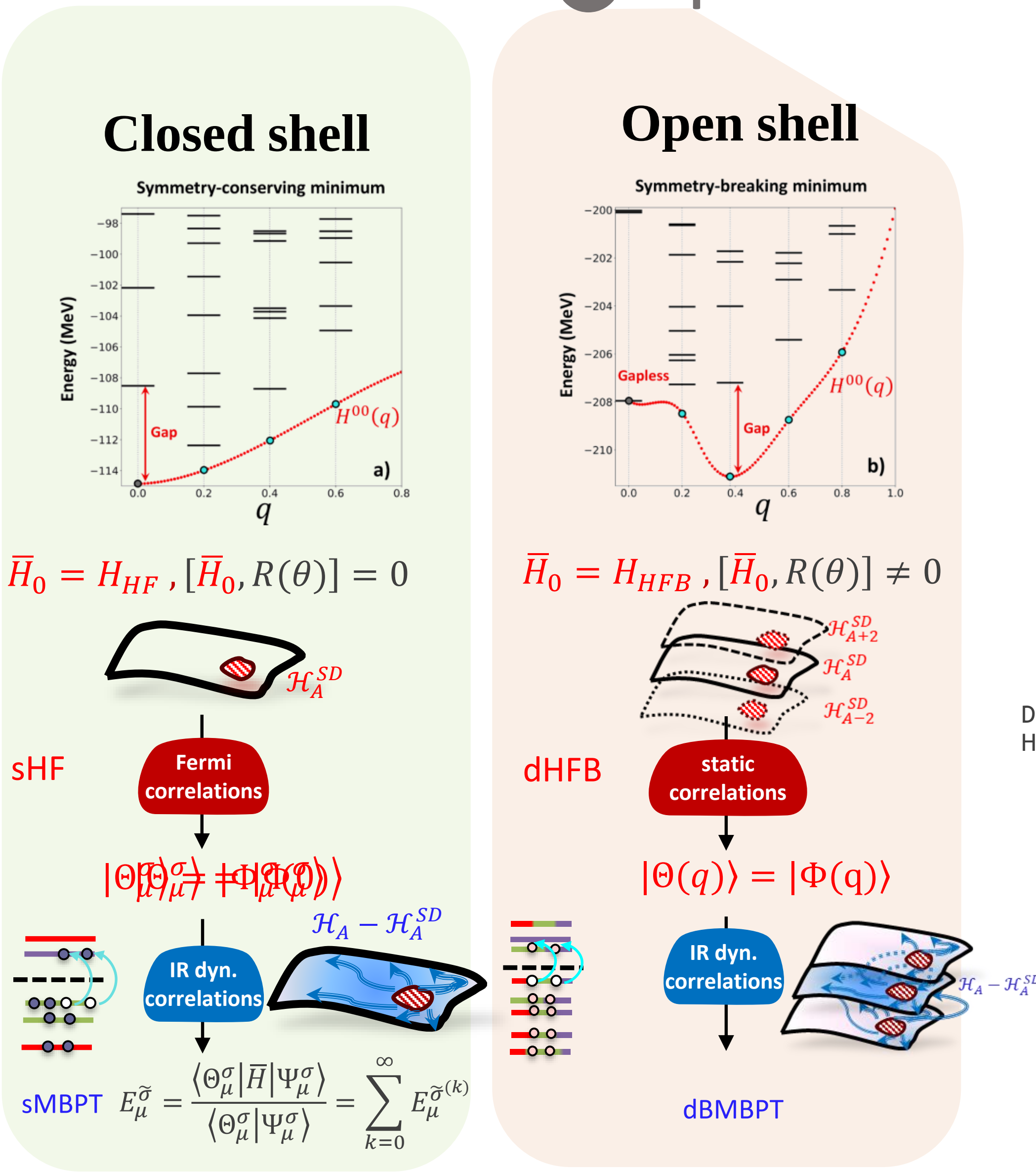


Tichai, Gebrerufael, Vobig, Roth, PLB (2018)



② Expansion scheme & SSB version 1





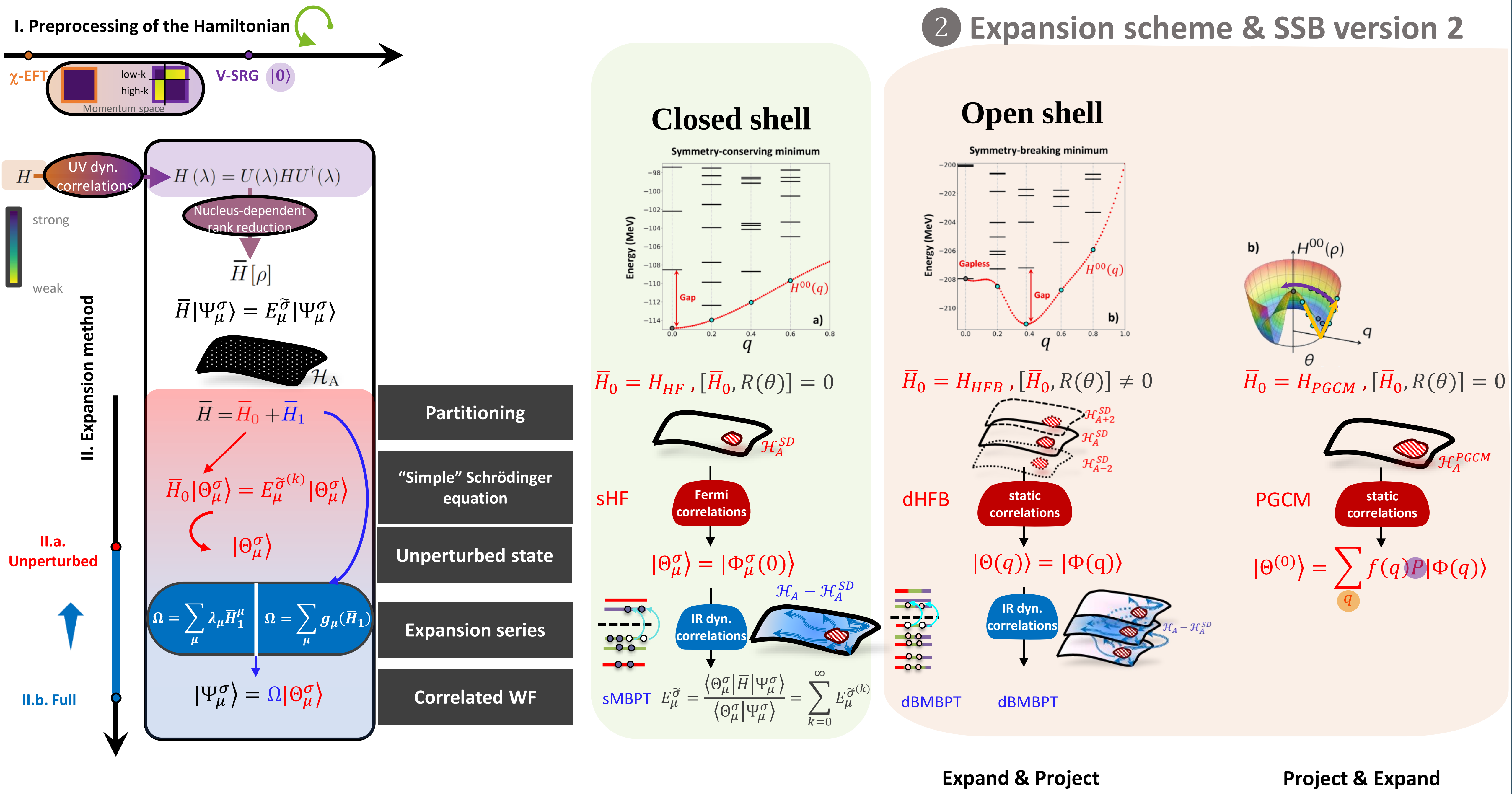
Need symmetry restoration !!

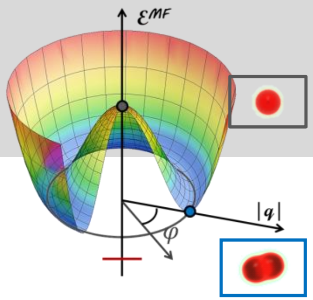
Duguet, Signoracci JPG (2017)
Hagen et al (2022)

Tichai, Arthuis, Duguet, Hergert, Somà, Roth PLB (2018)

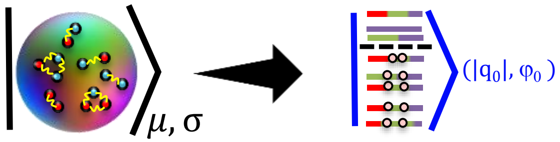
Expand & Project

2 Expansion scheme & SSB version 2





◈ dHFB treatment



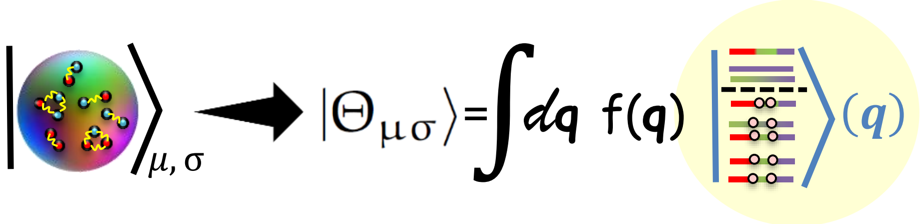
Correlated A-nucleon WF

Symmetry-breaking A independent quasinucleons WF

dHFB constrained calculations

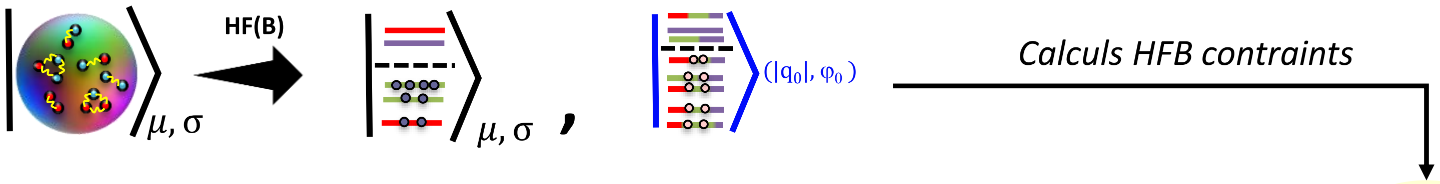
◈ Post-HFB treatment : PGCM

--> Symmetry-conserving (non orthogonal) mixture of symmetry-breaking HFB vacua



◉ Traitement HF(B)

--> Problème à *A* nucléons ⟶ *A* problèmes à 1 nucléon



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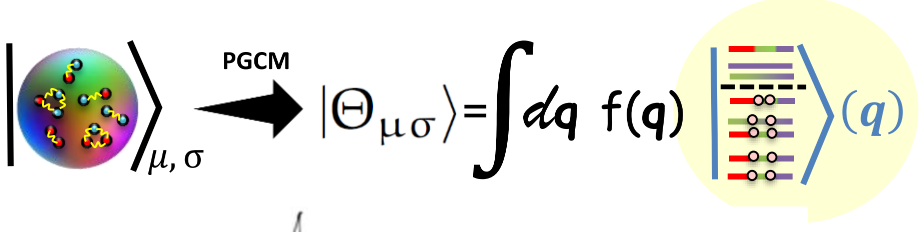

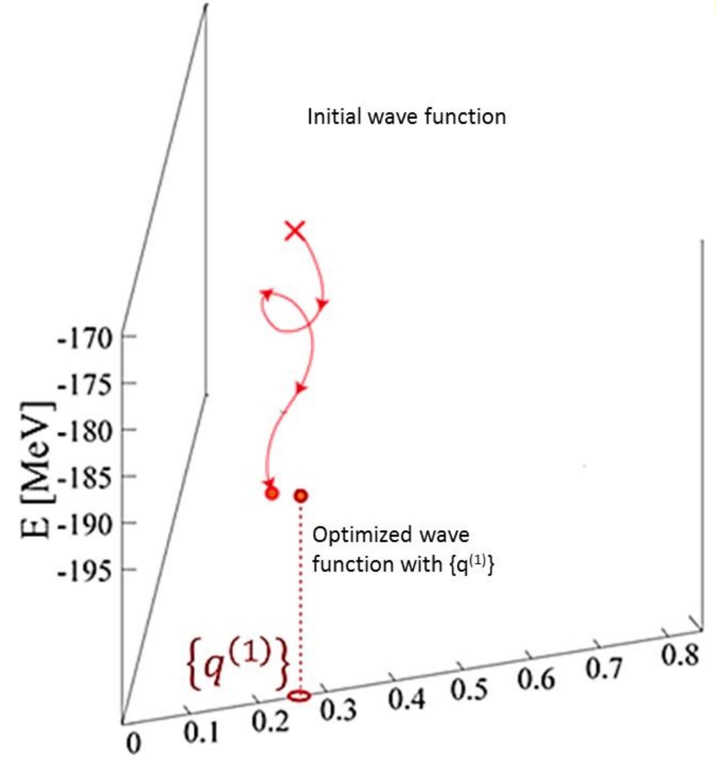

◉ Traitement HF(B)

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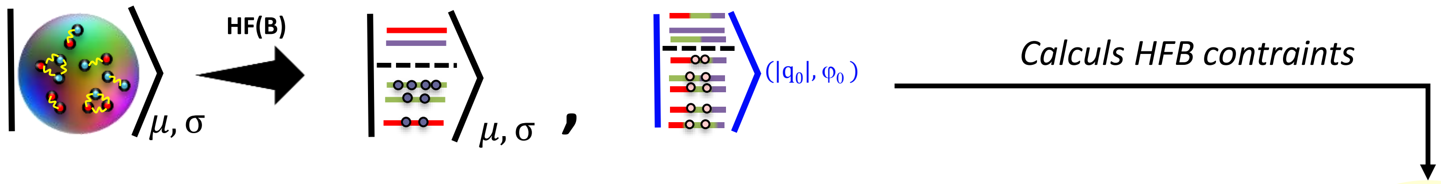
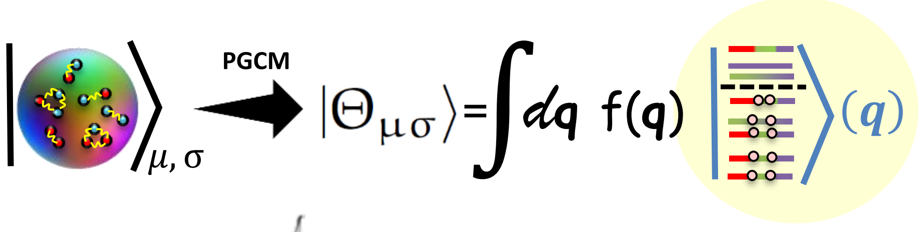
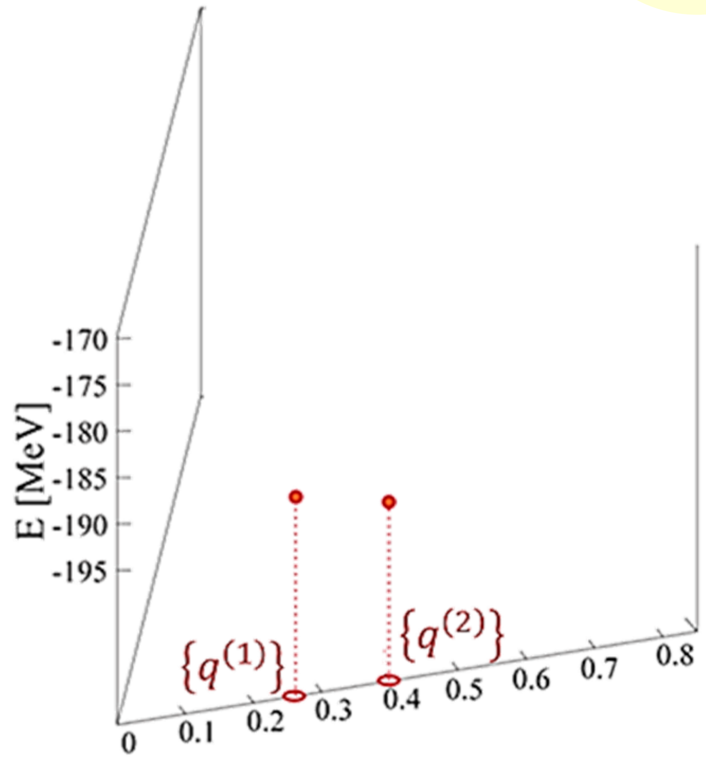


◈ Post-HFB treatment : PGCM

--> Symmetry-conserving (non orthogonal) mixture of symmetry-breaking HFB vacua





◉ Traitement HF(B)

--> Problème à *A* nucléons ⟶ *A* problèmes à 1 nucléon

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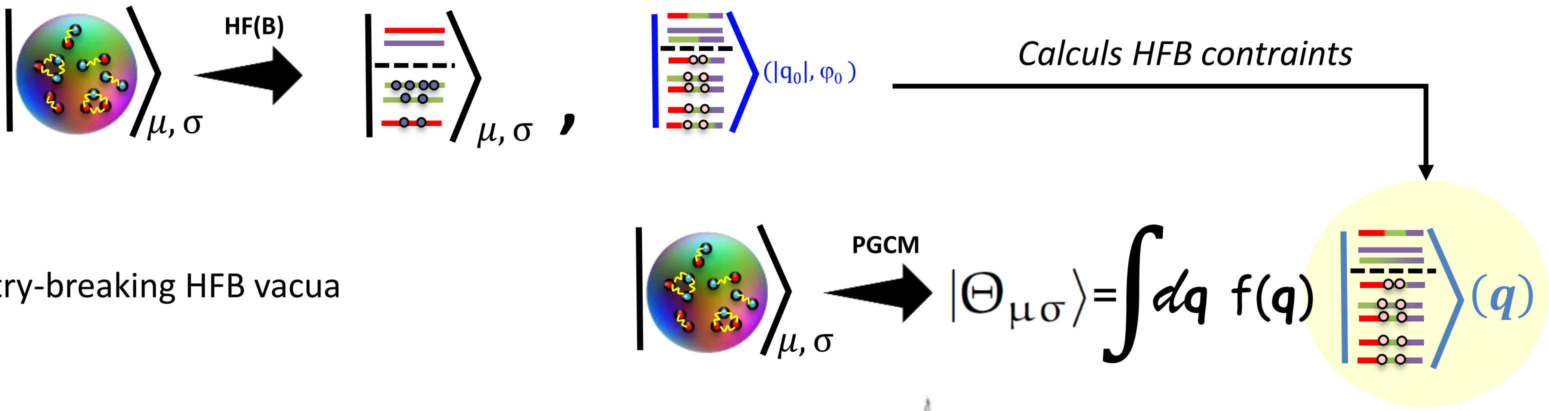
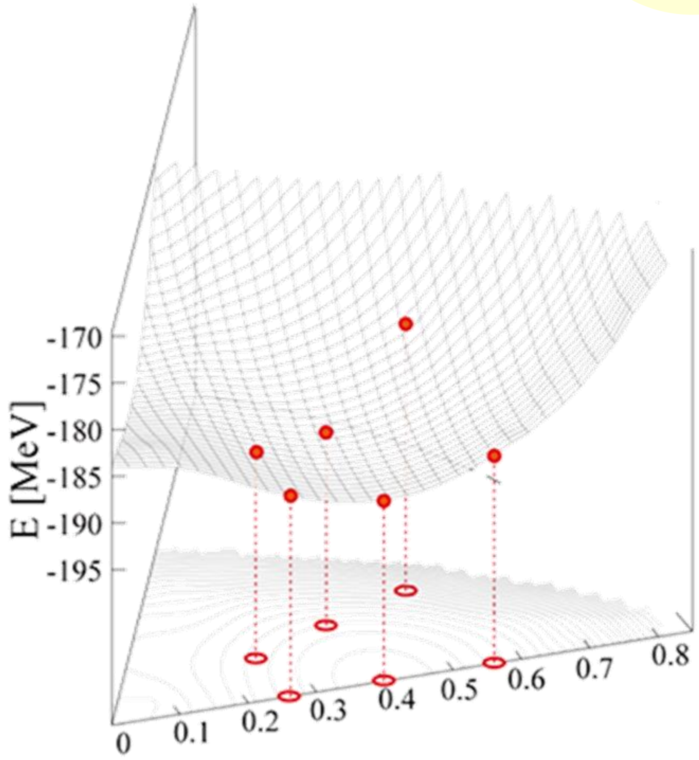
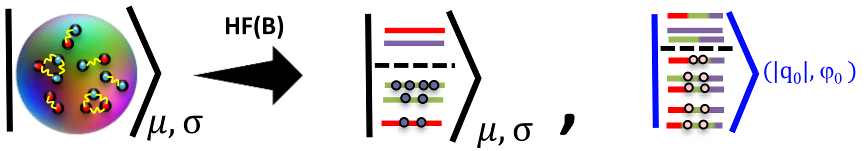




❸ Développements au niveau post-HFB : PGCM, généralités

◉ Traitement HF(B)

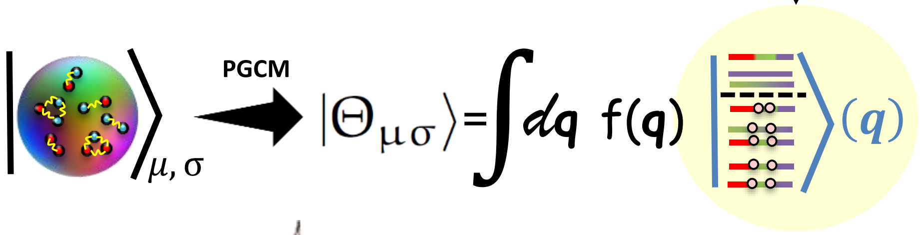
--> Problème à *A* nucléons ⟶ *A* problèmes à 1 nucléon

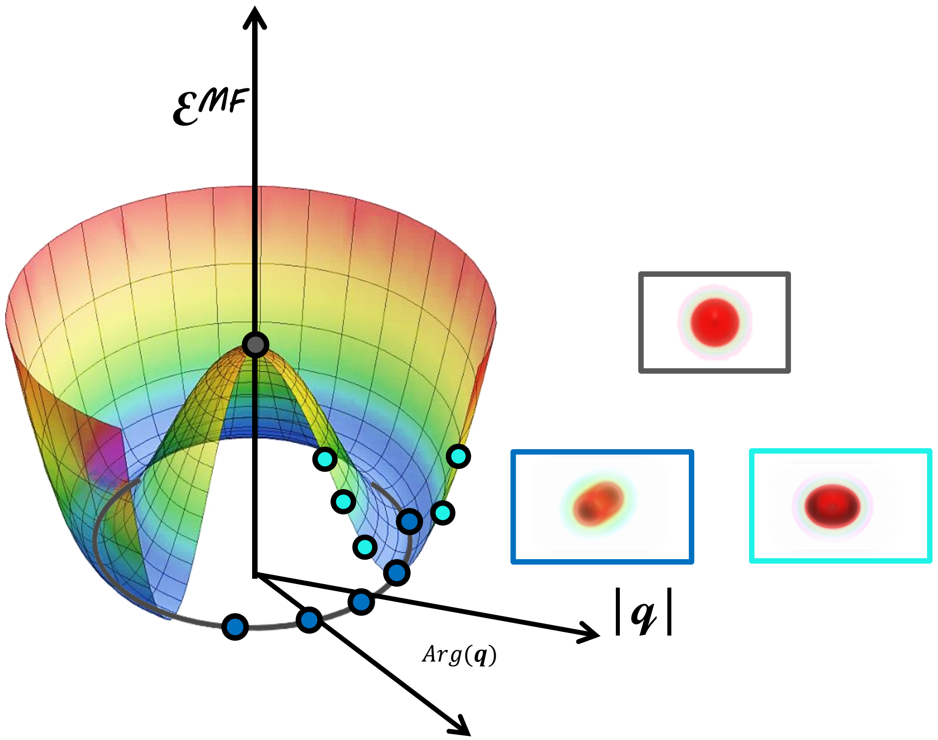


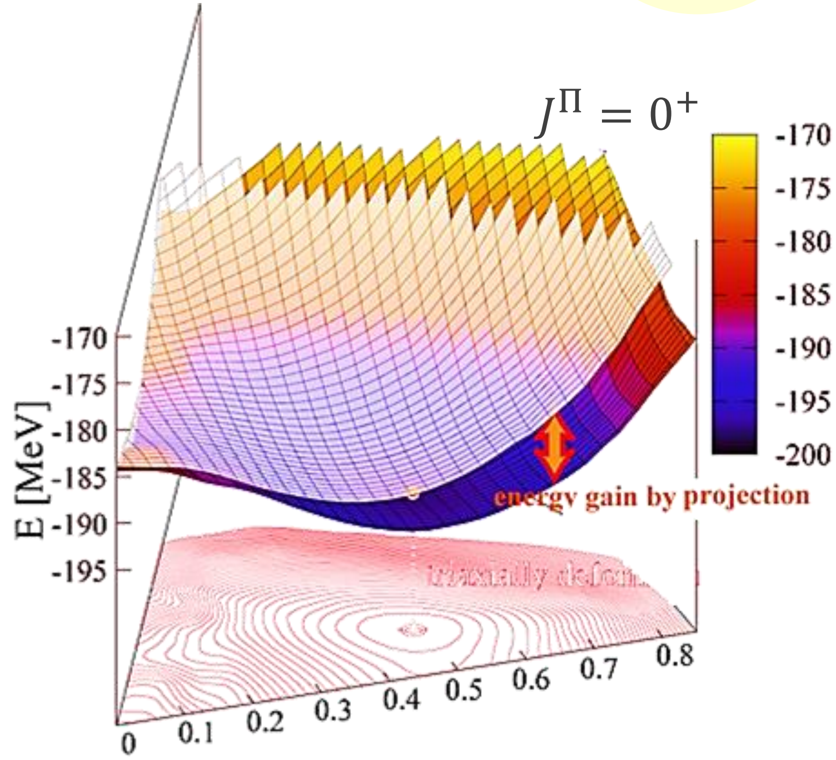
Calculs HFB contraints

◈ Post-HFB treatment : PGCM

--> Symmetry-conserving (non orthogonal) mixture of symmetry-breaking HFB vacua





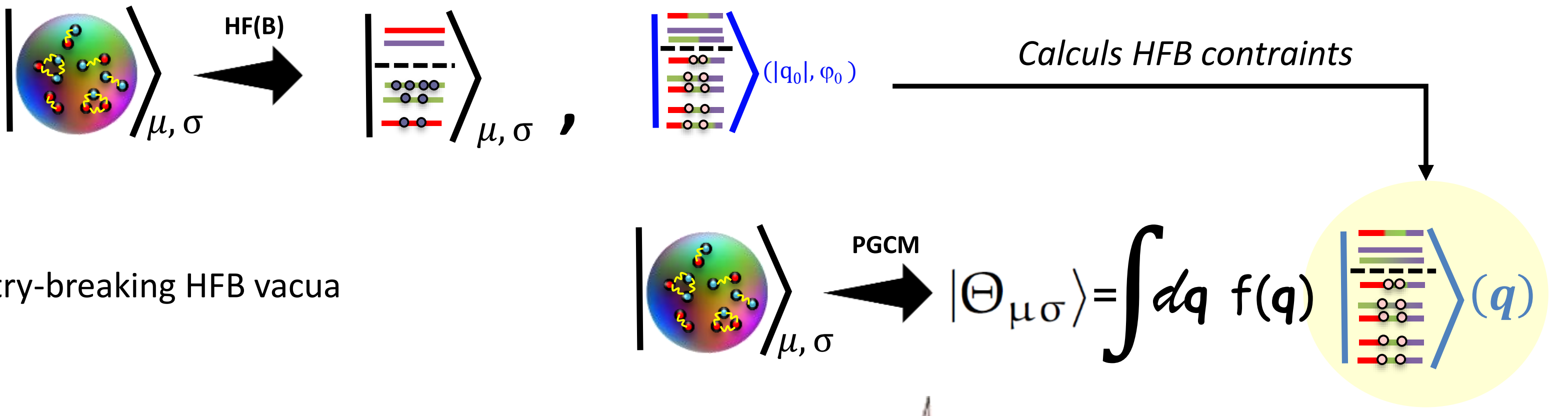


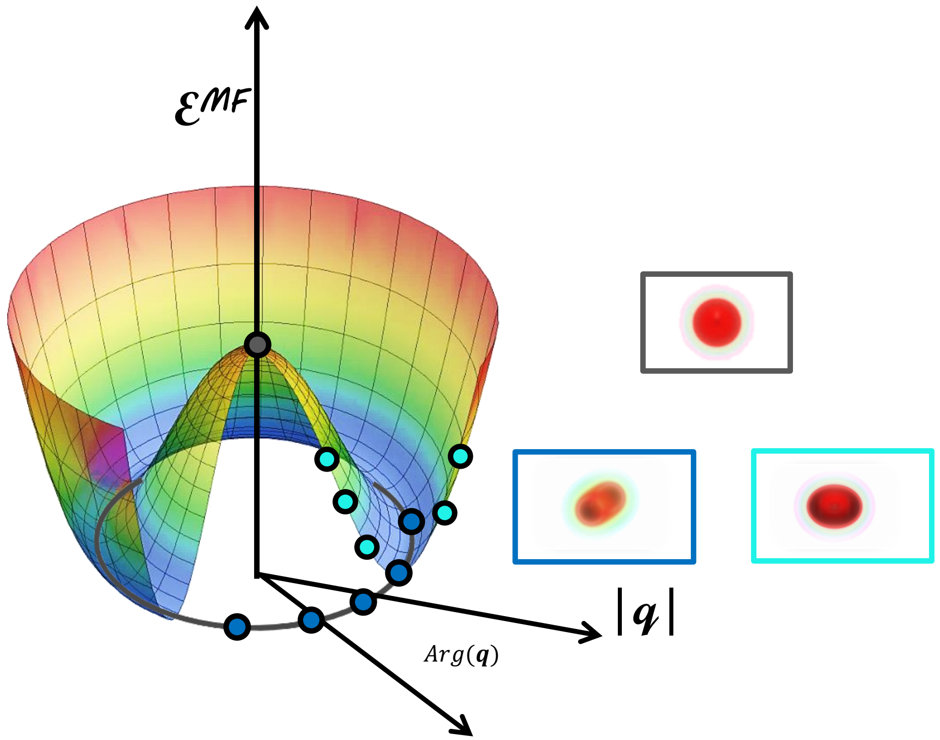
◉ Traitement HF(B)

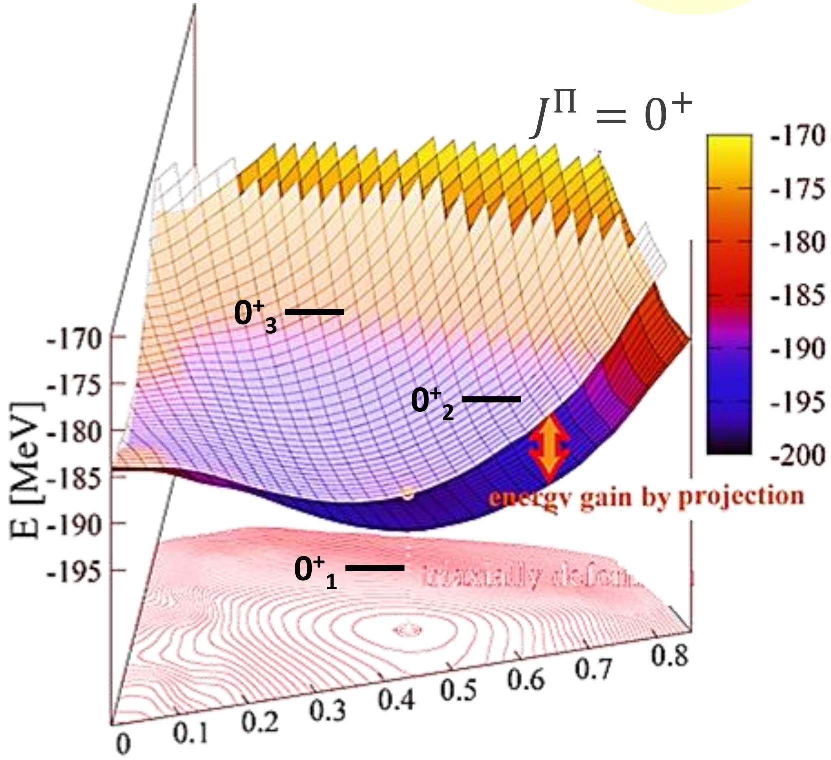
⇢ Problème à *A* nucléons ⟶ *A* problèmes à 1 nucléon

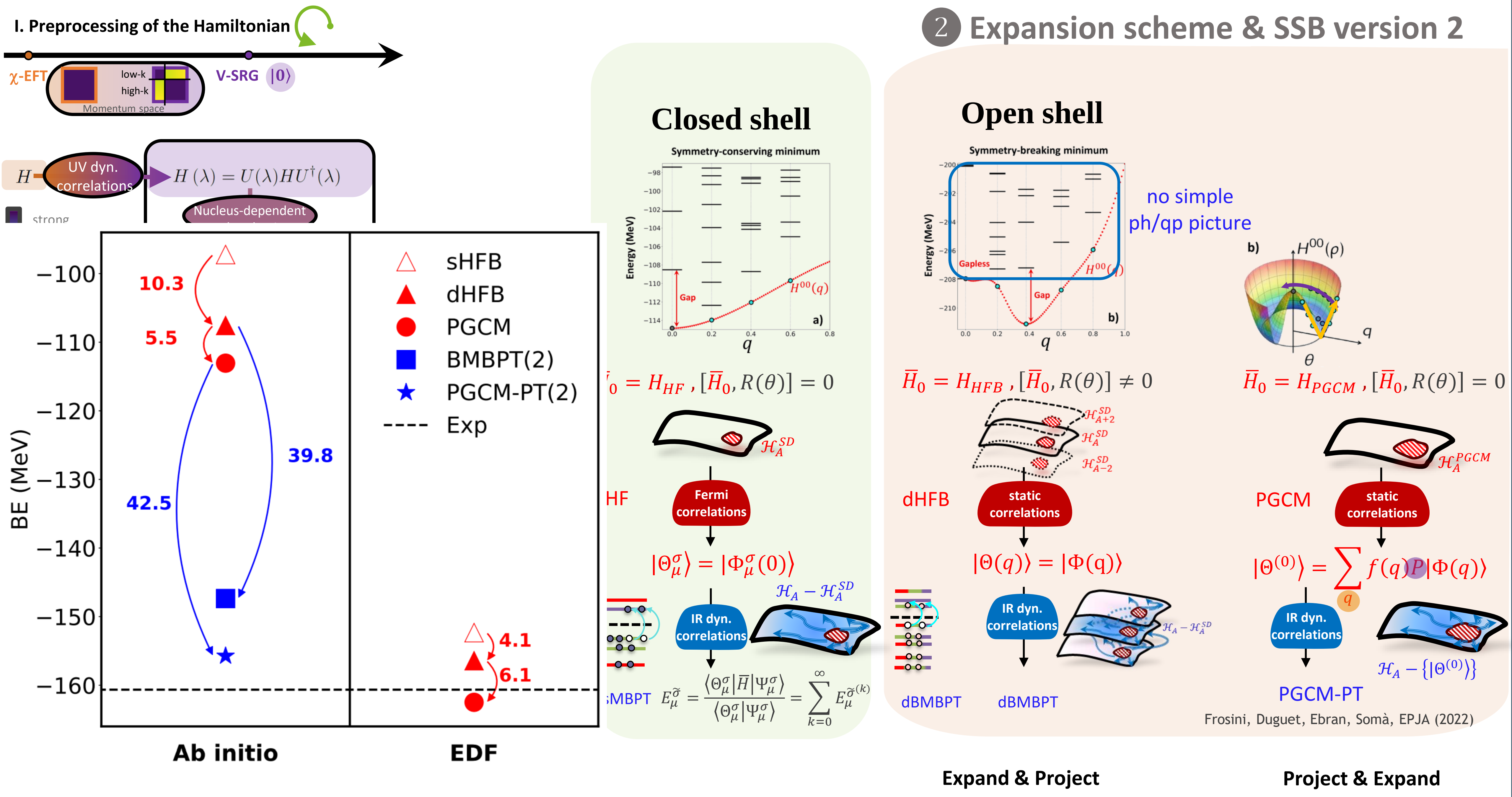
◈ Post-HFB treatment : PGCM

⇢ Symmetry-conserving (non orthogonal) mixture of symmetry-breaking HFB vacua









I. Preprocessing of the Hamiltonian
χ-EFT
low-k
high-k
Momentum space
V-SRG
|0⟩
H
UV dyn. correlations
H (λ) = U(λ)HU†(λ)
Nucleus-dependent
strong
2 Expansion scheme & SSB version 2
−100
−110
−120
−130
−140
−150
−160
BE (MeV)
10.3
5.5
39.8
42.5
4.1
6.1
sHFB
dHFB
PGCM
BMBPT(2)
PGCM-PT(2)
Exp
Ab initio
EDF
Closed shell
Symmetry-conserving minimum
Energy (MeV)
Gap
H00(q)
a)
q
H̄0 = HHF , [H̄0, R(θ)] = 0
HF
Fermi correlations
|Θ^σ_μ⟩ = |Φ^σ_μ(0)⟩
IR dyn. correlations
MBPT
Open shell
Symmetry-breaking minimum
Gapless
Gap
b)
no simple ph/qp picture
H00(ρ)
q
θ
H̄0 = HHFB , [H̄0, R(θ)] ≠ 0
H̄0 = HPGCM , [H̄0, R(θ)] = 0
dHFB
static correlations
|Θ(q)⟩ = |Φ(q)⟩
IR dyn. correlations
dBMBPT
dBMBPT
PGCM
static correlations
|Θ(0)⟩ = ∑ f(q)P|Φ(q)⟩
IR dyn. correlations
PGCM-PT
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Expand & Project
Project & Expand

❶ Context

Theoretical description of nuclear systems

❷ PGCM

How to best account for nucleons correlations

❸ Application

③ Application of PGCM-PT

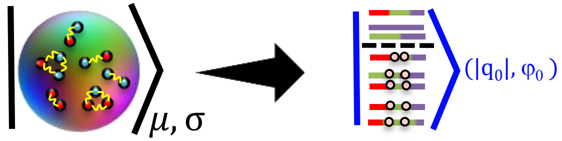
$$h^{q}_{ac} \equiv \sum_{bd} V^{(a)}_{abcd}\rho^{q}_{db}$$

$$\Delta^{q}_{ac} \equiv \sum_{bd} V^{(a)}_{acbd}\kappa^{q}_{bd}$$

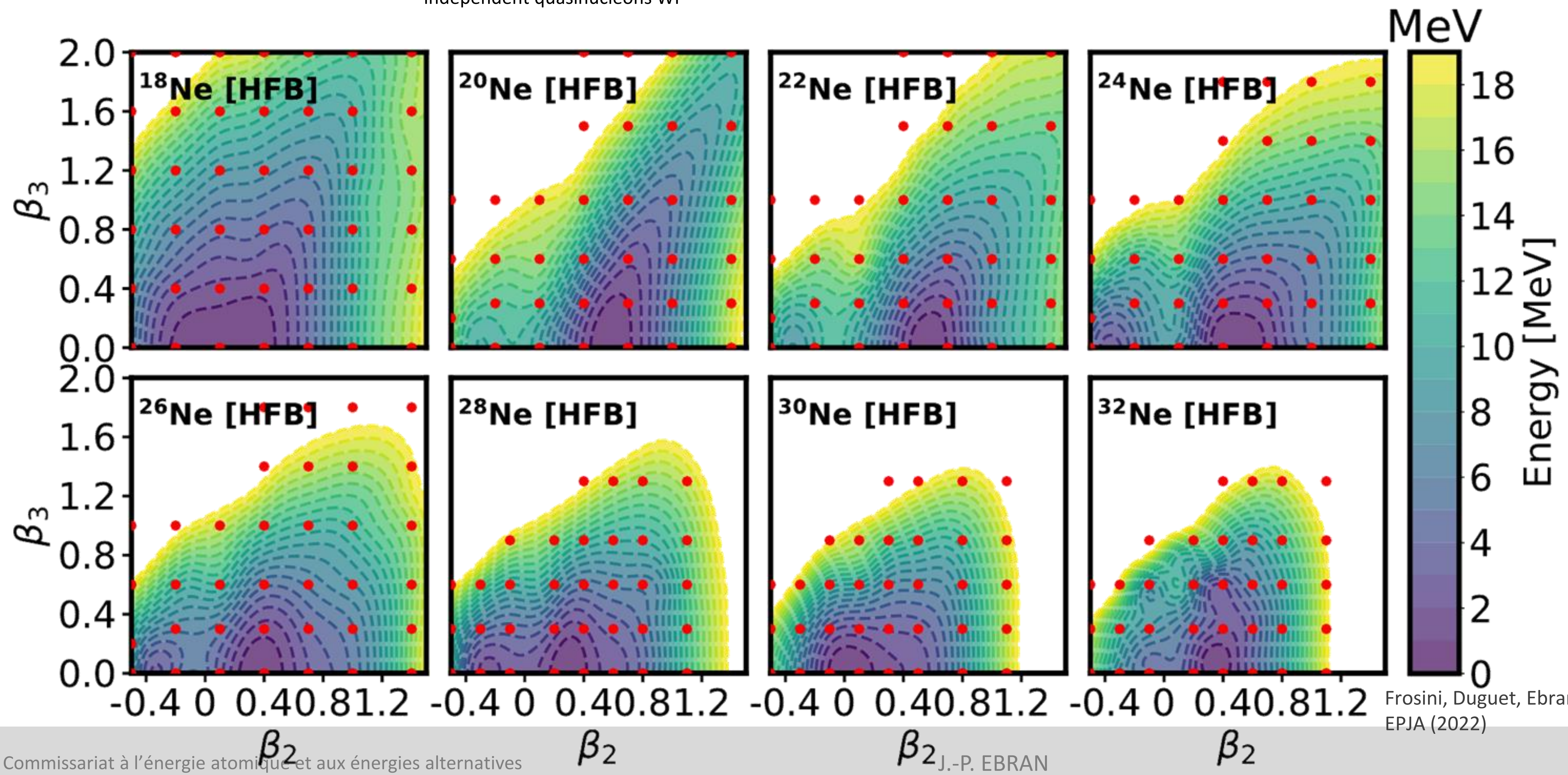
$$\rho^{q}_{ij} = \langle \Phi(\mathbf{q}) | c^{\dagger}_{j} c_{i} | \Phi(\mathbf{q}) \rangle$$

$$\kappa^{q}_{ij} = \langle \Phi(\mathbf{q}) | c_{j} c_{i} | \Phi(\boldsymbol{q}) \rangle$$

◈ dHFB treatment



$$\begin{pmatrix} h^{q} - \lambda^{q} & \Delta^{q} \\ -\Delta^{q*} & -h^{q*} + \lambda^{q} \end{pmatrix} \begin{pmatrix} U^{q} \\ V^{q} \end{pmatrix}_{\mu} = E^{q}_{\mu} \begin{pmatrix} U^{q} \\ V^{q} \end{pmatrix}_{\mu}$$



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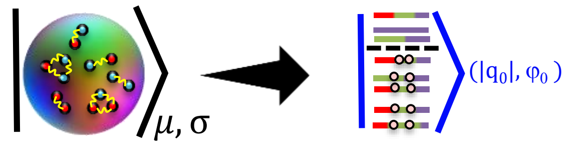
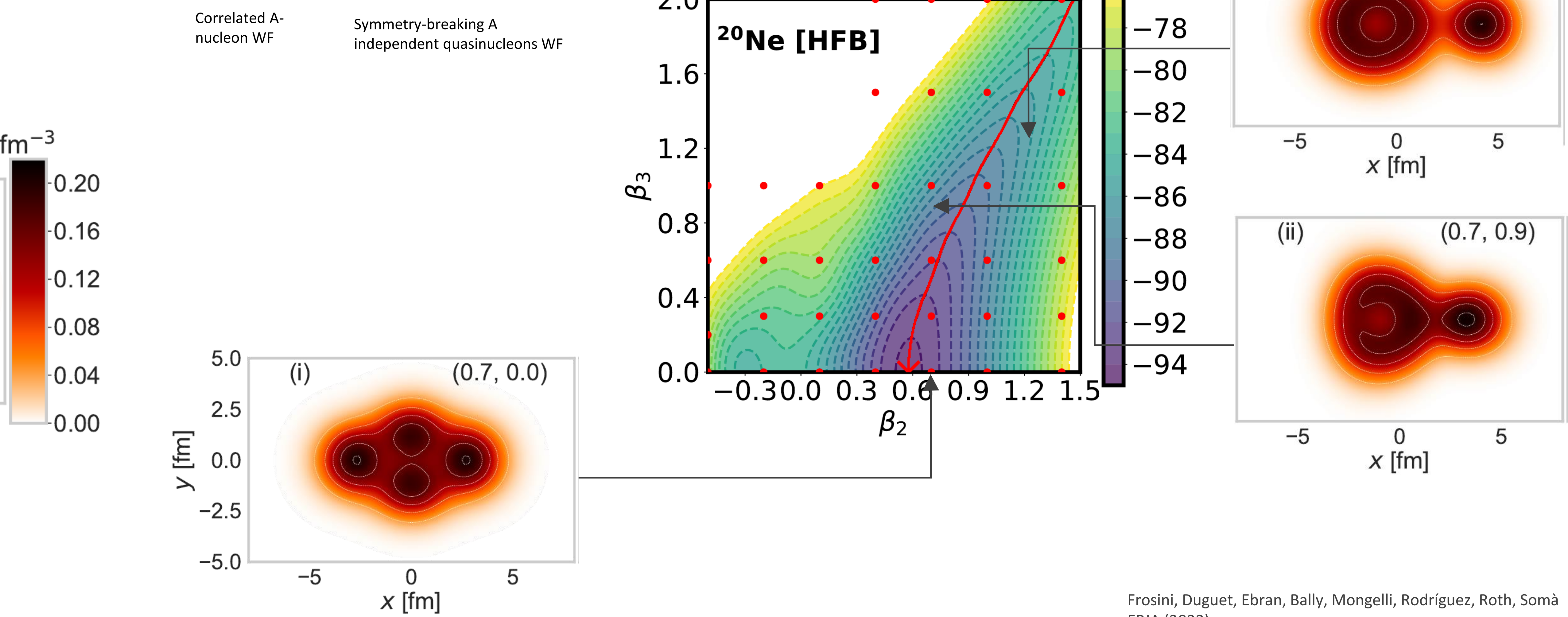
◈ dHFB treatment





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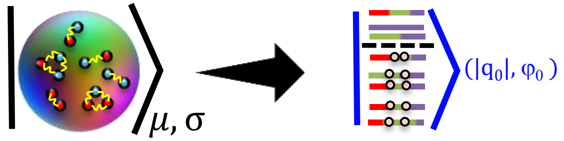
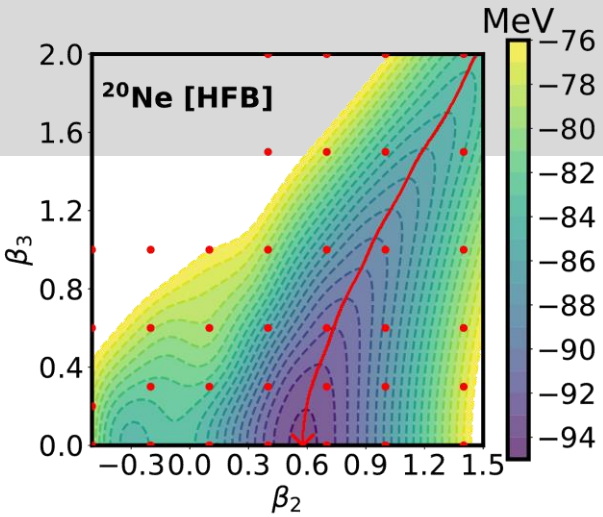
◈ dHFB treatment



Correlated A-nucleon WF

Symmetry-breaking A independent quasinucleons WF



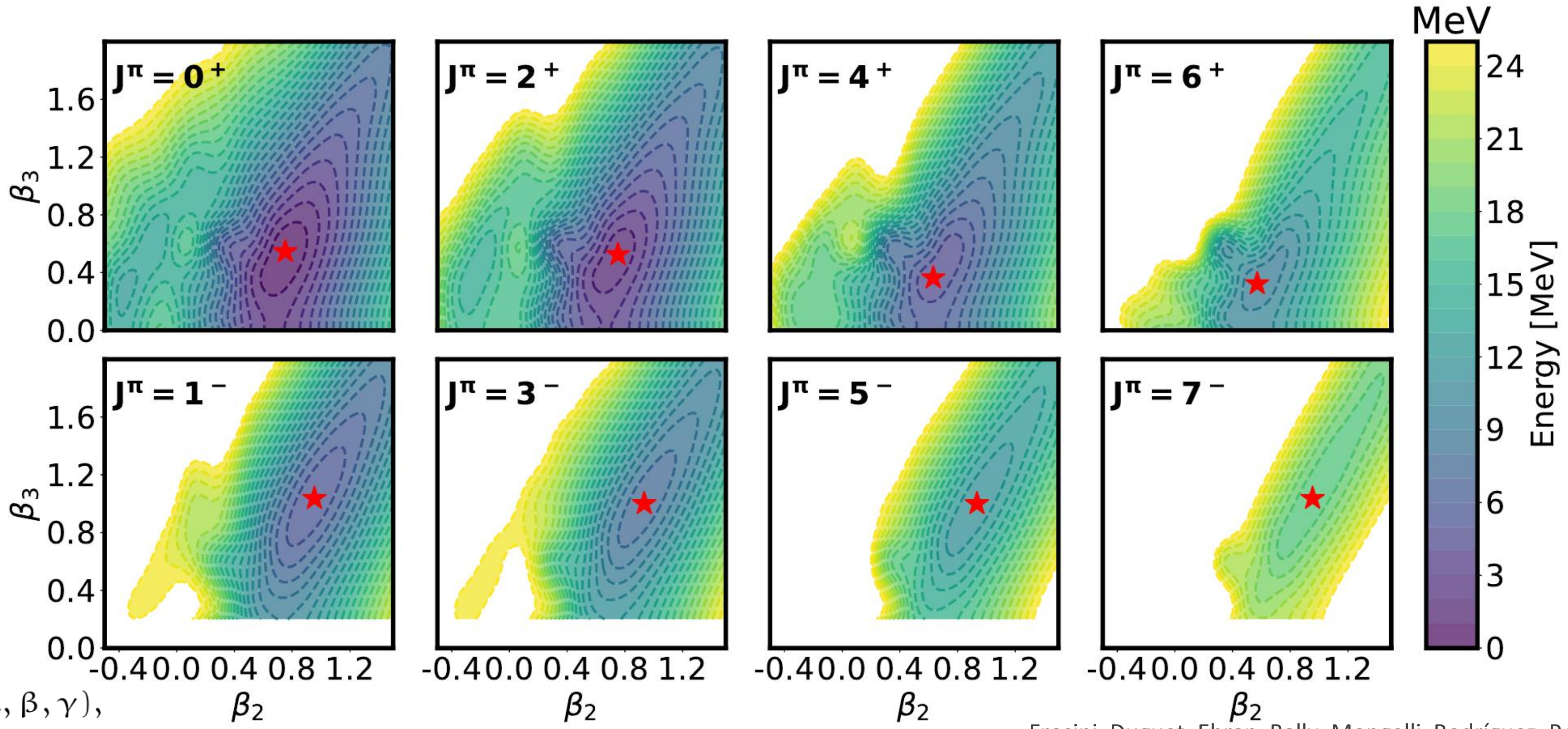
◈ Projection on good quantum numbers N,Z,J,π

$$|\Theta_{\mu\sigma}\rangle = \sum_{q}\sum_{K} f^{\tilde{\sigma}}_{\mu K}(\mathbf{q}) P^{\tilde{\sigma}}_{MK}(\mathbf{q})\,|\Phi(\mathbf{q})\rangle$$

$$P^{\tilde{\sigma}}_{MK} = P^{J}_{MK} P^{N_0} P^{Z_0}$$

$$P^{X_0} = \frac{1}{2\pi}\int_0^{2\pi} d\phi\, e^{-i\phi(X-X_0)}$$

$$P^{J}_{MK} = \frac{2J+1}{16\pi^2}\int_0^{2\pi} d\alpha \int_0^{\pi} d\beta \sin(\beta) \int_0^{4\pi} d\gamma D^{J*}_{MK}(\alpha,\beta,\gamma) R(\alpha,\beta,\gamma),$$



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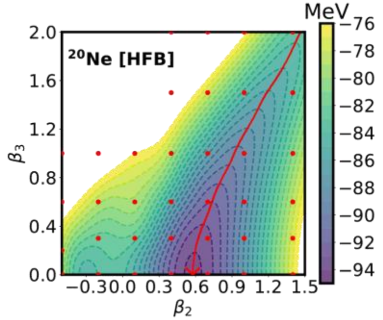
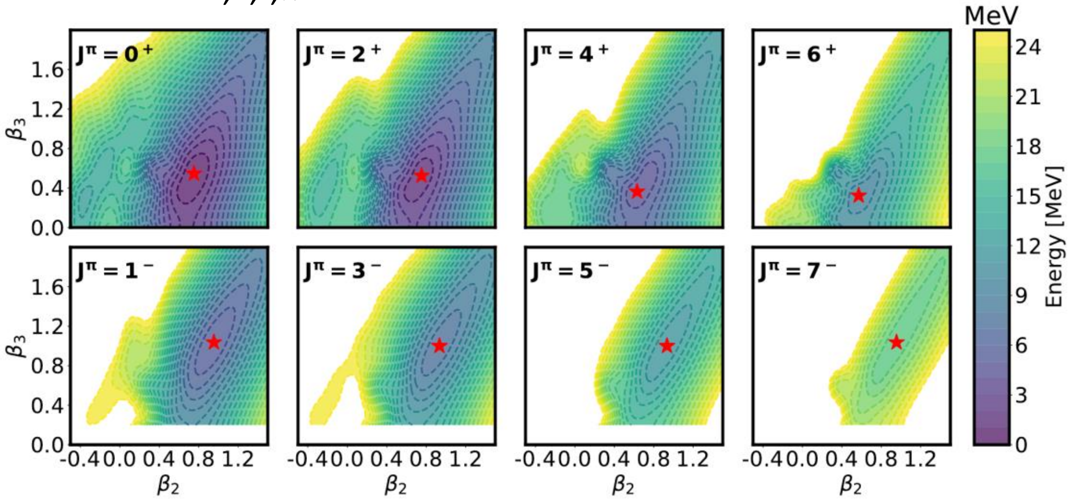
3 Application of PGCM-PT

◈ dHFB treatment



◈ Projection on good quantum numbers N,Z,J,π



◈ PGCM treatment $|\Theta_{\mu\sigma}\rangle = \sum_{\mathbf{q}} \sum_{K} f^{\tilde{\sigma}}_{\mu K}(\mathbf{q}) P^{\tilde{\sigma}}_{MK}(\mathbf{q}) \, |\Phi(\mathbf{q})\rangle$

$$\sum_{\mathbf{q}'K'} \left[\mathcal{H}^{JN_0Z_0}_{\mathbf{q}K\mathbf{q}'K'} - E_{\mu;JN_0Z_0} \mathcal{N}^{JN_0Z_0}_{\mathbf{q}K\mathbf{q}'K'} \right] f^{JN_0Z_0}_{\mu\mathbf{q}'K'} = 0.$$

$$\mathcal{T}^{\lambda\mu;JN_0Z_0}_{\mathbf{q}K\mathbf{q}'K'} = \frac{1}{2\pi}\int_0^{2\pi} d\varphi_N e^{i\varphi_N N_0} \frac{1}{2\pi}\int_0^{2\pi} d\varphi_Z e^{i\varphi_Z Z_0}$$
$$\frac{2J+1}{16\pi^2}\int_0^{4\pi} d\alpha \int_0^{\pi} d\beta \sin(\beta) \int_0^{2\pi} d\gamma D^{J*}_{KK'}(\alpha,\beta,\gamma) \mathcal{T}^{\lambda\mu}_{\varphi_N\varphi_Z\alpha\beta\gamma\mathbf{q}\mathbf{q}'},$$

$$\mathcal{T}^{\lambda\mu}_{\theta\mathbf{q}\mathbf{q}'} = \langle \Phi(\mathbf{q}) | T^{\lambda\mu} R(\theta) | \Phi(\mathbf{q}') \rangle$$

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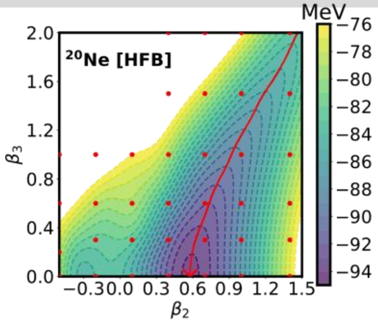
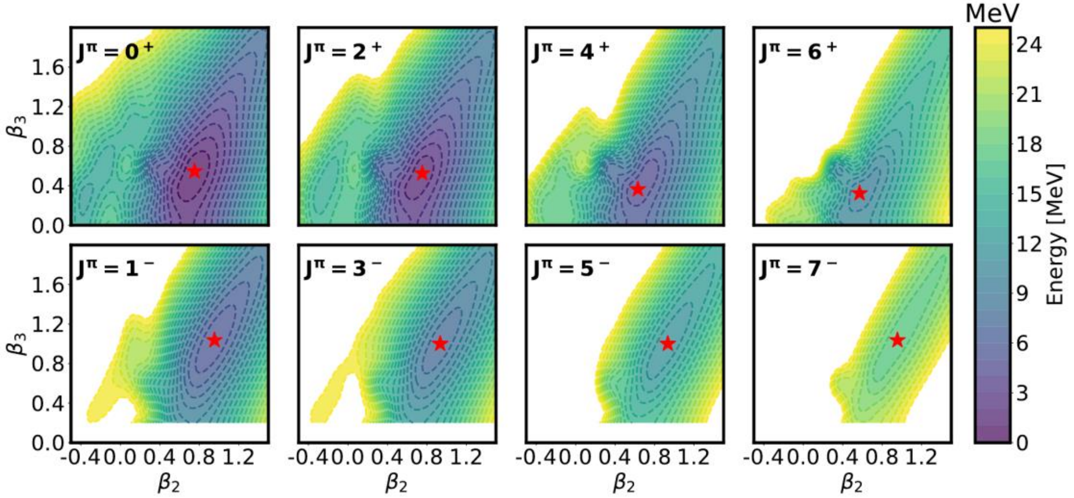
③ Application of PGCM-PT

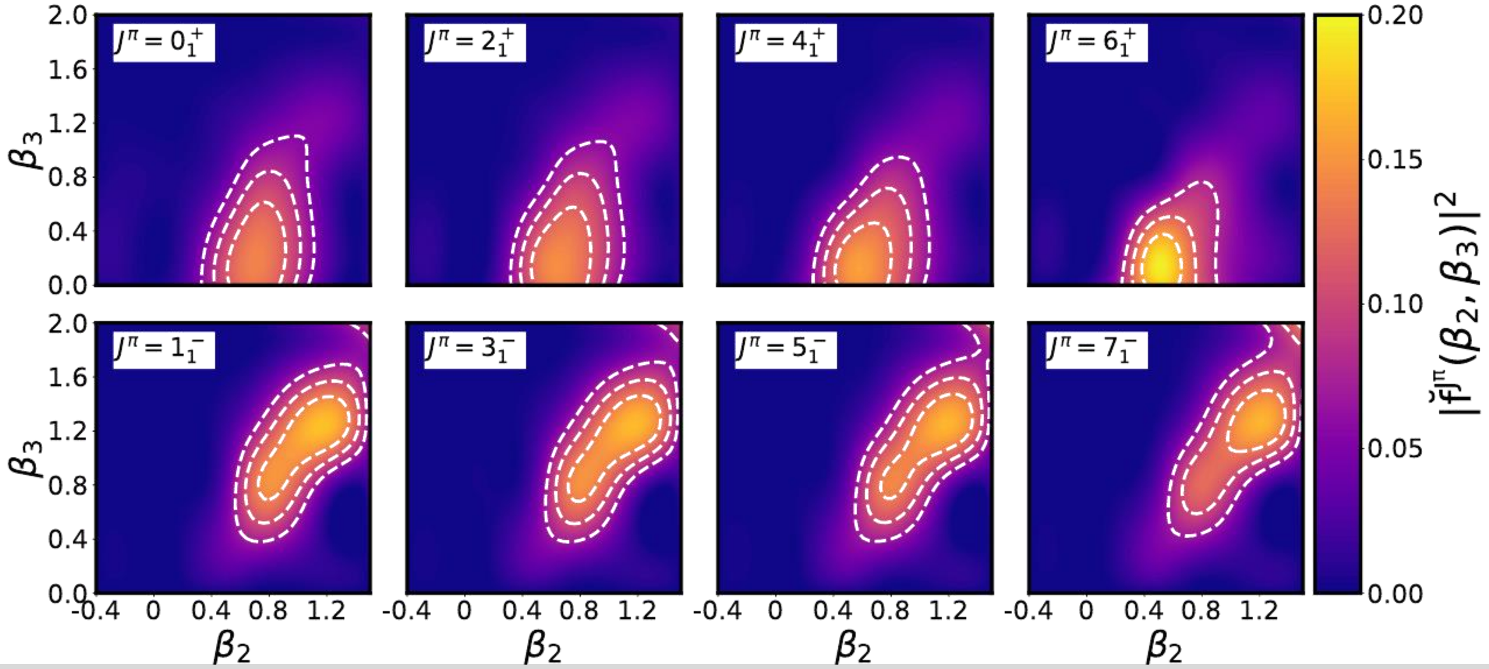
◈ dHFB treatment



◈ Projection on good quantum numbers N,Z,J,π



◈ PGCM treatment $|\Theta_{\mu\sigma}\rangle = \sum_{q} \sum_{K} f^{\tilde{\sigma}}_{\mu K}(\mathbf{q}) P^{\tilde{\sigma}}_{MK}(\mathbf{q})\, |\Phi(\mathbf{q})\rangle$



$$\sum_{q'K'} \left[\mathcal{H}^{JN_0Z_0}_{qKq'K'} - E_{\mu;JN_0Z_0} \mathcal{N}^{JN_0Z_0}_{qKq'K'} \right] f^{JN_0Z_0}_{\mu q'K'} = 0.$$

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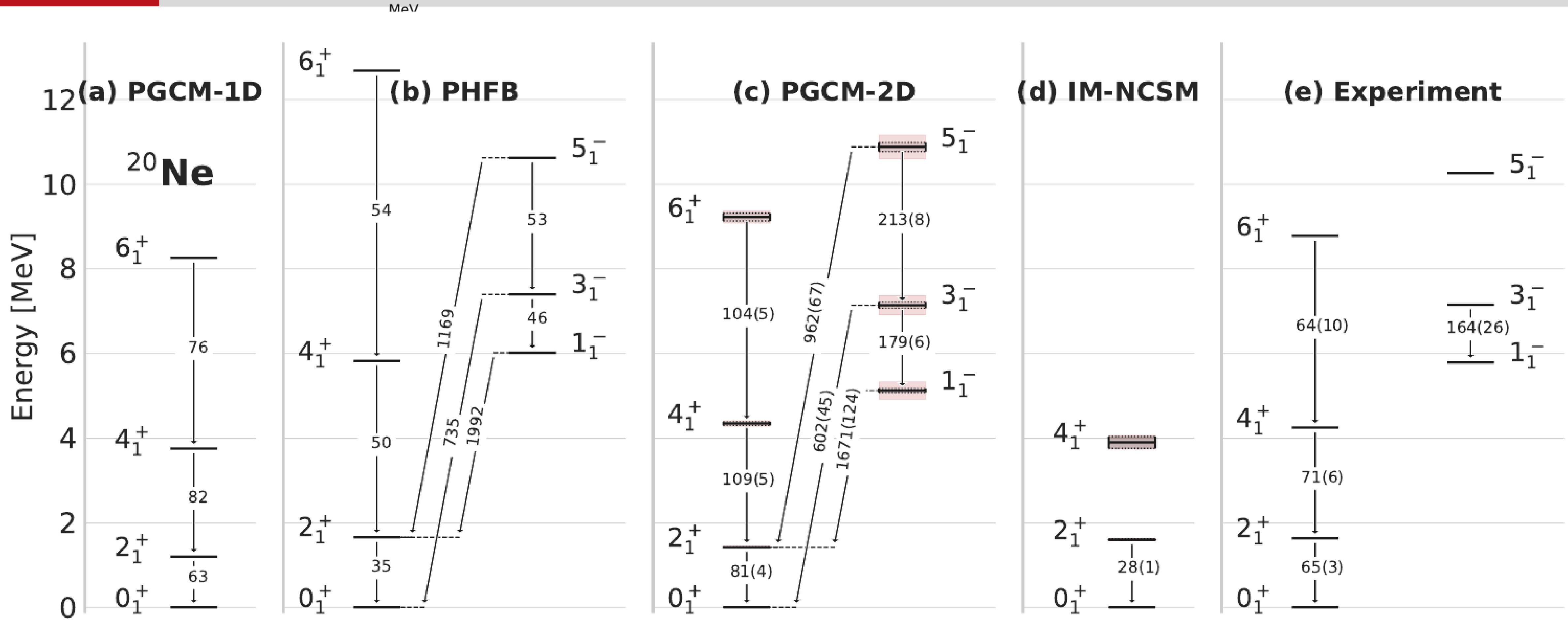

$$\sum_{q'K'} \left[\mathcal{H}^{JN_0Z_0}_{qKq'K'} - E_{\mu;JN_0Z_0} \mathcal{N}^{JN_0Z_0}_{qKq'K'} \right] f^{JN_0Z_0}_{\mu q'K'} = 0.$$

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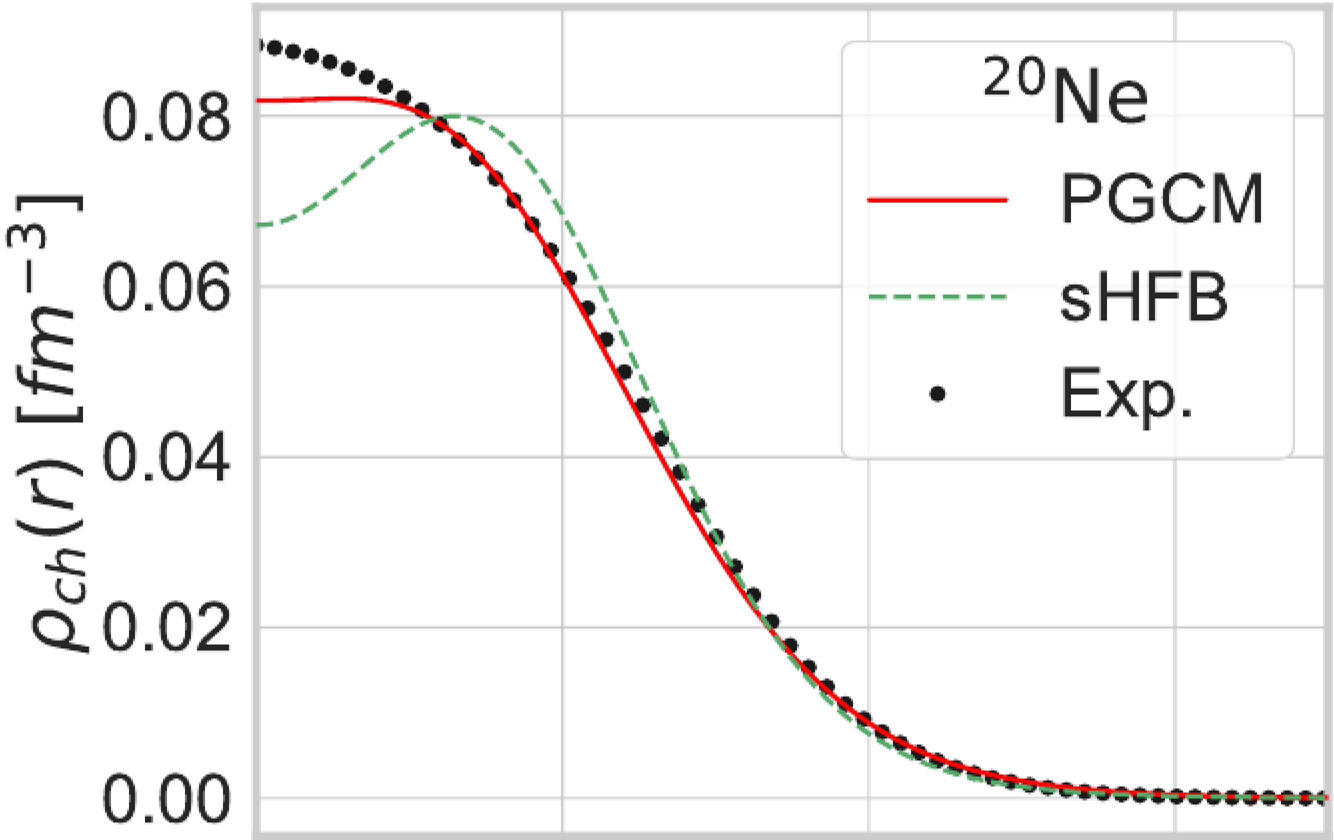

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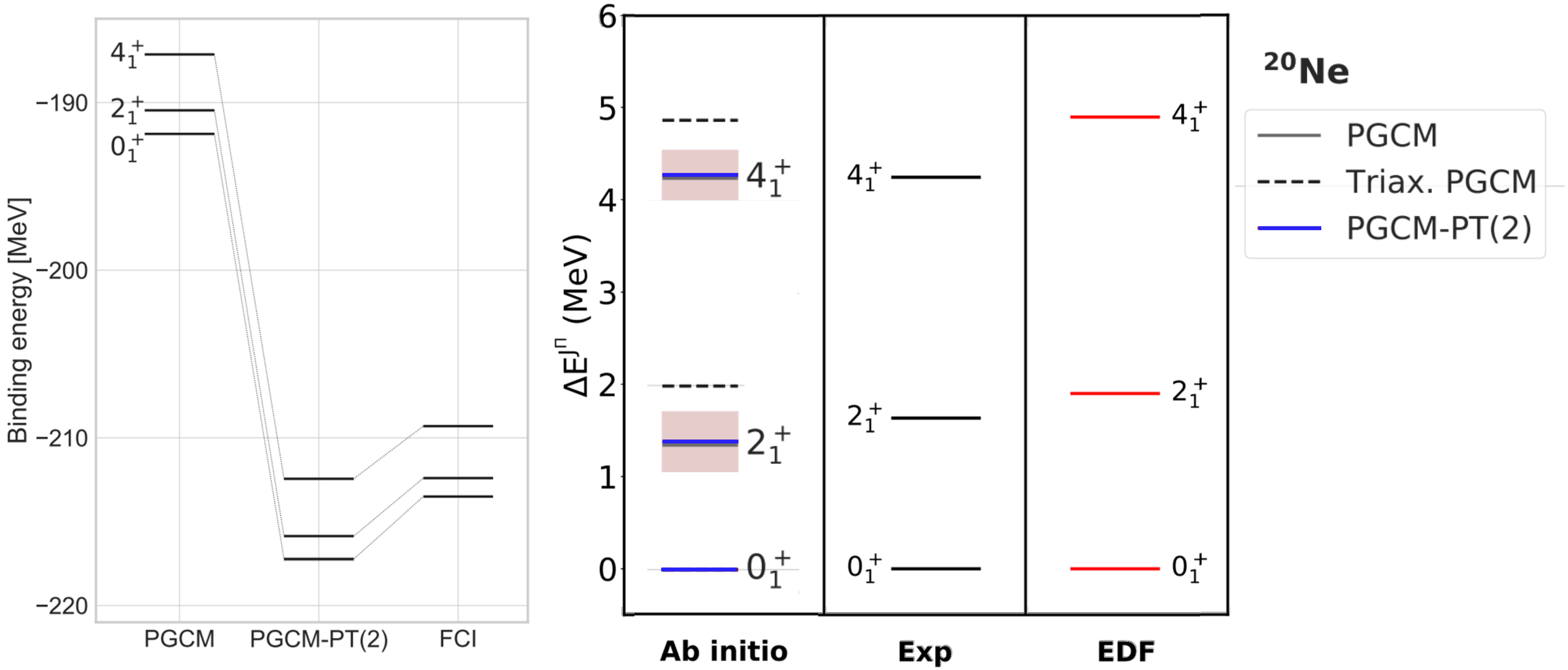
- PGCM : relevant ab initio tool for spectroscopy

- PGCM-PT : eventually needed for absolute energies + accuracy



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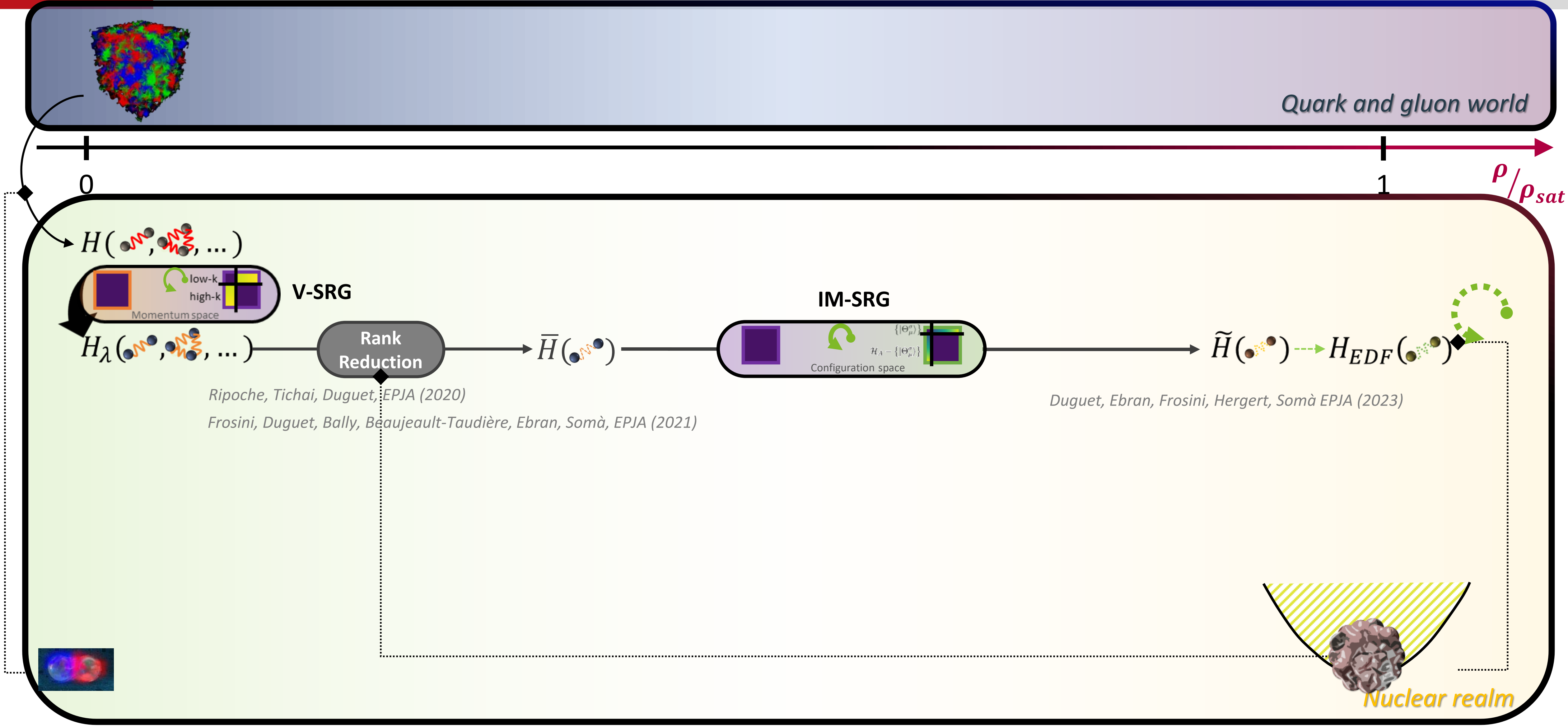
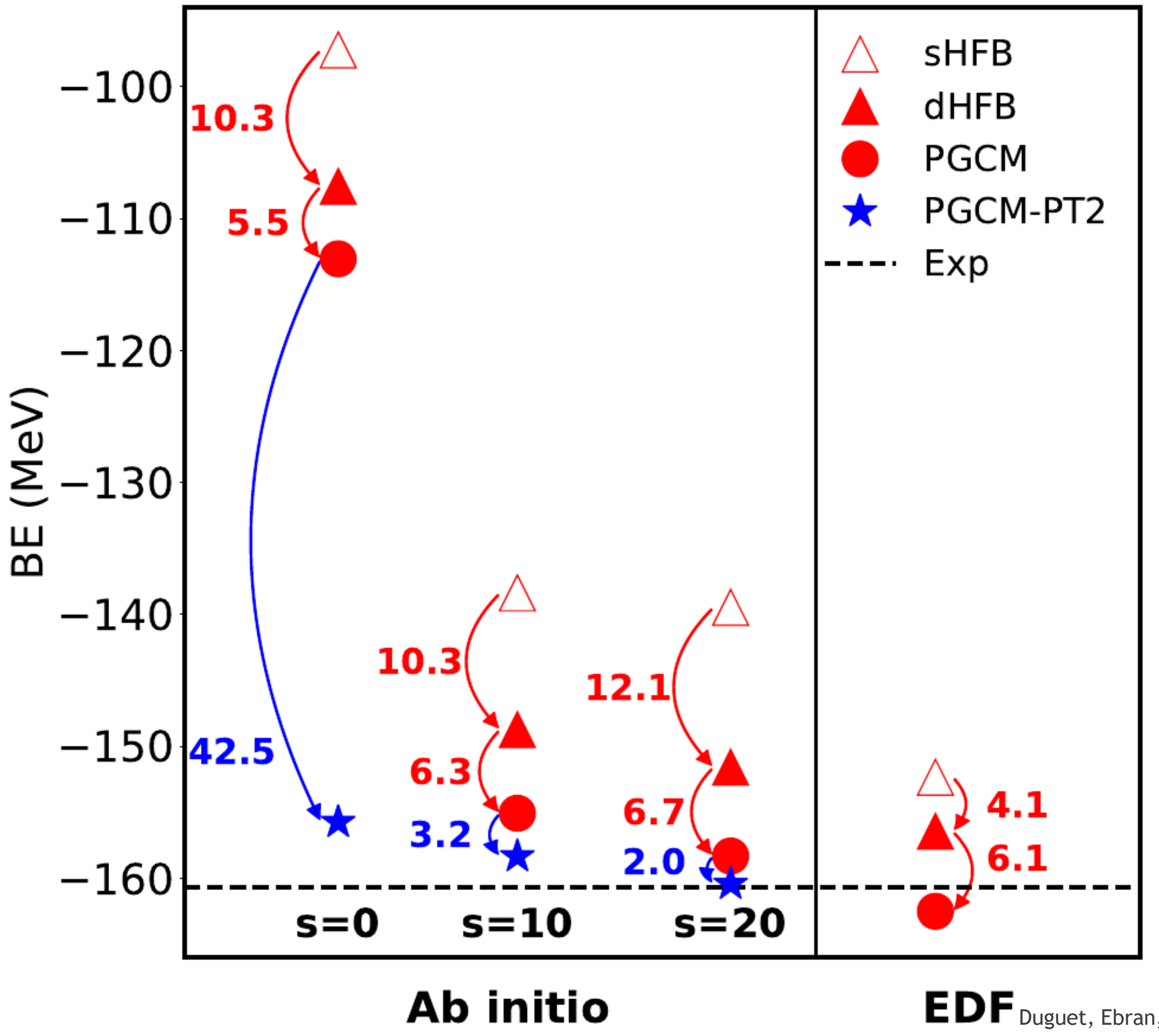

Quark and gluon world
0
1
ρ/ρsat
H(, , ...)
low-k
high-k
Momentum space
V-SRG
Hλ(, , ...)
Rank Reduction
H̄( )
IM-SRG
Configuration space
H̃( )
HEDF( )
Ripoche, Tichai, Duguet, EPJA (2020)
Frosini, Duguet, Bally, Beaujeault-Taudière, Ebran, Somà, EPJA (2021)
Duguet, Ebran, Frosini, Hergert, Somà EPJA (2023)
Nuclear realm

③ Application of PGCM-PT



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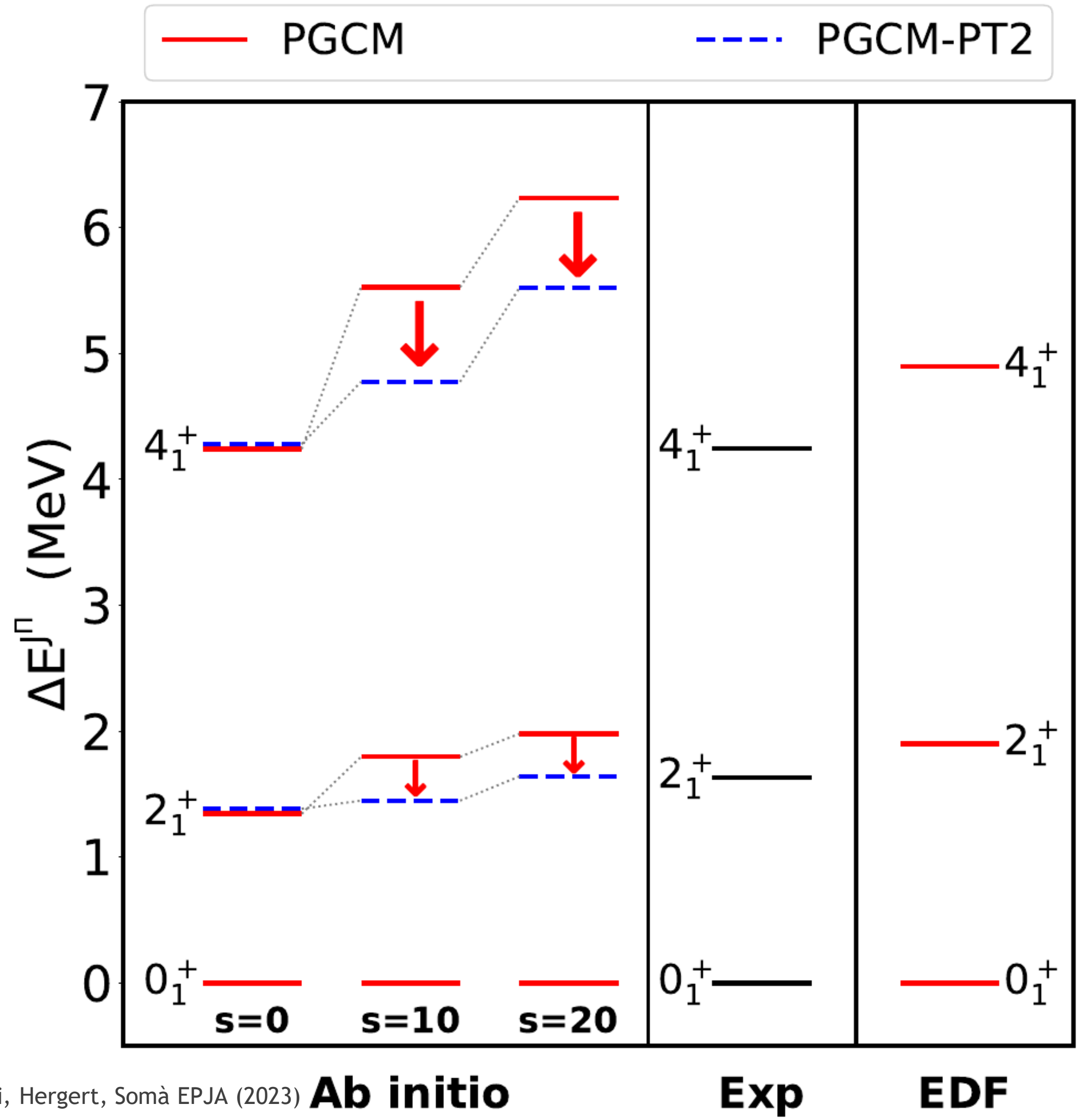

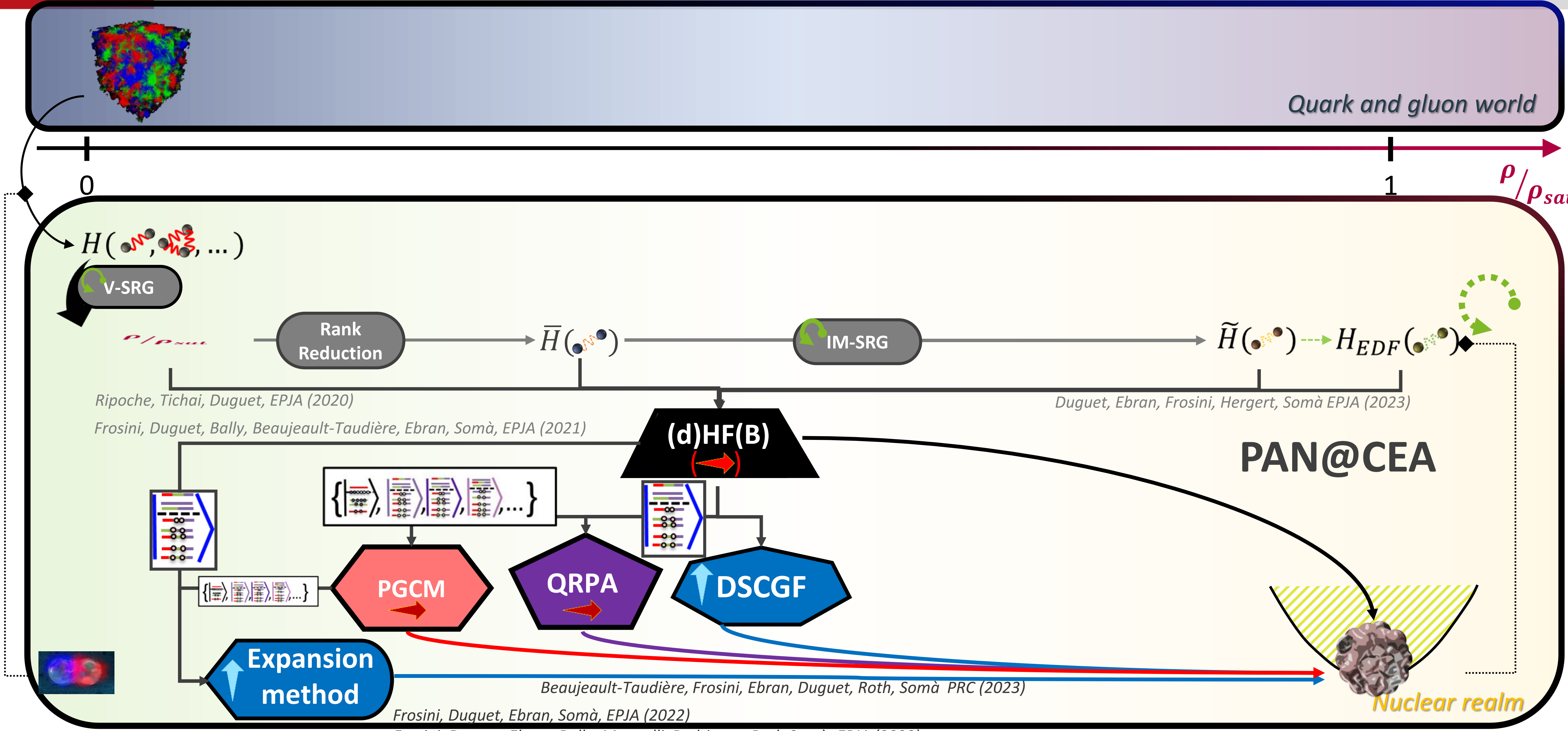

Ripoche, Tichai, Duguet, EPJA (2020)

Frosini, Duguet, Bally, Beaujeault-Taudière, Ebran, Somà, EPJA (2021)

Duguet, Ebran, Frosini, Hergert, Somà EPJA (2023)

Beaujeault-Taudière, Frosini, Ebran, Duguet, Roth, Somà PRC (2023)

Frosini, Duguet, Ebran, Somà, EPJA (2022)

Frosini, Duguet, Ebran, Bally, Mongelli, Rodriguez, Roth,Somà, EPJA (2022)

Frosini, Duguet, Ebran, Bally, Hergert, Rodriguez, Roth, Yao, Somà, EPJA (2022)