From the EDF method to Ab initio approaches and back again – A DRF-DAM success story –

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Problème à A nucleons au CEA

Séminaire DPhN

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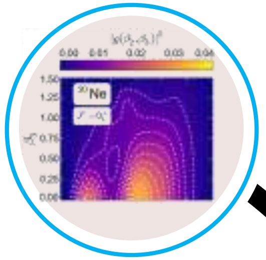
Outline

1. General context
2. Recent work on empirical EDFs
3. EDF-inspired ab initio methods
4. Towards a first-principle formulation of EDFs

1. General context

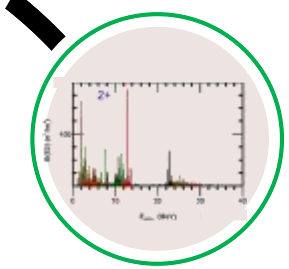
Context : General goal of nuclear structure theory

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



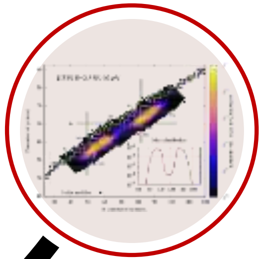
Ground-state

masses, radii, density profile, …



Excitation spectra

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

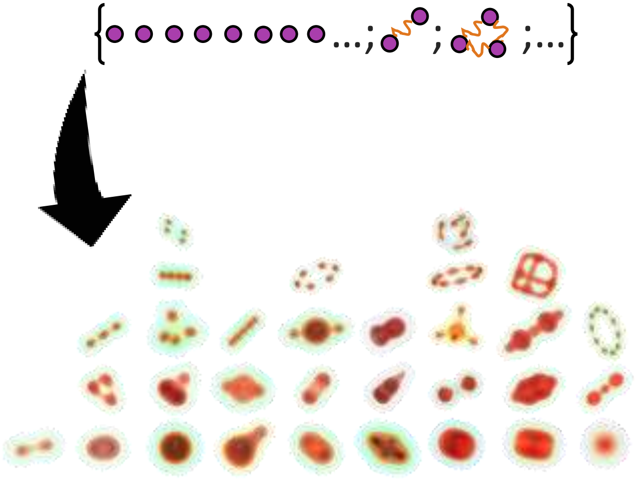


Decay modes

lifetime, yields, …

Reactions

cross sections, …



Intrinsic densities

Atomic nucleus

=

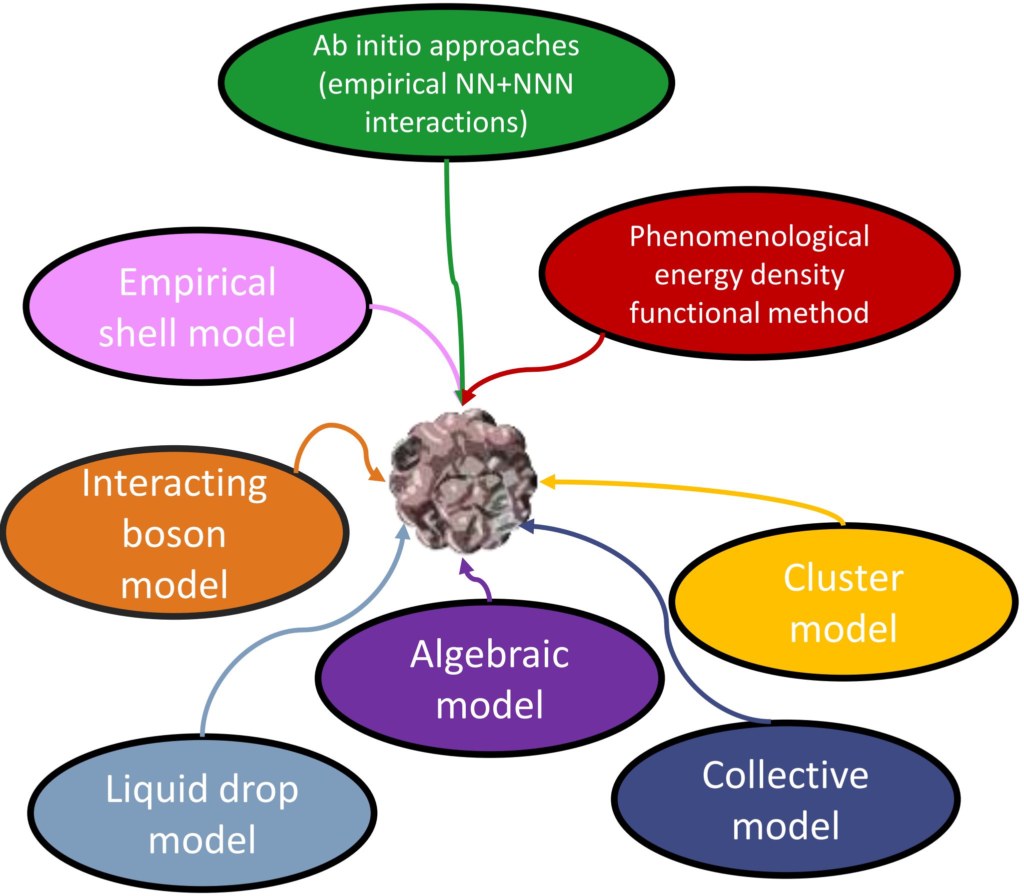
A mesoscopic, self-bound system of strongly correlated spin-1/2 and isospin-1/2 composite fermions in strong and electroweak interaction.

⇢ What is the nature of the force binding nucleons in nuclei and how all the richness of structure, decay and reactions properties emerge from it ?
⇢ How nucleon, cluster and collective dofs interfere/compete and how their coexistence evolve with mass number, neutron-proton asymmetry, excitation energy, … ?
⇢ What are the limit of existence of nuclei in terms of mass number and excitation energy, and what properties emerge near and beyond these frontiers ?
⇢ How structure properties impact nuclear decay and reactions features ?

Strategies

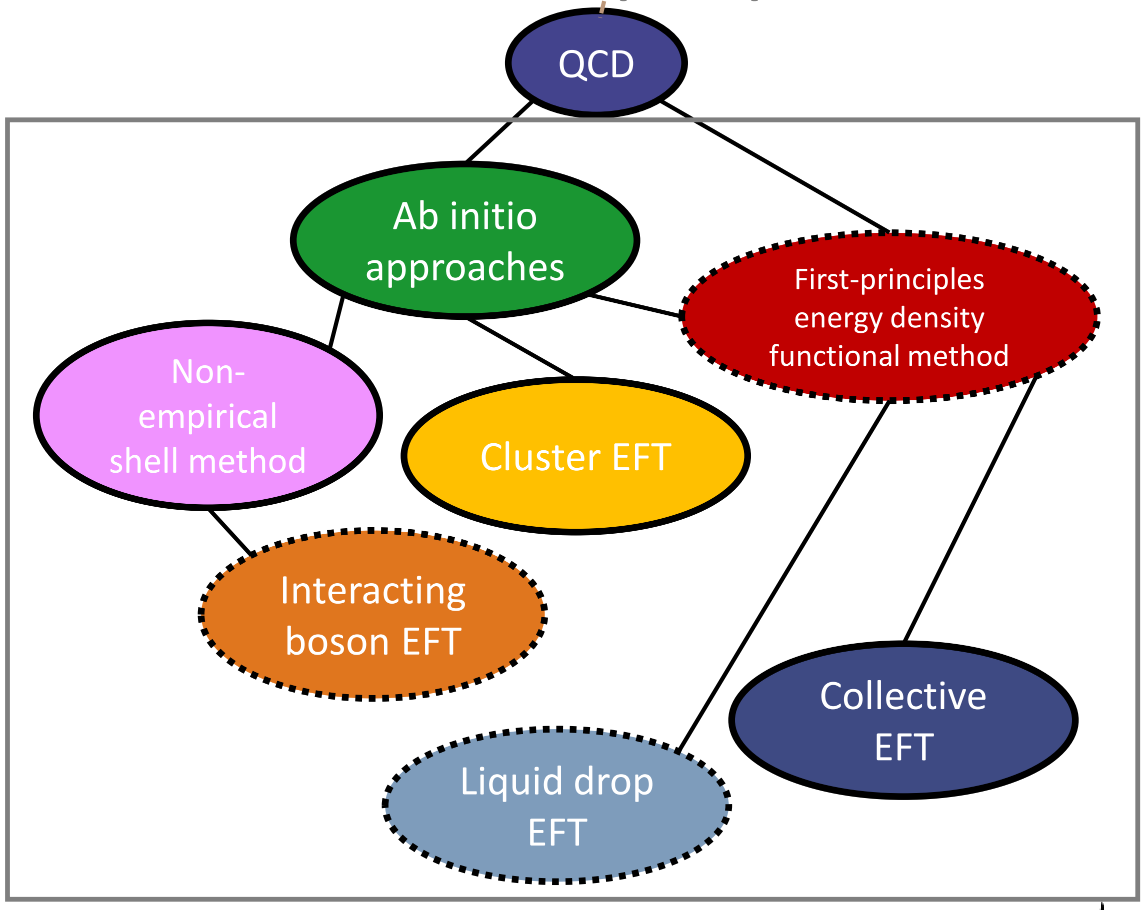
◉ Achieve a { *accurate* / *predictive* / *computationally affordable* } description ?

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

Microscopic viewpoint

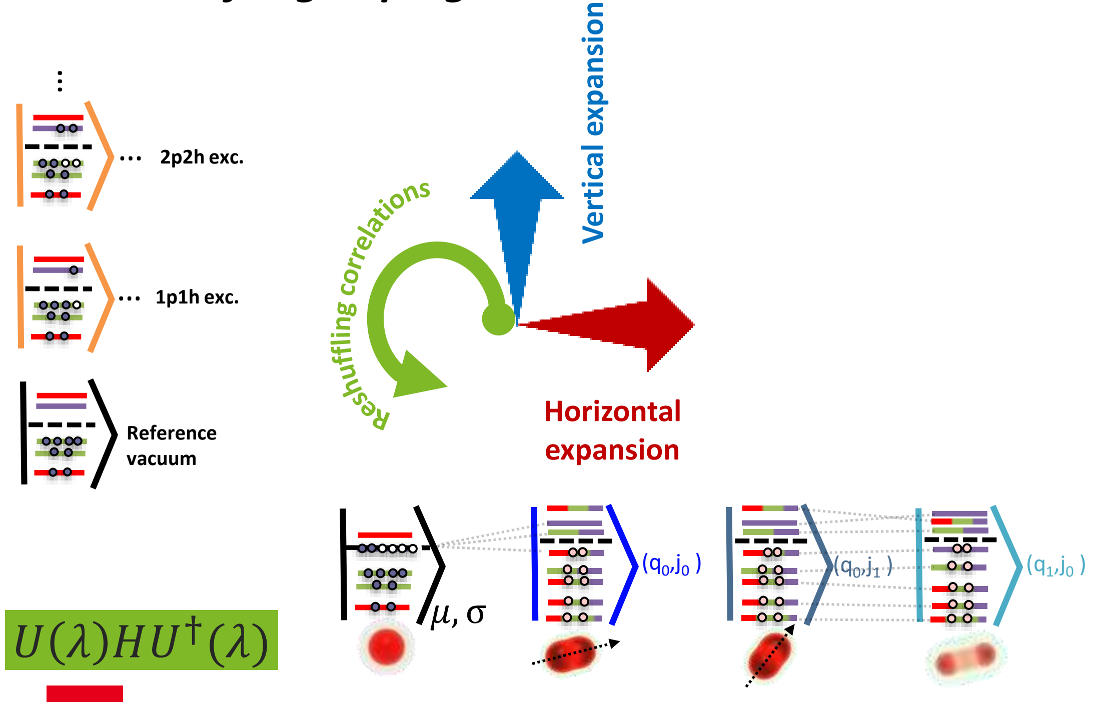
1) Nucleus: *A* interacting, structure-less nucleons
2) Structure & dynamic encoded in Hamiltonian, Functional, …
3) Solve *A*-nucleon Schrödinger/Dirac equation to desired accuracy

$$H(\ldots, \ldots, \ldots)|\Psi_{\mu,\sigma}\rangle = E_{\mu\tilde{\sigma}}|\Psi_{\mu,\sigma}\rangle \qquad N_{FCI} \propto \binom{I}{A}$$

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

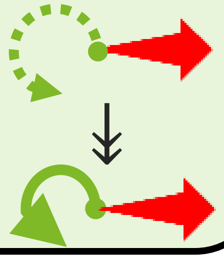
$|\Theta_{\mu\sigma}\rangle$ Simplified auxiliary WF

◉ **Various levels of realization**

⇢ *Hartree-Fock-Bogoliubov (HFB)*

⇢ *Projected Generator Coordinate Method (PGCM)*

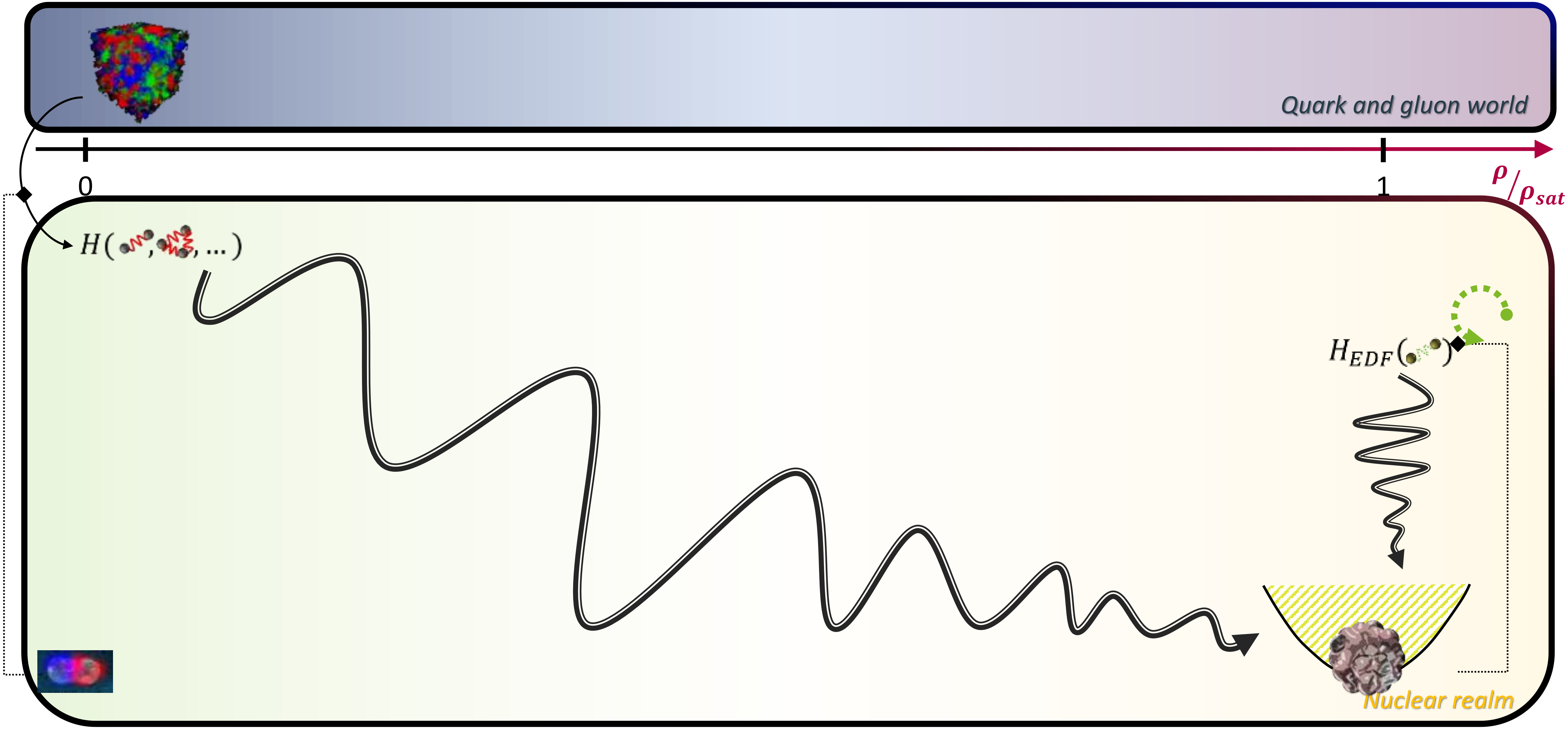
⇢ *Quasiparticule Random Phase Approximation (QRPA)*



⊗ *How to improve current EDFs*

⊗ *How to turn EDF in EFT ?*

Microscopic viewpoint



Outline

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3. EDF-inspired ab initio methods
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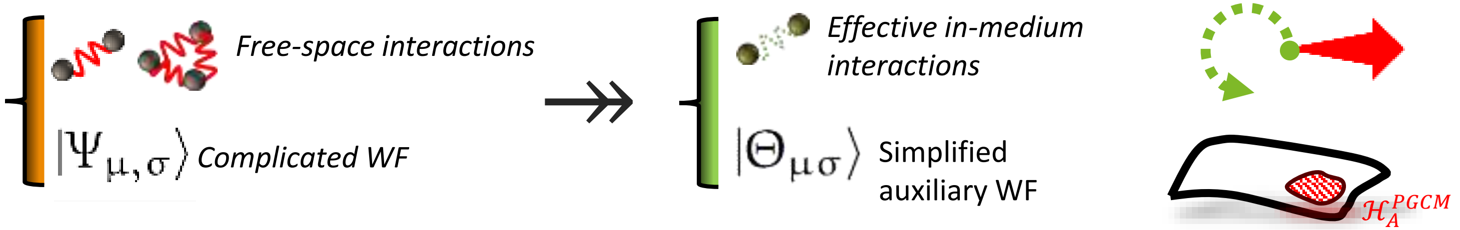
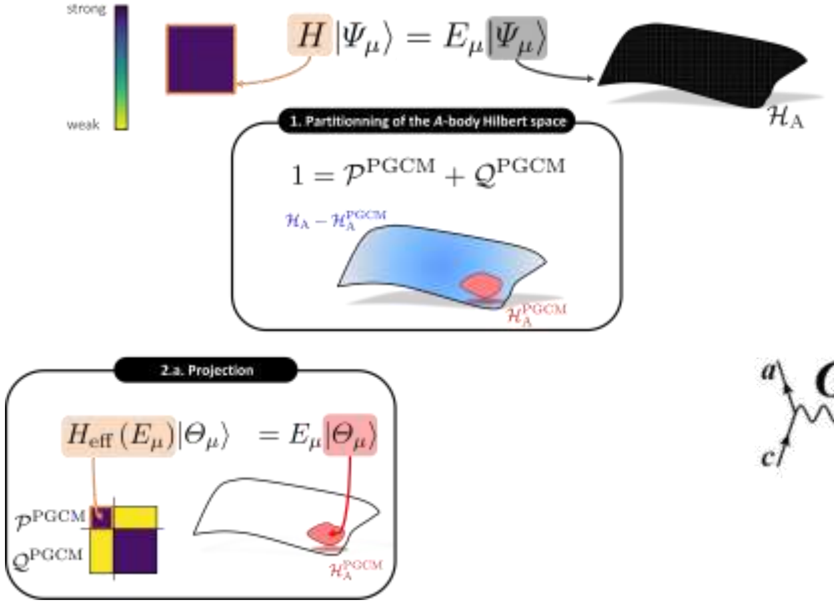
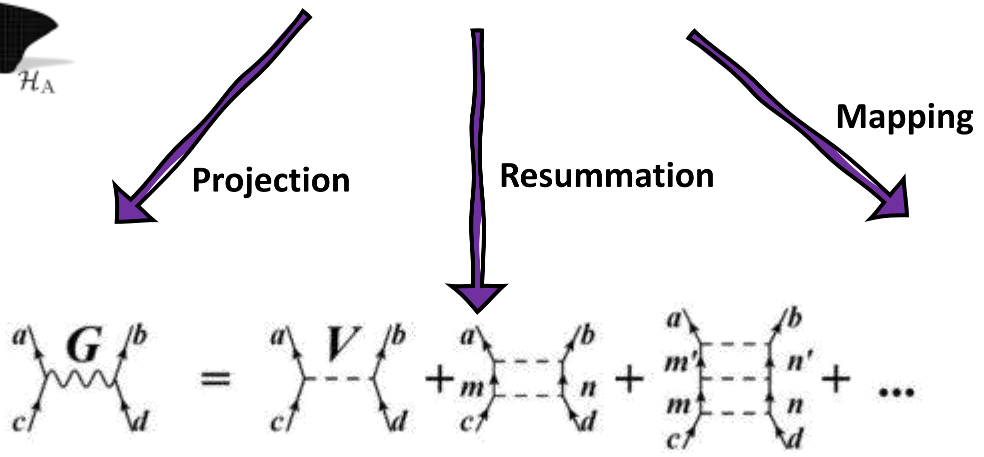
2. Recent work on empirical EDFs

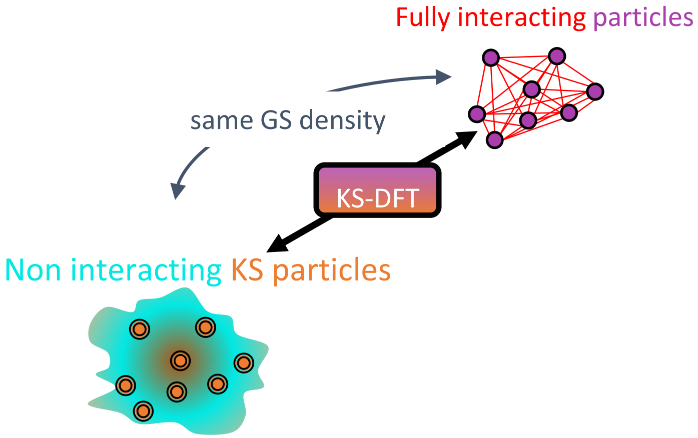
Empirical EDFs

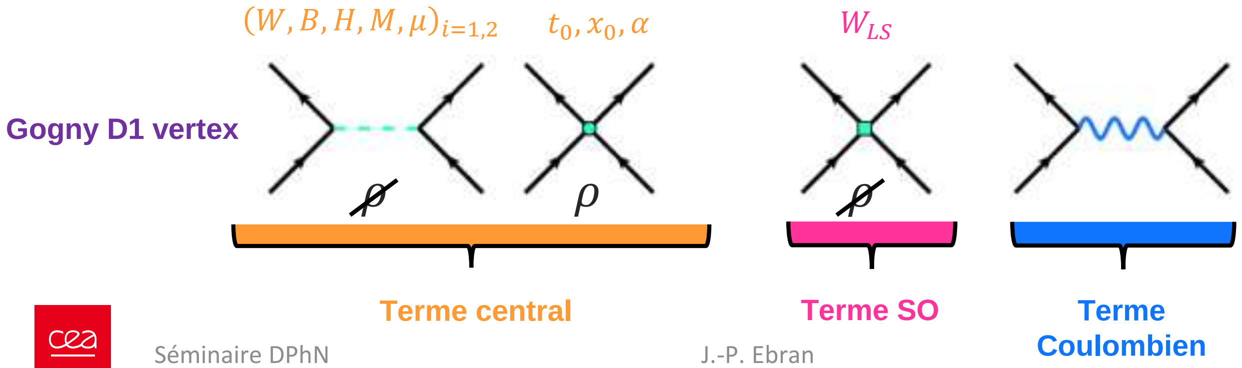


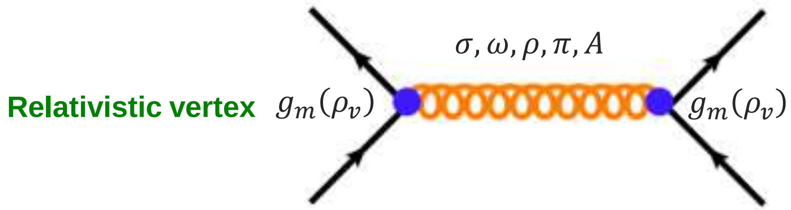
◉ Ground- and low-lying excited states computed from $H_{EDF}(\ldots)$ and $|\Theta_{\mu\sigma}\rangle \Leftrightarrow$ the ones computed from $H(\ldots, \ldots, \ldots)$ and $|\Psi_{\mu,\sigma}\rangle$







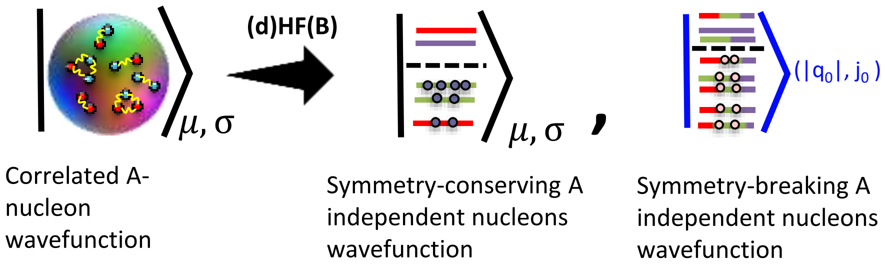




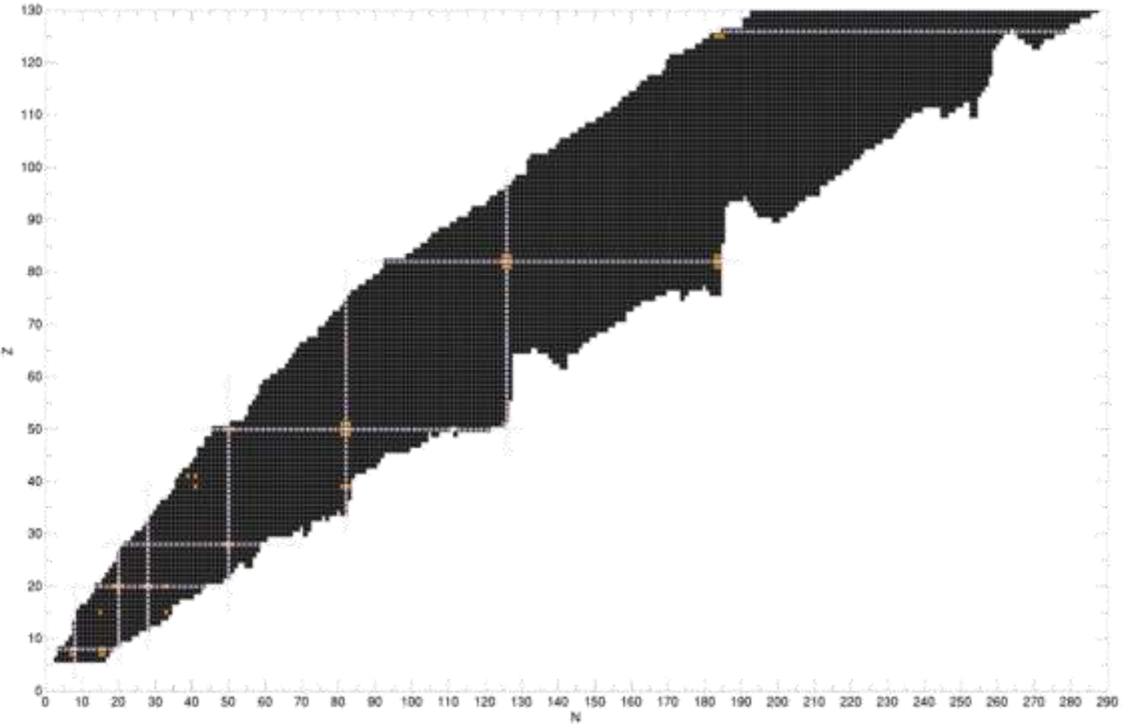
EDF : HFB realization

◉ HFB treatment

--> *A*-nucleon problem ⟶ *A* 1-nucleon problems



--> SSB : Efficient way for capturing so-called static correlations



No SSBs allowed : First level of description for ~30 nuclei

EDF : HFB realization

◉ HFB treatment

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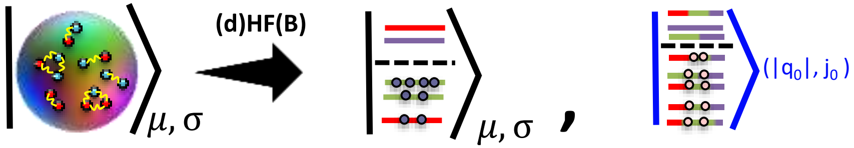
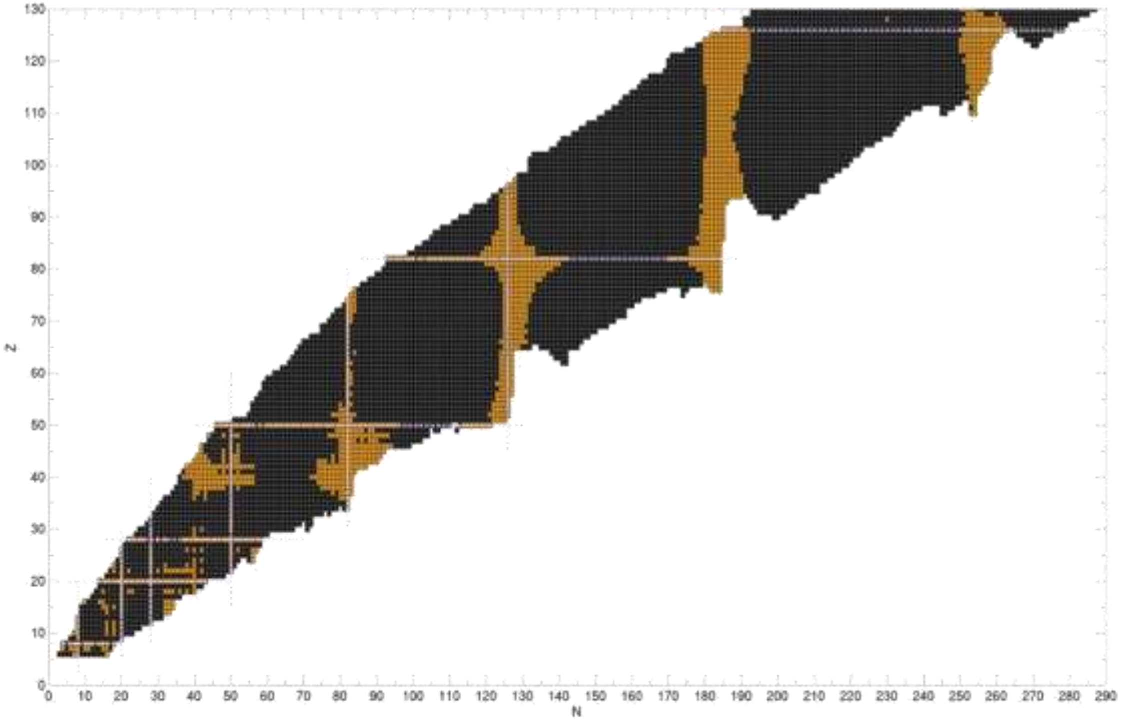


Correlated A-nucleon wavefunction

Symmetry-conserving A independent nucleons wavefunction

Symmetry-breaking A independent nucleons wavefunction

--> SSB : Efficient way for capturing so-called static correlations

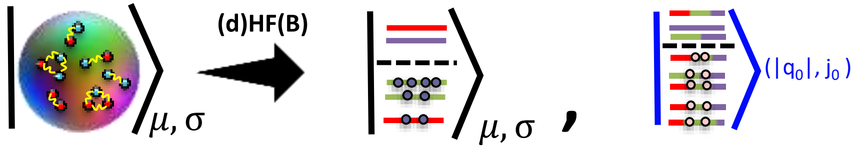


U(1) SSB allowed : First level of description for ~300 nuclei

EDF : HFB realization

◉ HFB treatment

--> *A*-nucleon problem ⟶ *A* 1-nucleon problems

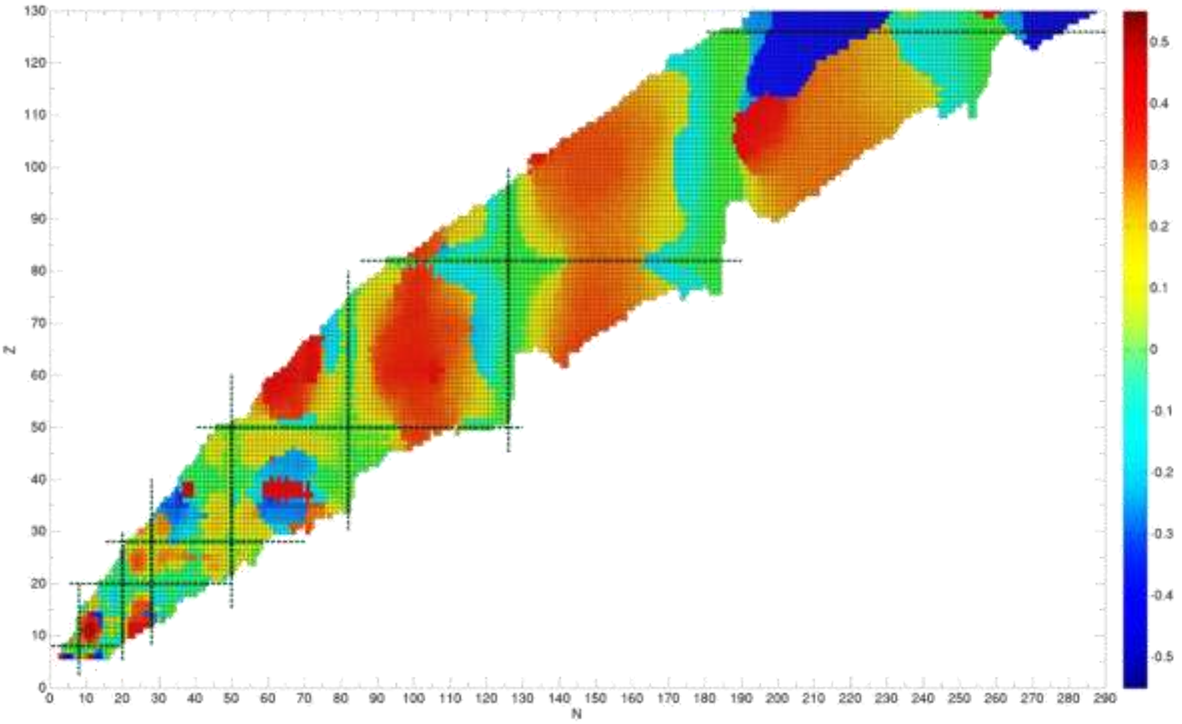


Correlated A-nucleon wavefunction

Symmetry-conserving A independent nucleons wavefunction

Symmetry-breaking A independent nucleons wavefunction

--> SSB : Efficient way for capturing so-called static correlations



SU(2) & U(1) SSB allowed : First level of description for all nuclei

◉ Typical physical quantities computed at the HFB level :

◈ Mass, radius, intrinsic density, … of the GS (and some isomeric states)

◈ Single-particle energies and wfs

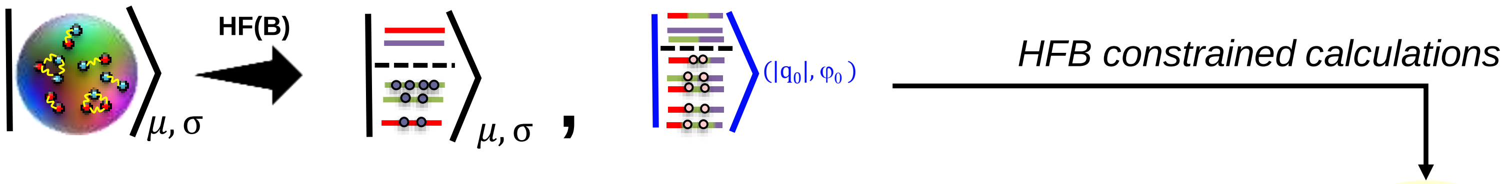
◈ Barrier, inertia tensor, …

◉ Refined description of properties already accessible at the HFB level, or access to new types of properties (essentially spectroscopic ones) require going beyond the HFB realization

Horizontal expansion

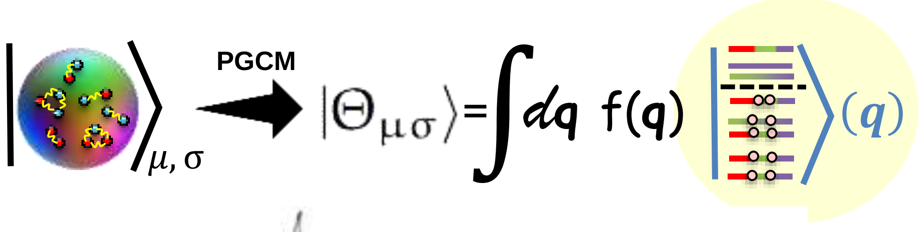
◉ HFB treatment

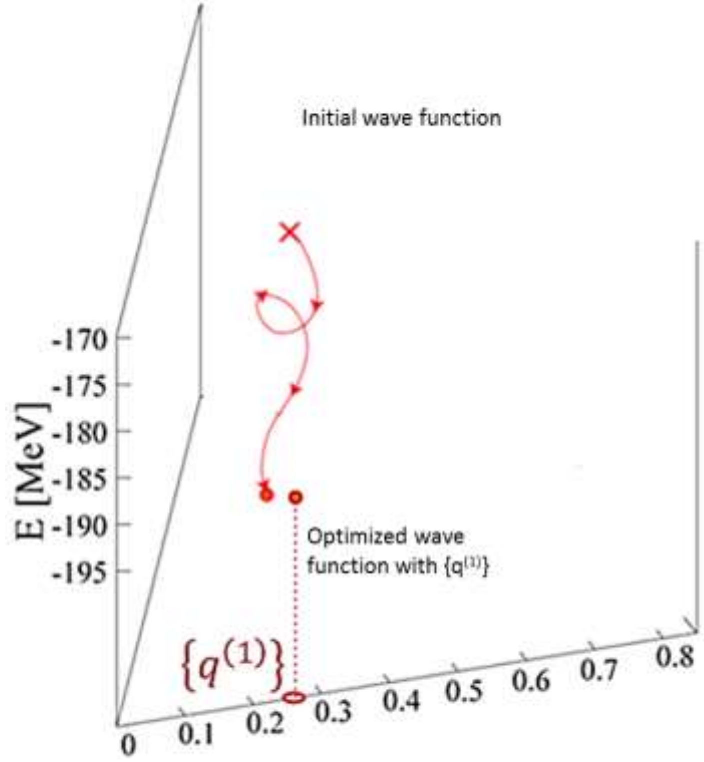
⇢ *A*-nucleon problem ⟶ *A* 1-nucleon problems



◉ Post-HFB treatment : PGCM

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





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◉ HFB treatment

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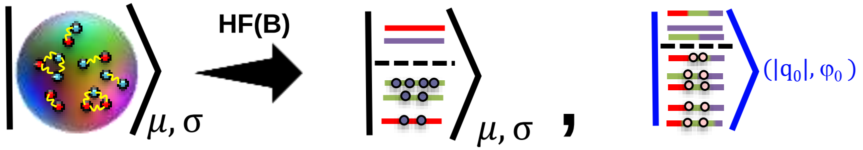

HFB constrained calculations

◉ Post-HFB treatment : PGCM

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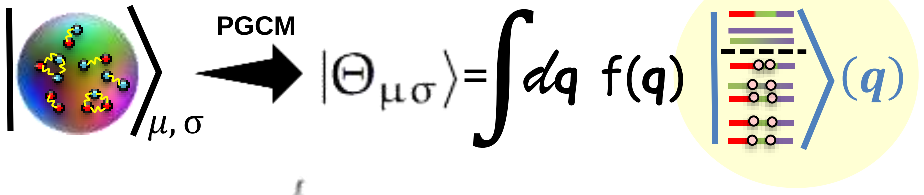

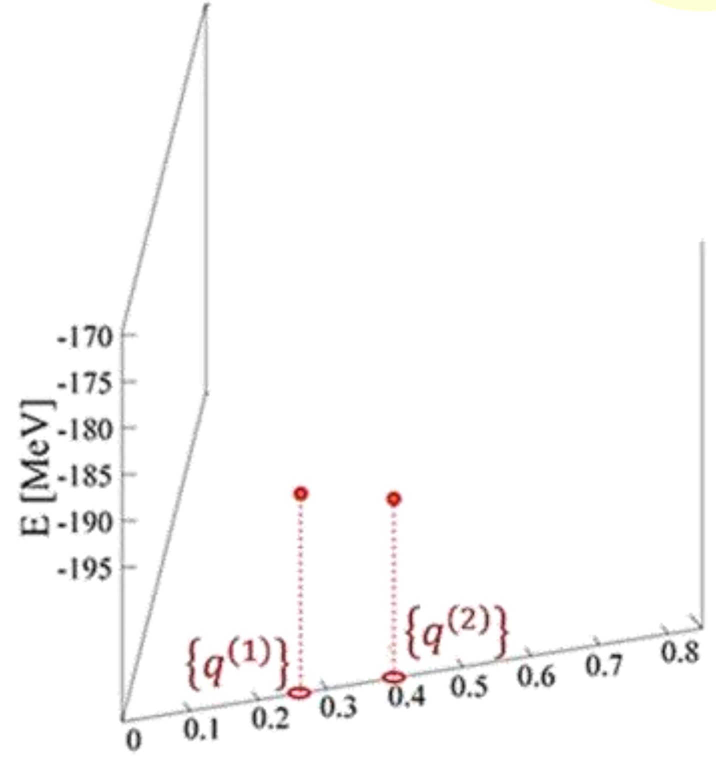

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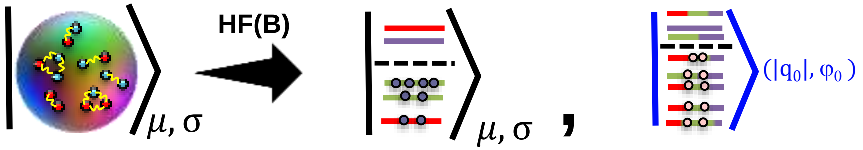

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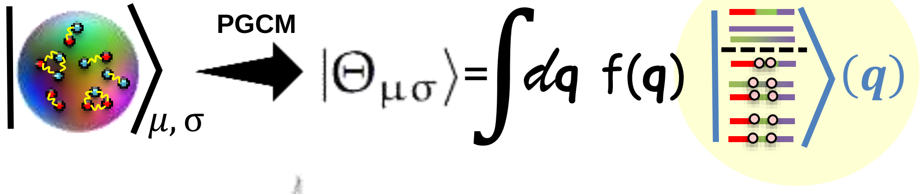

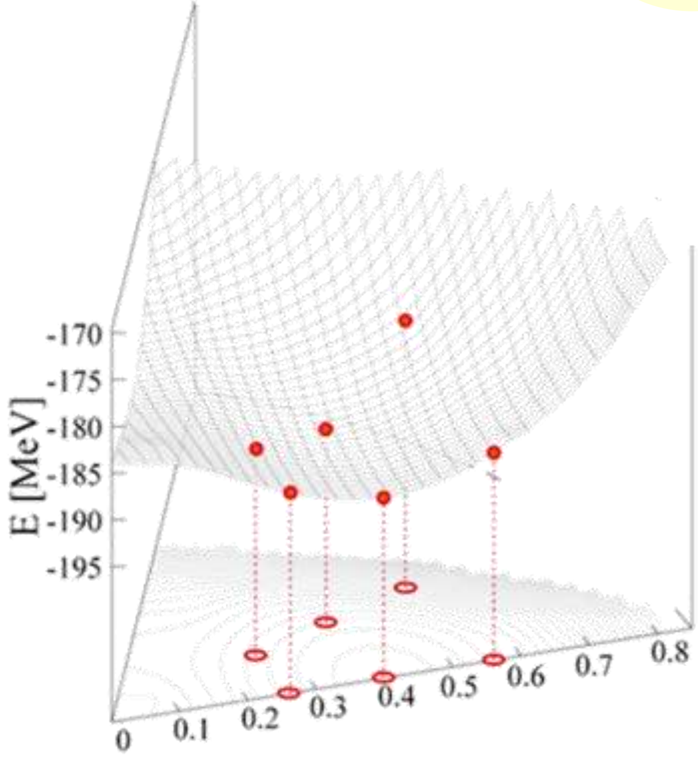

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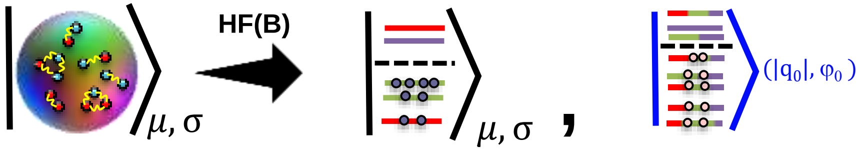

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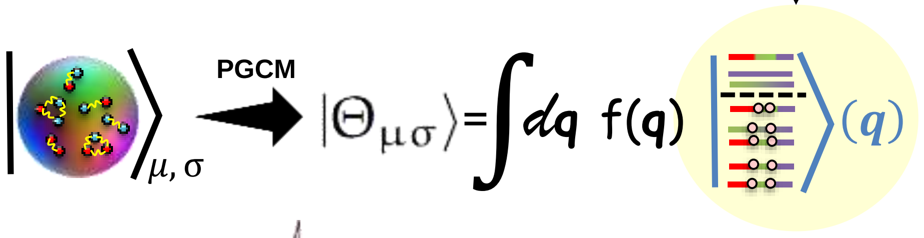

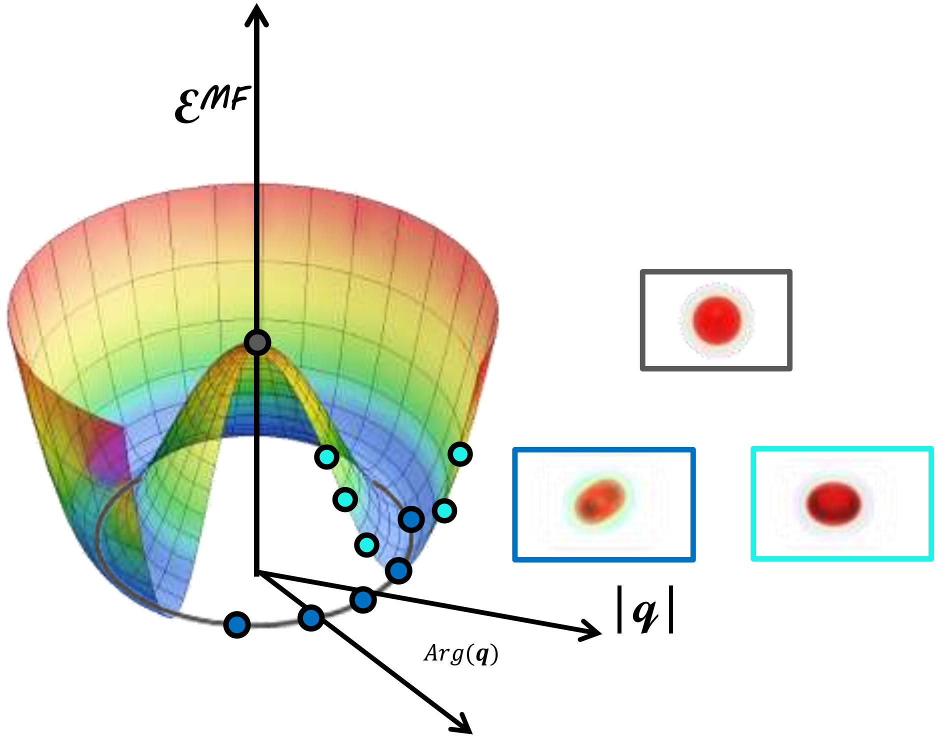

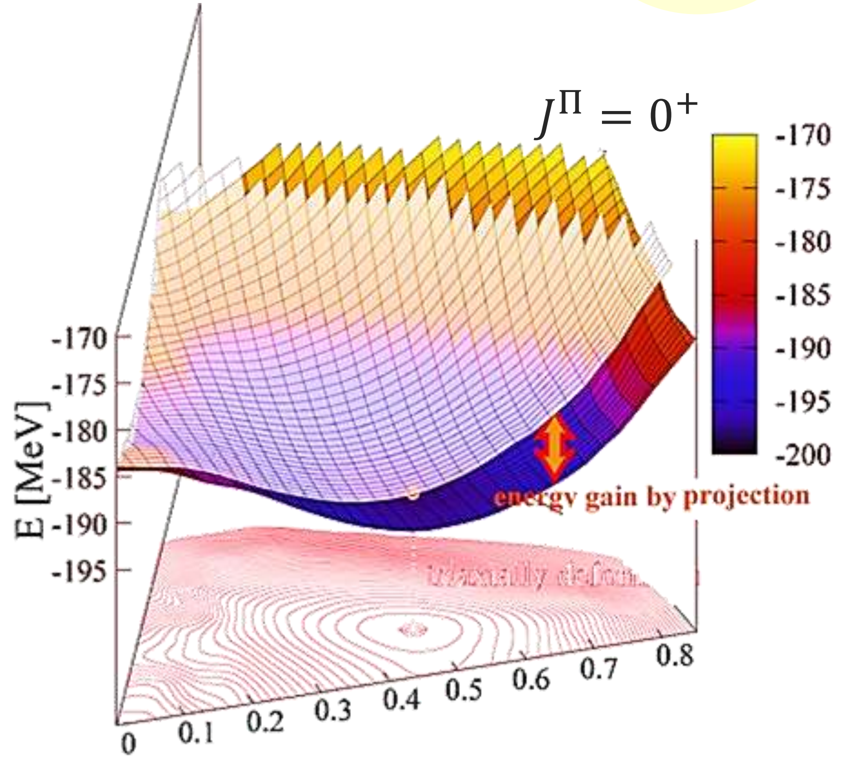

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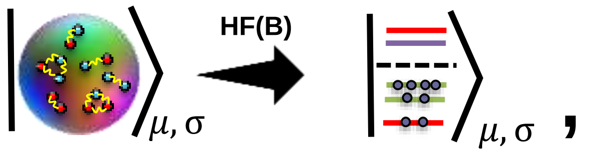

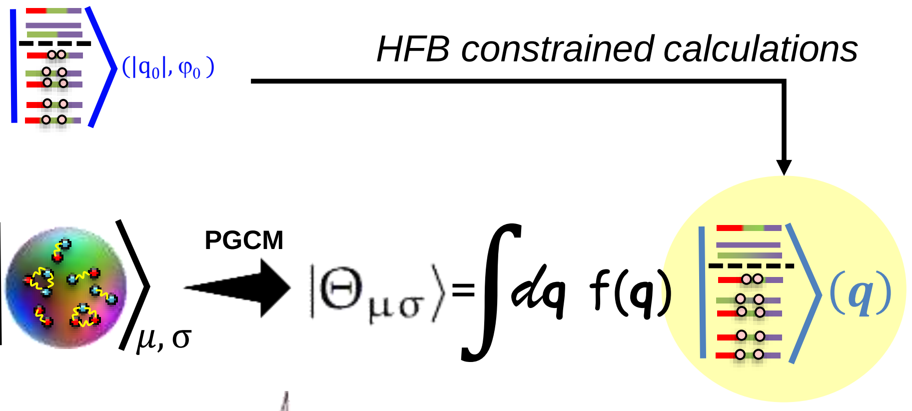

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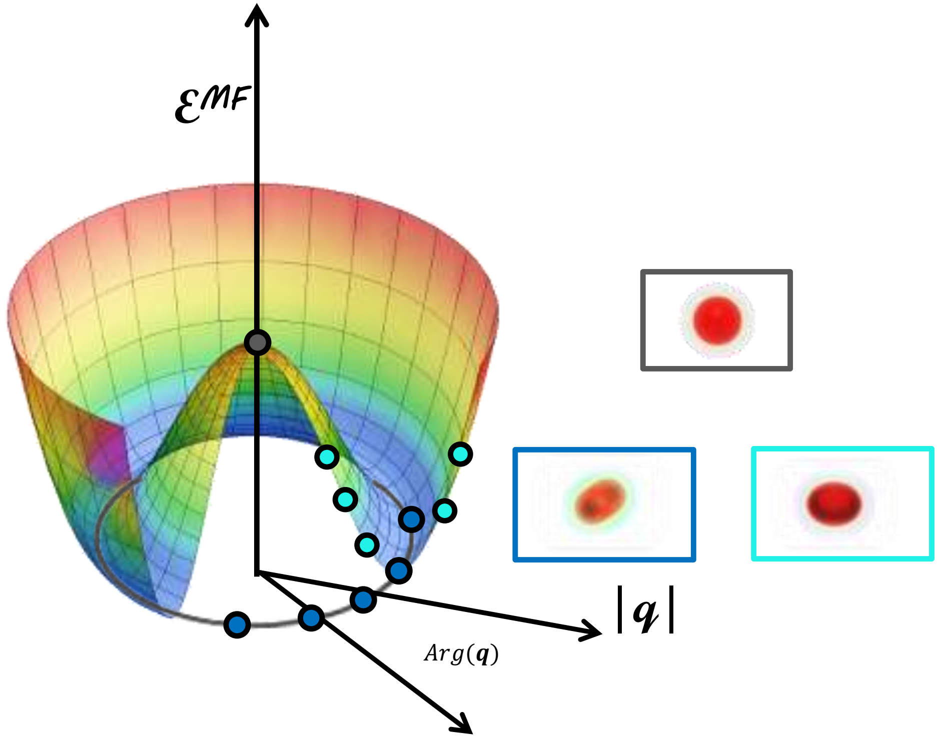
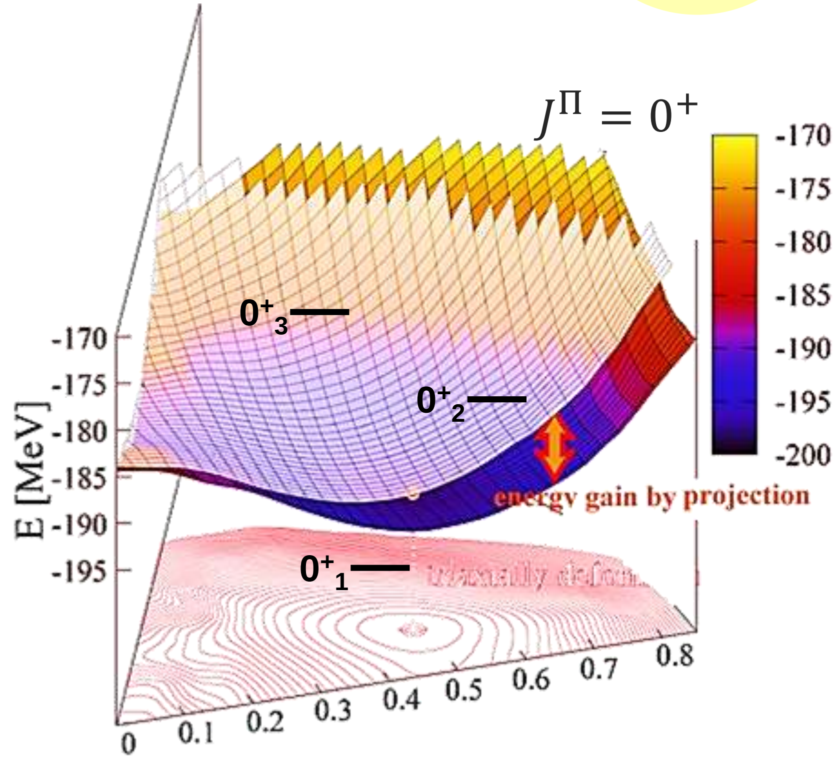




Horizontal expansion

◉ HFB treatment

⇢ *A*-nucleon problem ⟶ *A* 1-nucleon problems

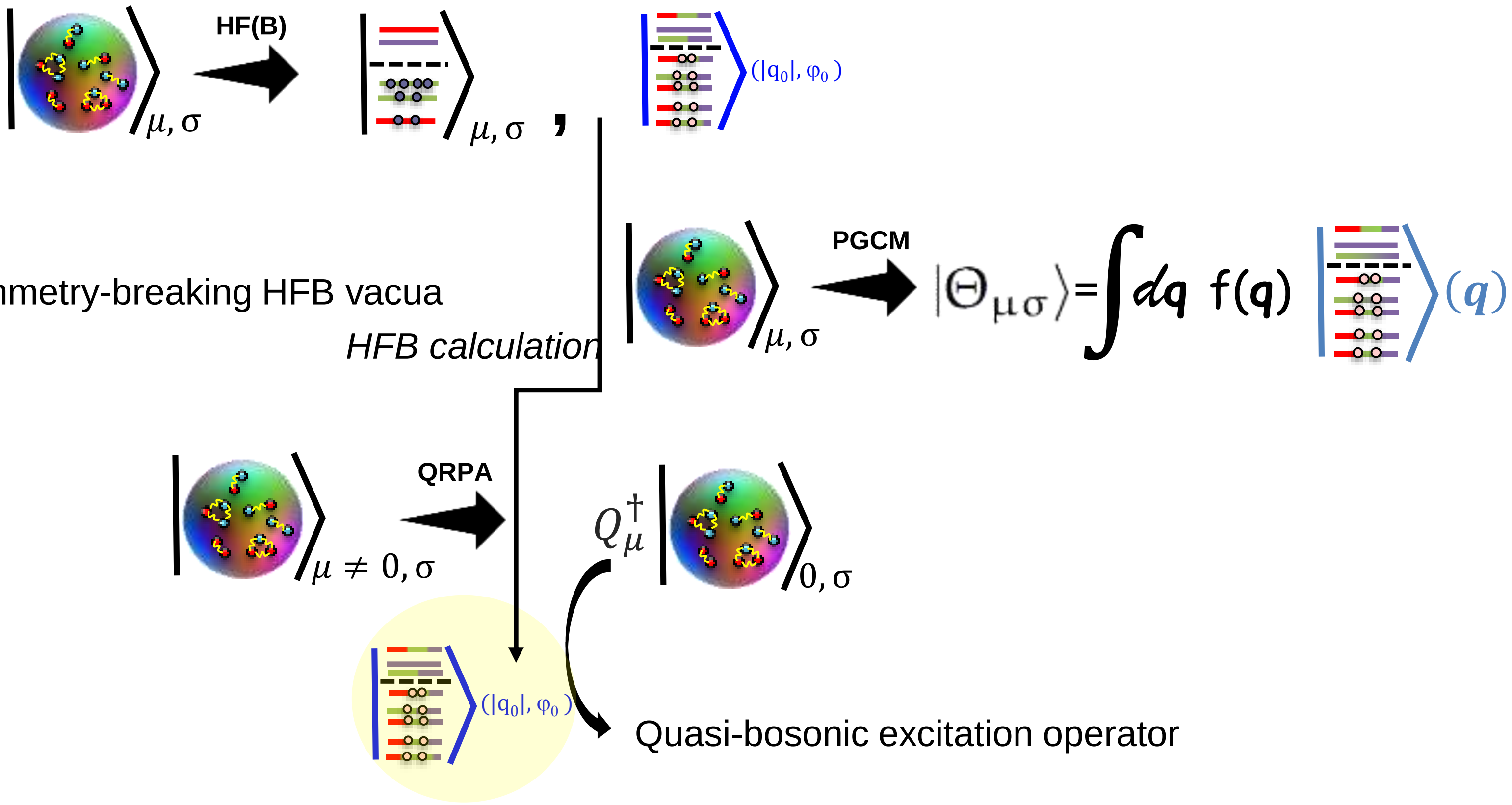
◉ Post-HFB treatment : PGCM

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

◉ Post-HFB : QRPA

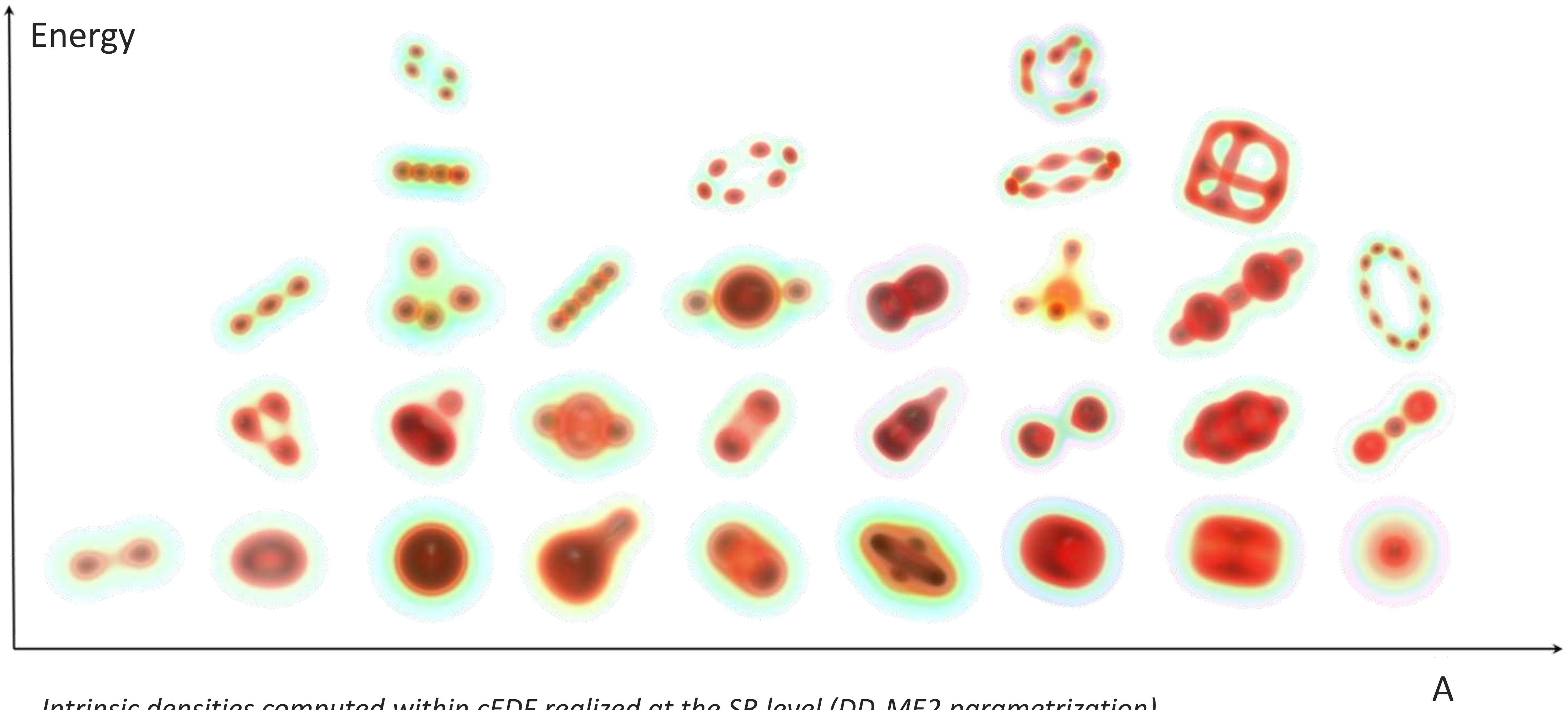
⇢ Excitations = coherent mixture of 2-qp excitations

⇢ Harmonic limit of the GCM



Example of applications : Nuclear clustering

- Clustering = nucleons clumping together into sub-groups within the nucleus



Intrinsic densities computed within cEDF realized at the SR level (DD-ME2 parametrization)

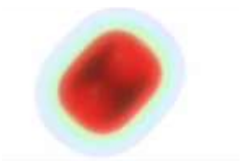
Strength of correlations

- Strength of correlations measured by dimensionless ratios

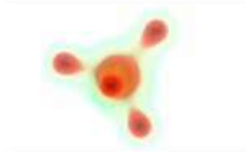
$$\sqrt{\Lambda} \equiv \sqrt{\frac{\langle V\rangle}{\langle T\rangle}} = \sqrt{2}\left(\frac{3}{4\pi}\right)^{\frac{1}{6}} (2MU)^{\frac{1}{4}} (An)^{-\frac{1}{6}} \sim \alpha_{loc}$$

Nucleon mass (M) — Number of nucleons (A) — Depth of the confining potential (U) — Mean density (n)

small



large



Clustering favored
- ⇢ For deep confining potential
- ⇢ For light nuclei
- ⇢ In regions at low-density

- Formation/dissolution of clusters : Mott parameter

Size of the nucleus X

$$\frac{R_X}{d^X_{Mott}} \sim 1 \Rightarrow n^X_{Mott} \sim \frac{\rho_{sat}}{A_X}$$

inter-nucleon average distance

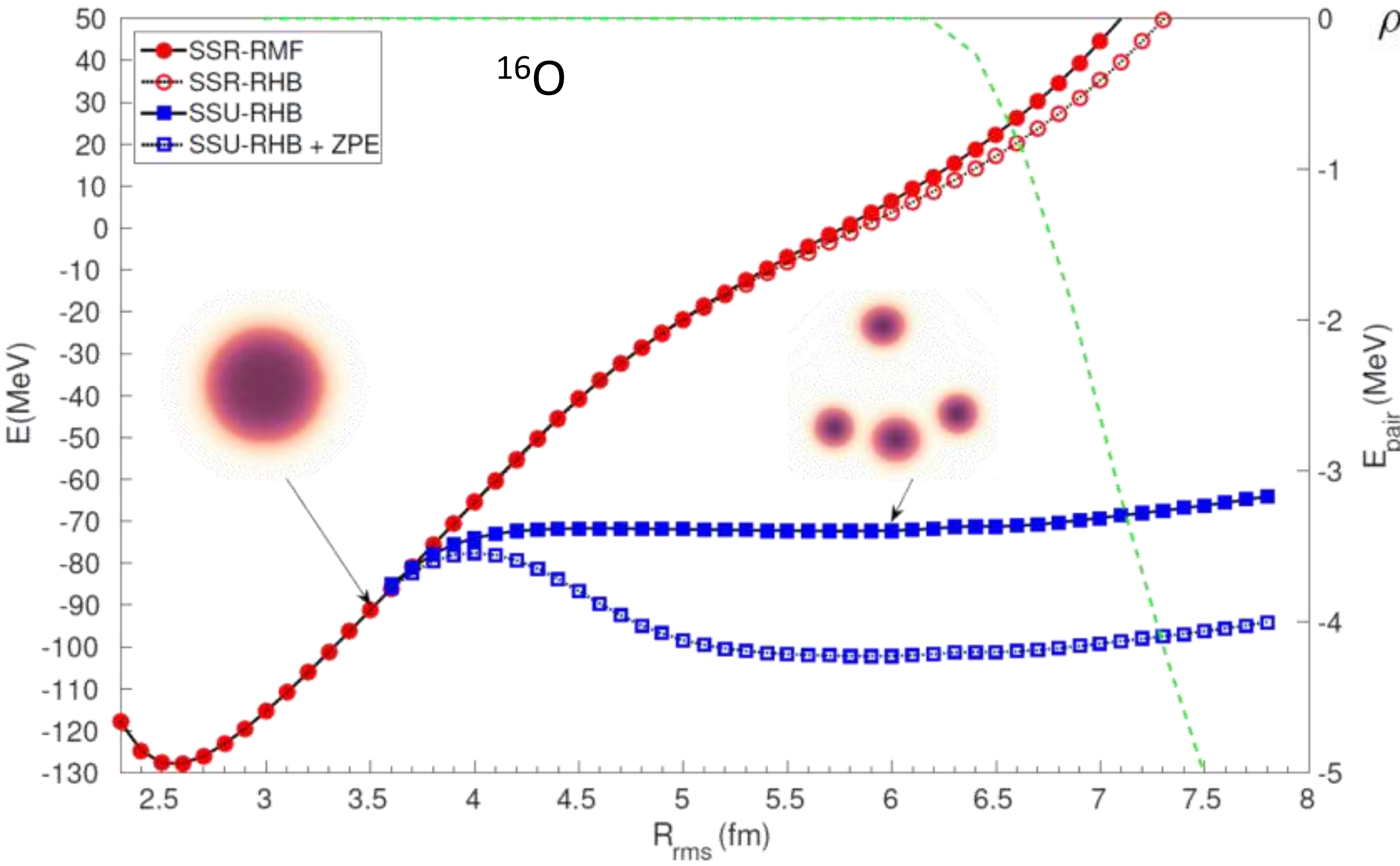
$n^{\alpha}_{Mott} \sim 0.25\rho_{sat}$ Size of an α in free-space

$\sim \frac{\rho_{sat}}{3}$ 0.9 size of an α in free-space

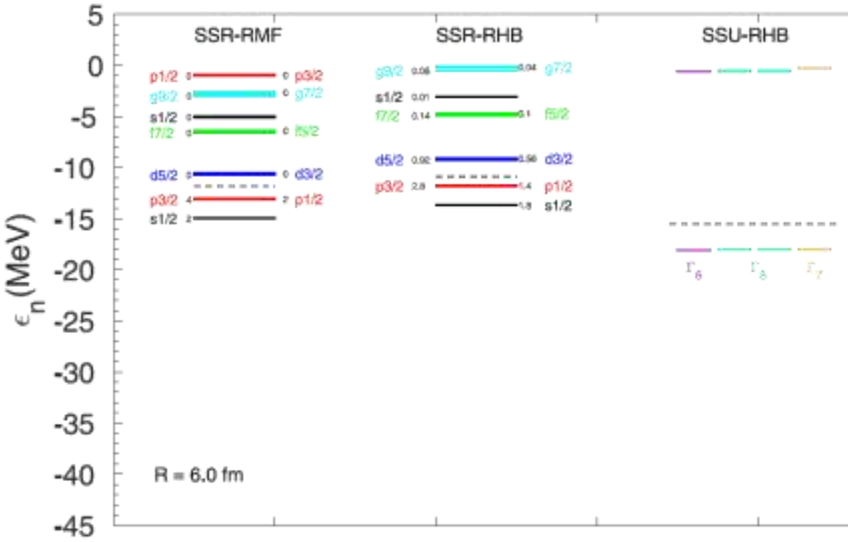
Ebran, Girod, Khan, Lasseri, Schuck, PRC 2020
Ebran, Khan, Niksic, Vretenar, PRC 2014
Ebran, Khan, Niksic & Vretenar PRC 2013
Ebran, Khan, Niksic & Vretenar Nature 2012

Quantum Mott-like phase transition

- Isotropically inflate ^{16}O by constraining its r.m.s. radius while imposing a global quadrupole moment to be zero

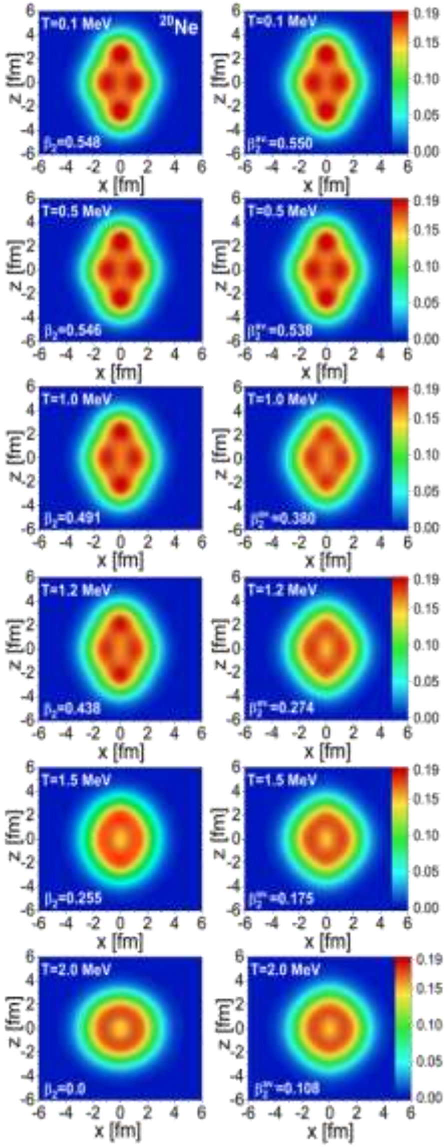


$$\rho_{\mathrm{Mott}}/\rho_0 = (R_{\mathrm{eq}}/R_c)^3 \approx \rho_0/3$$

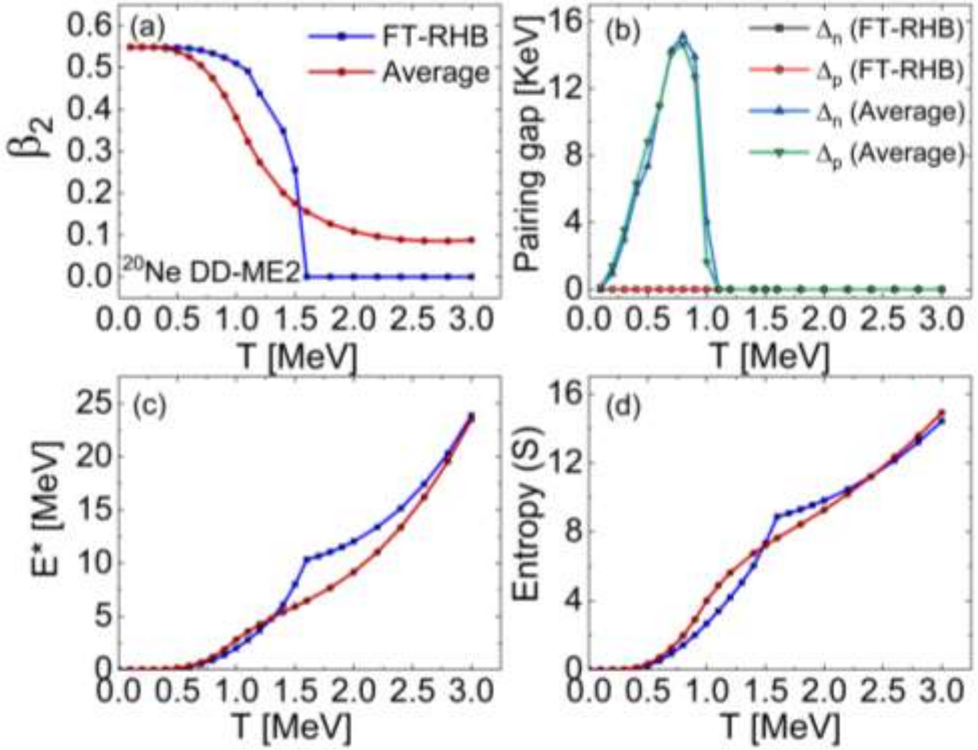


Thermal phase transition

- Isotropically inflate ^{16}O by constraining its r.m.s. radius while imposing a global quadrupole moment to be zero



$$\overline{O} = \frac{\int d\beta_2 O(\beta_2, T) \exp(-\Delta F(\beta_2, T)/T)}{\int d\beta_2 \exp(-\Delta F(\beta_2, T)/T)}.$$

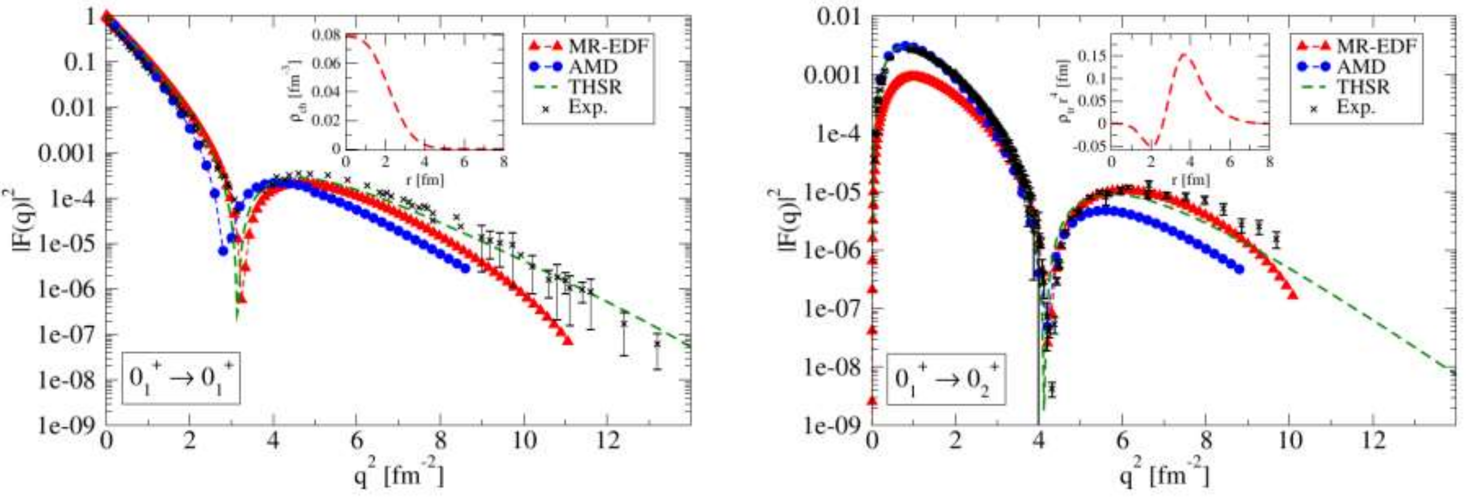


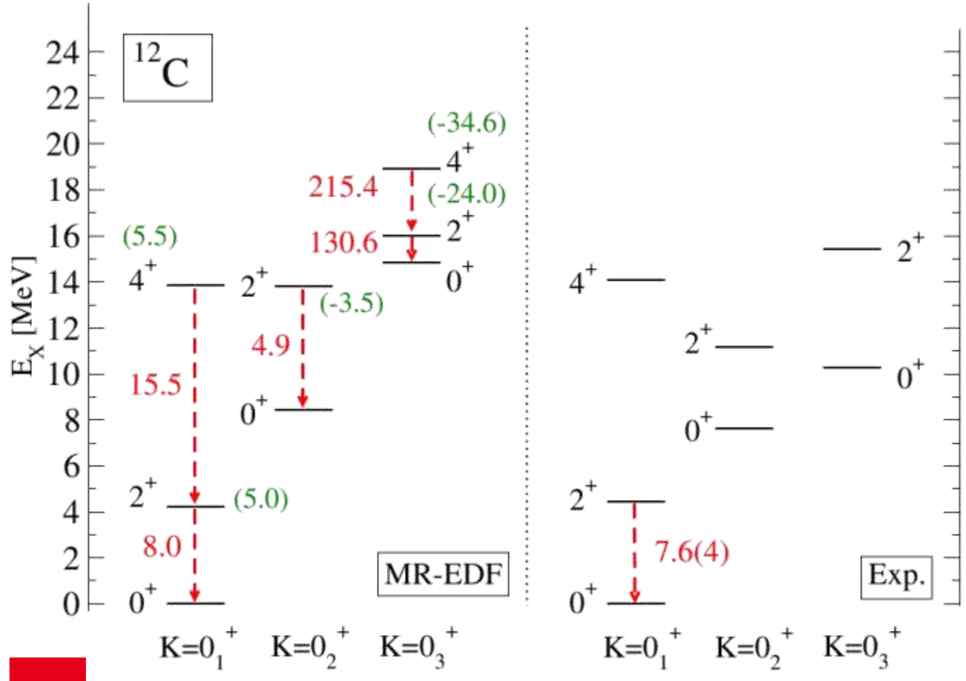
Yüksel, Mercier, Ebran, Khan PRC 2022

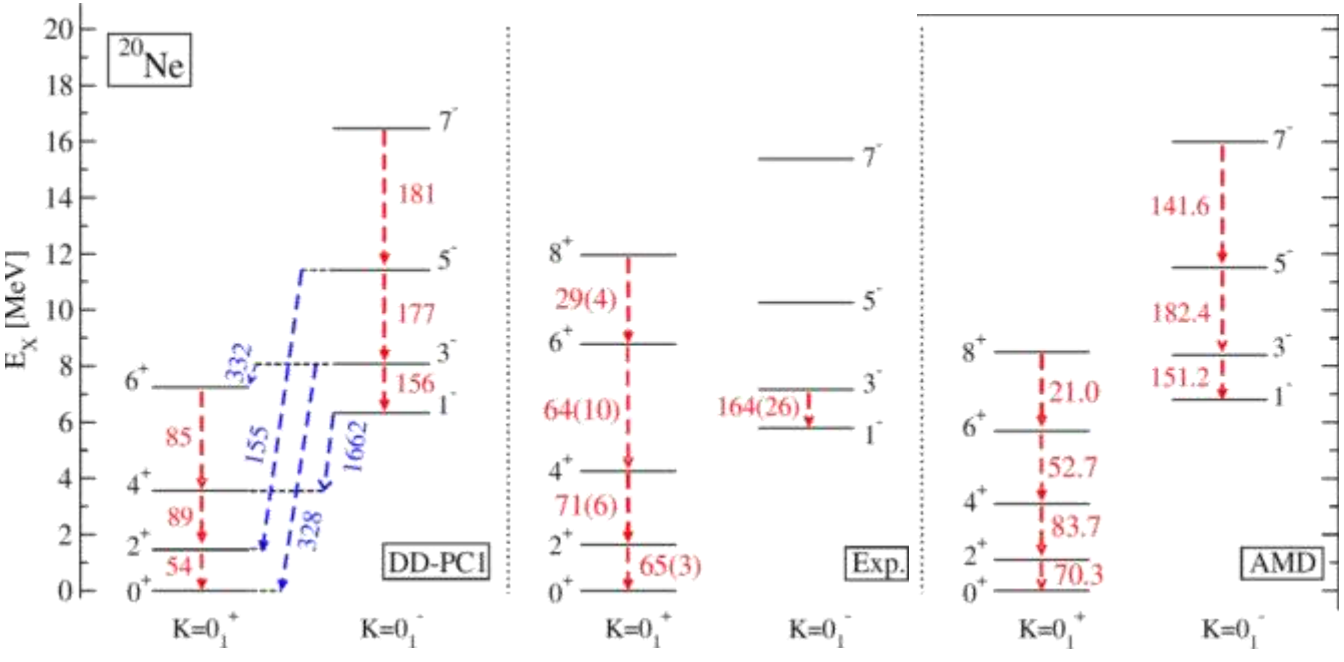
Nuclear clustering & PGCM

◉ Spectroscopy

Marević, Ebran, Khan, Nikšić, and Vretenar, 2019





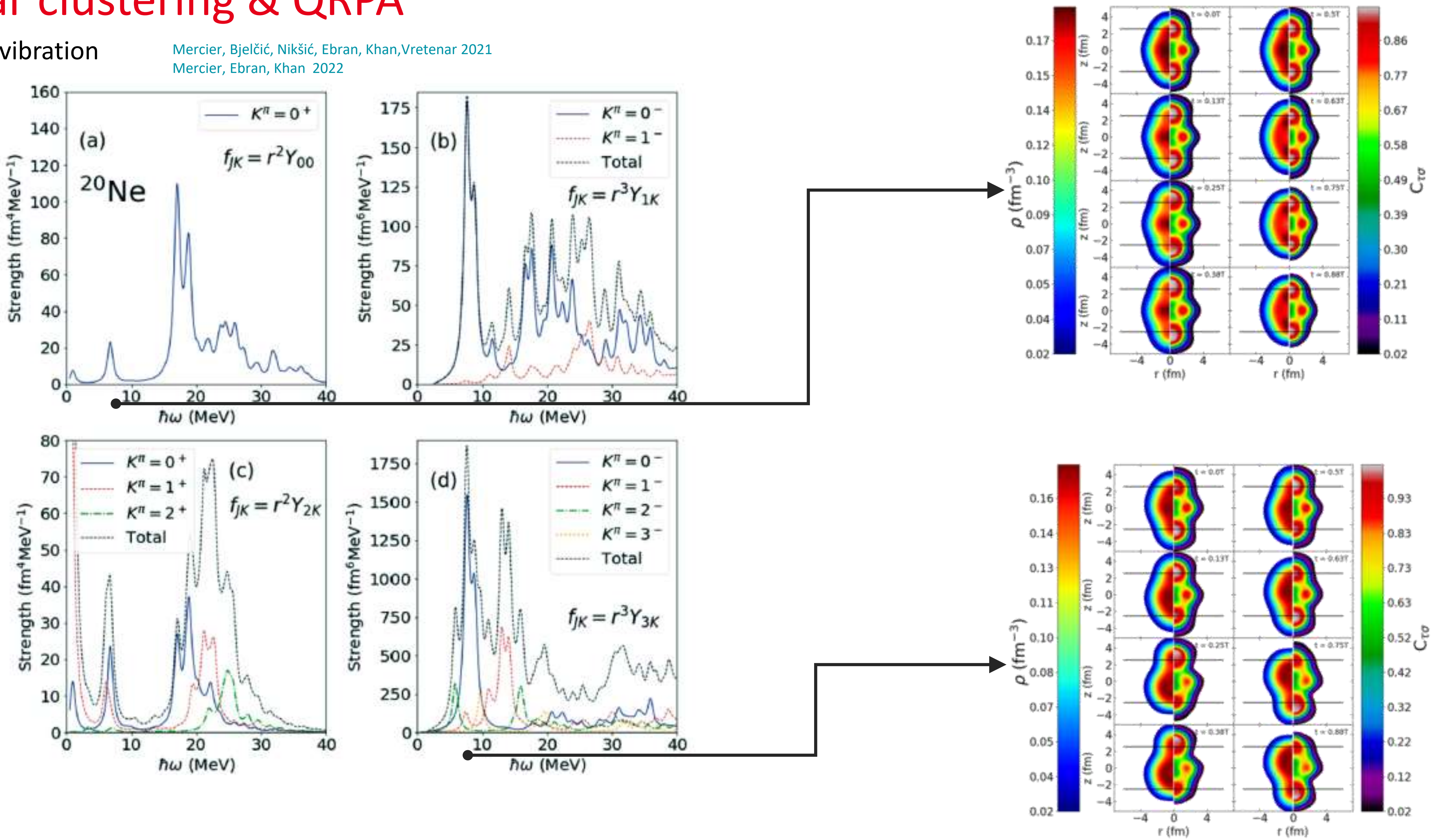


Marevic, Ebran, Khan, Niksic, Vretenar, 2018

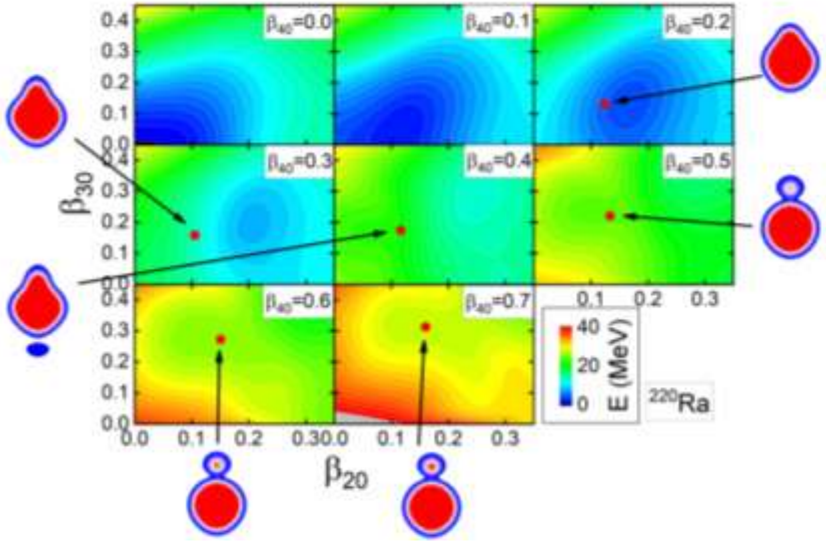
Nuclear clustering & QRPA

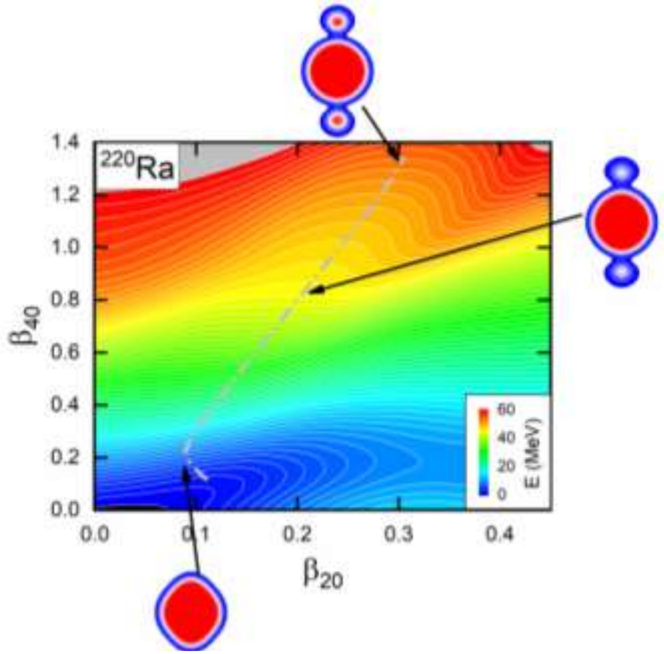
◉ Cluster vibration

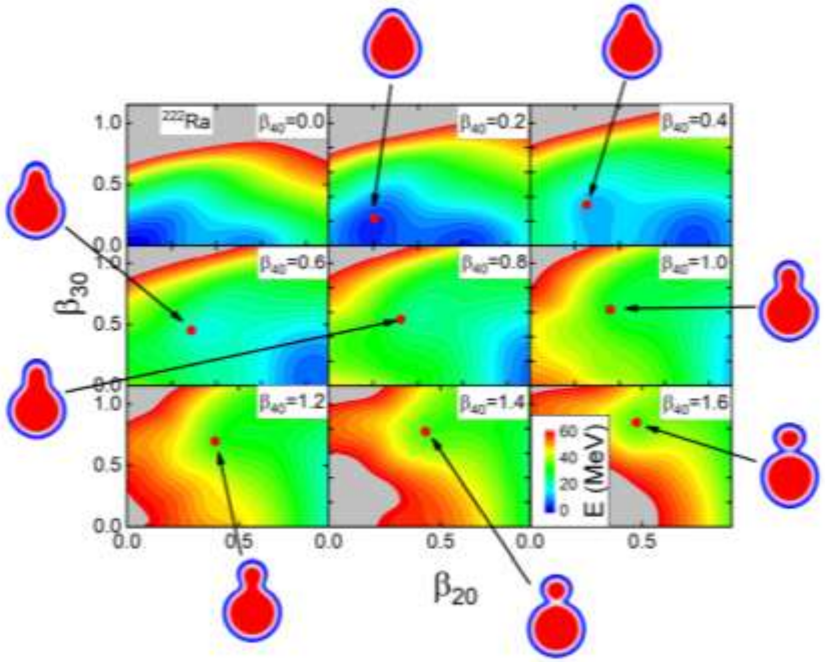
Mercier, Bjelčić, Nikšić, Ebran, Khan,Vretenar 2021
Mercier, Ebran, Khan 2022

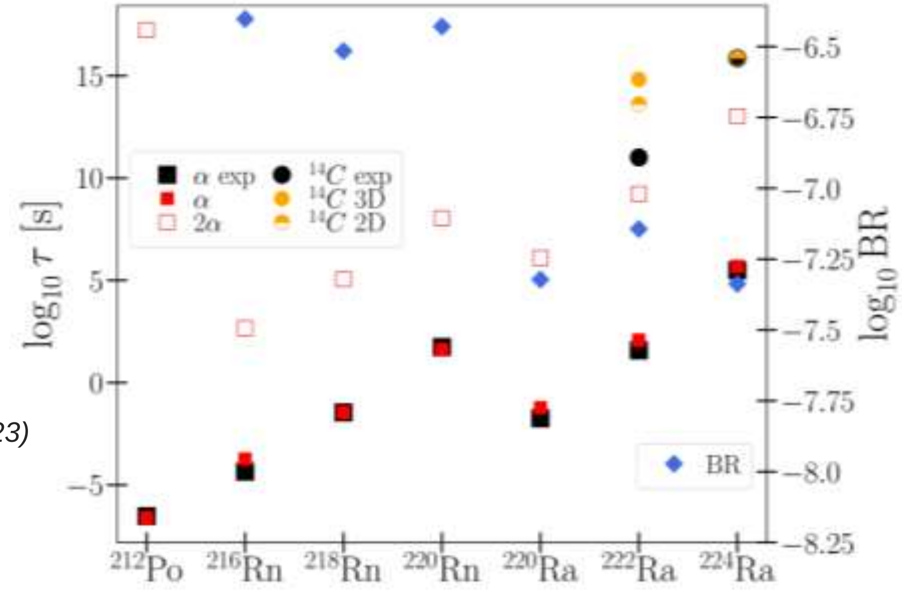


Cluster, α and 2α radioactivities



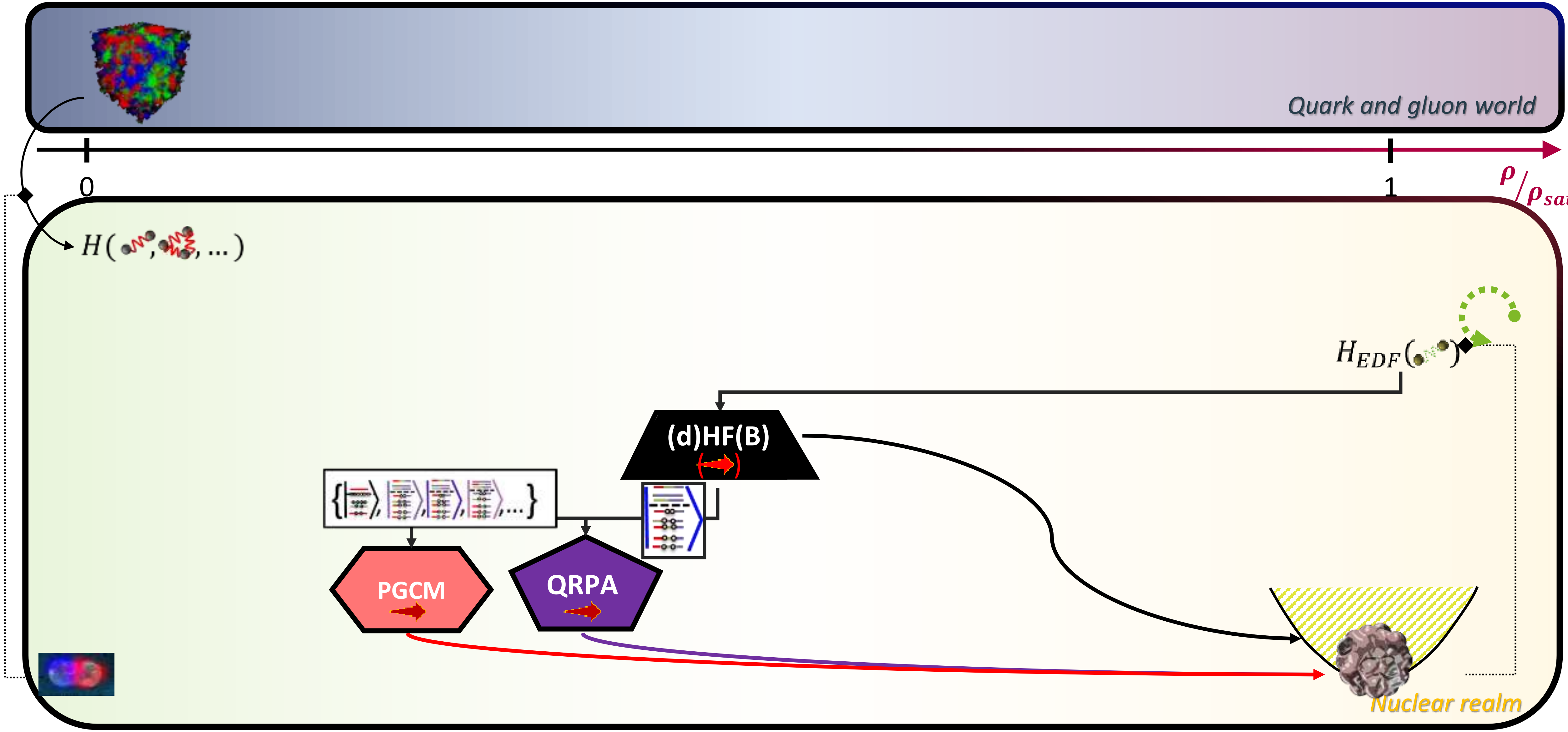






Zhao, Ebran, Heitz , Khan , Mercier, Nikšic,Vretenar PRC (2023)
Mercier, Zhao, Ebran, Khan, Nikšić, Vretenar PRL (2021)

EDF workflow



Outline

3. EDF-inspired ab initio metods

Ab initio strategy

◉ Solve in a controlled way, to some desired accuracy $H(\ldots, \ldots, \ldots)|\Psi_{\mu,\sigma}\rangle = E_{\mu\tilde{\sigma}}|\Psi_{\mu,\sigma}\rangle$

Which part of correlations should be treated here ?

--> Ab initio WFT : Expansion many-body methods

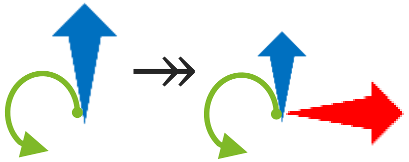
$$H = H_0 + H_1$$

$$|\Theta\rangle$$

$$|\Psi\rangle = \Omega|\Theta\rangle$$

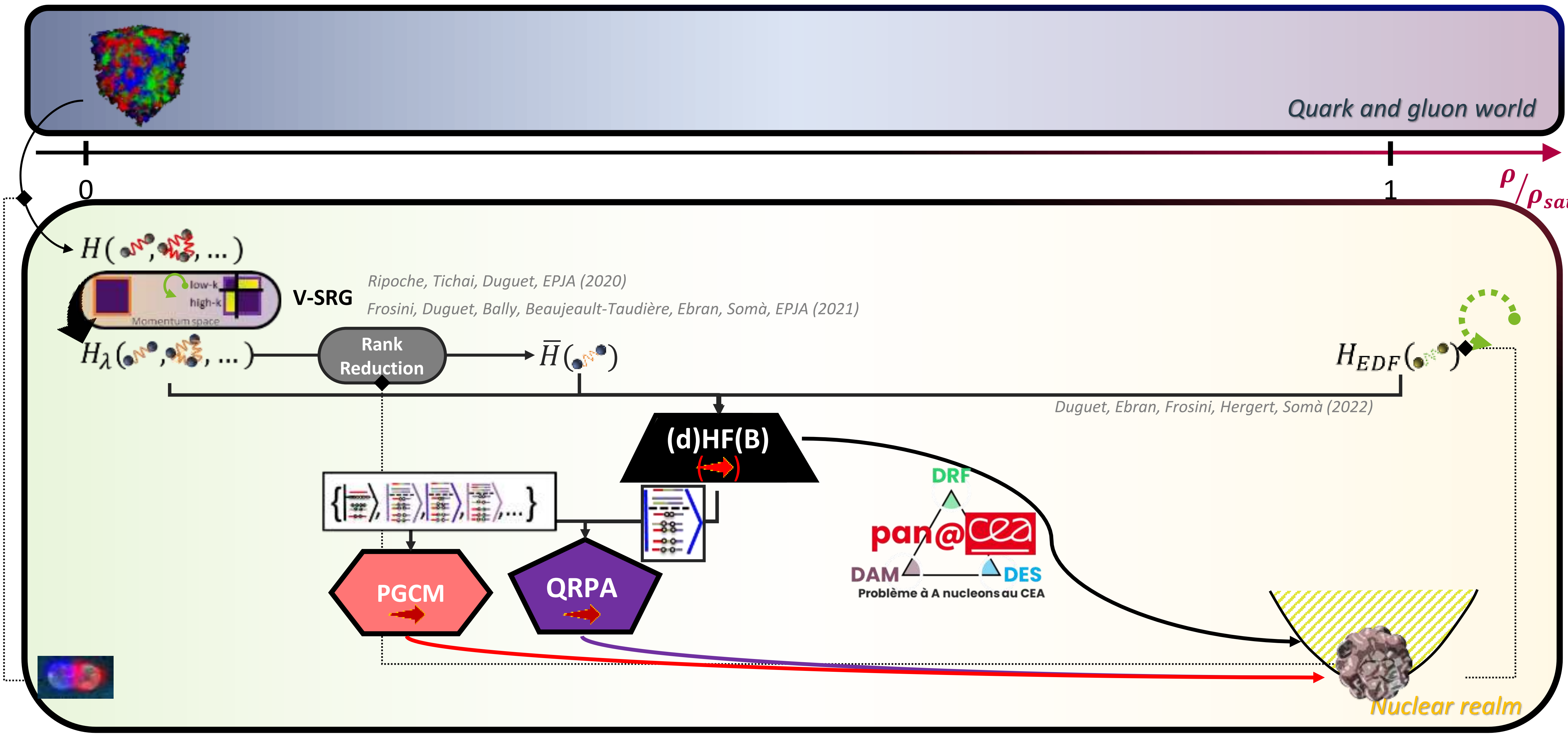
--> Get inspiration from EDFs to design new expansion methods working for both closed- and open-shell nuclei

Pioneering work by T. Duguet



Somà, Barbieri, Duguet, PRC (2014)
Duguet, JPG:NPP (2014)
Signoracci, Duguet, Hagen, Jansen PRC (2015)
Duguet, Signoracci JPG (2017)
Tichai, Arthuis, Duguet, Hergert, Somà, Roth PLB (2018)
Arthuis, Duguet, Tichai, Lasseri, Ebran CPC (2019)

DRF
pan@cea
DAM DES
Problème à A nucleons au CEA



Quark and gluon world
0
1
ρ/ρsat
H(, , ...)
low-k
high-k
Momentum space
V-SRG
Ripoche, Tichai, Duguet, EPJA (2020)
Frosini, Duguet, Bally, Beaujeault-Taudière, Ebran, Somà, EPJA (2021)
Hλ(, , ...)
Rank Reduction
H̄( )
HEDF( )
Duguet, Ebran, Frosini, Hergert, Somà (2022)
(d)HF(B)
DRF
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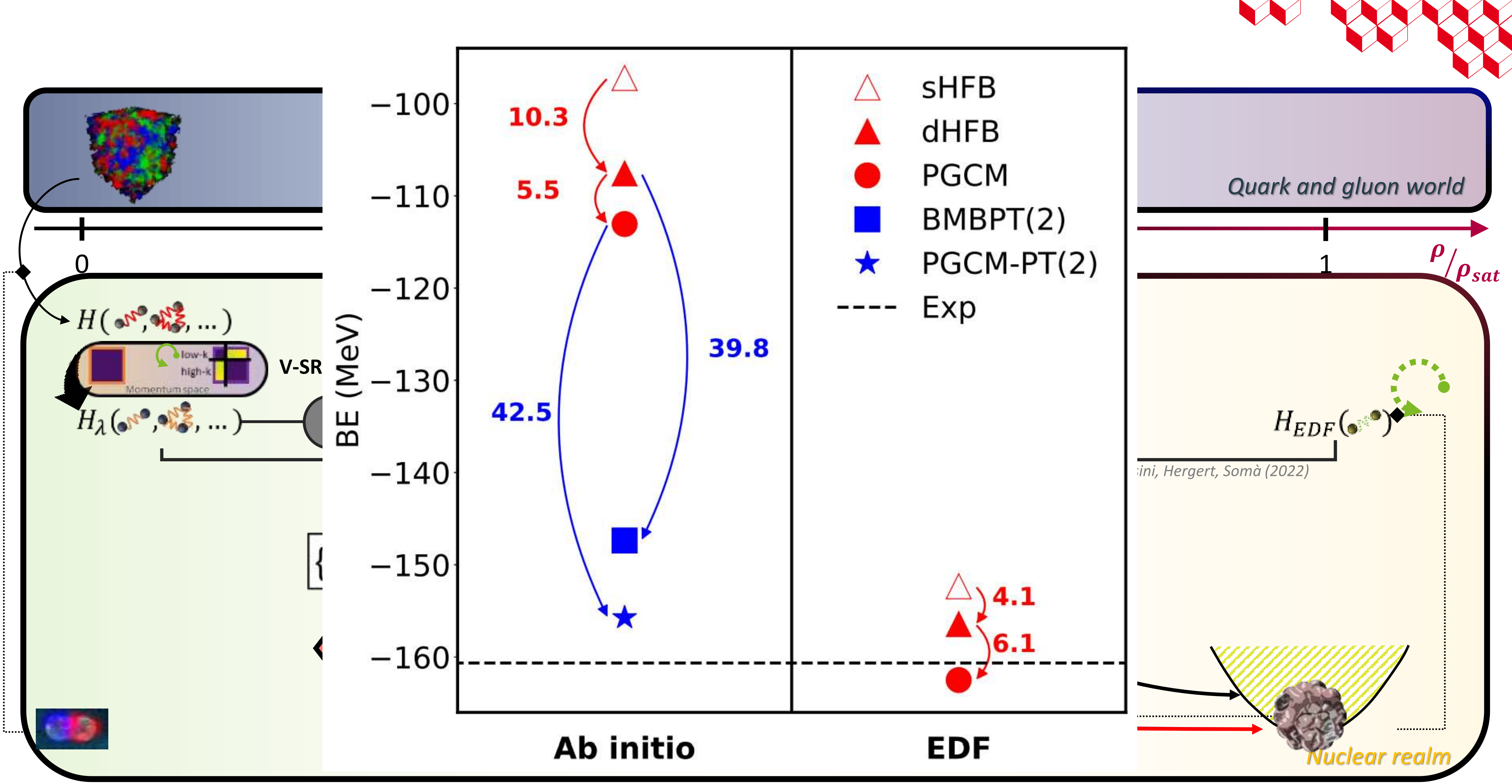
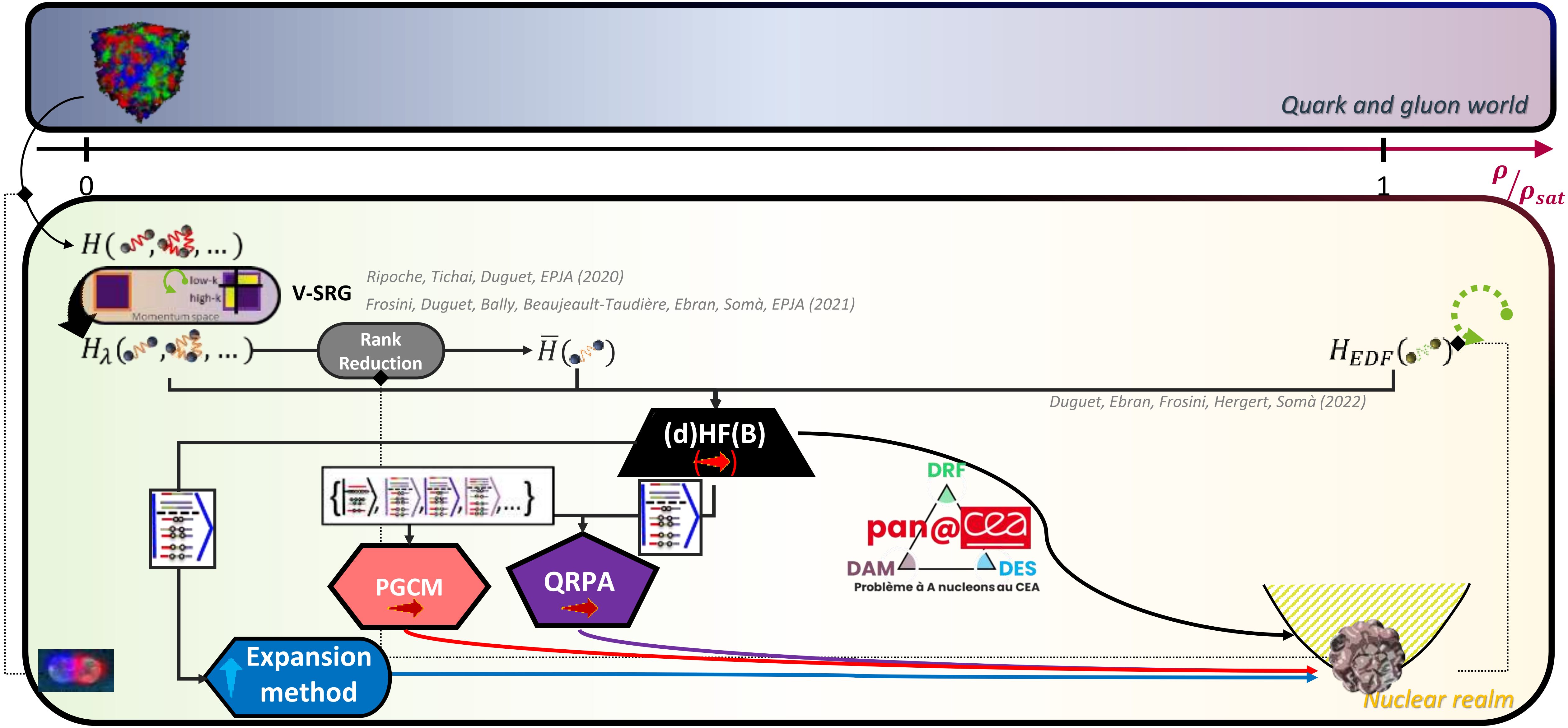
DAM
DES
Problème à A nucleons au CEA
PGCM
QRPA
Nuclear realm



Quark and gluon world
0
1
ρ/ρ_{sat}
$H(\ldots)$
low-k
high-k
Momentum space
V-SR
$H_\lambda(\ldots)$
$H_{EDF}(\ldots)$
…ini, Hergert, Somà (2022)
Nuclear realm
BE (MeV)
−100
−110
−120
−130
−140
−150
−160
10.3
5.5
42.5
39.8
4.1
6.1
sHFB
dHFB
PGCM
BMBPT(2)
PGCM-PT(2)
Exp
Ab initio
EDF


Quark and gluon world
0
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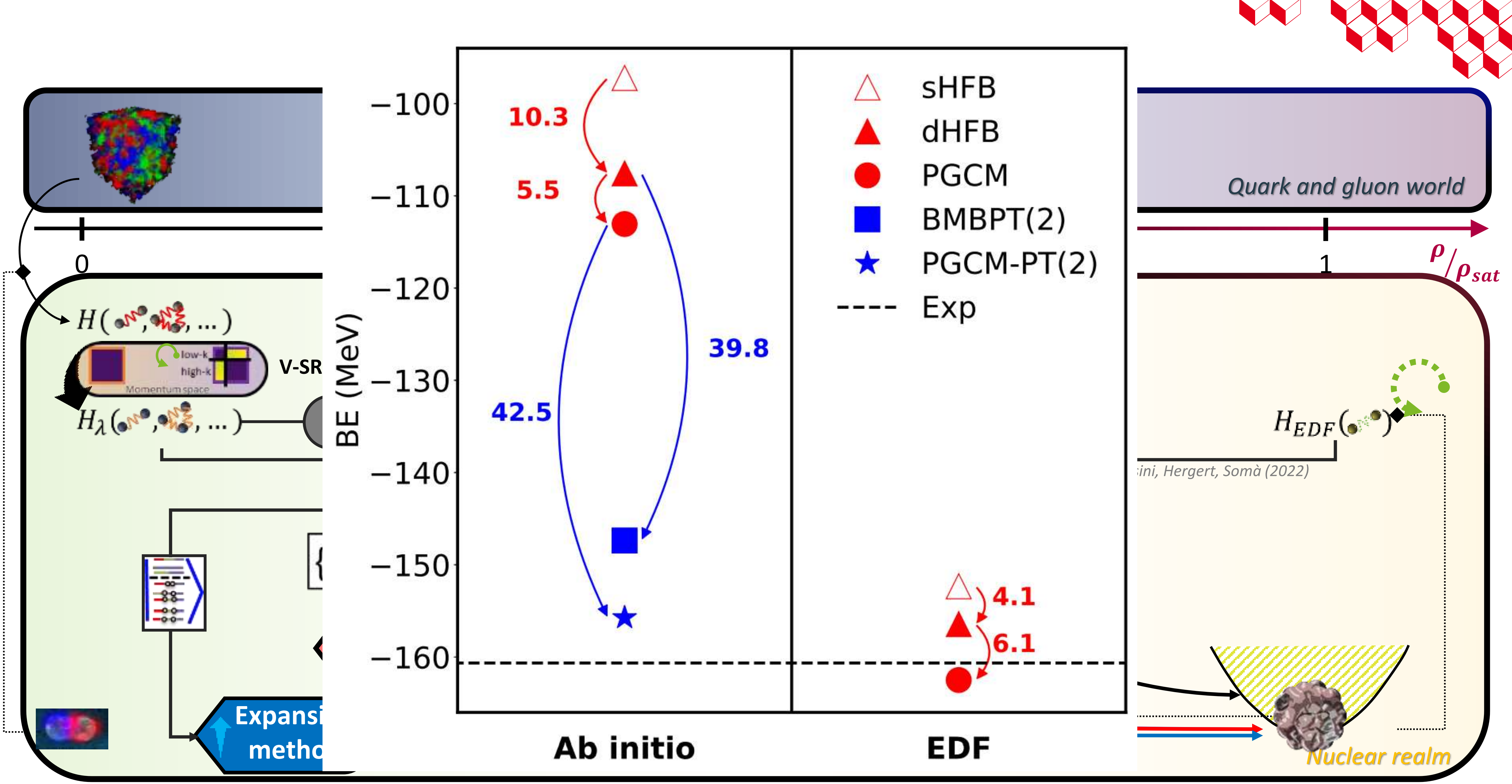
ρ/ρ_sat
H(, , ...)
low-k
high-k
Momentum space
V-SRG
Ripoche, Tichai, Duguet, EPJA (2020)
Frosini, Duguet, Bally, Beaujeault-Taudière, Ebran, Somà, EPJA (2021)
H_λ(, , ...)
Rank Reduction
H̄( )
H_EDF( )
Duguet, Ebran, Frosini, Hergert, Somà (2022)
(d)HF(B)
PGCM
QRPA
Expansion method
DRF
pan@cea
DAM
DES
Problème à A nucleons au CEA
Nuclear realm



Quark and gluon world
0
1
ρ/ρ_{sat}
$H($…$)$
V-SR
low-k
high-k
Momentum space
$H_\lambda($…$)$
Expansi
metho
$H_{EDF}($…$)$
…ini, Hergert, Somà (2022)
Nuclear realm
BE (MeV)
−100
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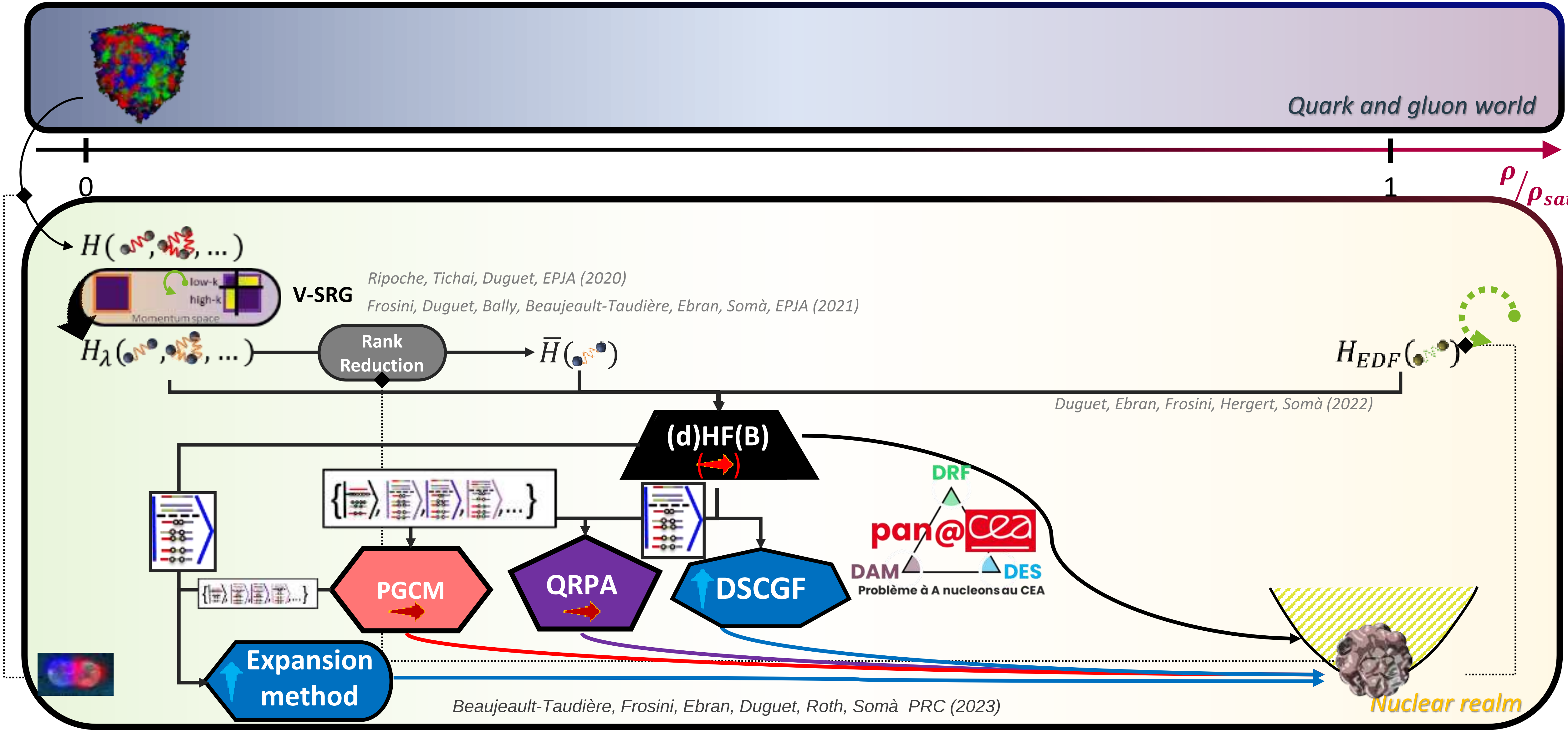
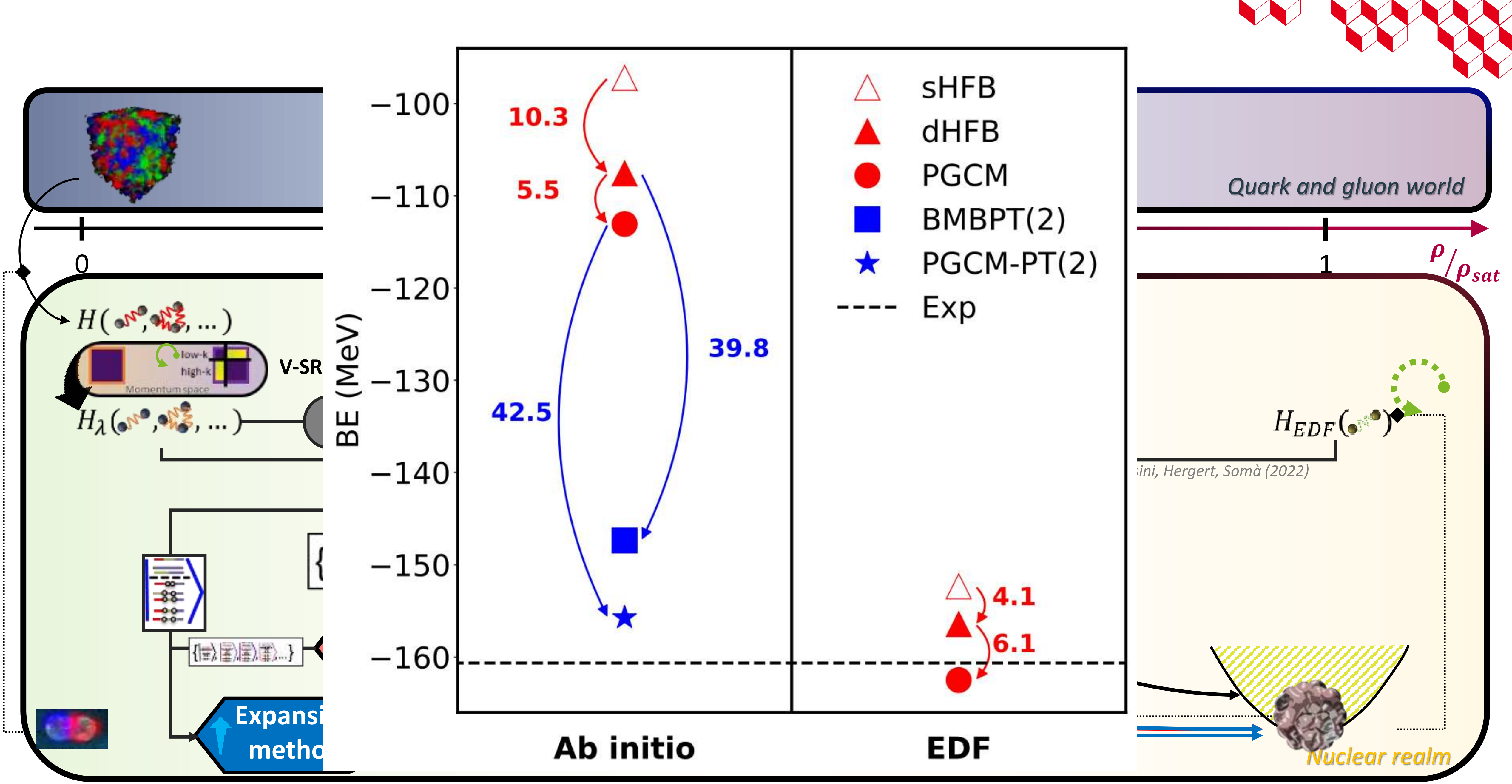
PGCM
BMBPT(2)
PGCM-PT(2)
Exp
Ab initio
EDF



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)

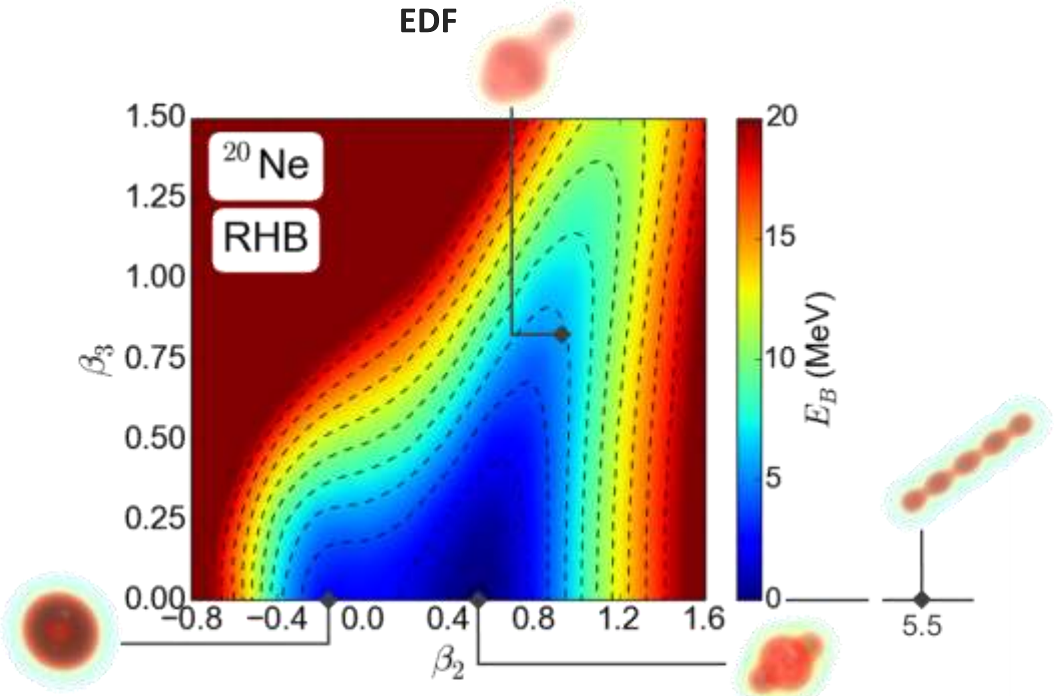


Frosini, Duguet, Ebran, Somà, EPJA (2022)
Frosini, Duguet, Ebran, Bally, Mongelli, Rodriguez, Roth,Somà, EPJA (2022)
Frosini, Duguet, Ebran, Bally, Hergert, Rodriguez, Roth, Yao, Somà, EPJA (2022)

PGCM-PT

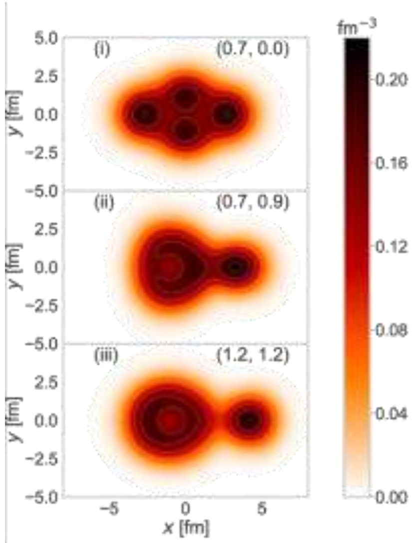
◉ Correlated GS

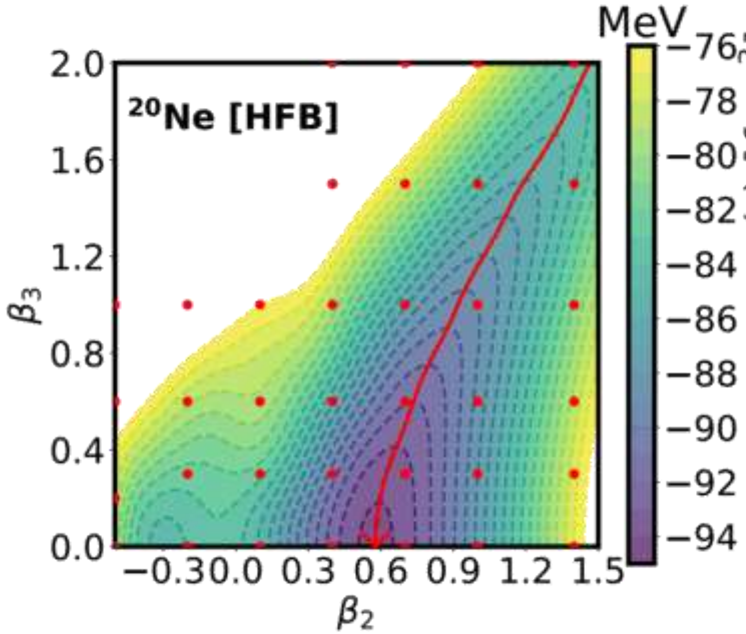
EDF

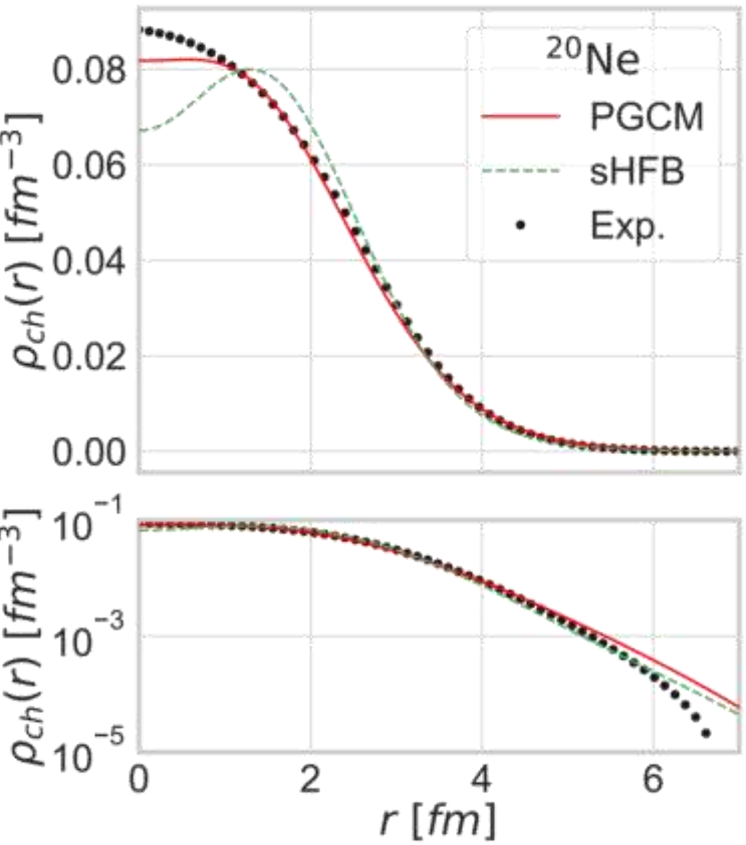


Marevic, Ebran, Khan, Niksic, Vretenar, PRC 97 (2018)

Ab initio



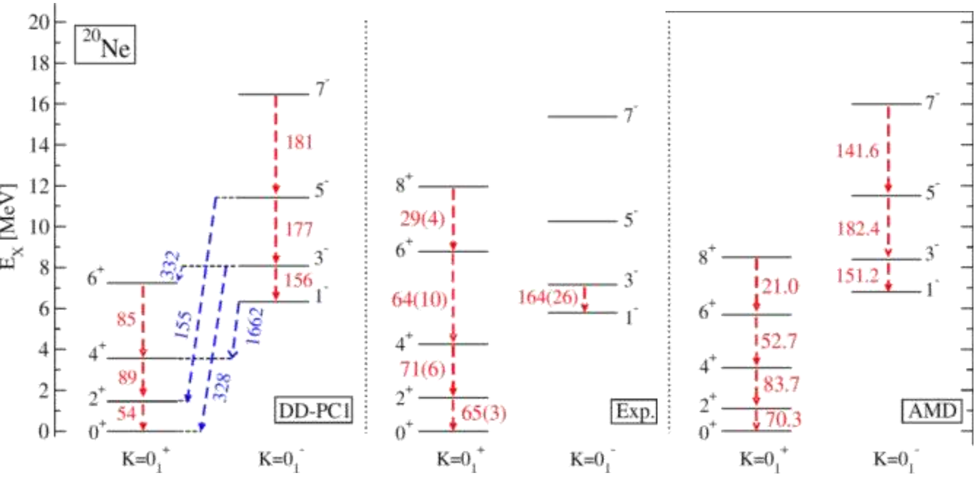




Frosini, Duguet, Ebran, Bally, Mongelli, Rodriguez, Roth, Somà, EPJA 2022

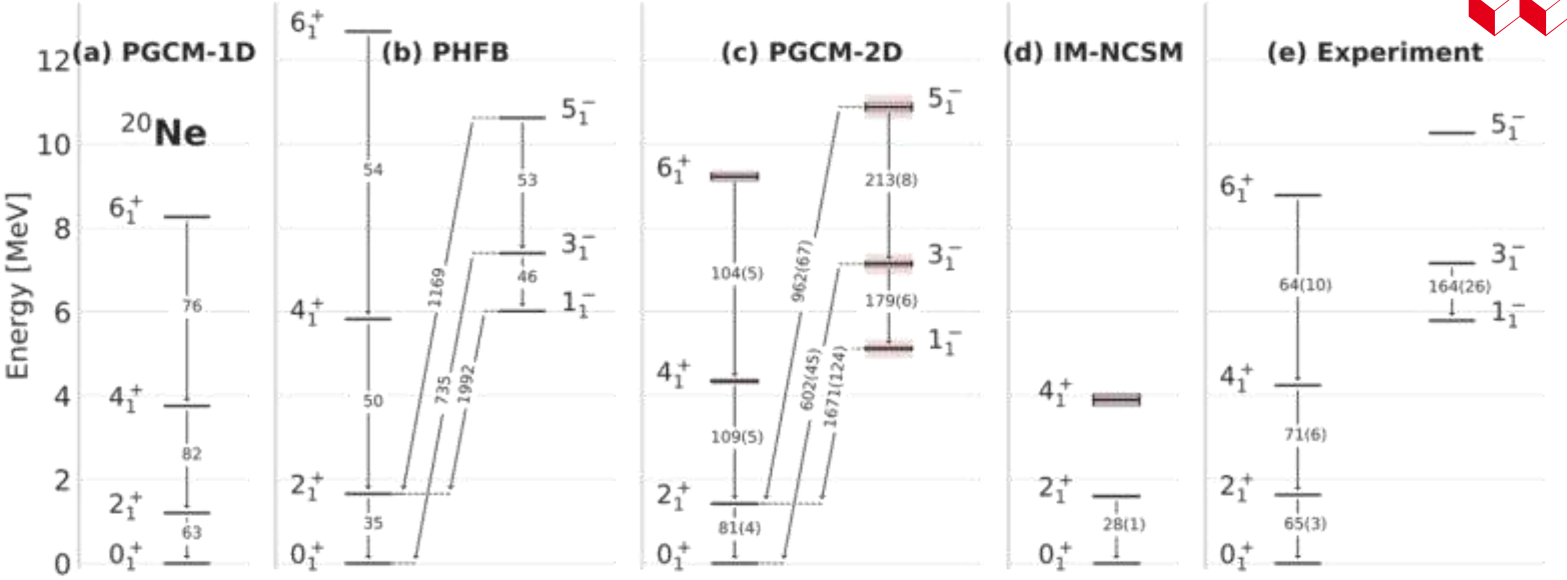
PGCM-PT

EDF

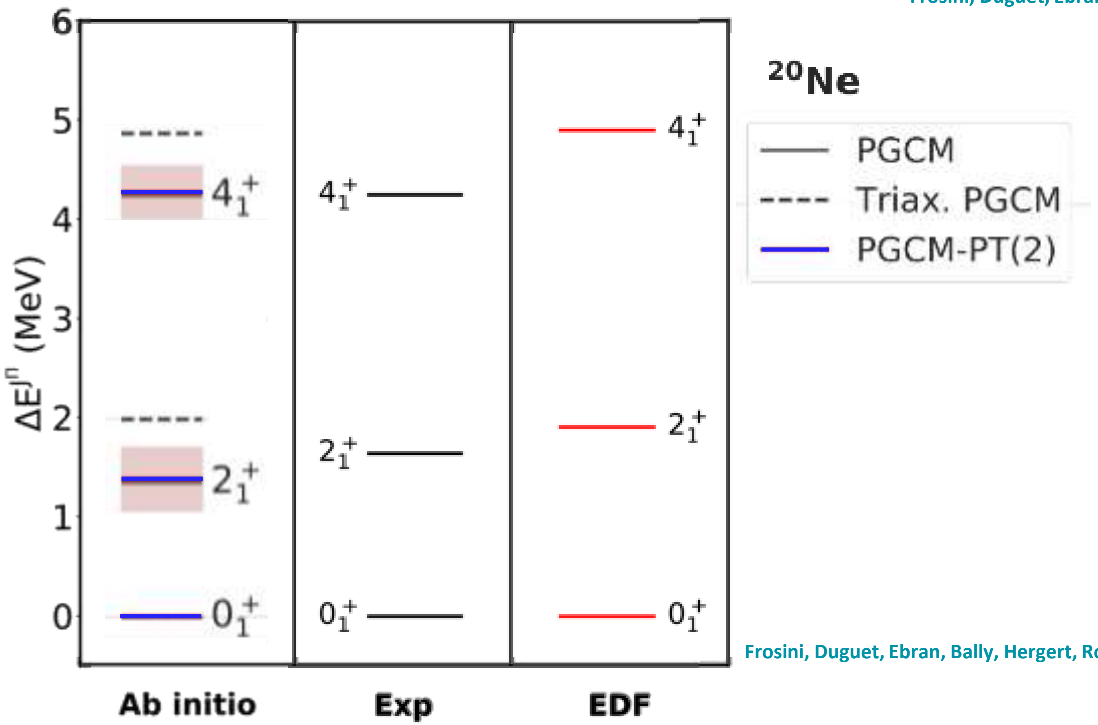


Marevic, Ebran, Khan, Niksic, Vretenar, 2018

Ab initio



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

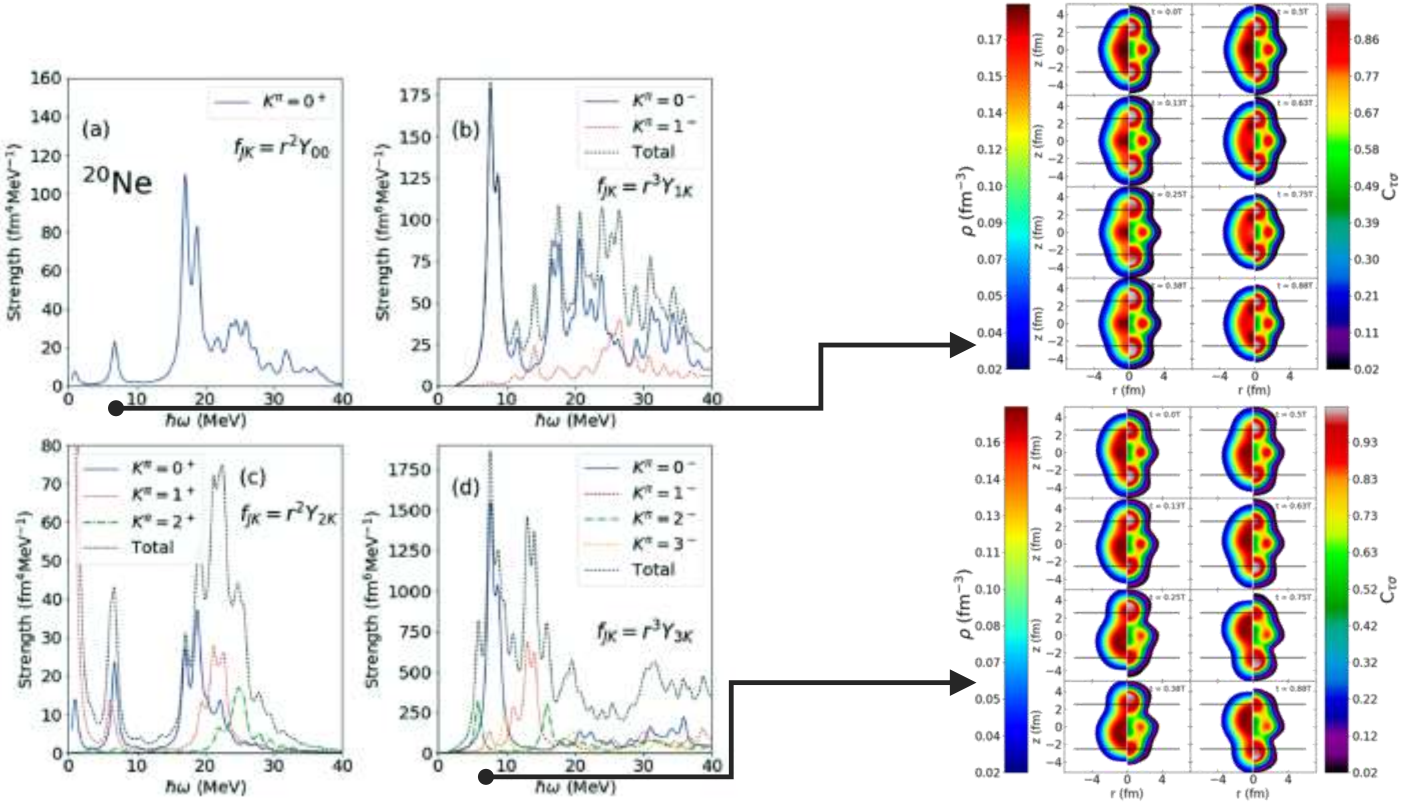


Frosini, Duguet, Ebran, Bally, Hergert, Rodriguez, Roth, Yao, Somà, EPJA 2022

QRPA (FAM)

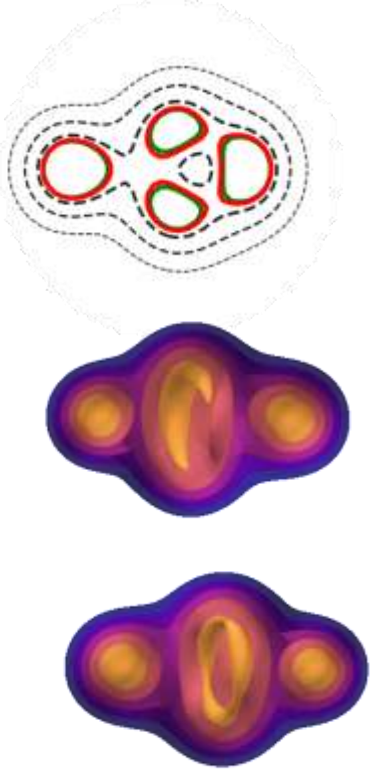
- Cluster vibration

EDF



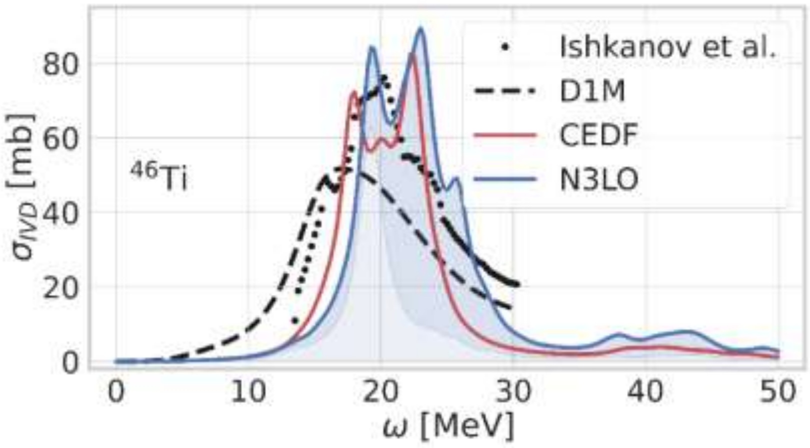
Mercier, Bjelčić, Nikšić, Ebran, Khan,Vretenar 2021
Mercier, Ebran, Khan 2022

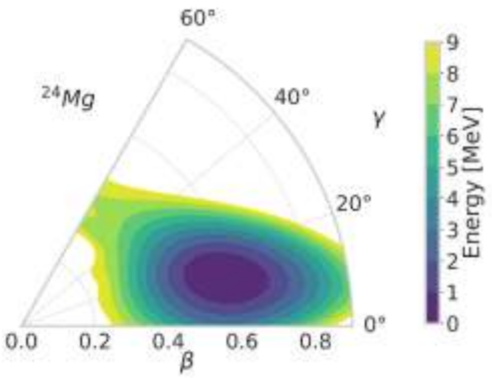
Ab initio

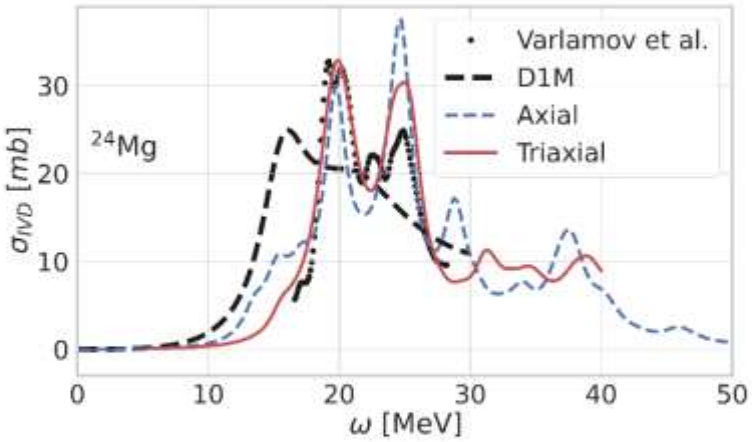


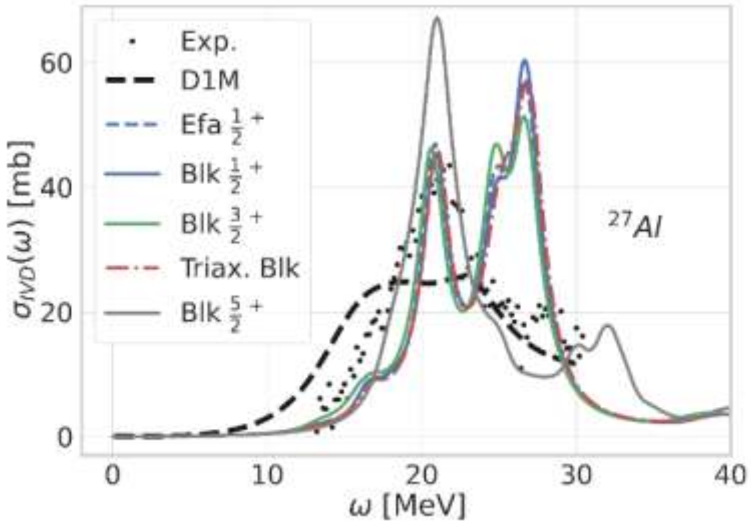
Ab initio QFAM time-dependent intrinsic density
Frosini, Ebran, Duguet, Somà, unpublished

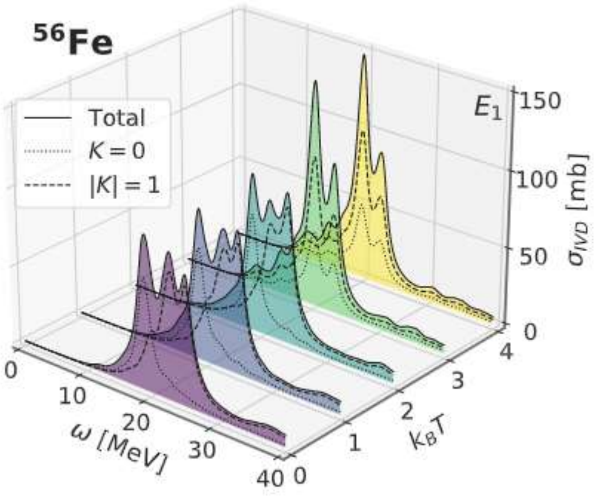
QRPA (FAM)











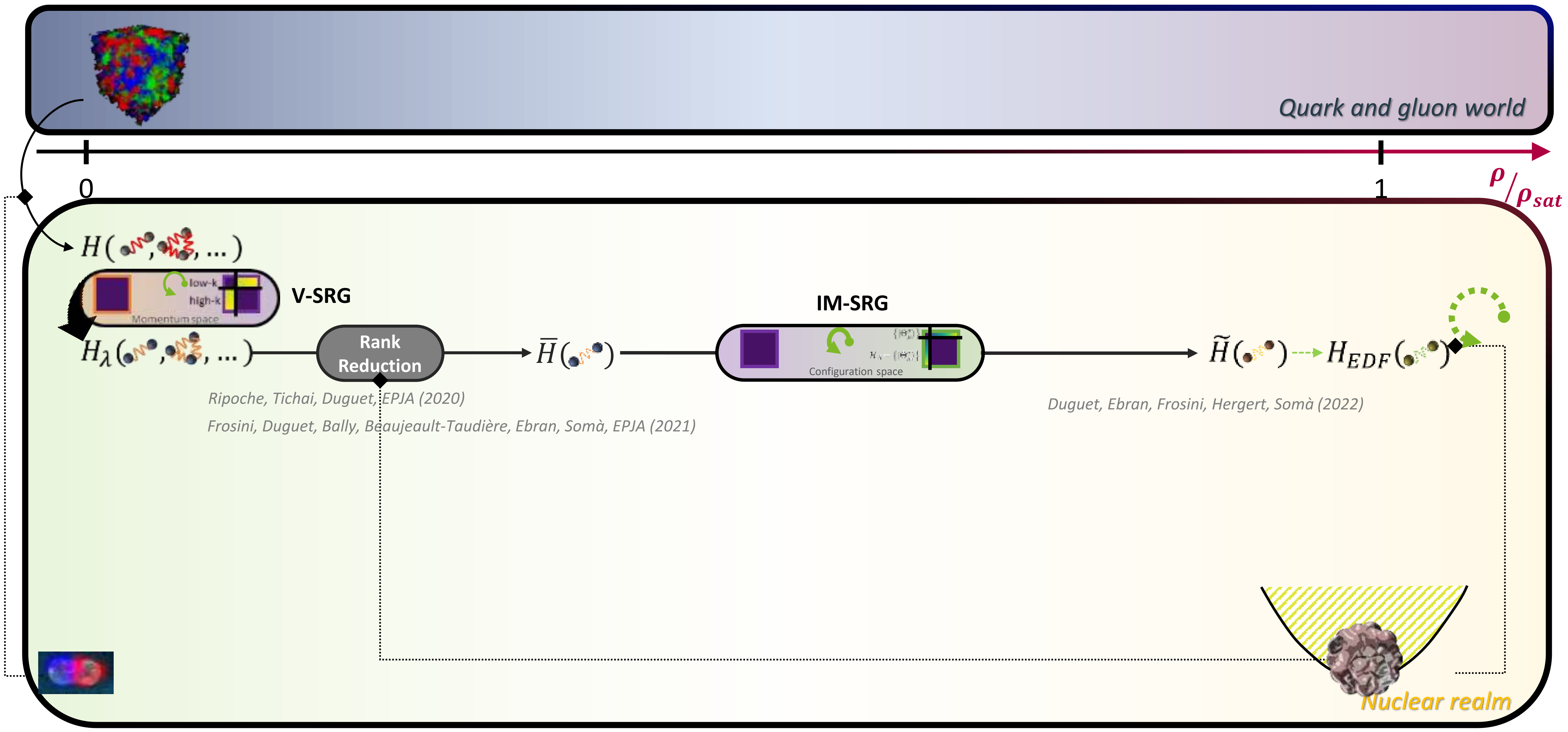
Beaujeault-Taudière, Frosini, Ebran, Duguet, Roth, Somà PRC (2023)
Frosini, Duguet, Ebran, Somà, unpublished

Outline

1. **General context**
2. **Recent work on empirical EDFs**
3. **EDF-inspired ab initio methods**
4. **Towards a first-principle formulation of EDFs**

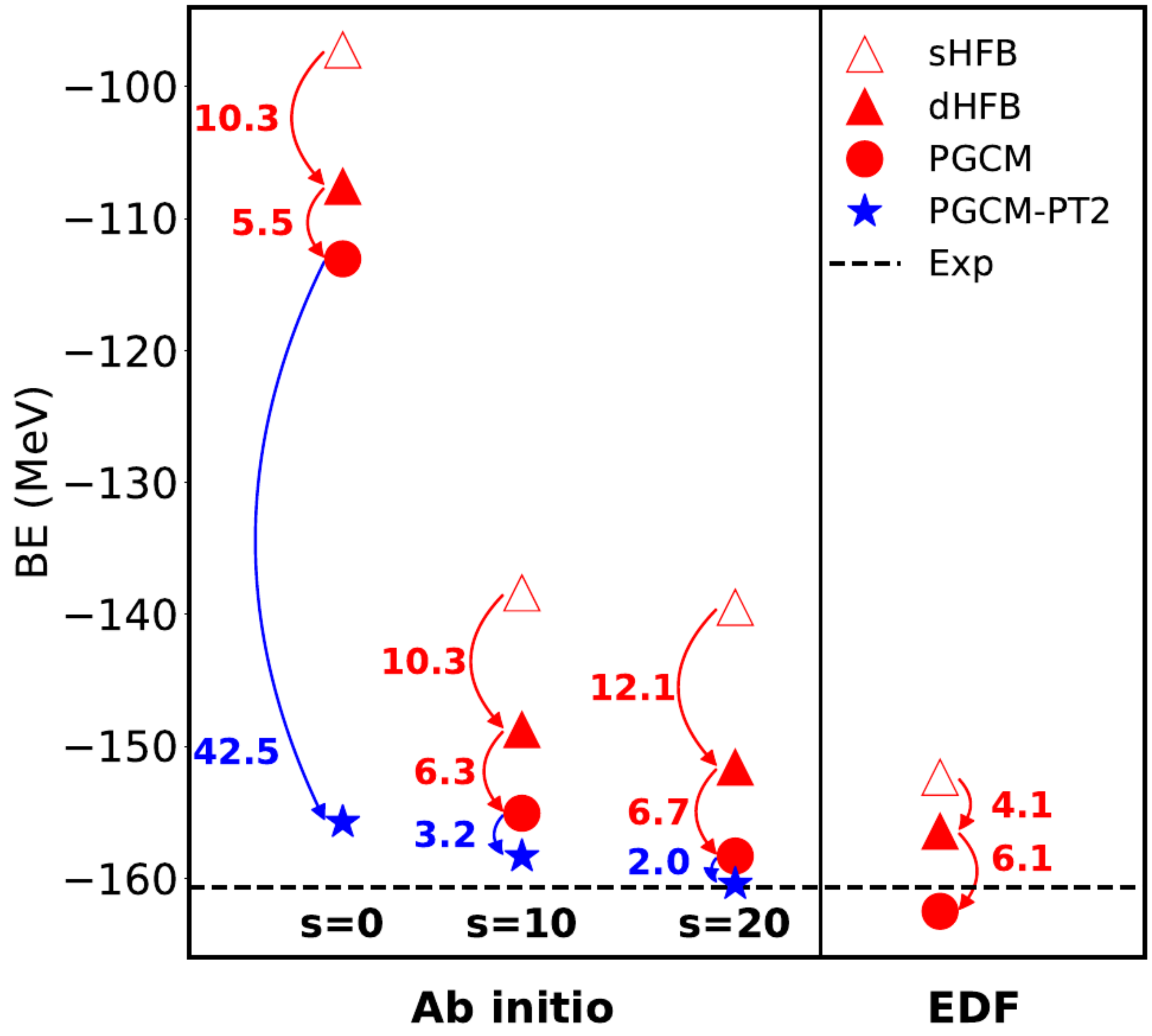
4. Towards a first-principle formulation of EDFs

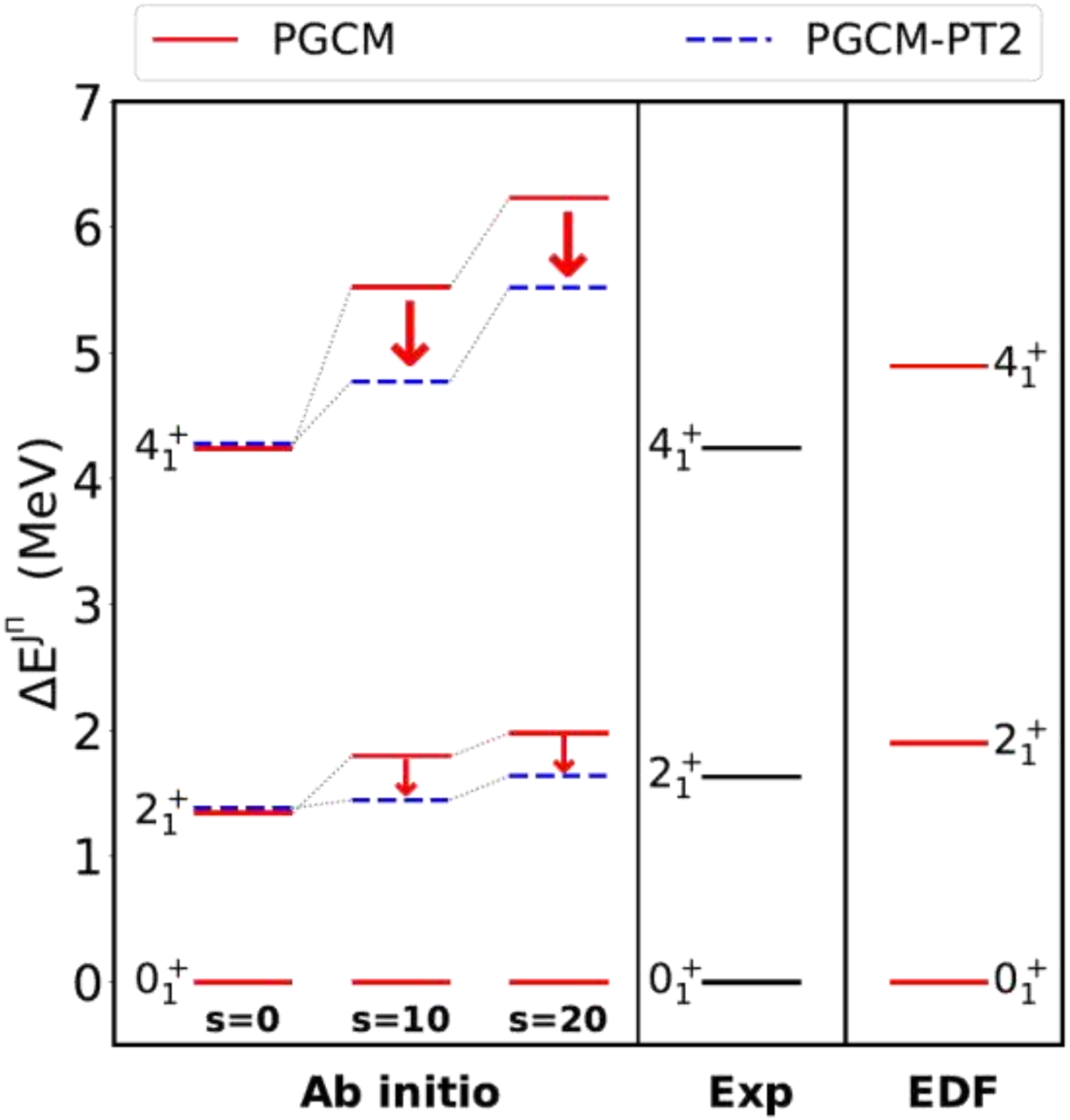
(EDF-inspired ab initio method)-inspired EDFs



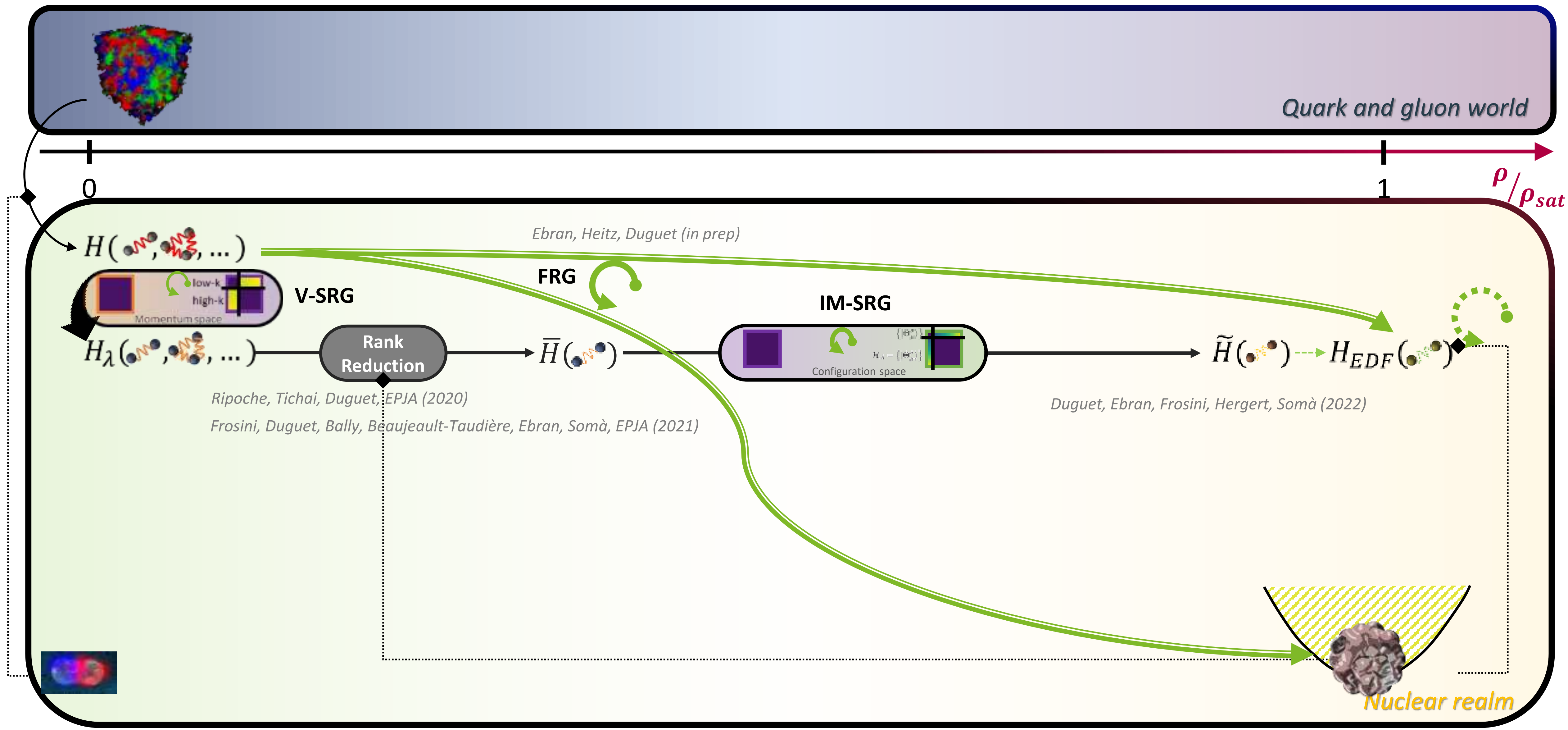
Quark and gluon world
0
1
ρ/ρ_{sat}
$H(\ldots)$
low-k
high-k
Momentum space
V-SRG
$H_\lambda(\ldots)$
Rank Reduction
$\overline{H}$
IM-SRG
Configuration space
$\widetilde{H}$
H_{EDF}
Ripoche, Tichai, Duguet, EPJA (2020)
Frosini, Duguet, Bally, Beaujeault-Taudière, Ebran, Somà, EPJA (2021)
Duguet, Ebran, Frosini, Hergert, Somà (2022)
Nuclear realm

Non empirical EDFs via IM-SRG





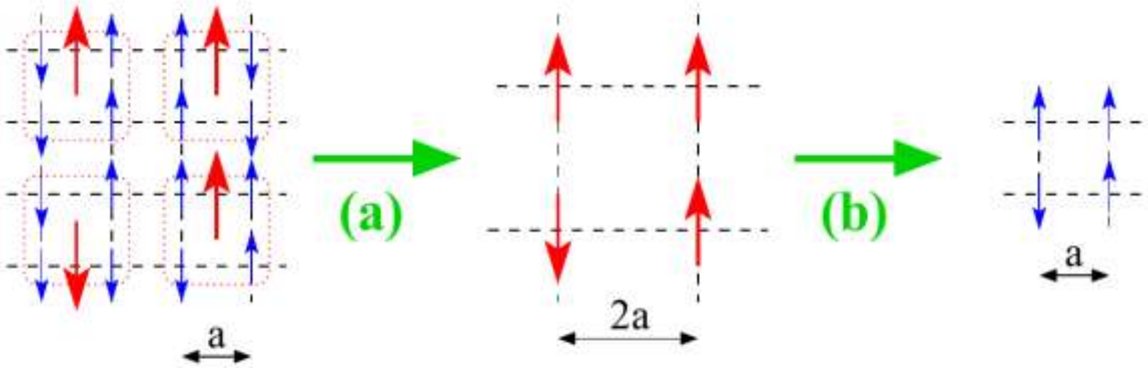
Duguet, Ebran, Frosini, Hergert, Somà EPJA (2023)



Quark and gluon world
0
1
ρ/ρ_{sat}
$H(\ldots)$
Ebran, Heitz, Duguet (in prep)
FRG
V-SRG
low-k
high-k
Momentum space
$H_\lambda(\ldots)$
Rank Reduction
$\bar{H}(\ldots)$
IM-SRG
Configuration space
$\tilde{H}(\ldots)$
$H_{EDF}(\ldots)$
Ripoche, Tichai, Duguet, EPJA (2020)
Frosini, Duguet, Bally, Beaujeault-Taudière, Ebran, Somà, EPJA (2021)
Duguet, Ebran, Frosini, Hergert, Somà (2022)
Nuclear realm

Non empirical EDFs via FRG

◉ Renormalization group transformation : Wilson-Kadanoff procedure



$\mathcal{H}_k[\{S_i^k\}]$

$\mathcal{H}_0[\{S_i^0\}]$ Decimation Renormalization $\mathcal{H}_1[\{S_i^1\}]$

◉ Renormalization group transformation : FRG

--> Central object of FRG : scale-dependent (or average) effective action Γ_k interpolating between the S and Γ

$\Gamma_{k=\Lambda}[\varphi_\Lambda] = S[\psi]$ $\quad k = \Lambda$

↓

$\Gamma_k[\varphi_k]$ $\quad k$

↓

$\Gamma_{k=0}[\varphi_0] = \Gamma[\varphi]$ $\quad k = 0$

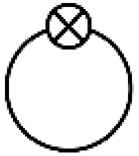
Incorporation of fluctuations of modes with $q > k$

--> Mass term $\quad S + \Delta S_k \qquad \Delta S_k = \frac{1}{2}\int \psi^\dagger(q) R_k(q) \psi(-q)$

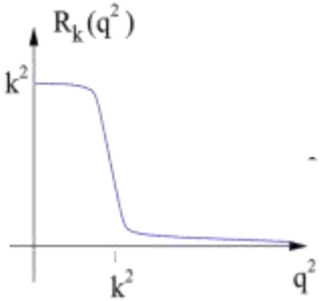
--> Exact RG (or Wetterich) equation

$$\partial_k \Gamma_k[\varphi] = \frac{1}{2}\,\mathrm{tr}\left\{\partial_k R_k \left(\Gamma_k^{(2)}[\varphi] + R_k\right)^{-1}\right\}$$

$$\partial_k \Gamma_k[\overline{\psi}, \psi] = -\,\mathrm{tr}\left\{\partial_k R_k \left(\Gamma_k^{(1,1)}[\overline{\psi}, \psi] + R_k\right)^{-1}\right\} =$$

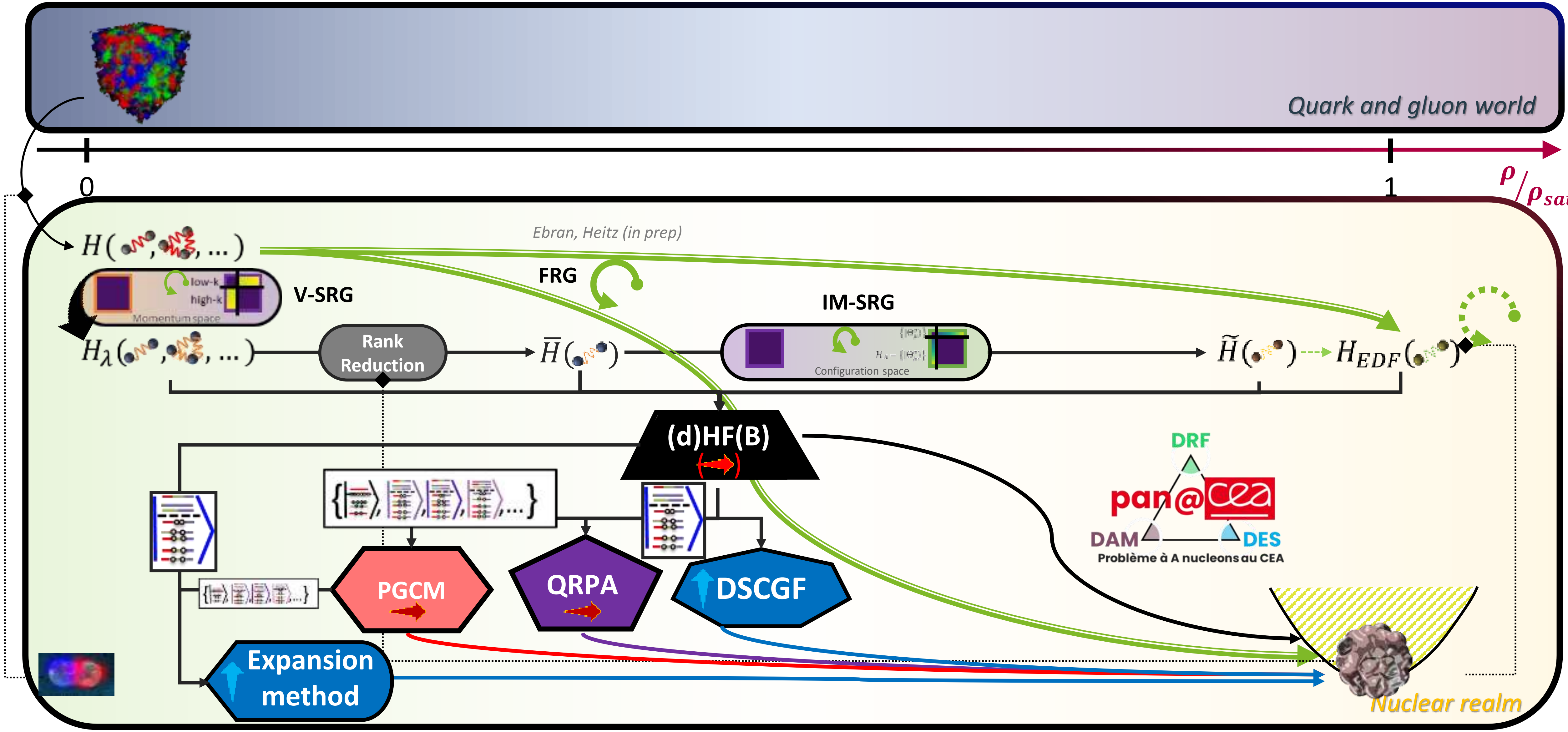


$$\Gamma_k^{(a)}[\varphi] = \frac{\delta^a}{\delta \varphi^a}\Gamma_k[\varphi]$$



$$\Gamma_k^{(a,b)}[\psi, \overline{\psi}] = \frac{\overrightarrow{\delta^a}}{\delta \overline{\psi}^a}\Gamma_k[\psi, \overline{\psi}]\frac{\overleftarrow{\delta^b}}{\delta \psi^b}$$

Conclusion



Quark and gluon world
0
1
ρ/ρ_{sat}
Ebran, Heitz (in prep)
$H(\ldots)$
low-k
high-k
Momentum space
V-SRG
FRG
IM-SRG
$H_\lambda(\ldots)$
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DRF
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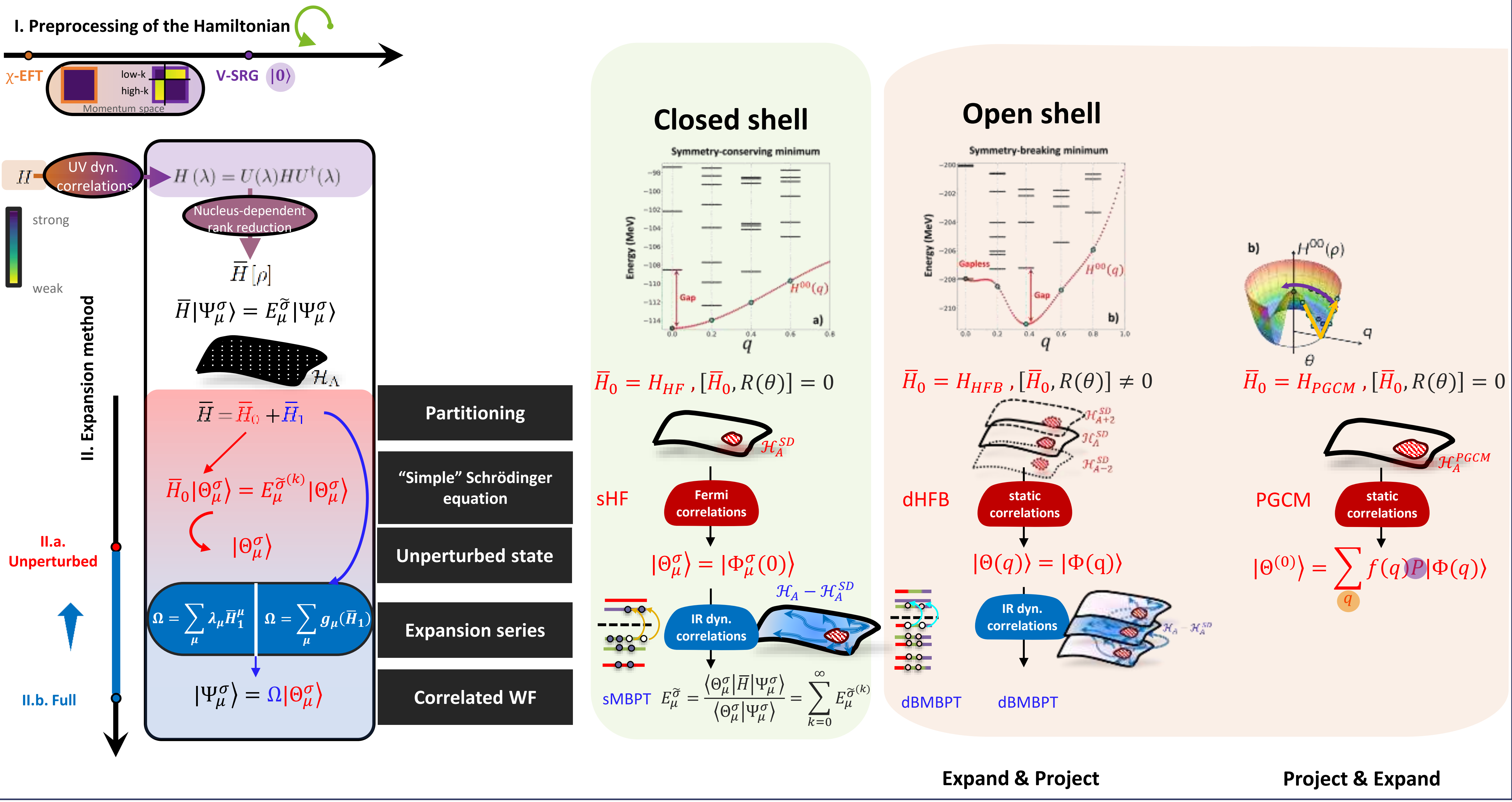
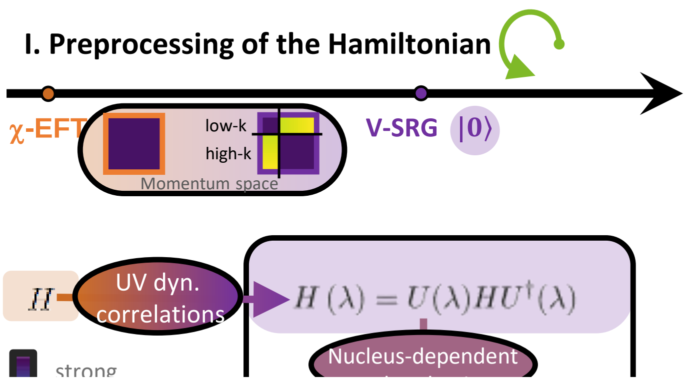
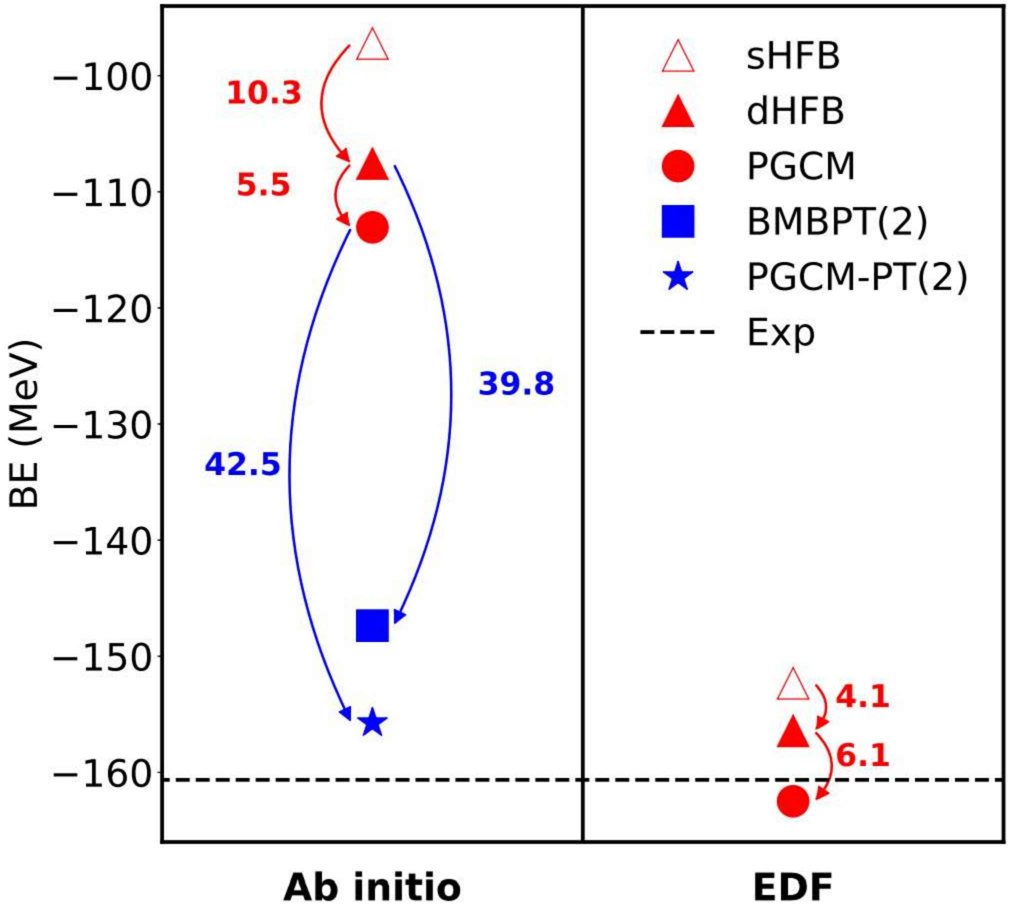
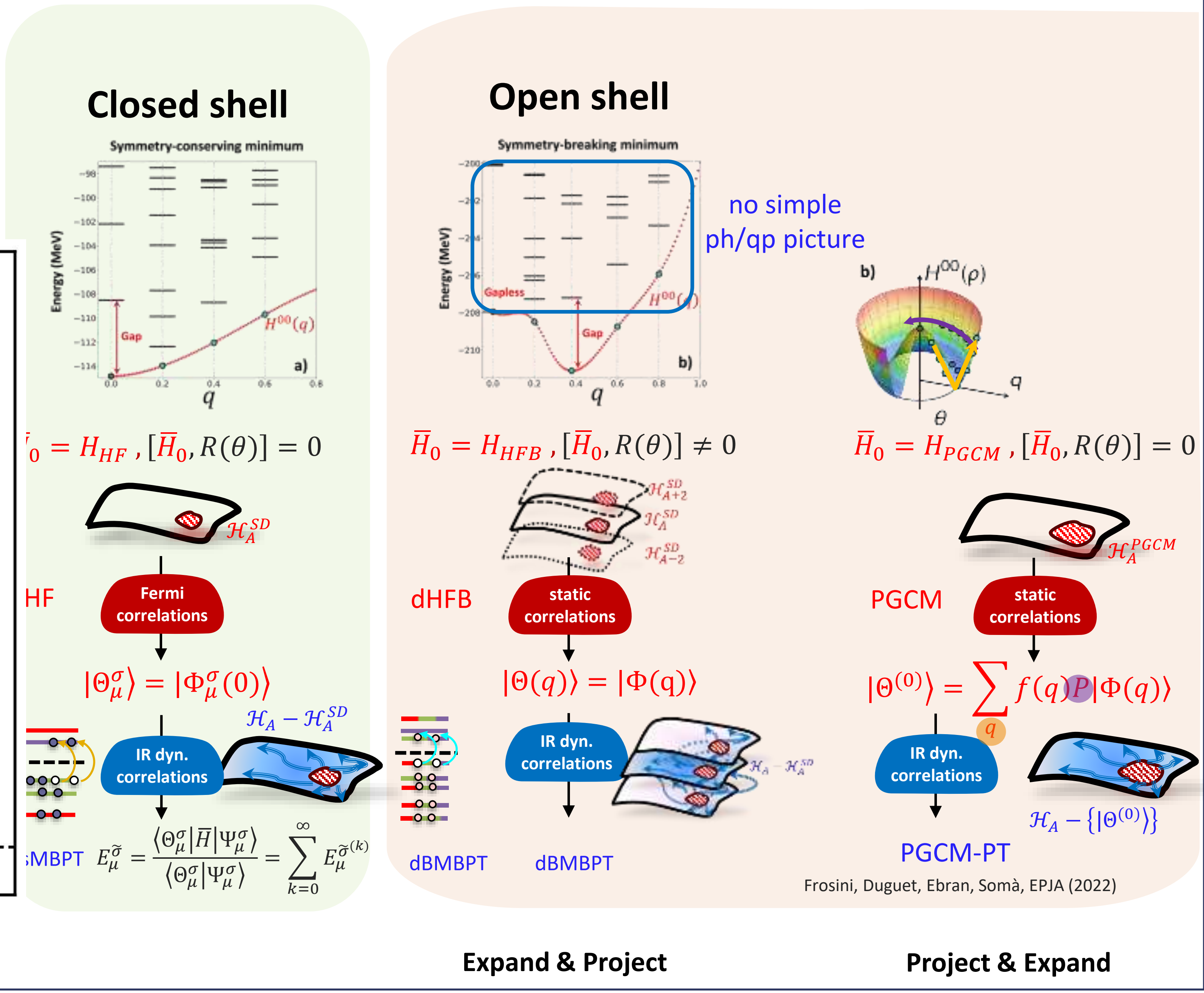
DAM
DES
Problème à A nucleons au CEA
PGCM
QRPA
DSCGF
Expansion method
Nuclear realm

Thank you for your attention


I. Preprocessing of the Hamiltonian
χ-EFT
low-k
high-k
Momentum space
V-SRG
|0⟩
UV dyn. correlations
strong
weak
II. Expansion method
Nucleus-dependent rank reduction
Partitioning
"Simple" Schrödinger equation
Unperturbed state
Expansion series
Correlated WF
II.a. Unperturbed
II.b. Full
Closed shell
Symmetry-conserving minimum
Energy (MeV)
Gap
a)
Open shell
Symmetry-breaking minimum
Gapless
Gap
b)
sHF
Fermi correlations
IR dyn. correlations
sMBPT
dHFB
static correlations
IR dyn. correlations
dBMBPT
dBMBPT
PGCM
static correlations
Expand & Project
Project & Expand



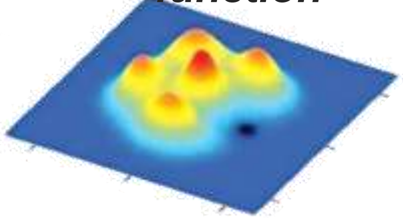




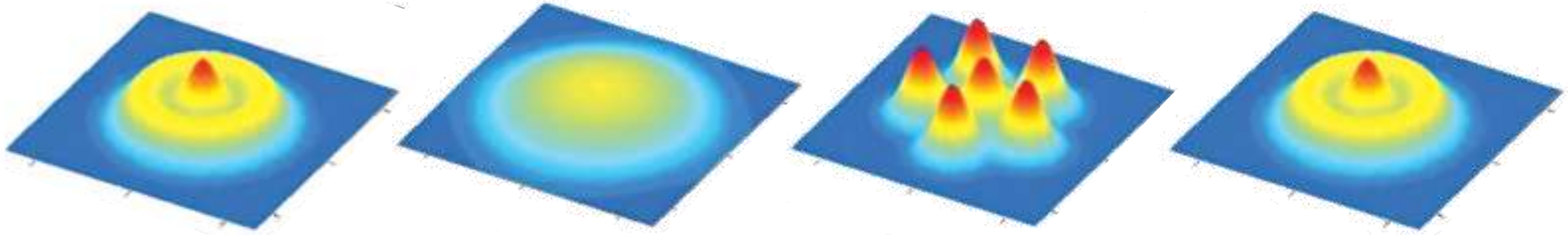
Frosini, Duguet, Ebran, Somà, EPJA (2022)

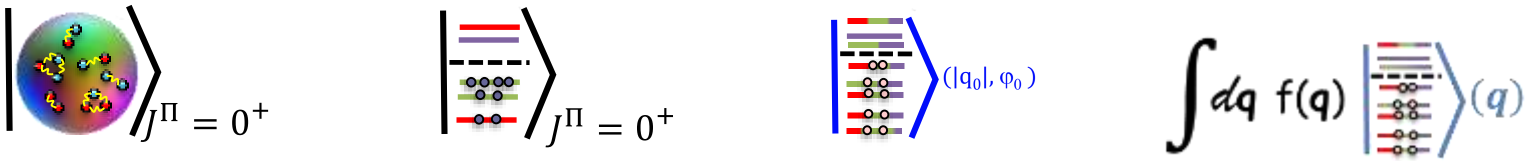
Nuclear clustering & PGCM

2-point correlation function



Density profile



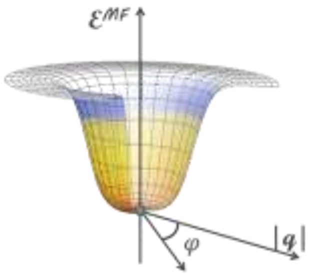


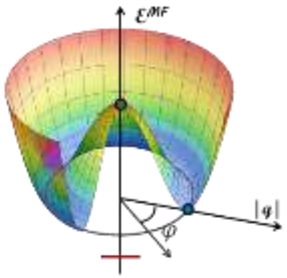
Exact WF

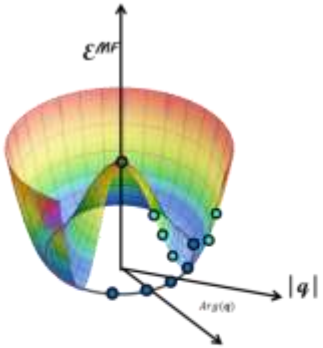
Approx :
Symmetry-preserving HF WF

Approx :
Symmetry-broken HFB WF

Approx :
PGCM WF



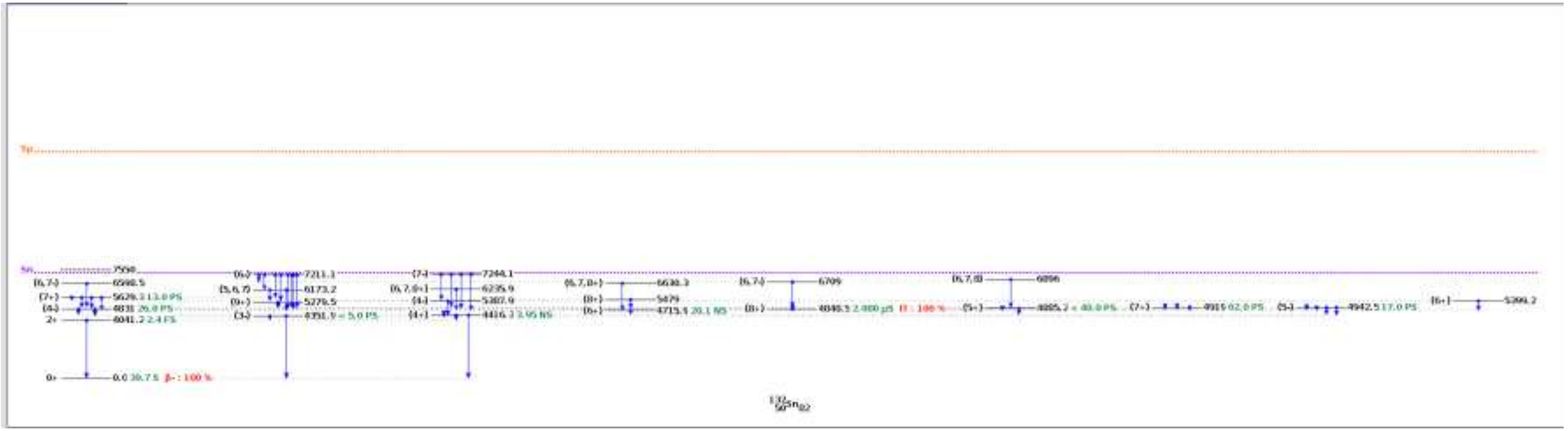


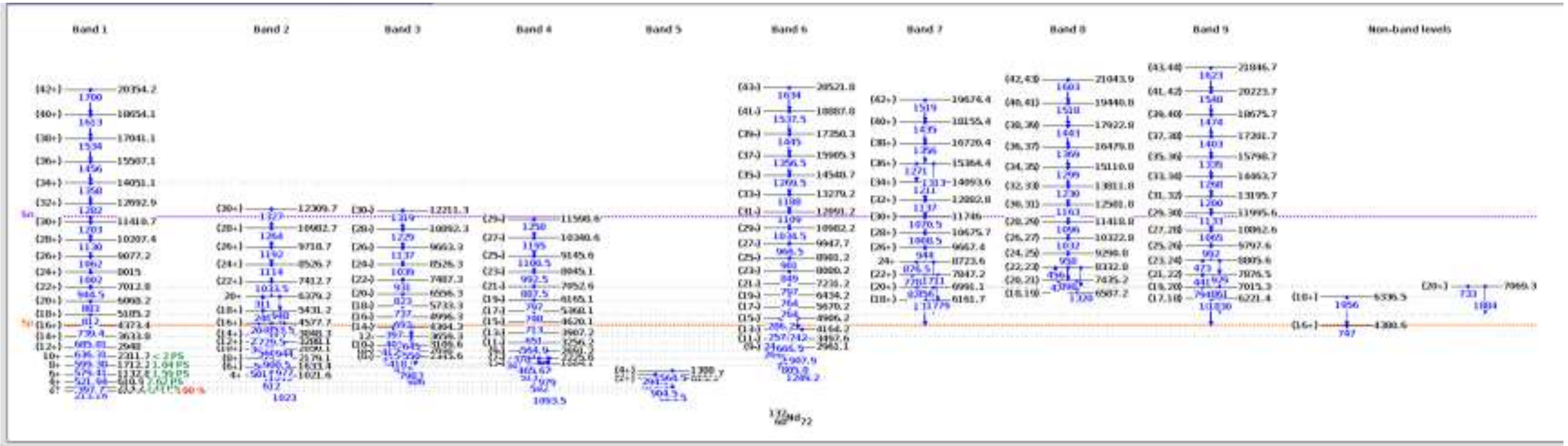


Spectroscopy

Yannouleas & Landman, 2017

Nuclear clustering & PGCM





DRF

pan@

DAM DES

Problème à A nucleons au CEA