Causes and consequences of the emergence of clusters in nuclei

J.-P. Ebran

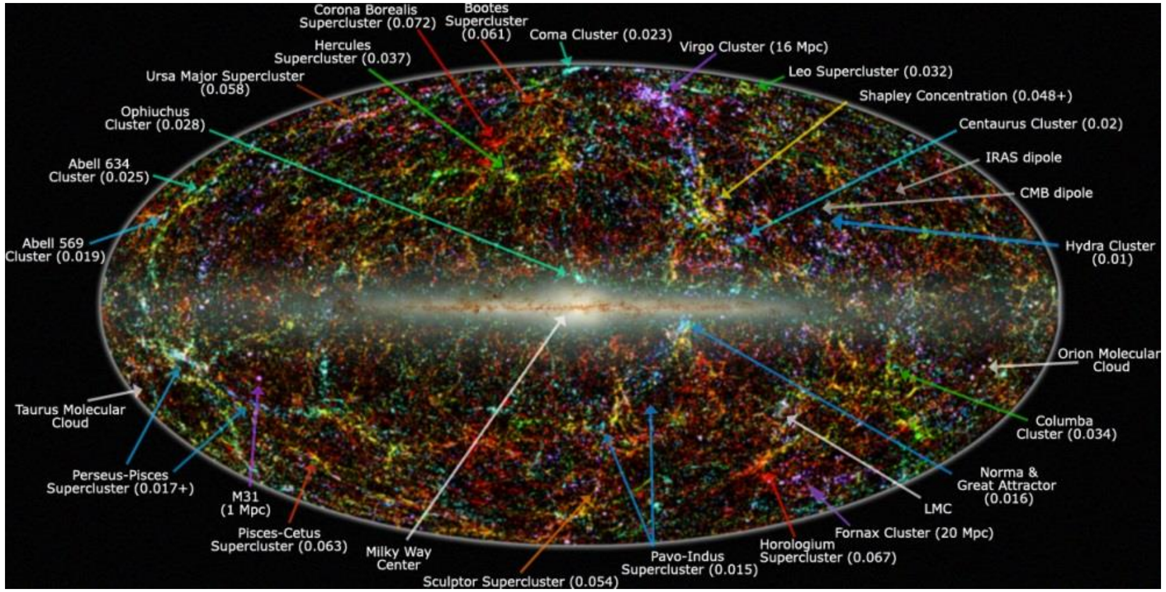
CEA,DAM,DIF

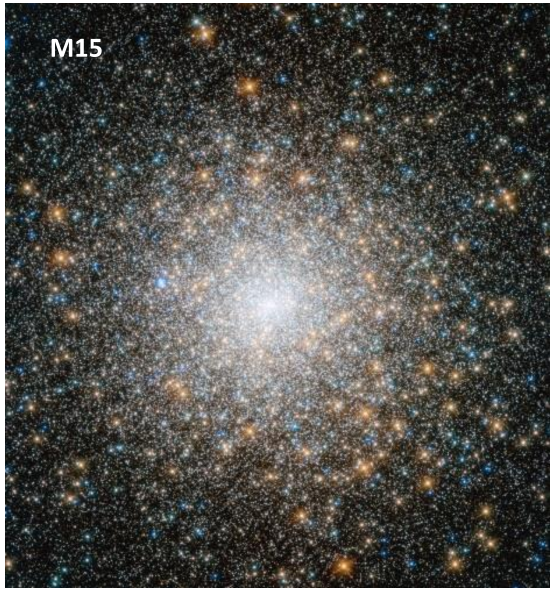
Conference on Quantum-Many-Body Correlations in memory of Peter Schuck

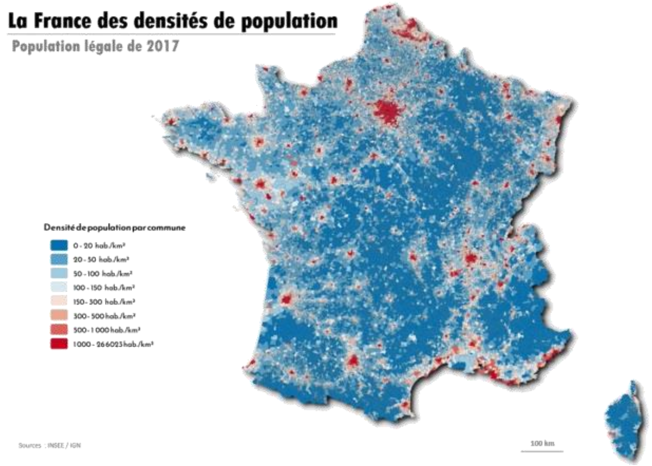
21-23 March 2023

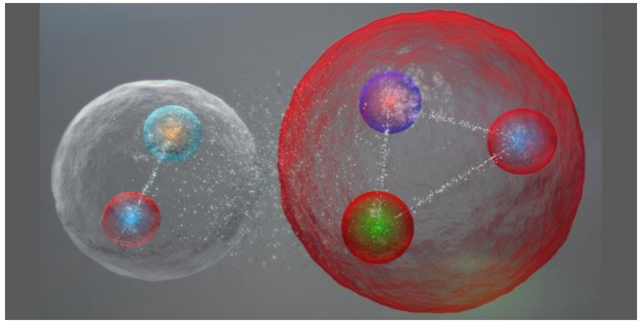
Clustering

◉ Clustering : an ubiquitous phenomenon



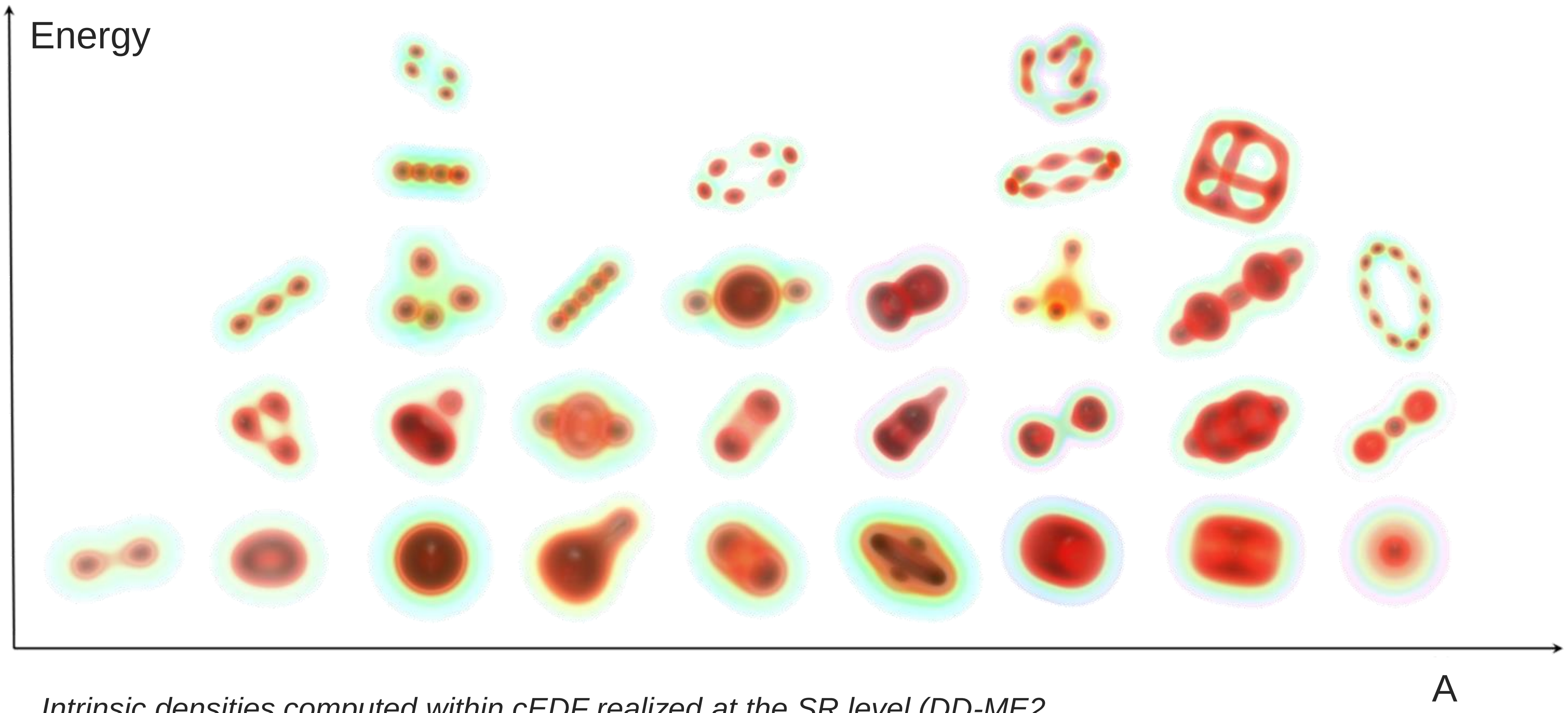






Nuclear clustering

◉ Nuclear clustering = nucleons clumping together into sub-groups within the nucleus



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

Outline

1. Nuclear structure from a microscopic viewpoint
2. What causes the nuclear clustering phenomenon ?
3. What are the consequences of the nuclear clustering phenomenon ?

1. Nuclear structure from a microscopic viewpoint

1 Nuclear structure from a microscopic viewpoint

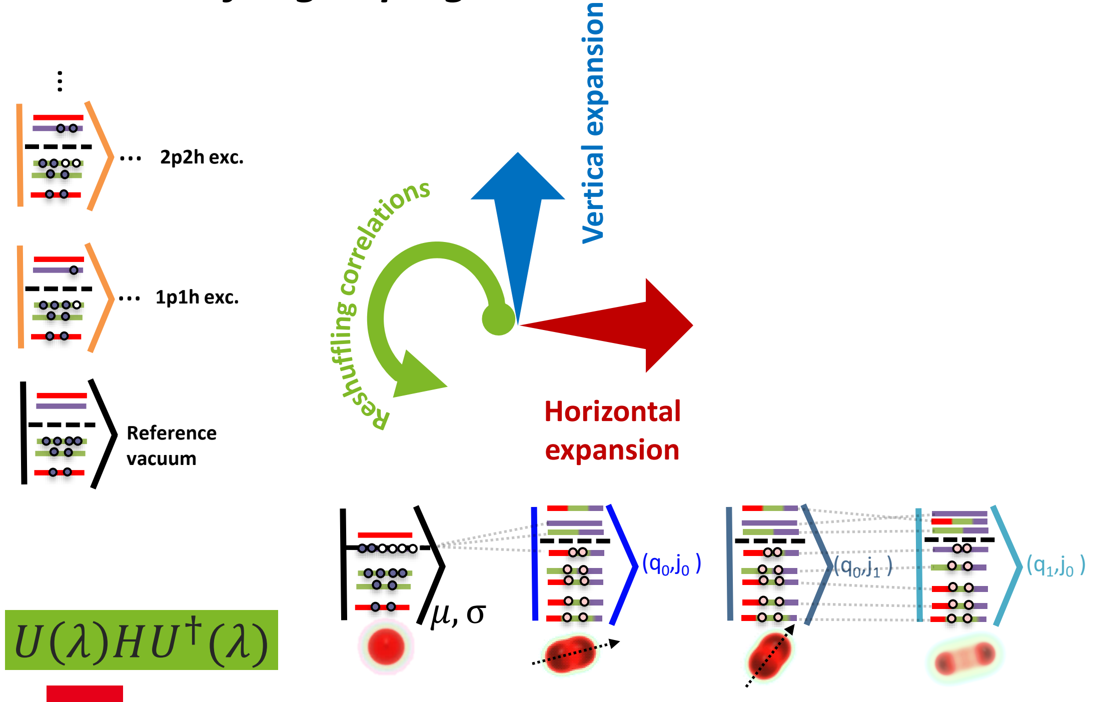
1) Nucleus: *A* interacting, structure-less nucleons
2) Structure & dynamic encoded in Hamiltonian, Functional, …
3) Solve *A*-nucleon Schrödinger/Dirac equation to desired accuracy

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

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

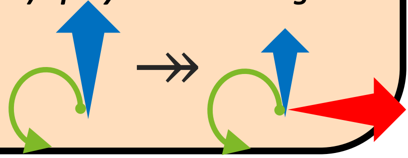


$U(\lambda)HU^{\dagger}(\lambda)$

Ab initio

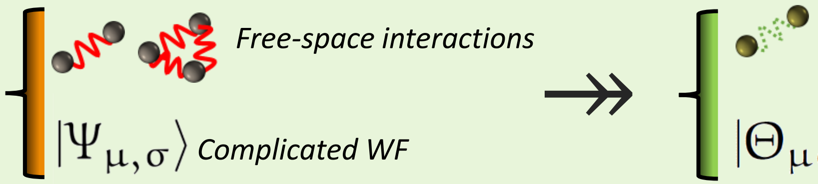
- **Systematically improvable free-space Hamiltonian in χEFT**
- **Solving Schrödinger equation**
  - Pre-processing H
  - Refined many-body schemes with controlled uncertainties
    - --> *CI (full space diag.) : exponential scaling*
    - --> *Hybrids (valence space diag.) : mixed scaling*
    - -->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

How to challenge ab initio frontiers



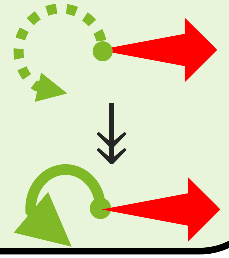
EDF

- **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)*



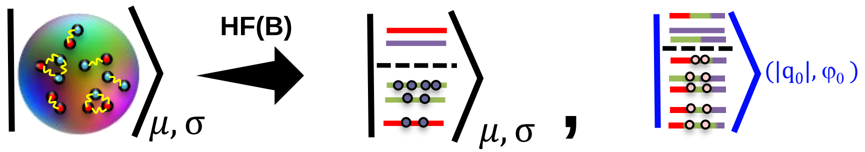
How to improve current EDFs

How to turn EDF in EFT ?

The Energy Density Functional Method

◉ 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

The Energy Density Functional Method

◉ HFB treatment

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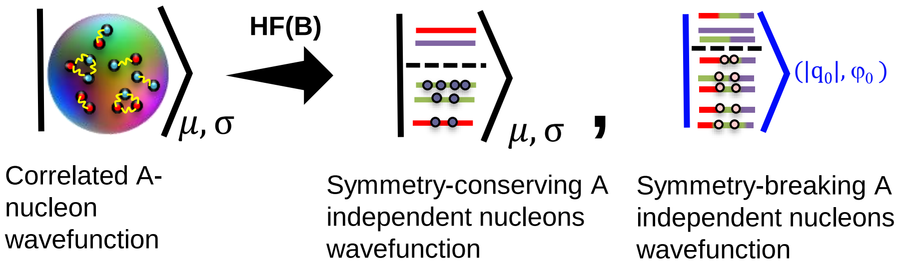

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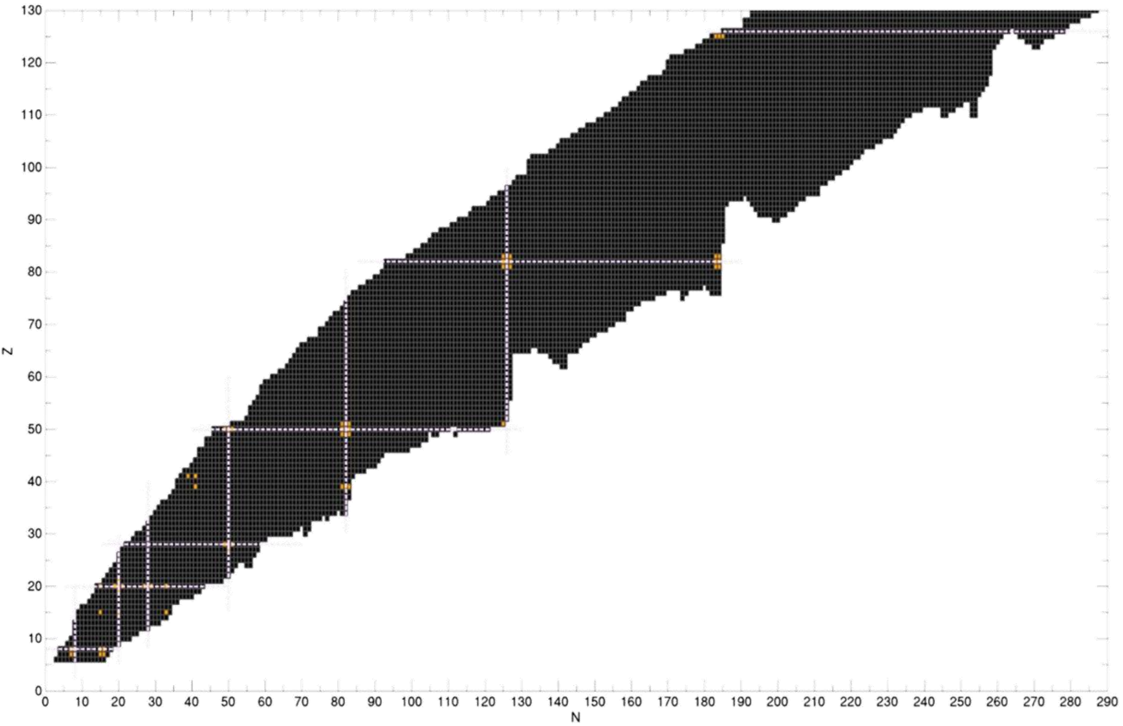
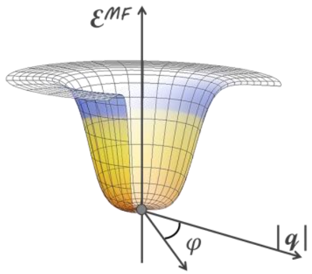
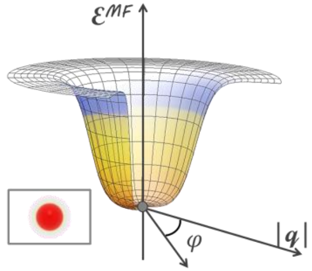


Symmetry-restriced HF : good description of GS of doubly closed-shell nuclei & neighbors (~30 nuclei)





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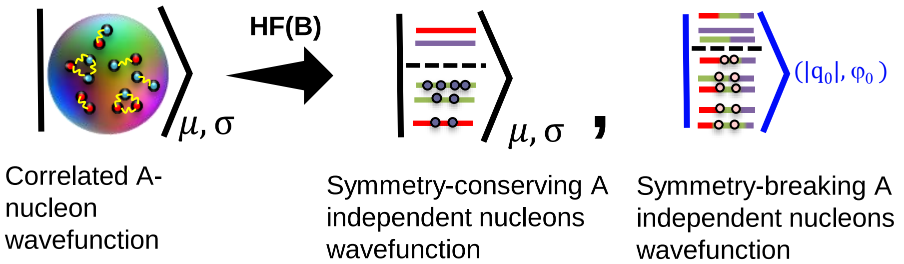

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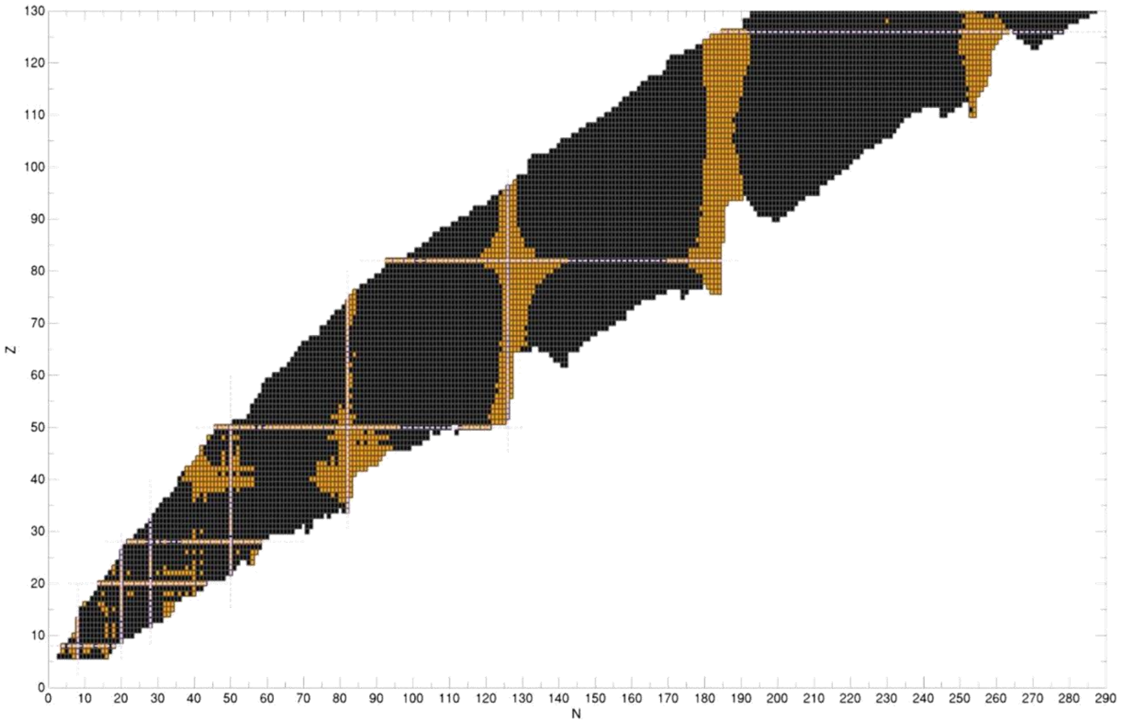
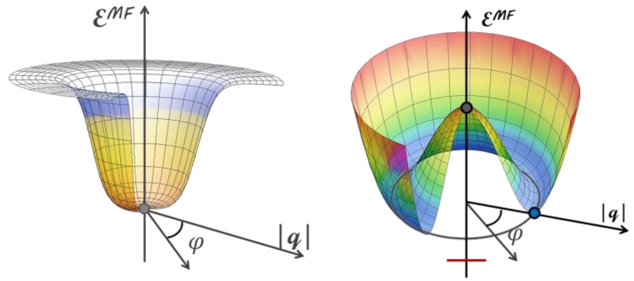
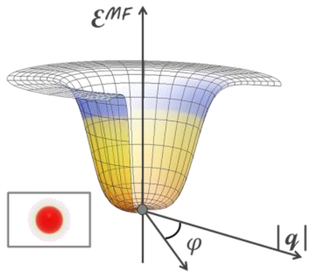




Spatial symmetry-restricted HFB: good description of GS of doubly and singly closed-shell nuclei & neighbors (~300 nuclei)



The Energy Density Functional Method

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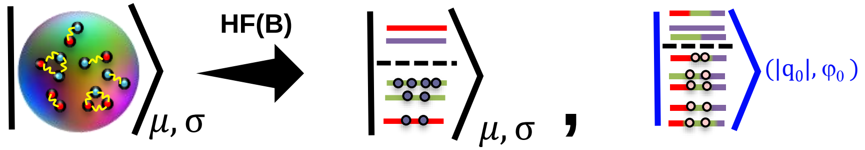
⇢ A-nucleon problem ⟶ A 1-nucleon problems



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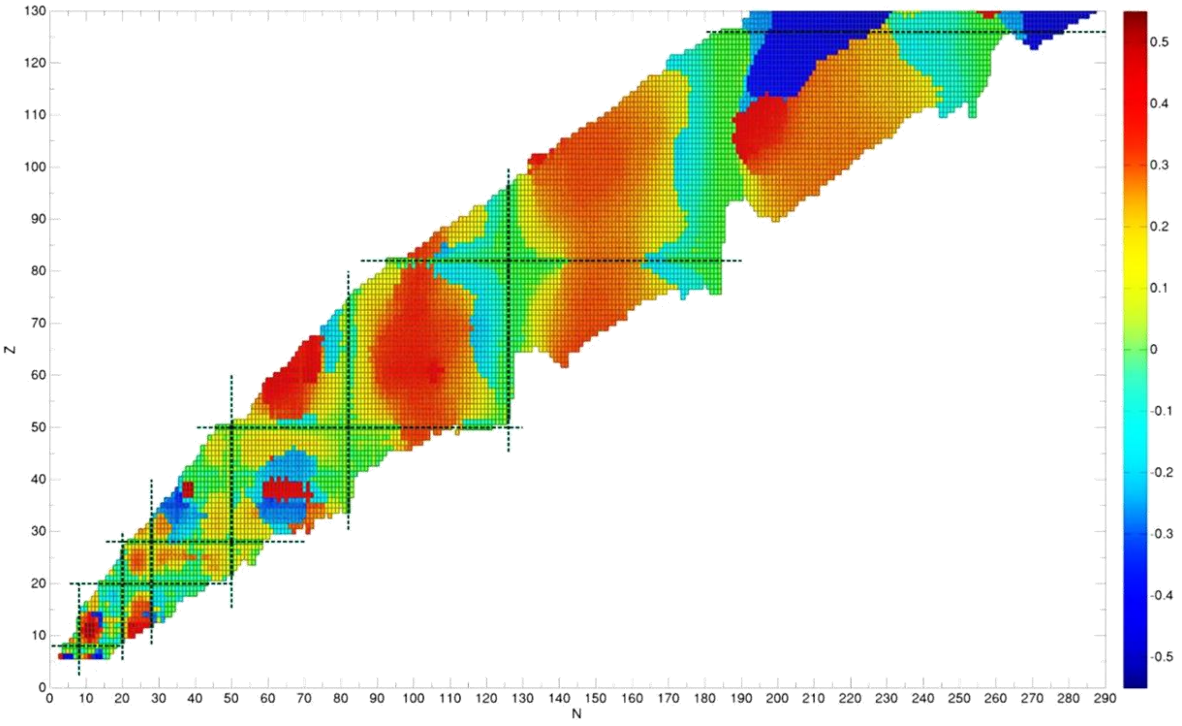
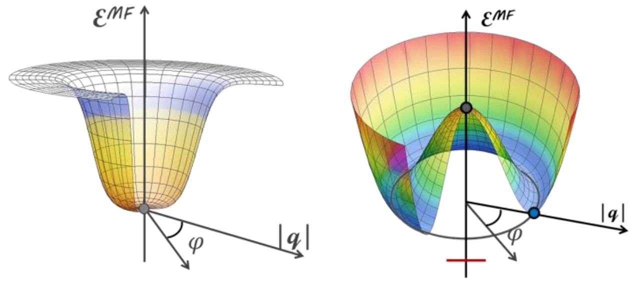
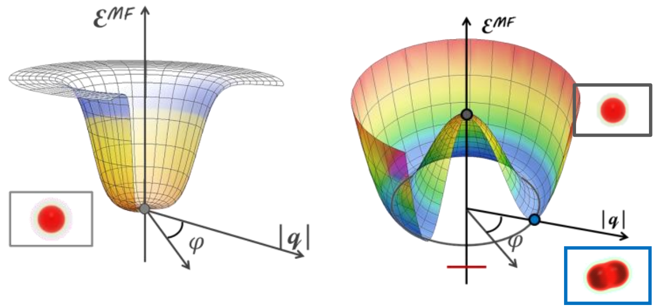




Symmetry-unrestricted HFB: good description of GS of all nuclei



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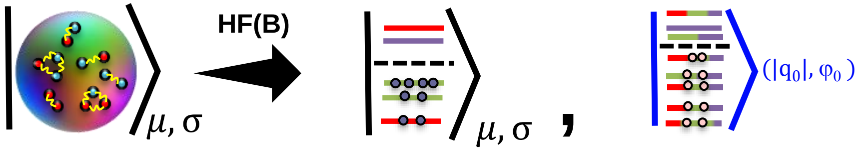
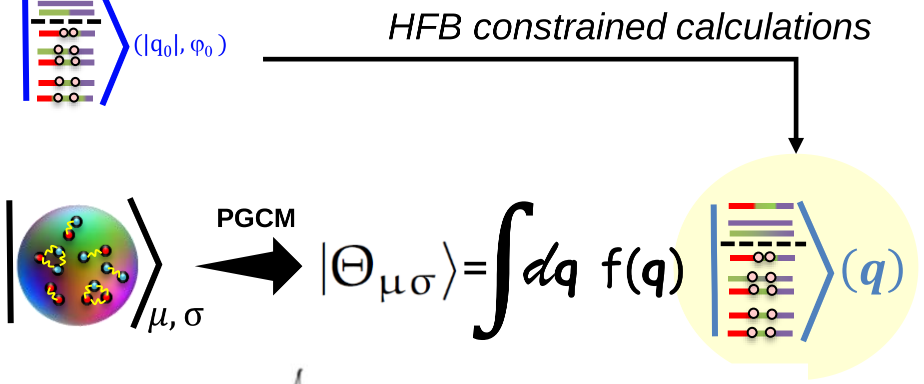
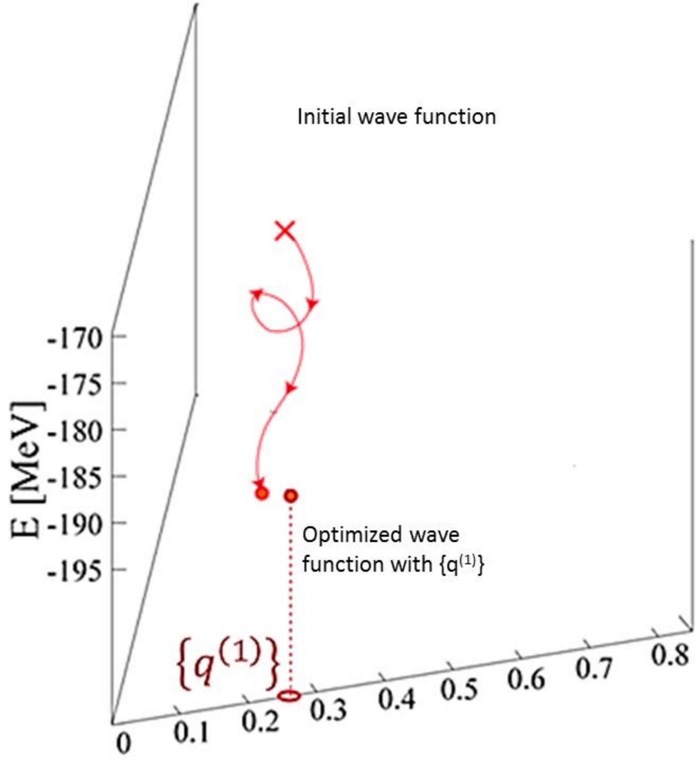


◉ Post-HFB treatment : PGCM

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





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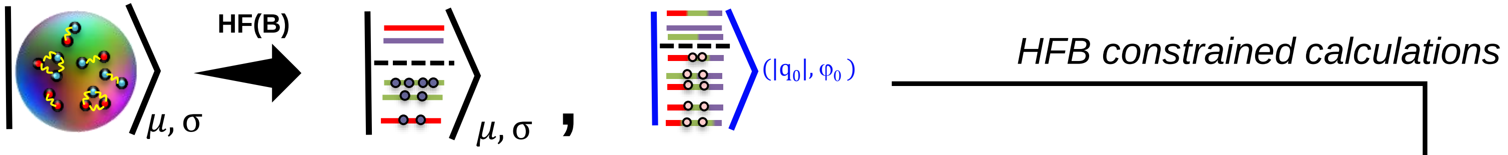

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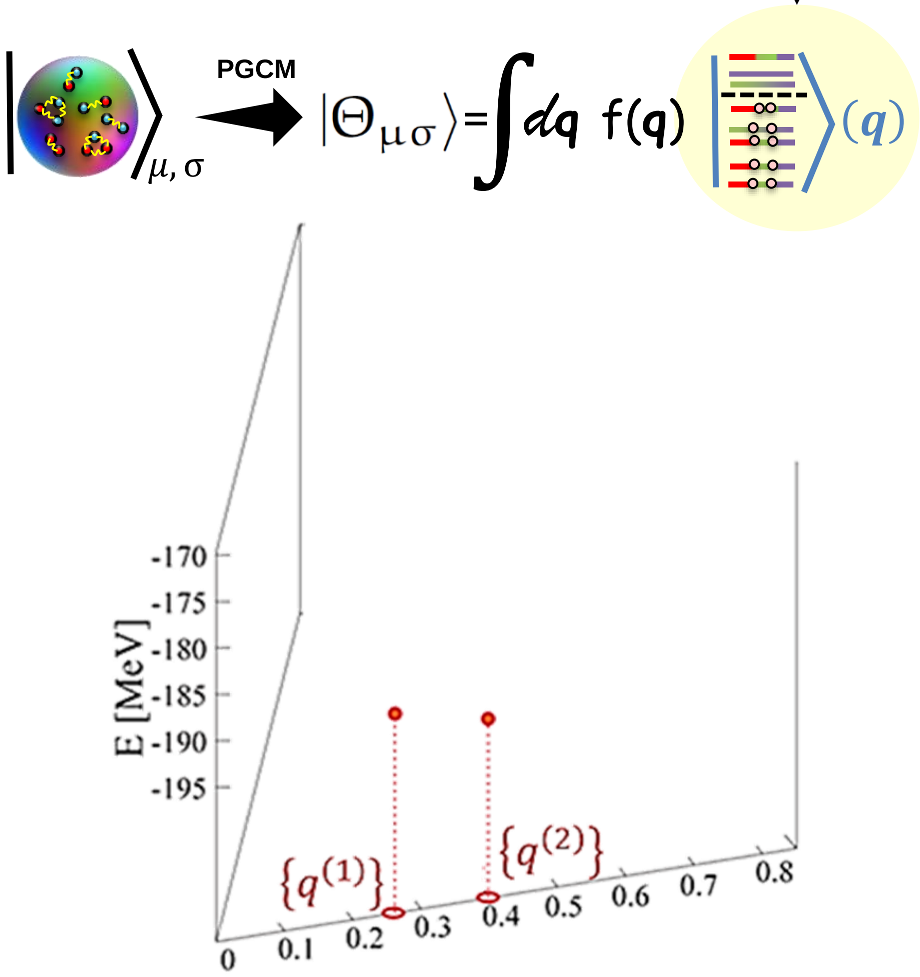

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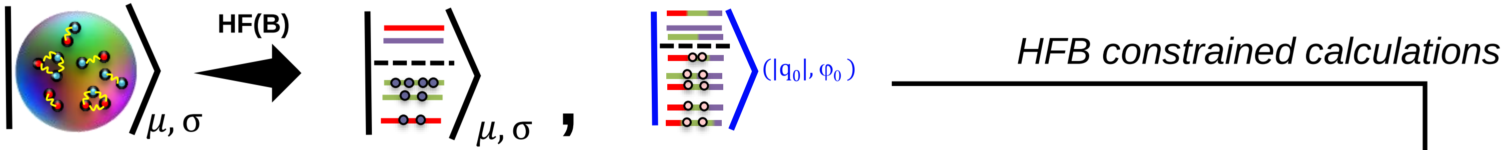

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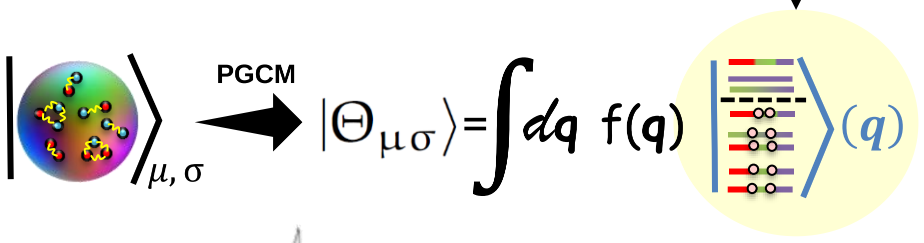

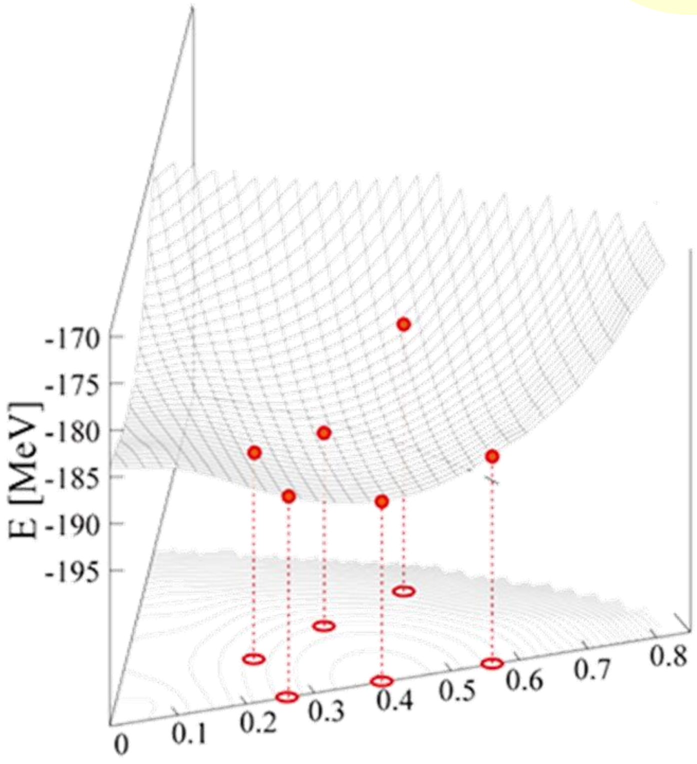

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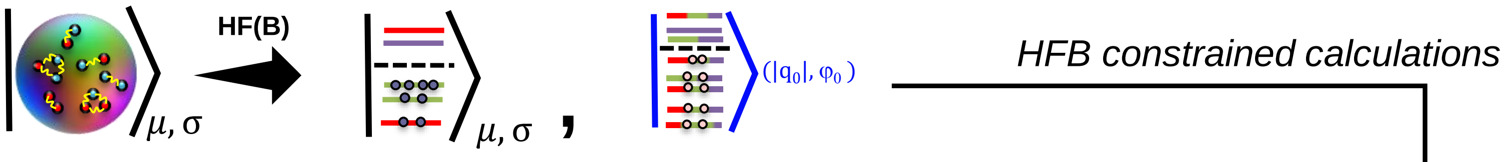

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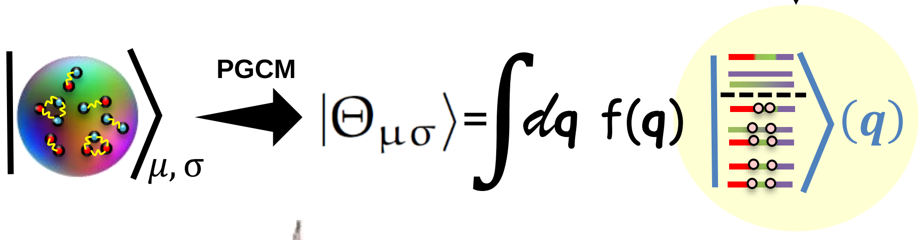

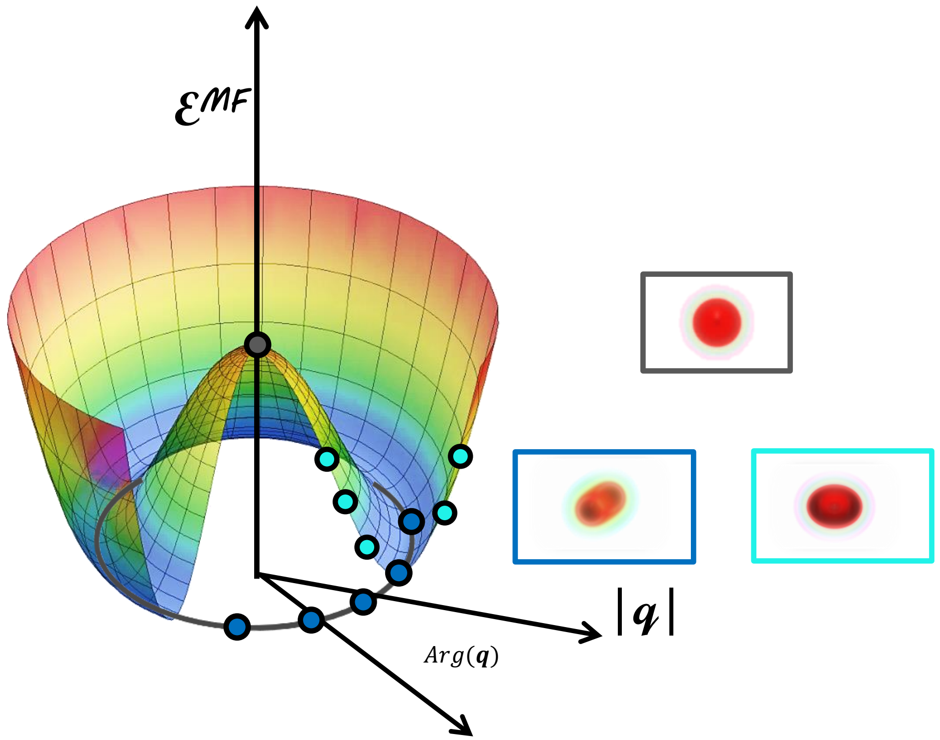

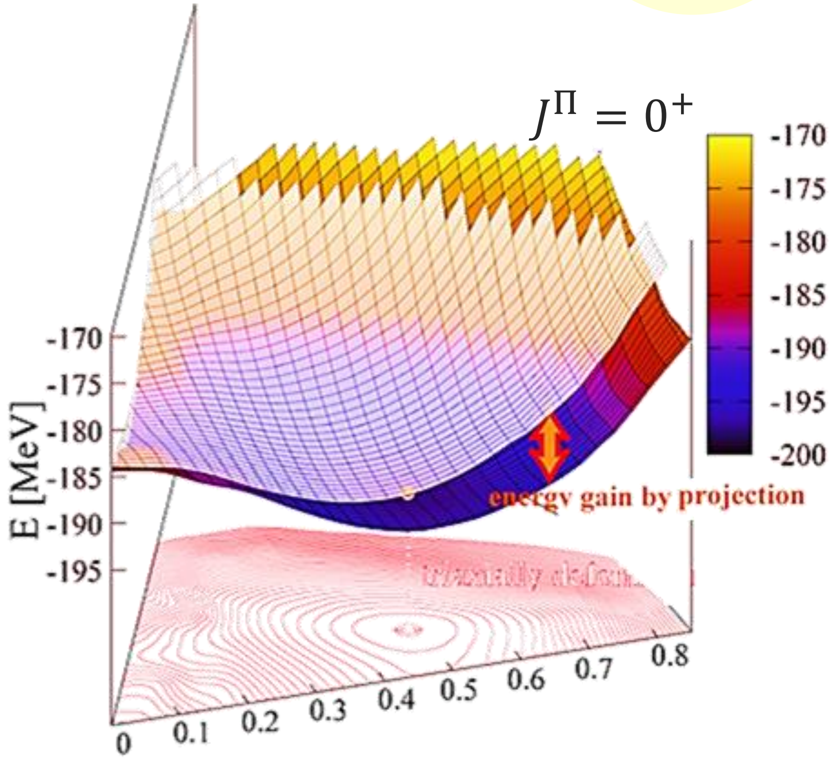

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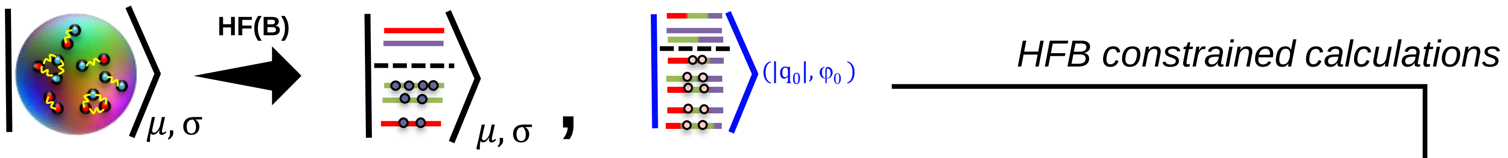

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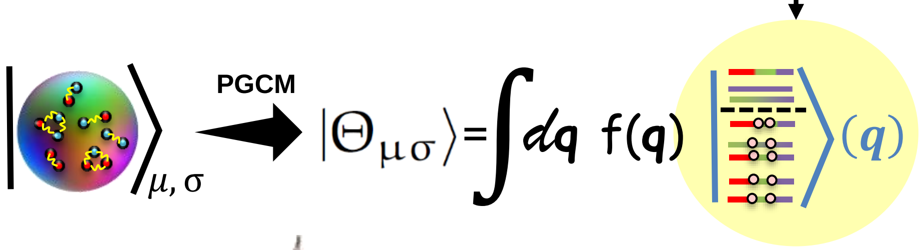

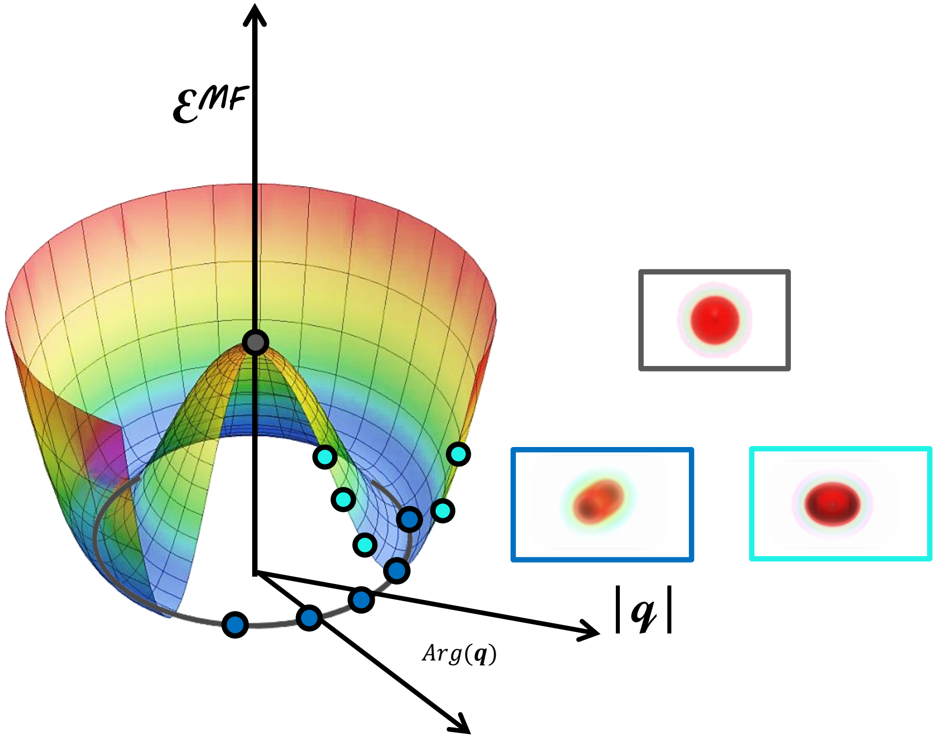

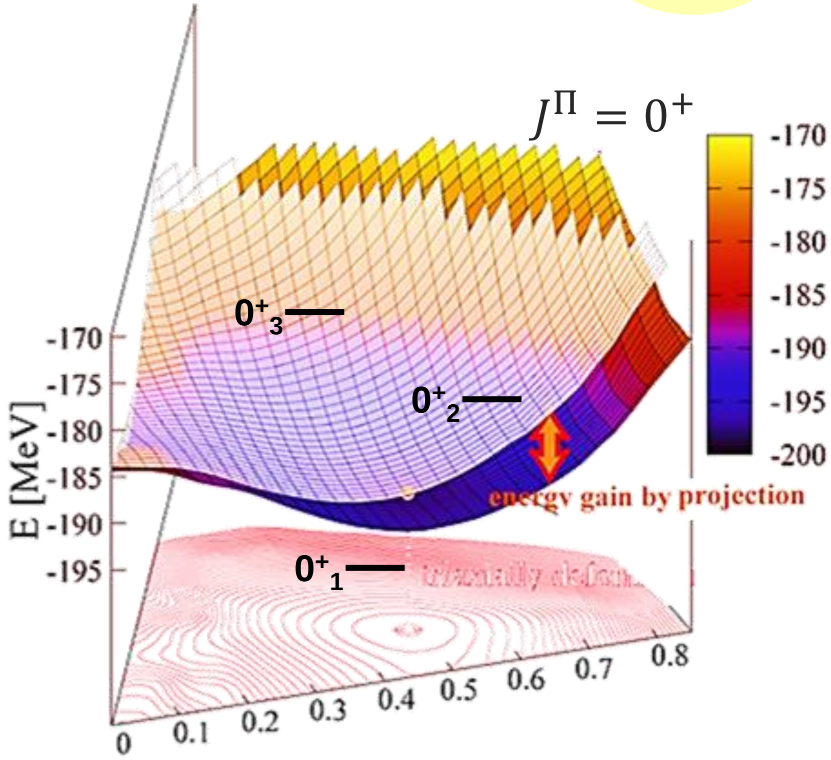

The Energy Density Functional Method

◉ HFB treatment

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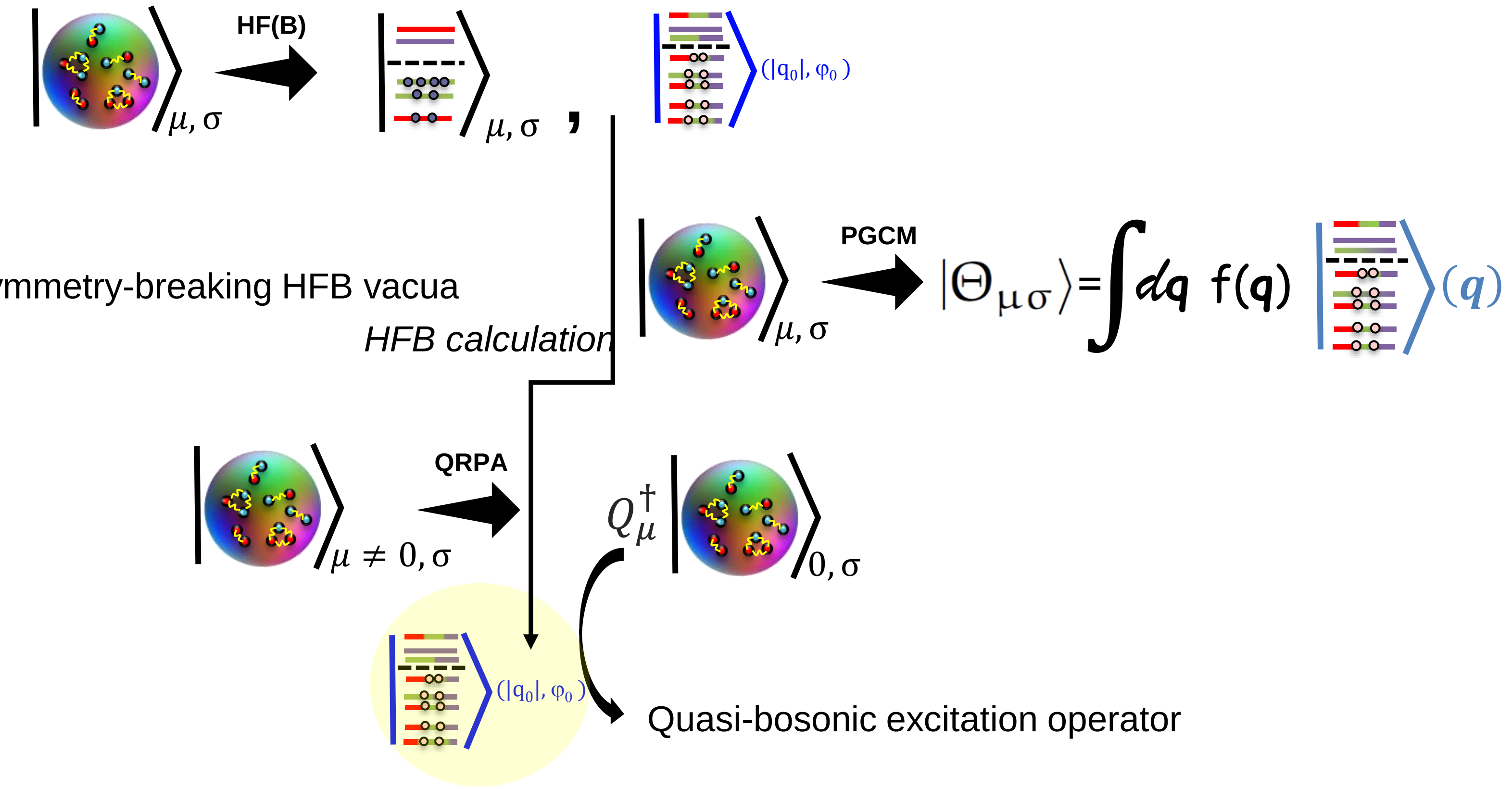
◉ Post-HFB treatment : PGCM

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

◉ Post-HFB : QRPA

--> Excitations = coherent mixture of 2-qp excitations

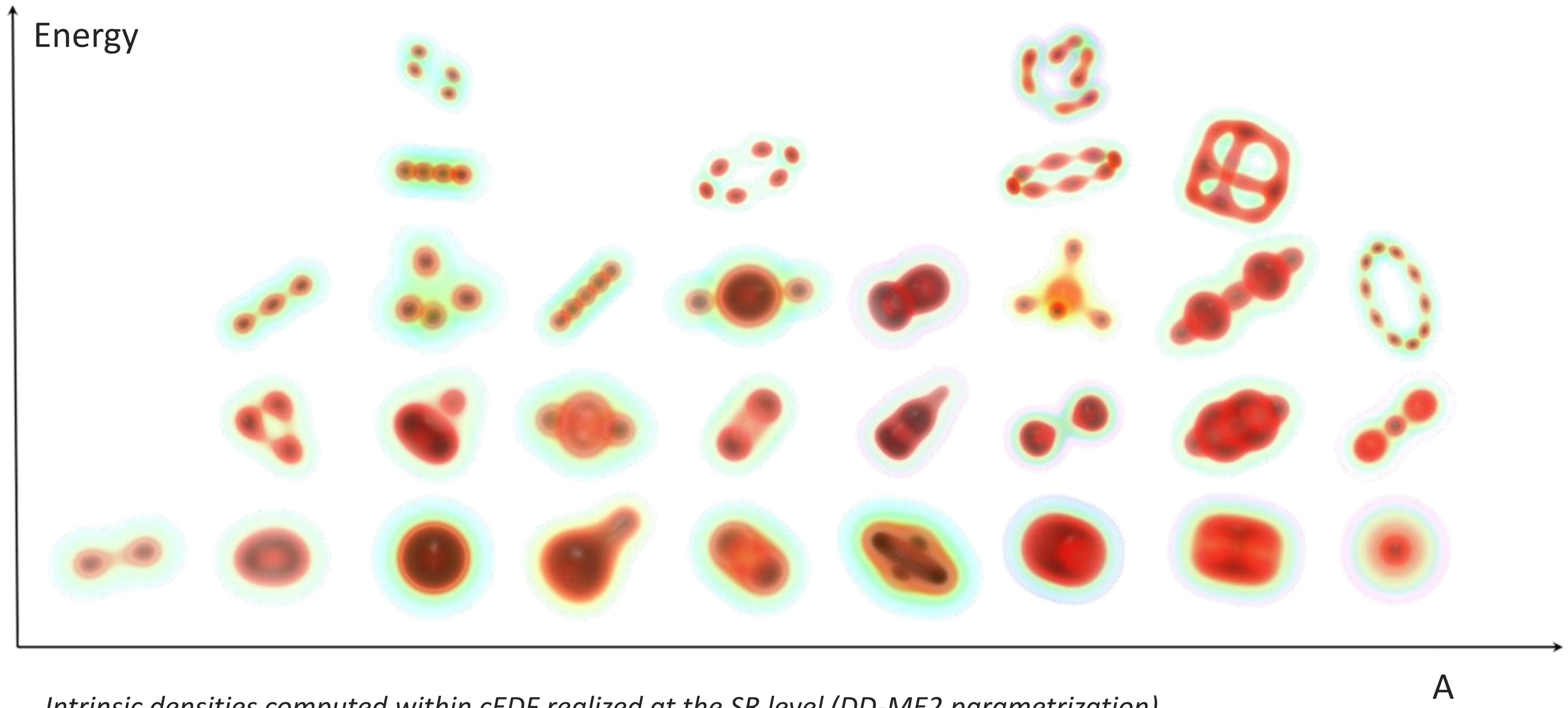
--> Harmonic limit of the GCM



2. What causes the nuclear clustering phenomenon ?

Nuclear clustering

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

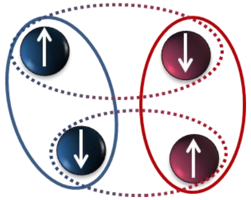


Intrinsic densities computed within cEDF realized at the SR level (DD-ME2 parametrization)

EDF & Nuclear clustering

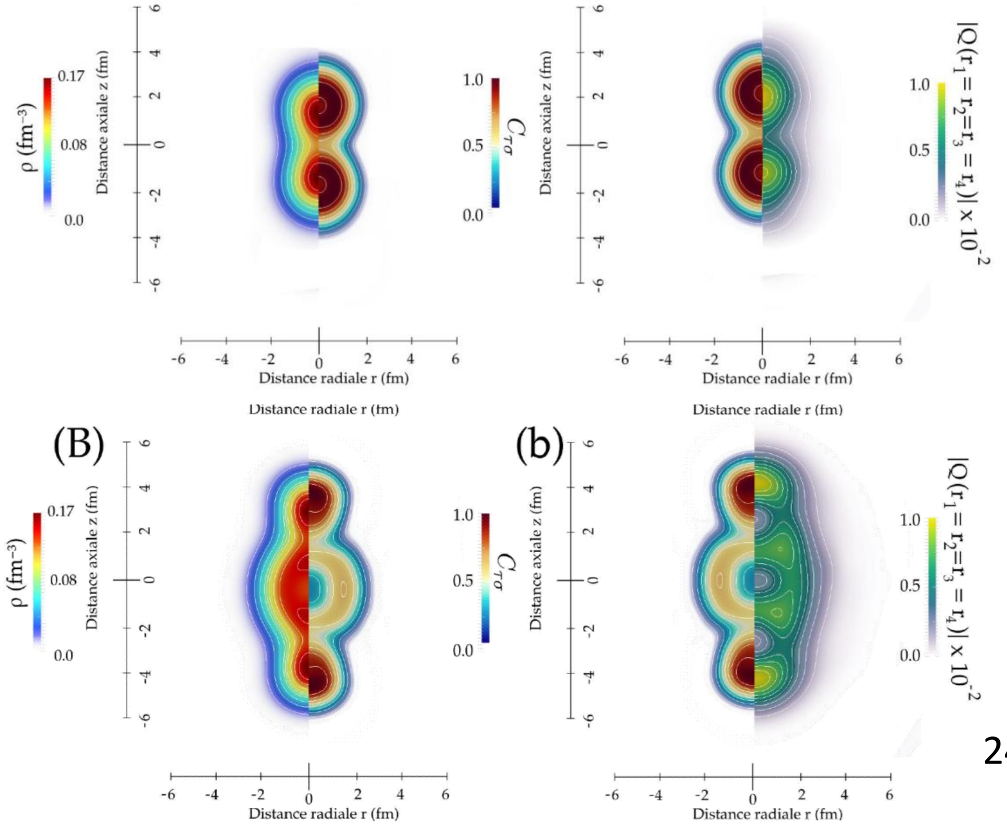
- How to account for correlations underpinning α-clustering ?

    i) Explicitly treat 4-nucleon correlations : RMF + QCM



$$|\Psi\rangle = \left(\mathcal{Q}^\dagger\right)^{n_q}|0\rangle \qquad \mathcal{Q}^\dagger = 2\Gamma_1^\dagger\Gamma_{-1}^\dagger - \left(\Gamma_0^\dagger\right)^2 \qquad \Gamma_t^\dagger = \sum_k x_k P_{k,t}^\dagger$$

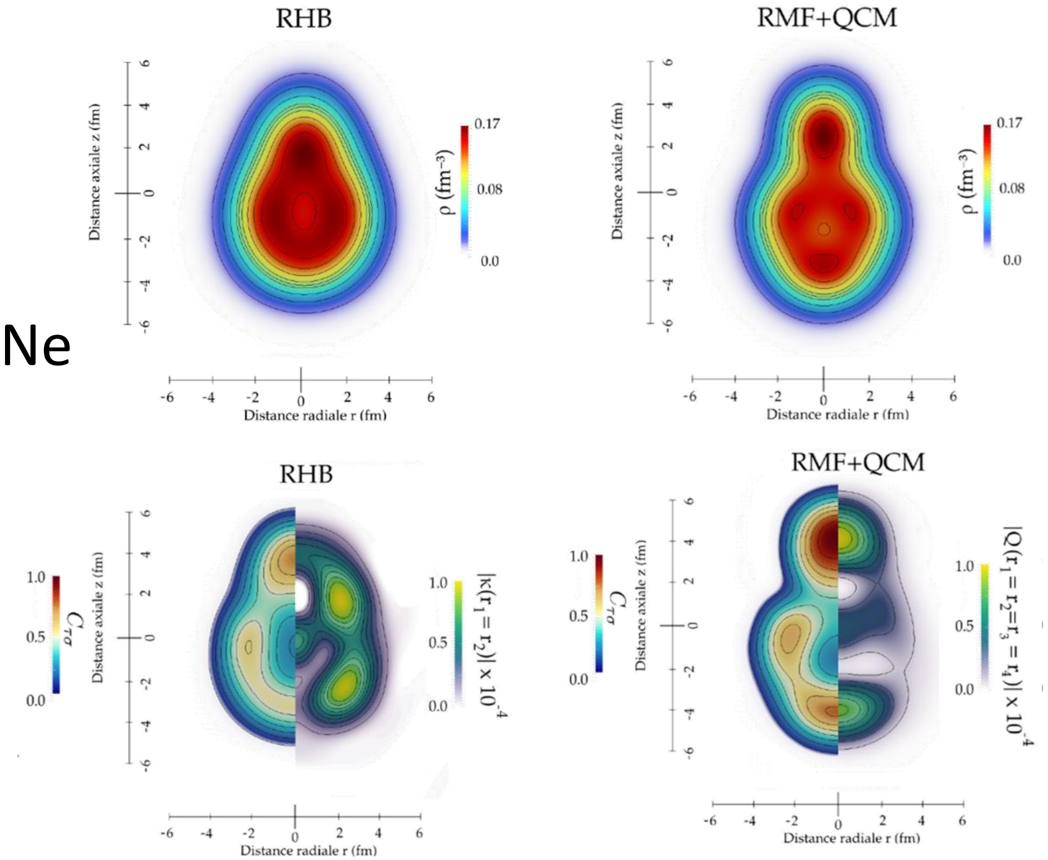
Lasseri, Ebran, Khan, Sandulescu



^{8}Be

^{24}Mg

^{20}Ne

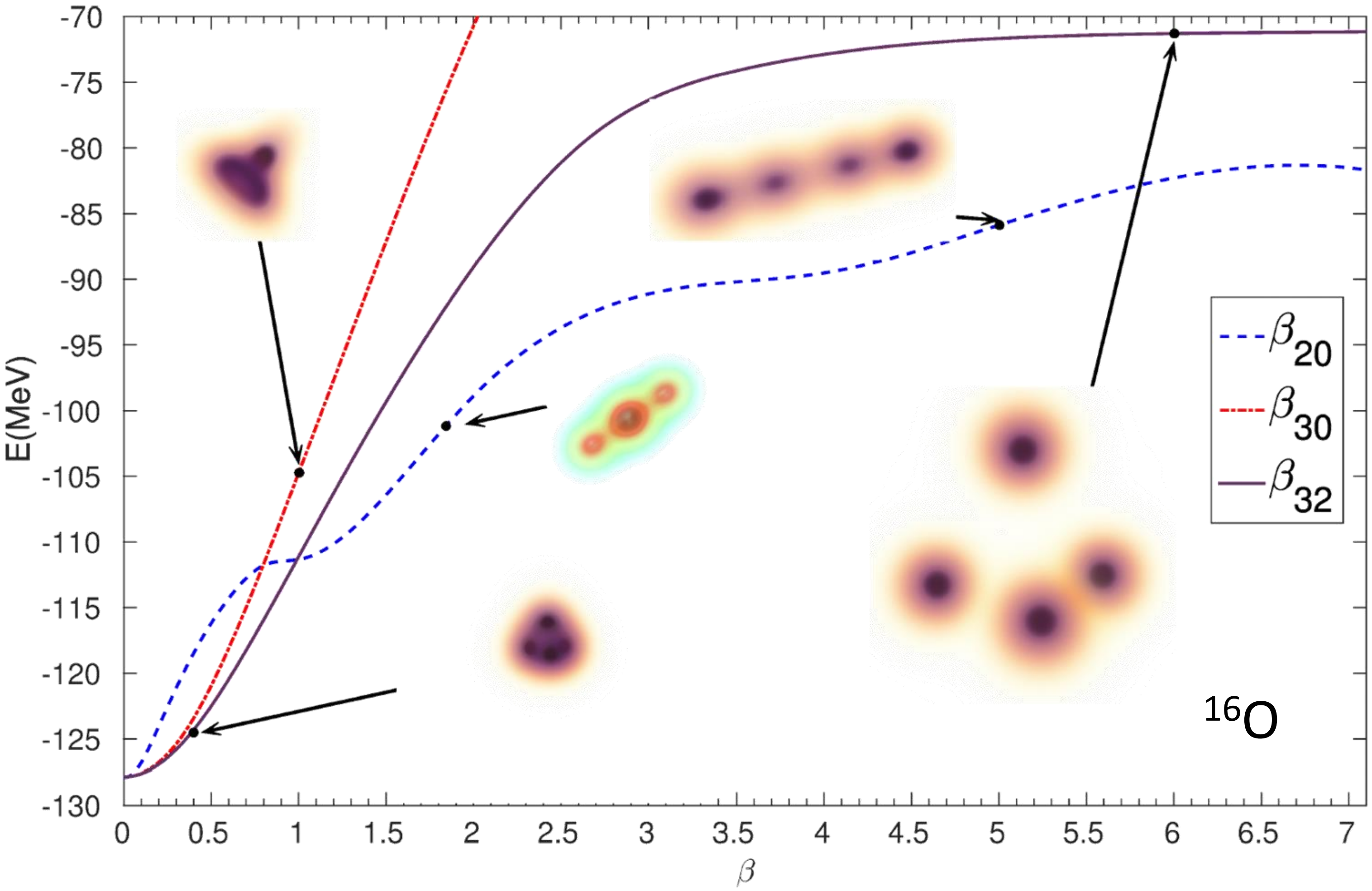


EDF & Nuclear clustering

◉ How to account for correlations underpinning α-clustering ?

i) Explicitly treat 4-nucleon correlations : RMF + QCM
ii) Look for a collective field whose fluctuations cause nucleon to aggregate into α dofs

(Mott) transition from delocalized to totally localized nucleons takes the form of a transition from O(3) (or continuous subgroup) to a discrete point-group

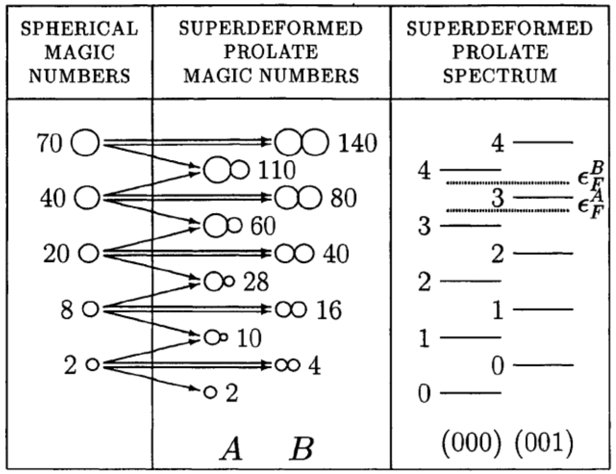


Deformation & Nuclear clustering

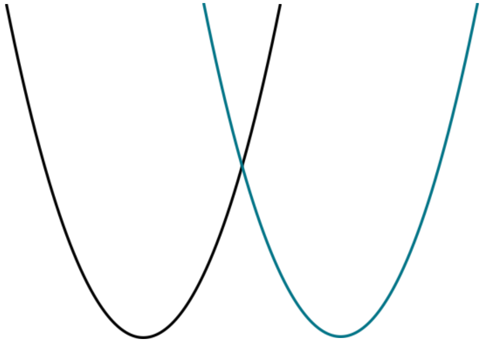
◉ Role of deformation

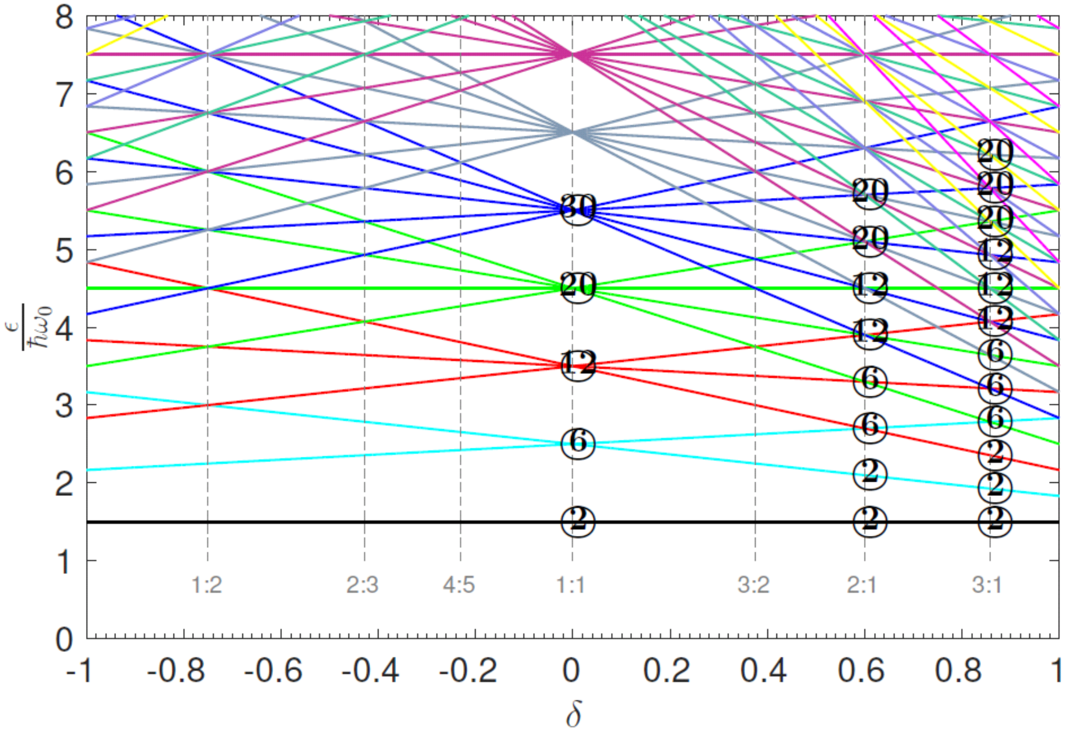
N-dimensional anisotropic HO with commensurate frequencies enjoys dynamical symmetries involving multiple independent copies of SU(N) irreps

Susceptibility of nucleons in deformed nuclei to arrange into multiple spherical fragments



Nazarewicz & *Dobaczewski*, PRL 1992





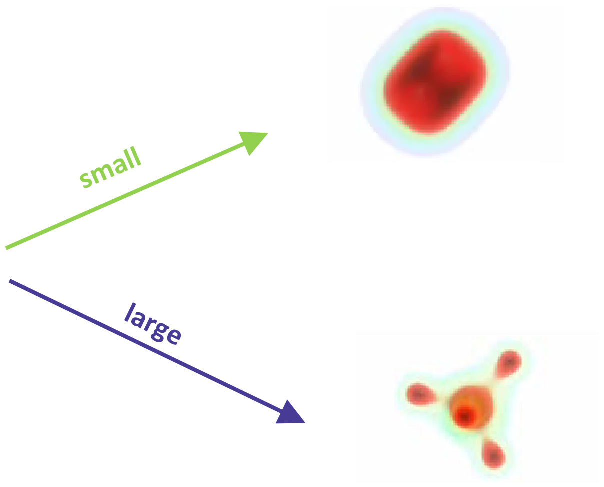
Deformation = necessary condition, but not a sufficient one

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)



Ebran, Khan, Niksic & Vretenar Nature 2012
Ebran, Khan, Niksic & Vretenar PRC 2013

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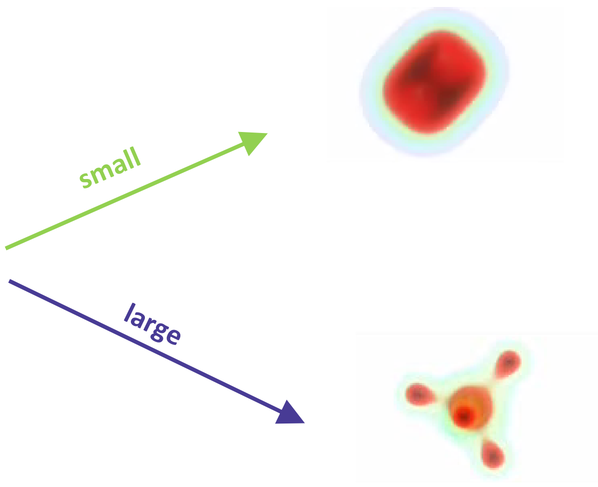
Depth of the confining potential — Mean density

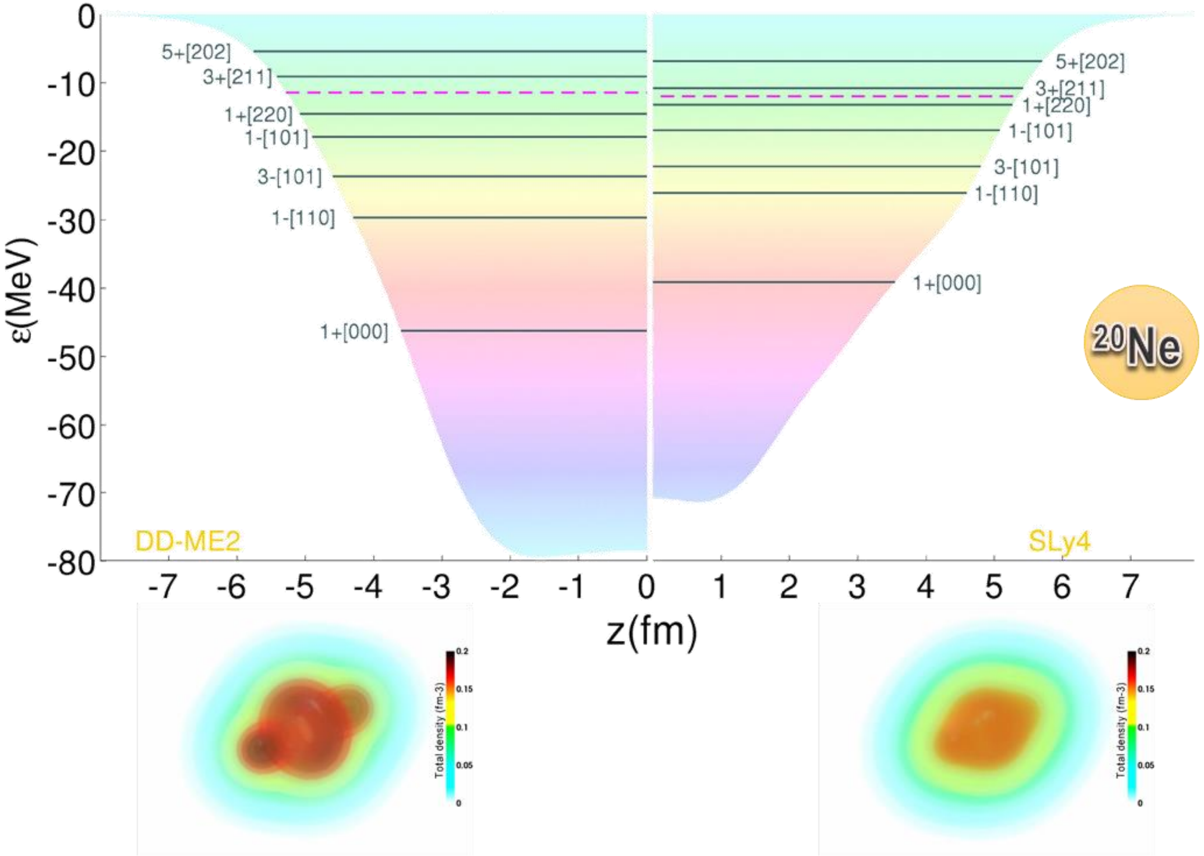


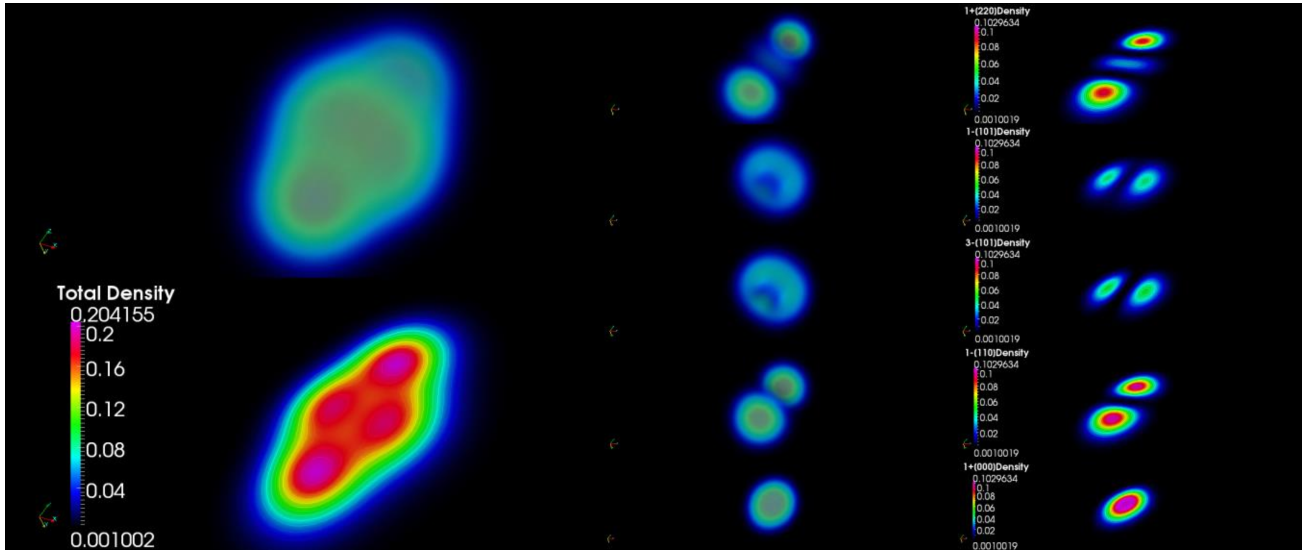
Clustering favored
- ⇢ For deep confining potential
- ⇢ For light nuclei
- ⇢ In regions at low-density

Ebran, Khan, Niksic & Vretenar Nature 2012
Ebran, Khan, Niksic & Vretenar PRC 2013

Effect of the depth of the confining potential

- Deeper potential yielding the same nuclear radii ⇒ more localized single-nucleon orbitals





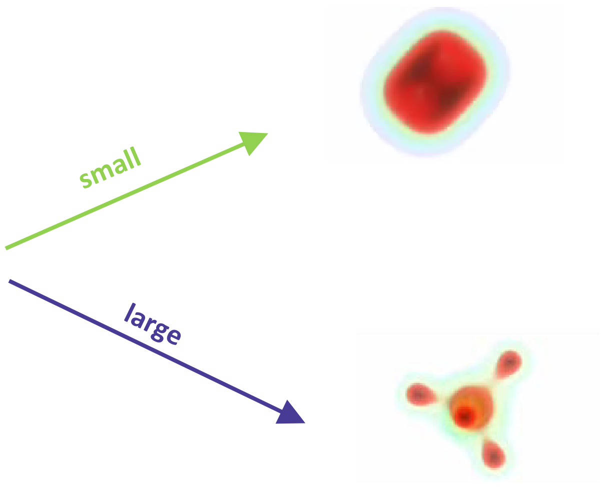
- When Coulomb effects are not too important and owing to Kramers degeneracy, proton ↑, proton ↓, neutron ↑, neutron ↓ share the same spatial properties

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



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◉ Formation/dissolution of clusters : Mott parameter

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

R_X: Size of the nucleus X

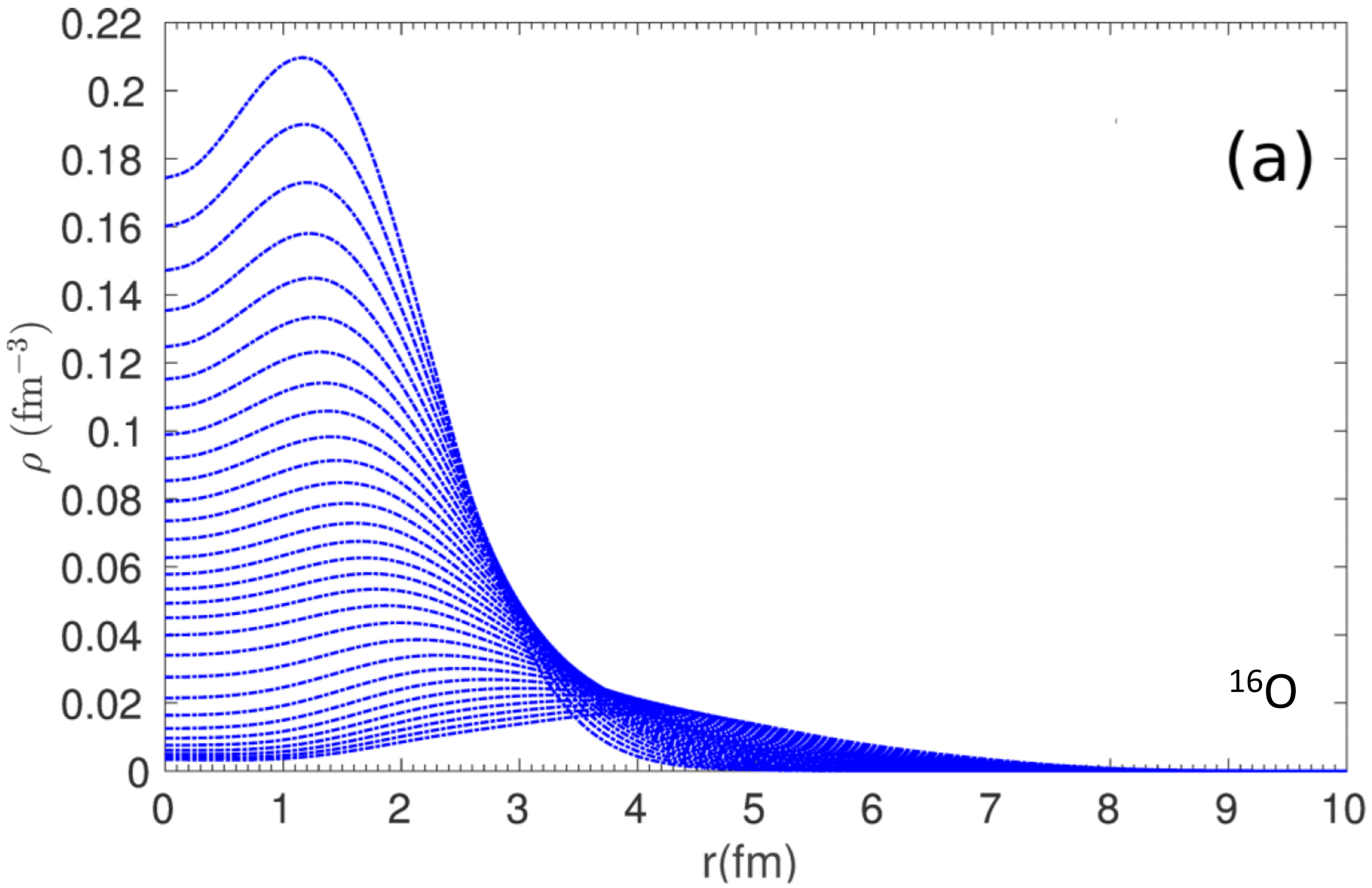
d^X_{Mott}: inter-nucleon average distance

n^{α}_{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

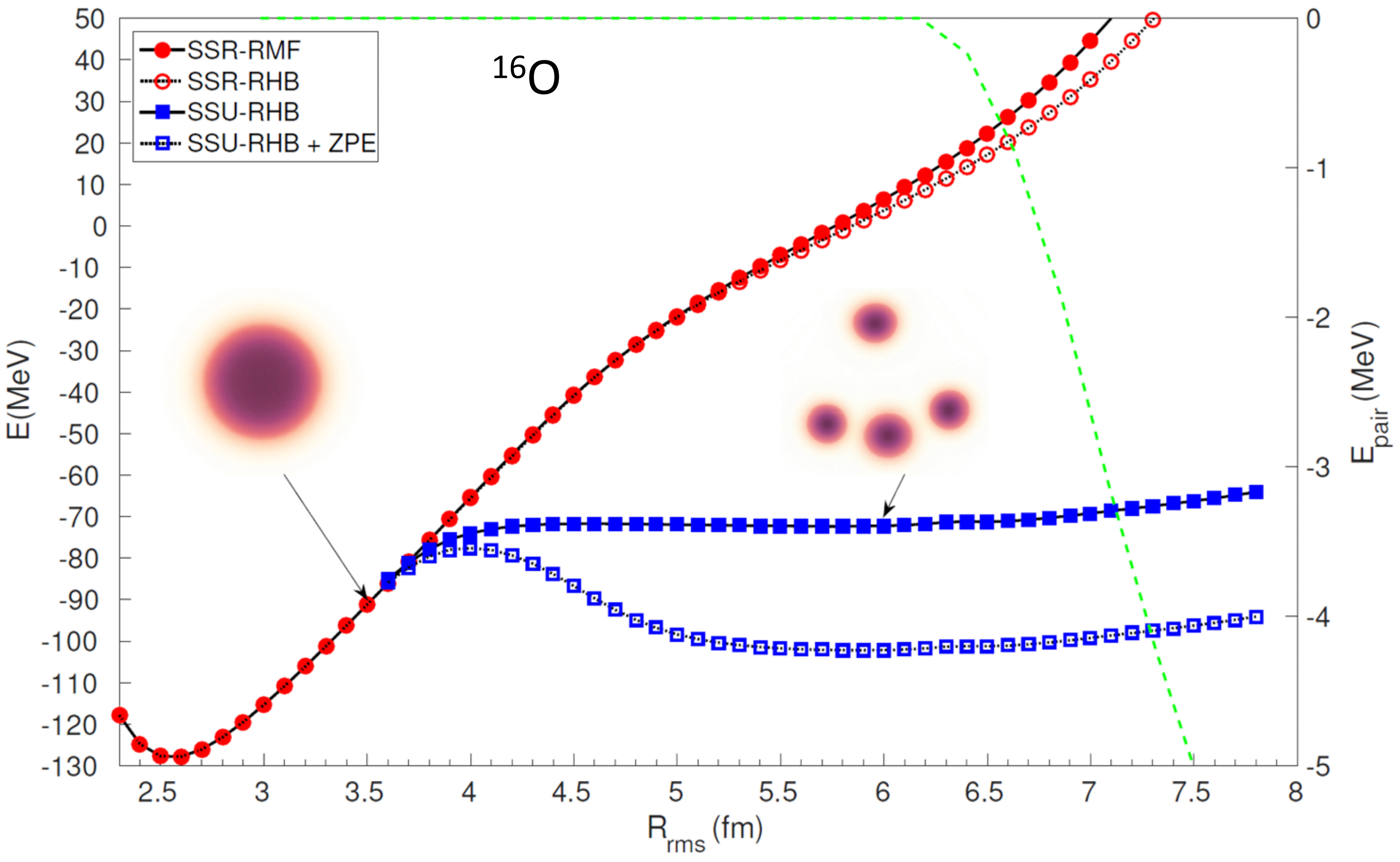
Effect of the density

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



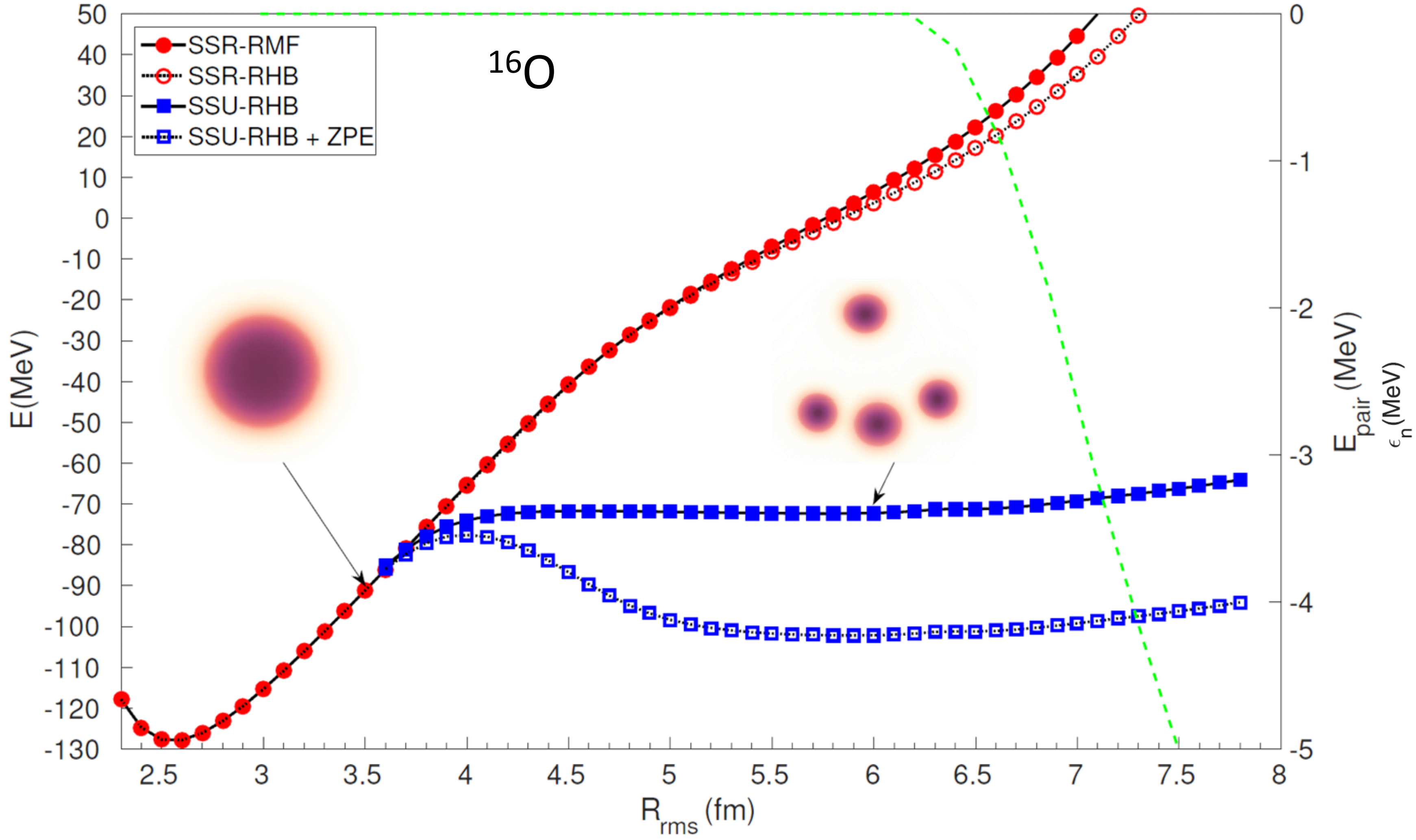
Effect of the density

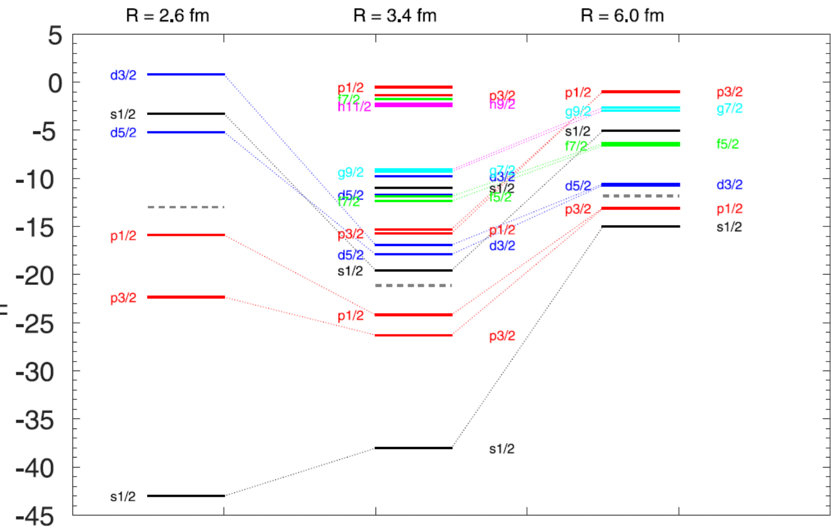
- Isotropically inflate ^{16}O by constraining its r.m.s. radius while imposing a global quadrupole moment to be zero



Effect of the density

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





Effect of the density

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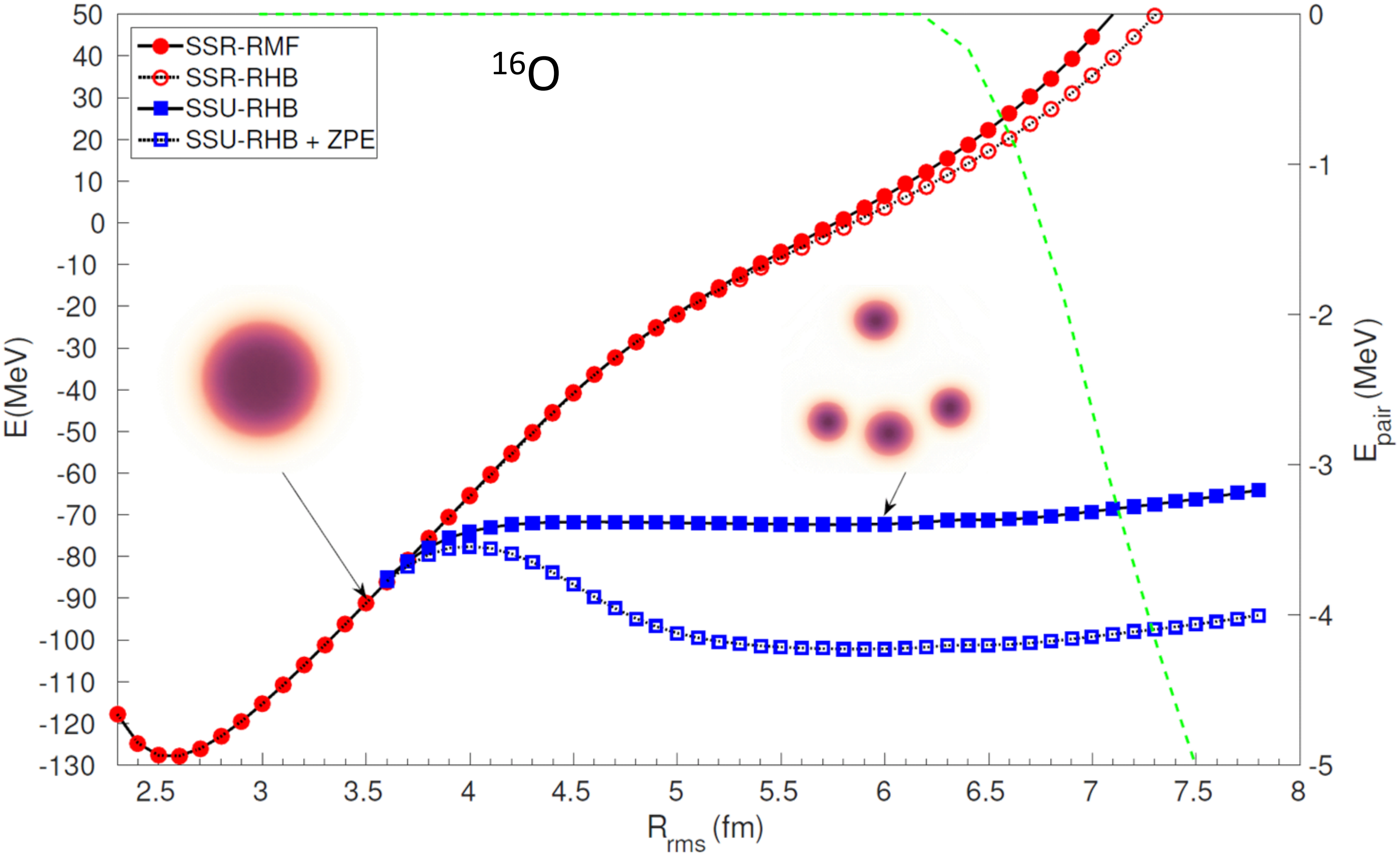
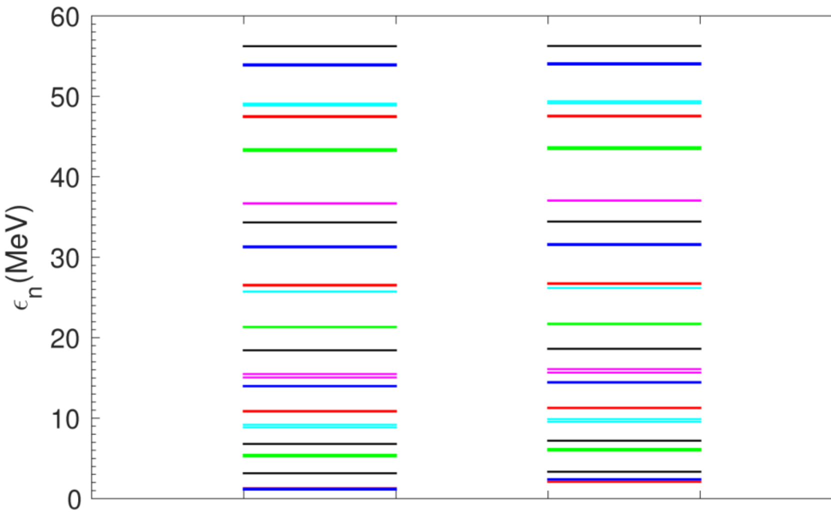
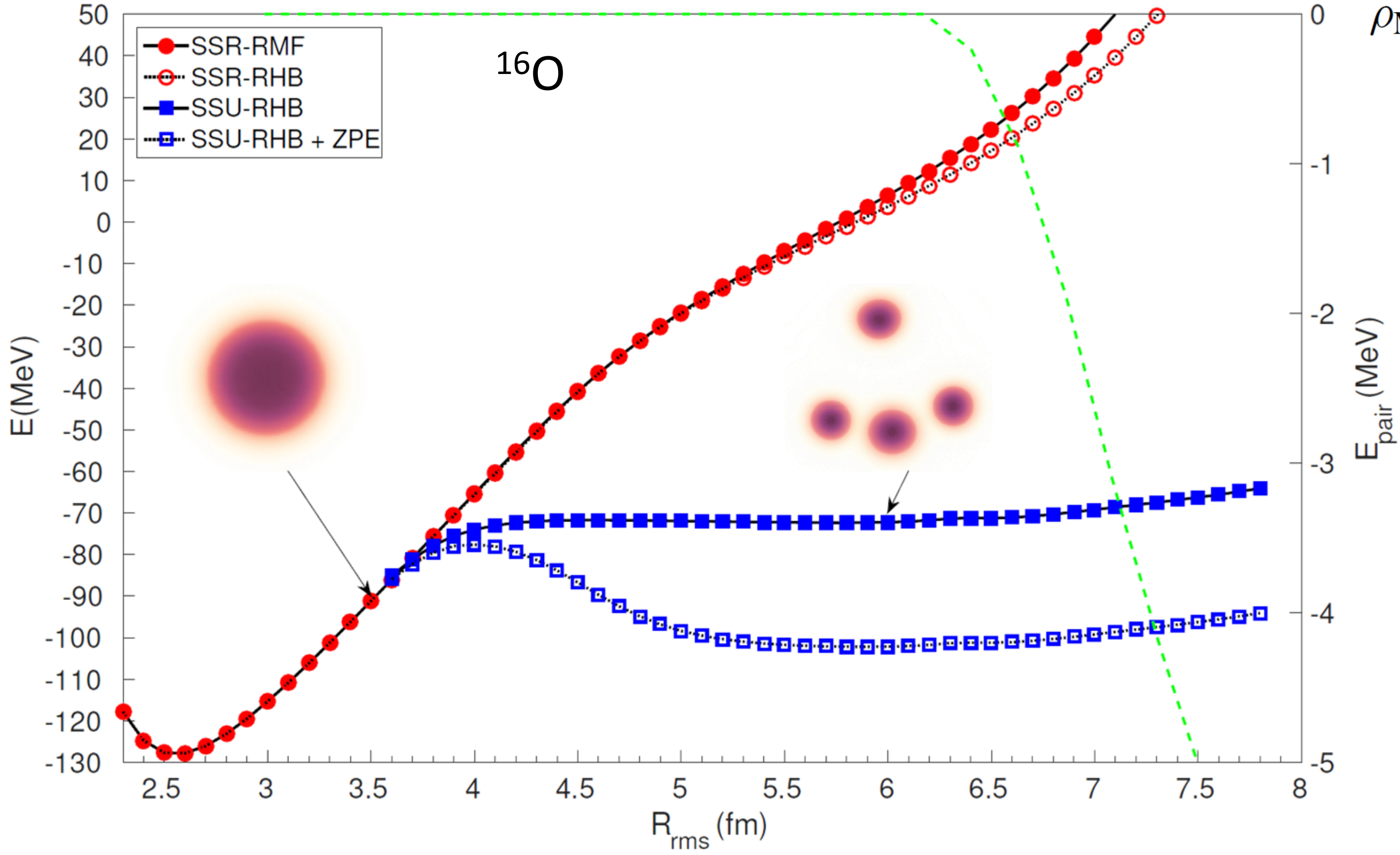


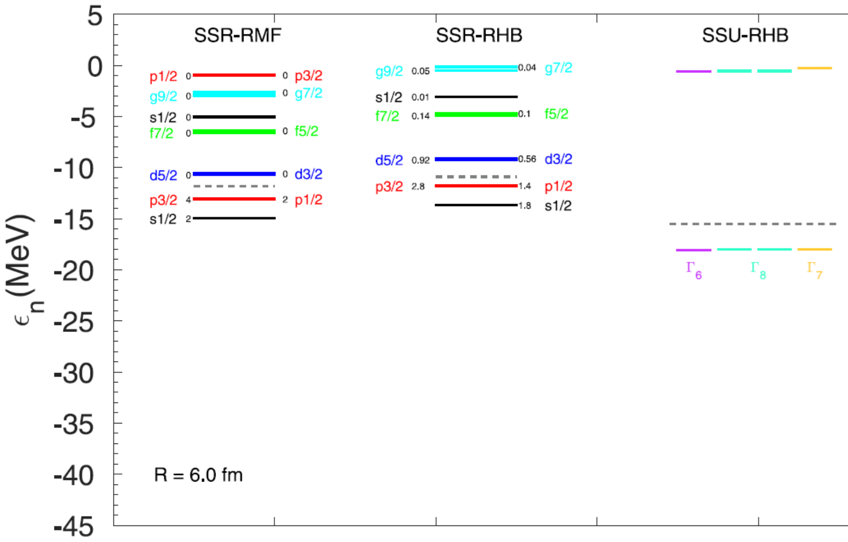


Effect of the density

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

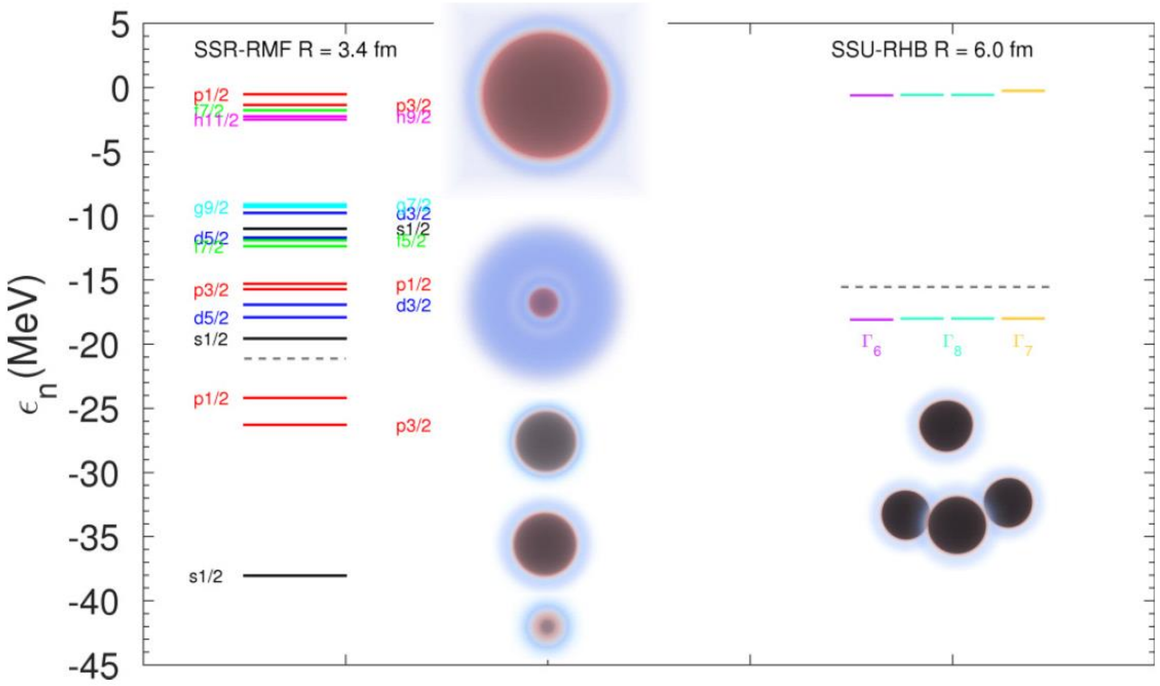


$$\rho_{\text{Mott}}/\rho_0 = (R_{\text{eq}}/R_c)^3 \approx \rho_0/3$$

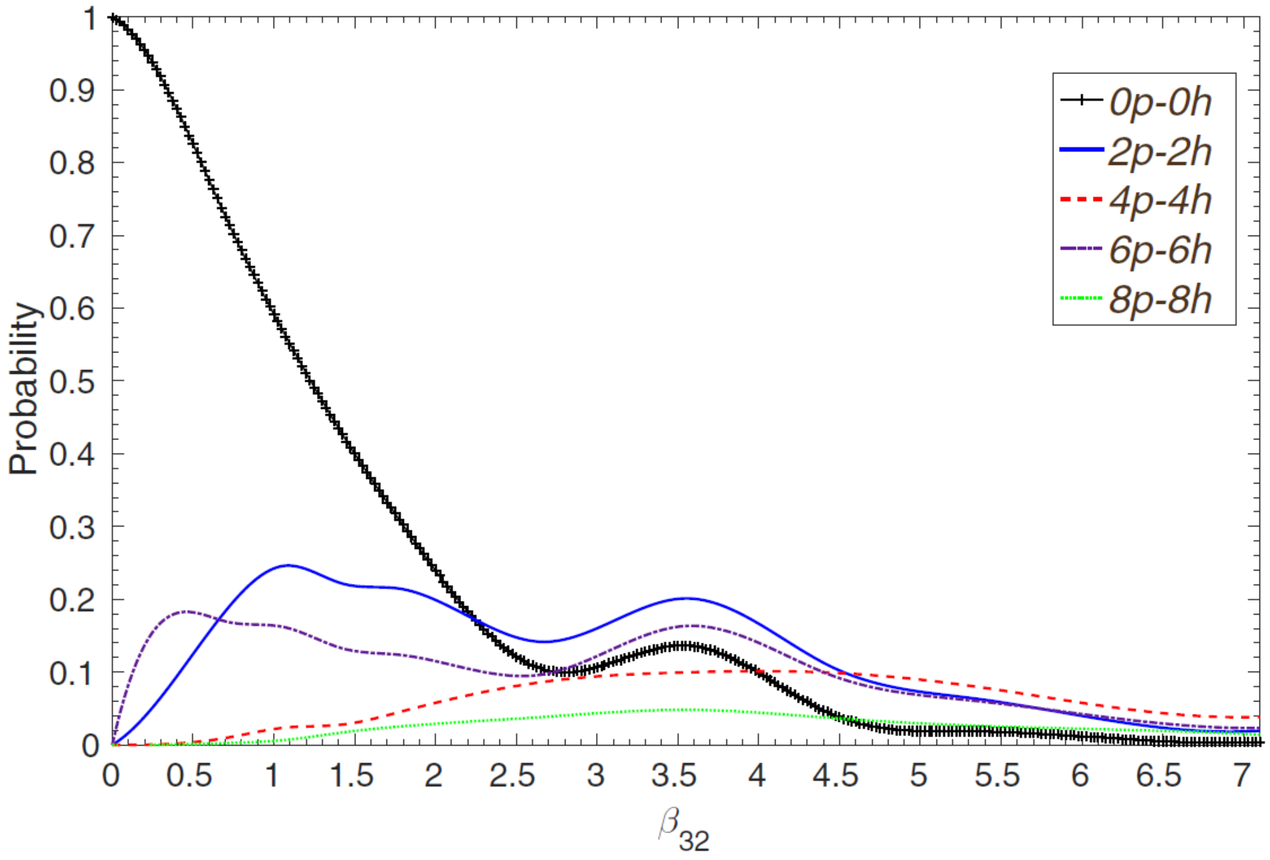


Effect of the density

- mp-mh content of a tetrahedrally-deformed Slater determinant

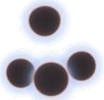


Symmetry breaking : O(3) → Td



LCAO-MO

- Borrowing the LCAO-MO language, on can think of the 16O thetrahedrally-deformed SD as a MO built from 4 1s α AOs



$$\psi_i = \sum_{j=1}^{4} f_j^i \phi_j$$

- Find the unknowns f in the Hückel approximation : $\mathcal{N}_{ij} = 0 \forall i, j$

$\epsilon \equiv \mathcal{H}_{ii}$; $-\mu \equiv \mathcal{H}_{ij}$ for adjacent i,j ; $\mathcal{H}_{ij} = 0$ otherwise

$$\begin{pmatrix} \epsilon & -\mu & -\mu & -\mu \\ -\mu & \epsilon & -\mu & -\mu \\ -\mu & -\mu & \epsilon & -\mu \\ -\mu & -\mu & -\mu & \epsilon \end{pmatrix} \begin{pmatrix} f_1^i \\ f_2^i \\ f_3^i \\ f_4^i \end{pmatrix} = E_i \begin{pmatrix} f_1^i \\ f_2^i \\ f_3^i \\ f_4^i \end{pmatrix}$$

$$\psi_1 = \frac{1}{2}(\phi_1 + \phi_2 + \phi_3 + \phi_4) \qquad E_1 = \epsilon - 3\mu$$

$$\psi_2 = \frac{1}{\sqrt{2}}(-\phi_1 + \phi_2) \qquad E_2 = \epsilon + \mu$$

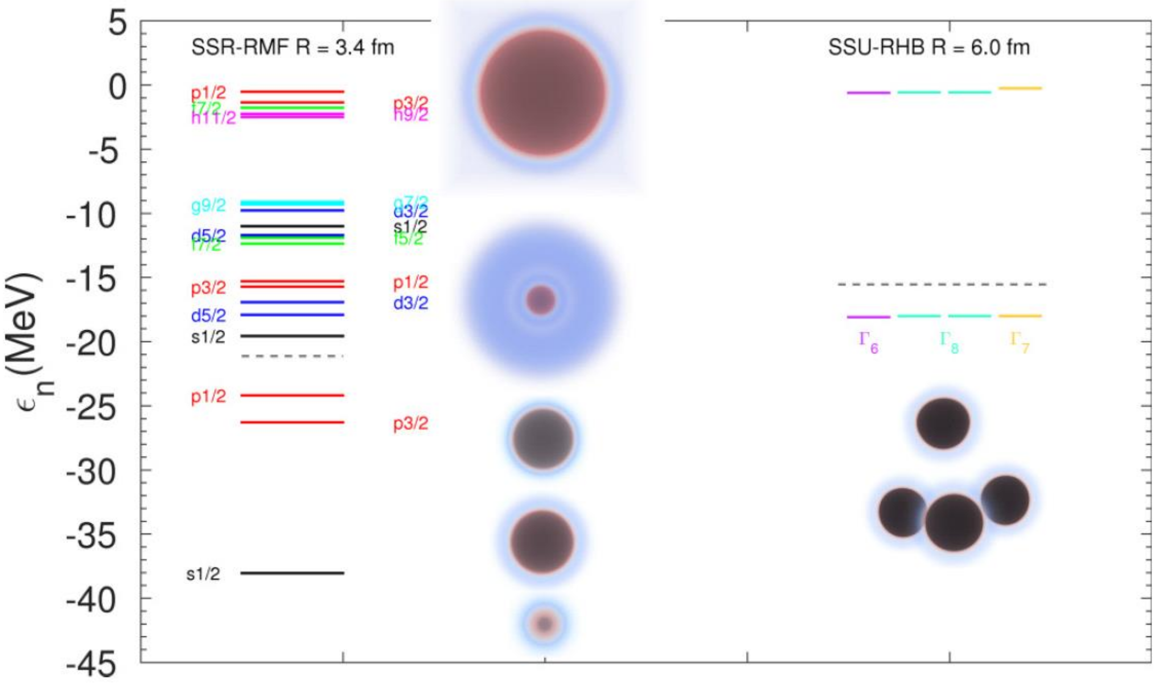
$$\psi_3 = \frac{1}{\sqrt{2}}(-\phi_1 + \phi_3) \qquad E_3 = E_2$$

$$\psi_4 = \frac{1}{\sqrt{2}}(-\phi_1 + \phi_4) \qquad E_4 = E_3 = E_2$$

$$\psi'_2 = \frac{1}{2}(\phi_1 - \phi_2 - \phi_3 + \phi_4),$$

$$\psi'_3 = \frac{1}{2}(\phi_1 + \phi_2 - \phi_3 - \phi_4),$$

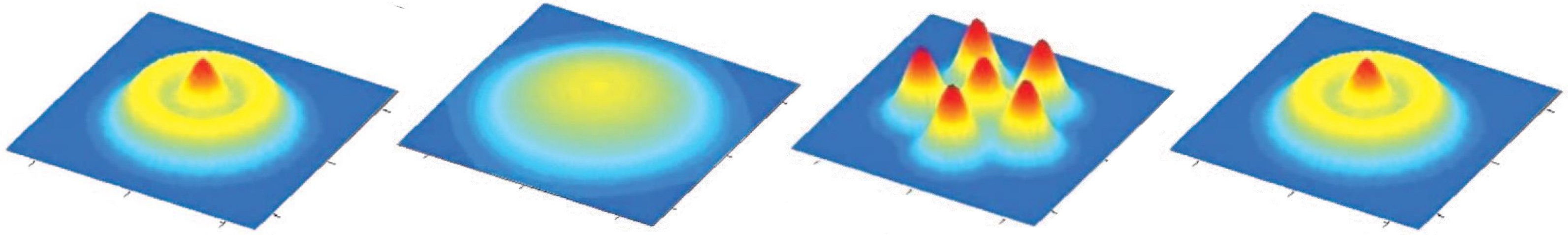
$$\psi'_4 = \frac{1}{2}(-\phi_1 + \phi_2 - \phi_3 + \phi_4).$$



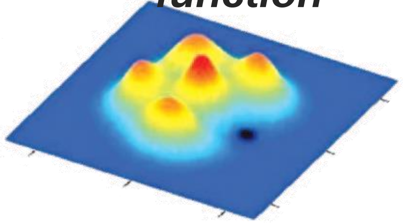
3. What are the consequences of the nuclear clustering phenomenon ?

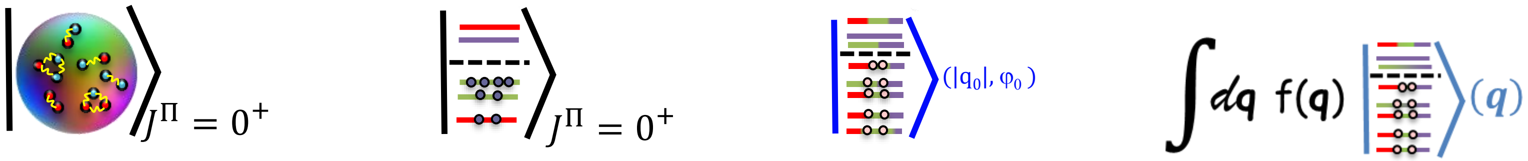
Nuclear clustering & PGCM

Density profile



2-point correlation function



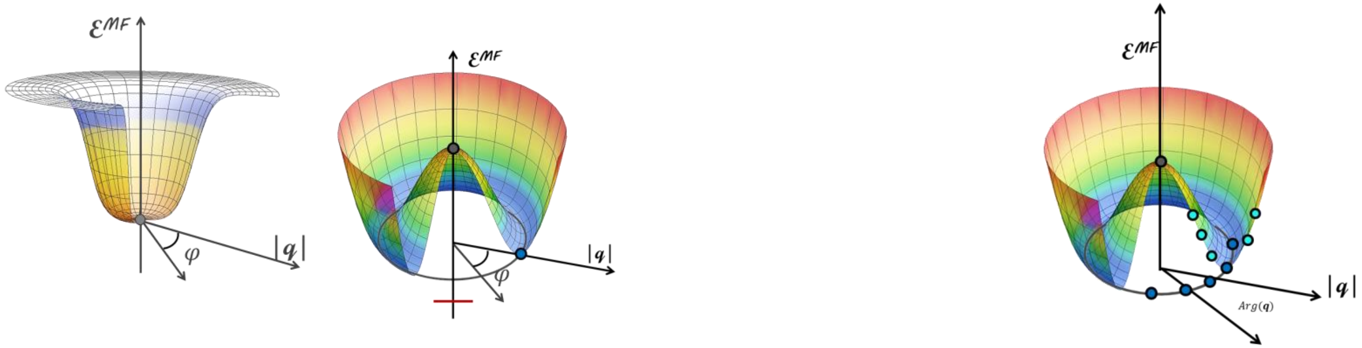


Exact WF

Approx :
Symmetry-preserving HF WF

Approx :
Symmetry-broken HFB WF

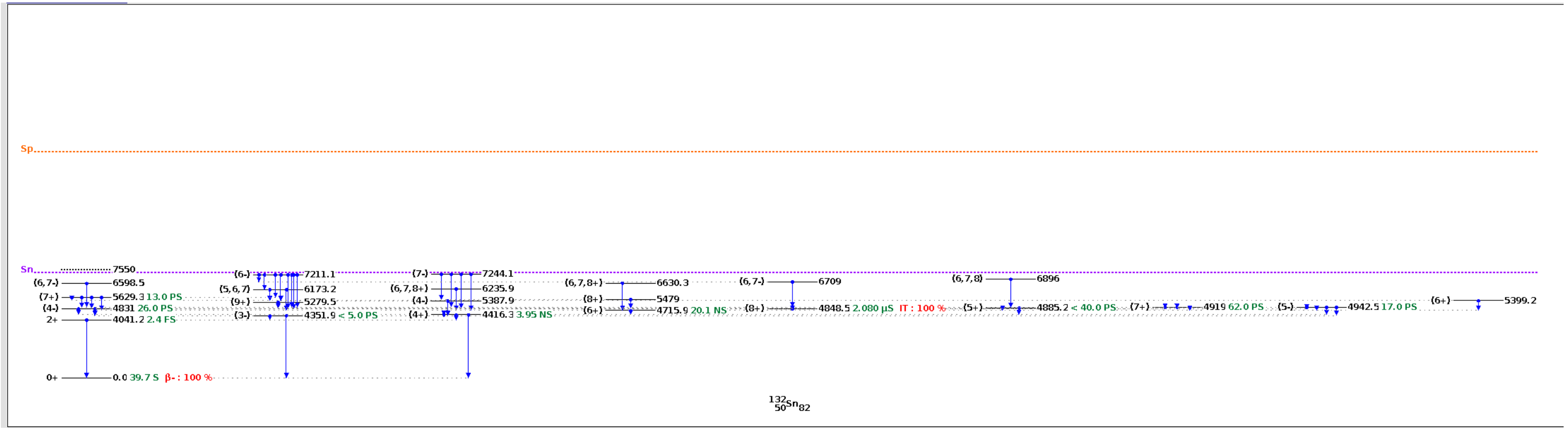
Approx :
PGCM WF

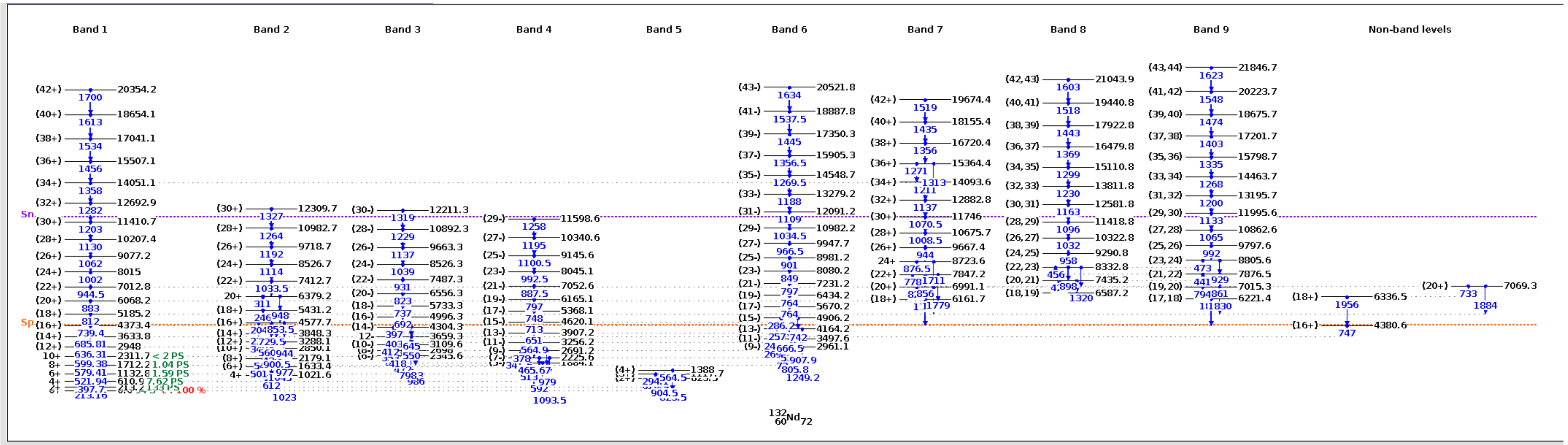


Spectroscopy

Yannouleas & Landman, 2017

Nuclear clustering & PGCM

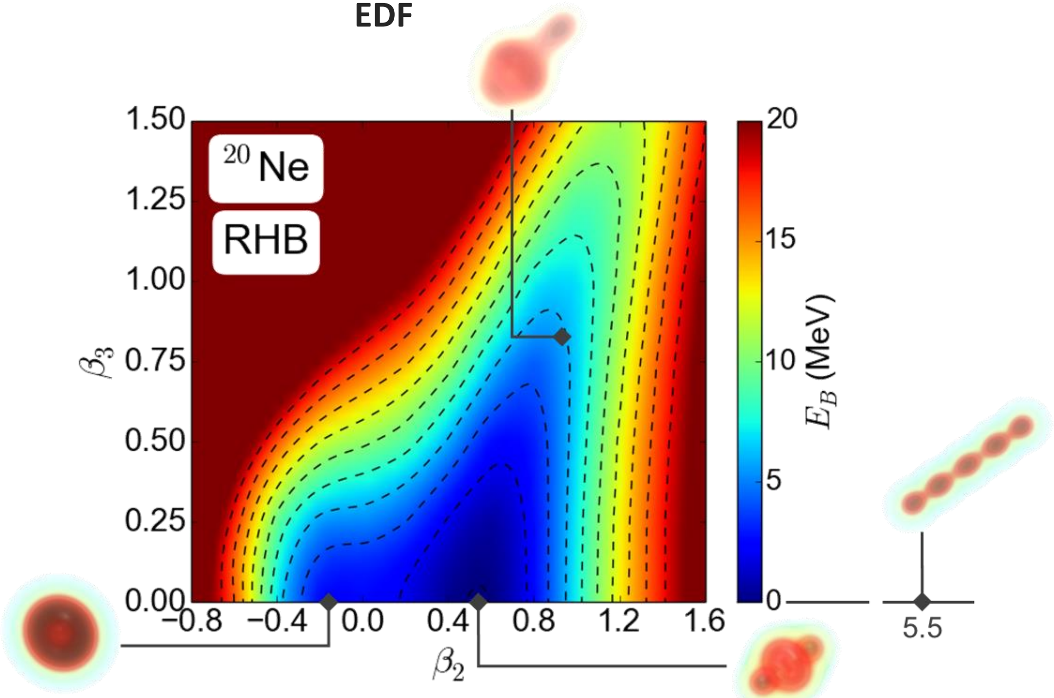




Nuclear clustering & PGCM

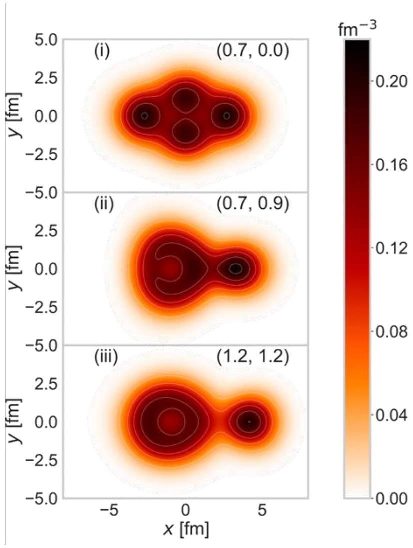
- Correlated GS

EDF

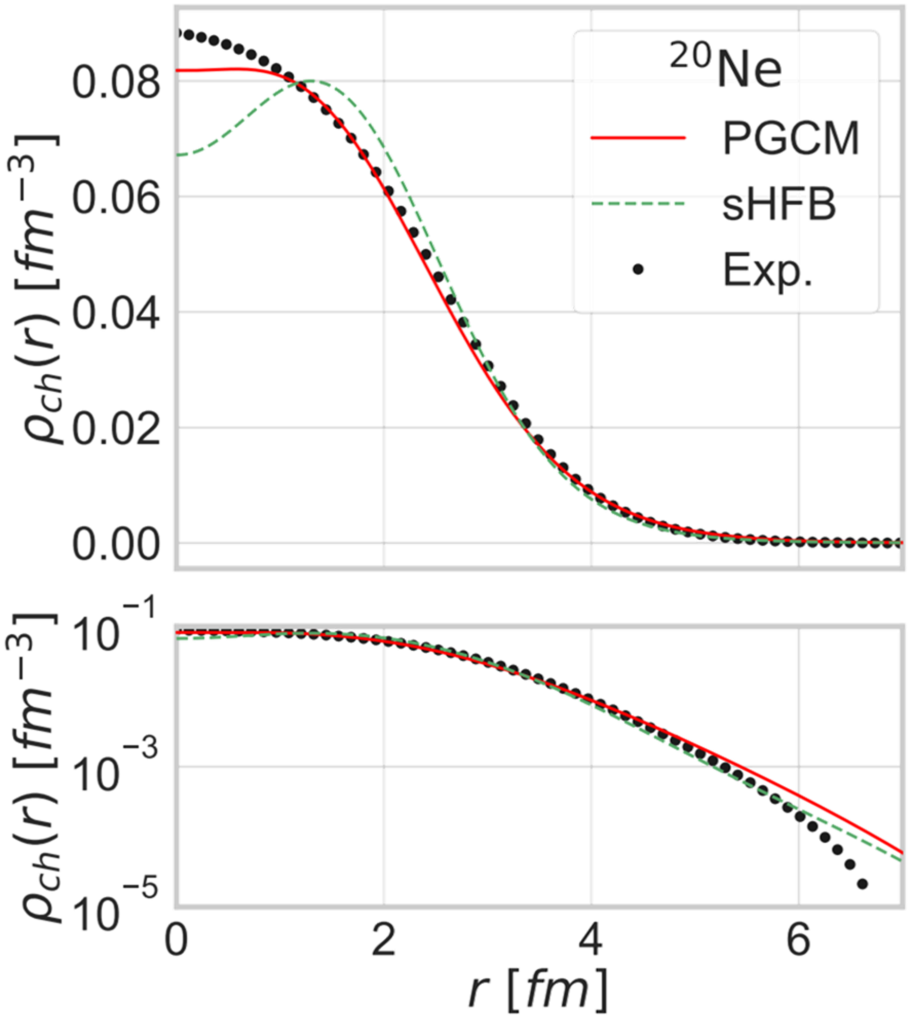


Marevic, Ebran, Khan, Niksic, Vretenar, PRC 97 (2018)

Ab initio



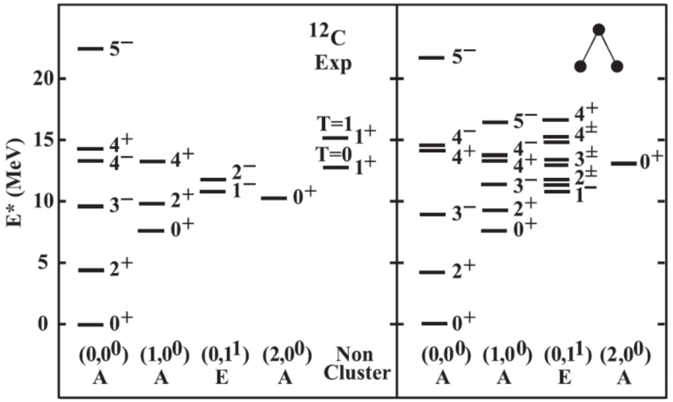
Frosini, Duguet, Ebran, Somà

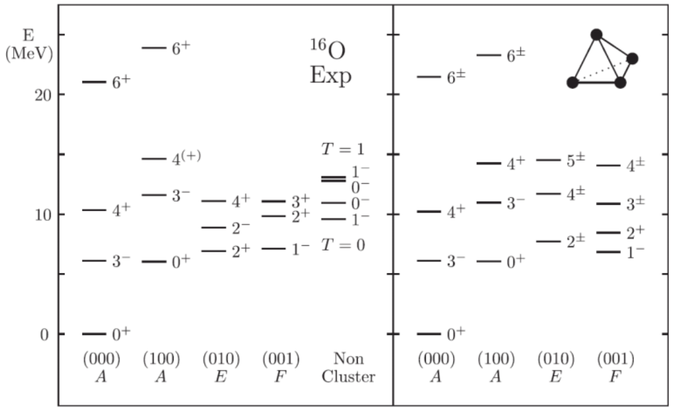


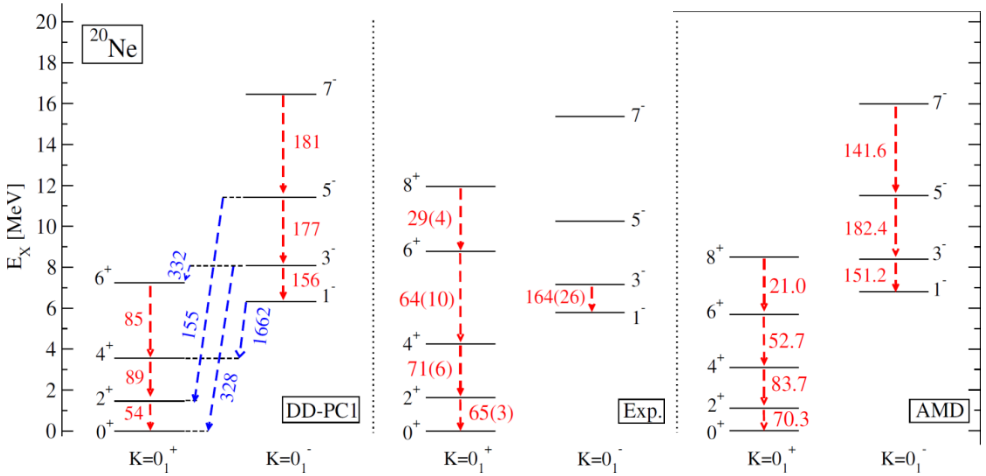
Nuclear clustering & PGCM

◉ Spectroscopy

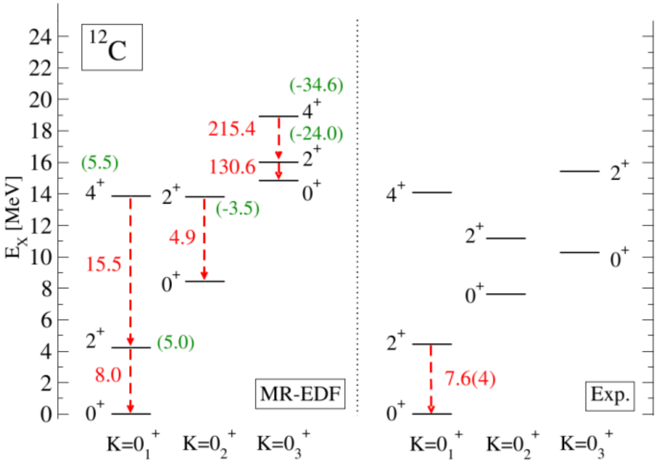
Bijker (2016)

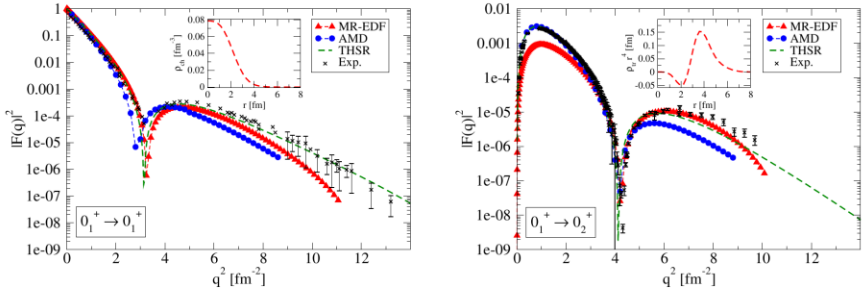




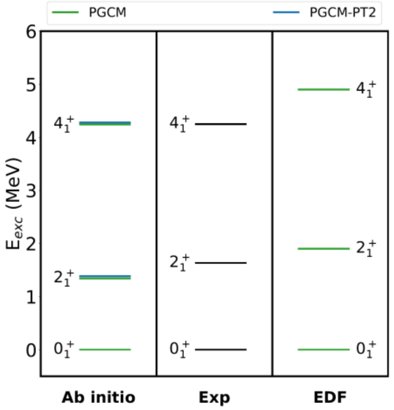


Marevic, Ebran, Khan, Niksic, Vretenar, PRC 2018





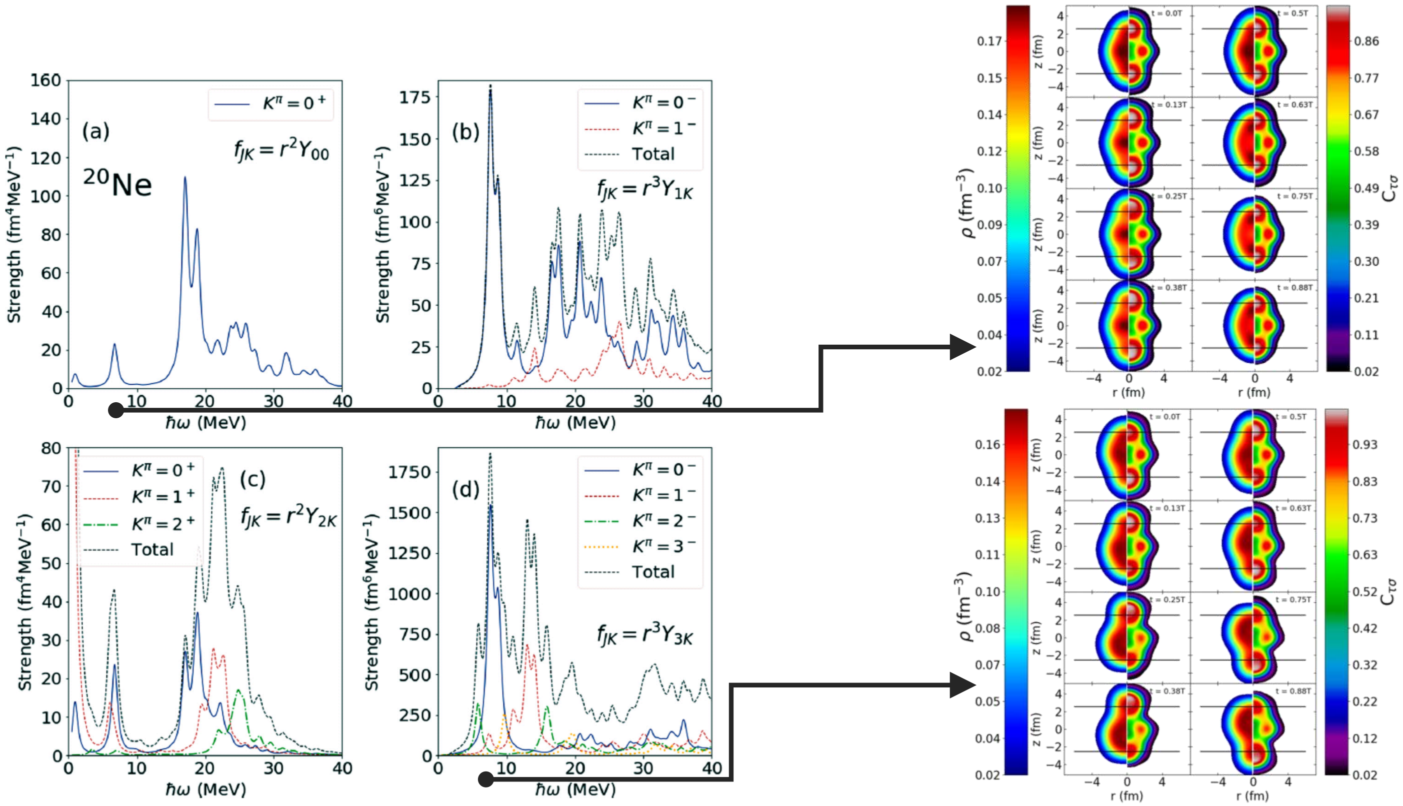
Marević, Ebran, Khan, Nikšić, and Vretenar PRC 2019



Frosini, Duguet, Ebran, Somà, EPJA 2022

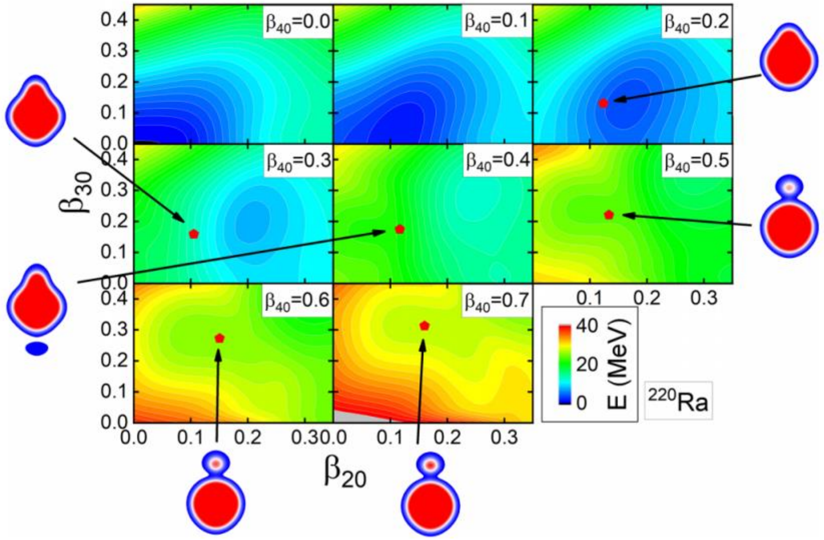
Nuclear clustering & QRPA

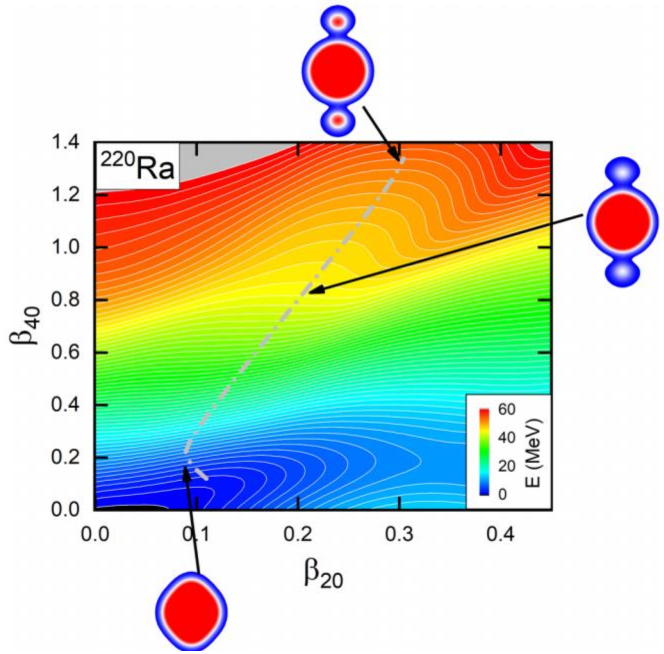
◉ Cluster vibration

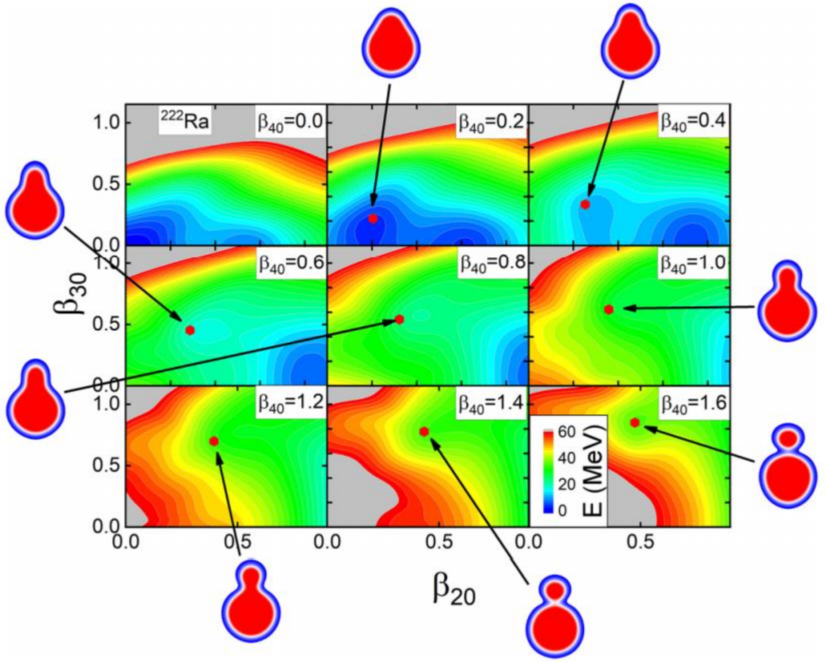


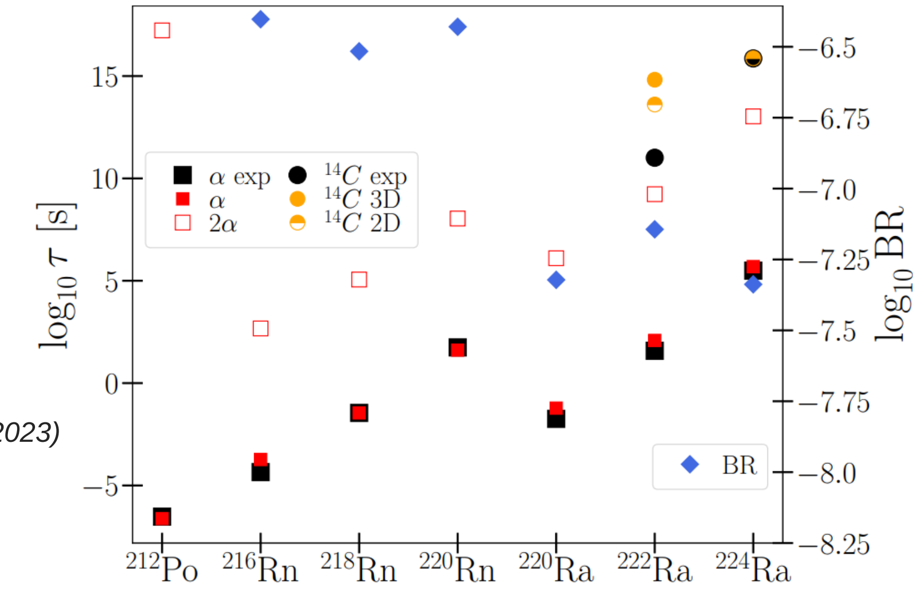
Mercier, Bjelčić, Nikšić, Ebran, Khan,Vretenar PRC 2021
Mercier, Ebran, Khan PRC 2022

Cluster, α and 2α radioactivities







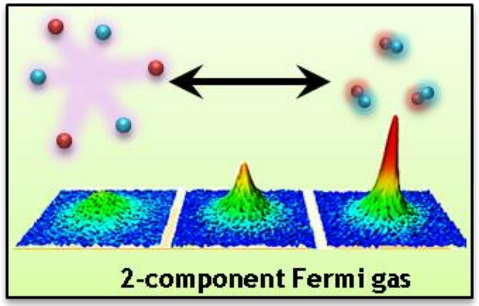


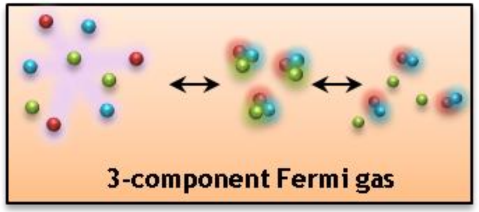
Zhao , Ebran, Heitz , Khan , Mercier, Nikšic,Vretenar, PRC (2023)

Thank you for your attention

N-component Fermi systems

◉ BCS/BEC crossover + phases stabilized by internal dofs





◉ How does this translate in nuclei = 4-component Fermi systems ?

Group theory considerations

- Schematic Hamiltonian $H = H_0 + \mathcal{V}_{\text{res}}$

$$H_0 = \int d^3r \sum_\alpha \varepsilon_\alpha \psi^\dagger_\alpha(\boldsymbol{r})\psi_\alpha(\boldsymbol{r})$$

$$\mathcal{V}_{\text{res}} \sim V_{\text{pair}} = -\int d^3r \left[g^{\text{T}=1} \sum_{\nu=\pm1,0} P^\dagger_\nu(\boldsymbol{r})P_\nu(\boldsymbol{r}) + g^{\text{T}=0} \sum_{\mu=\pm1,0} Q^\dagger_\mu(\boldsymbol{r})Q_\mu(\boldsymbol{r}) \right]$$

Correlated pair operators

$$P^\dagger_\nu(\boldsymbol{r}) \equiv \sqrt{\frac{1}{2}} \sum_l \sqrt{2l+1} \left\{ \psi^\dagger_{l,s=\frac{1}{2},t=\frac{1}{2}}(\boldsymbol{r}) \psi^\dagger_{l,s=\frac{1}{2},t=\frac{1}{2}}(\boldsymbol{r}) \right\}^{(L=0,S=0,T=1)}_{M_L=0,M_S=0,M_T=\nu}$$

$$Q^\dagger_\mu(\boldsymbol{r}) \equiv \sqrt{\frac{1}{2}} \sum_l \sqrt{2l+1} \left\{ \psi^\dagger_{l,\frac{1}{2},\frac{1}{2}}(\boldsymbol{r}) \psi^\dagger_{l,\frac{1}{2},\frac{1}{2}}(\boldsymbol{r}) \right\}^{(L=0,S=1,T=0)}_{M_L=0,M_S=\mu,M_T=0}$$

Group theory considerations

proton
neutron

◉ One-to-one correspondence with a system of spin-3/2 fermions with the Hamiltonian

$$H = \int d^3r \left\{ \sum_\alpha \varepsilon_\alpha \varphi_\alpha^\dagger(\boldsymbol{r})\varphi_\alpha(\boldsymbol{r}) - g_0 S_{0,0}^\dagger(\boldsymbol{r}) S_{0,0}(\boldsymbol{r}) - \sum_{m=\pm2,\pm1,0} g_{2,m} D_{2,m}^\dagger(\boldsymbol{r}) D_{2,m}(\boldsymbol{r}) \right\}$$

Singlet (S=0) pairing operator $S_{0,0}^\dagger = \sum_{\alpha\beta} \langle \tfrac{3}{2}\tfrac{3}{2};00|\tfrac{3}{2}\tfrac{3}{2}\alpha\beta\rangle \varphi_\alpha^\dagger \varphi_\beta^\dagger$

Quintet (S=2) pairing operator $D_{2,m}^\dagger = \sum_{\alpha\beta} \langle \tfrac{3}{2}\tfrac{3}{2};2m|\tfrac{3}{2}\tfrac{3}{2}\alpha\beta\rangle \varphi_\alpha^\dagger \varphi_\beta^\dagger$

with $S_{0,0}^\dagger = P_0^\dagger,\ D_{2,0}^\dagger = Q_0^\dagger,\ D_{2,\pm1}^\dagger = P_{\pm1}^\dagger \text{ and } D_{2,\pm2}^\dagger = Q_{\pm1}^\dagger$

Group theory considerations

- Sp(4) ~ SO(5) symmetry without fine tuning the coupling constants

- Generators of $\mathfrak{so}(5)$ $\quad \Gamma^{ab} \equiv -\frac{i}{2}\left[\Gamma^a, \Gamma^b\right] \quad (1 \leq a, b \leq 5)$ $\quad \Gamma^1 = \begin{pmatrix} 0 & -iI \\ iI & 0 \end{pmatrix}, \quad \Gamma^{2,3,4} = \begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & -\boldsymbol{\sigma} \end{pmatrix}, \quad \Gamma^1 = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}$

- Bilinears of fermions can be classified according to their behavior under SO(5)

Particle-hole channel

$$
\begin{aligned}
n(\boldsymbol{r}) &= \sum_{\alpha} \varphi_\alpha^\dagger(\boldsymbol{r}) \varphi_\alpha(\boldsymbol{r}), \\
n_a(\boldsymbol{r}) &= \frac{1}{2} \sum_{\alpha\beta} \varphi_\alpha^\dagger(\boldsymbol{r}) \Gamma^a_{\alpha\beta} \varphi_\beta(\boldsymbol{r}), \\
L_{ab}(\boldsymbol{r}) &= -\frac{1}{2} \sum_{\alpha\beta} \varphi_\alpha^\dagger(\boldsymbol{r}) \Gamma^{ab}_{\alpha\beta} \varphi_\beta(\boldsymbol{r}).
\end{aligned}
$$

Particle-particle channel

$$
\begin{aligned}
\eta^\dagger(\boldsymbol{r}) &= \frac{1}{2} \sum_{\alpha\beta} \varphi_\alpha^\dagger(\boldsymbol{r}) C_{\alpha\beta} \varphi_\beta^\dagger(\boldsymbol{r}), \\
\xi_a^\dagger(\boldsymbol{r}) &= -\frac{i}{2} \sum_{\alpha\beta} \varphi_\alpha^\dagger(\boldsymbol{r}) \left(\Gamma^a C\right)_{\alpha\beta} \varphi_\beta^\dagger(\boldsymbol{r}),
\end{aligned}
$$

$$C = \Gamma^1 \Gamma^3$$

$$S_{0,0}^\dagger = -\frac{\eta^\dagger}{\sqrt{2}} \quad D_{2,0}^\dagger = -i\frac{\xi_4^\dagger}{\sqrt{2}}, \quad D_{2,\pm1}^\dagger = -\frac{\xi_3^\dagger \mp i\xi_2^\dagger}{\sqrt{2}}, \quad D_{2,\pm2}^\dagger = \frac{\mp\xi_1^\dagger + i\xi_5^\dagger}{\sqrt{2}}$$

C. Wu PRL 2005

Group theory considerations

$$H = \int d^3r \left\{ \sum_\alpha \varepsilon_\alpha \varphi^\dagger_\alpha(\boldsymbol{r})\varphi_\alpha(\boldsymbol{r}) - g_0 S^\dagger_{0,0}(\boldsymbol{r}) S_{0,0}(\boldsymbol{r}) - \sum_{m=\pm 2,\pm 1,0} g_{2,m} D^\dagger_{2,m}(\boldsymbol{r}) D_{2,m}(\boldsymbol{r}) \right\}$$

- If $g_0 = g_2 \equiv g$, singlet and quintet pairing states are degenerate and can be recast into a sextet pairing state $\Rightarrow$ SU(4) symmetry

- 2 different superfluid orders : i) Sp(4)-singlet BCS pairing phas $\eta^\dagger(\boldsymbol{r})$

  ii) SU(4) molecular superfluid phase formed from bound states ($A^\dagger(\boldsymbol{r}) \equiv \varphi^\dagger_{\frac{3}{2}}(\boldsymbol{r})\varphi^\dagger_{\frac{1}{2}}(\boldsymbol{r})\varphi^\dagger_{-\frac{1}{2}}(\boldsymbol{r})\varphi^\dagger_{-\frac{3}{2}}(\boldsymbol{r})$

- Competition manifested by a $\mathbb{Z}_2$ discrete symmetry (coset between the center of SU(4) and the center of Sp(4)) $\mathcal{U}_n = e^{in_4\pi}$

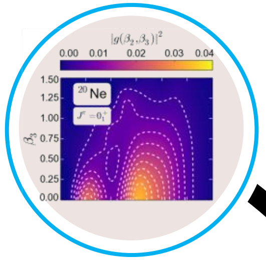
$$\begin{aligned} \eta^\dagger &\mapsto \mathcal{U}_n \eta^\dagger \mathcal{U}_n^{-1} = -\eta^\dagger, \\ A^\dagger &\mapsto \mathcal{U}_n A^\dagger \mathcal{U}_n^{-1} = A^\dagger. \end{aligned}$$

$\mathbb{Z}_2$ needs to be spontaneously broken to stabilize the BCS quasi-long range order.

$\mathbb{Z}_2$ remaining unbroken $\Rightarrow$ strong quantum fluctuations in the spin channel suppressing Cooper pairing (2 fermions can't form a $\mathbb{Z}_2$ singlet) $\Rightarrow$ leading superfluid instability = quartetting

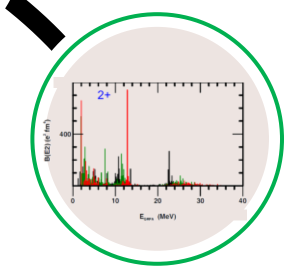
1 General goal of nuclear structure theory

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



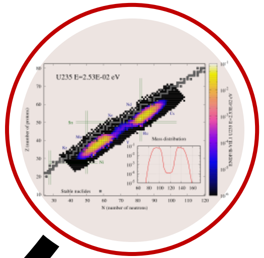
Ground-state

masses, radii, density profile, …



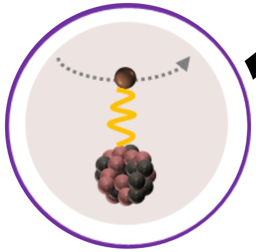
Excitation spectra

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



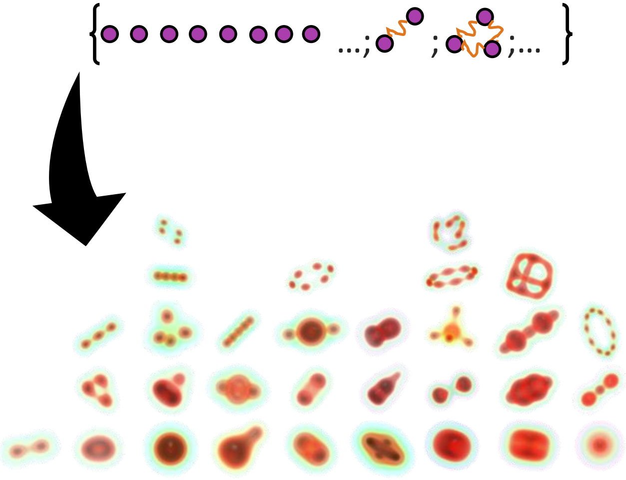
Decay modes

lifetime, yields, …



Reactions

cross sections, …



Intrinsic densities

Atomic nucleus

=

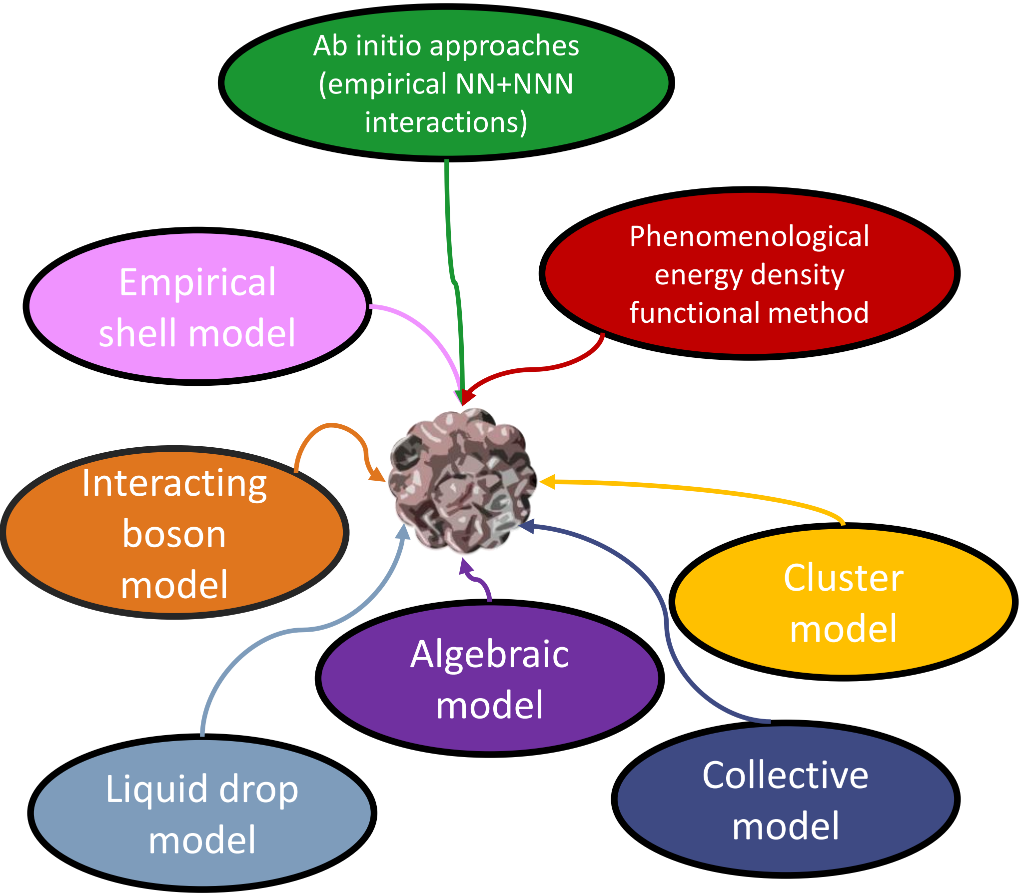
A mesoscopic, self-bound system of strongly correlated spin-1/2 and isospin-1/2 composite fermions in strong and electroweak interaction.

Emergent SSBs

1 Strategies

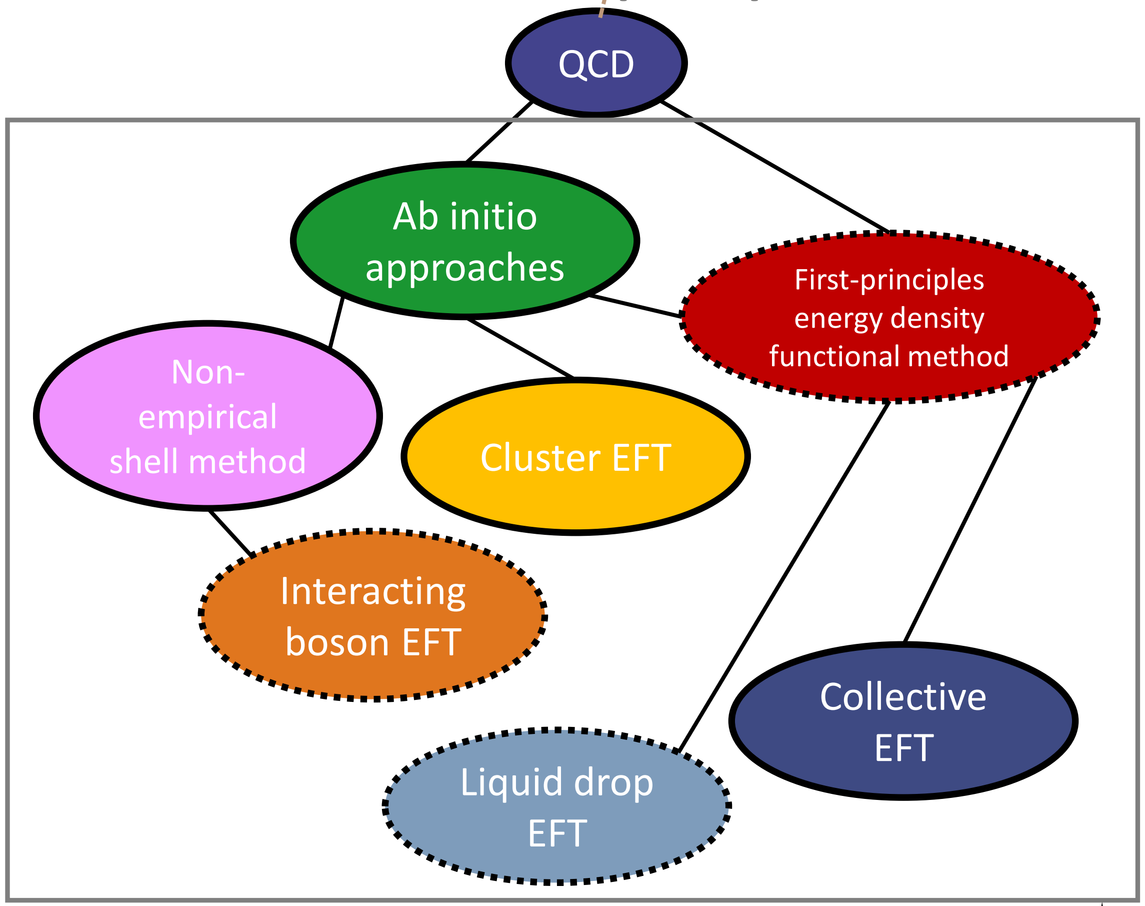
◉ Achieve a { *accurate* / *predictive* / *computationally affordable* } description ?

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