



DE LA RECHERCHE À L'INDUSTRIE

The nuclear clustering phenomenon

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EMMI Taskforce

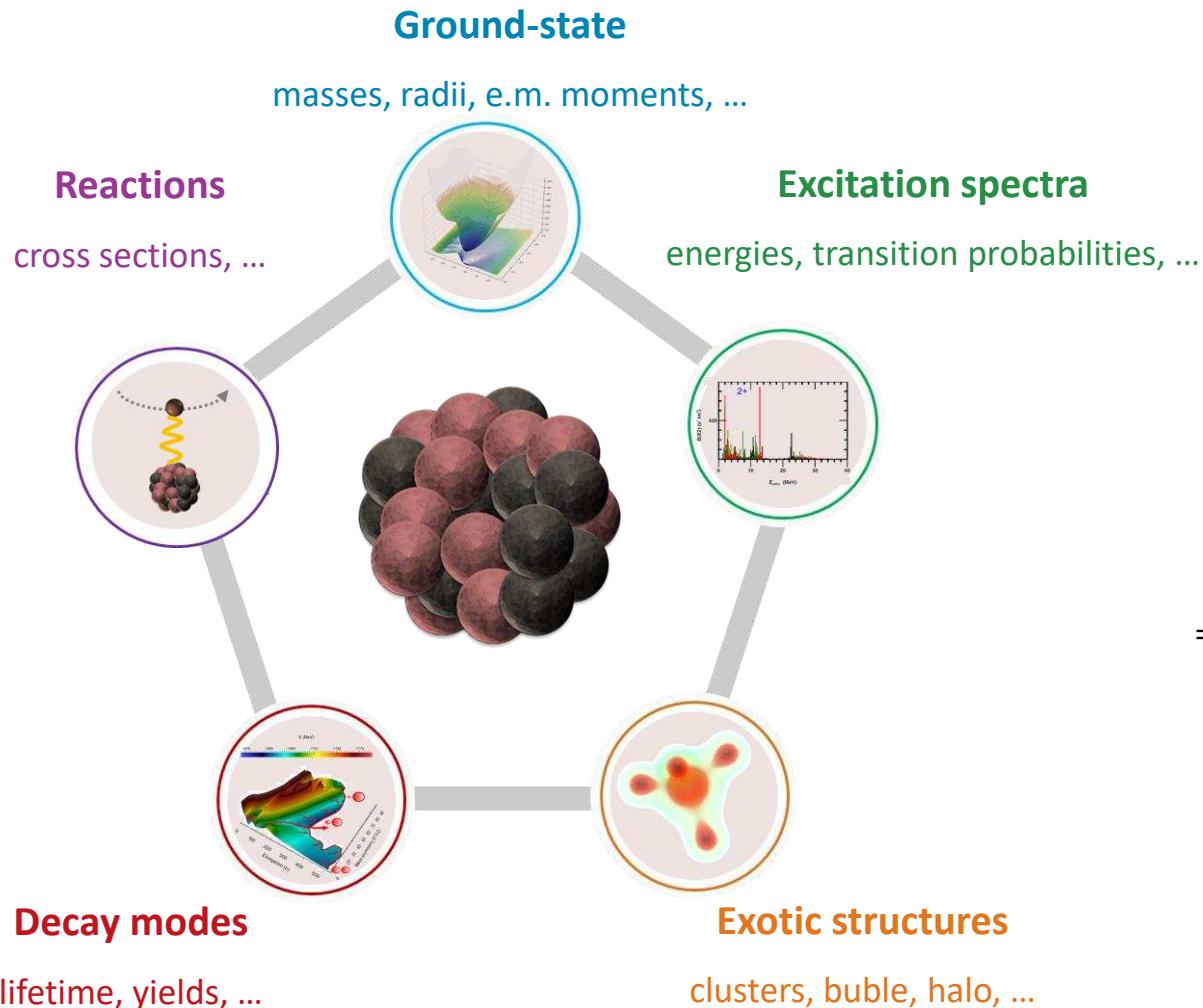
2022 May 30th-June 3rd

1 Few words on nuclear structure theory

2 Microscopic description of nuclear clustering

What is nuclear structure theory about ?

- How nucleons self-organize and become disorganized ?



Nuclei are complex systems

- Many characteristic scales :

→ p & n momenta	~	100 MeV
→ separation energies	~	10 MeV
→ vibration modes	~	1MeV
→ rotation modes	~	0.01-5 MeV

- Strongly correlated:

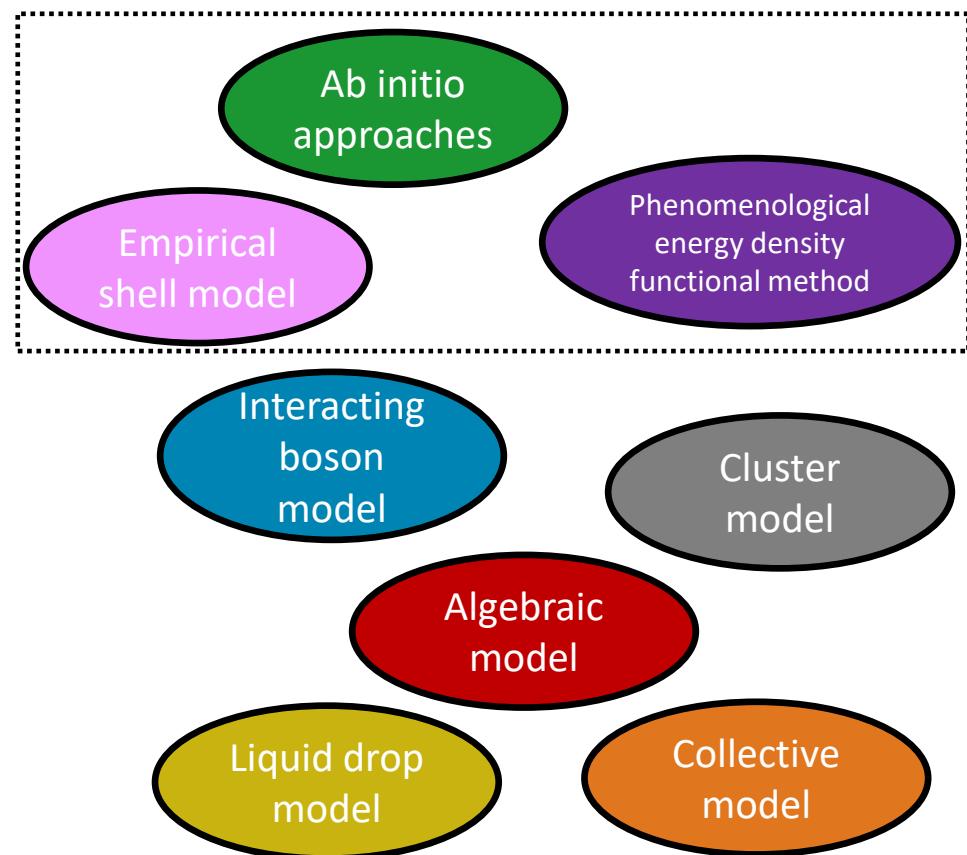
→ angular correlations	⇒ deformation
→ pairing correlations	⇒ superfluidity
→ quartetting correlations	⇒ clustering

⇒ Rich diversity of nuclear phenomena, among which the clustering phenomenon

Best strategy ?

- What is the best strategy to achieve a **robust, predictive, yet computationally affordable** description of nuclear structure properties ?

--> Richness of nuclear phenomena propelled the formulation of a plethora of models, in general born from systematics of regularities in the behavior of nuclei



- Popular misconception : The more microscopic the more predictive

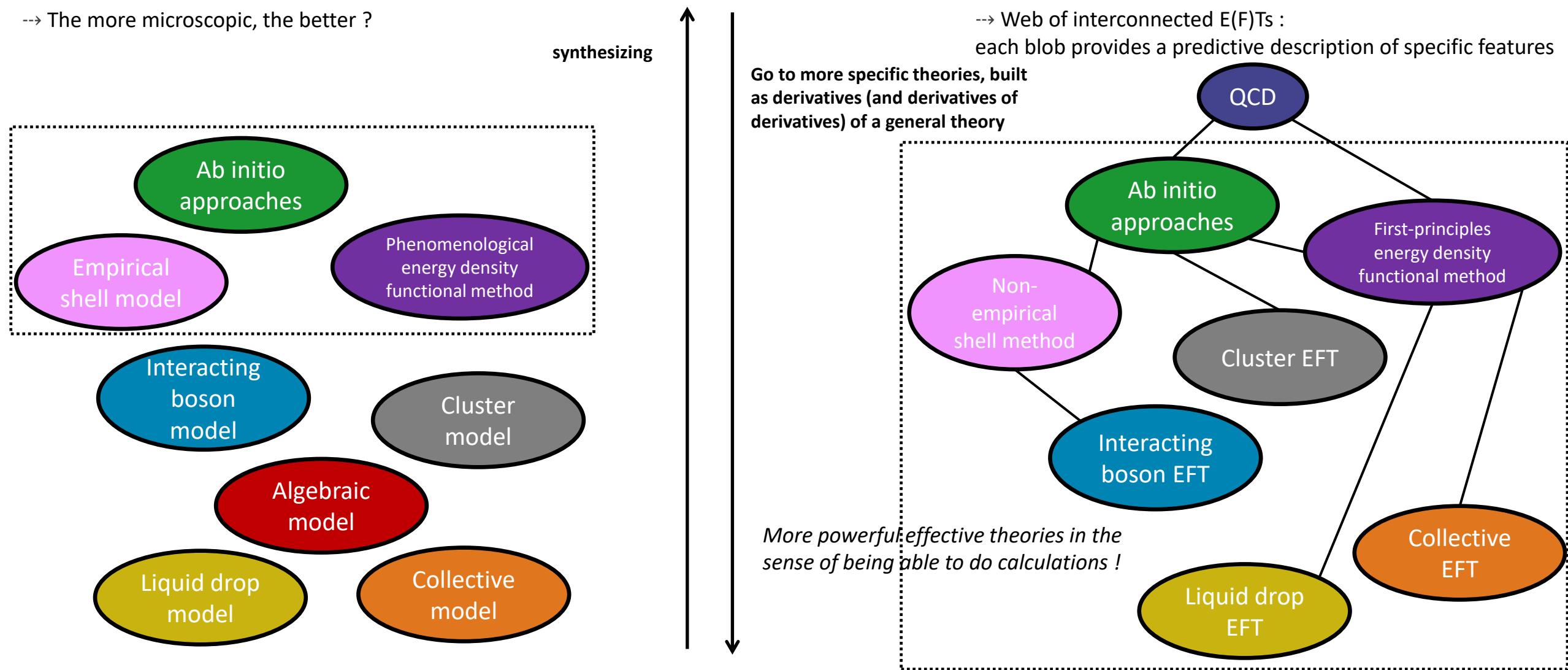
--> Confusion between the resolution of the language – **microscopic/coarse grain** – on the one hand
and
the nature of the description – **effective theory/phenomenological model** – on the other hand

Precious empirical knowledge about various phenomena and associated relevant dofs

Best strategy ?

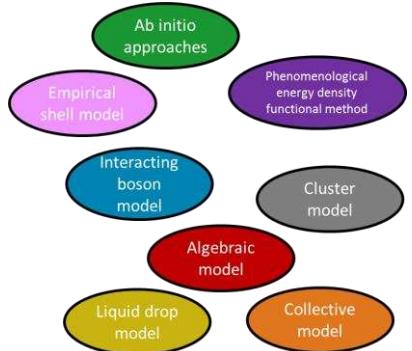
● What is the best strategy to achieve a **robust, predictive, yet computationally affordable** description of nuclear structure properties ?

--> The more microscopic, the better ?



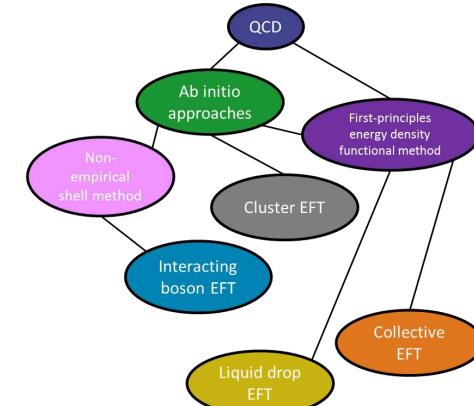
Best strategy ?

- In what aspect(s) empirical models and EFTs differ ?



--> As we get more microscopic, things become harder to compute

--> Want the **simplest** framework that captures the essential physics
 => identification of relevant dofs + dynamics constrained by symmetry arguments



--> As we move up, it becomes harder to compute

--> Want the **simplest** framework that captures the essential physics
 => identification of relevant **scales** & dofs + dynamics constrained by symmetry arguments

--> At the same time, we don't want to give up anything , in the sense that even if we're giving up smthg at our LO description, we want to retain the ability to correct that LO description order by order in some expansions, so that it can be corrected to arbitrary precision

● To describe a physical system :

--> Determine the **relevant** dofs/scales (*"everything should be made as simple as possible, but no simpler," Einstein*)

In QFT language :

might be obvious or very tricky

What fields ?

--> Identify the symmetry pattern (global, gauged, accidental, spontaneously broken, anomalous, approximate, ...) you want to be consistent with (*Totalitarian principle : "everything that is not forbidden is compulsory" Gell-Mann — Folk Theorem : "If one writes down the most general possible Lagrangian, including all terms consistent with assumed symmetry principles, and then calculates matrix elements with this Lagrangian to any given order of perturbation theory, the result will simply be the most general possible S-matrix consistent with perturbative unitarity, analyticity, cluster decomposition, and the assumed symmetry properties" Weinberg*)

What interactions/dynamics ?

EFT can have more symmetries than the original theory

--> Specify what is (are) your expansion parameter(s) as well as your LO description

Ensures that only a finite number of terms contribute at any given order in an expansion $\frac{E}{\Lambda'}$, and that we can decide upfront which terms to keep in the action based on the desired level of accuracy

What power counting ?

--> Constrain LECs

Matching

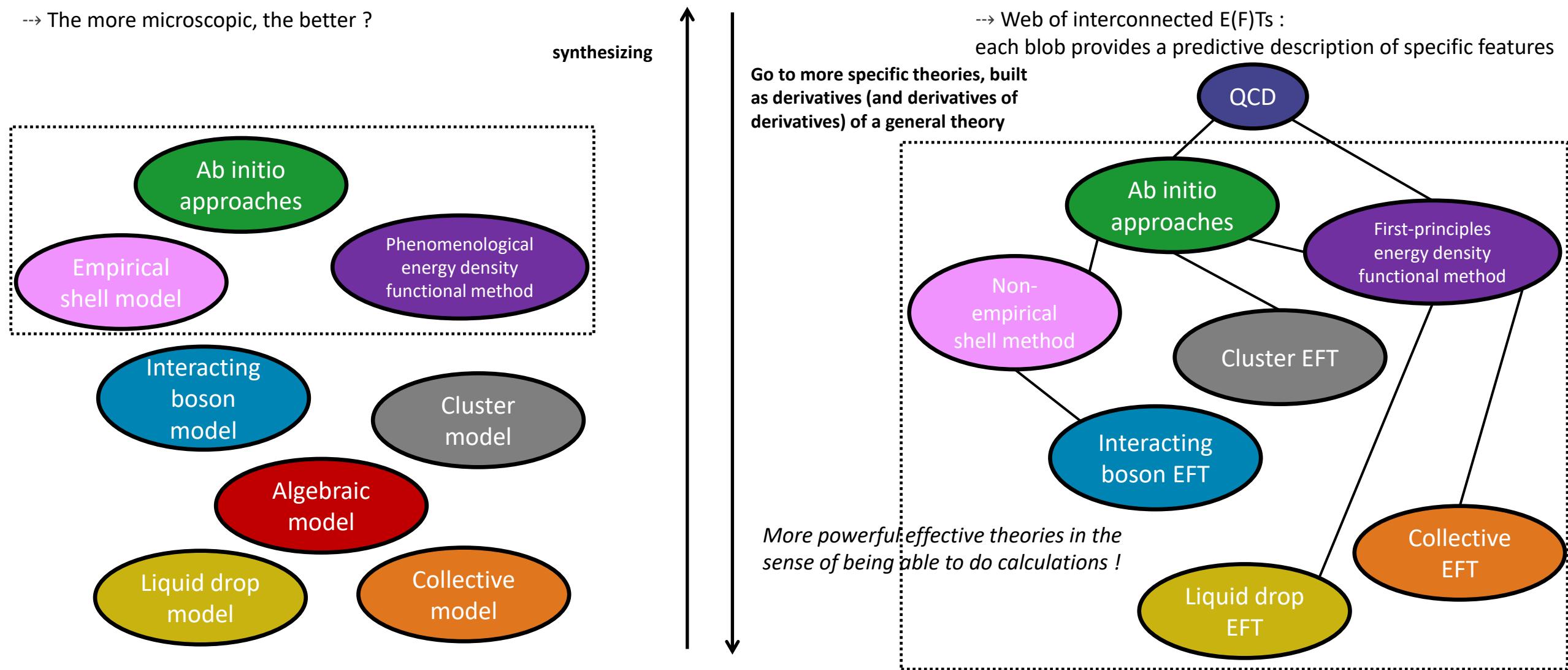
--> Make predictions



Best strategy ?

● What is the best strategy to achieve a **robust, predictive, yet computationally affordable** description of nuclear structure properties ?

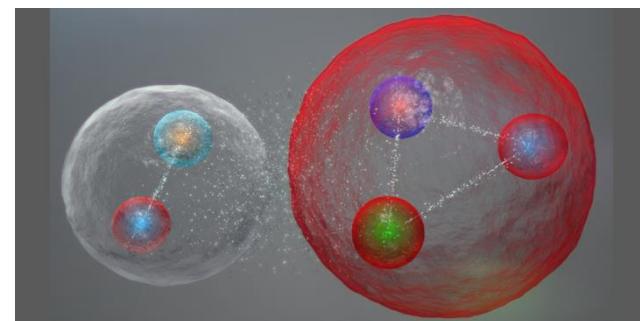
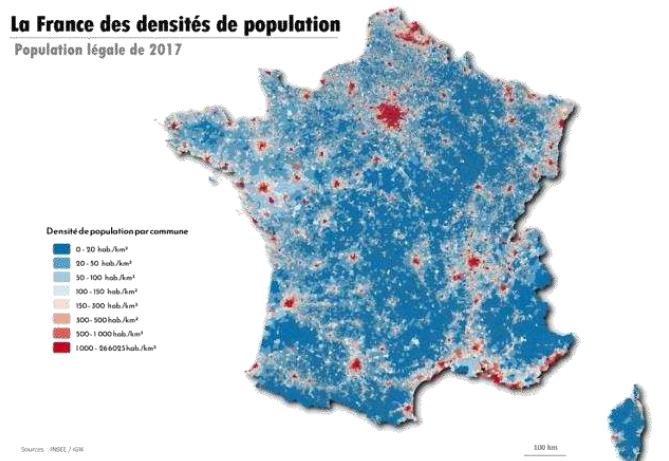
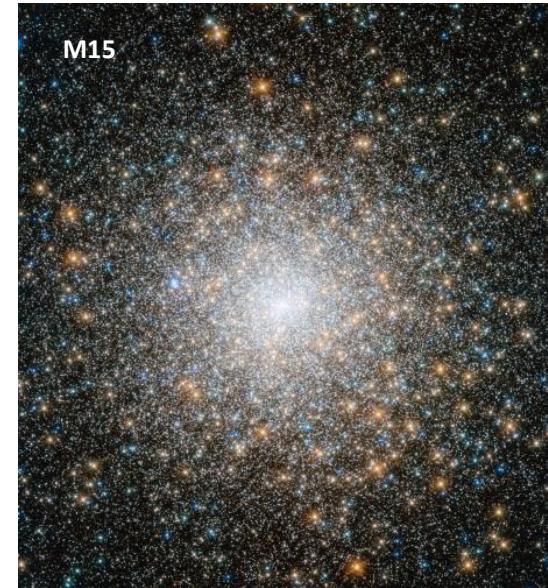
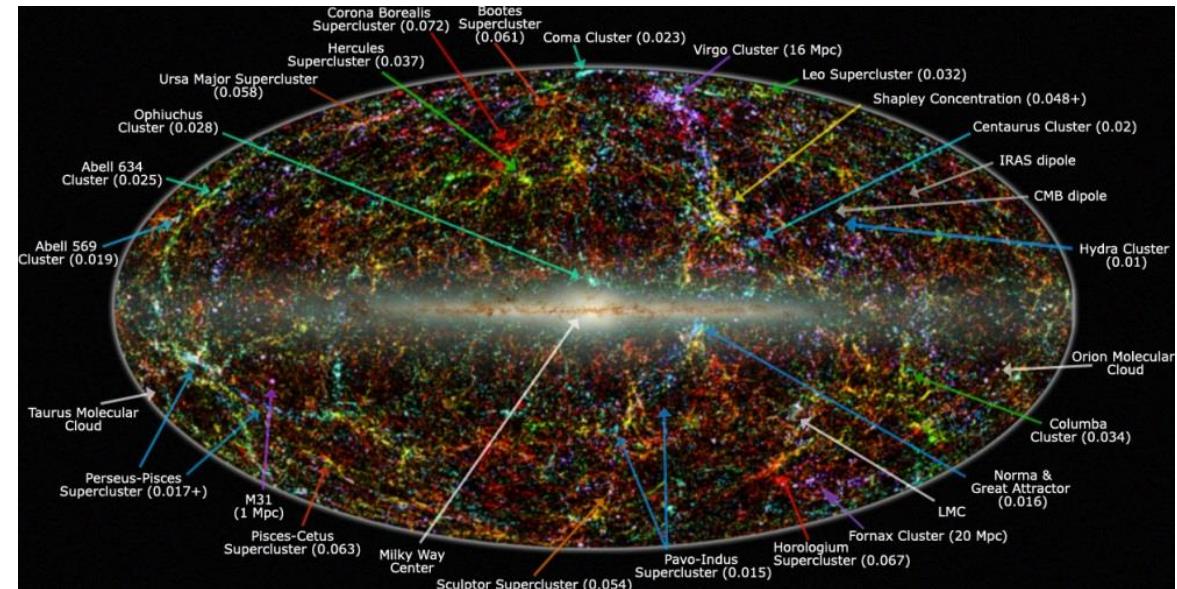
--> The more microscopic, the better ?



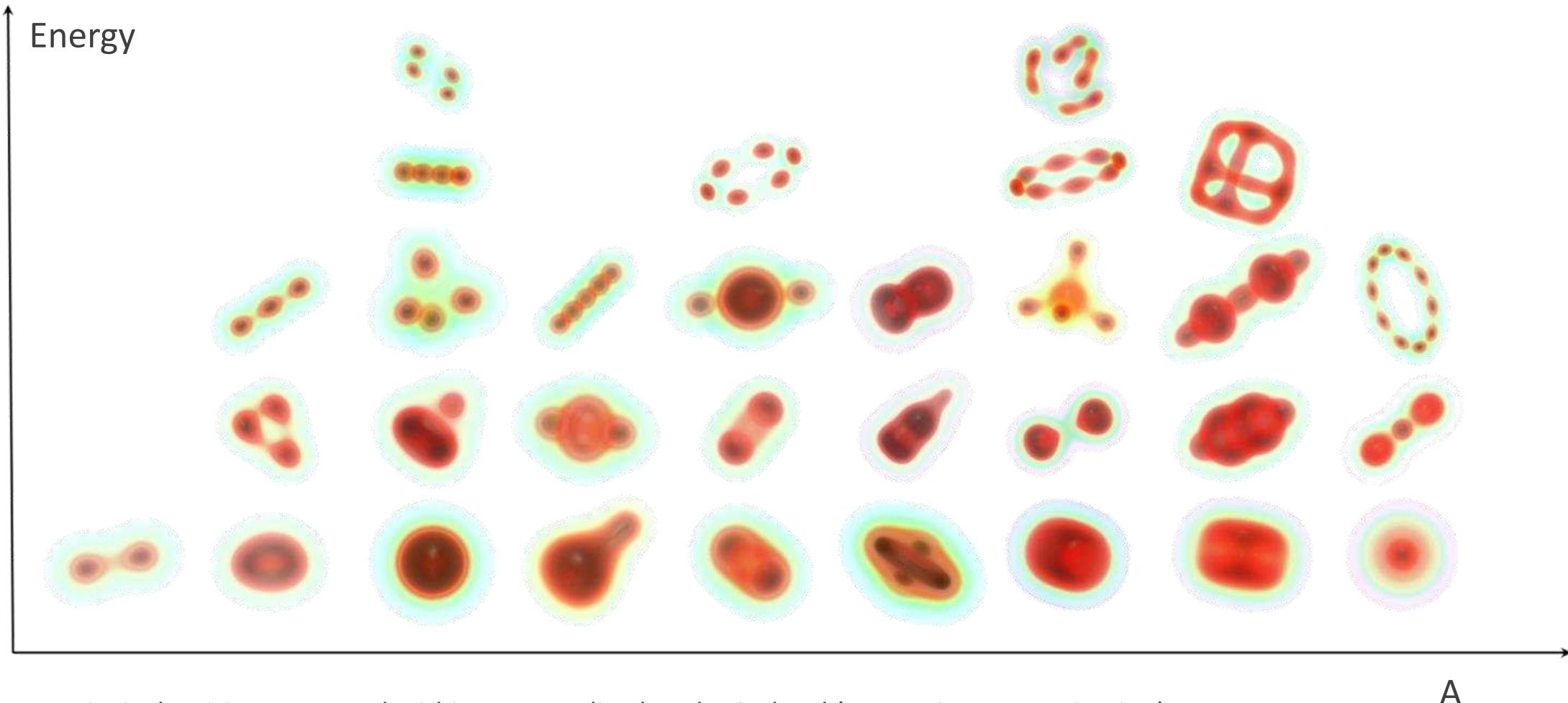
1 Few words on nuclear structure theory

2 Microscopic description of nuclear clustering

● Clustering : an ubiquitous phenomenon



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



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

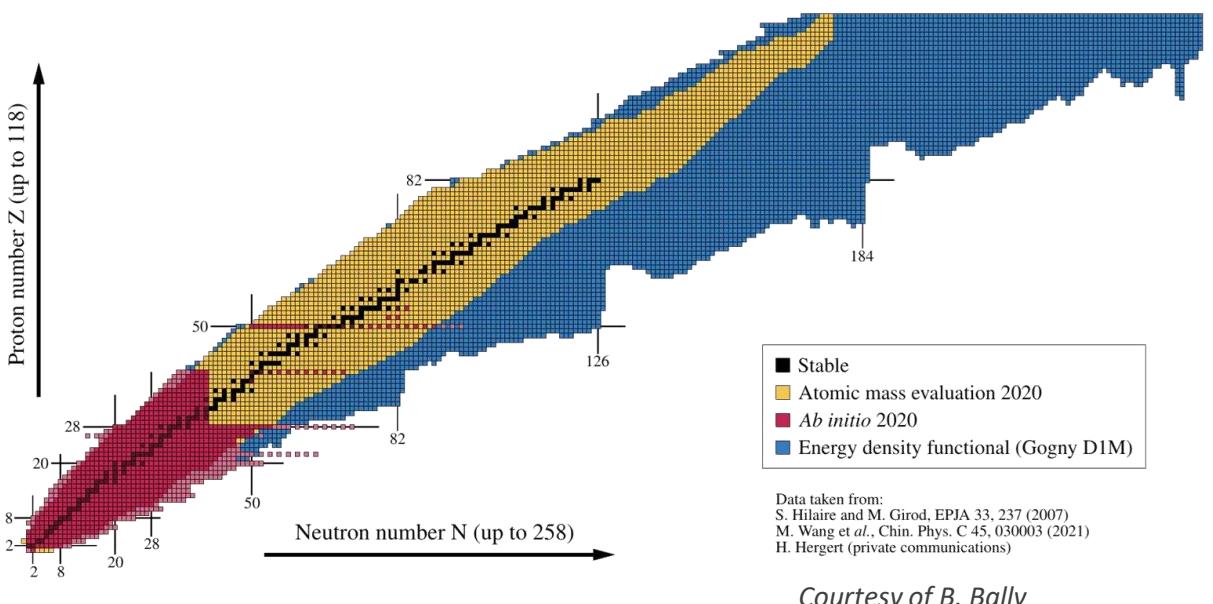
A

Microscopic treatment of nuclear systems

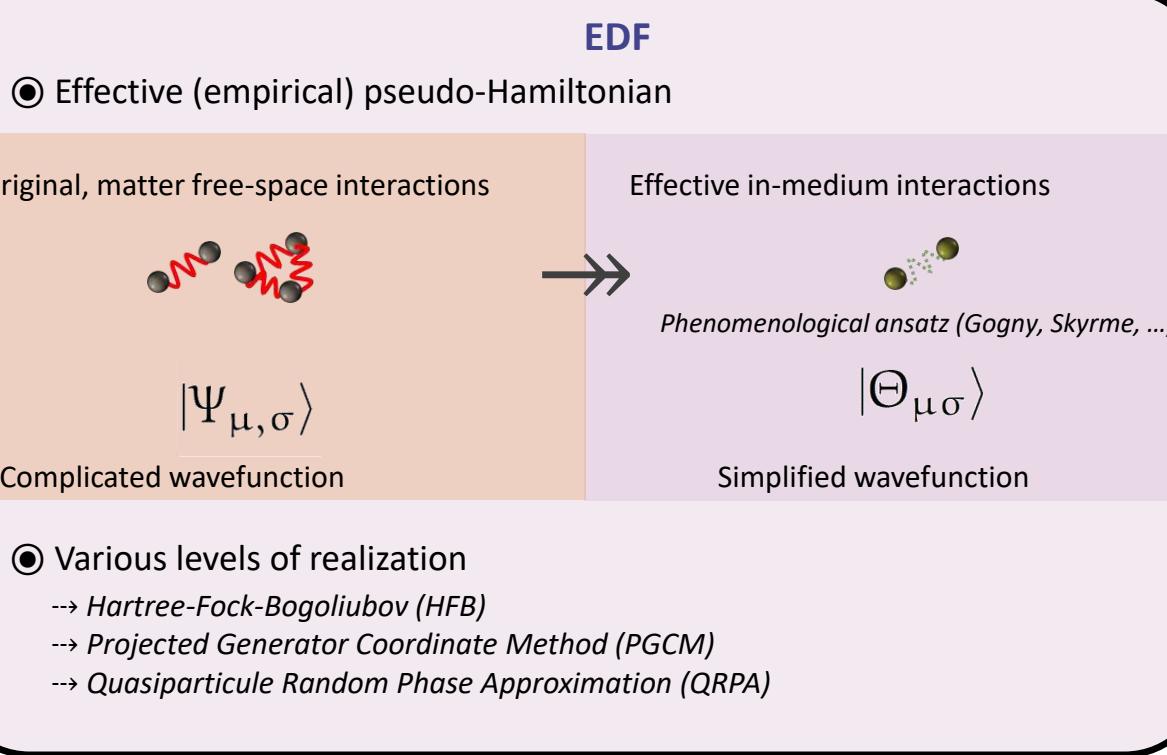
- 1) Nucleus: A interacting, structure-less nucleons
- 2) Structure & dynamic encoded in a Hamiltonien
- 3) Solve A -nucleon Schrödinger/Dirac equation to desired accuracy

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

Strongly correlated wavefunction



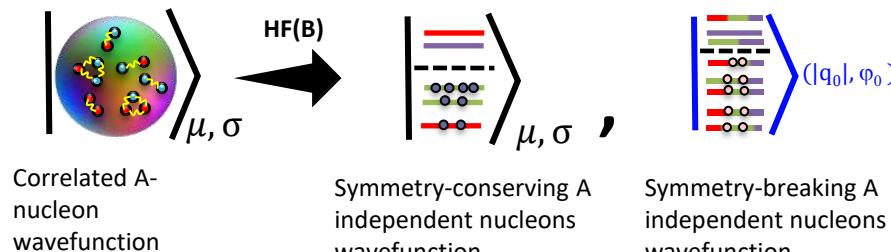
- Ab initio**
- Chiral Hamiltonian rooted in QCD
 - Bunch of many-body methods
 - CI (full space diag.) : exponential scaling
 - Hybrids (valence space diag.) : mixed scaling
 - Expansion methods (partition, expand and truncate) : polynomial scaling



The Energy Density Functional Method

● HFB treatment

--> A -nucleon problem $\rightarrow A$ 1-nucleon problems

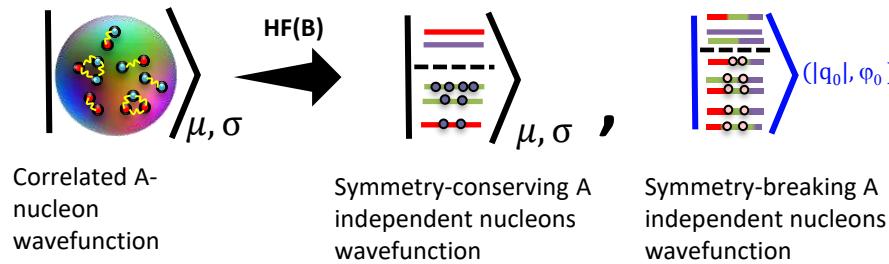


--> SSB : Efficient way for capturing so-called static correlations

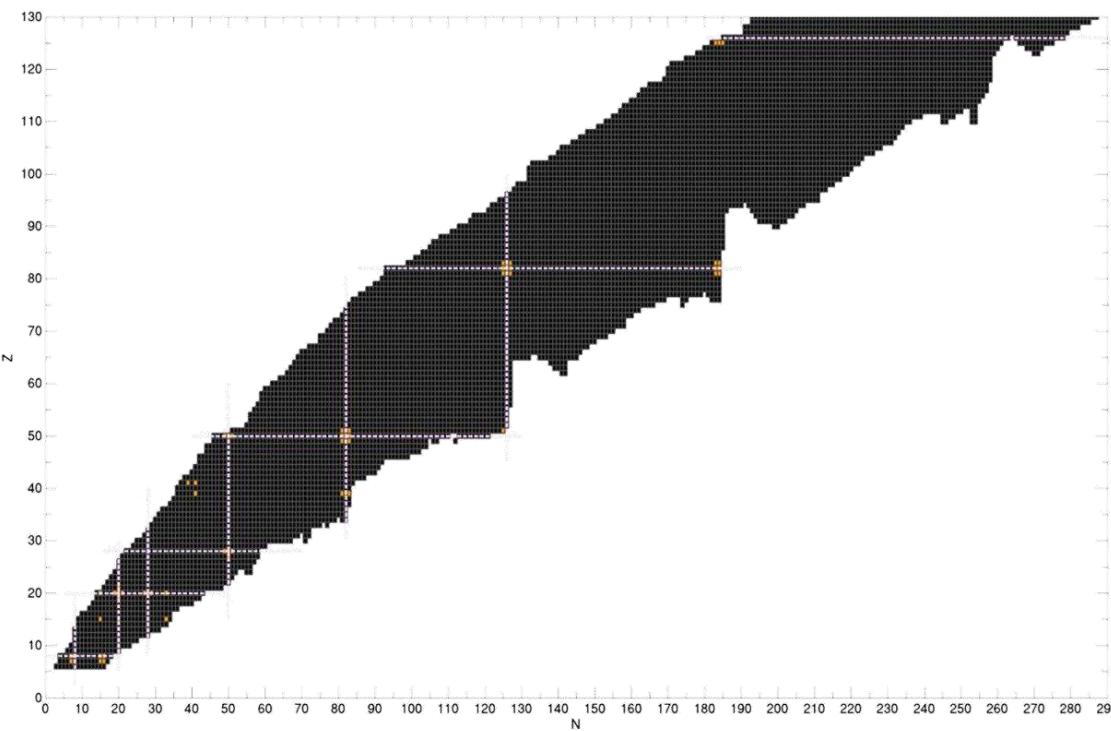
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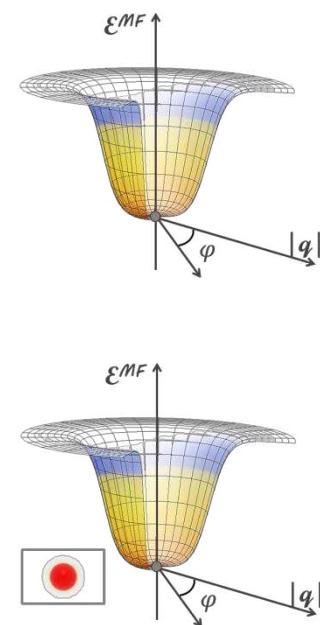
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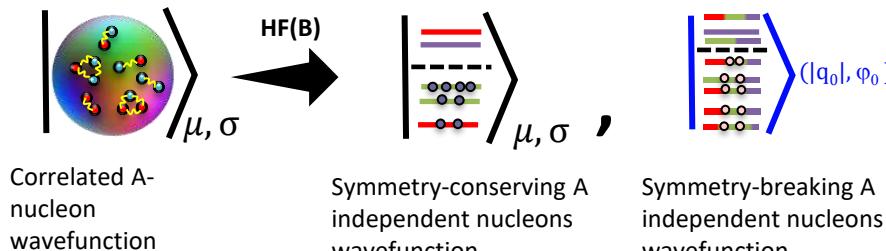
Symmetry-restricted HF : good description of GS of doubly closed-shell nuclei & neighbors (~ 30 nuclei)



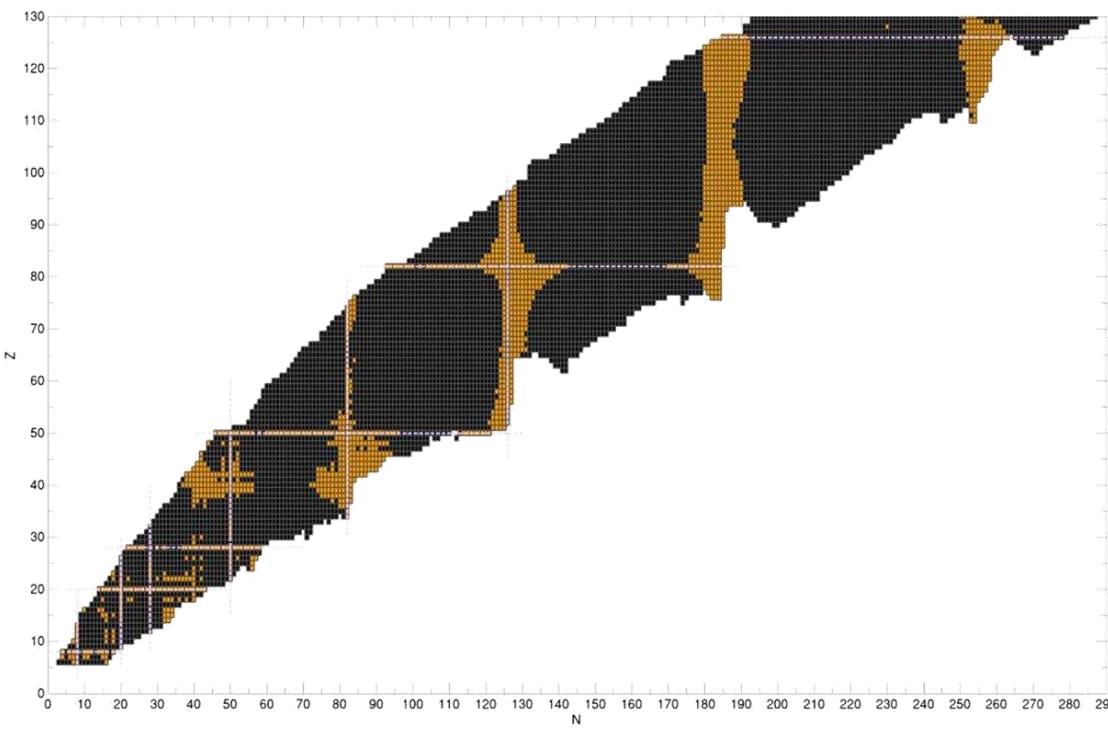
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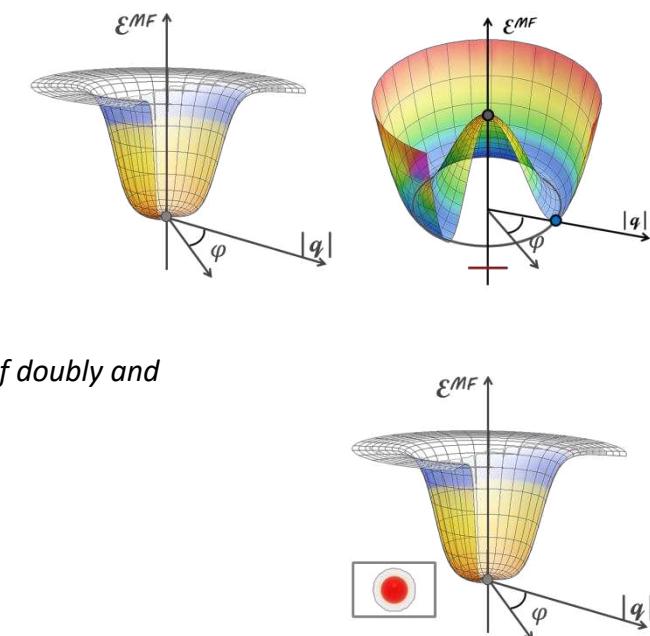
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--> SSB : Efficient way for capturing so-called static correlations



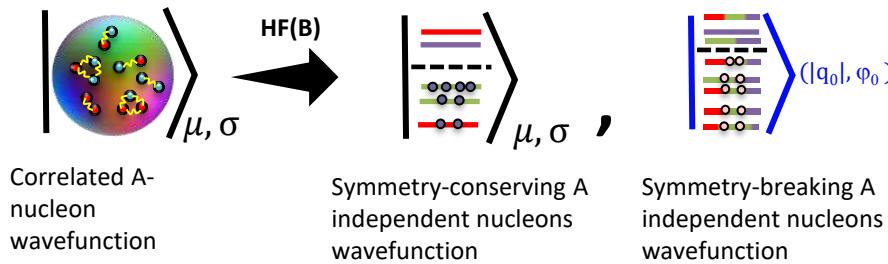
Spatial symmetry-restricted HFB: good description of GS of doubly and singly closed-shell nuclei & neighbors (~ 300 nuclei)



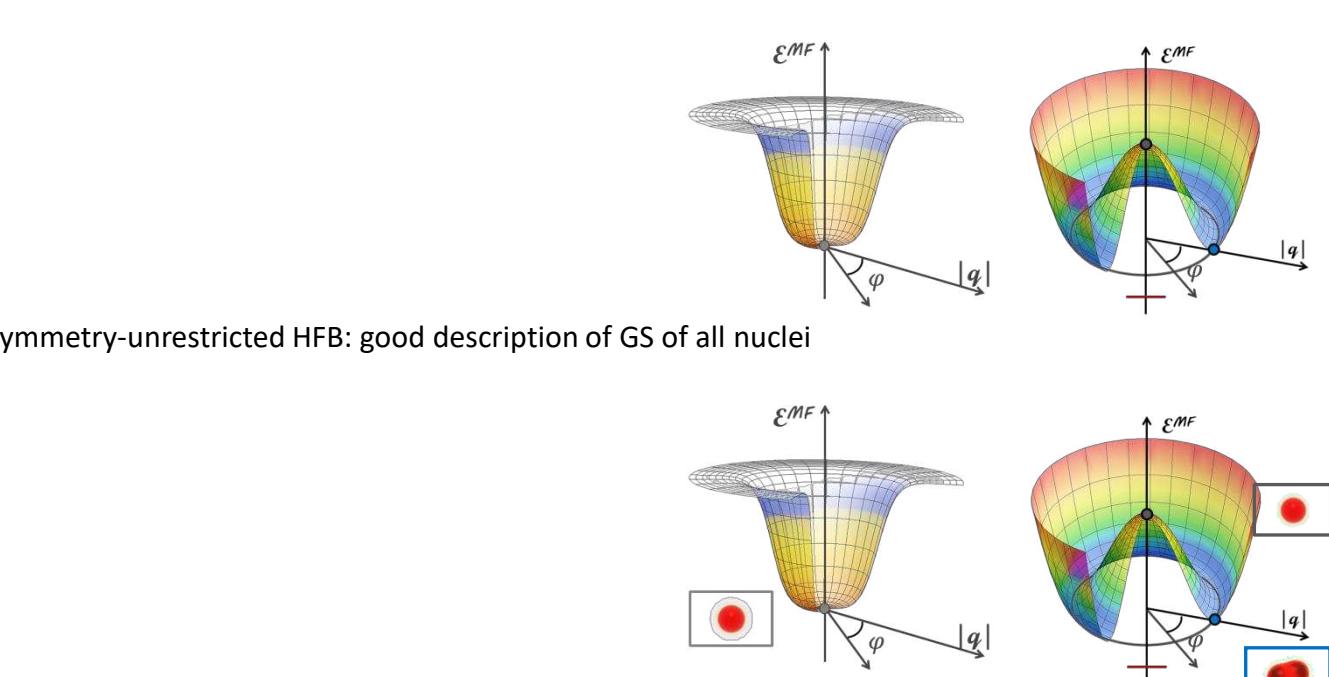
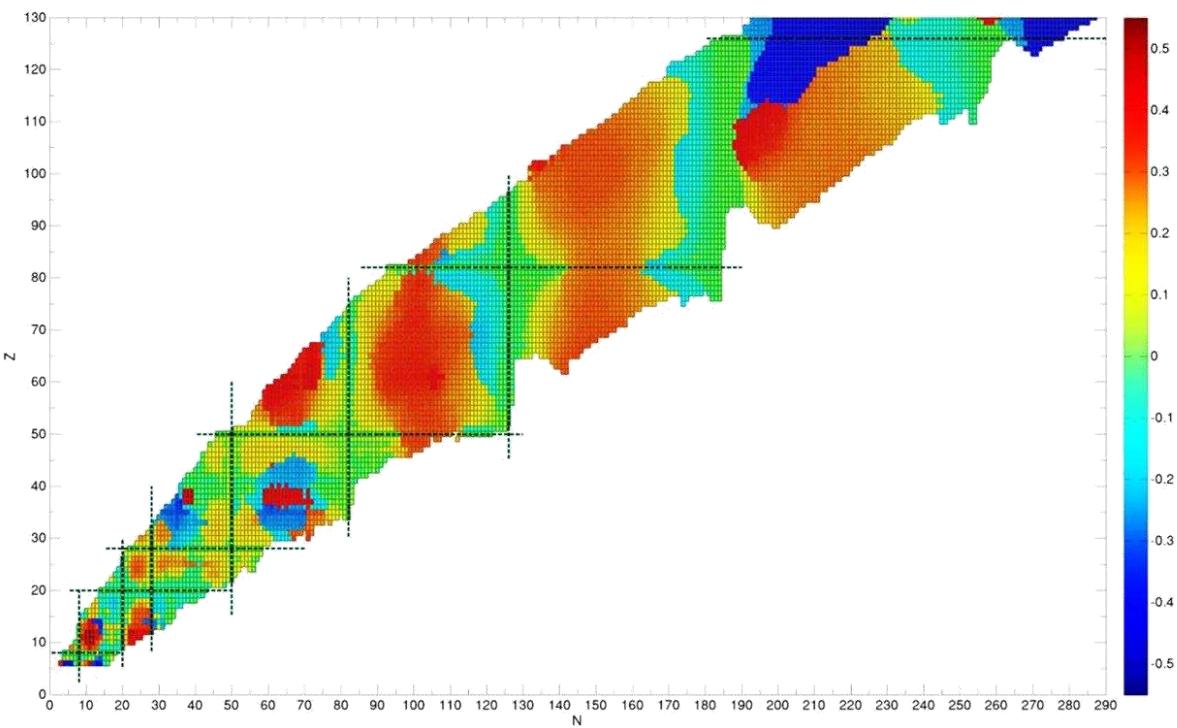
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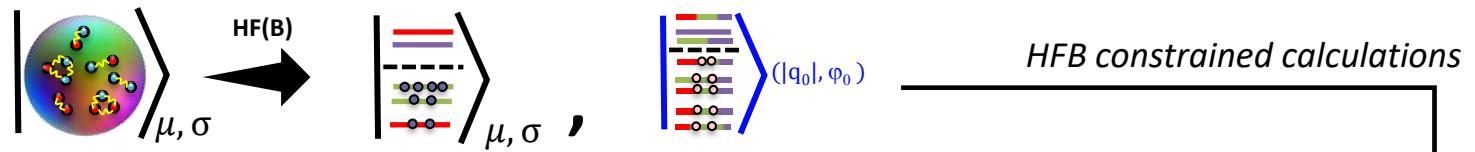
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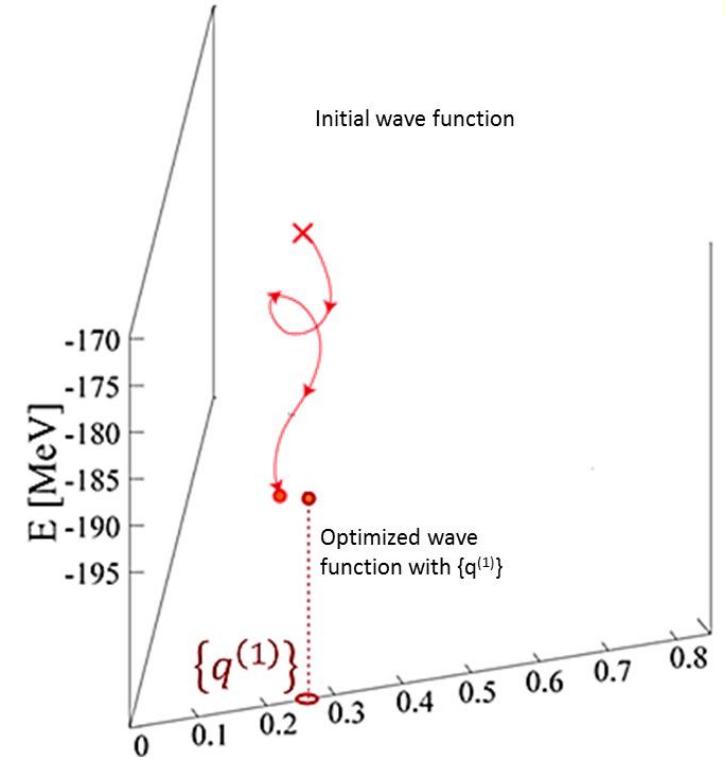
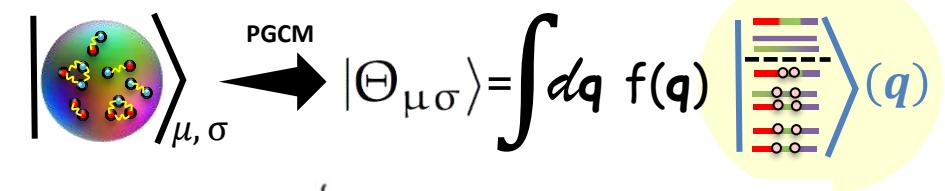
- HFB treatment

→ A -nucleon problem → A 1-nucleon problems



- Post-HFB treatment : PGCM

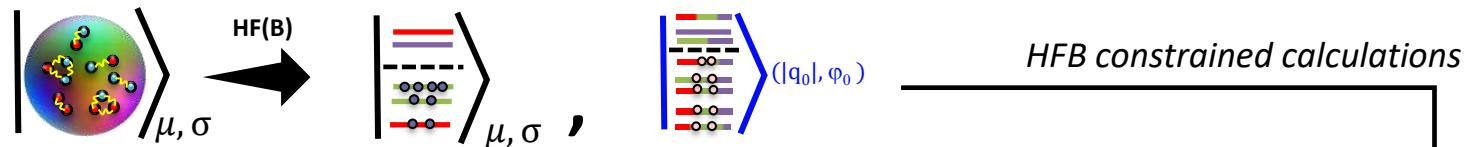
→ Symmetry-conserving (non orthogonal) mixture of symmetry-breaking HFB vacua



The Energy Density Functional Method

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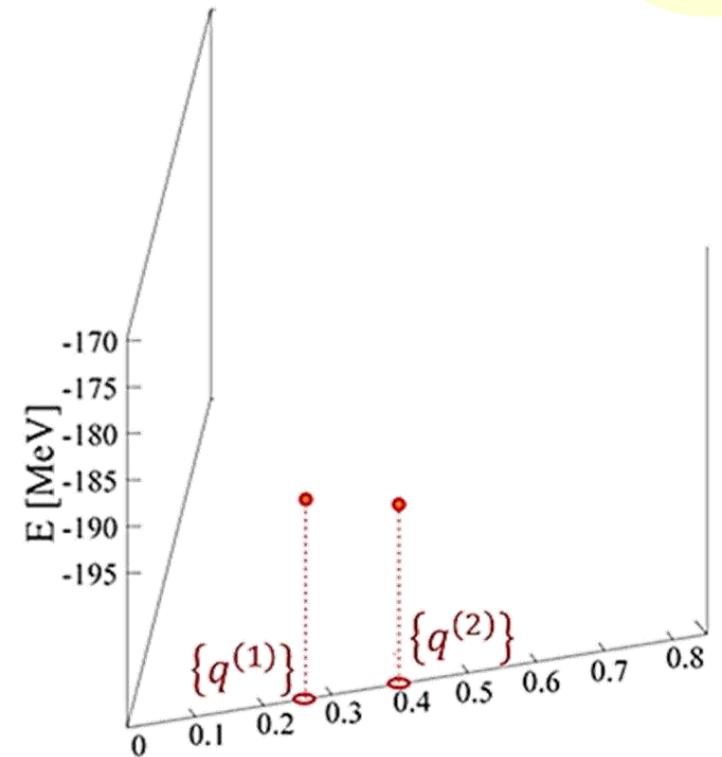
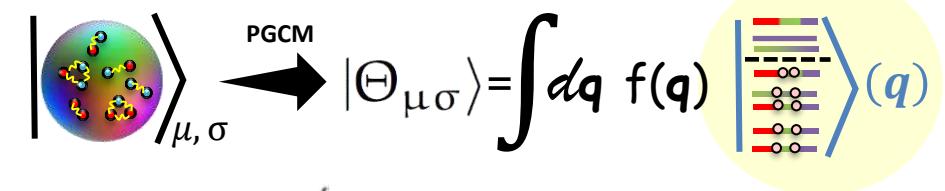
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HFB constrained calculations

- Post-HFB treatment : PGCM

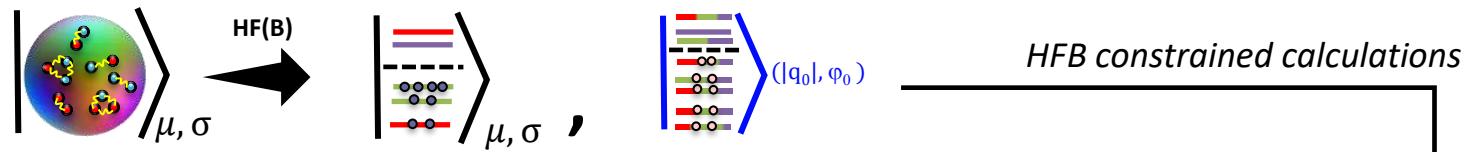
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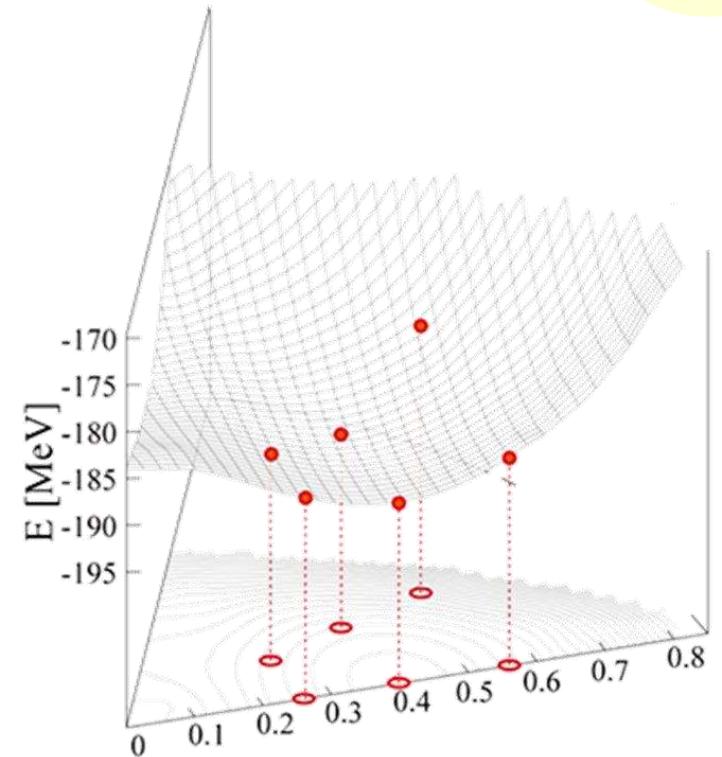
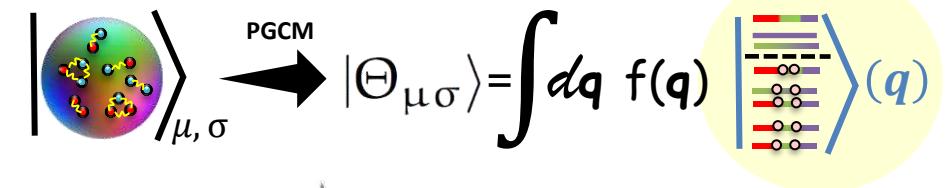
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- Post-HFB treatment : PGCM

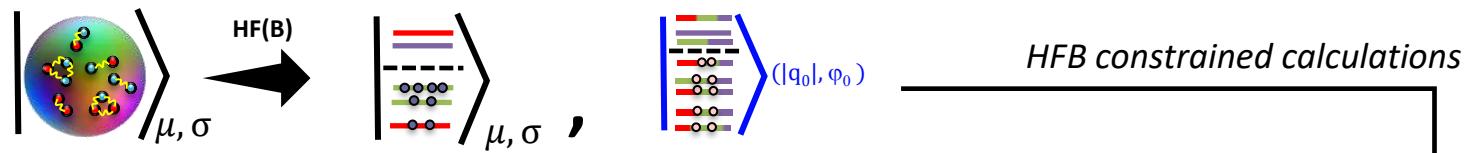
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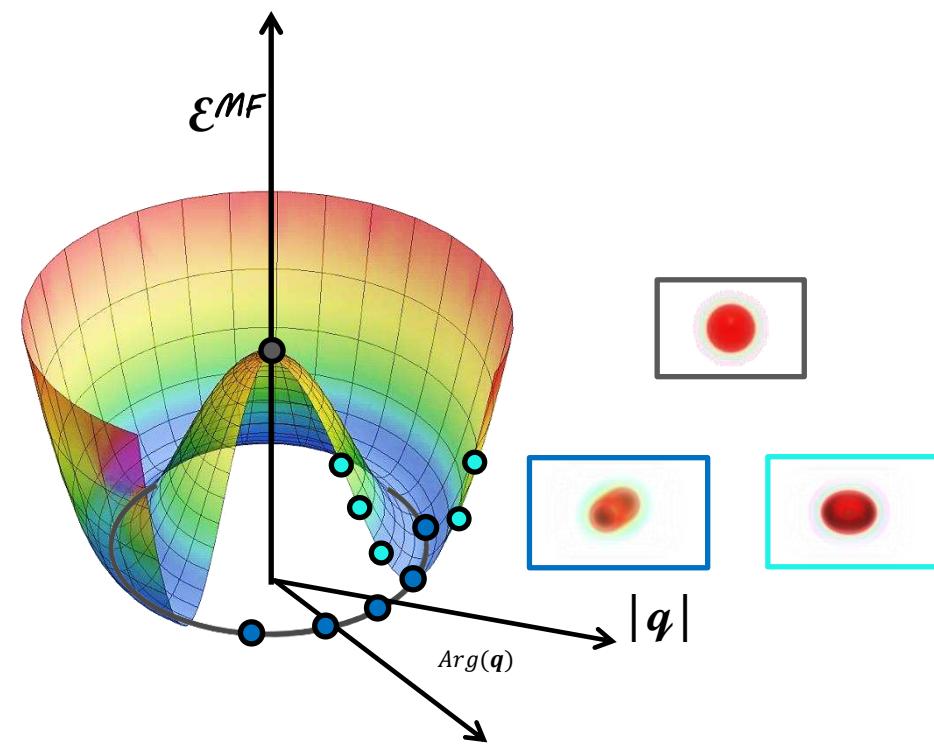
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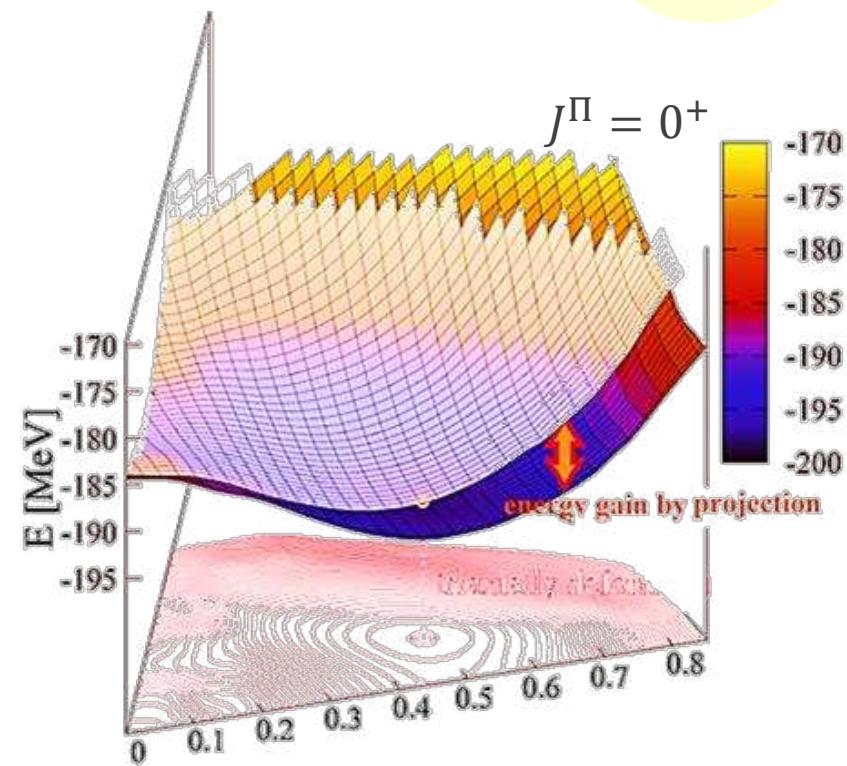


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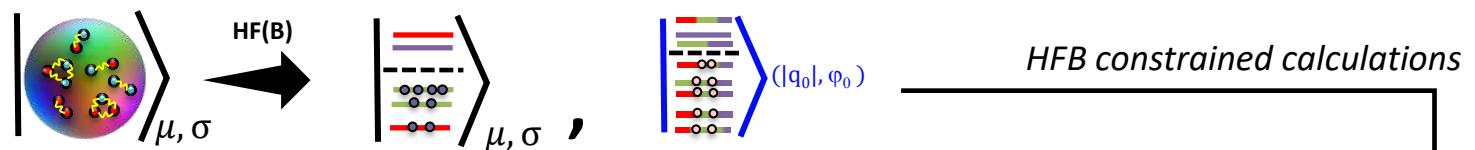
$$|\Theta_{\mu\sigma}\rangle = \int d\mathbf{q} f(\mathbf{q}) |\langle \mathbf{q} | (q)\rangle_{\mu\sigma}$$



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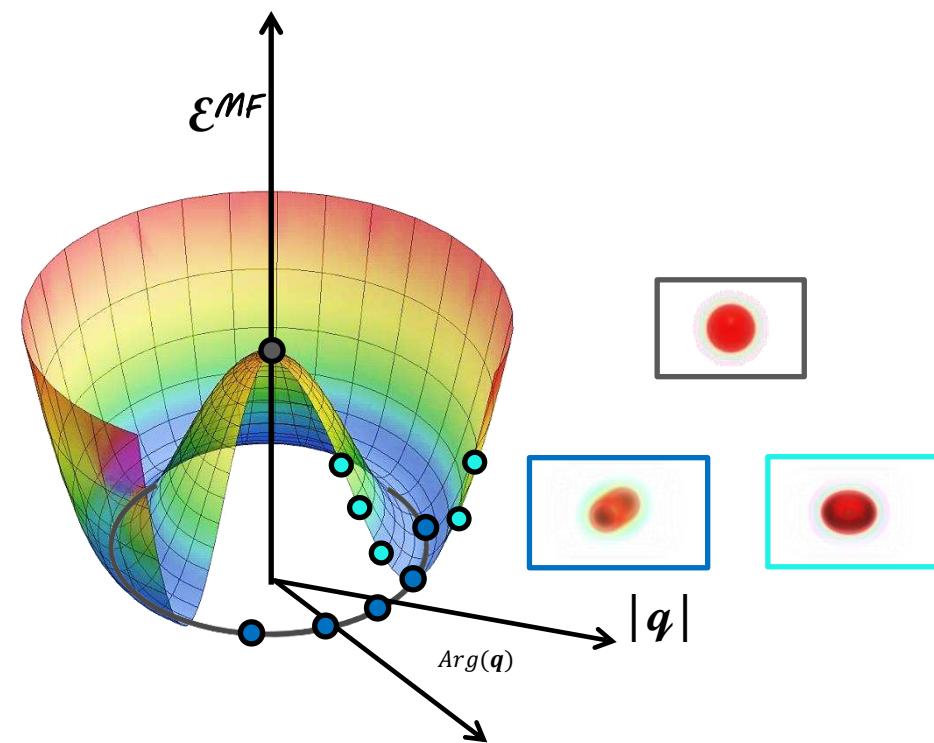
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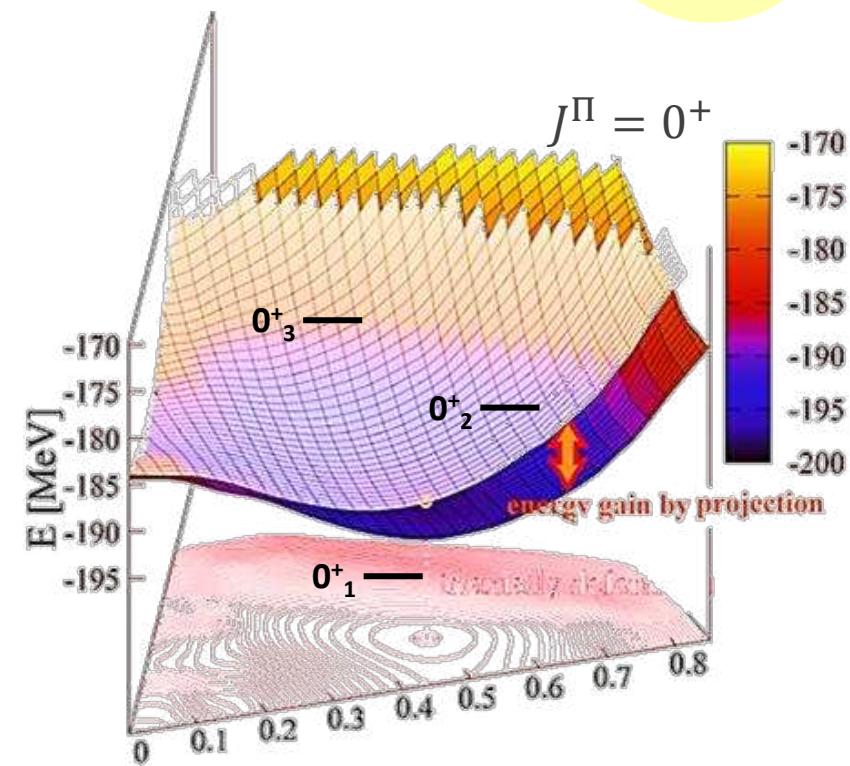
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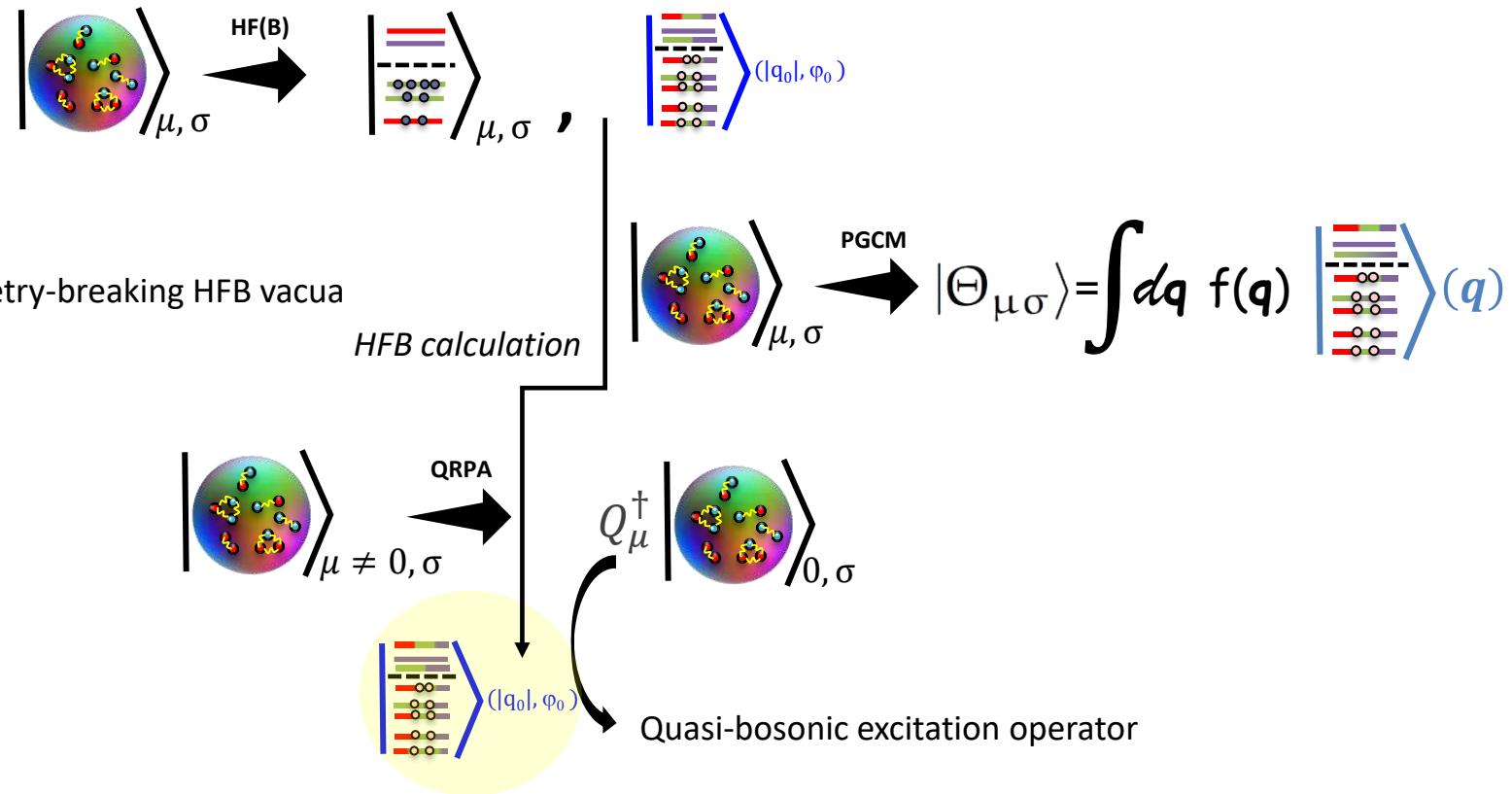
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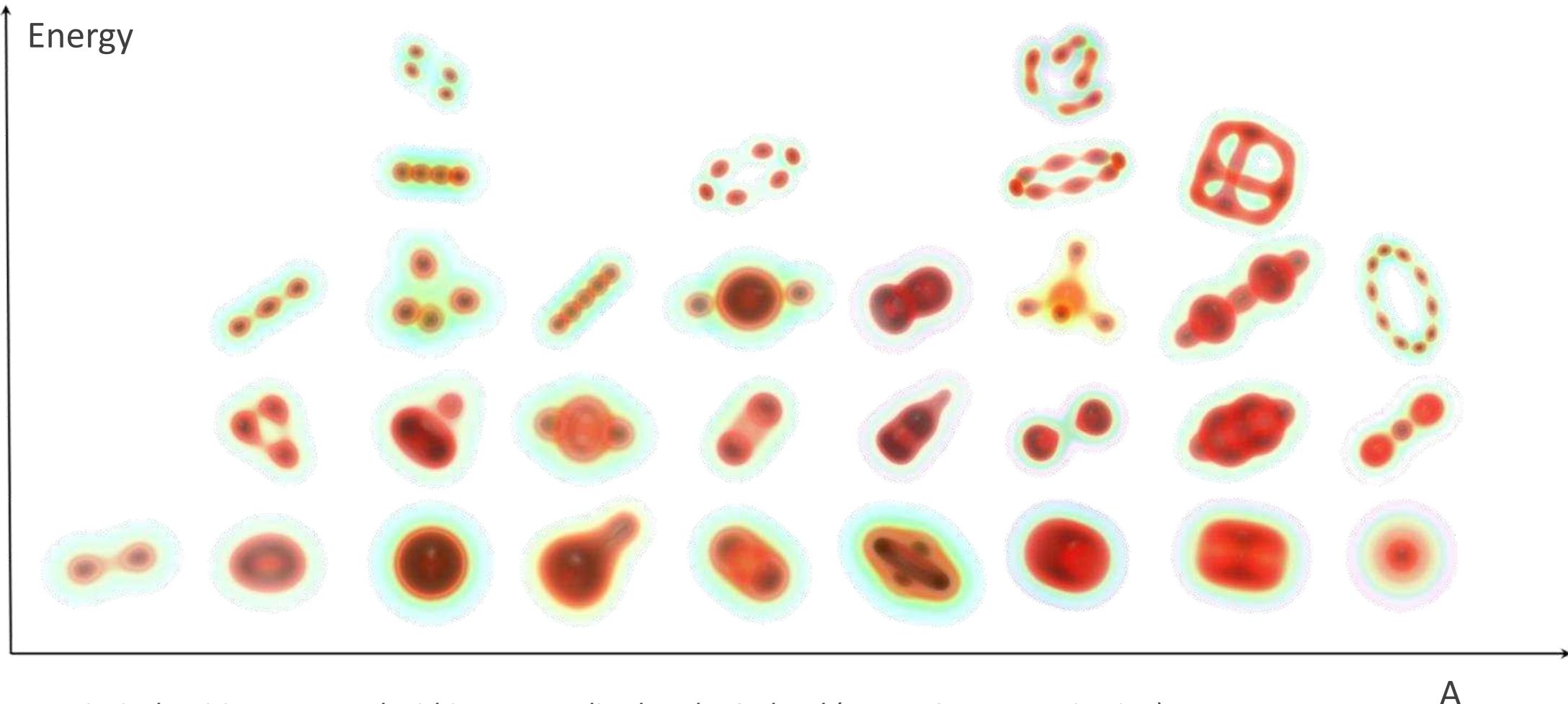
The Energy Density Functional Method

- HFB treatment

→ A-nucleon problem → A 1-nucleon problems



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

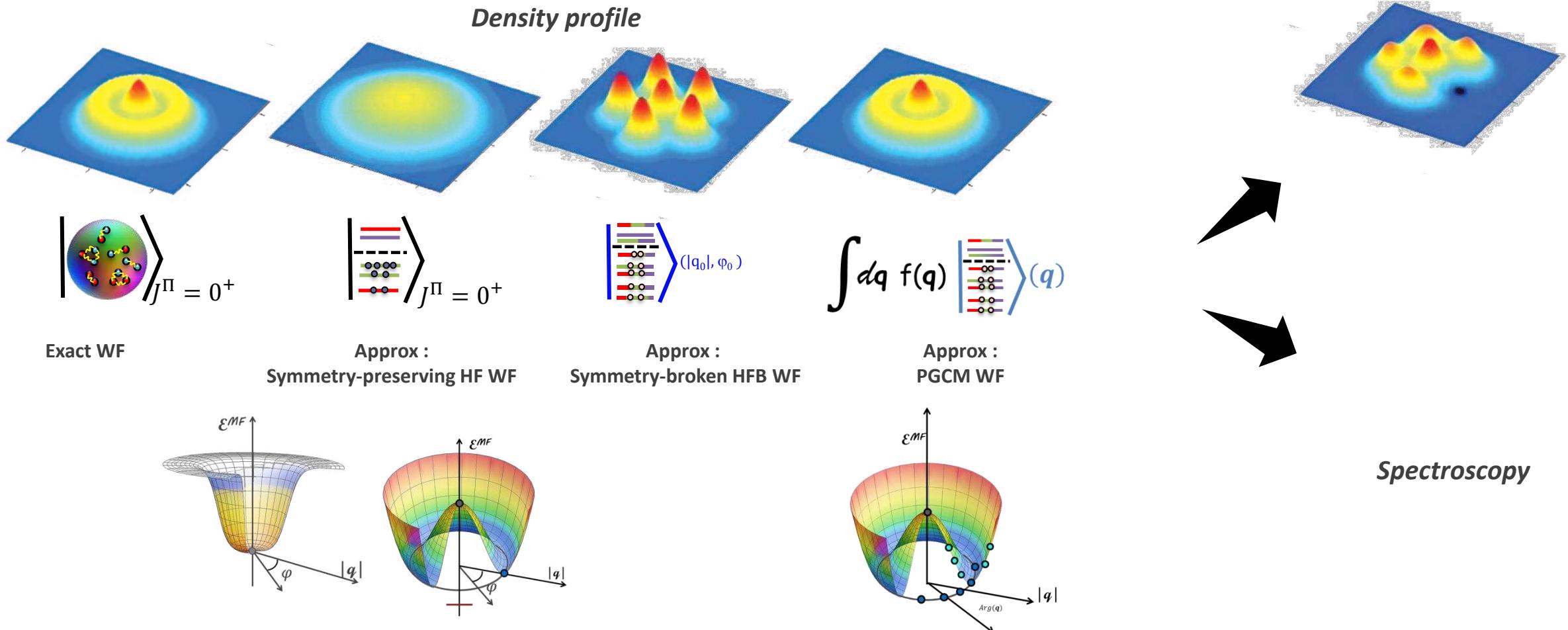


Intrinsic densities computed within cEDF realized at the SR level (DD-ME2 parametrization)

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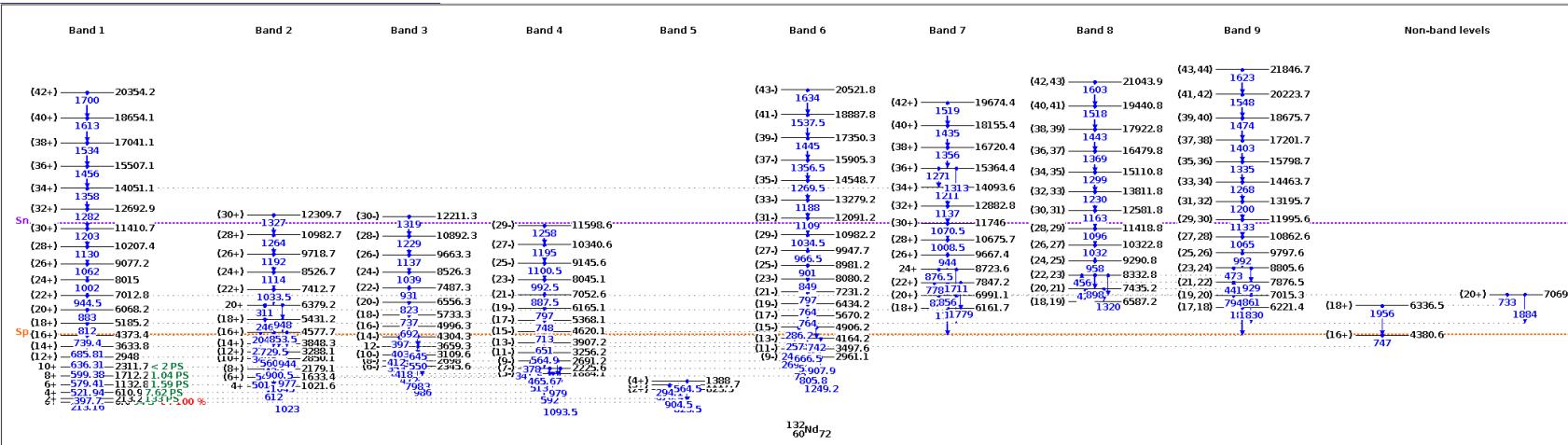
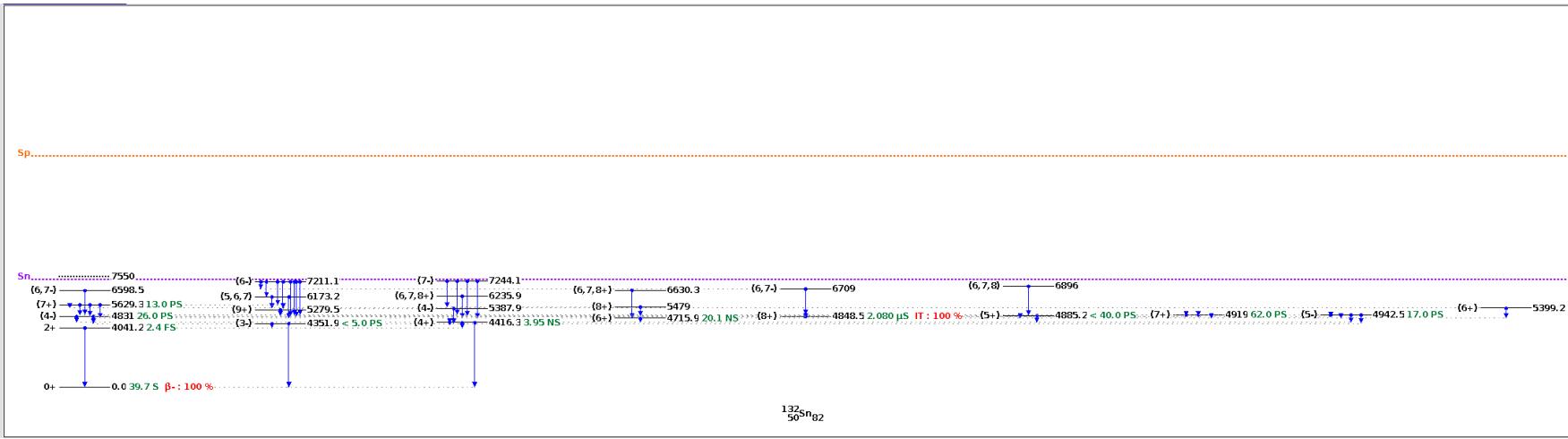
- Nuclear shapes : Take the case of a doubly open-shell system with strong angular correlation

2-point correlation function



Yannouleas & Landman, 2017

Nuclear clustering & PGCM



● How to account for correlations underpinning α -clustering ?

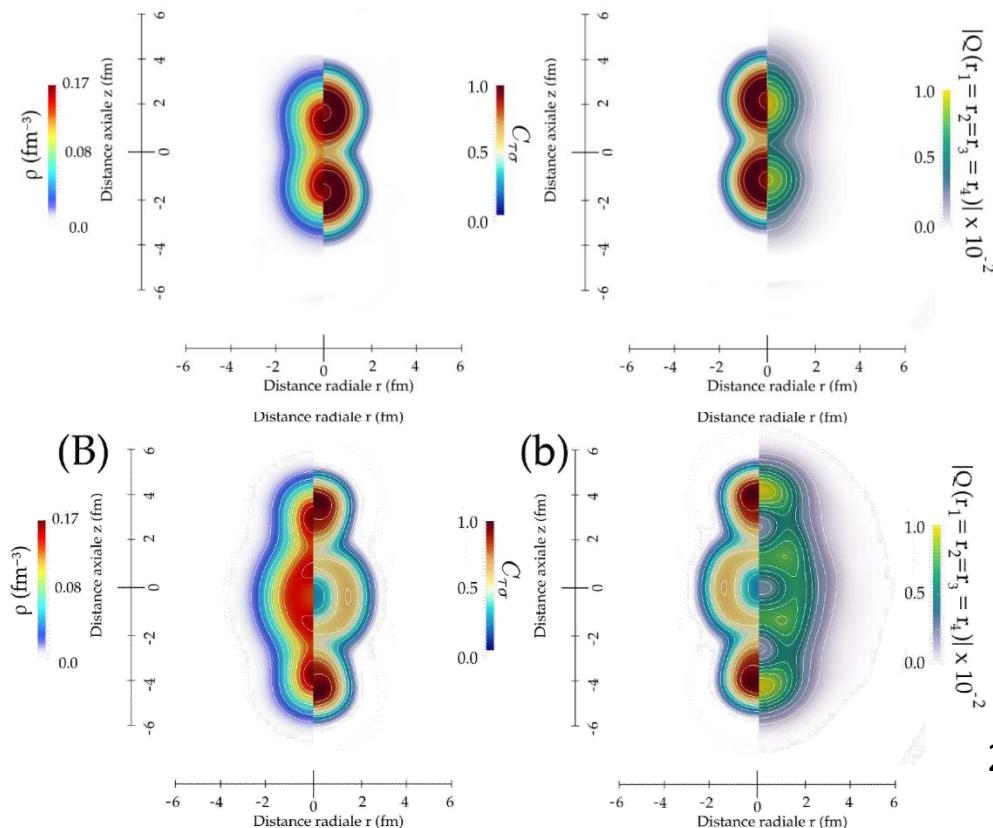
i) Explicitly treat 4-nucleon correlations : RMF + QCM

$$|\Psi\rangle = (Q^\dagger)^{n_q} |0\rangle$$

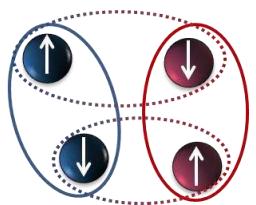
$$Q^\dagger = 2\Gamma_1^\dagger \Gamma_{-1}^\dagger - (\Gamma_0^\dagger)^2$$

$$\Gamma_t^\dagger = \sum_k x_k P_{k,t}^\dagger$$

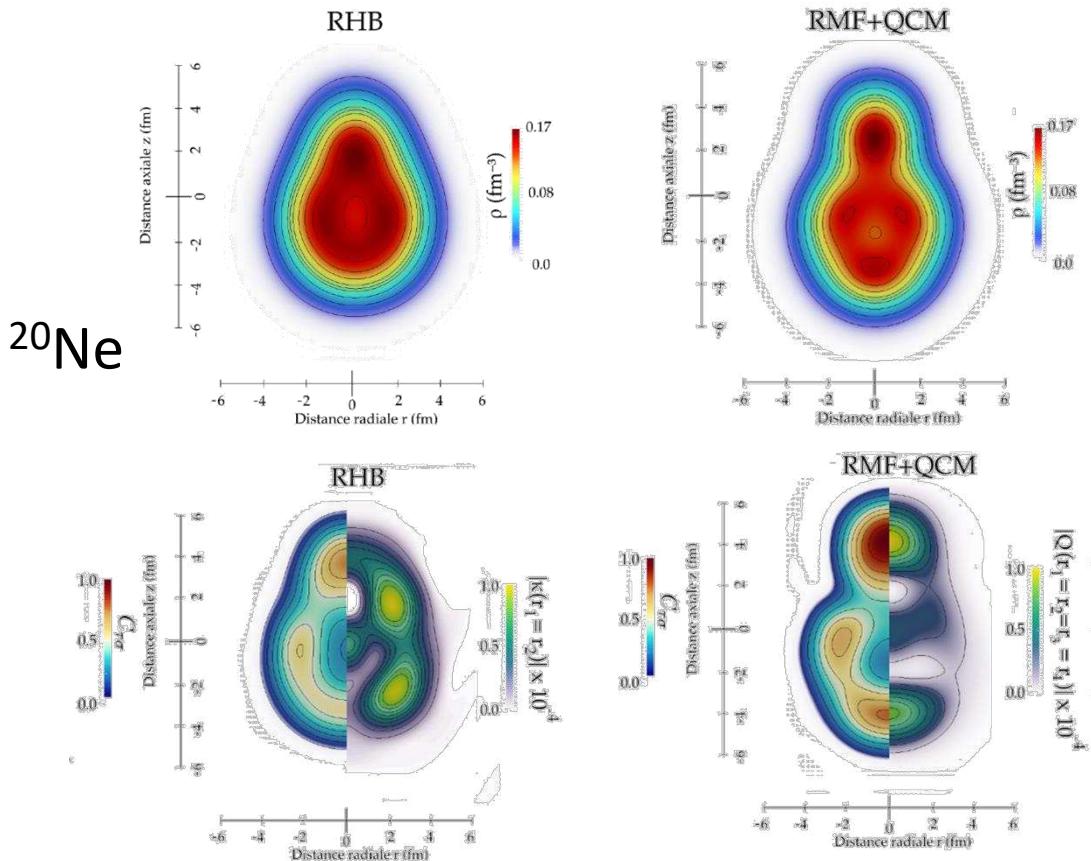
Lasseri, Ebran, Khan, Sandulescu



^{24}Mg



J.-P. EBRAN



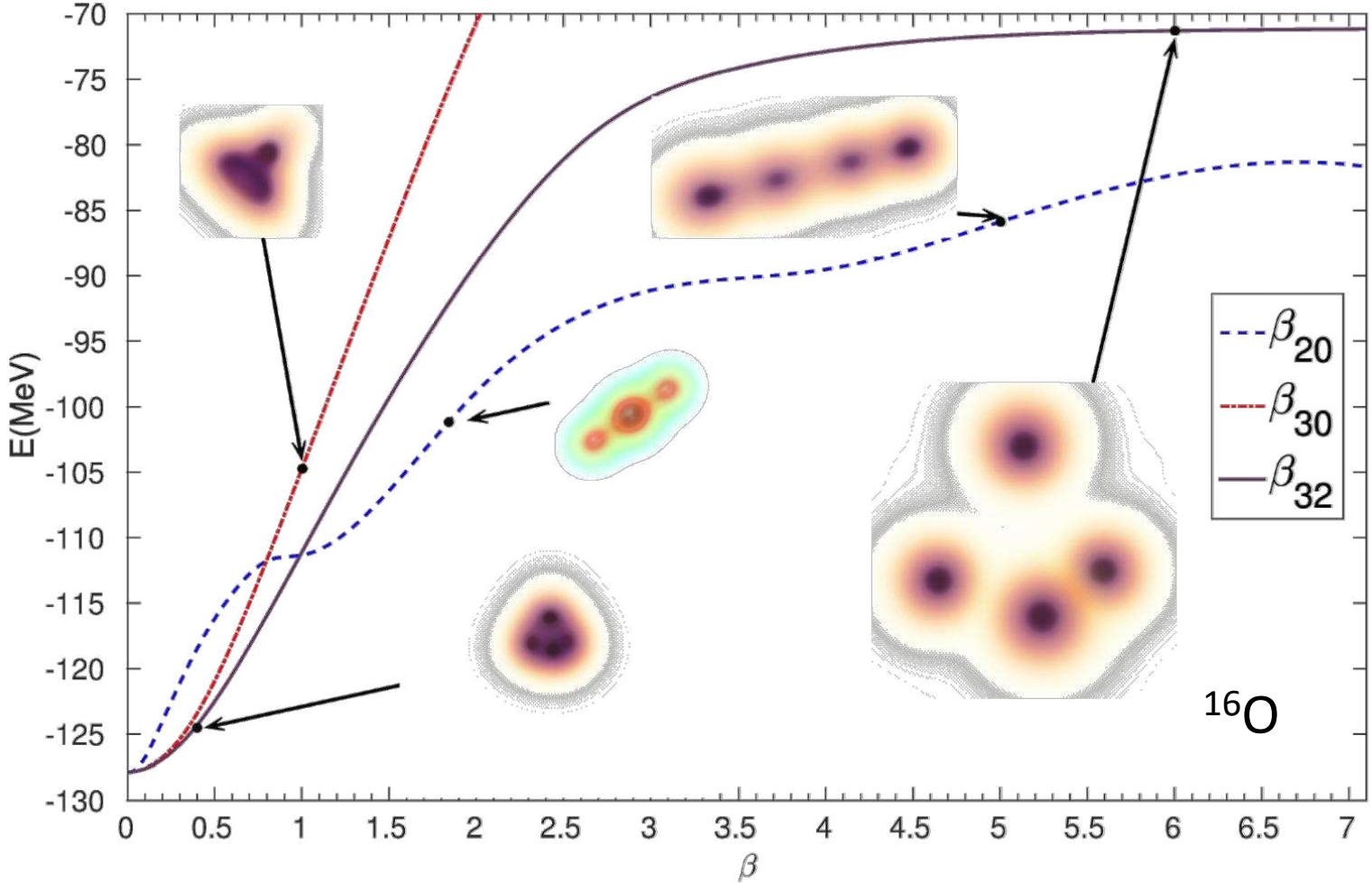
31 mai 2022

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● 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 SO(3) (or continuous subgroup) to a discrete point-group

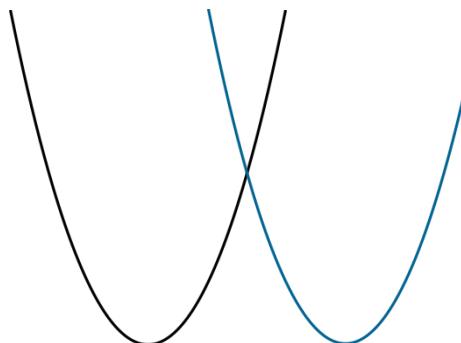


● Role of deformation

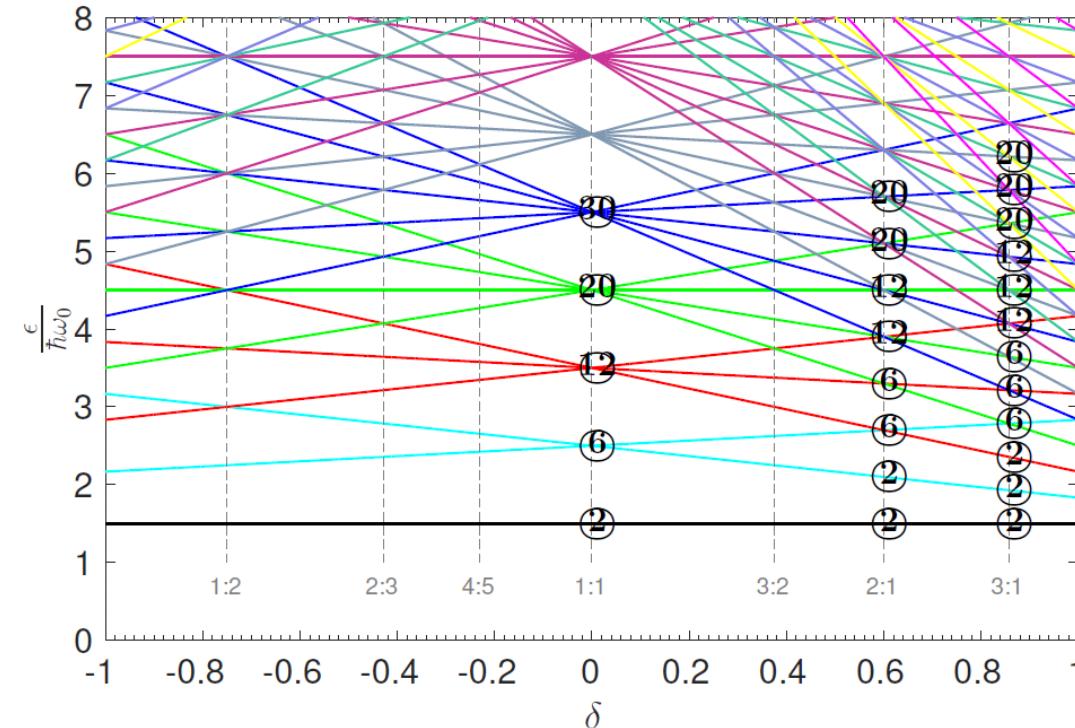
N-dimensional anisotropic HO with commensurate frequencies enjoys dynamical symmetries involving multiple independent copies of SU(N) irreps

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

SPHERICAL MAGIC NUMBERS	SUPERDEFORMED PROLATE MAGIC NUMBERS	SUPERDEFORMED PROLATE SPECTRUM
70	140	4
40	110	4
20	80	3
20	60	3
8	40	2
8	28	2
2	16	1
2	10	1
2	4	0
A	B	(000) (001)



Nazarewicz & Dobaczewski, PRL 1992



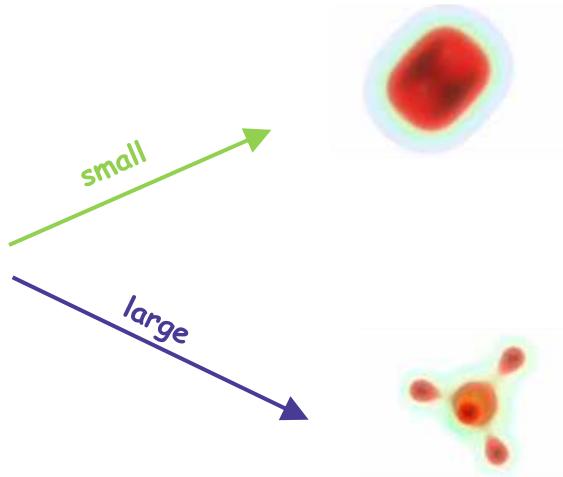
Deformation = necessary condition, but not a sufficient one

Strength of correlations

- Strength of correlations measured by dimensionless ratios

$$\sqrt{\lambda} \equiv \sqrt{\frac{\langle V \rangle}{\langle T \rangle}} = \sqrt{2} \left(\frac{3}{4\pi} \right)^{\frac{1}{6}} (2M_U)^{\frac{1}{4}} (\bar{A}_n)^{-\frac{1}{6}} \sim \alpha_{loc}$$

Nucleon mass Number of nucleons
 Depth of the confining potential Mean density



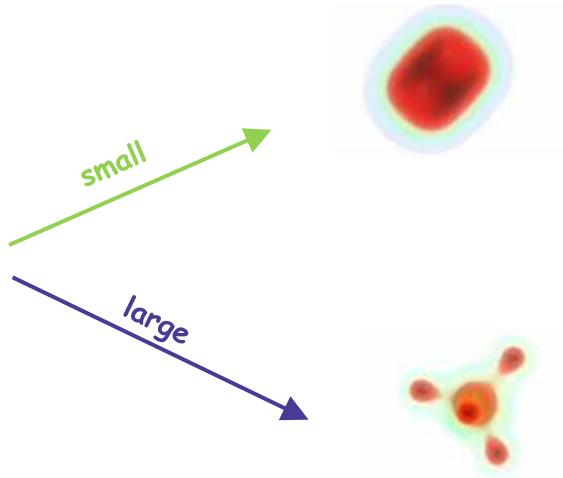
Ebran, Khan, Niksic & Vretenar *Nature* 2012
 Ebran, Khan, Niksic & Vretenar *PRC* 2013

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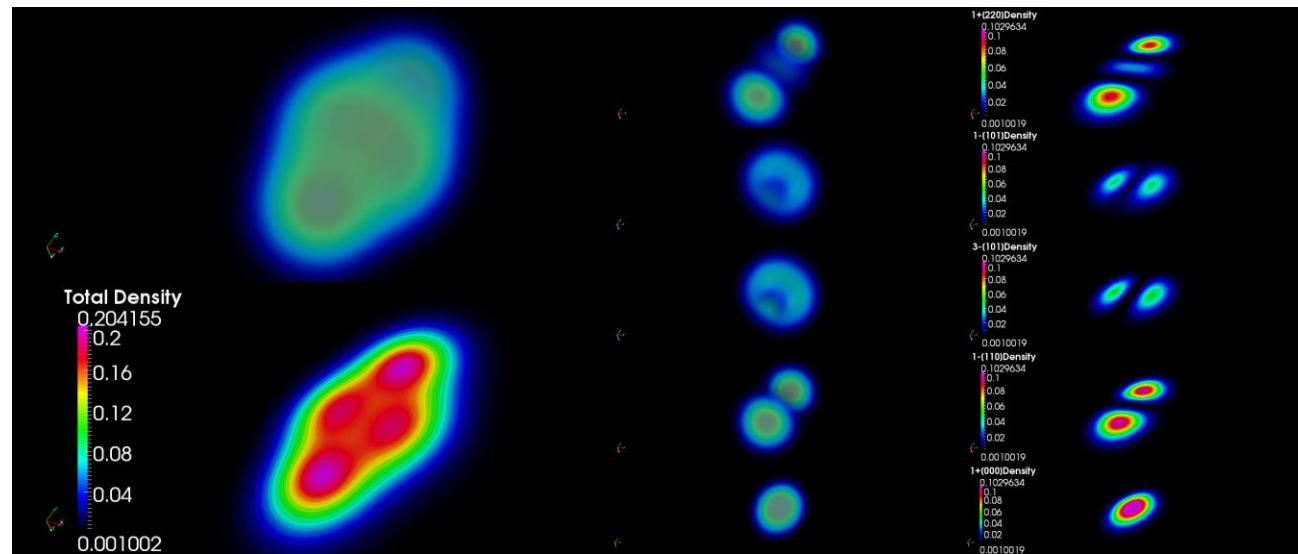
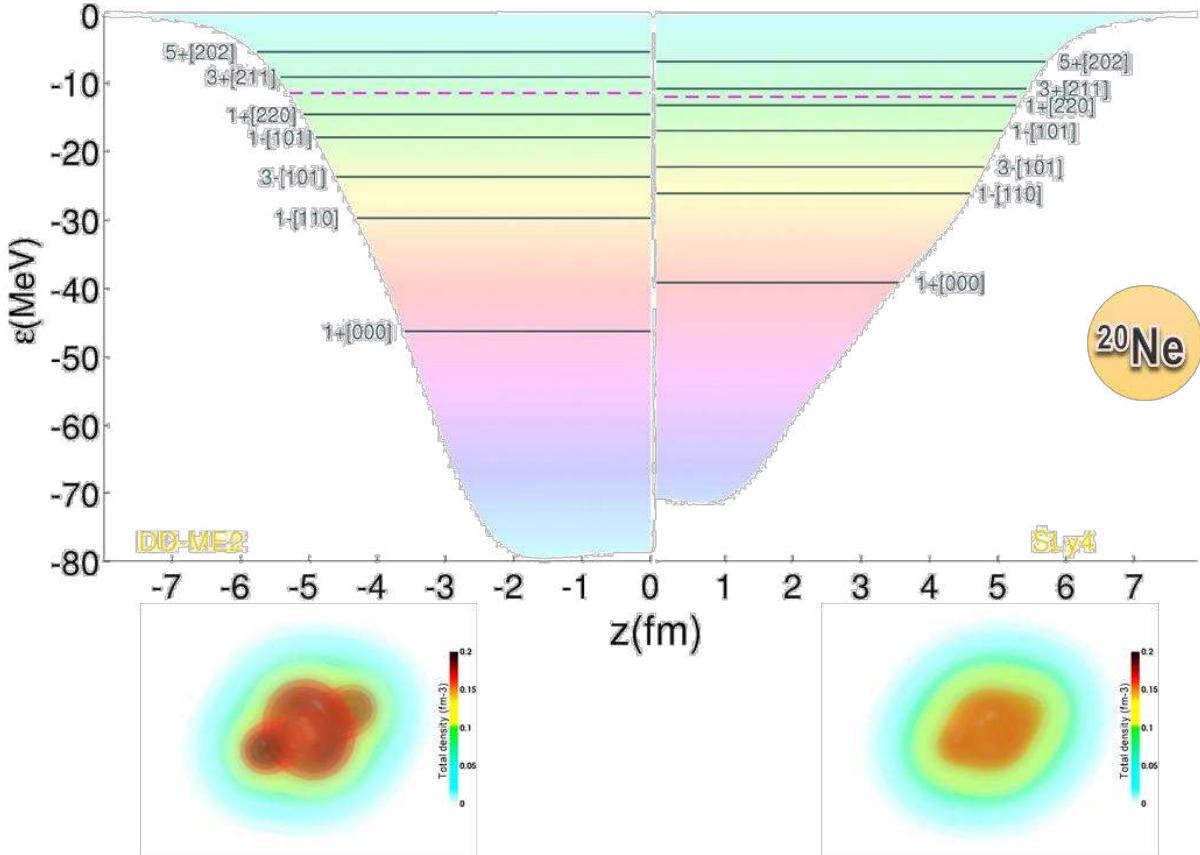
Nucleon mass Number of nucleons
 Depth of the confining potential Mean density



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

Effect of the depth of the confining potential

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



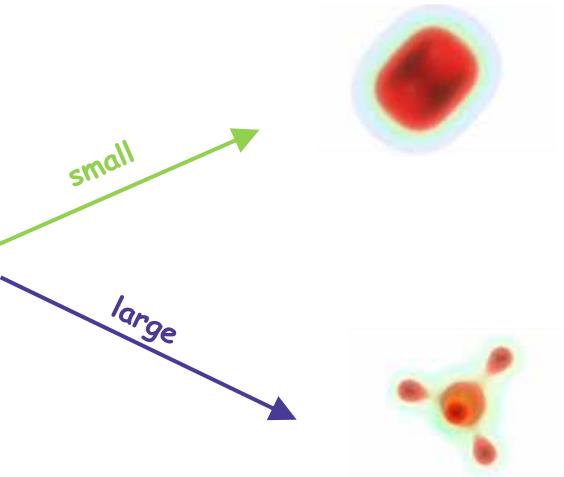
- When Coulomb effects are not too important and owing to Kramers degeneracy, proton \uparrow , proton \downarrow , neutron \uparrow , neutron \downarrow share the same spatial properties

Strength of correlations

● Strength of correlations measured by dimensionless ratios

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Nucleon mass Number of nucleons
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- Clustering favored
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● Formation/dissolution of clusters : Mott parameter

$$\frac{R_X}{d_{Mott}^X} \sim 1 \Rightarrow n_{Mott}^X \sim \frac{\rho_{sat}}{A_X}$$

Size of the nucleus X
inter-nucleon average distance

$$n_{Mott}^\alpha \sim 0.25\rho_{sat}$$

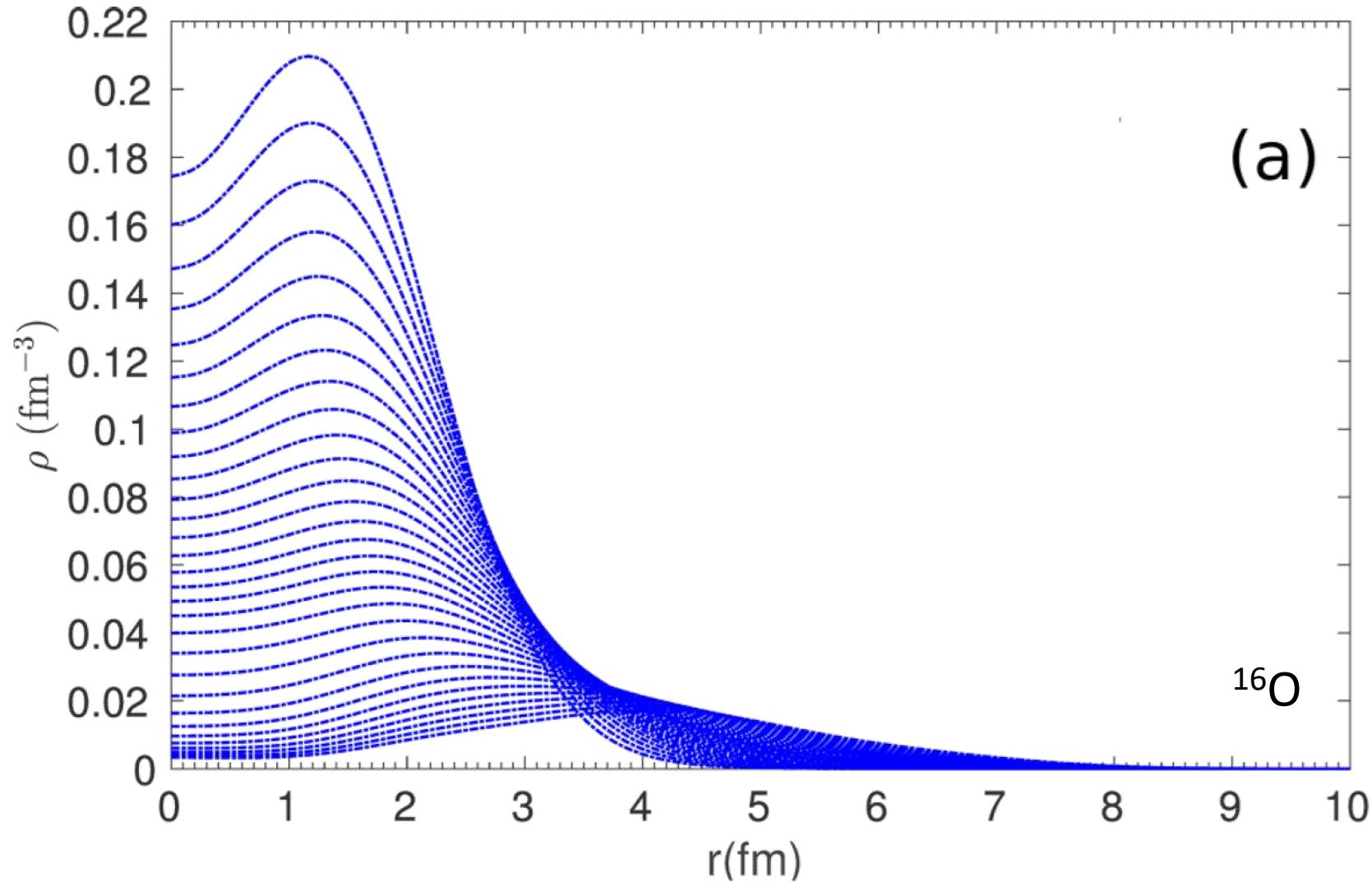
Size of an α in free-space

$$\sim \frac{\rho_{sat}}{3}$$

0.9 size of an α in free-space

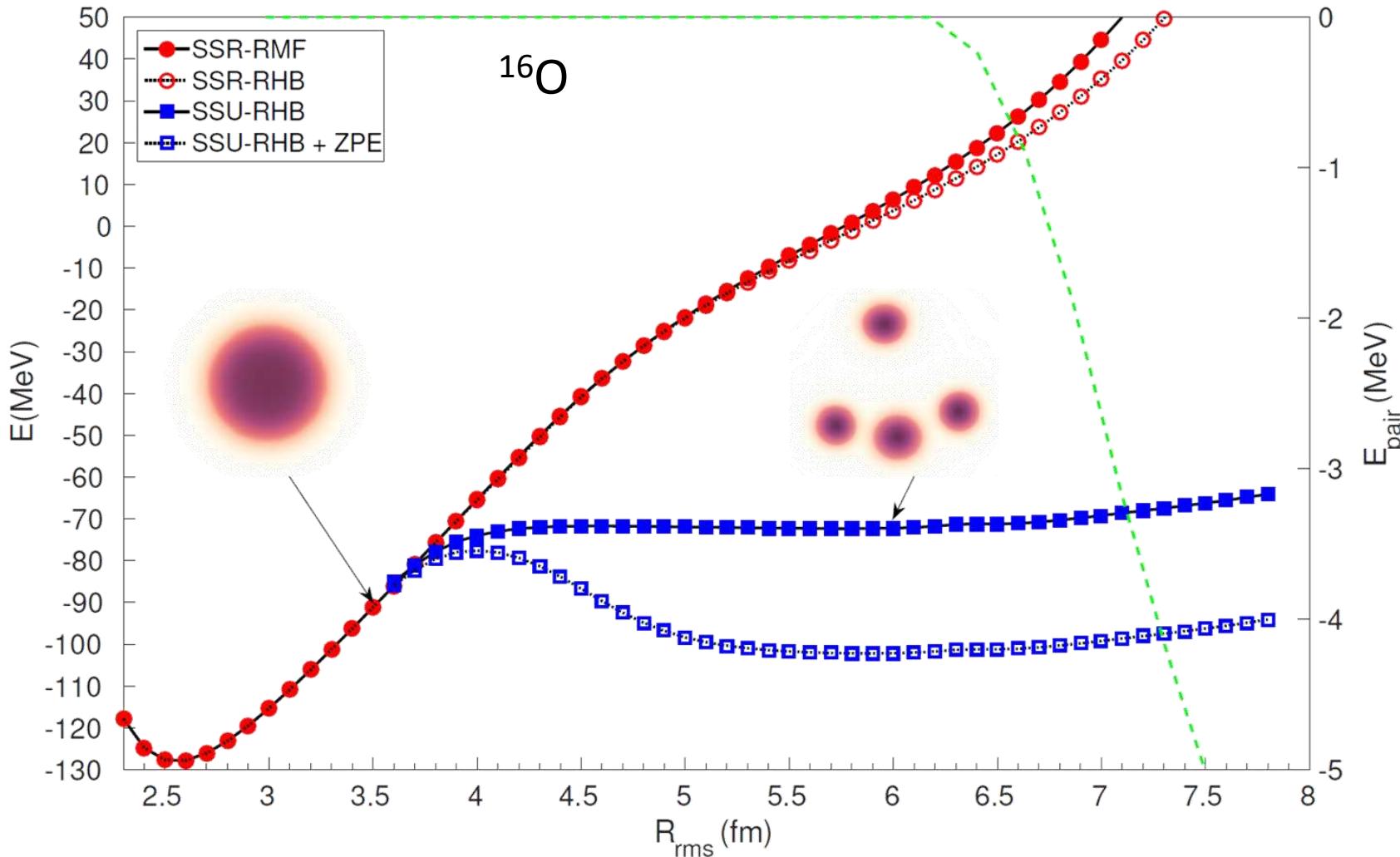
Effect of the density

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



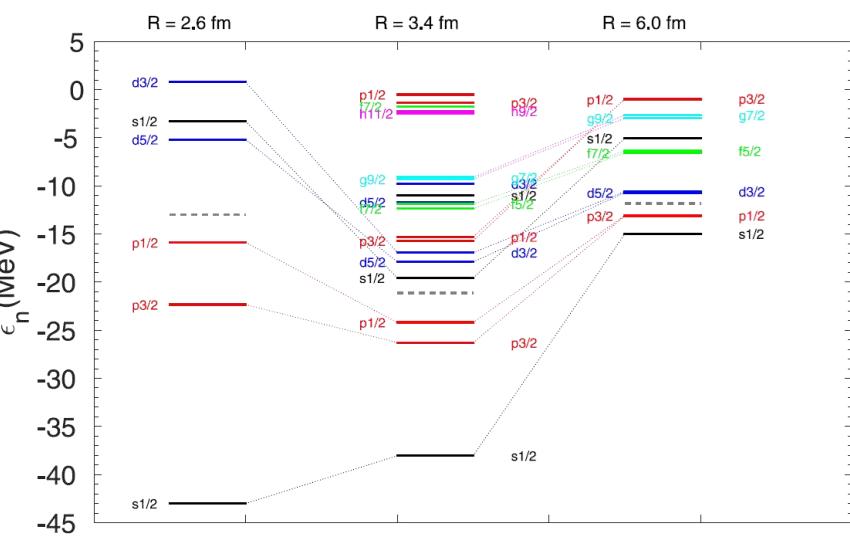
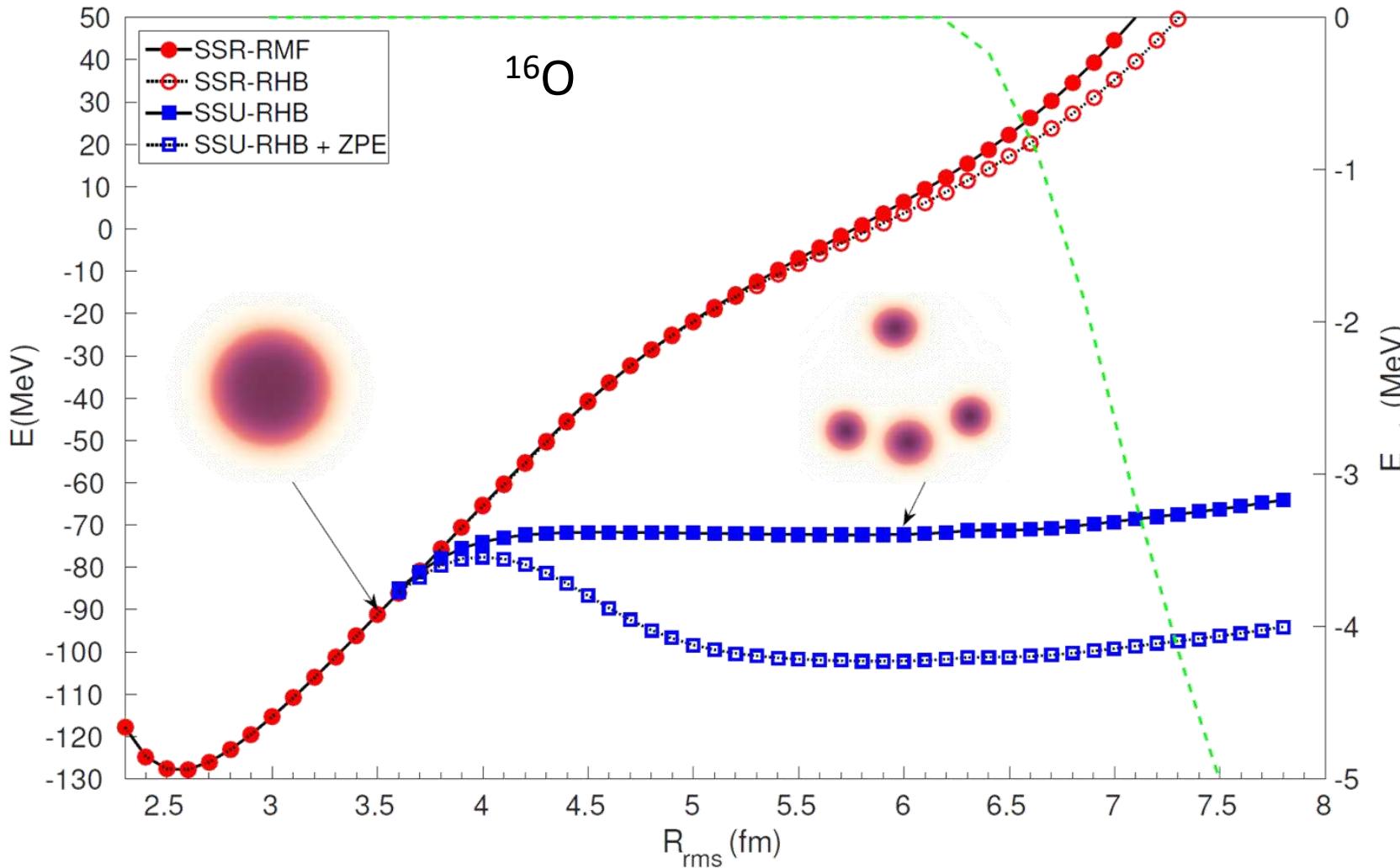
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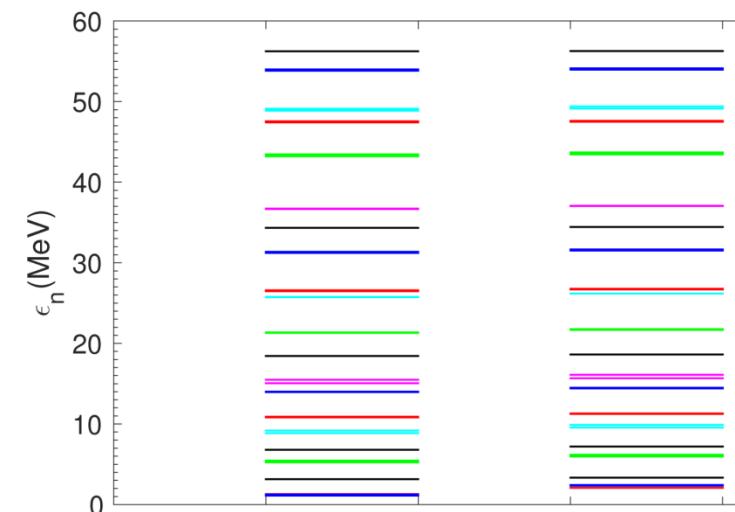
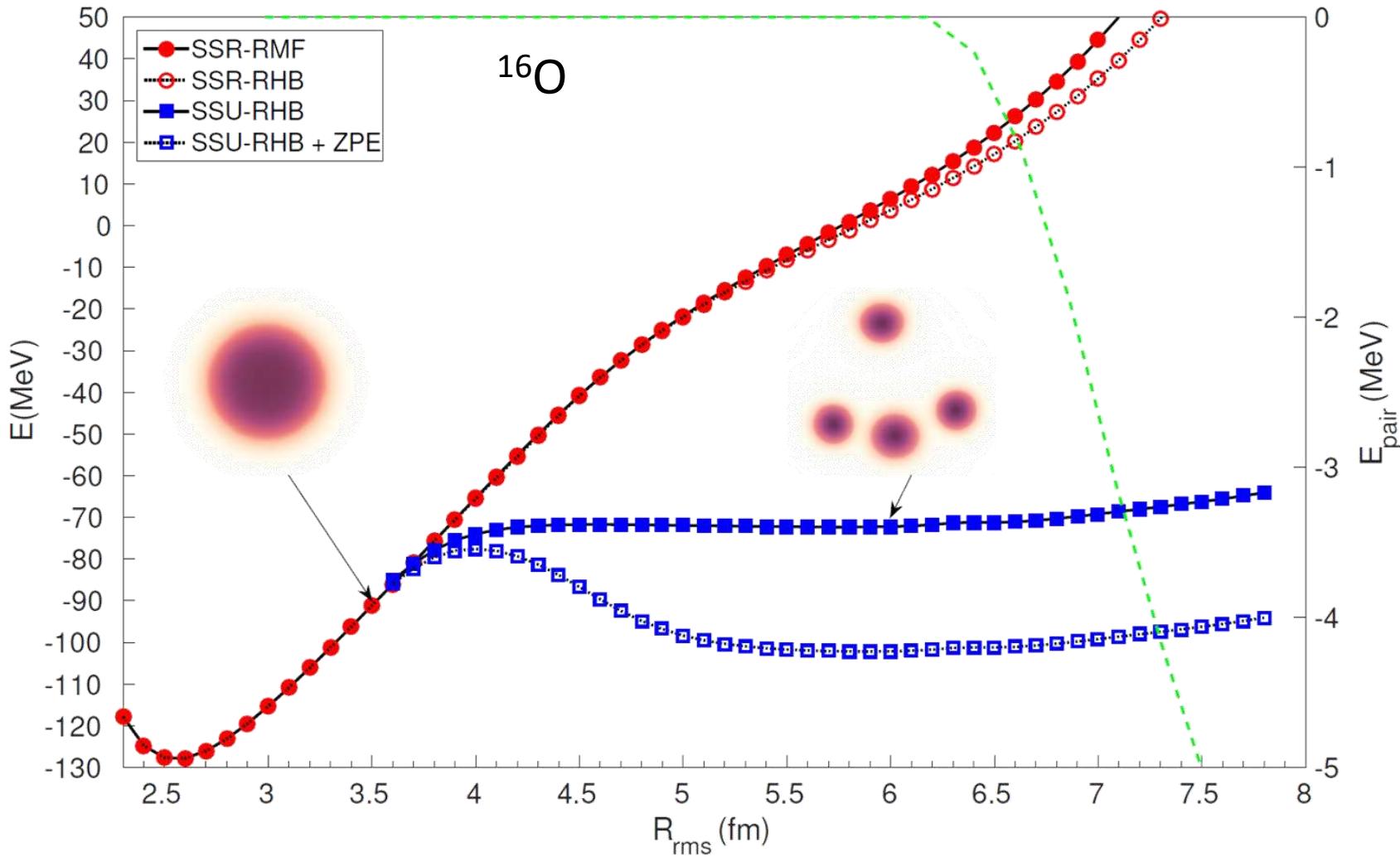
Effect of the density

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



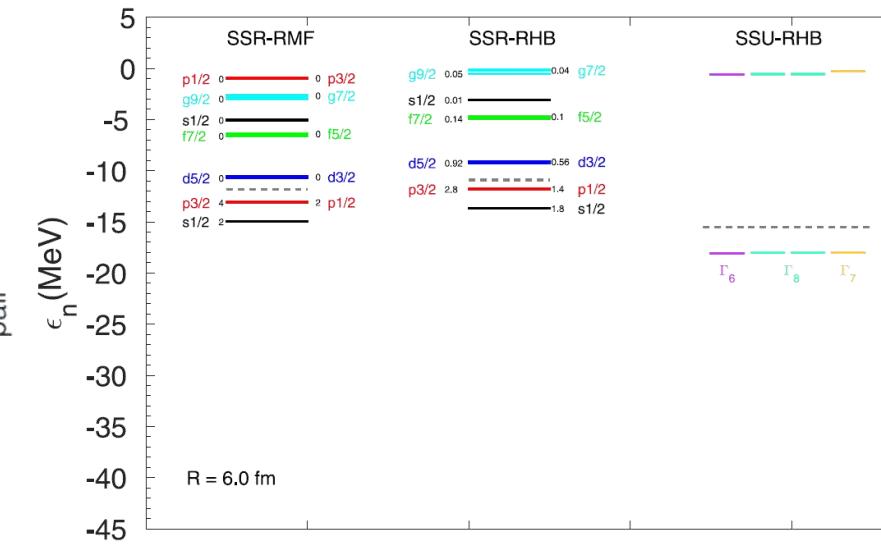
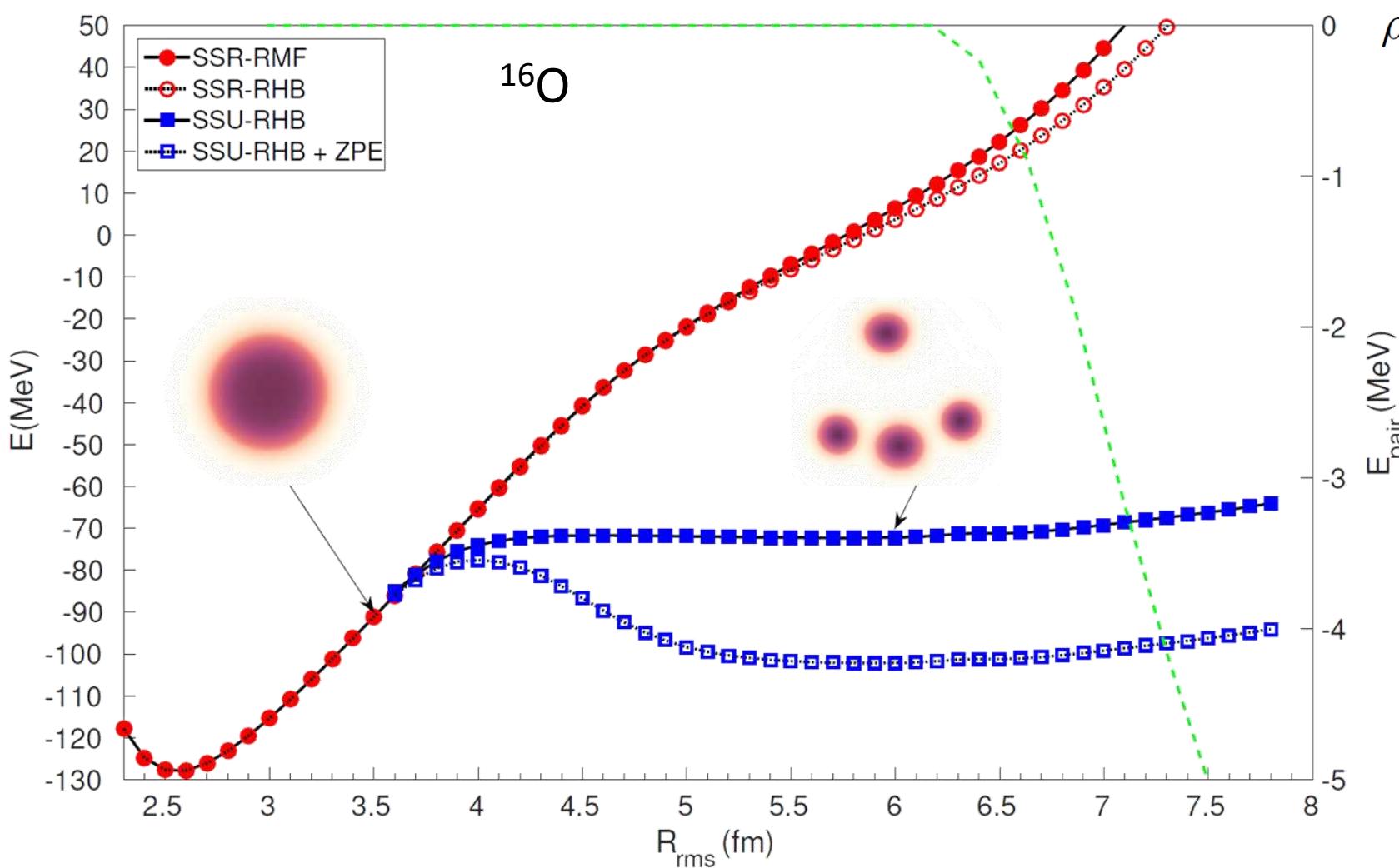
Effect of the density

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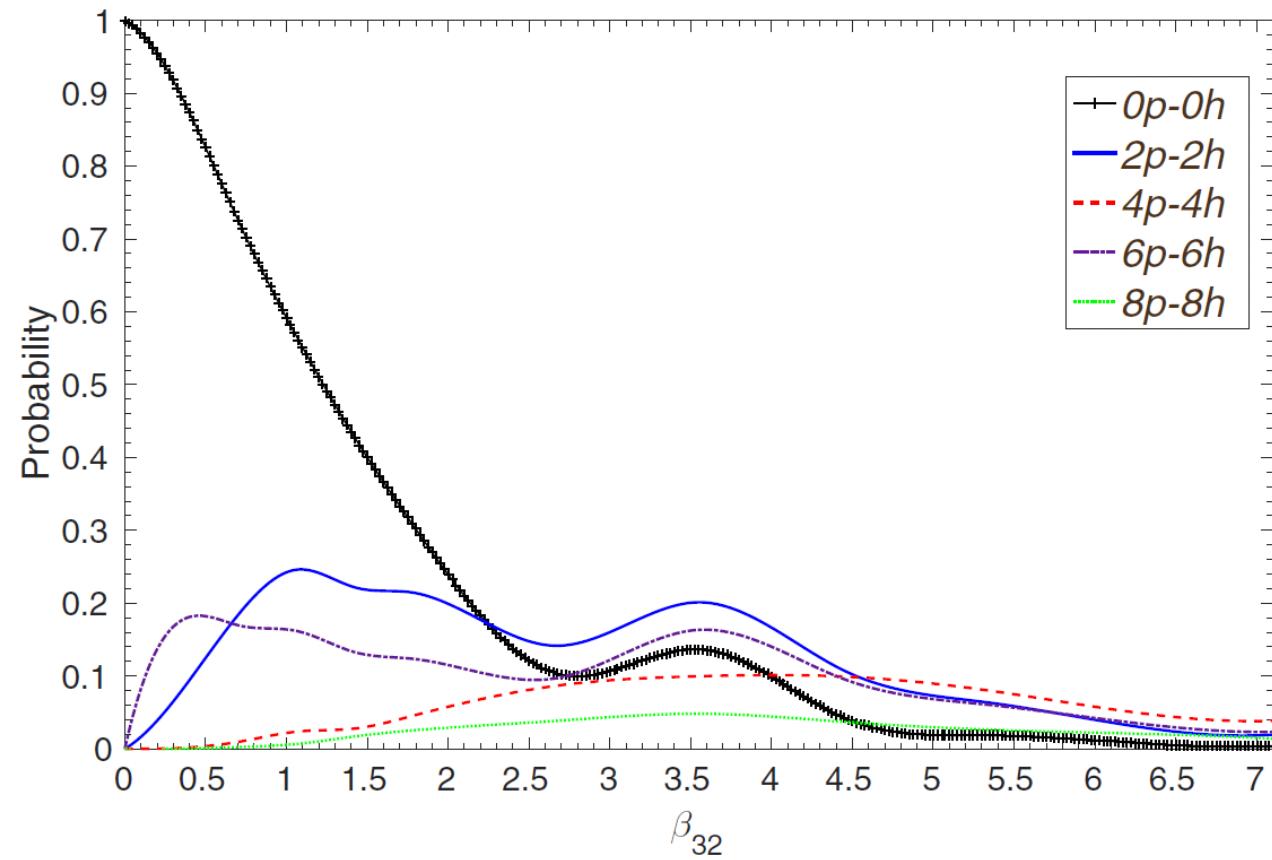
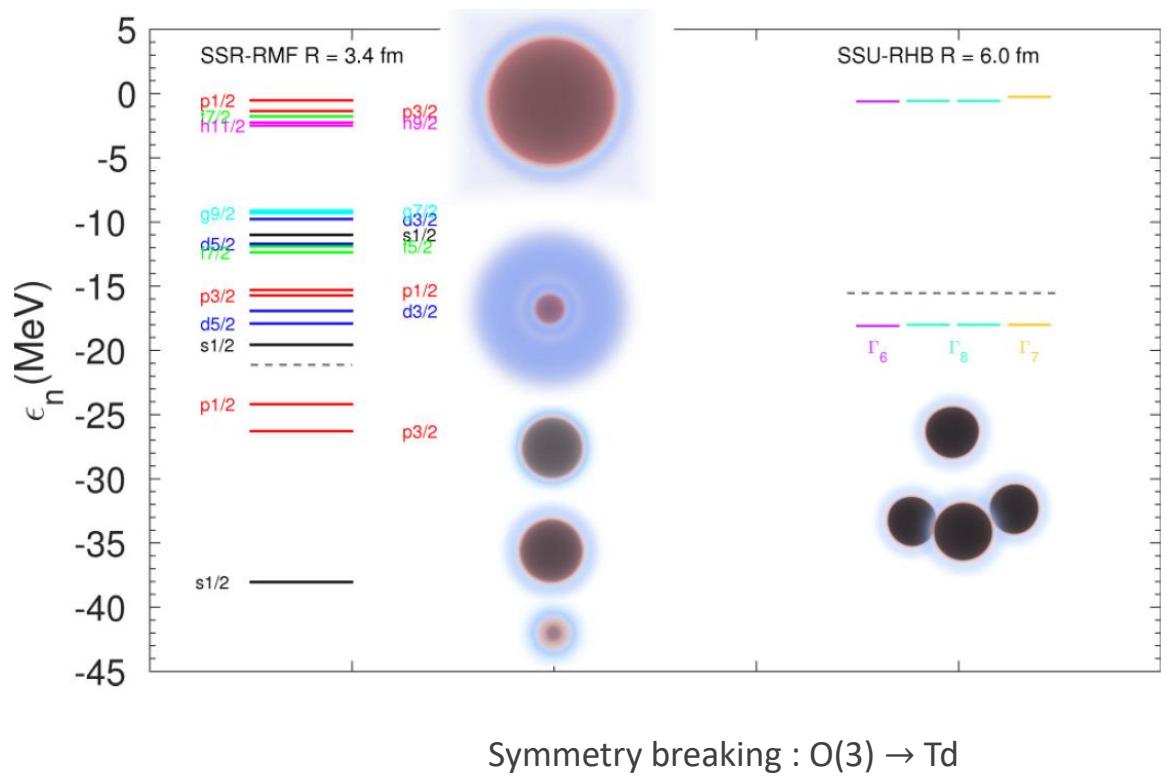
Effect of the density

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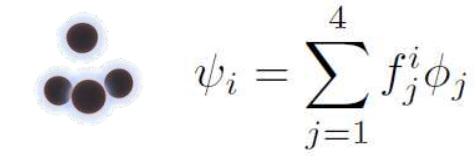


Effect of the density

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



- Borrowing the LCAO-MO language, one can think of the ^{16}O tetrahedrally-deformed SD as a MO built from 4 $1s \alpha$ AOs



- 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

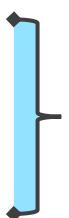
$$\begin{pmatrix} \epsilon & -\mu & -\mu & -\mu \\ -\mu & \epsilon & -\mu & -\mu \\ -\mu & -\mu & \epsilon & -\mu \\ -\mu & -\mu & -\mu & \epsilon \end{pmatrix} \begin{pmatrix} f_1^i \\ f_2^i \\ f_3^i \\ f_4^i \end{pmatrix} = E_i \begin{pmatrix} f_1^i \\ f_2^i \\ f_3^i \\ f_4^i \end{pmatrix}$$

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

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

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

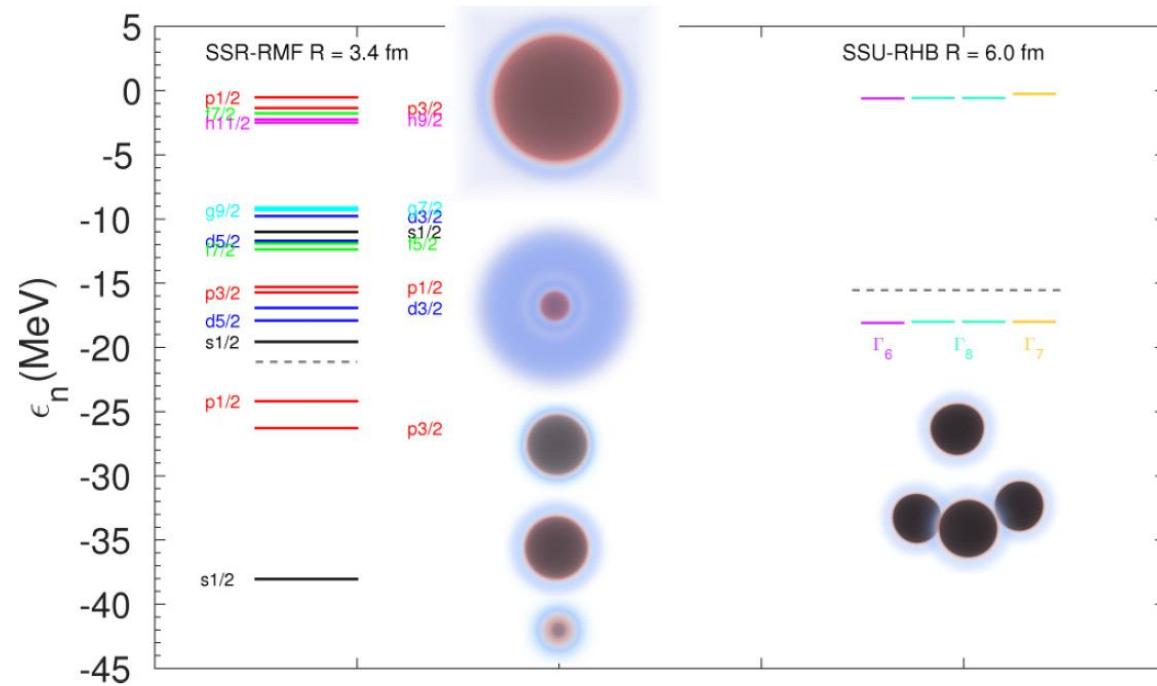
$$\psi_4 = \frac{1}{\sqrt{2}} (-\phi_1 + \phi_4) \quad E_4 = E_3 = E_2$$



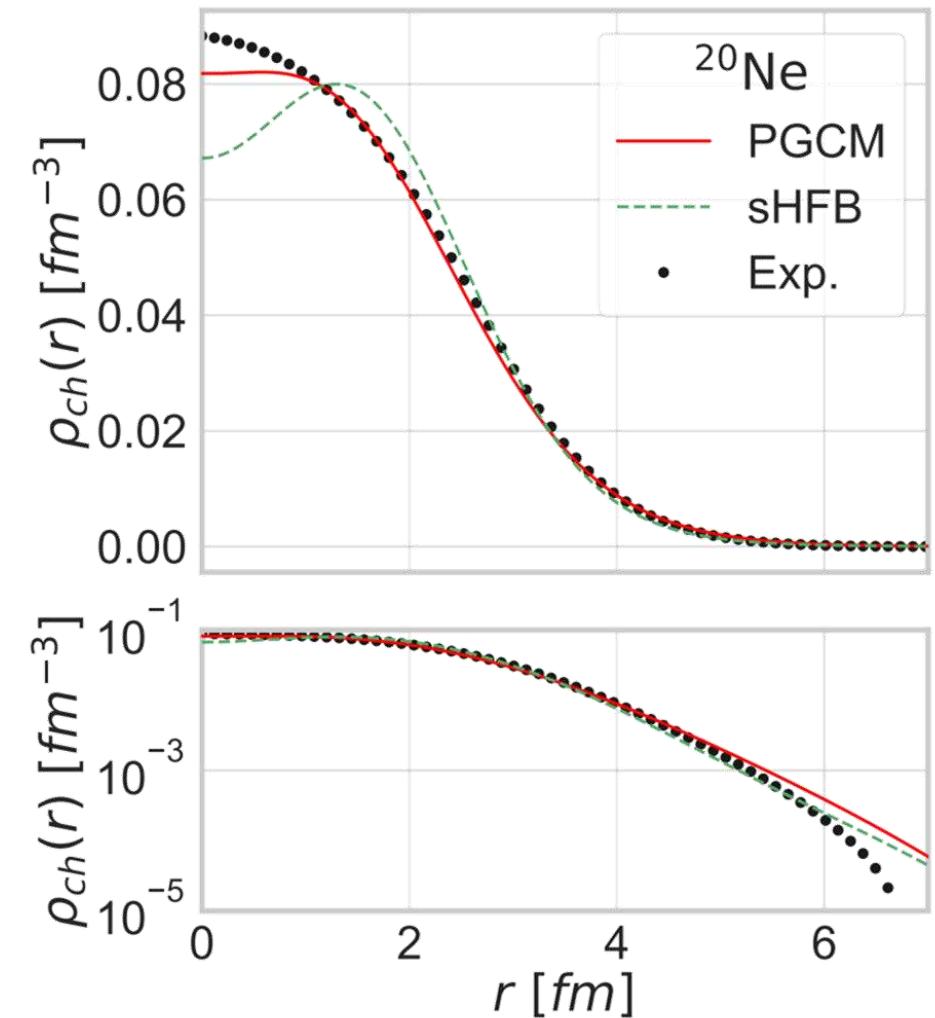
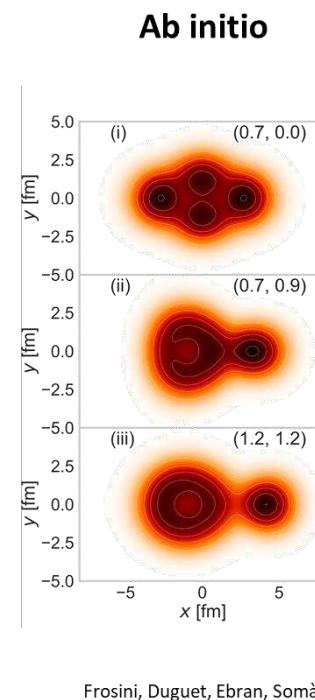
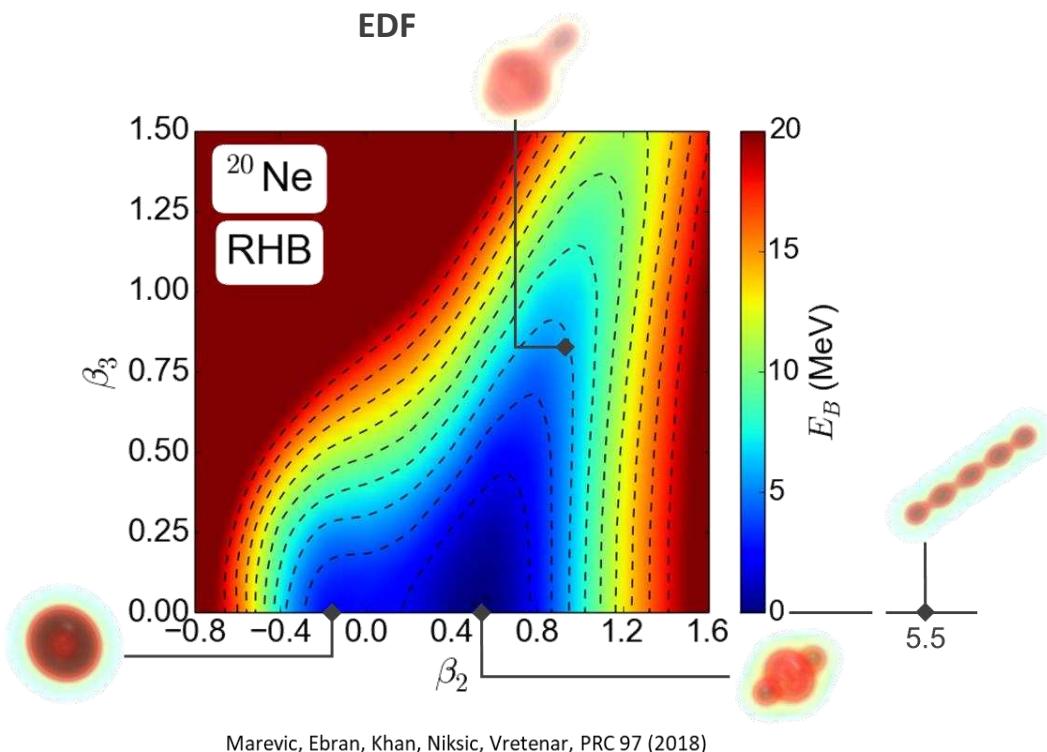
$$\psi'_2 = \frac{1}{2} (\phi_1 - \phi_2 - \phi_3 + \phi_4),$$

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

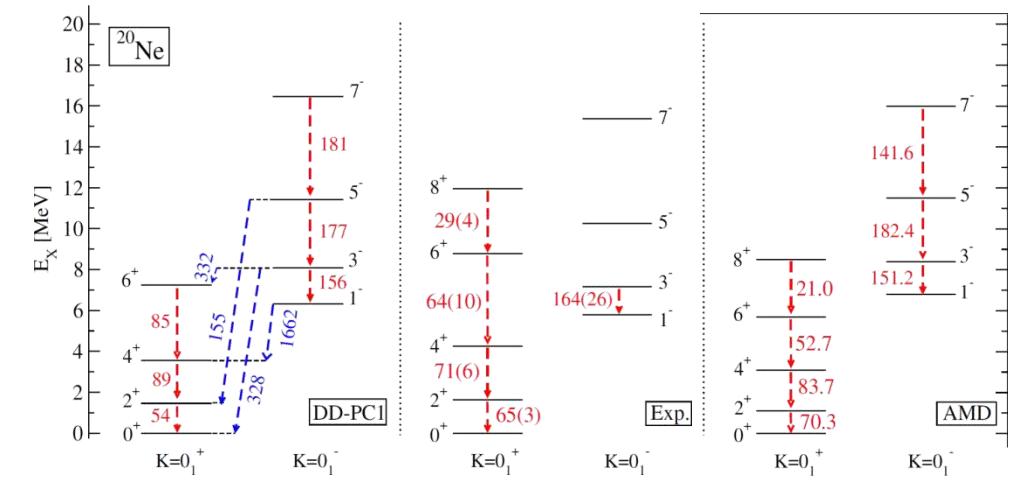
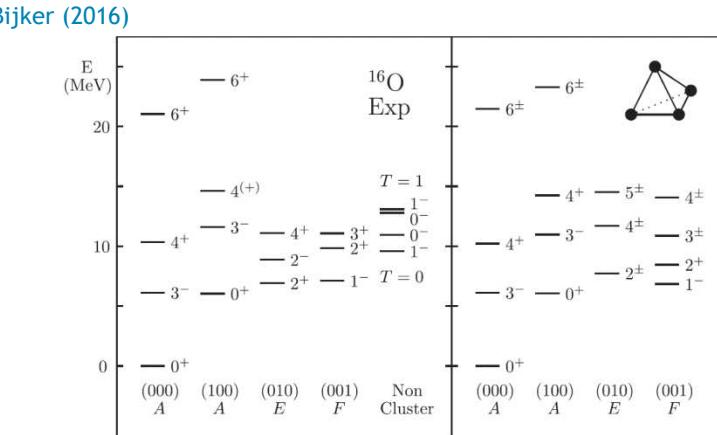
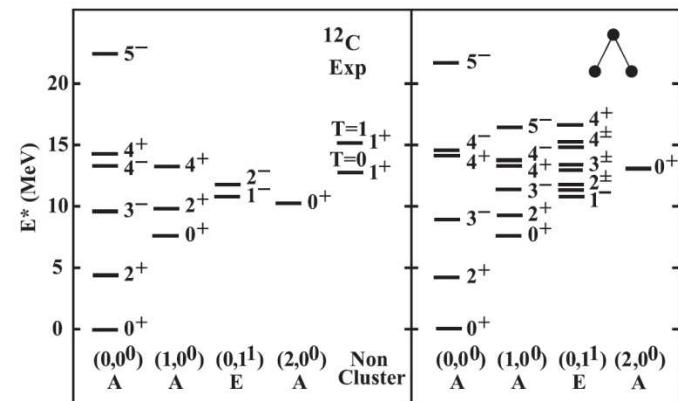
$$\psi'_4 = \frac{1}{2} (-\phi_1 + \phi_2 - \phi_3 + \phi_4).$$



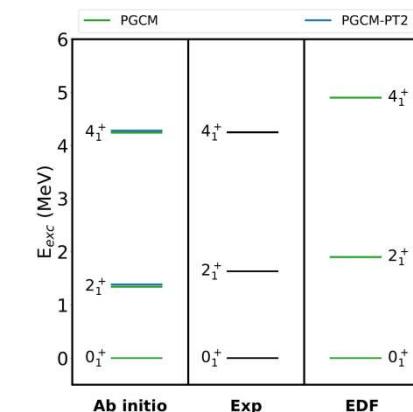
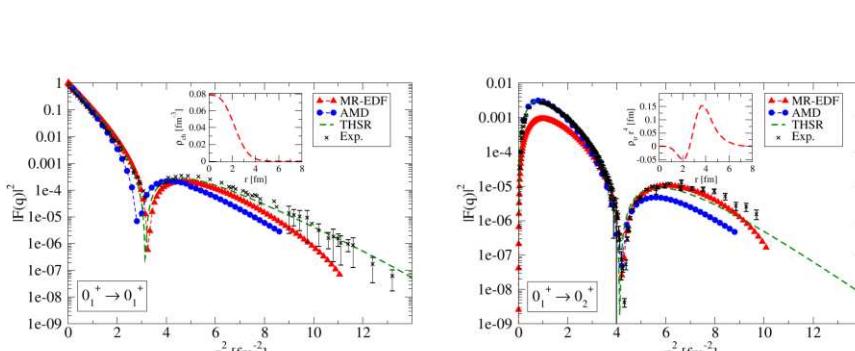
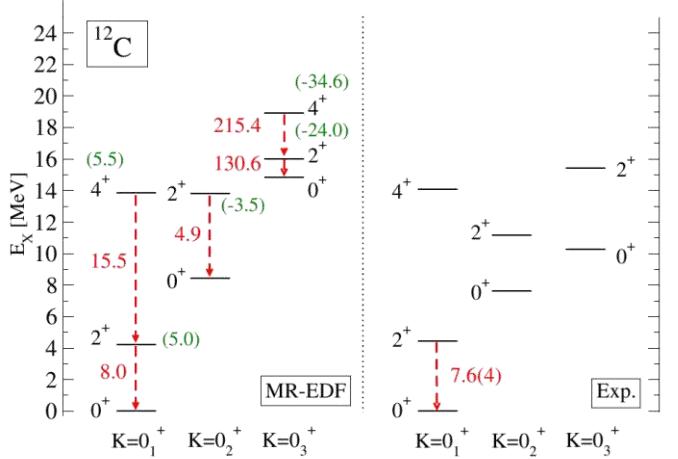
● Correlated GS



● Spectroscopy

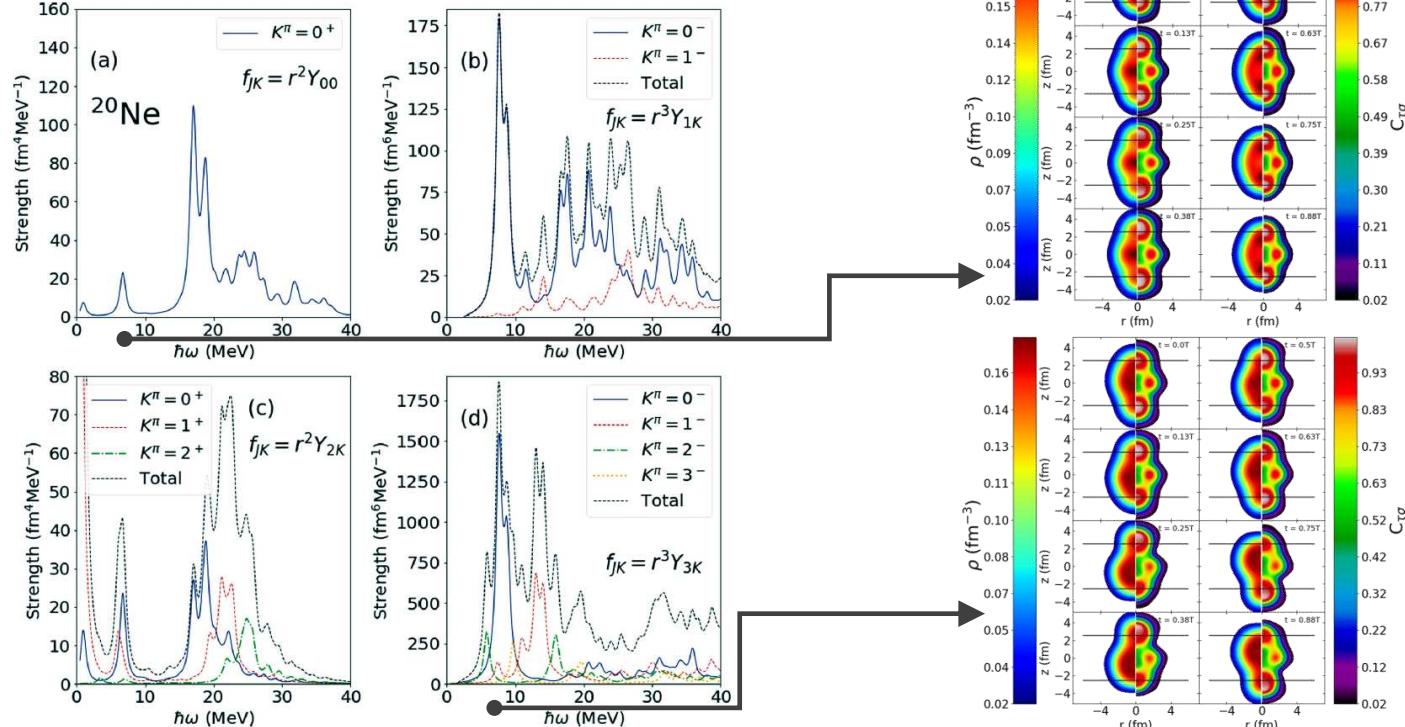


Marević, Ebran, Khan, Nikšić, Vretenar, PRC 2018



Frosini, Duguet, Ebran, Somà, EPJA 2022

● Cluster vibration

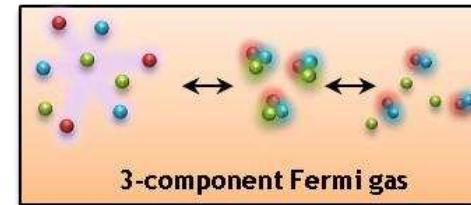
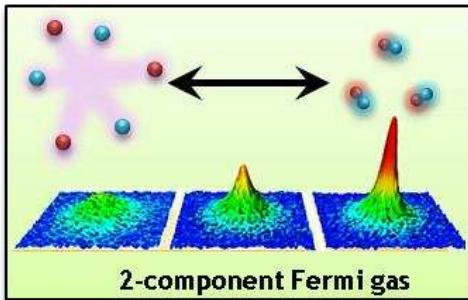


Mercier, Bjelčić, Nikšić, Ebran, Khan, Vretenar PRC 2021
 Mercier, Ebran, Khan PRC 2022

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 ?





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

$$H_0 = \int d^3r \sum_{\alpha} \varepsilon_{\alpha} \psi_{\alpha}^{\dagger}(\mathbf{r}) \psi_{\alpha}(\mathbf{r})$$

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

Correlated pair operators

$$P_{\nu}^{\dagger}(\mathbf{r}) \equiv \sqrt{\frac{1}{2}} \sum_l \sqrt{2l+1} \left\{ \psi_{l,s=\frac{1}{2},t=\frac{1}{2}}^{\dagger}(\mathbf{r}) \psi_{l,s=\frac{1}{2},t=\frac{1}{2}}^{\dagger}(\mathbf{r}) \right\}_{M_L=0,M_S=0,M_T=\nu}^{(L=0,S=0,T=1)}$$

$$Q_{\mu}^{\dagger}(\mathbf{r}) \equiv \sqrt{\frac{1}{2}} \sum_l \sqrt{2l+1} \left\{ \psi_{l,\frac{1}{2},\frac{1}{2}}^{\dagger}(\mathbf{r}) \psi_{l,\frac{1}{2},\frac{1}{2}}^{\dagger}(\mathbf{r}) \right\}_{M_L=0,M_S=\mu,M_T=0}^{(L=0,S=1,T=0)}$$



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

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

Singlet ($S=0$) pairing operator

$$S_{0,0}^{\dagger} = \sum_{\alpha\beta} \langle \frac{3}{2} \frac{3}{2}; 00 | \frac{3}{2} \frac{3}{2} \alpha\beta \rangle \varphi_{\alpha}^{\dagger} \varphi_{\beta}^{\dagger}$$

Quintet ($S=2$) pairing operator

$$D_{2,m}^{\dagger} = \sum_{\alpha\beta} \langle \frac{3}{2} \frac{3}{2}; 2m | \frac{3}{2} \frac{3}{2} \alpha\beta \rangle \varphi_{\alpha}^{\dagger} \varphi_{\beta}^{\dagger}$$

with $S_{0,0}^{\dagger} = P_0^{\dagger}$, $D_{2,0}^{\dagger} = Q_0^{\dagger}$, $D_{2,\pm 1}^{\dagger} = P_{\pm 1}^{\dagger}$ and $D_{2,\pm 2}^{\dagger} = Q_{\pm 1}^{\dagger}$



- $\text{Sp}(4) \sim \text{SO}(5)$ symmetry without fine tuning the coupling constants

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

- Bilinears of fermions can be classified according to their behavior under $\text{SO}(5)$

Particle-hole channel

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

Particle-particle channel

$$\begin{aligned} \eta^{\dagger}(\mathbf{r}) &= \frac{1}{2} \sum_{\alpha\beta} \varphi_{\alpha}^{\dagger}(\mathbf{r}) C_{\alpha\beta} \varphi_{\beta}^{\dagger}(\mathbf{r}), \\ \xi_a^{\dagger}(\mathbf{r}) &= -\frac{i}{2} \sum_{\alpha\beta} \varphi_{\alpha}^{\dagger}(\mathbf{r}) (\Gamma^a C)_{\alpha\beta} \varphi_{\beta}^{\dagger}(\mathbf{r}), \\ \dot{C} &= \Gamma^1 \Gamma^3 \\ S_{0,0}^{\dagger} &= -\frac{\eta^{\dagger}}{\sqrt{2}}, \quad D_{2,0}^{\dagger} = -i \frac{\xi_4^{\dagger}}{\sqrt{2}}, \quad D_{2,\pm 1}^{\dagger} = -\frac{\xi_3^{\dagger} \mp i \xi_2^{\dagger}}{\sqrt{2}}, \quad D_{2,\pm 2}^{\dagger} = \frac{\mp \xi_1^{\dagger} + i \xi_5^{\dagger}}{\sqrt{2}} \end{aligned}$$



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

● 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 phase : $\eta^{\dagger}(\mathbf{r})$

ii) SU(4) molecular superfluid phase formed from bound states of 4 fermions: $A^{\dagger}(\mathbf{r}) \equiv \varphi_{\frac{3}{2}}^{\dagger}(\mathbf{r}) \varphi_{\frac{1}{2}}^{\dagger}(\mathbf{r}) \varphi_{-\frac{1}{2}}^{\dagger}(\mathbf{r}) \varphi_{-\frac{3}{2}}^{\dagger}(\mathbf{r})$

● 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