Theoretical description of the nuclear clustering phenomenon – An introduction –

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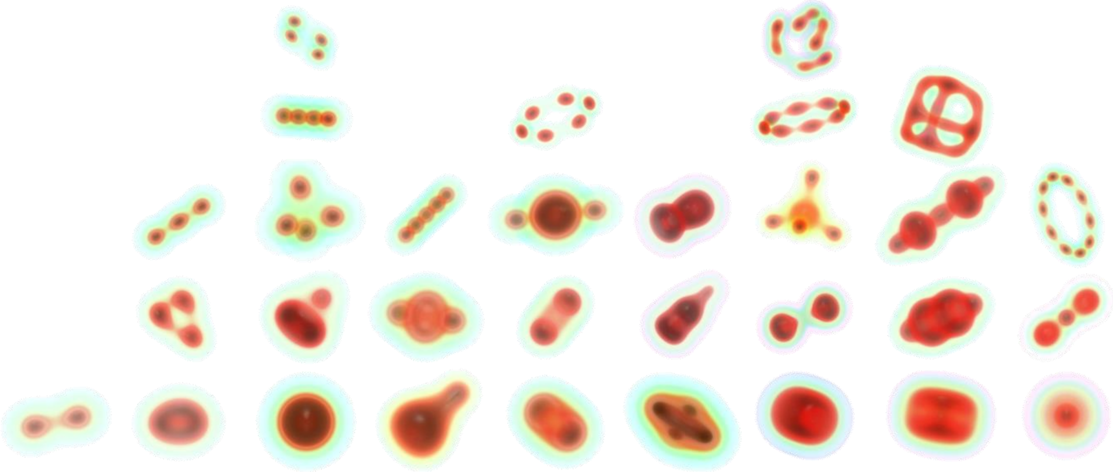
CEA,DAM,DIF



2nd Rencontre PhyNuBE : clustering and symmetries in nuclear physics

26-31 March 2023

Outline

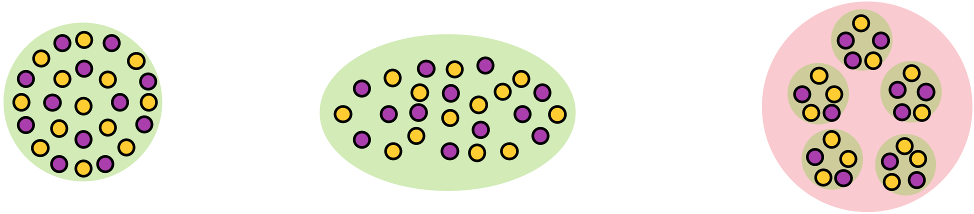
1. General context
2. Qualitative understanding of the nuclear clustering phenomenon
3. Theoretical description of the nuclear clustering phenomenon

1. General context

1 Context

◉ Take a bunch of interacting classical or quantal dofs, coming in different species {●●● … ●●●…} and forming a bound state

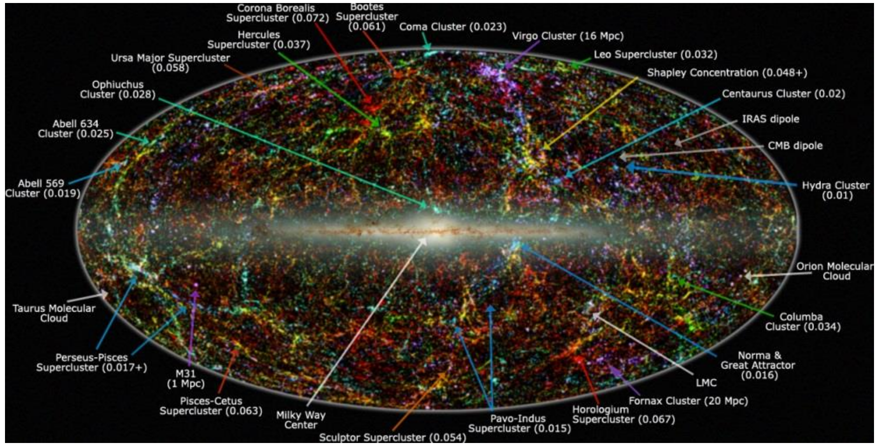
i) How do these dofs arrange themselves ? (helps interpreting ground state/excitation/decay/reaction features)
⇒ Competition between kinetic (delocalization/disorder) and potential (localization/order) energies

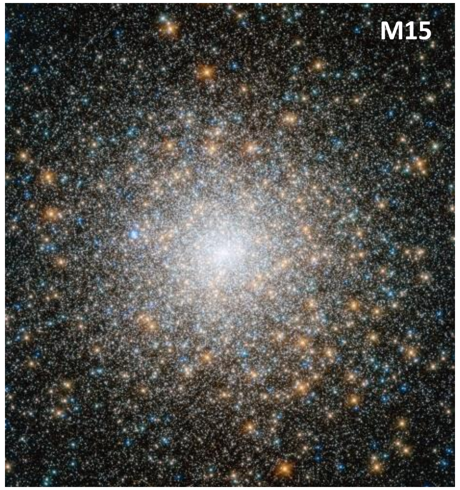


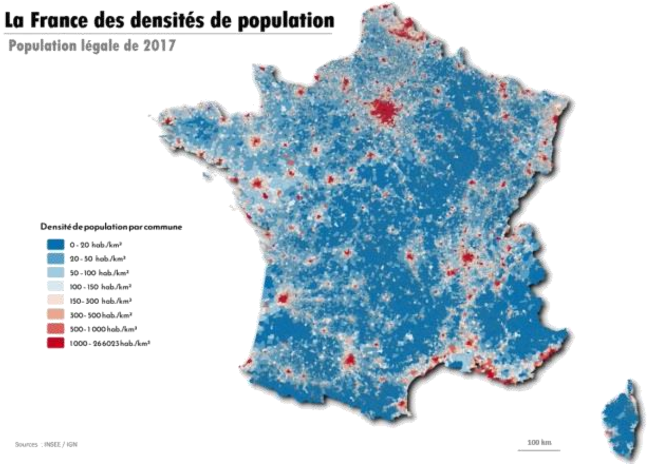
ii) How emerging structures evolve with E*, T, number of particles, species unbalance, … ?

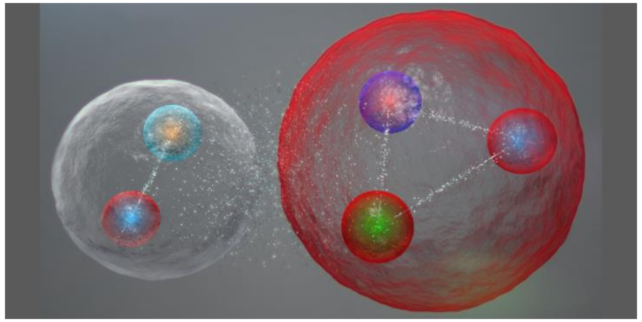
1 Clustering

◉ Clustering : an ubiquitous phenomenon



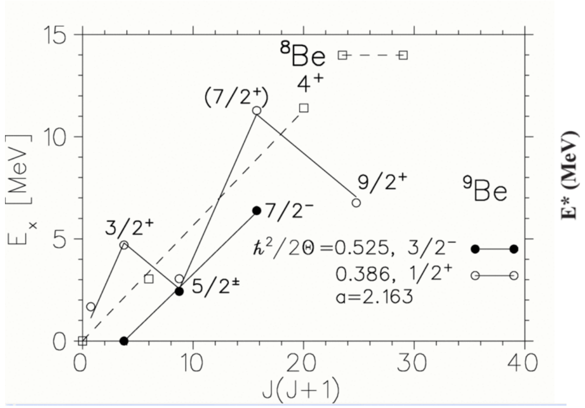


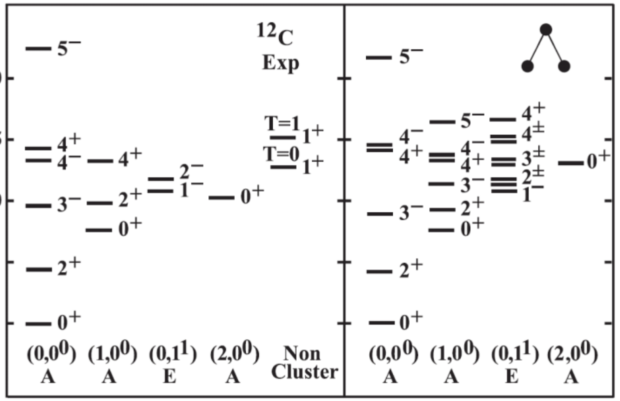


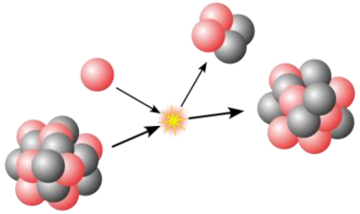


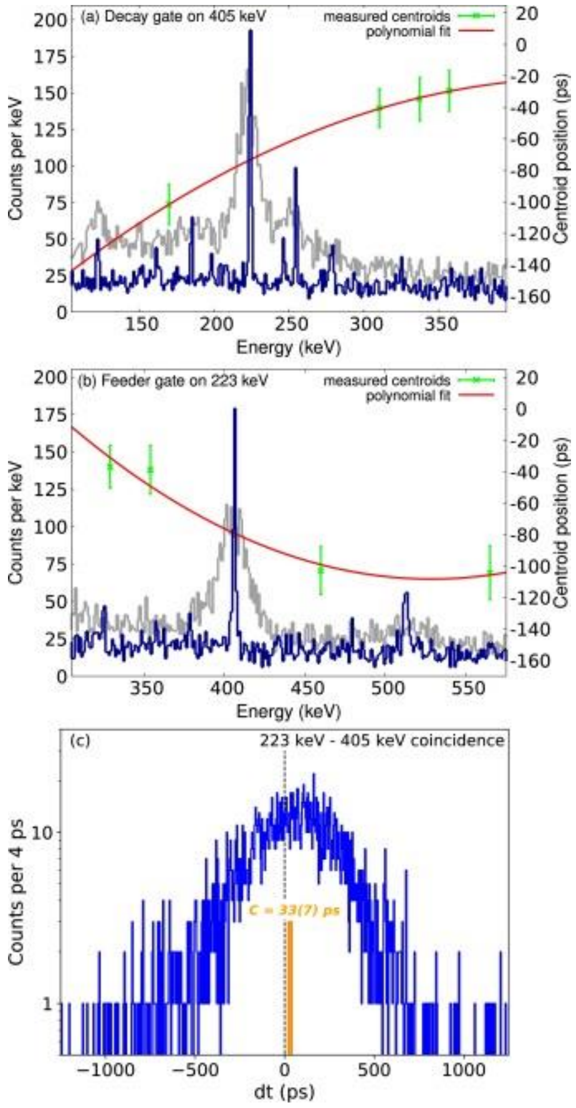
❶ Nuclear clustering

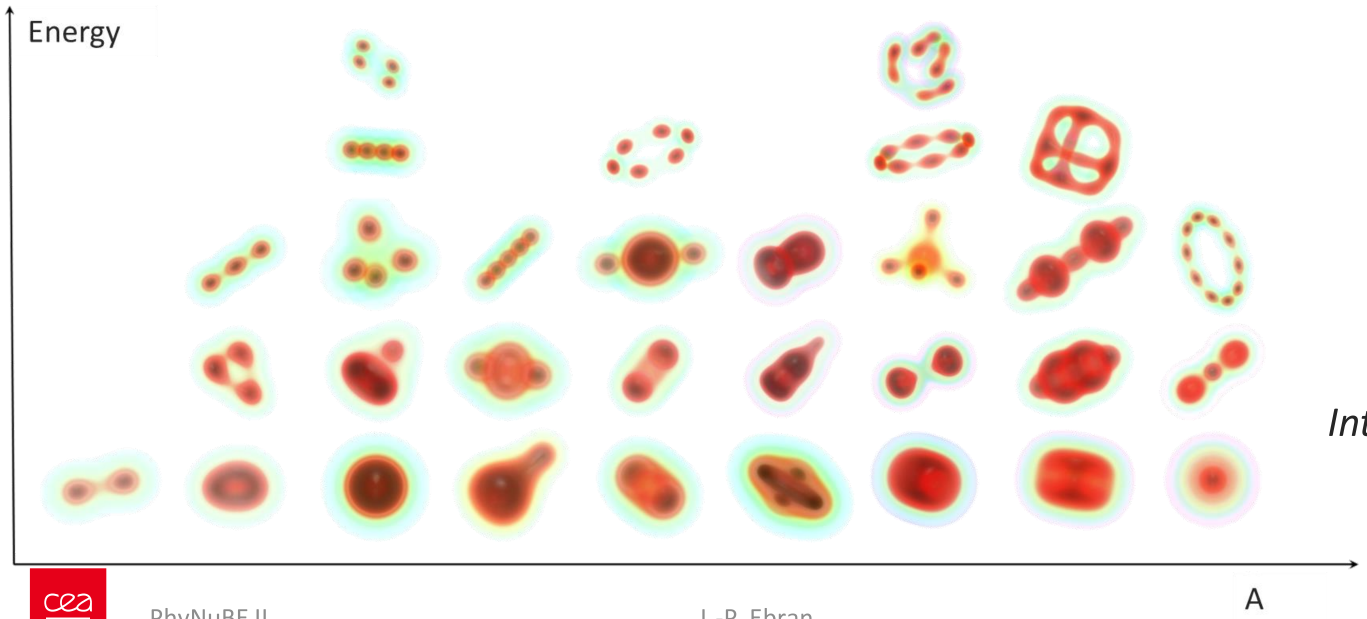
- Nuclear clustering = nucleons clumping together into sub-groups within the nucleus









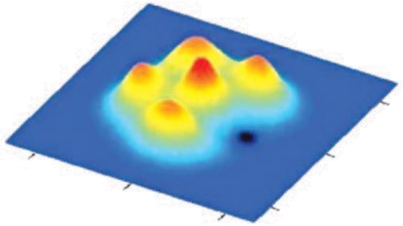


Intrinsic densities

1 Probing cluster correlations

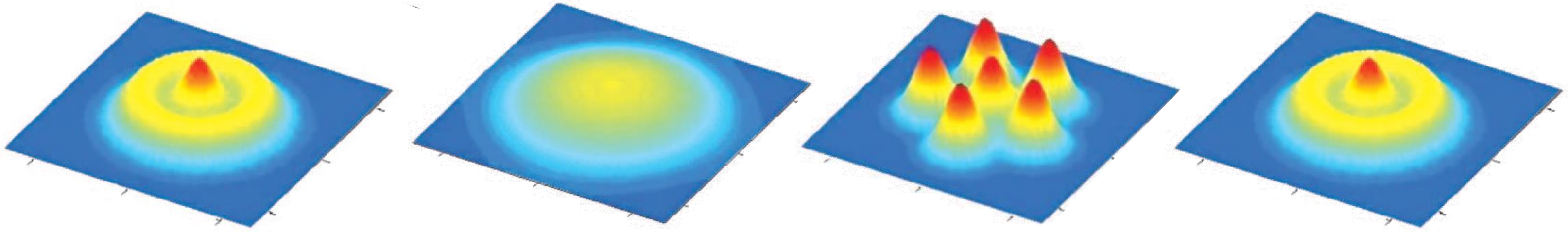
- Emergent SSBs : SSBs obscured by non-negligible fluctuations of order parameters but still leave traces

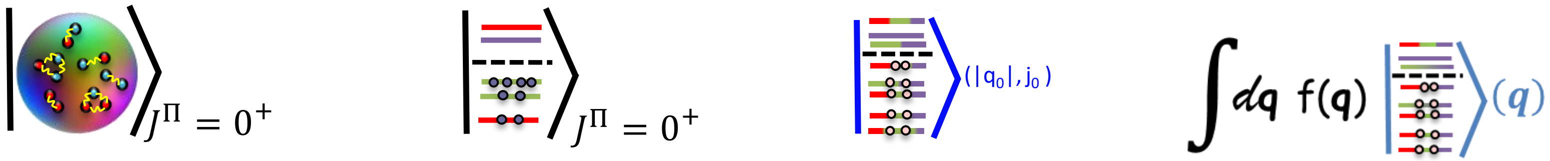
2-point correlation function



Revealing back long-range order

Density profile





Exact WF

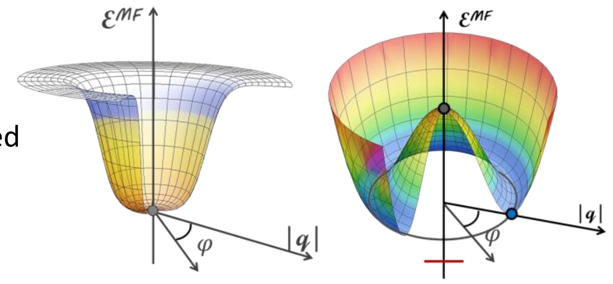
Approx :
Symmetry-preserving HF WF

Approx :
Symmetry-broken HFB WF

Approx :
PGCM WF

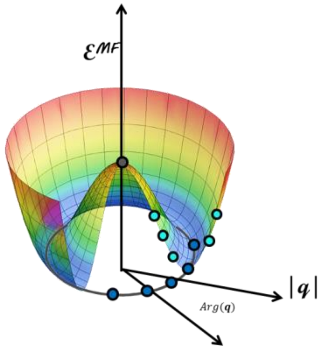
Spectroscopy

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



Closed-shell system

Open-shell system

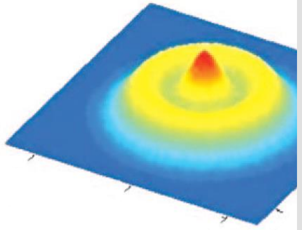


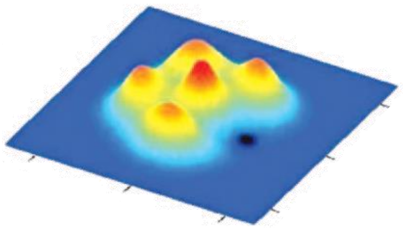
Yannouleas & Landman, 2017

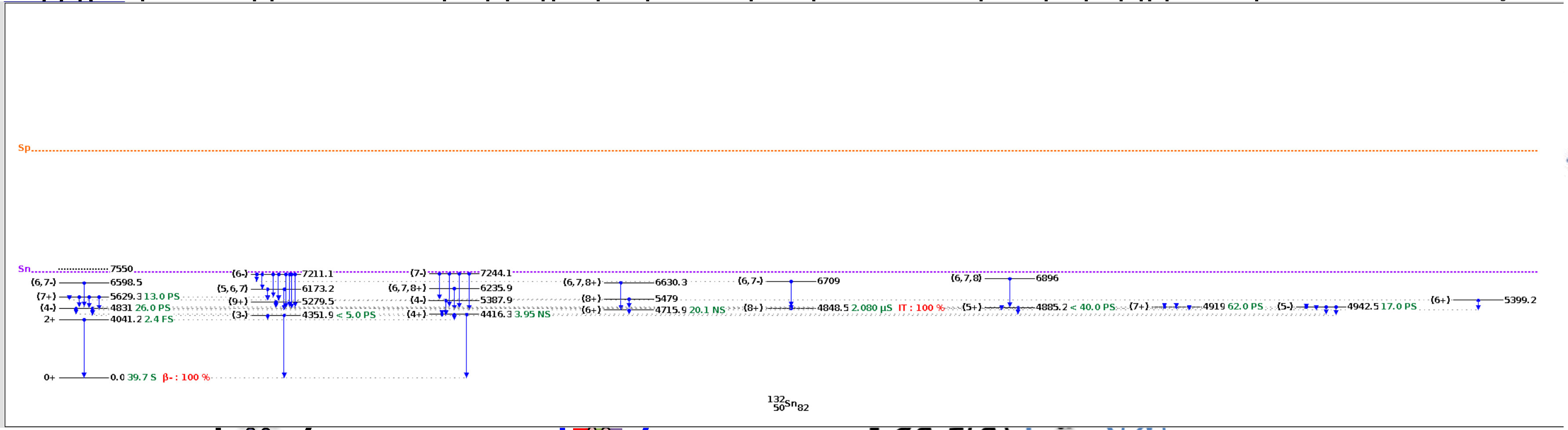
1 Probing cluster correlations

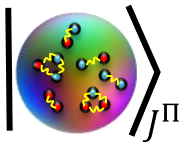
- Emergent SSB

2-point correlation function









$J^\Pi = 0^+$

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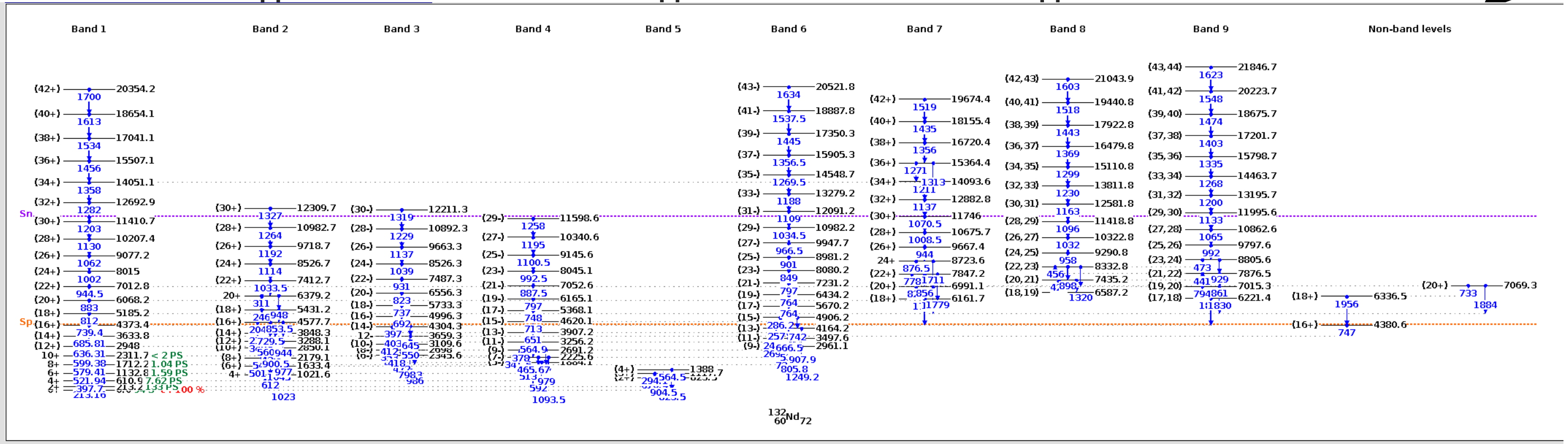
Exact WF

Approx :

Approx :

Approx :

Spectroscopy



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Yannouleas & Landman, 2017

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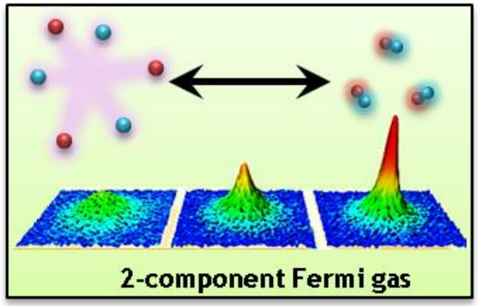
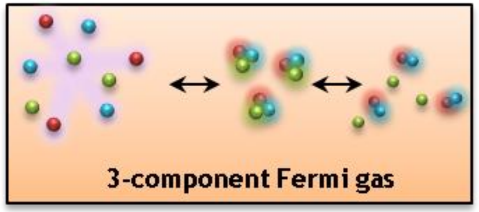
2. Qualitative understanding of the nuclear clustering phenomenon

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

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

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

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

Quintet (S=2) pairing operator $\quad D^\dagger_{2,m} = \sum_{\alpha\beta} \langle \tfrac{3}{2}\tfrac{3}{2};2m|\tfrac{3}{2}\tfrac{3}{2}\alpha\beta\rangle\, \varphi^\dagger_\alpha \varphi^\dagger_\beta$

with $S^\dagger_{0,0} = P^\dagger_0,\ D^\dagger_{2,0} = Q^\dagger_0,\ D^\dagger_{2,\pm1} = P^\dagger_{\pm1}$ and $D^\dagger_{2,\pm2} = Q^\dagger_{\pm1}$

Group theory considerations

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

- Generators of $\mathfrak{so}(5)$

$$\Gamma^{ab} \equiv -\frac{i}{2}\left[\Gamma^a, \Gamma^b\right] \quad (1 \leq a, b \leq 5)$$

$$\Gamma^1 = \begin{pmatrix} 0 & -iI \\ iI & 0 \end{pmatrix}, \quad \Gamma^{2,3,4} = \begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & -\boldsymbol{\sigma} \end{pmatrix}, \quad \Gamma^1 = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}$$

- 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

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

- 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 : $\eta^\dagger(\boldsymbol{r})$

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

- 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.

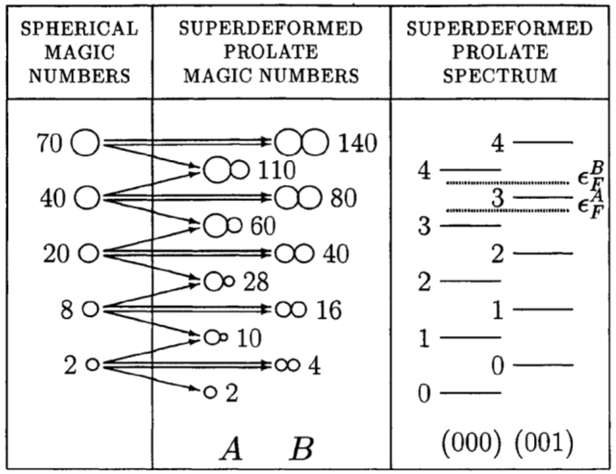
$\mathbb{Z}_2$ remaining unbroken $\Rightarrow$ strong quantum fluctuations in the spin channel suppressing Cooper pairing (2 fermions can't form a $\mathbb{Z}_2$ singlet) $\Rightarrow$ leading superfluid instability = quartetting

Deformation & Nuclear clustering

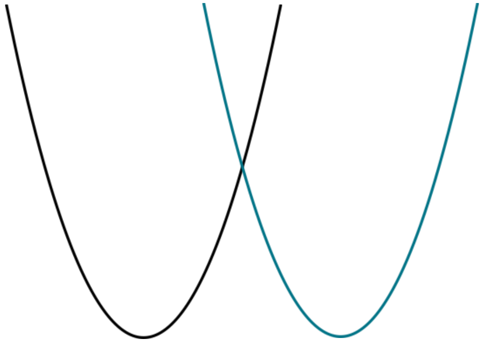
◉ Role of deformation

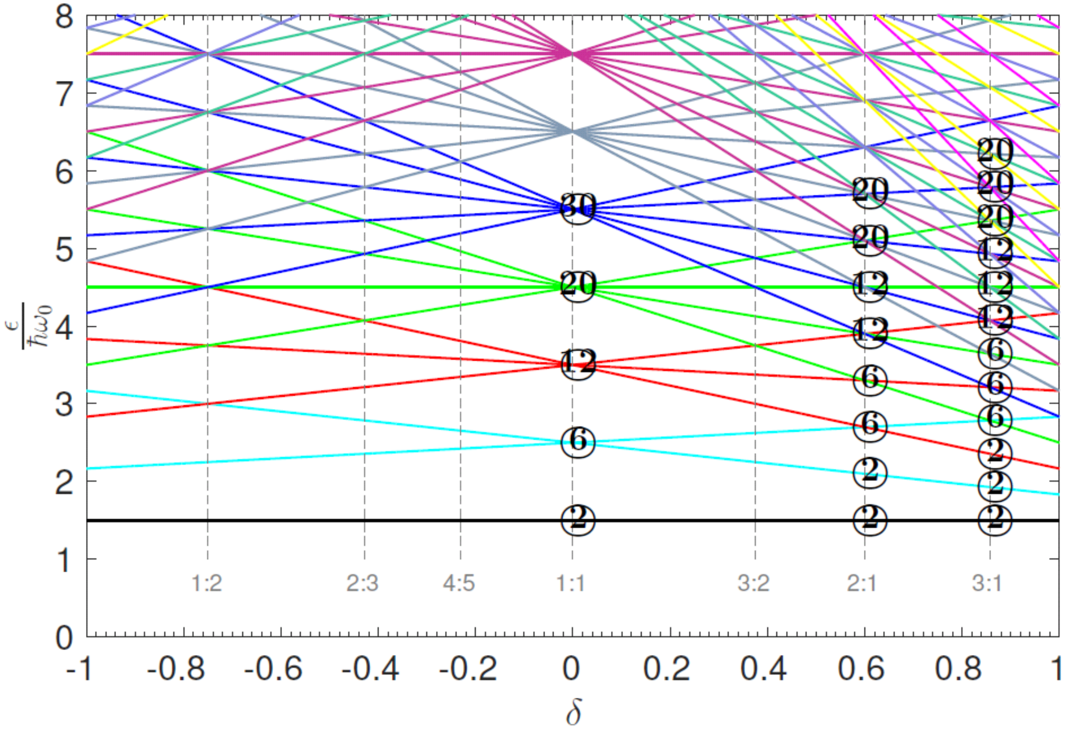
N-dimensional anisotropic HO with commensurate frequencies enjoys dynamical symmetries involving multiple independent copies of SU(N) irreps

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

Nucleon mass

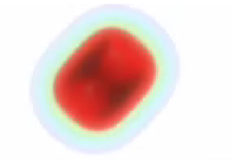
Number of nucleons

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

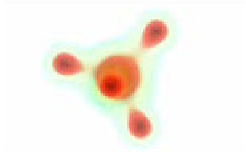
Depth of the confining potential

Mean density

small



large



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

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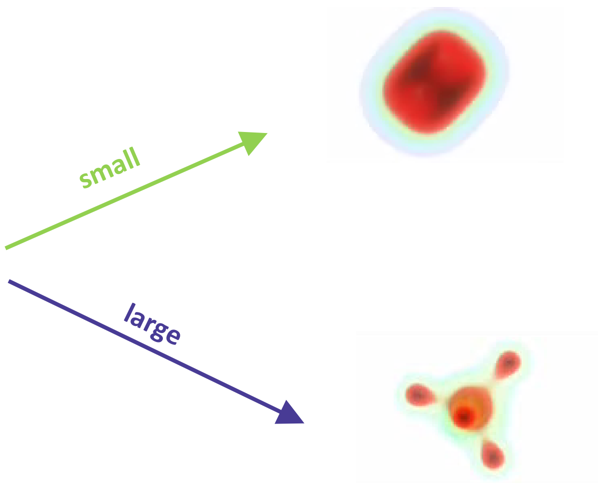
Depth of the confining potential — Mean density



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

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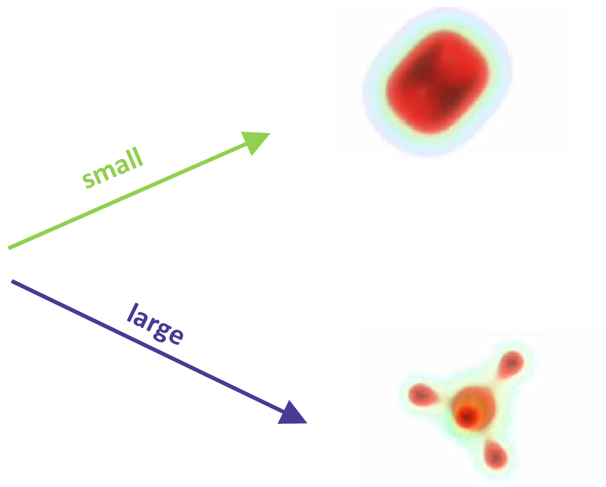

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- Formation/dissolution of clusters : Mott parameter

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

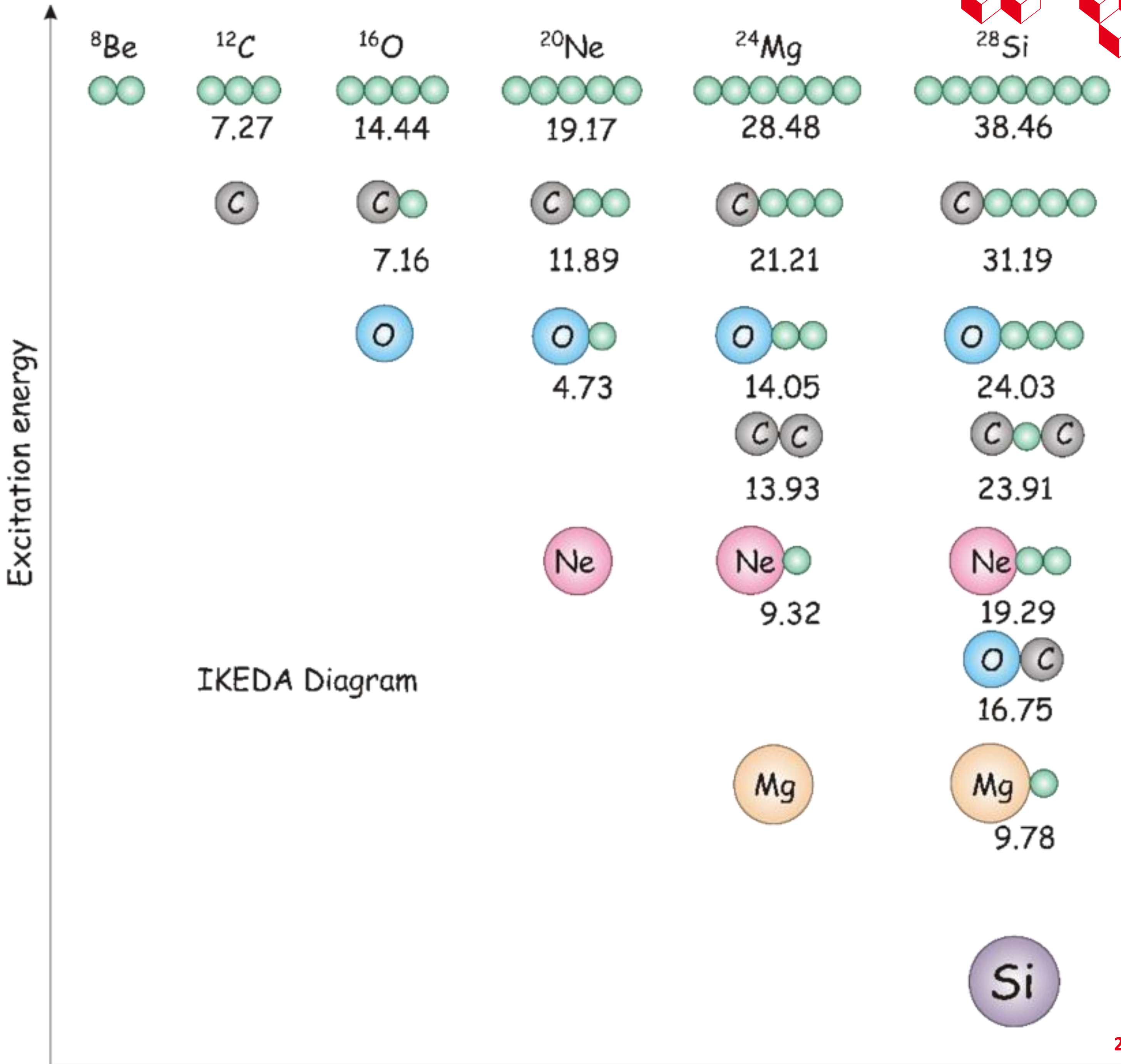
$\sim \frac{\rho_{sat}}{3}$ — 0.9 size of an α in free-space

Ebran, Girod, Khan, Lasseri, Schuck, PRC 2020
Ebran, Khan, Niksic, Vretenar, PRC 2014

Coupling to the continuum

◉ Clustering as threshold effect
Strong impact of the continuum (Ploszajczak)

◉ But at the same time, clustering correlations impact structure of compact states



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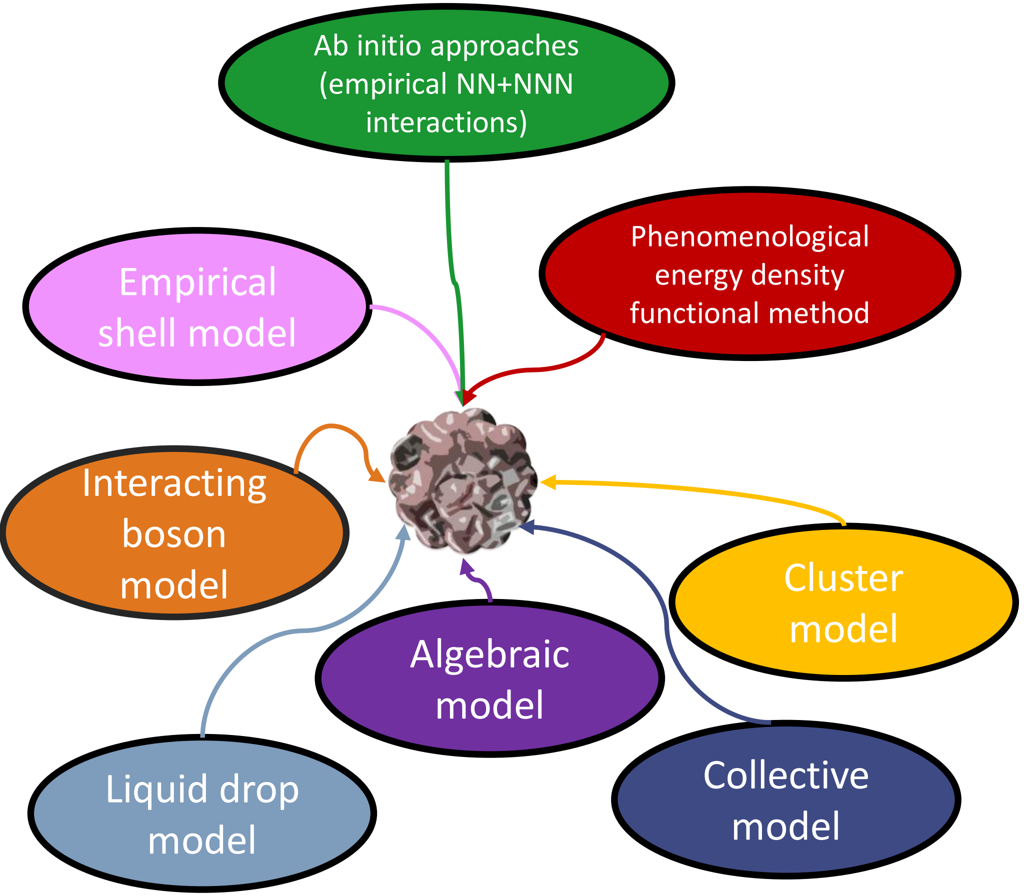
Strategies

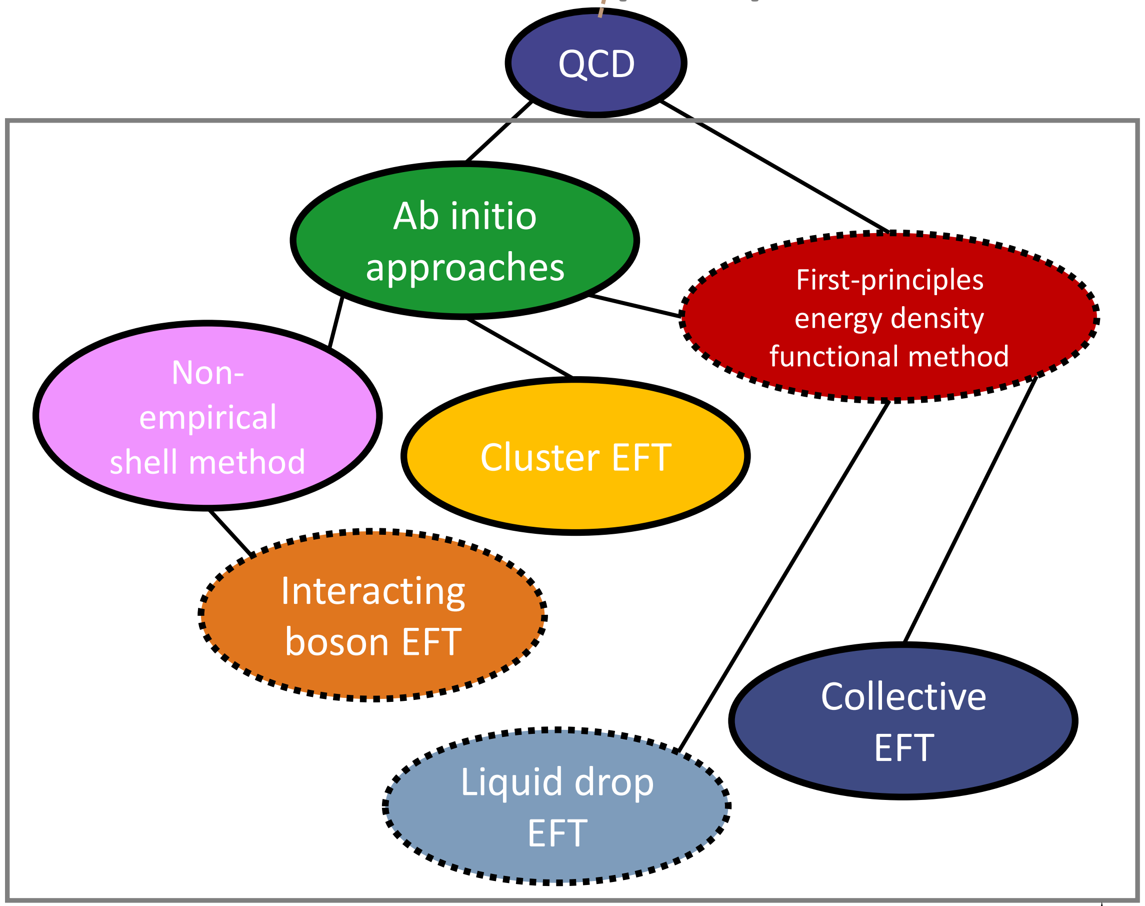
◉ Achieve a { *accurate* / *predictive* / *computationally affordable* } description ?

Era of models

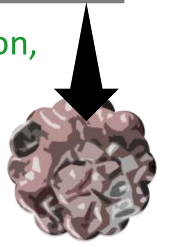


- ☑ Gives insight about relevant scales/dofs
- ☑ Ready to be used
- ☒ Lack of control
  ⇒ double counting issues, error compensation, no error assessment

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



2 possible viewpoints for describing nuclear clustering

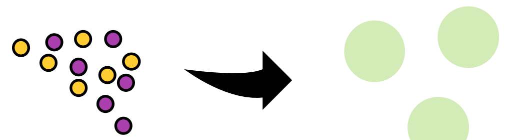
- Relevant dofs = inert clusters + possibly single nucleons

- Relevant dofs = nucleons

"non-microscopic" approaches : empirical perspective

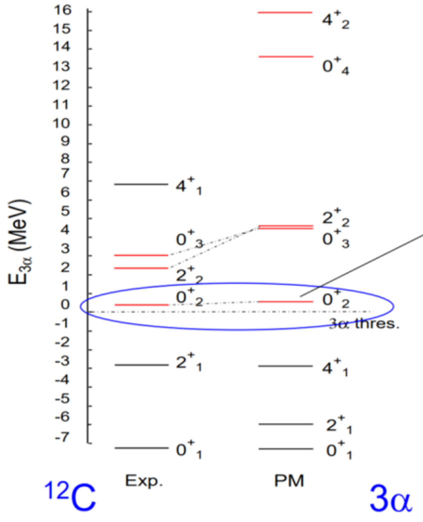
⦿ View the nucleus as a system of N "elementary" clusters in which the A nucleons are distributed and solve $H\Psi = E\Psi$ with

$$H = \sum_{i=1}^{N} \frac{\boldsymbol{P}_i^2}{2M_i} + \sum_{i<j=1}^{N} V_{ij}\left(\boldsymbol{R}_i - \boldsymbol{R}_j\right)$$



--> Potentials fitted on binding energies and nucleus-nucleus phase shifts

--> Models rather simple for N=2. For N=3, hyperspherical or Faddeev methods are efficient techniques.



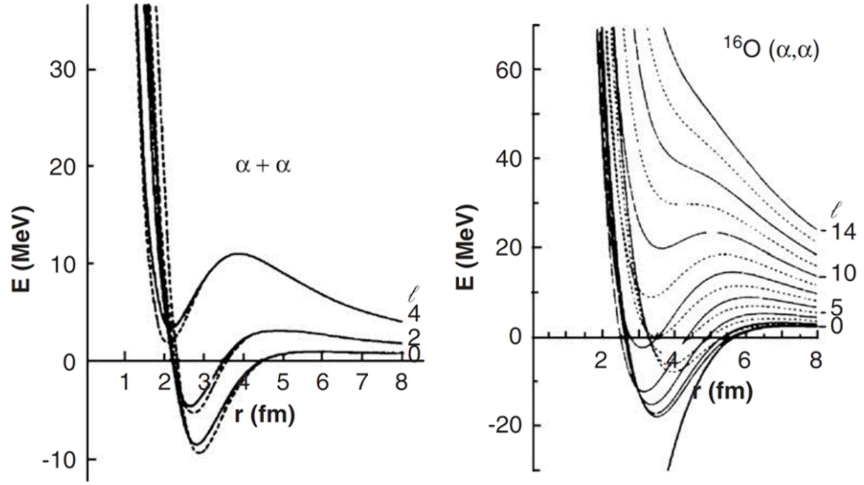
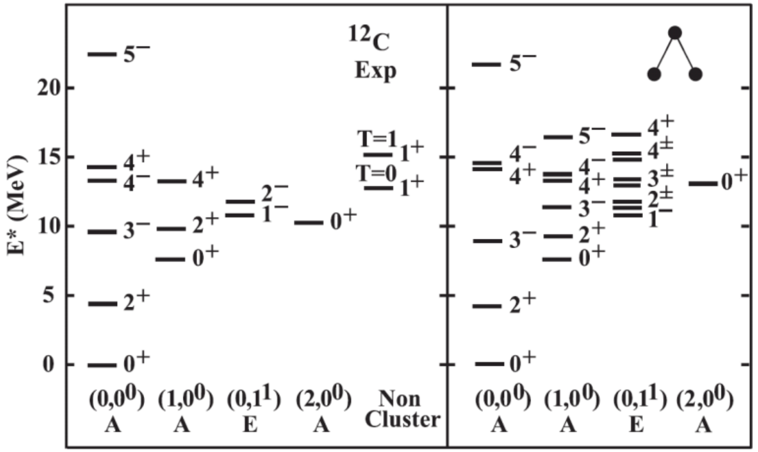


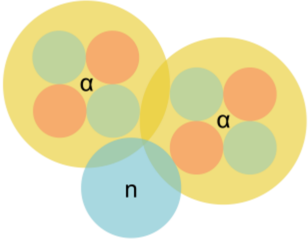
Fig. 12. Two examples of molecular local potentials for the α–α interaction, i.e. for ^{8}Be, and for the α-^{16}O system, forming ^{20}Ne. Different partial waves are shown. Figure adapted from Ref. [206].

Bijker, Iachello (2002)



“non-microscopic” approaches : EFT perspective

◉ Loosely bound cluster nuclei like ^{9}Be (Borromean nucleus)



⇢ Energy needed to separate ^{9}Be into $\alpha + \alpha + n$: ~1.5 MeV

⇢ Proton separation energy of ^{4}He: ~19.8 MeV

⇒Separation of scale calling for an EFT (cf Halo/Cluster EFT by Bira van Kolck)

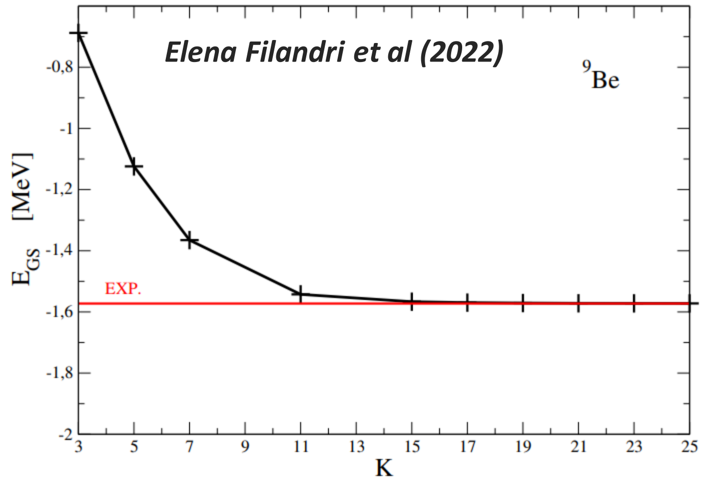


FIGURE 6.15: Ground state energy of ^{9}Be increasing the hyperangular momentum K with the three-body force.

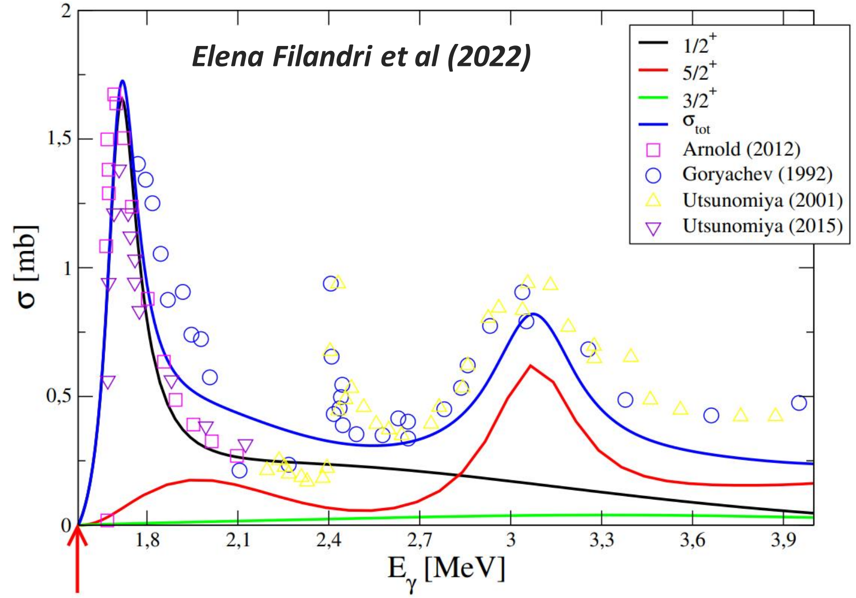


FIGURE 6.33: Comparison of our result obtained for the ^{9}Be photodisintegration cross-section and the experimental data shown in Figure 1.2. The red arrow indicates the threshold.

Microscopic viewpoint

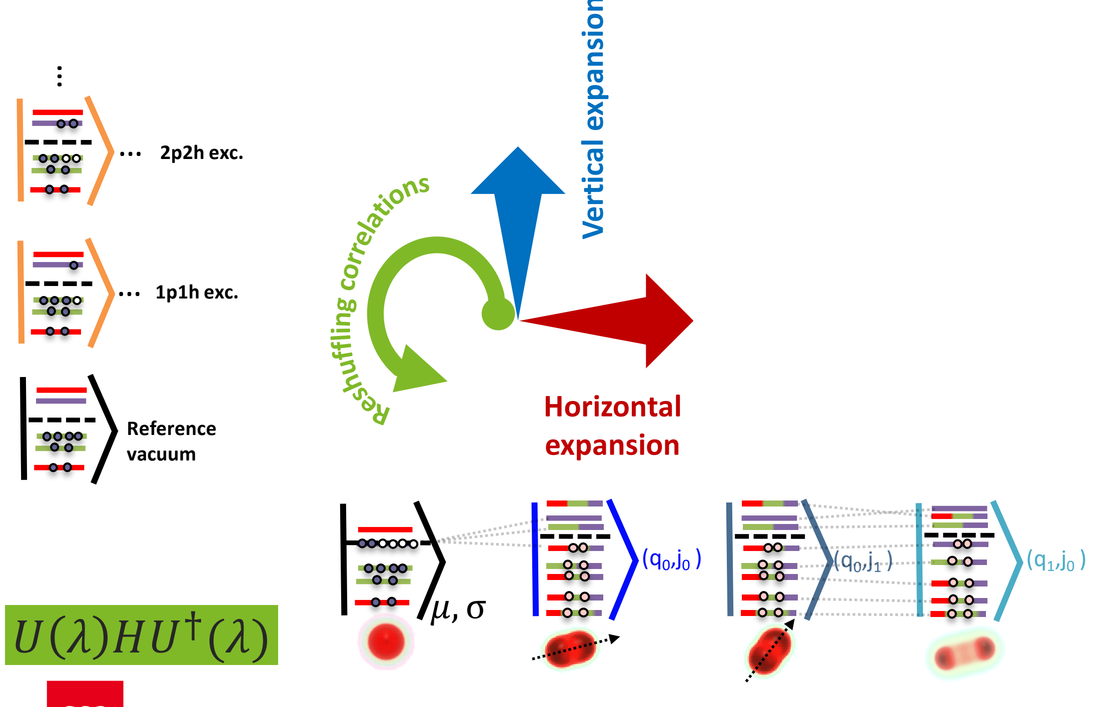
1) Nucleus: *A* interacting, structure-less nucleons
2) Structure & dynamic encoded in Hamiltonian, Functional, …
3) Solve *A*-nucleon Schrödinger/Dirac equation to desired accuracy

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

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

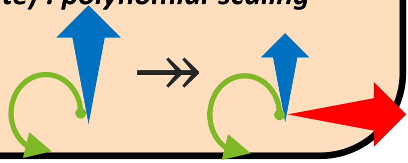
◈ Refined many-body schemes with controlled uncertainties

--→ *CI (full space diag.) : exponential scaling*

--→ *Hybrids (valence space diag.) : mixed scaling*

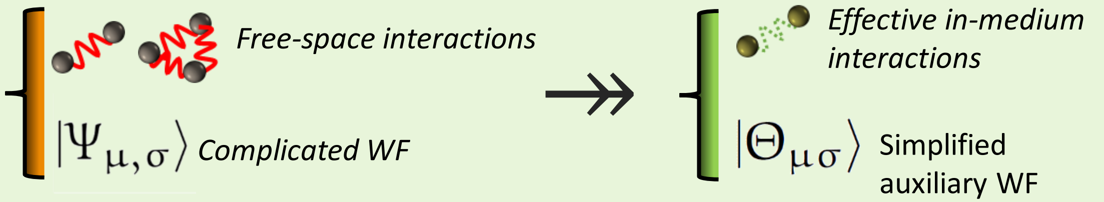
--→ ***Expansion methods (partition, expand and truncate) : polynomial scaling***

⊗ *How to challenge ab initio frontiers*



EDF

◉ **Effective pseudo-Hamiltonian**

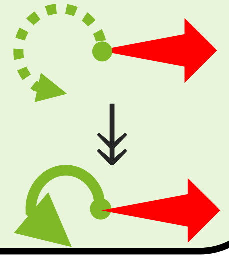


◉ **Various levels of realization**

--→ *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 ?*

Capture clustering in a microscopic framework

◉ Cluster approximation : assume that A nucleons organize into N clusters
⇒Impose a specific form for the nucleus total wavefunction

⇢ Resonating group method (Wheeler, Descouvement, …) : For 2 clusters

$$\Psi_{\mathrm{RGM}} = \mathcal{A}\left\{\phi(C_1)\phi(C_2)\chi(\boldsymbol{\xi})\right\}$$

Nucleon antisymmetrizer

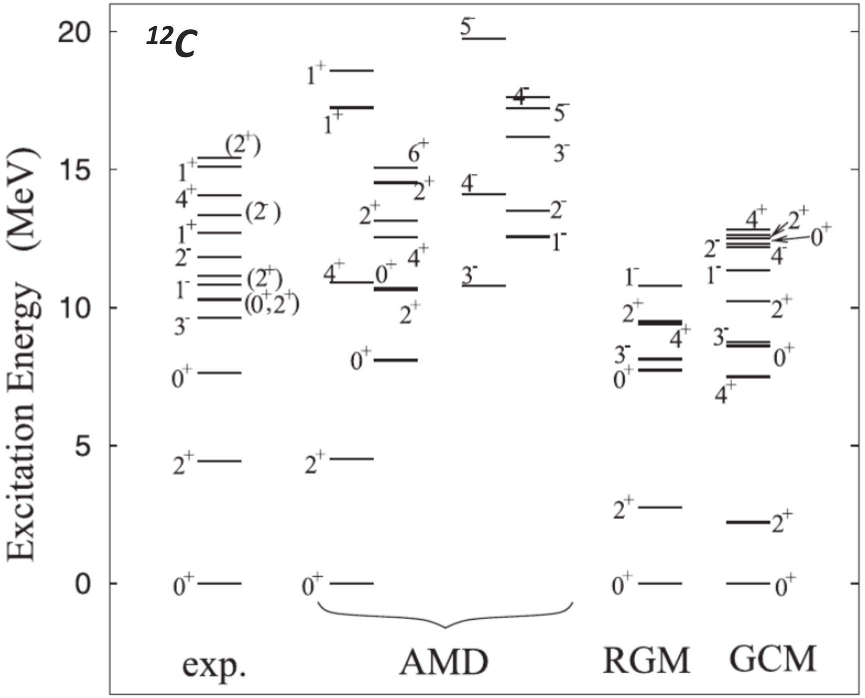
(A-C)-body internal WF of the 2nd cluster : $\boldsymbol{x}_{C+1}, \boldsymbol{x}_{C+2}, \dots, \boldsymbol{x}_A$

C-body internal WF of the 1st cluster : $\boldsymbol{x}_1, \boldsymbol{x}_2, \dots, \boldsymbol{x}_C$

A-body WF : $\boldsymbol{x}_1, \boldsymbol{x}_2, \dots, \boldsymbol{x}_A$

Inter-cluster WF depending on the relative coordinate between the coms of the clusters

Phenomenological

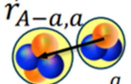


Ab initio : Navratiln Hupin, Romero, …

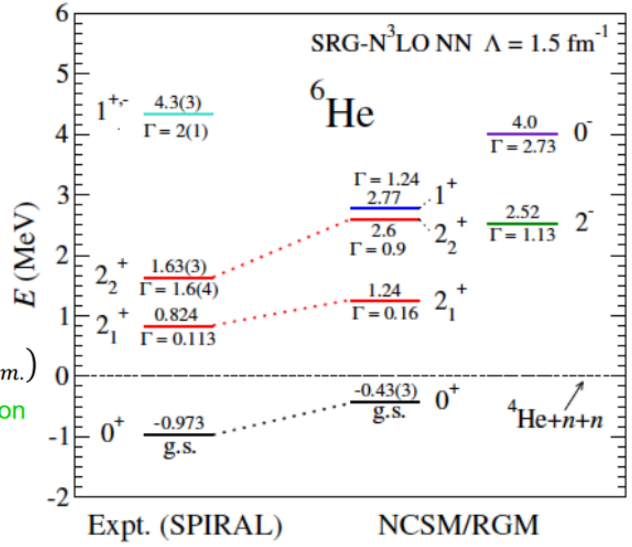
$$\Psi^{(A)}_{NCSM} = |A\lambda J^\pi T\rangle = \sum_\alpha c_\alpha \, |A\alpha j_z{}^\pi t_z\rangle \Leftrightarrow |A\lambda J^\pi T\rangle_{SD}\phi_{00}(\vec{R}^A_{c.m.})$$

Mixing coefficients(unknown) — A-body harmonic oscillator states — Second quantization

$$\Psi^{(A)}_{RGM} = \sum_\nu \int d\vec{r}\, g_\nu(\vec{r})\, \hat{A}_\nu \left|\Phi^{(A-a,a)}_{\nu\vec{r}}\right\rangle \Leftrightarrow \psi^{(A-a)}_{\alpha_1}\psi^{(a)}_{\alpha_2}\,\delta(\vec{r}-\vec{r}_{A-a,a})$$



Relative wave function (unknown) — Antisymmetrizer — Channel basis — Cluster expansion technique



Capture clustering in a microscopic framework

◉ Cluster approximation : assume that A nucleons organize into N clusters
⇒Impose a specific form for the nucleus total wavefunction

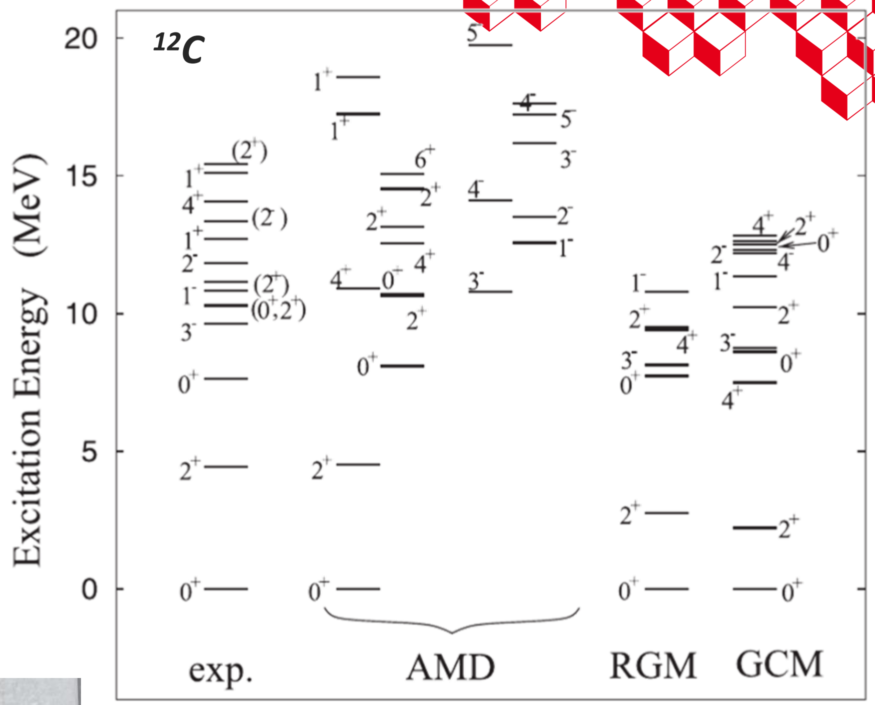
⇢ Resonating group method (Wheeler, Descouvemont, …)

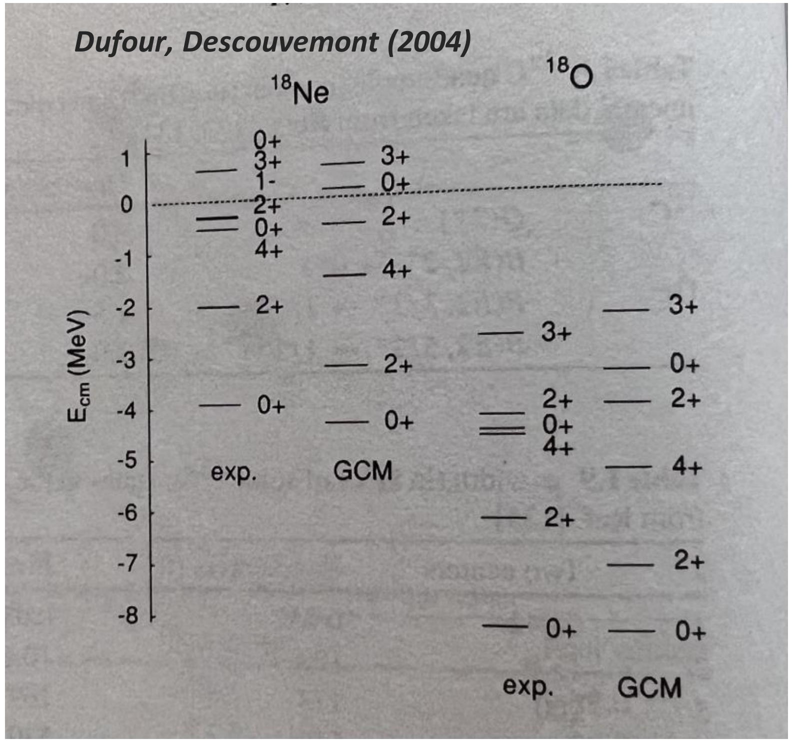
⇢ Generator Coordinate Method with Bloch-Brink cluster WF (Descouvemont, Dufour, …)

$$\Phi_{\rm BB}(\boldsymbol{S}_1,\ldots,\boldsymbol{S}_k) = n_0\mathcal{A}\left\{\psi(C_1;\boldsymbol{S}_1)\cdots\psi(C_k;\boldsymbol{S}_k)\right\}$$

Written in terms of HO WF

$$\Psi_{\rm GCM} = \int d\boldsymbol{S}_1,\ldots,d\boldsymbol{S}_k f(\boldsymbol{S}_1,\ldots,\boldsymbol{S}_k) \times P^{J\pi}_{MK}\Phi_{\rm BB}(\boldsymbol{S}_1,\ldots,\boldsymbol{S}_k),$$





Capture clustering in a microscopic framework

◉ Cluster approximation : assume that A nucleons organize into N clusters
⇒Impose a specific form for the nucleus total wavefunction

- Resonating group method (Wheeler, Descouvemont, …) : For 2 clusters $$\Psi_{\mathrm{RGM}} = \mathcal{A}\left\{\phi(C_1)\phi(C_2)\chi(\boldsymbol{\xi})\right\}$$

- Generator Coordinate Method with Bloch-Brink cluster WF (Descouvemont, Dufour, …)

$$\Phi_{\mathrm{BB}}(\boldsymbol{S}_1,\ldots,\boldsymbol{S}_k) = n_0\mathcal{A}\left\{\psi(C_1;\boldsymbol{S}_1)\cdots\psi(C_k;\boldsymbol{S}_k)\right\},$$

$$\Psi_{\mathrm{GCM}} = \int d\boldsymbol{S}_1,\ldots,d\boldsymbol{S}_k f(\boldsymbol{S}_1,\ldots,\boldsymbol{S}_k) \times P^{J\pi}_{MK}\Phi_{\mathrm{BB}}(\boldsymbol{S}_1,\ldots,\boldsymbol{S}_k),$$

- THSR WF (Tohsaki, Horiuchi, Schuck, Röpke, Funaki, Zhou,…)

$$\Phi_{THSR} = \mathscr{A}\left[\phi_\alpha(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3,\mathbf{r}_4)\phi_\alpha(\mathbf{r}_5,\mathbf{r}_6,\mathbf{r}_7,\mathbf{r}_8)\phi_\alpha(\mathbf{r}_{N-3},\ldots,\mathbf{r}_N)\right]$$

$$\phi_\alpha(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3,\mathbf{r}_4) = e^{-\mathbf{R}^2/B^2}\phi(\mathbf{r}_1-\mathbf{r}_2,\mathbf{r}_1-\mathbf{r}_3,\ldots)$$

$$\phi(\mathbf{r}_1-\mathbf{r}_2,\mathbf{r}_1-\mathbf{r}_3,\ldots) = \exp\left(-[\mathbf{r}_1-\mathbf{r}_2,\mathbf{r}_1-\mathbf{r}_3,\ldots]^2/b^2\right)$$

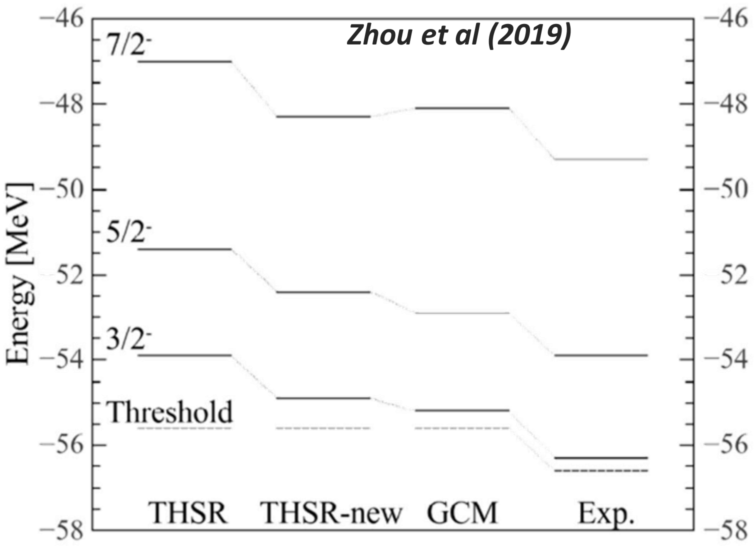


Fig. 49 Theoretical and experimental results of the energy spectrum of ^{9}B [131].

Table 2 Comparison of the binding energies E, r.m.s. radii of matter (R_{rms}), and monopole matrix elements ($M(0_2^+ \to 0_1^+)$) between calculated with the THSR wave function given by solving Hill-Wheeler equation, Eq. (20), calculated with the RGM/GCM wave function, and of the corresponding experimental data. $E^{\mathrm{th.}}_{3\alpha}$ is the calculated 3α threshold energy. Force 1 and 2 denote Volkov No.1 [42] and slightly modified Volkov No.2 forces, respectively [2].

		Force 1, ($E^{\mathrm{th.}}_{3\alpha} = -81.01$ MeV)		Force 2, ($E^{\mathrm{th.}}_{3\alpha} = -82.04$ MeV)		
		THSR (Hill-Wheeler)	GCM	THSR (Hill-Wheeler)	RGM	Exp.
E (MeV)	0_1^+	−87.81	−87.9	−89.52	−89.4	−92.2
	0_2^+	−79.97	−79.3	−81.79	−81.7	−84.6
R_{rms} (fm)	0_1^+	2.40	2.40	2.40	2.40	2.44
	0_2^+	4.44	3.40	3.83	3.47	
$M(0_2^+ \to 0_1^+)$ (fm^2)		5.36	6.6	6.45	6.7	5.4

Capture clustering in a microscopic framework

⦿ Cluster approximation : assume that A nucleons organize into N clusters
⇒Impose a specific form for the nucleus total wavefunction

⦿ Don't assume that A nucleons organize into N clusters but still impose some restrictions on the shape of the wavefunction : AMD/FMD

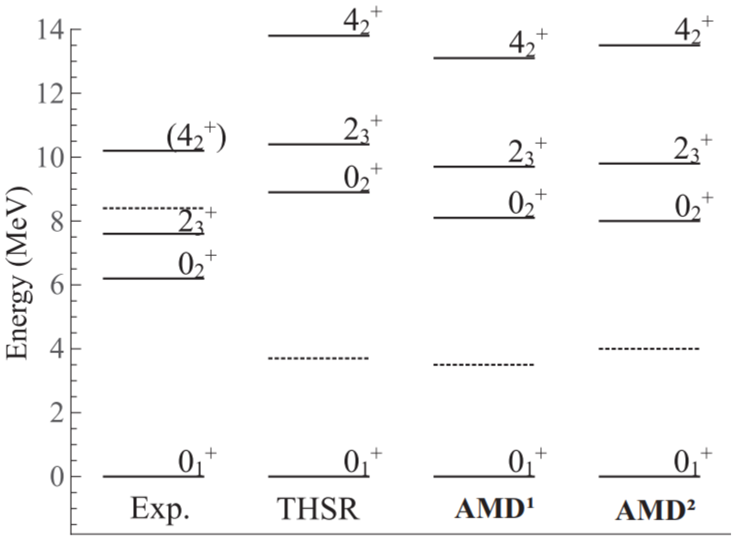
$$\Phi_{\mathrm{AMD}}(\mathbf{Z}) = \frac{1}{\sqrt{A!}}\mathscr{A}\{\varphi_1, \varphi_2, \ldots, \varphi_A\} \qquad \mathbf{Z} \equiv \{X_{ni}, \xi_i\}$$

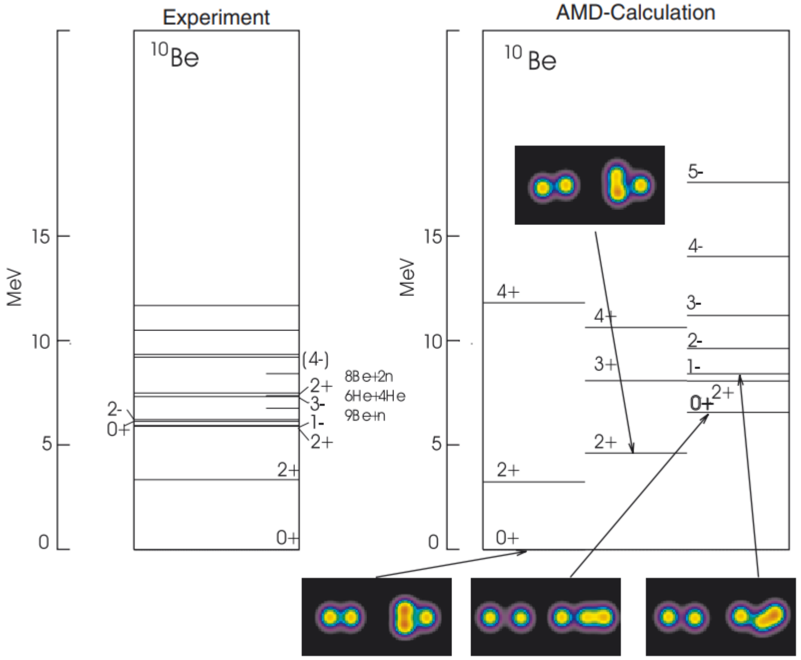
$$\varphi_i = \phi_{\mathbf{X}_i}\chi_i\tau_i,$$

$$\phi_{\mathbf{X}_i}(\mathbf{r}_j) \propto \exp\left\{-\nu\left(\mathbf{r}_j - \frac{\mathbf{X}_i}{\sqrt{\nu}}\right)^2\right\},$$

$$\chi_i = \left(\frac{1}{2} + \xi_i\right)\chi_\uparrow + \left(\frac{1}{2} - \xi_i\right)\chi_\downarrow,$$

$$\Phi = P^{J\pm}_{MK'}\Phi_{\mathrm{AMD}}(\mathbf{Z})$$





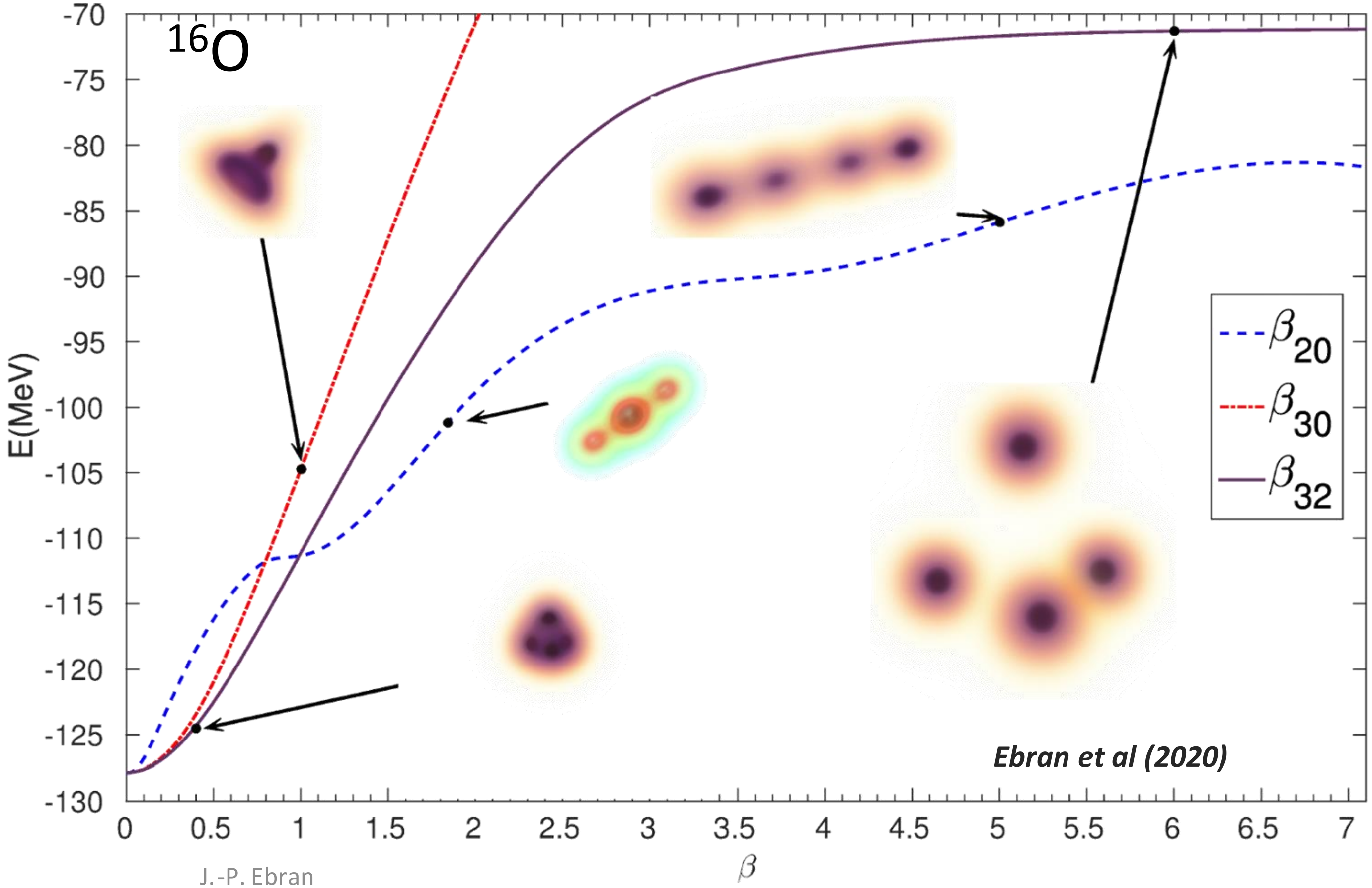
Kanada-En'yo (2006)

Capture clustering in a microscopic framework

⦿ Cluster approximation : assume that A nucleons organize into N clusters
⇒Impose a specific form for the nucleus total wavefunction

⦿ Don't assume that A nucleons organize into N clusters but still impose some restrictions on the shape of the wavefunction : AMD/FMD

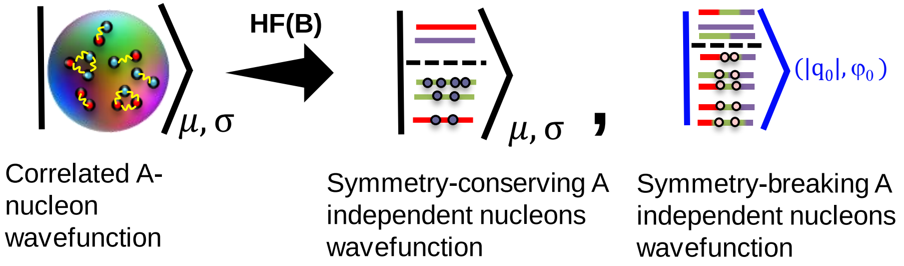
⦿ Don't assume that A nucleons organize into N clusters and use horizontal expansion (look for a bosonic order parameter whose fluctuations cause nucleons to aggregate into clusters) : can be done in both ab initio and EDF



Horizontal expansion

◉ HFB treatment

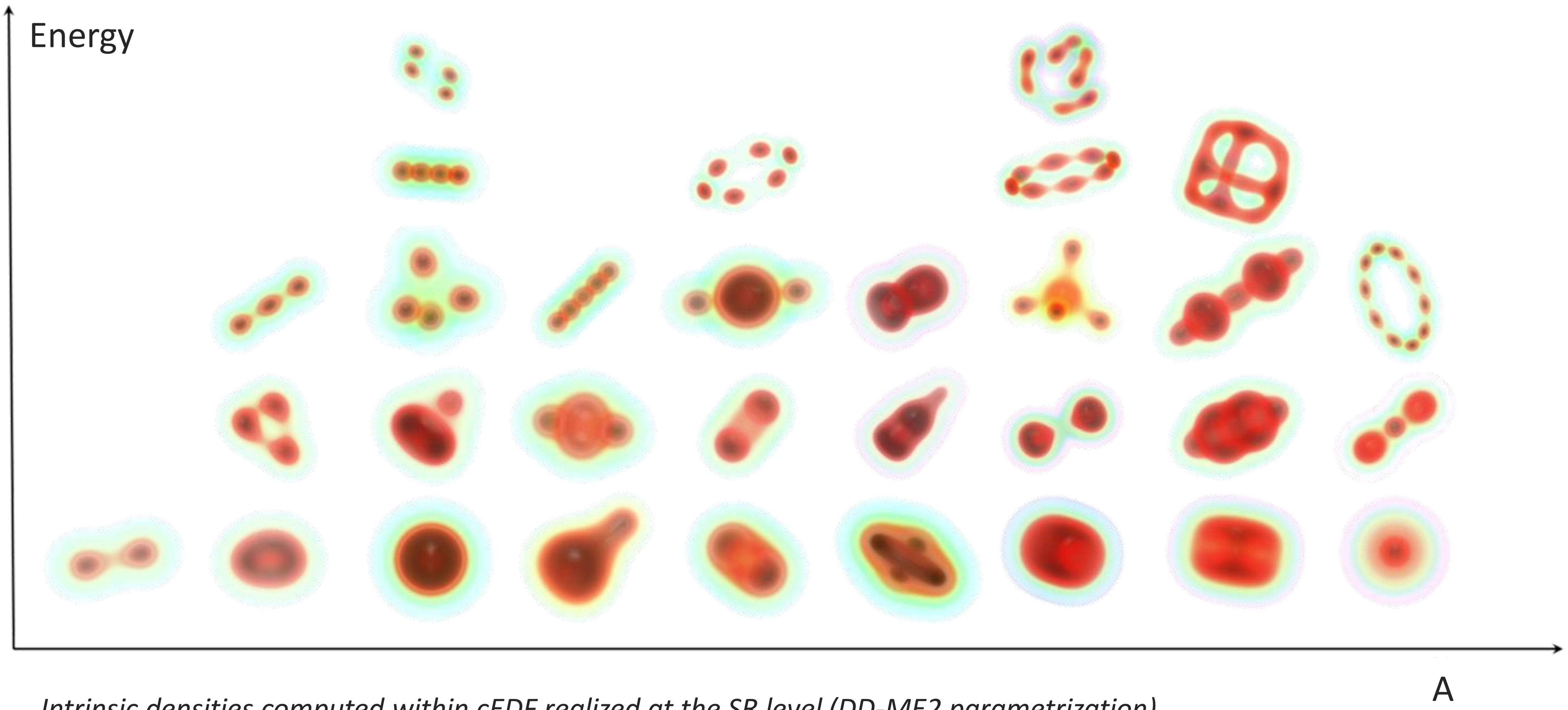
⇢ A-nucleon problem ⟶ A 1-nucleon problems



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

Nuclear clustering at the SR level

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

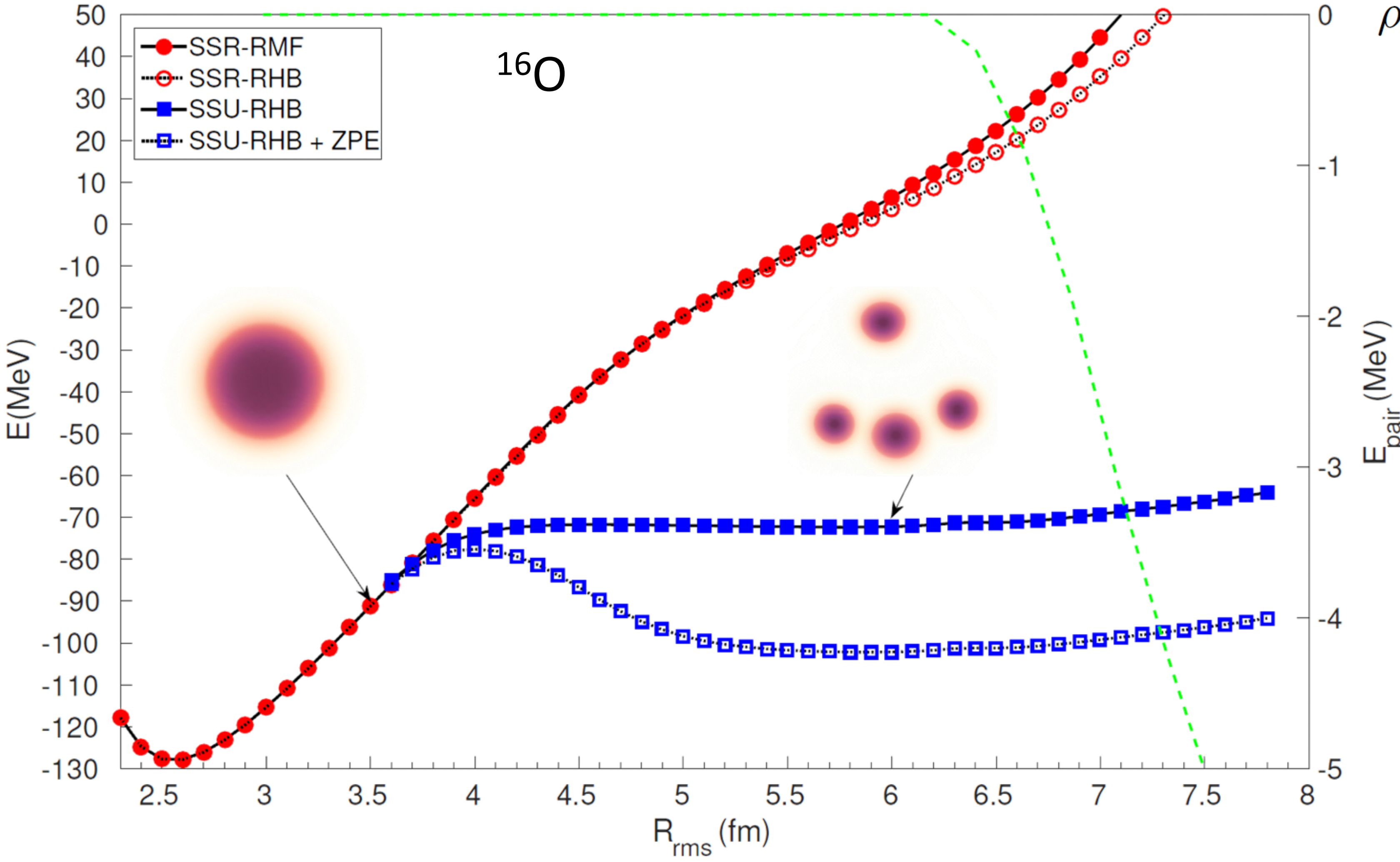


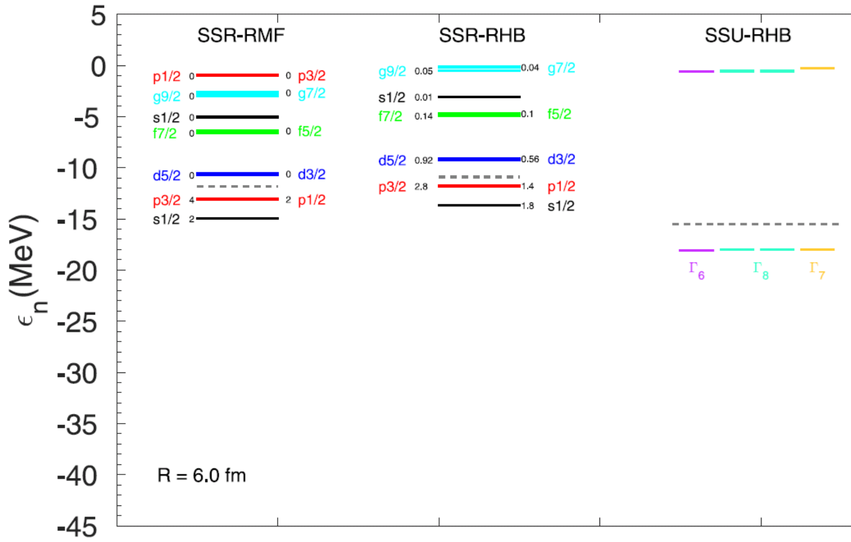
Intrinsic densities computed within cEDF realized at the SR level (DD-ME2 parametrization)

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

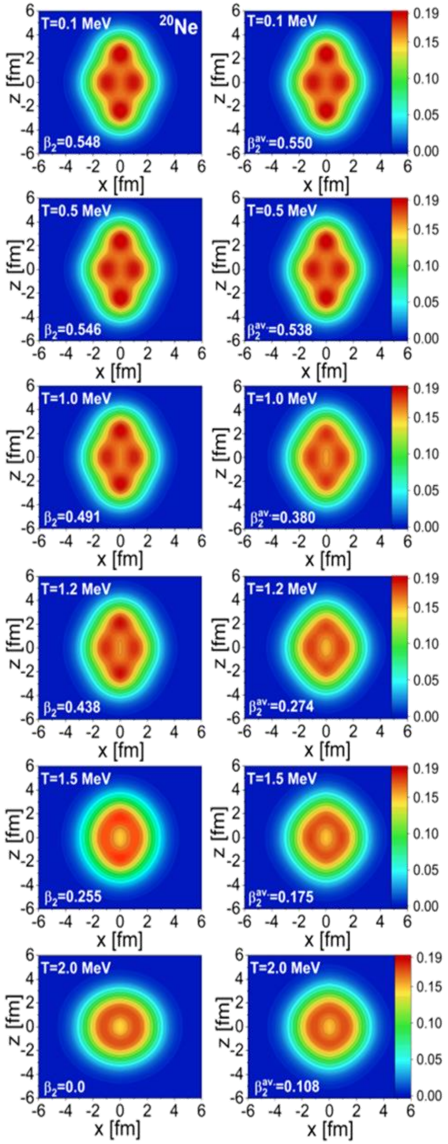
$$\rho_{\mathrm{Mott}}/\rho_0 = (R_{\mathrm{eq}}/R_c)^3 \approx \rho_0/3$$



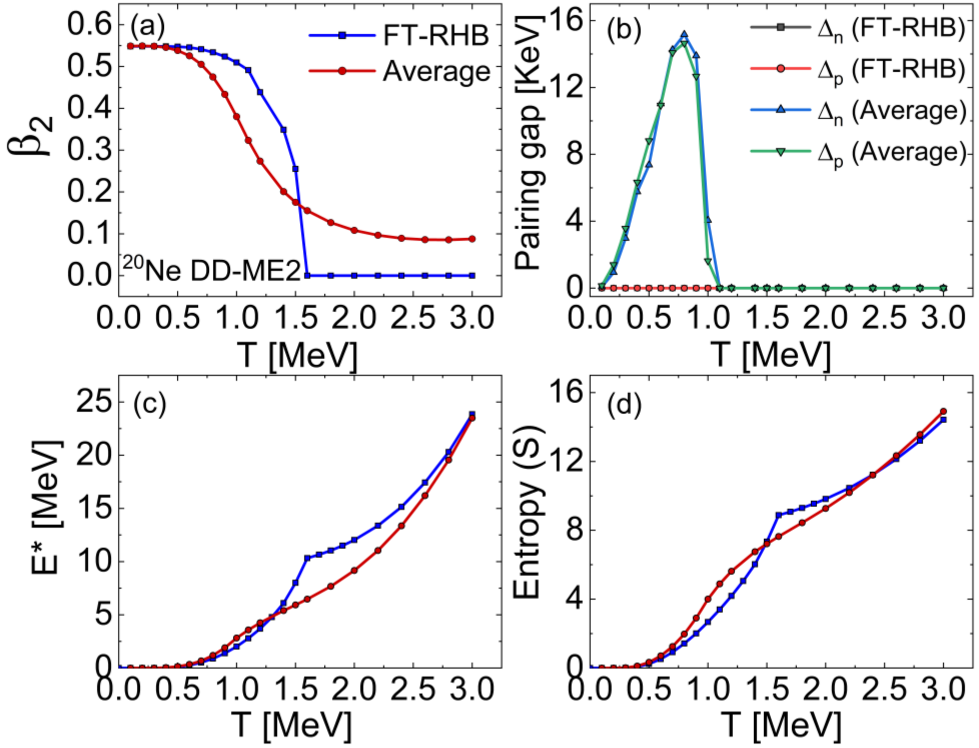


Thermal phase transition

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



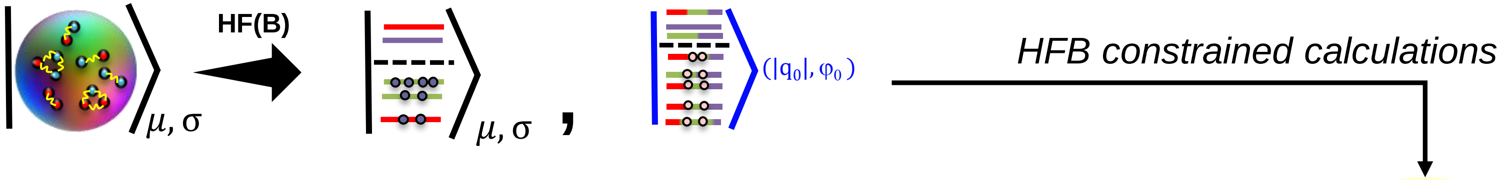
$$\overline{O} = \frac{\int d\beta_2 O(\beta_2, T) \exp(-\Delta F(\beta_2, T)/T)}{\int d\beta_2 \exp(-\Delta F(\beta_2, T)/T)}.$$



Horizontal expansion

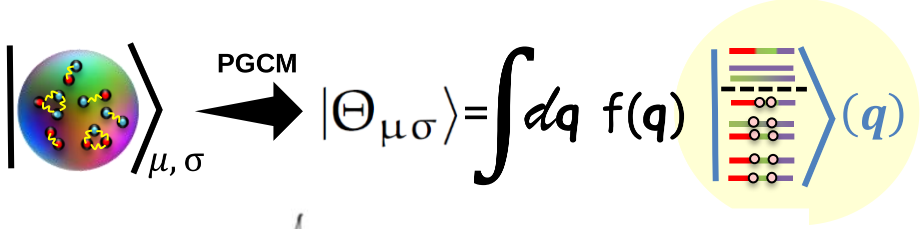
◉ HFB treatment

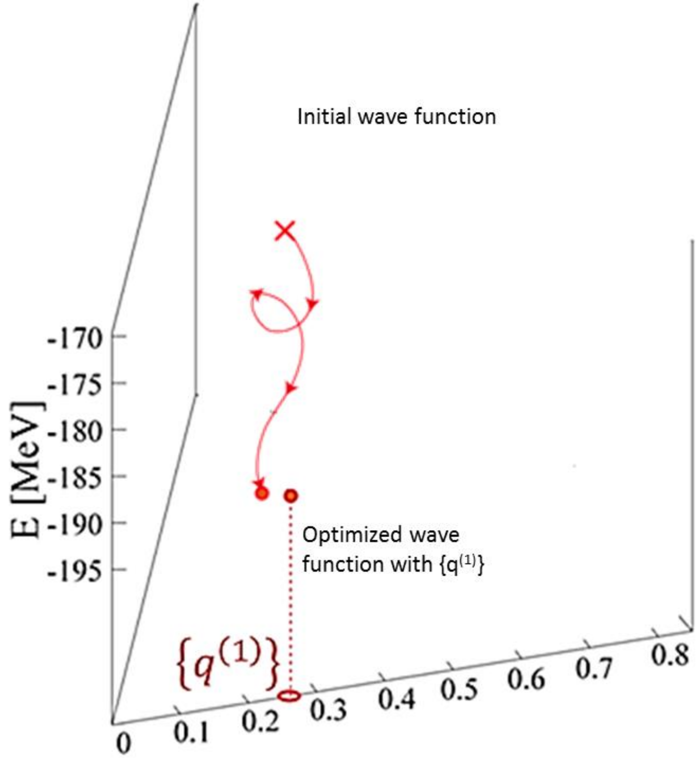
⇢ *A*-nucleon problem ⟶ *A* 1-nucleon problems



◉ Post-HFB treatment : PGCM

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





Horizontal expansion

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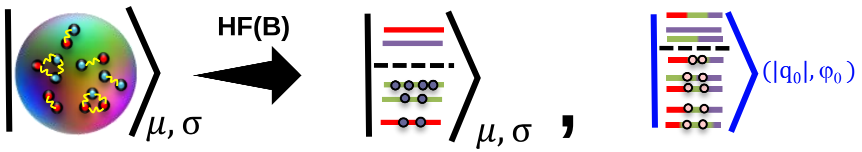

HFB constrained calculations

◉ Post-HFB treatment : PGCM

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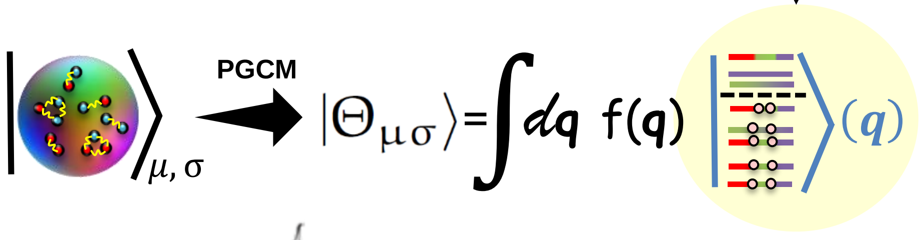

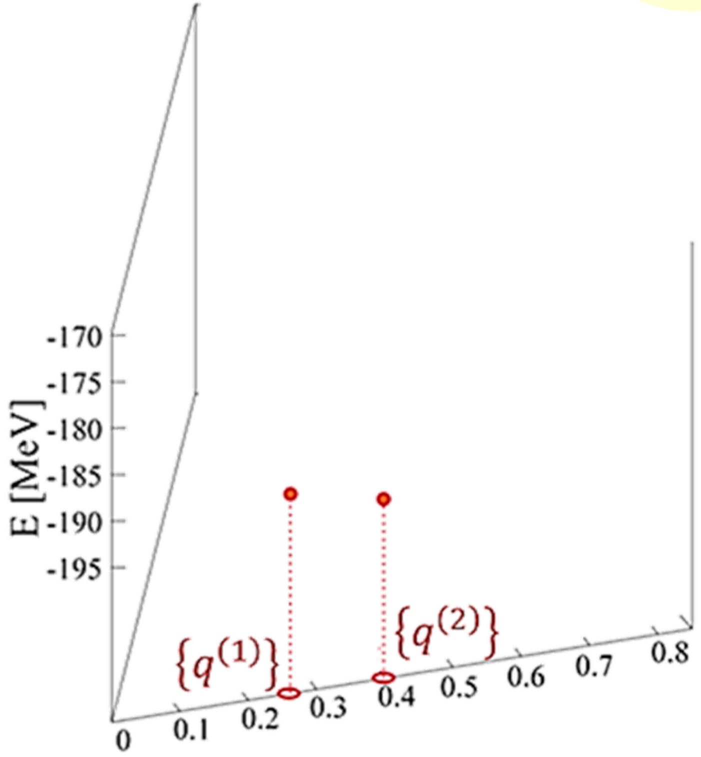

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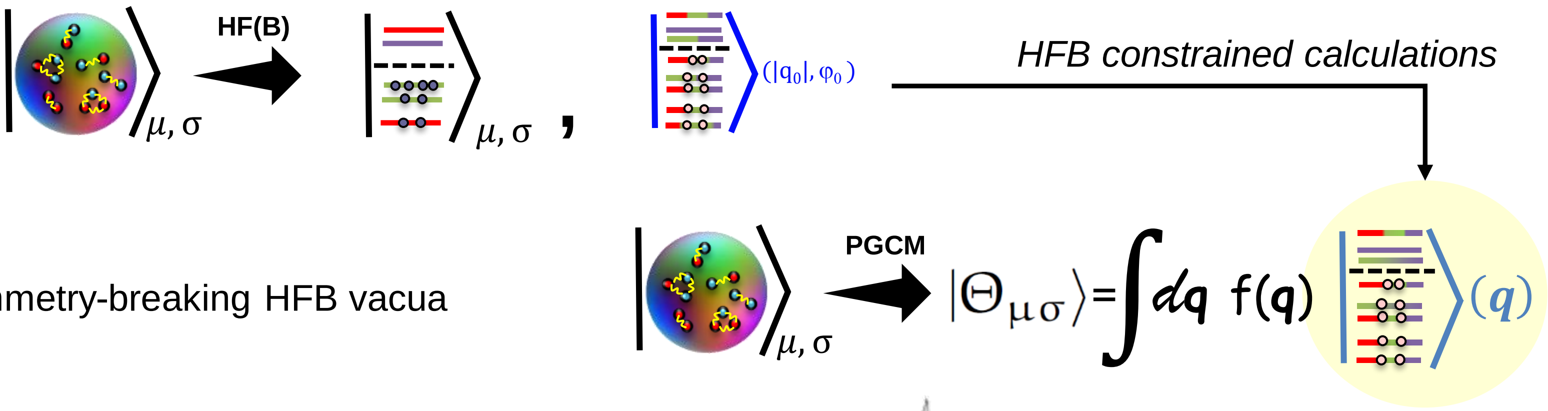

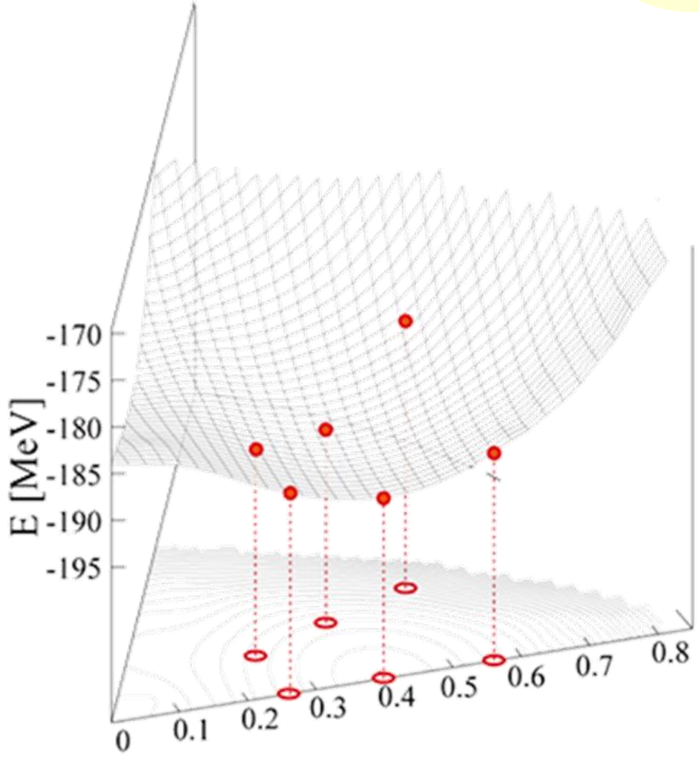

Horizontal expansion

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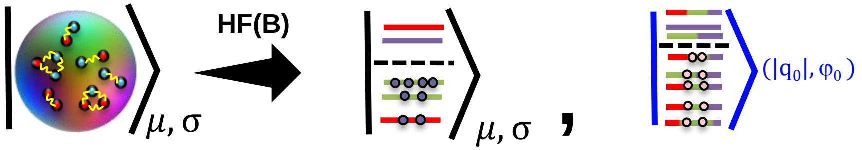

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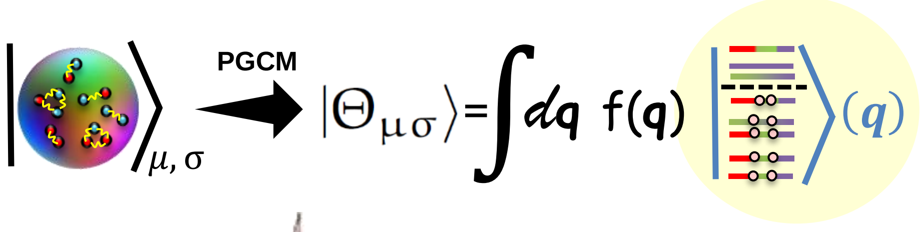

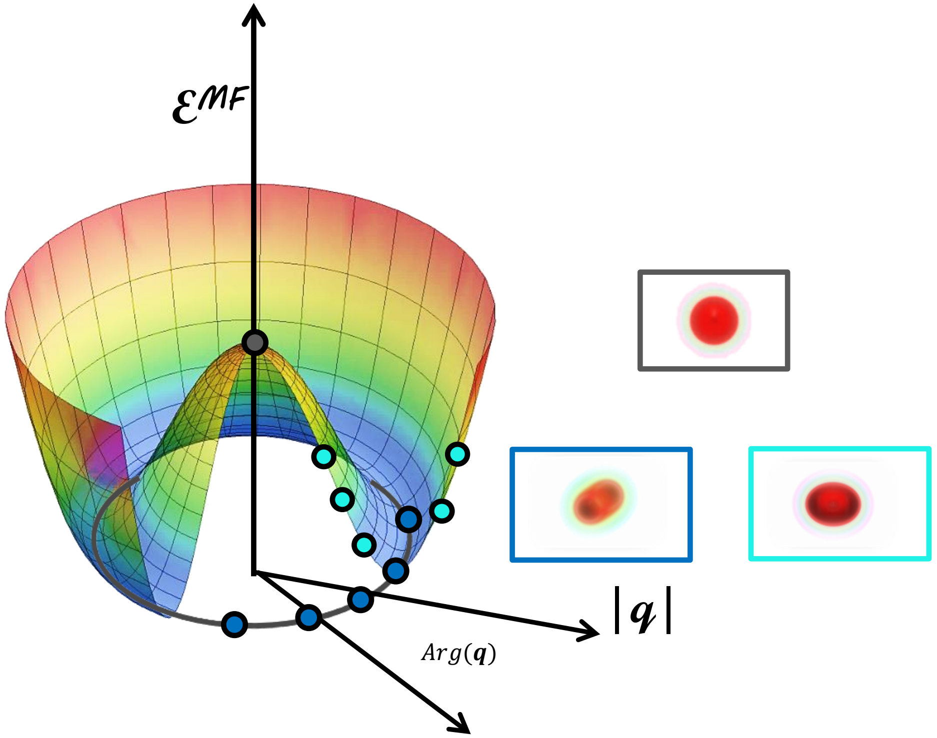

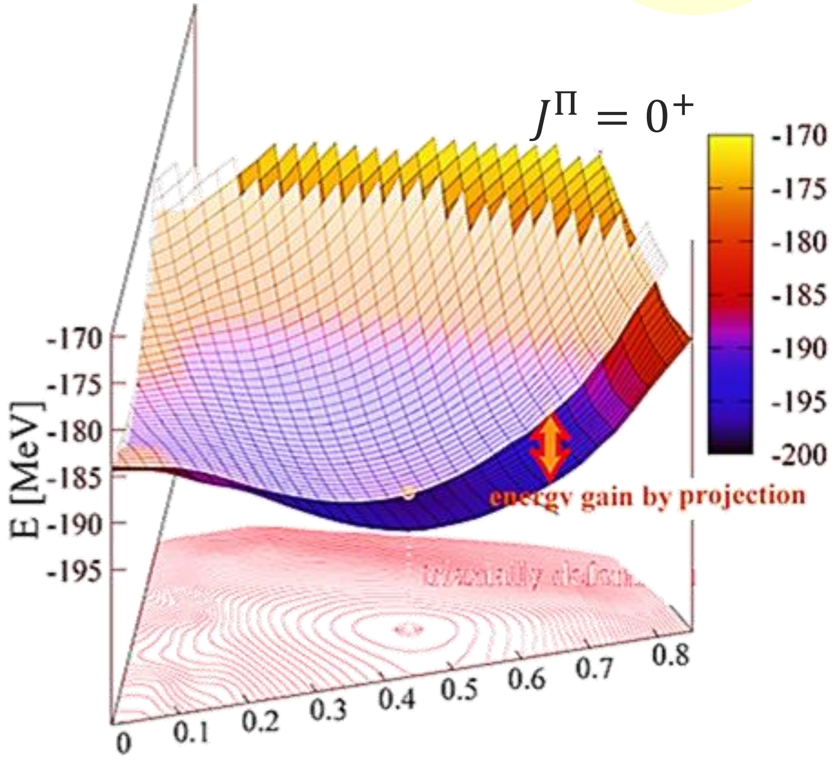

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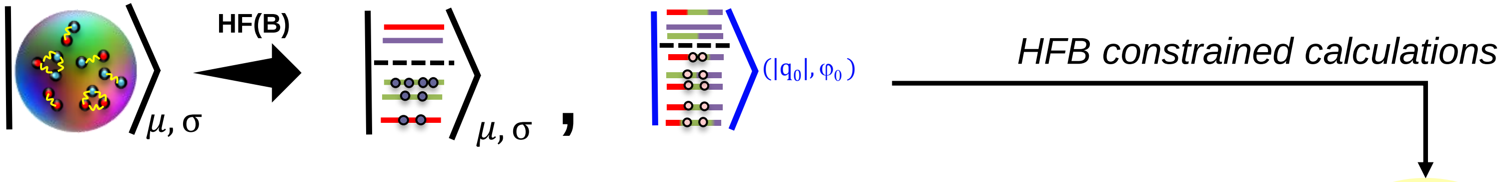

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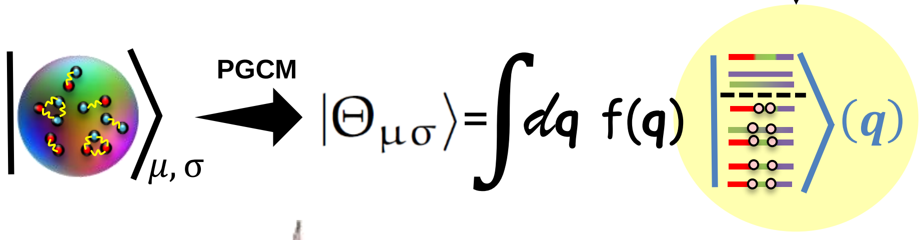
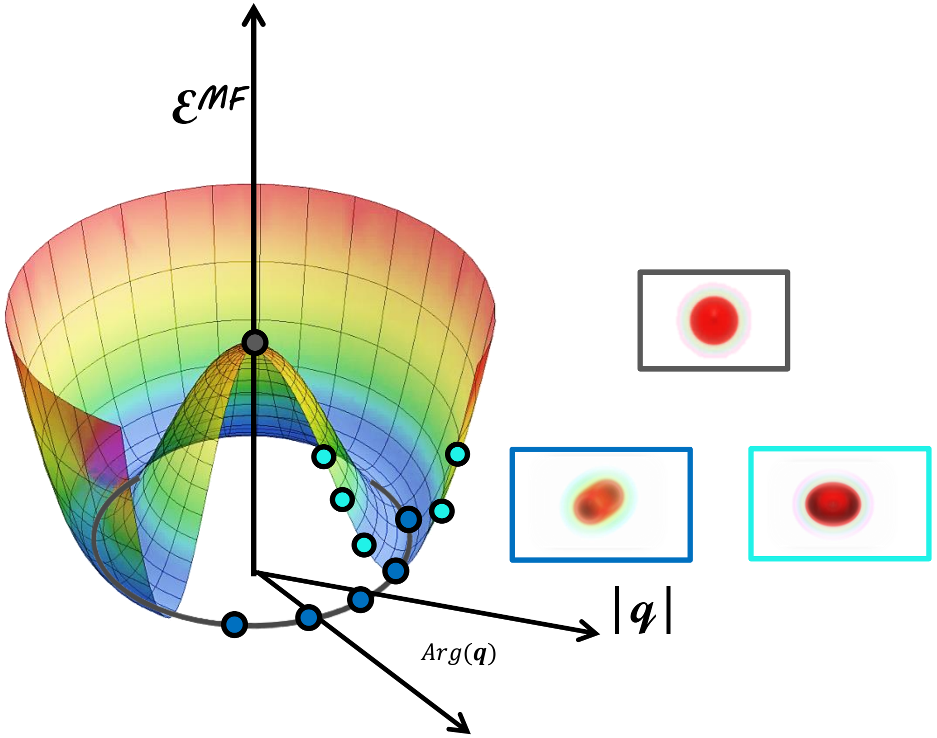
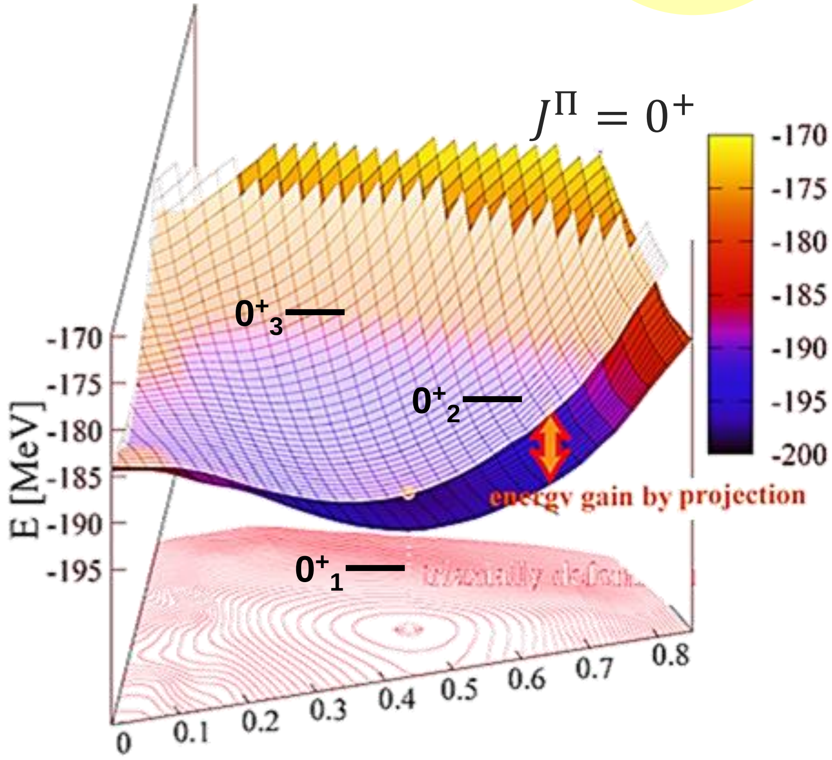


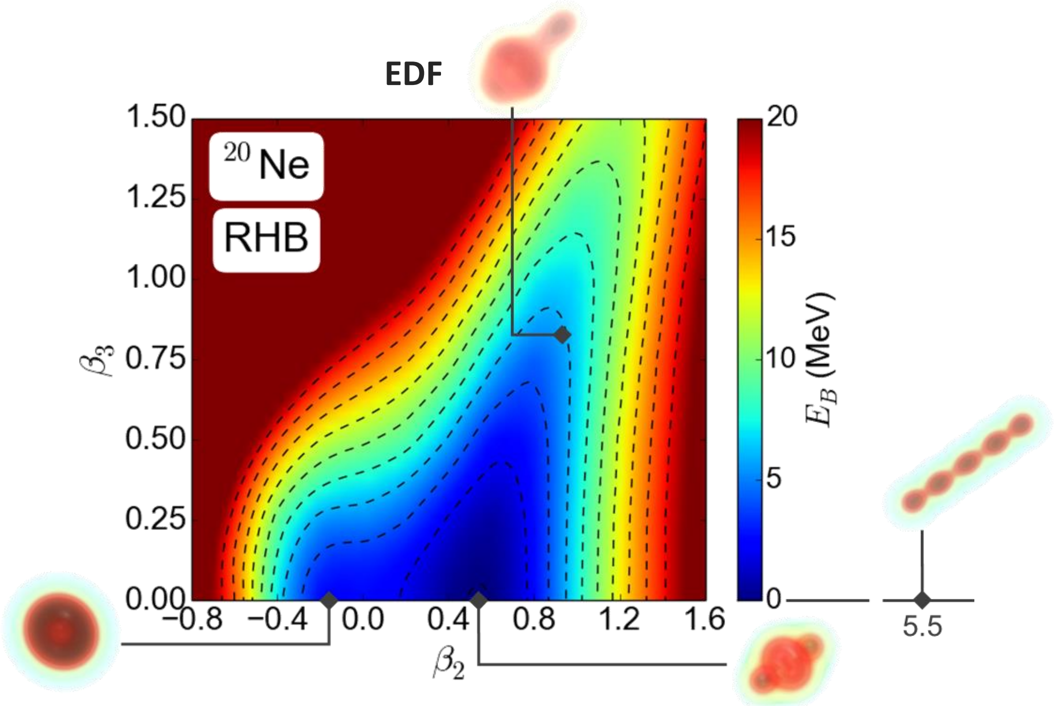




Nuclear clustering & PGCM

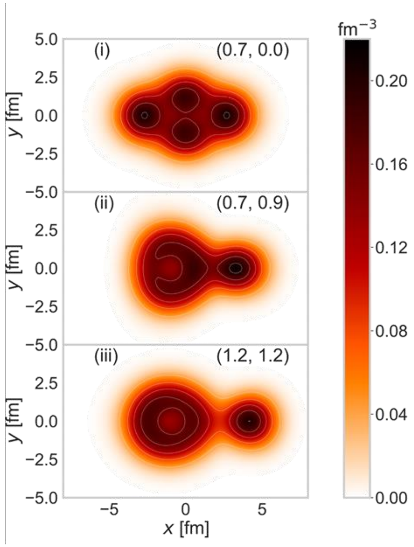
◉ Correlated GS

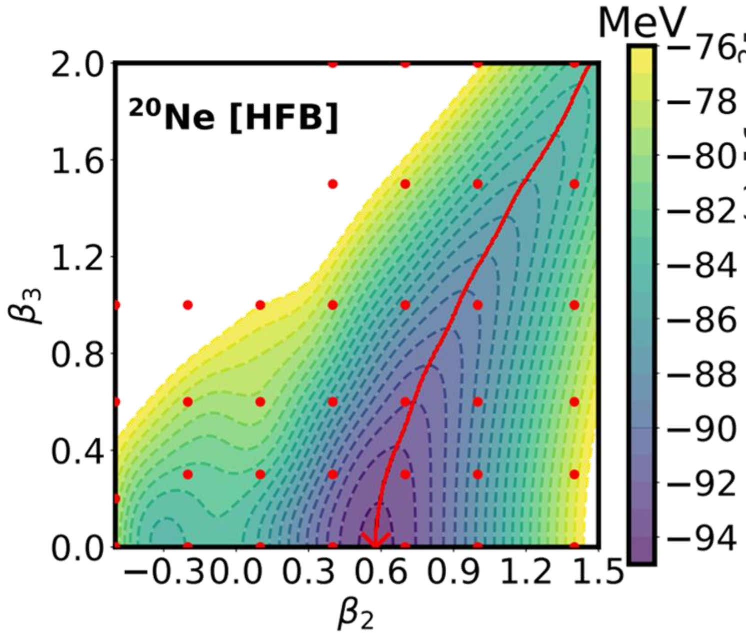
EDF

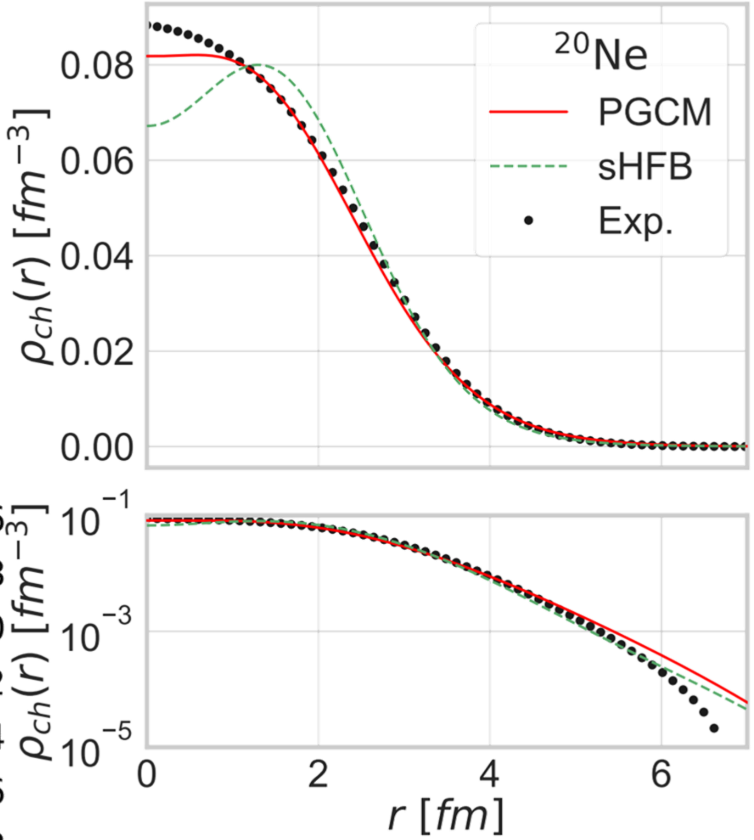


Marevic, Ebran, Khan, Niksic, Vretenar, PRC 97 (2018)

Ab initio



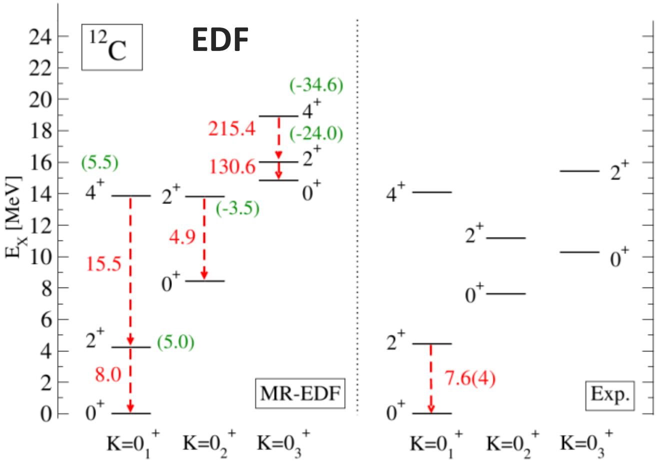




Frosini, Duguet, Ebran, Bally, Mongelli, Rodriguez, Roth, Somà, EPJA 2022

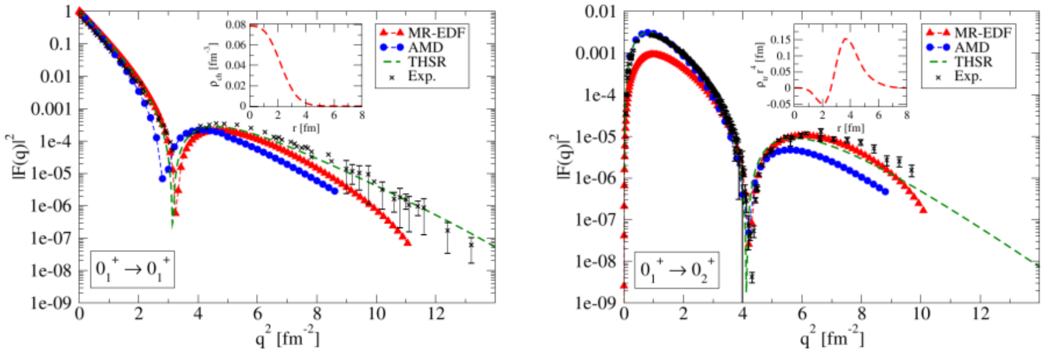
Nuclear clustering & PGCM

◉ Spectroscopy

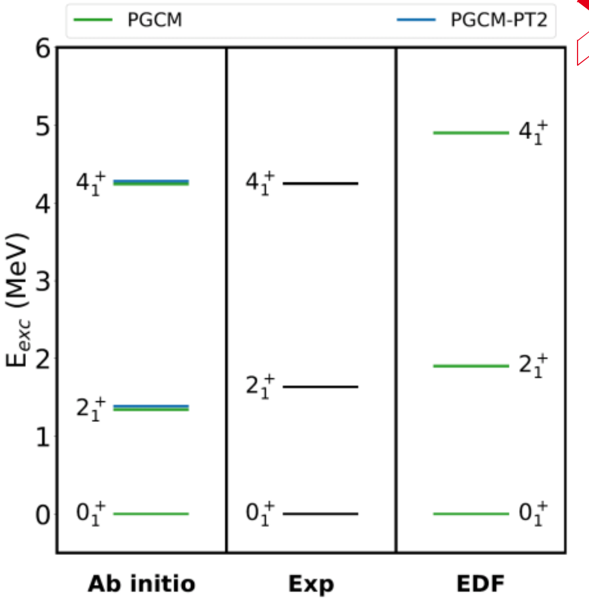


Marević, Ebran, Khan, Nikšić, and Vretenar, 2019

EDF



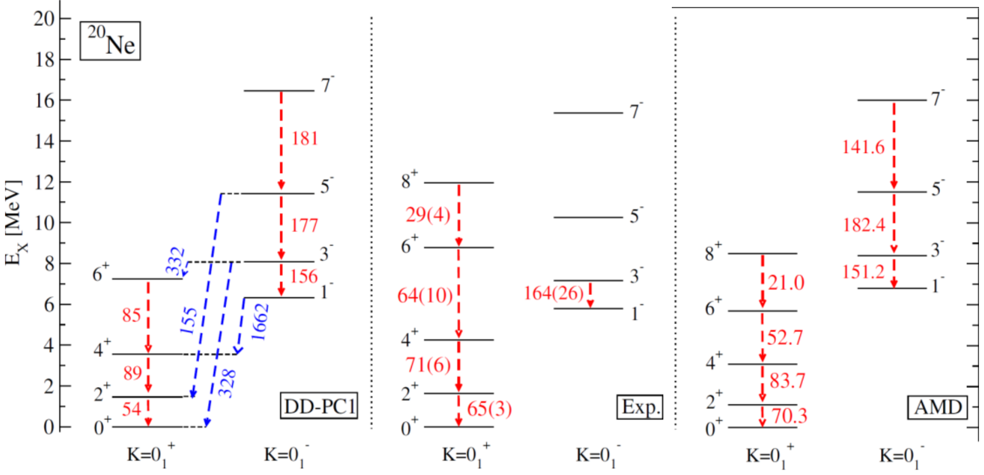
Ab initio



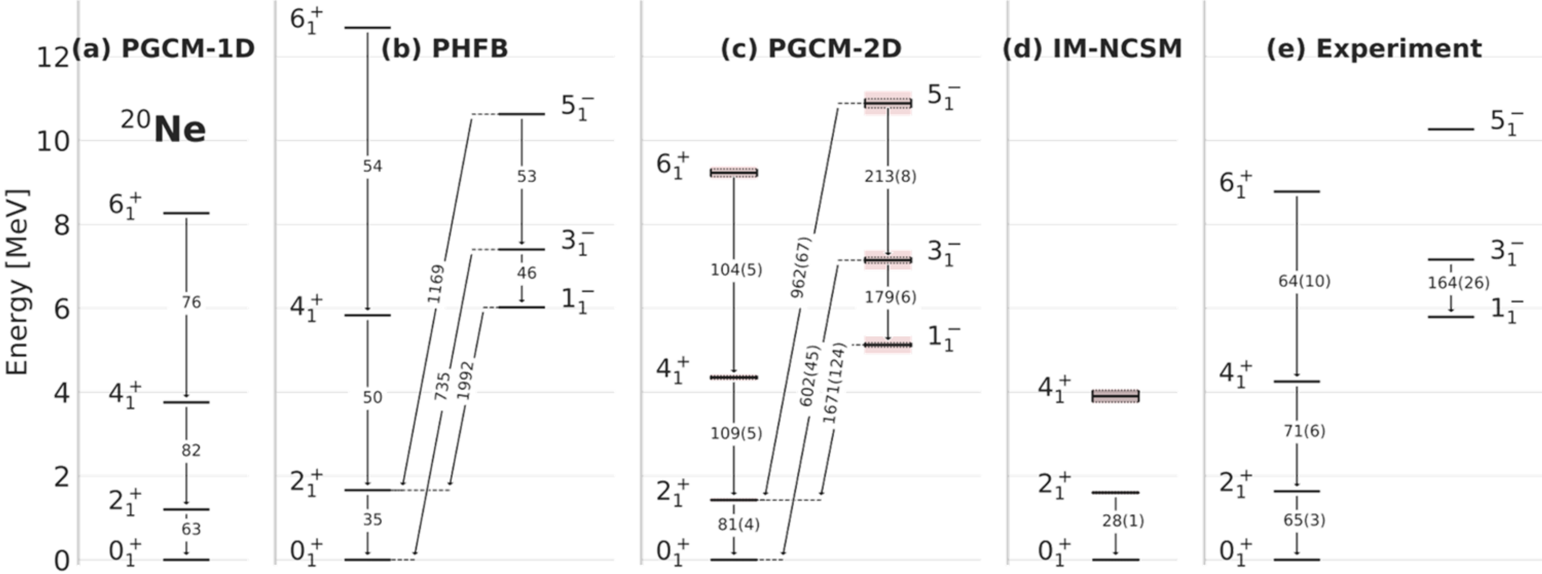
Frosini, Duguet, Ebran, Bally, Hergert, Rodriguez, Roth, Yao, Somà, EPJA 2022

EDF

Marevic, Ebran, Khan, Niksic, Vretenar, 2018



Ab initio



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

Horizontal expansion

◉ HFB treatment

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

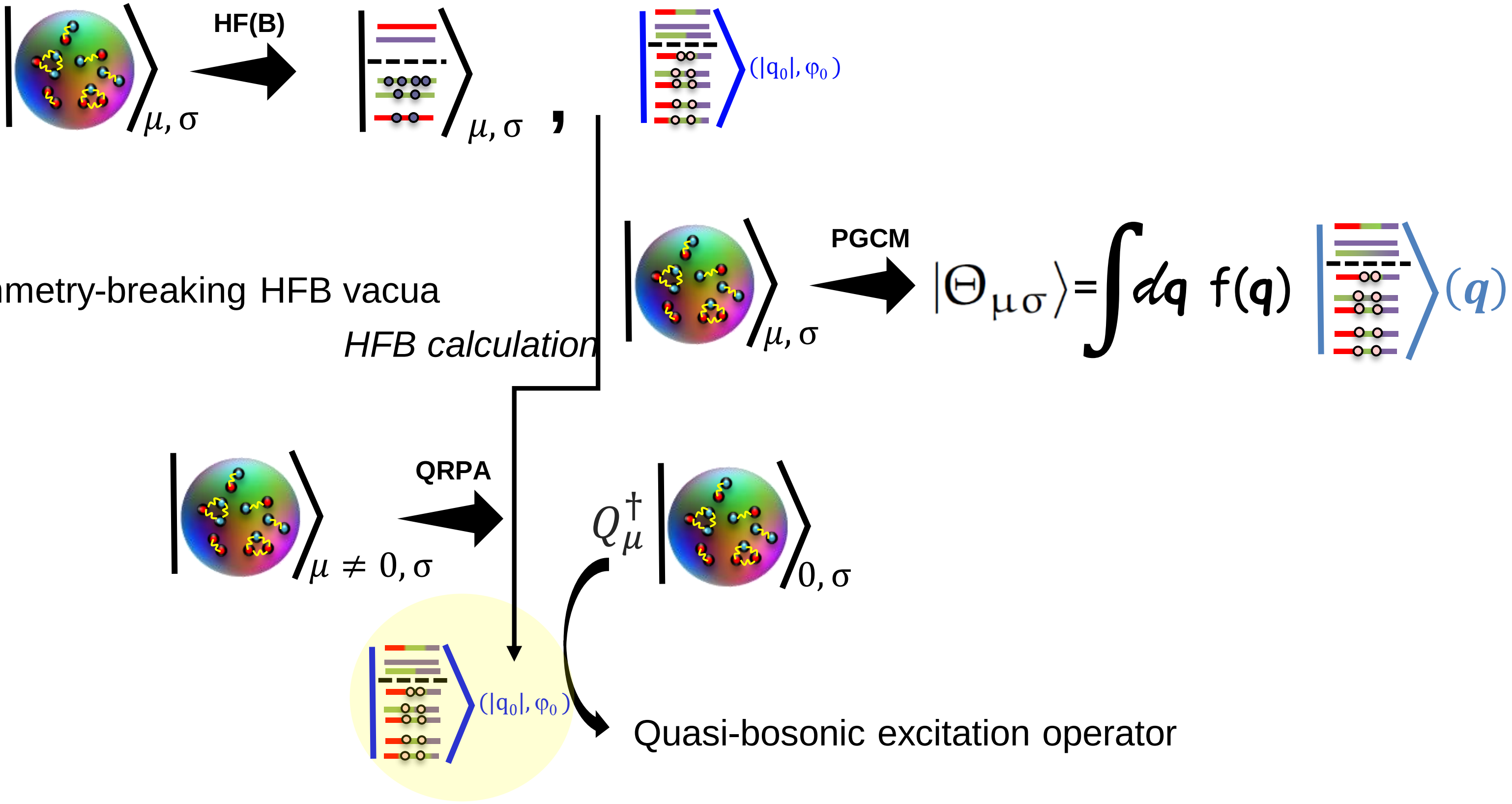
◉ Post-HFB treatment : PGCM

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

◉ Post-HFB : QRPA

⇢ Excitations = coherent mixture of 2-qp excitations

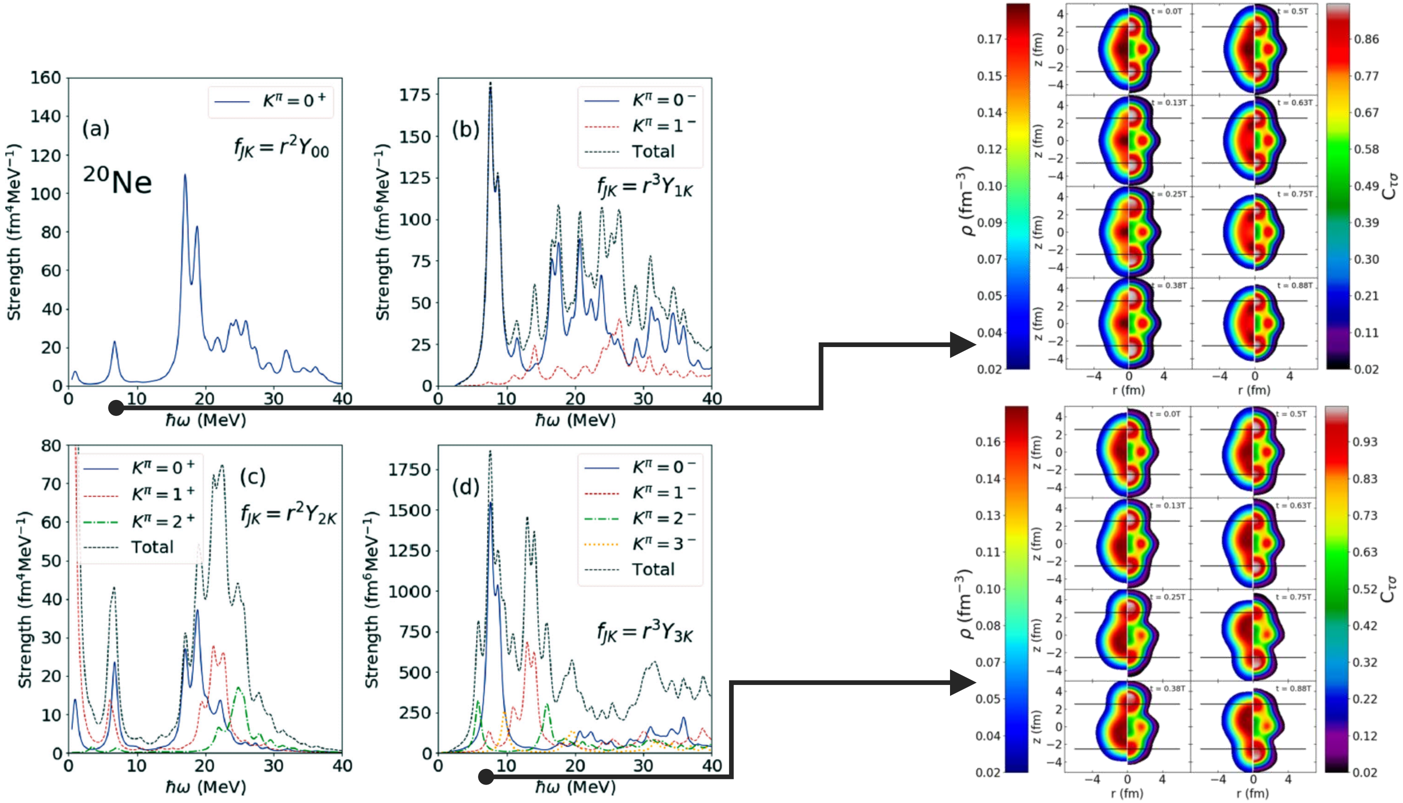
⇢ Harmonic limit of the GCM



Nuclear clustering & QRPA

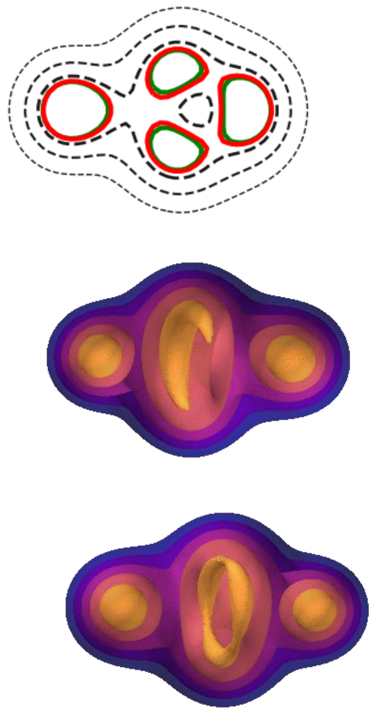
◉ Cluster vibration

EDF



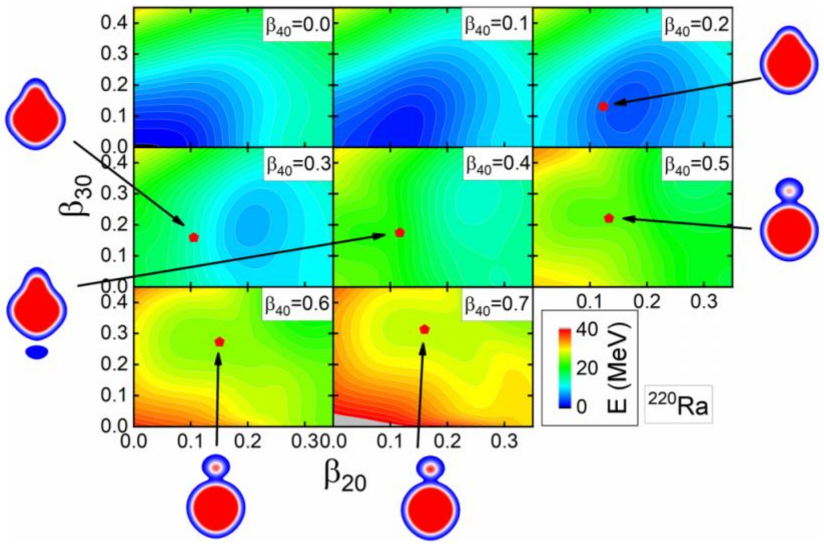
Mercier, Bjelčić, Nikšić, Ebran, Khan,Vretenar 2021
Mercier, Ebran, Khan 2022

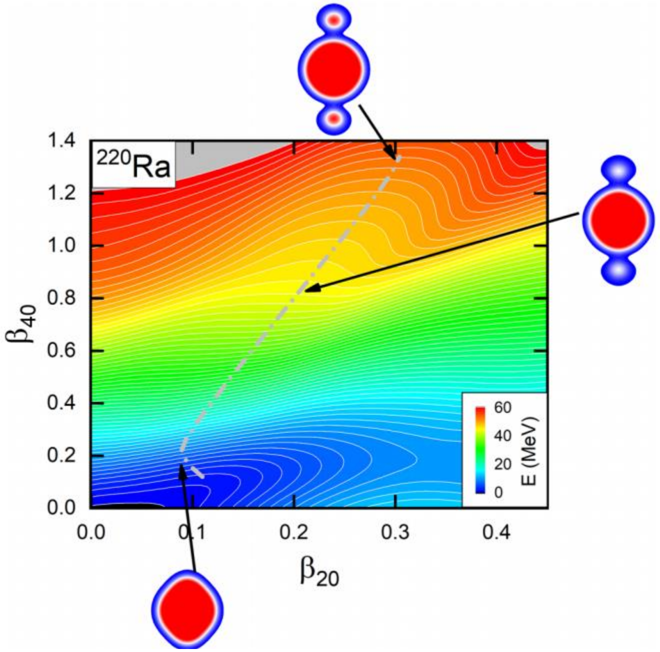
Ab initio

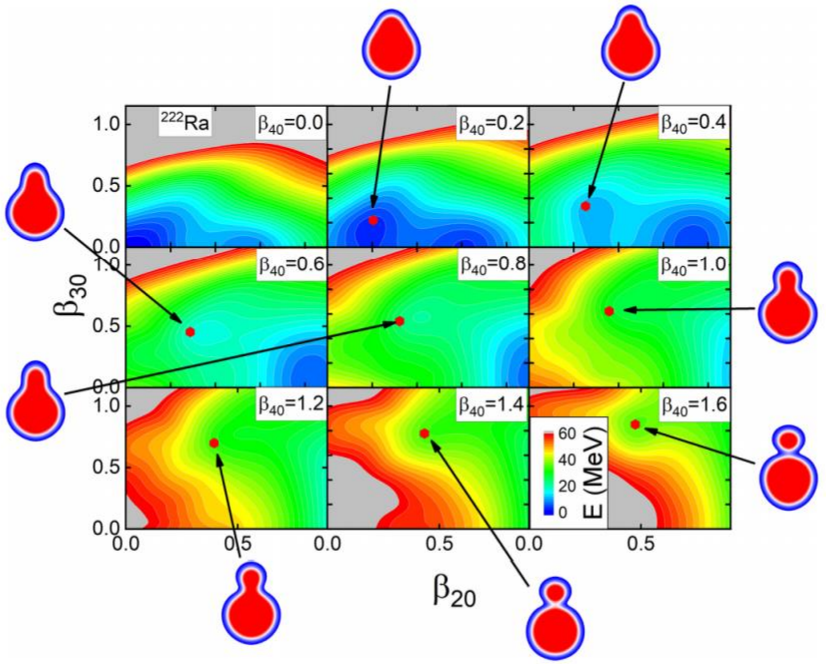


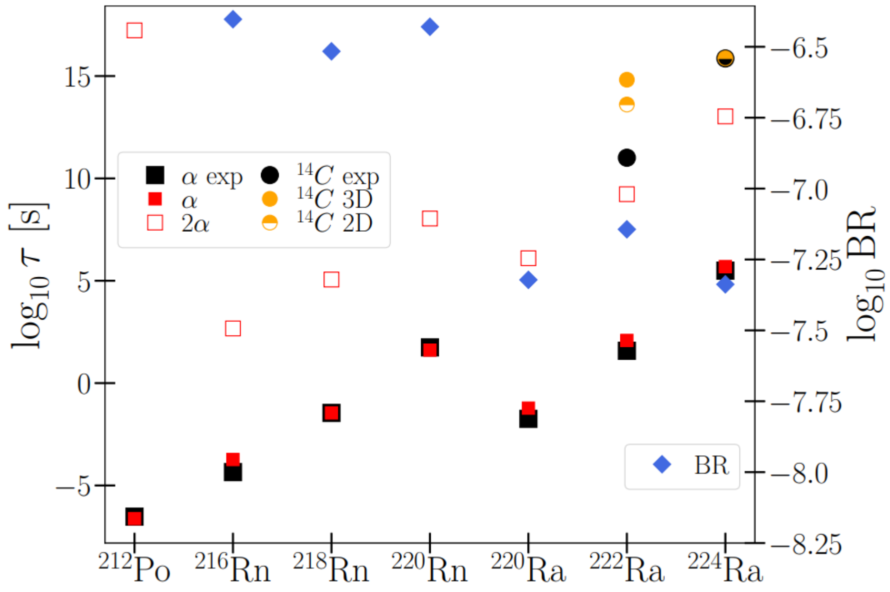
Ab initio QFAM time-dependent intrinsic density
Frosini, Ebran, Duguet, Somà, unpublished

Cluster, α and 2α radioactivities









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

Capture clustering in a microscopic framework

◉ Cluster approximation : assume that A nucleons organize into N clusters
⇒Impose a specific form for the nucleus total wavefunction

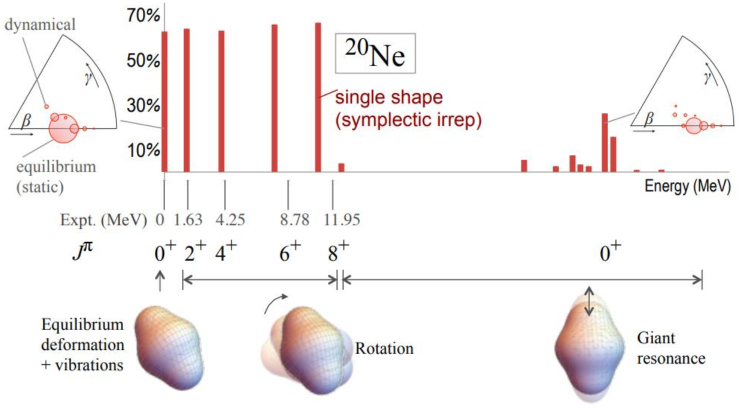
◉ Don't assume that A nucleons organize into N clusters but still impose some restrictions on the shape of the wavefunction : AMD/FMD

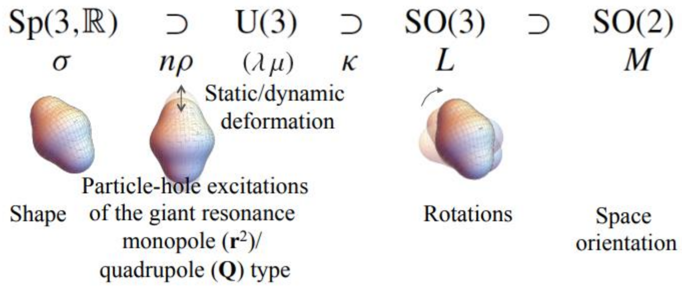
◉ Don't assume that A nucleons organize into N clusters and use horizontal expansion (look for a bosonic order parameter whose fluctuations cause nucleons to aggregate into clusters) : can be done in both ab initio and EDF

◉ Don't assume that A nucleons organize into N clusters and use vertical expansion

Symmetry-adapted NCSM

⦿ Exploits approximate symmetry of the collective nuclear many-body dynamics to reorganize the model space into a physically relevant basis
⇒ Tames down the scaling explosion problem of NCSM





K. D. Launey et al (2018)

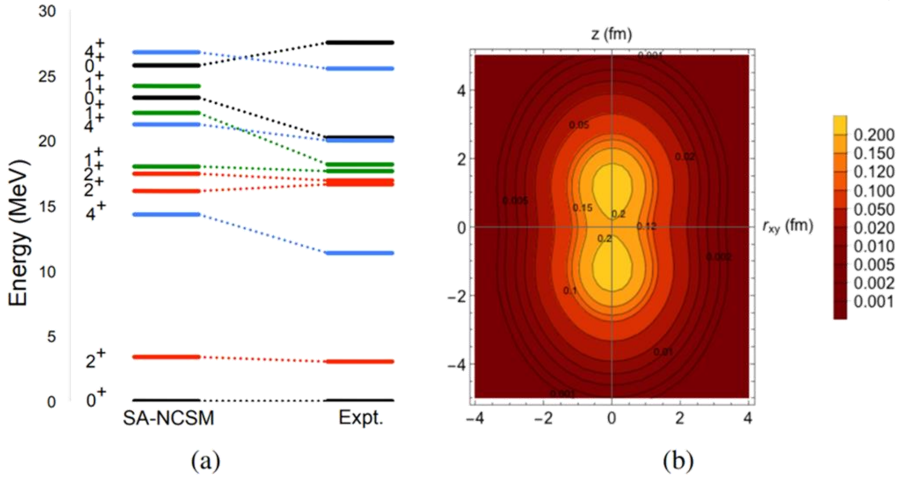


FIGURE 2. (a) Energy spectrum of ^{8}Be, calculated in the *ab initio* SA-NCSM and compared to experiment. (b) The corresponding one-body density profile (in the body-fixed frame) of the ^{8}Be ground state (*gs*) clearly reveals two alpha clusters. SA-NCSM calculations are performed using the realistic JISP16 *NN* [25] in a model space of 14 HO major shells ($\hbar\Omega$ = 20 MeV).

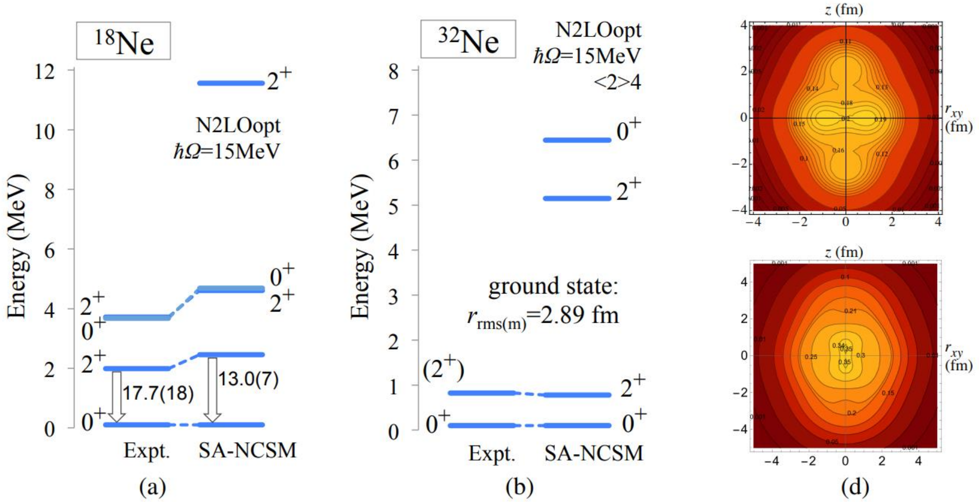


FIGURE 3. *Ab initio* SA-NCSM calculations using the chiral NNLO$_{opt}$ *NN* [26] in ultra-large model spaces ($\hbar\Omega$ = 15 MeV). Energy spectrum of (a) ^{18}Ne in 9 HO major shells, along with the $B(E2; 2^+ \rightarrow 0^+)$ strength in W.u. reported for 33 shells, and (b) ^{32}Ne in 7 shells. (c) Density profile of the *gs* of ^{20}Ne (top) and ^{48}Ti (bottom). Simulations are performed on the Blue Waters system.

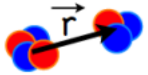
NCSMC

⦿ Exploits approximate symmetry of the collective nuclear many-body dynamics to reorganize the model space into a physically relevant basis
⇒ Tames down the scaling explosion problem of NCSM

NCSM

$$\left|\Psi_A^{J^\pi T}\right\rangle = \sum_{Ni} c_{Ni} \left|ANiJ^\pi T\right\rangle$$

NCSM/RGM



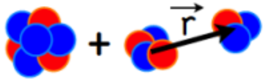
$$|\Psi_A^{J^\pi T}\rangle = \sum_\nu \int d\vec{r}\, \chi_\nu(\vec{r}) \hat{A}\Phi_{\nu\vec{r}}^{J^\pi T(A-a,a)}$$

$$\mathcal{H}\chi = E\mathcal{N}\chi$$

$$\bar{\chi} = \mathcal{N}^{+\frac{1}{2}}\chi$$

$$(\mathcal{N}^{-\frac{1}{2}}\mathcal{H}\mathcal{N}^{-\frac{1}{2}})\bar{\chi} = E\bar{\chi}$$

NCSMC

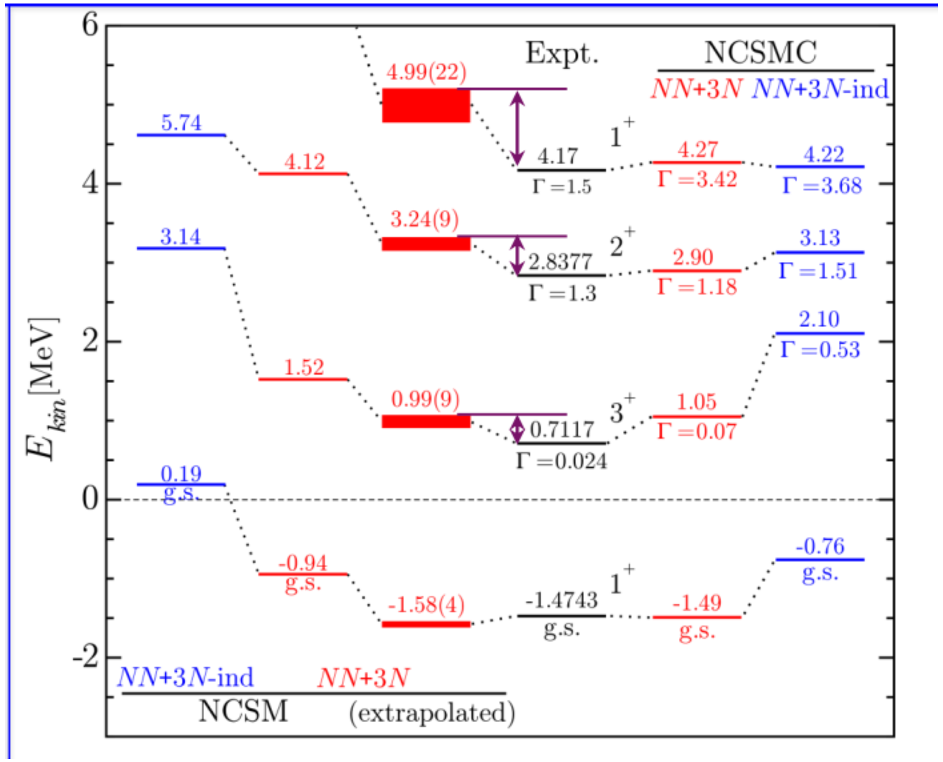


S. Baroni, P. N., and S. Quaglioni,
PRL **110**, 022505 (2013); PRC **87**, 034326 (2013).

$$|\Psi_A^{J^\pi T}\rangle = \sum_\lambda c_\lambda |A\lambda J^\pi T\rangle + \sum_\nu \int d\vec{r} \left(\sum_{\nu'} \int d\vec{r}\,' \mathcal{N}_{\nu\nu'}^{-\frac{1}{2}}(\vec{r},\vec{r}\,')\bar{\chi}_{\nu'}(\vec{r}\,') \right) \hat{A}\Phi_{\nu\vec{r}}^{J^\pi T(A-a,a)}$$

$$\begin{pmatrix} H_{NCSM} & \bar{h} \\ \bar{h} & \mathcal{N}^{-\frac{1}{2}}\mathcal{H}\mathcal{N}^{-\frac{1}{2}} \end{pmatrix} \begin{pmatrix} c \\ \bar{\chi} \end{pmatrix} = E \begin{pmatrix} 1 & \bar{g} \\ \bar{g} & 1 \end{pmatrix} \begin{pmatrix} c \\ \bar{\chi} \end{pmatrix}$$

Hupin et al (2015)



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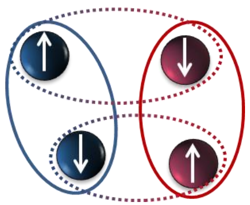
◉ Don't assume that A nucleons organize into N clusters and use vertical expansion

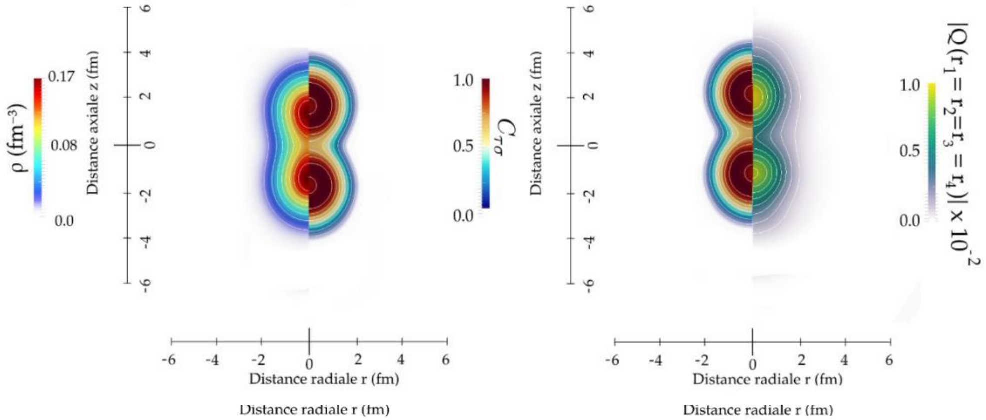
◉ Don't assume that A nucleons organize into N clusters and consider in-medium C-body wavefunctions : QCM, Green's function theory, …

QMC

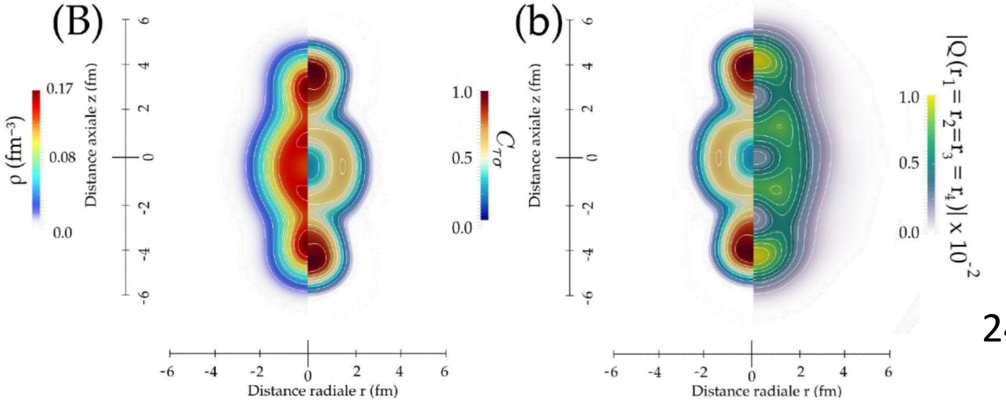


$$|\Psi\rangle = \left(\mathcal{Q}^\dagger\right)^{n_q}|0\rangle \qquad \mathcal{Q}^\dagger = 2\Gamma_1^\dagger\Gamma_{-1}^\dagger - \left(\Gamma_0^\dagger\right)^2 \qquad \Gamma_t^\dagger = \sum_k x_k P_{k,t}^\dagger$$

Lasseri, Ebran, Khan, Sandulescu

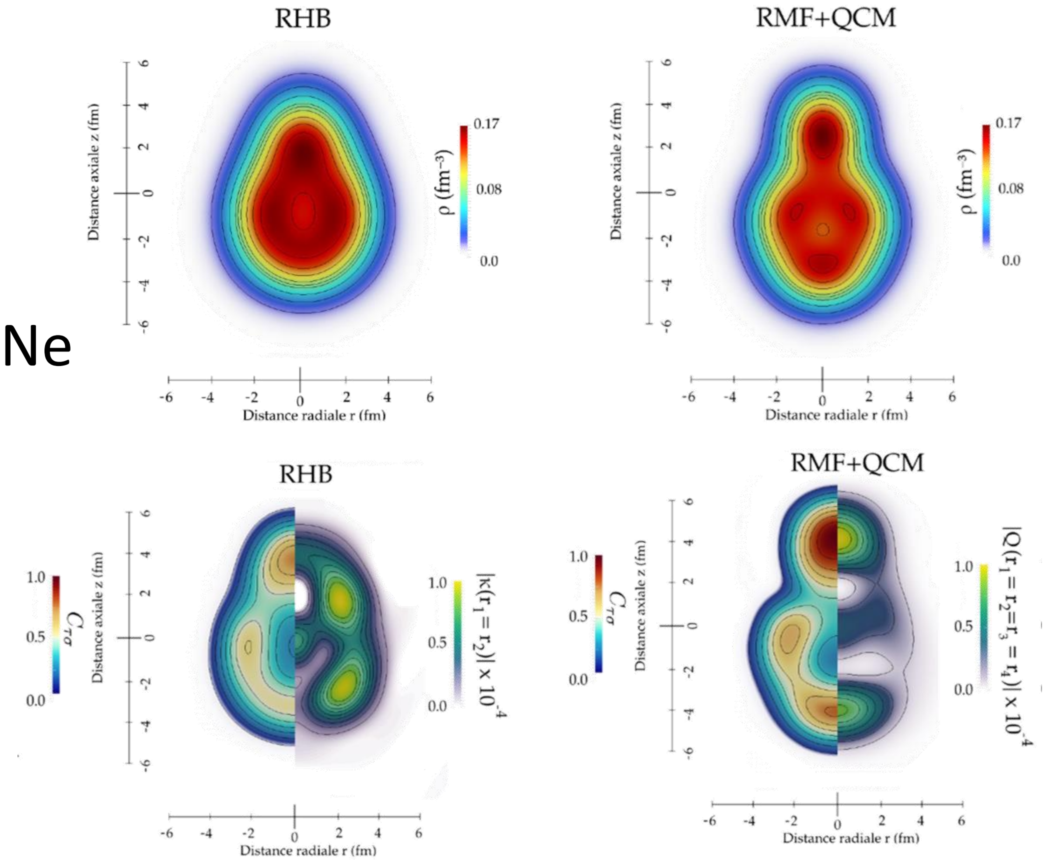


^{8}Be

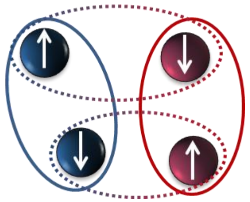


^{24}Mg

^{20}Ne



Quartet BCS-like theory

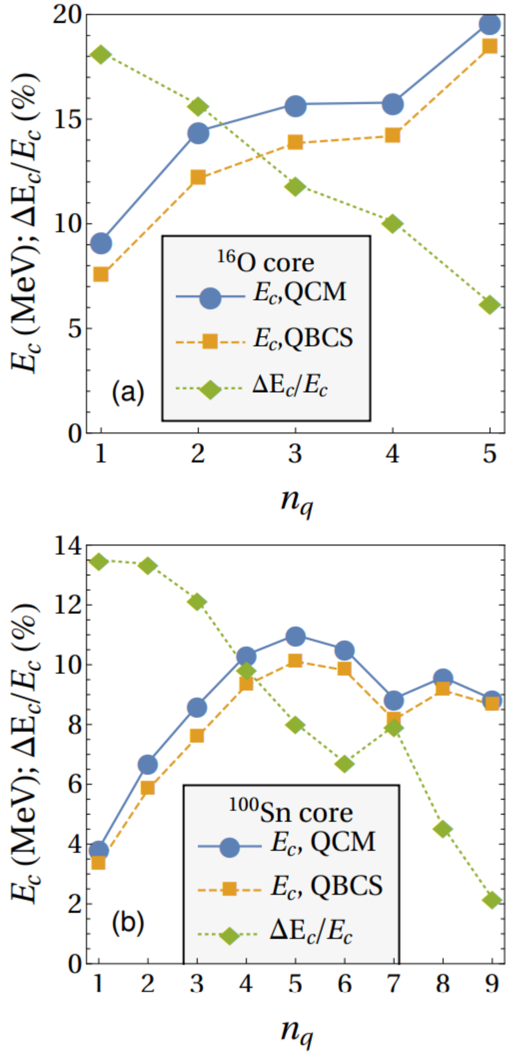


$$|\Psi\rangle = \left(\mathcal{Q}^\dagger\right)^{n_q} |0\rangle \qquad \mathcal{Q}^\dagger = 2\Gamma_1^\dagger \Gamma_{-1}^\dagger - \left(\Gamma_0^\dagger\right)^2 \qquad \Gamma_t^\dagger = \sum_k x_k P_{k,t}^\dagger$$

Lasseri, Ebran, Khan, Sandulescu

$$|QBCS\rangle \equiv \exp(Q^\dagger)|0\rangle = \sum_{n=0}^{N_{\mathrm{lev}}} \frac{1}{n!}(Q^\dagger)^n|0\rangle$$

Baran, Delion, 2019



Conclusion

⦿ Capturing nucleons correlations governing clustering is challenging

⦿ If one is interested to states with well developed clusters : clusters + nucleons or nucleons as relevant dofs

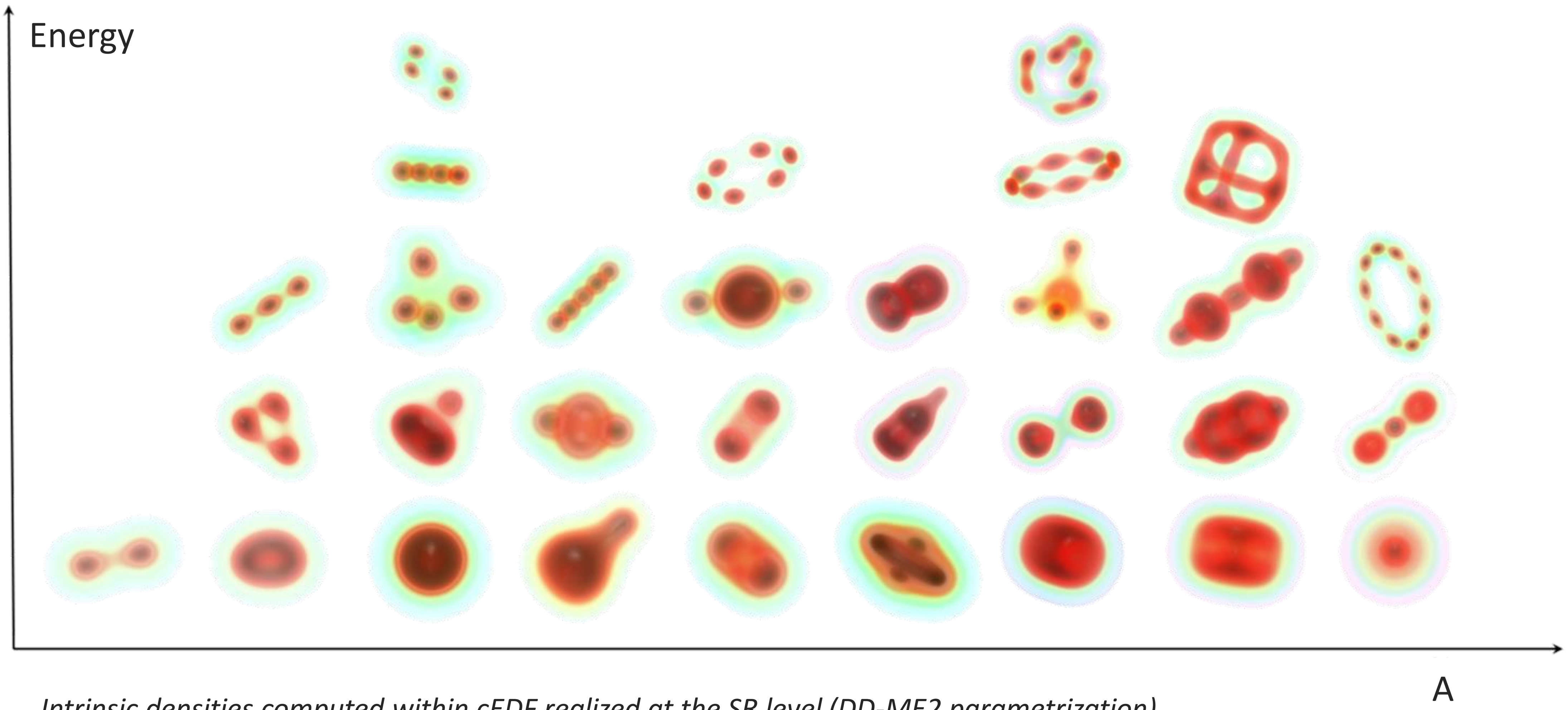
⦿ Clustering correlations seem to play a role in structural properties of compact states (seeds for clusterinsation already there): nucleons as relevant dofs
Tame down the complexity of treating corresponding correlations by:

i) Presupposing that nucleons arrange into clusters (RGM, BB-GCM, THSR-GCM)
ii) Imposing a localized gaussian form for nucleon wfs (AMD/FMD)
iii) Let the nucleons wfs be what they are, and catch correlations via horizontal expansion (symmetry breaking and restauration) : ab initio and EDF PGCM/QRPA
iv) Let the nucleons wfs be what they are, and catch correlations via symmetry-guided vertical expansion : SA-NCSM
v) Let the nucleons wfs be what they are, catch correlations via vertical expansion, take into account arrangement into clusters : NCSMc, Gamow SM
vi) Let the nucleons wfs be what they are, see how correlations translate into an in-medium 4-body wf : QCM, GF

Thank you for your attention

❶ Nuclear clustering

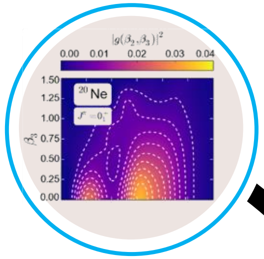
◉ Nuclear clustering = nucleons clumping together into sub-groups within the nucleus



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

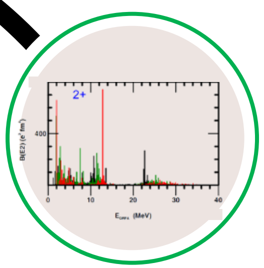
1 General goal of nuclear structure theory

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



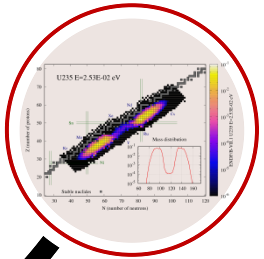
Ground-state

masses, radii, density profile, …



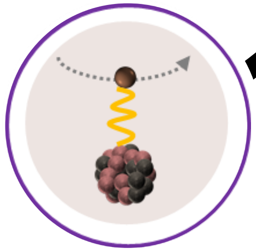
Excitation spectra

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



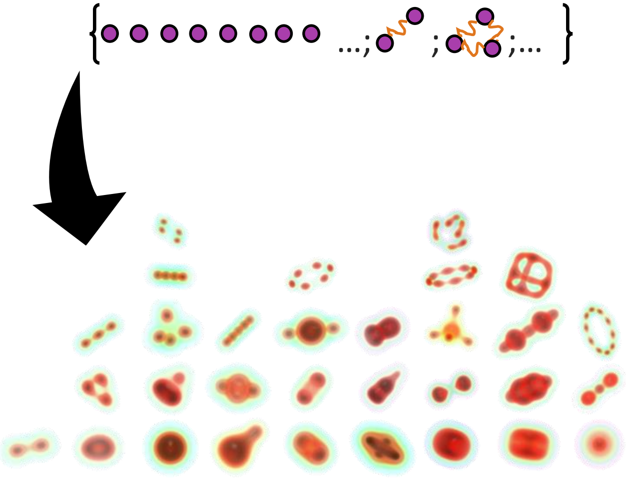
Decay modes

lifetime, yields, …



Reactions

cross sections, …



Intrinsic densities

Atomic nucleus

=

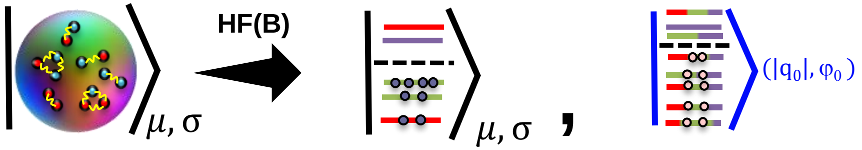
A mesoscopic, self-bound system of strongly correlated spin-1/2 and isospin-1/2 composite fermions in strong and electroweak interaction.

Emergent SSBs

The Energy Density Functional Method

◉ HFB treatment

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

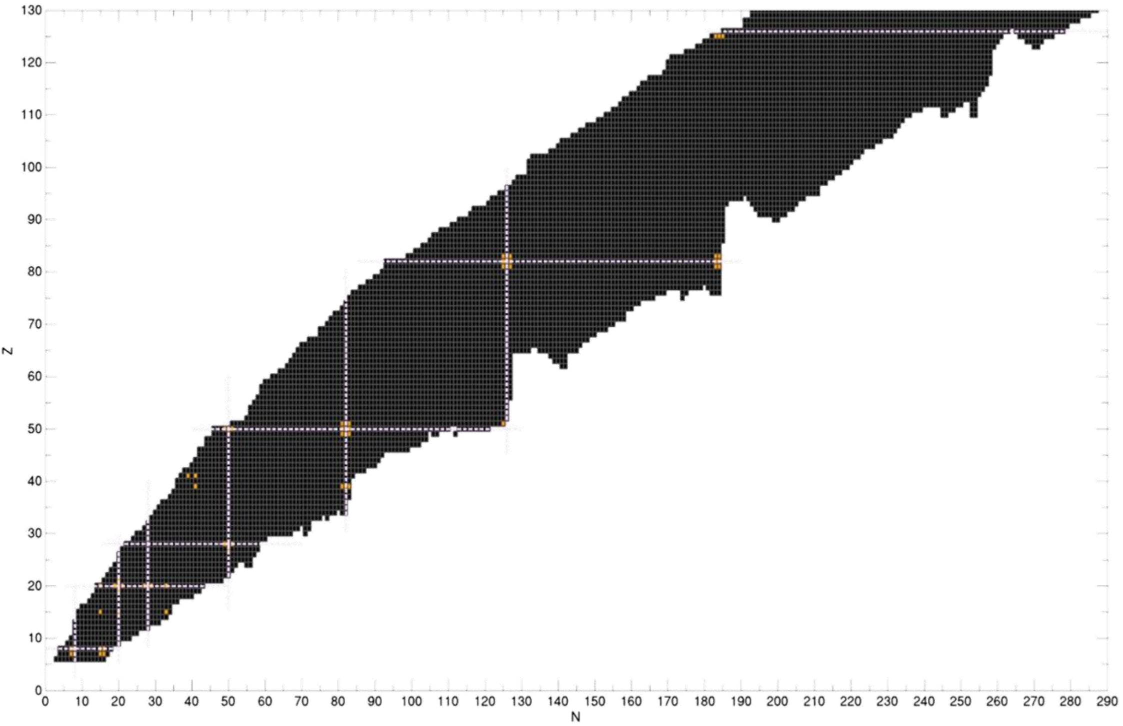


Correlated A-nucleon wavefunction

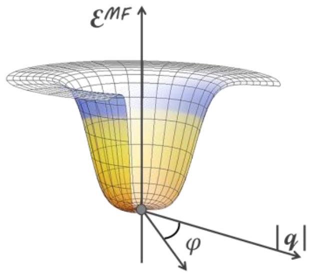
Symmetry-conserving A independent nucleons wavefunction

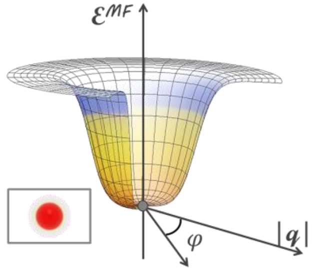
Symmetry-breaking A independent nucleons wavefunction

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



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





The Energy Density Functional Method

◉ HFB treatment

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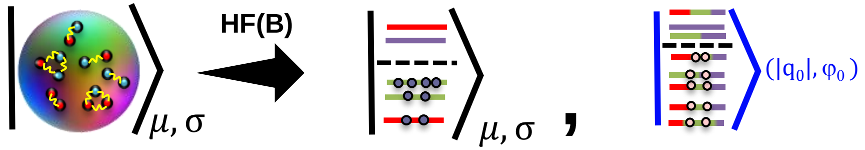

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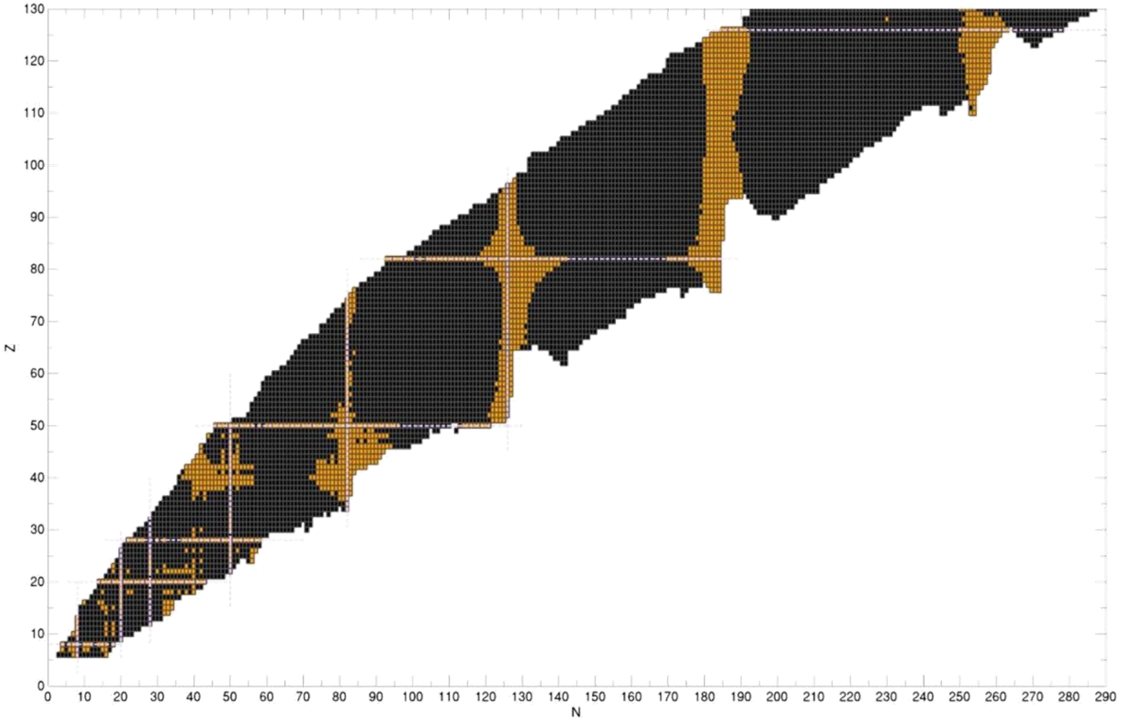
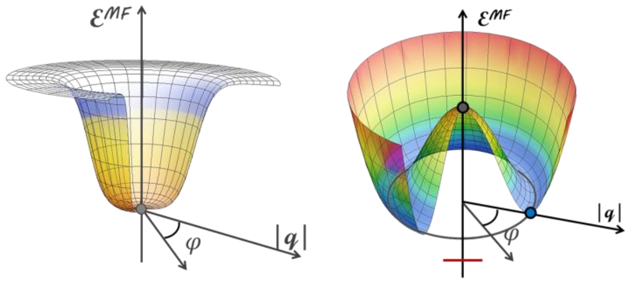
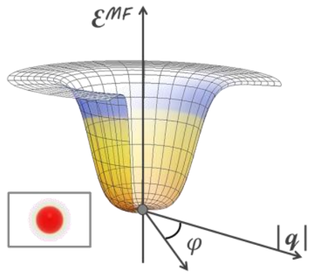




Spatial symmetry-restricted HFB: good description of GS of doubly and singly closed-shell nuclei & neighbors (~300 nuclei)



The Energy Density Functional Method

◉ HFB treatment

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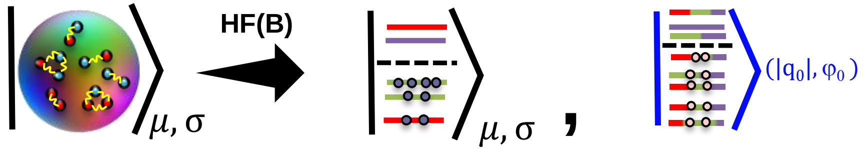

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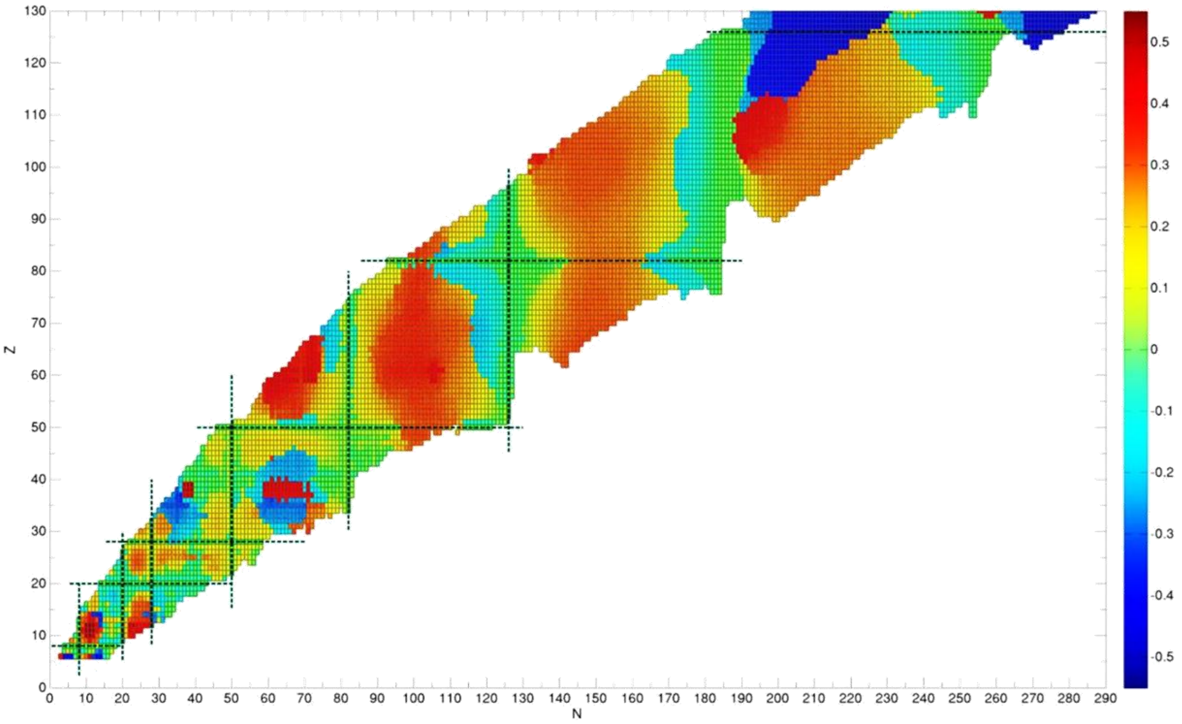
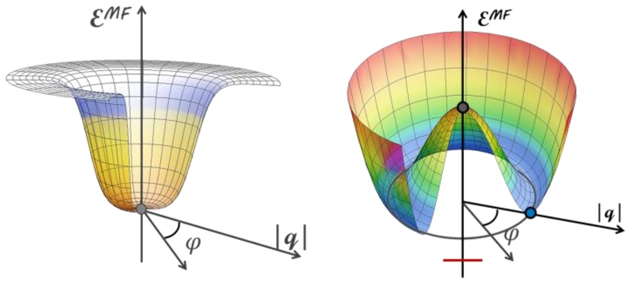
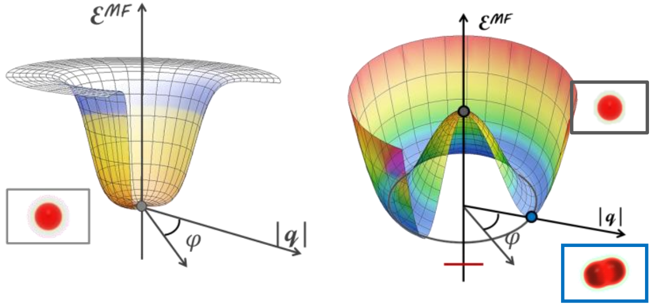


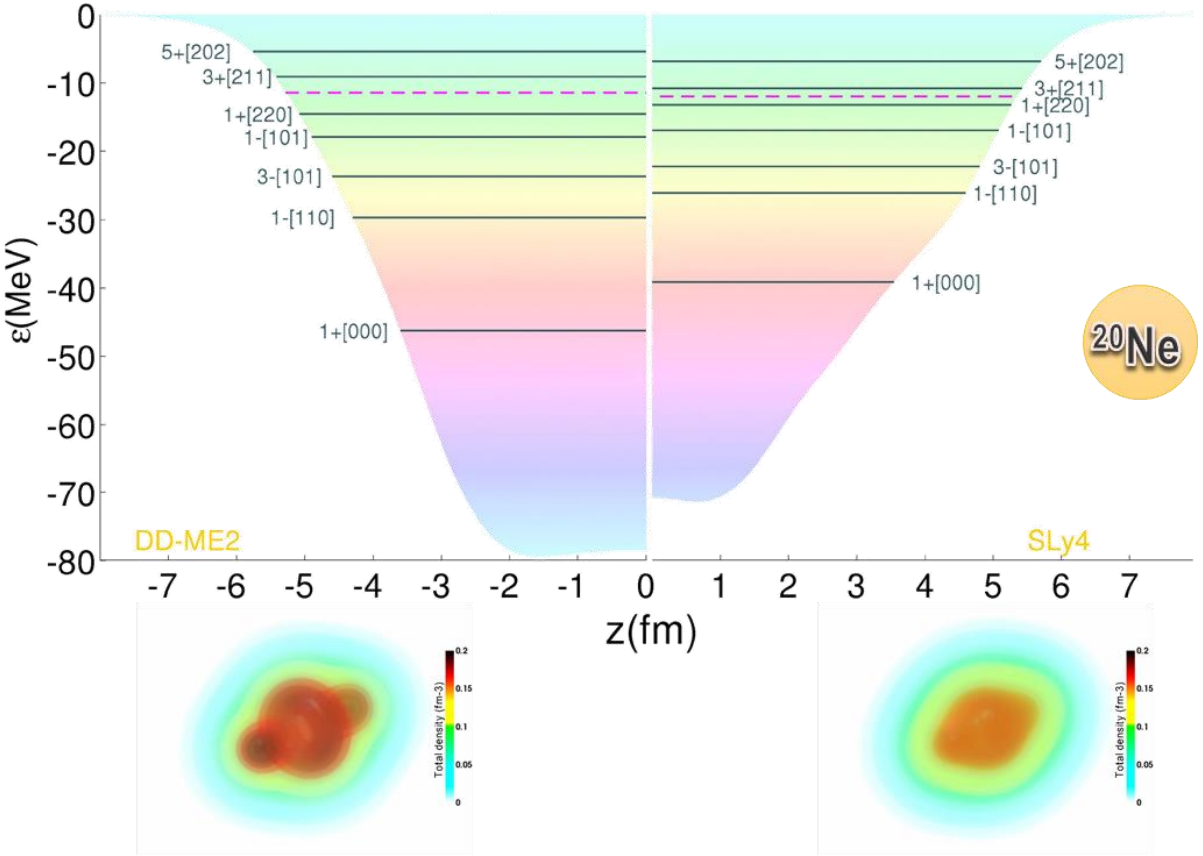


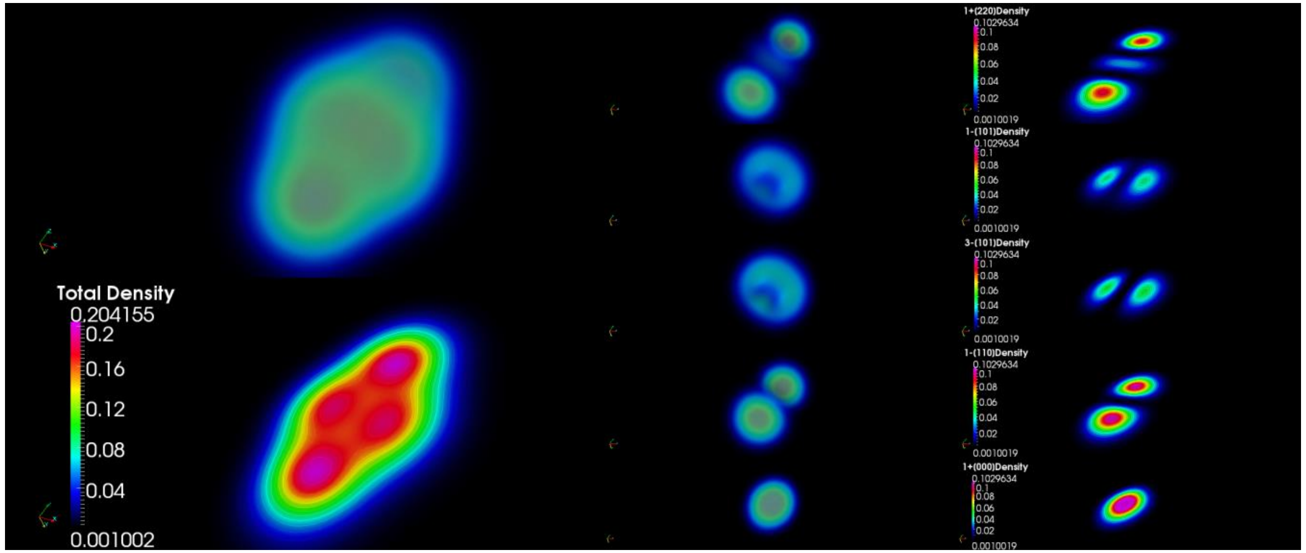
Symmetry-unrestricted HFB: good description of GS of all nuclei



Effect of the depth of the confining potential

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

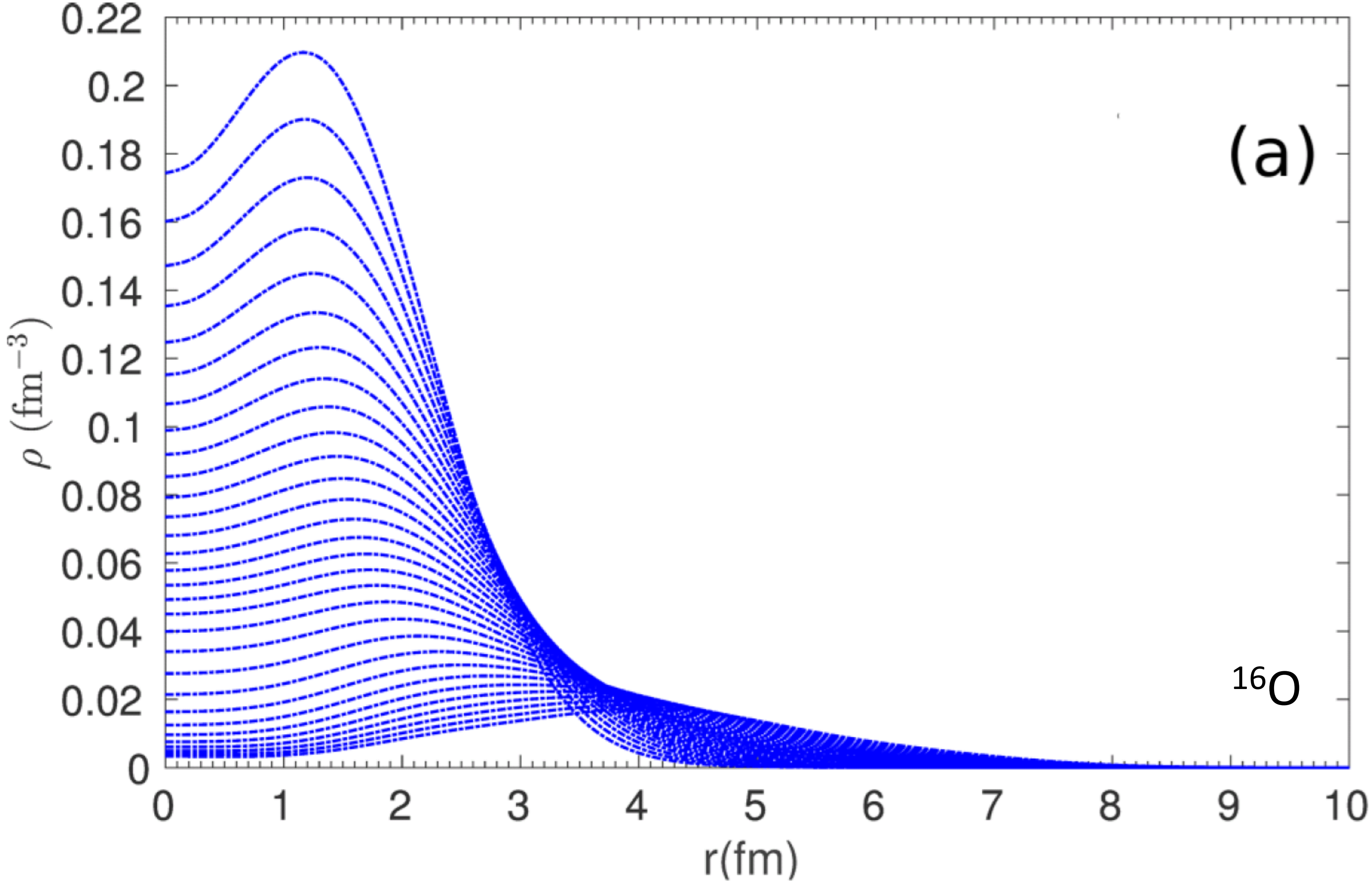




⦿ When Coulomb effects are not too important and owing to Kramers degeneracy, proton ↑, proton ↓, neutron ↑, neutron ↓ share the same spatial properties

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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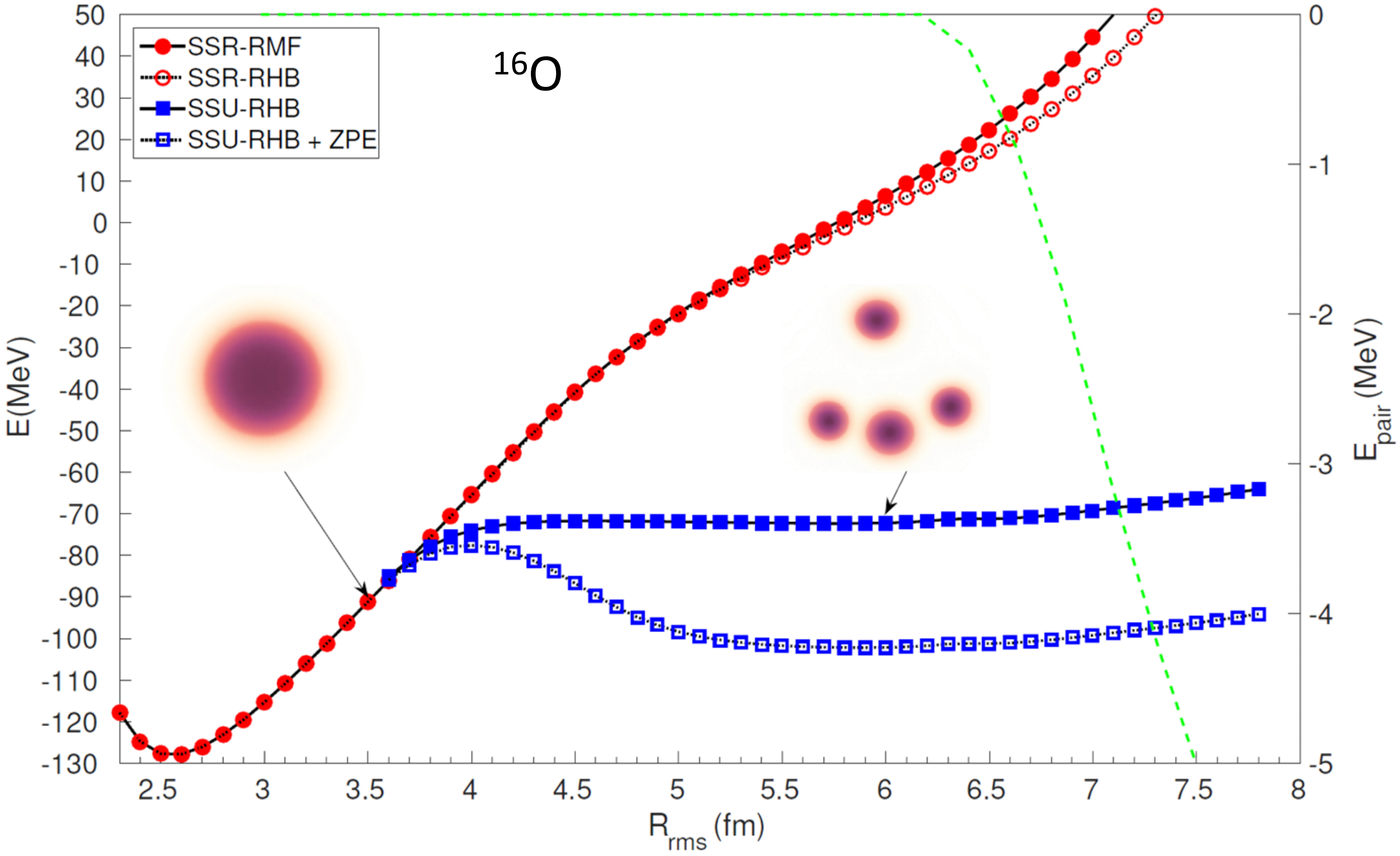

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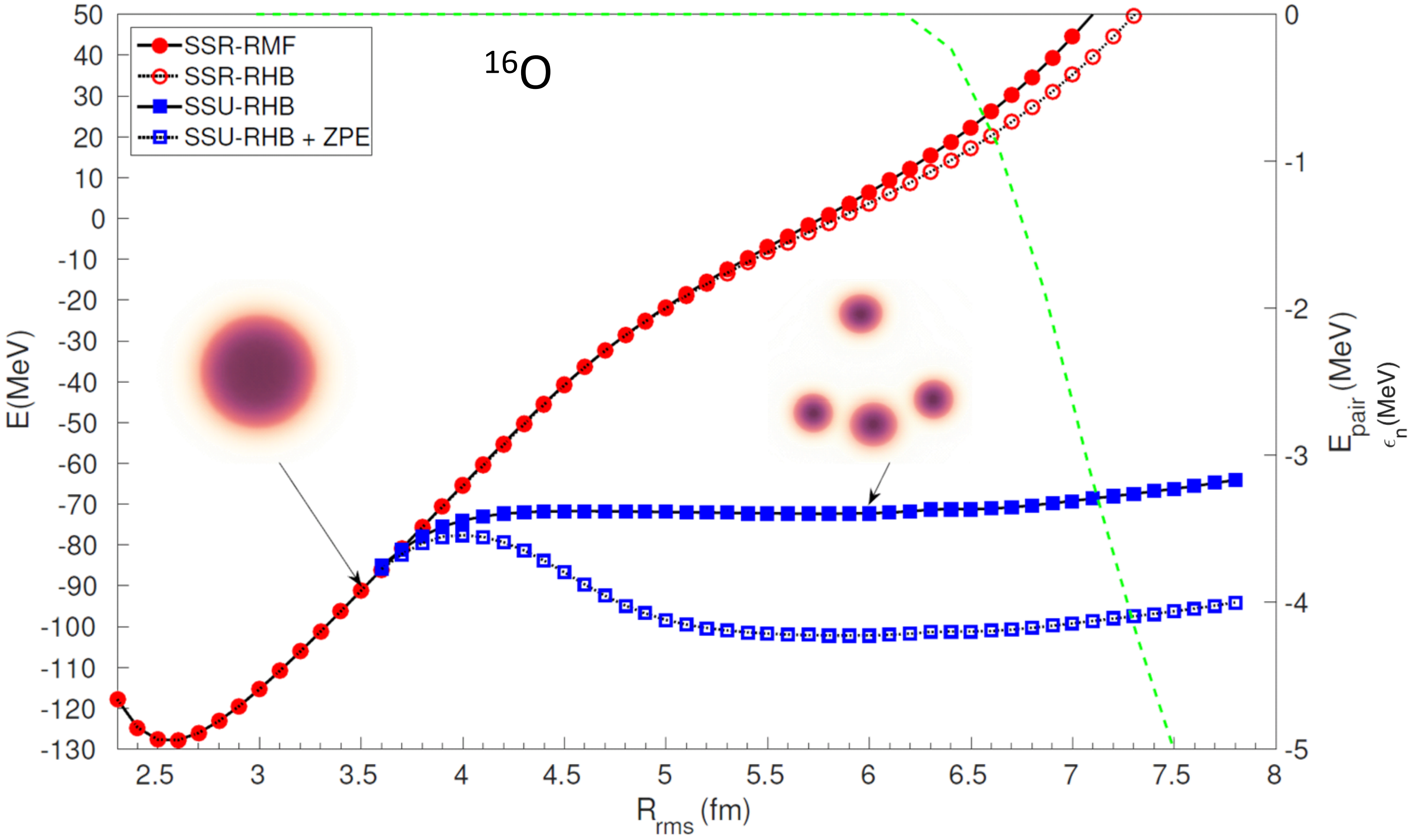

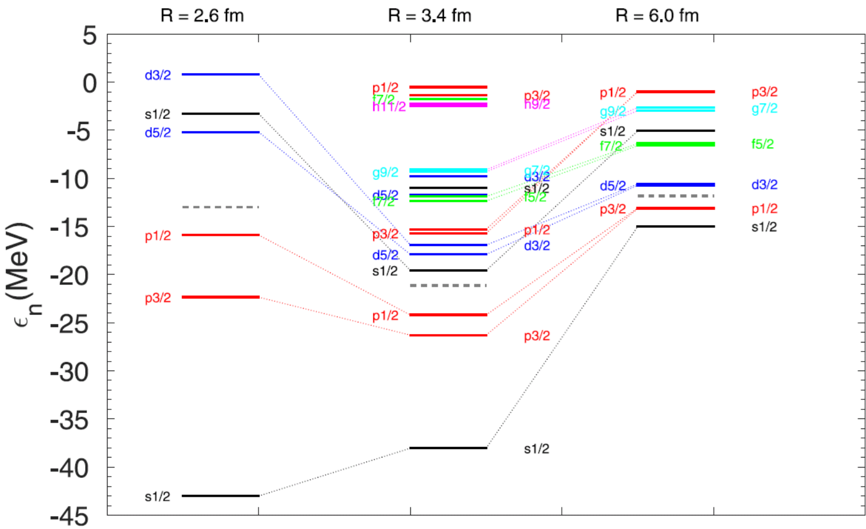

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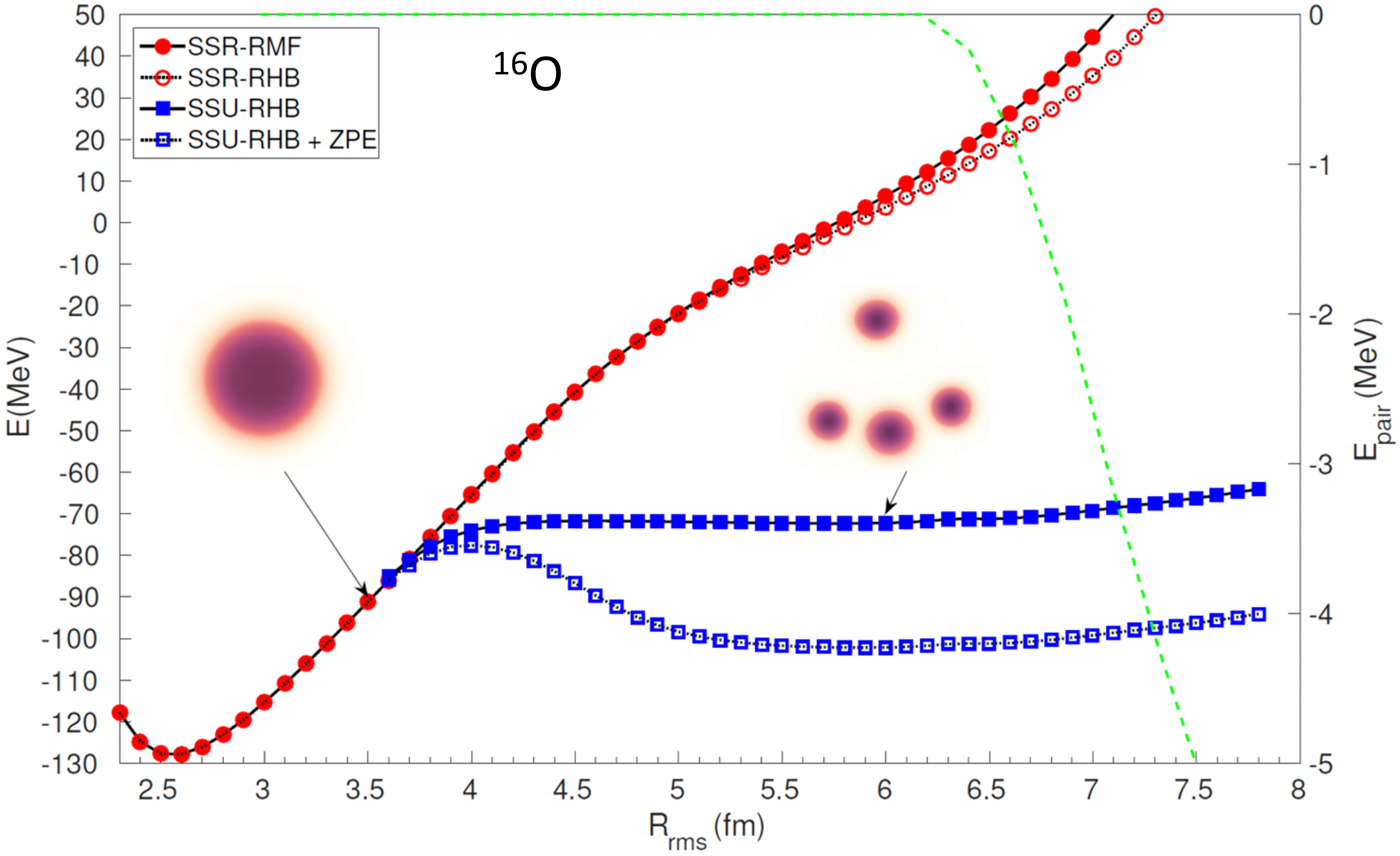
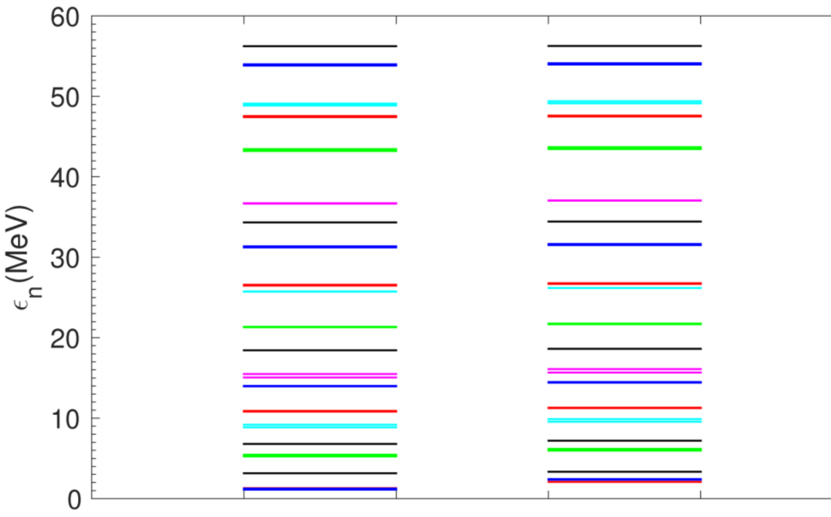
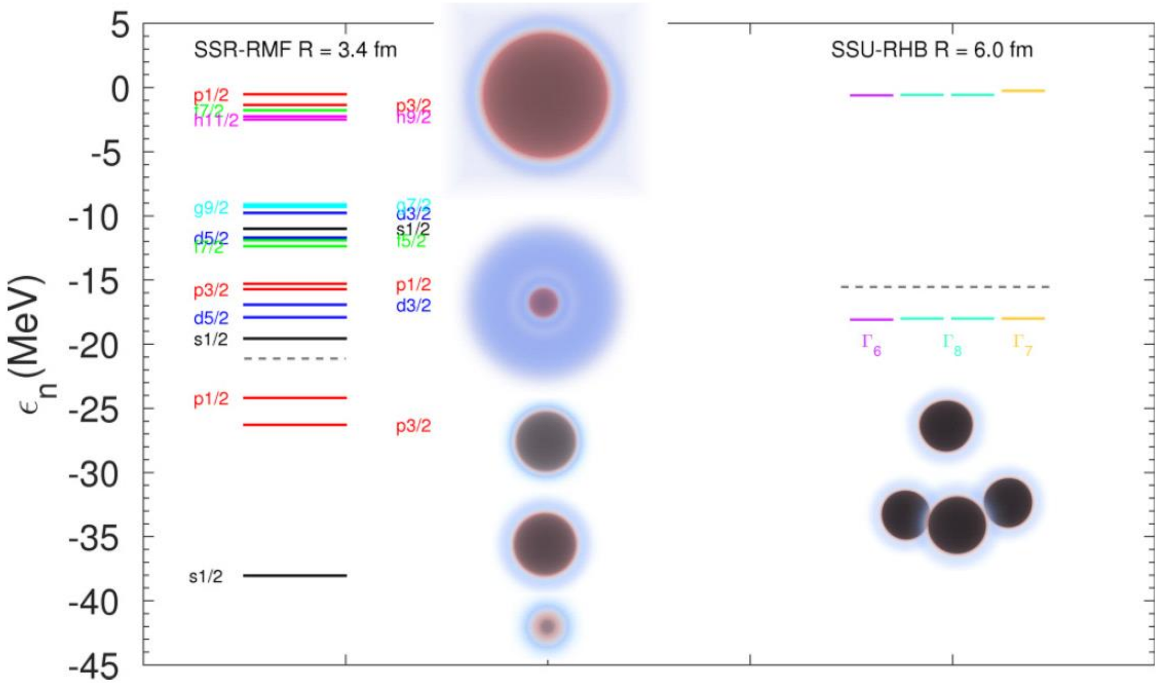


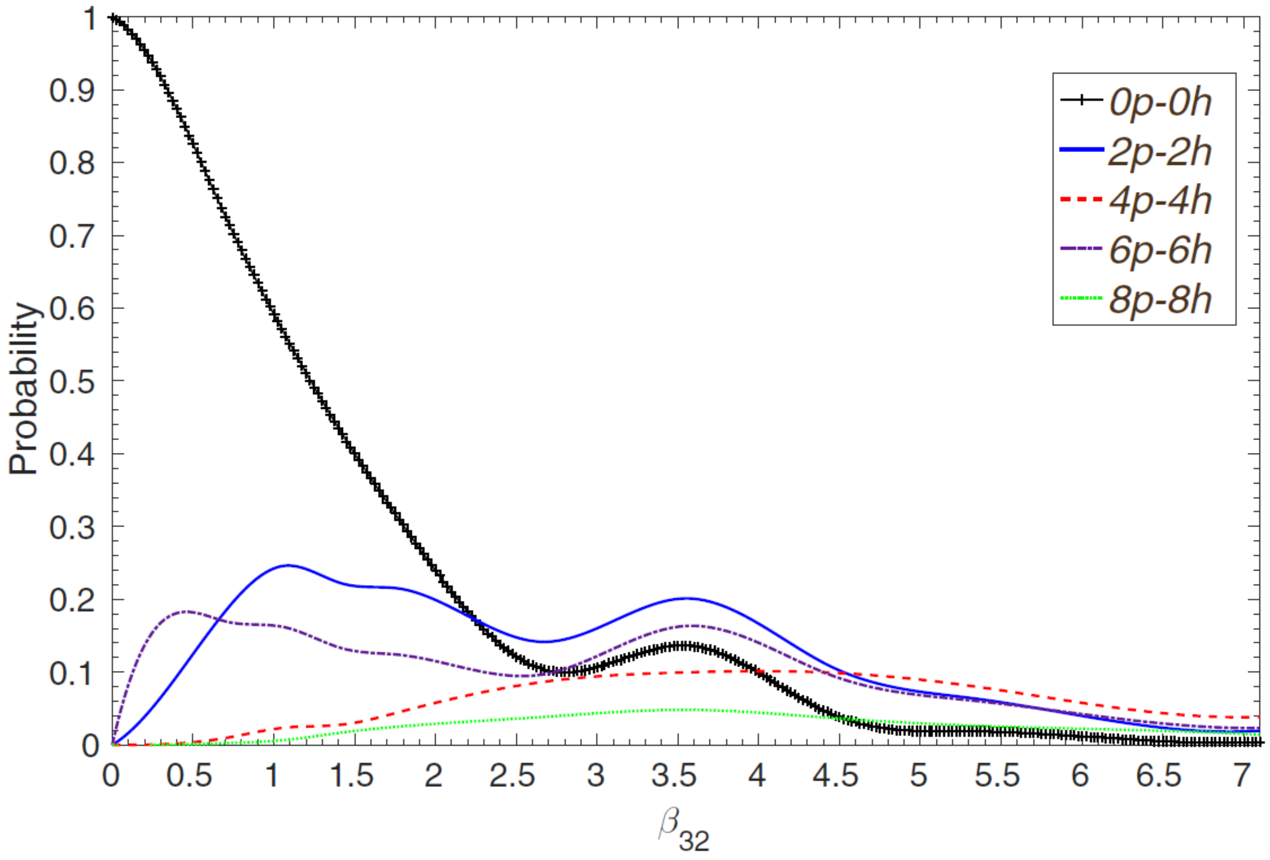


Effect of the density

- 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

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

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

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

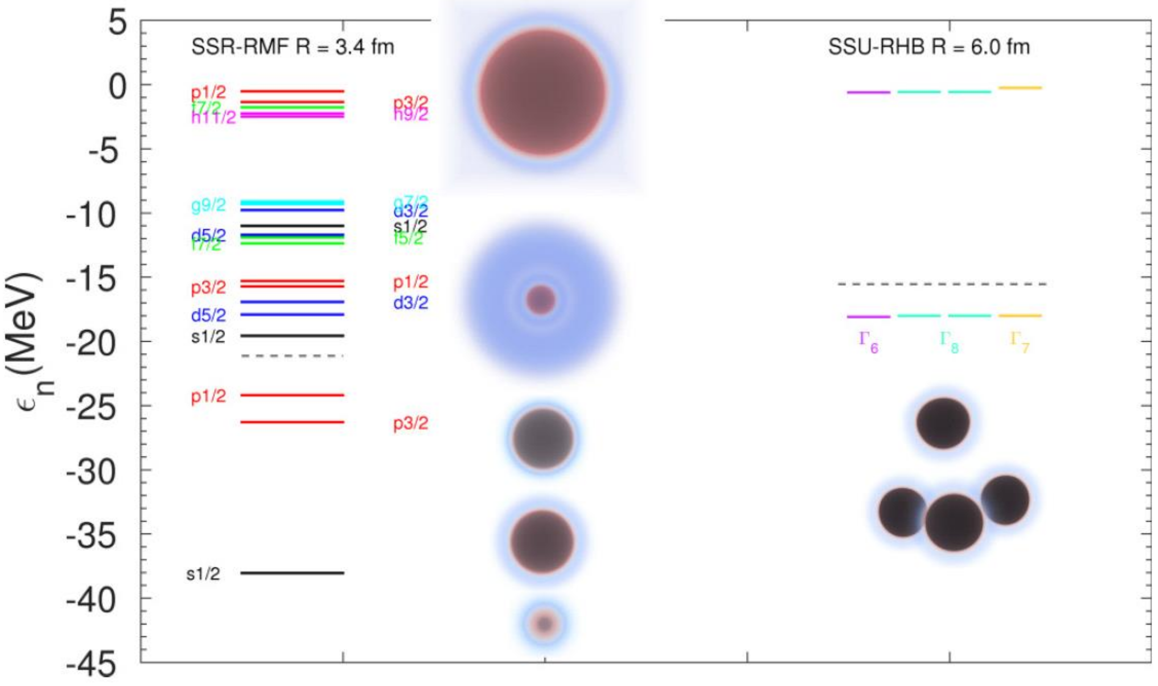
$$\psi_3 = \frac{1}{\sqrt{2}}(-\phi_1 + \phi_3) \qquad E_3 = E_2$$

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

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

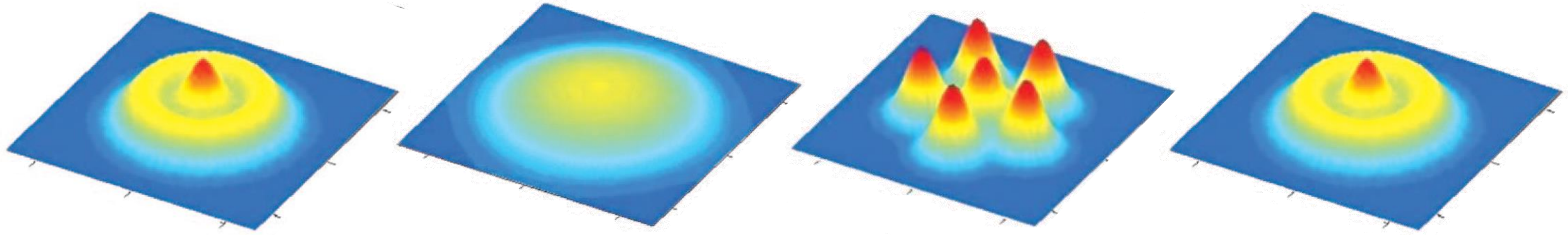
$$\psi'_3 = \frac{1}{2}(\phi_1 + \phi_2 - \phi_3 - \phi_4),$$

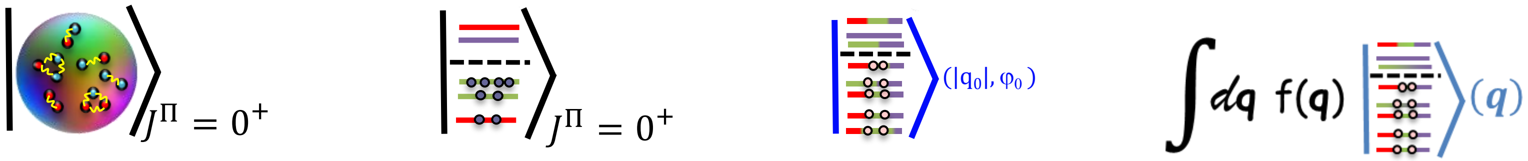
$$\psi'_4 = \frac{1}{2}(-\phi_1 + \phi_2 - \phi_3 + \phi_4).$$



Nuclear clustering & PGCM

Density profile



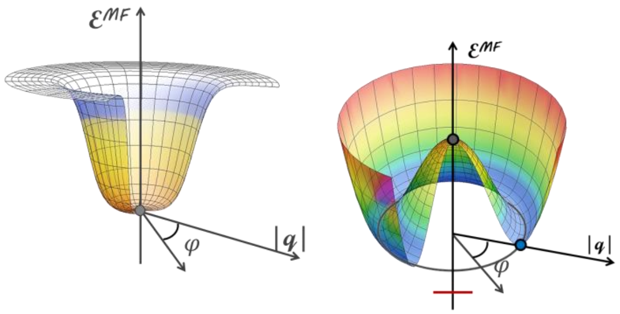


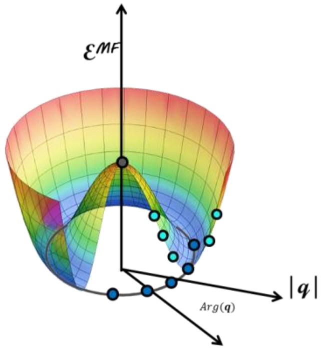
Exact WF

Approx : Symmetry-preserving HF WF

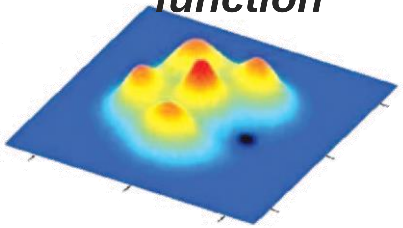
Approx : Symmetry-broken HFB WF

Approx : PGCM WF





2-point correlation function



Spectroscopy

Yannouleas & Landman, 2017

Nuclear clustering & PGCM