Nuclear clustering within the Energy Density Functional approach

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CEA,DAM,DIF

Light nuclei between single-particle and clustering features

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Introduction

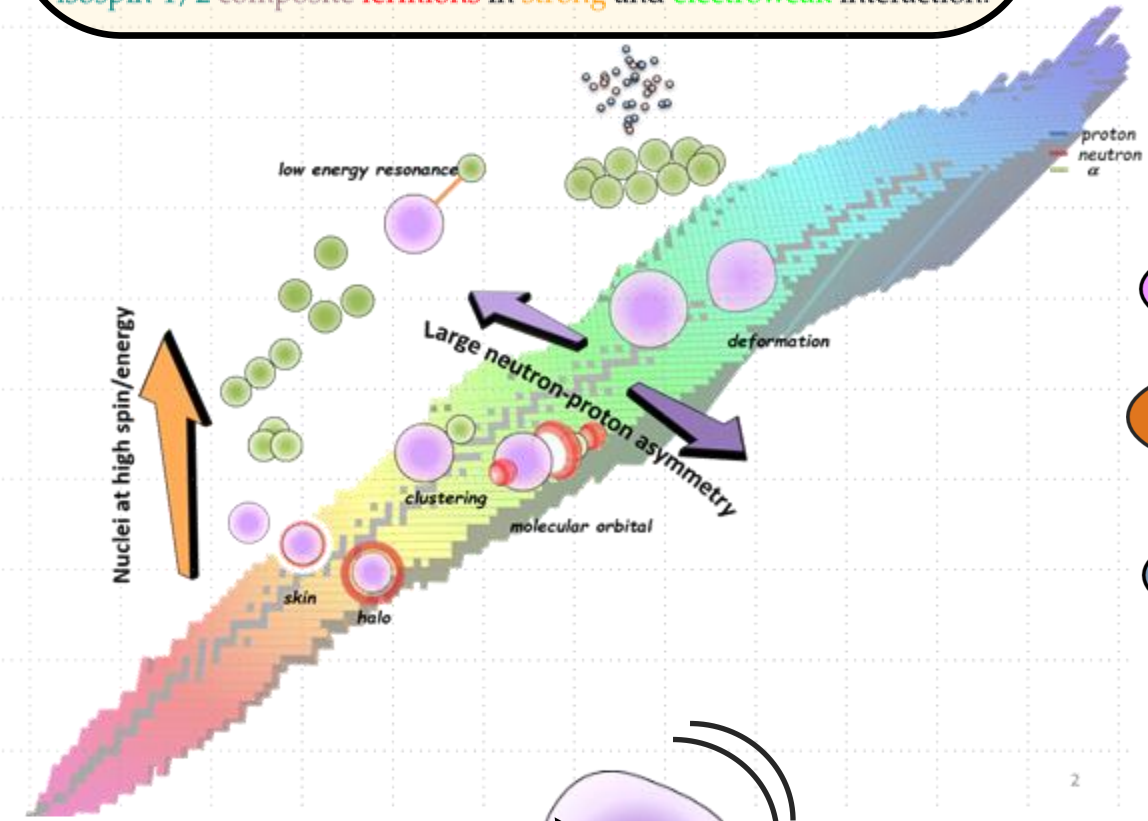
Atomic nucleus

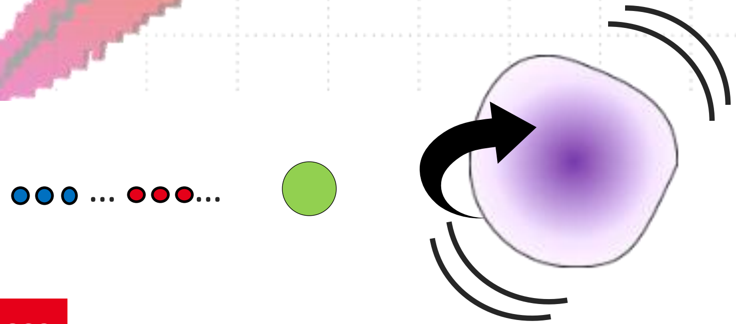
=

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

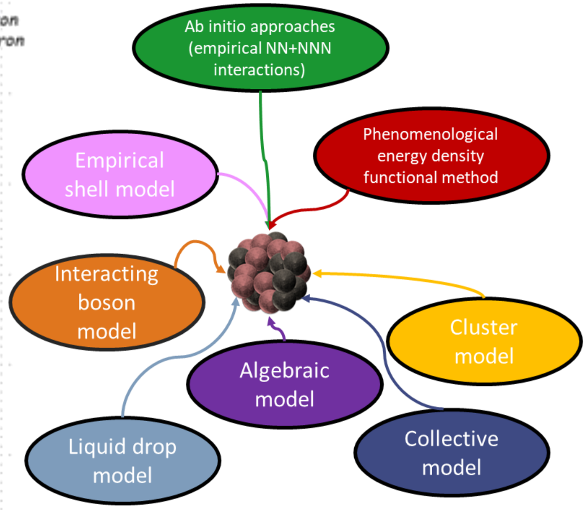
◉ Many characteristic scales :

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

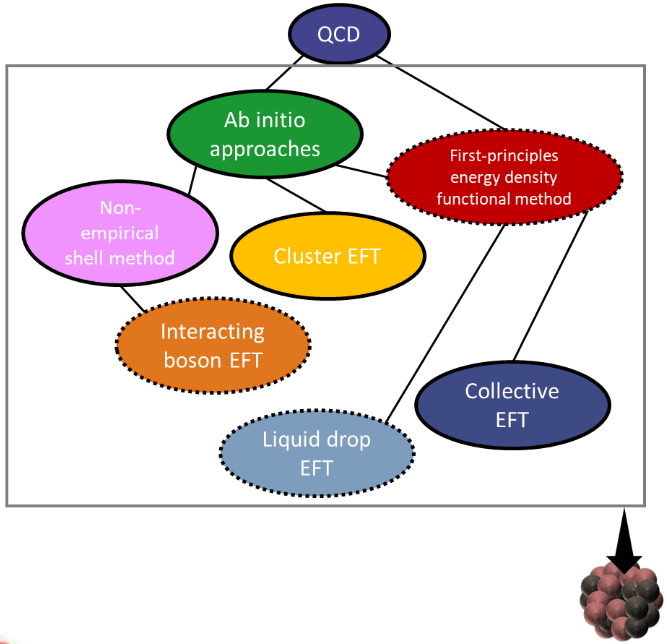


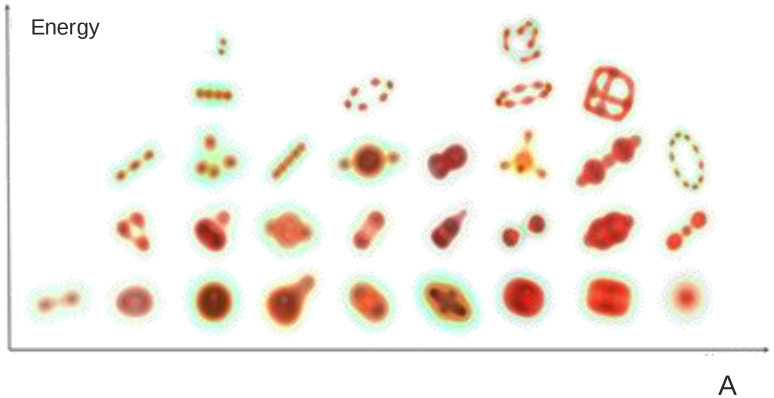


Era of models



Era of effective (field) theories





Outline

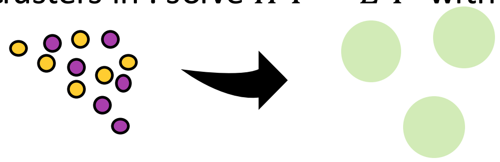
1. What strategies to account for nuclear clustering
2. EDF in a nutshell
3. EDF & clustering

2 main descriptions

Relevant dofs = inert clusters + possibly single nucleons

◉ Nucleus = system of N “elementary” clusters in : solve $H\Psi = E\Psi$ with

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



12 spin-1/2 fermions *3 spin-0 bosons*

⇢ 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.

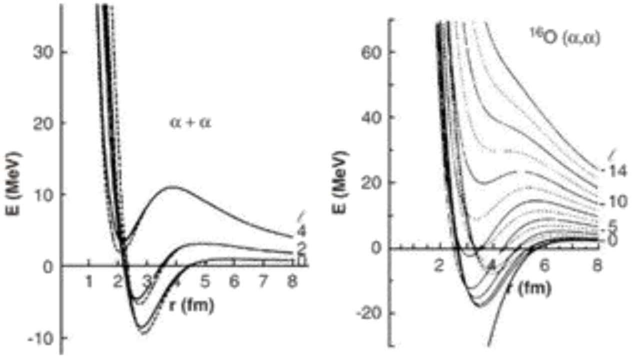


Fig. 12. Two examples of molecular local potentials for the α–α interaction, i.e. for ^{8}Be, and for the α-^{16}O system, forming ^{20}Ne. Different partial waves are shown. Figure adapted from Ref. [206].

Relevant dofs = nucleons

2 main descriptions

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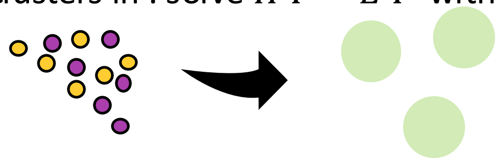

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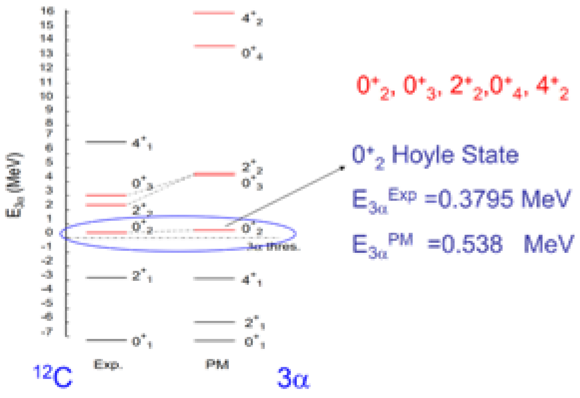
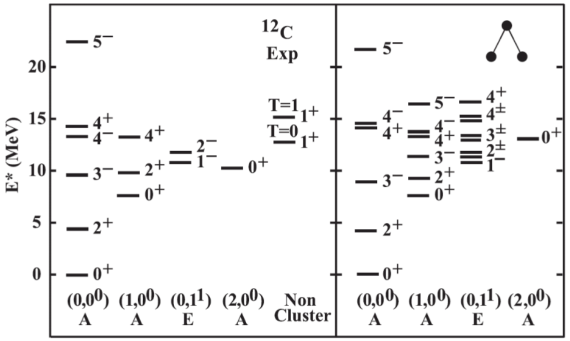
Lazauskas, Dufour (2011)



Bijker, Iachello (2002)



2 main descriptions

Relevant dofs = inert clusters + possibly single nucleons

- Empirical formulation
- EFT formulation

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

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

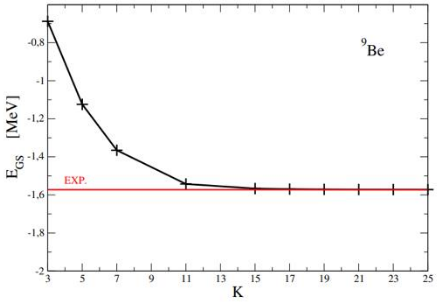
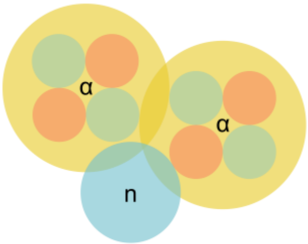


FIGURE 6.15: Ground state energy of ^{9}Be increasing the hyperangular momentum K with the three-body force.



Elena Filandri et al (2022)

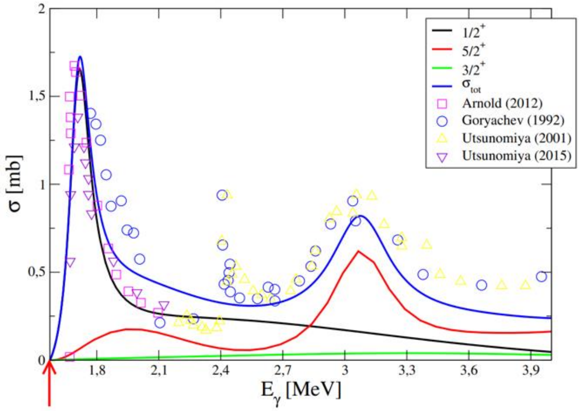


FIGURE 6.33: Comparison of our result obtained for the ^{9}Be photodisintegration cross-section and the experimental data shown in Figure 1.2. The red arrow indicates the threshold.

Relevant dofs = nucleons

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Relevant dofs = nucleons

- 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

Nucleon antisymmetrizer

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

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

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

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

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

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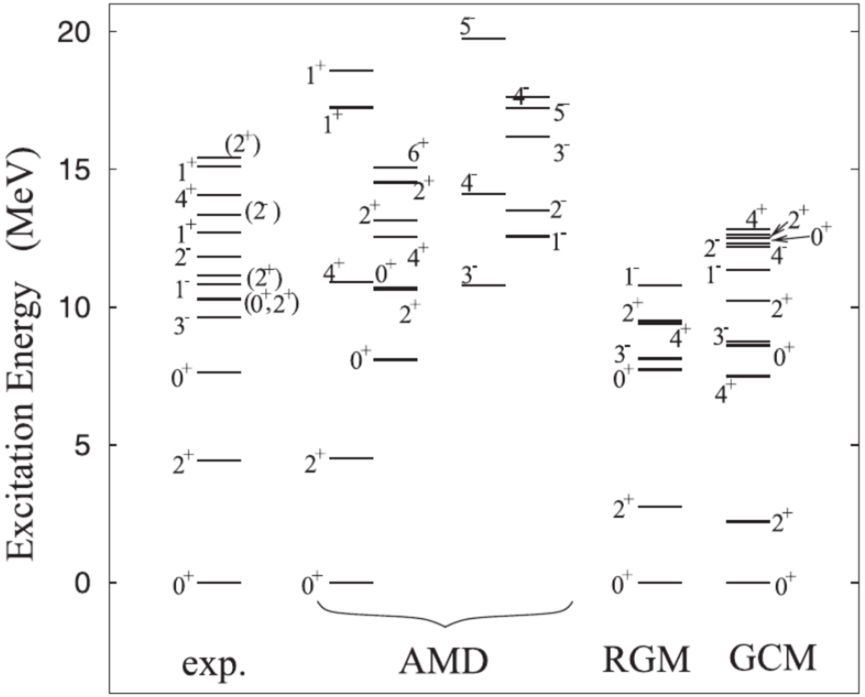

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--> Resonating group method (Wheeler, Descouvemont, …)

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

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

Written in terms of HO WF

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

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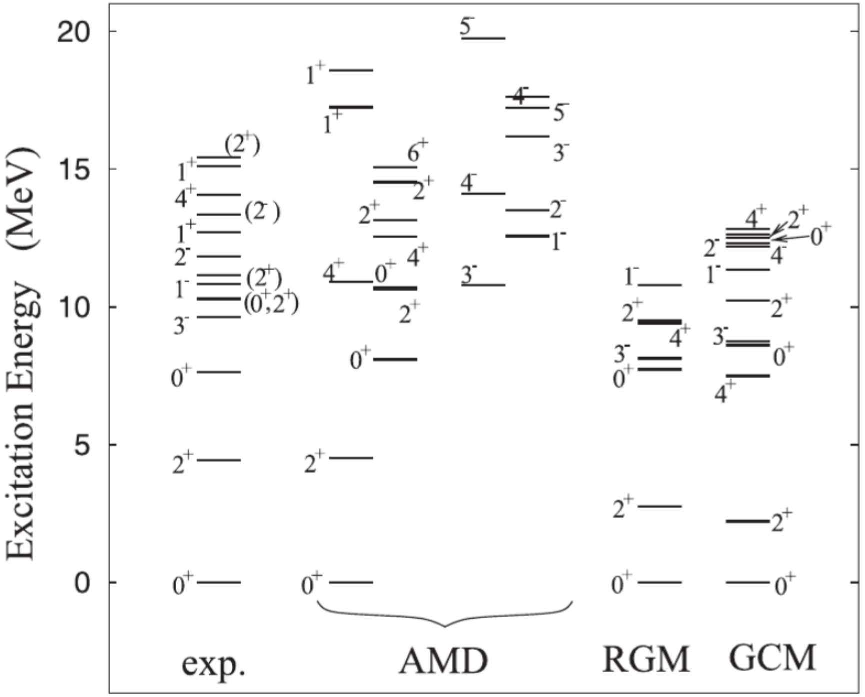

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--> THSR WF (Tohsaki, Horiuchi, Schuck, Röpke, Funaki, Zhou,...)

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

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

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

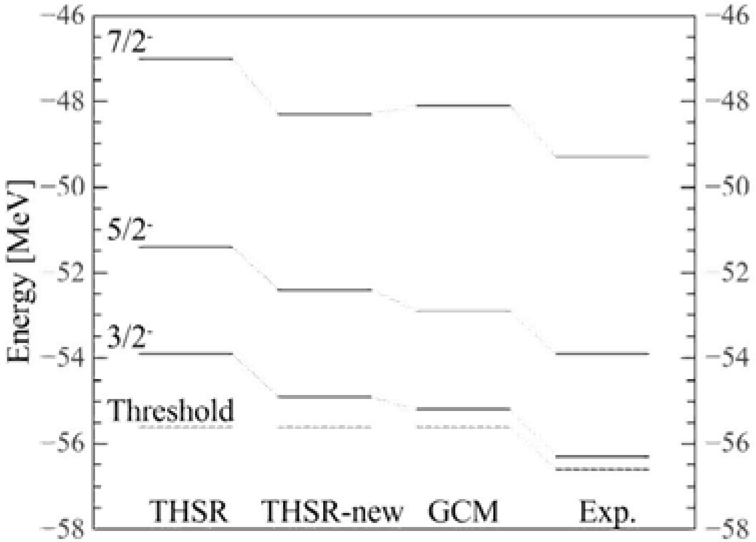

Fig. 49 Theoretical and experimental results of the energy spectrum of ^{9}B [131].

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- Favor nucleonic localization : AMD/FMD

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

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

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

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

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

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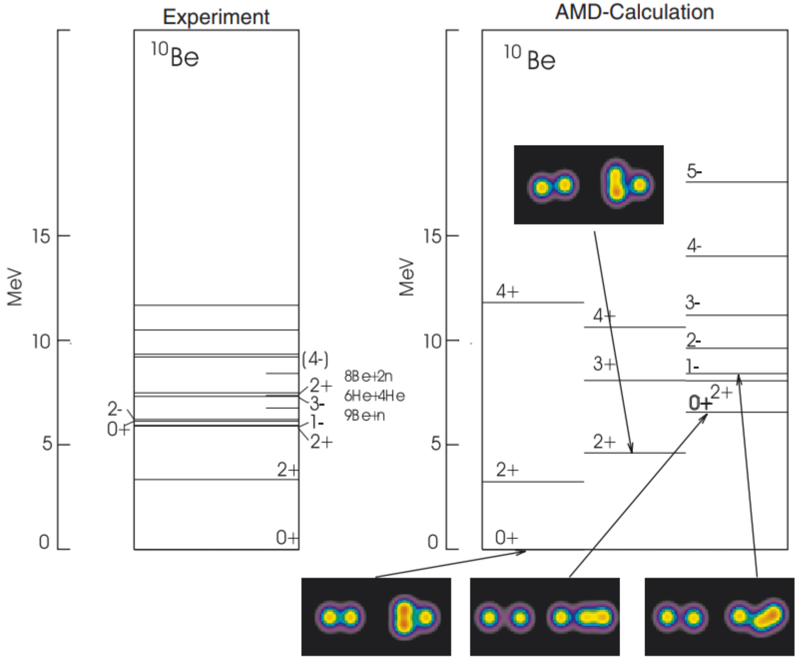

Kanada-En'yo (2006)

2 main descriptions

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- Favor nucleonic localization : AMD/FMD

- Account for correlations

  --> χEFT : Start from chiral Hamiltonian and try grasping correlations in a computationally tractable way

  - NLEFT *(Lee et al)*
  - SA-NCSM *(Launey et al)*
  - PGCMPT (+ IMSRG) *(Duguet et al)*

  --> EDF : Empirical microscopic method ($\approx$IMSRG+PGCMPT^0)

Outline

1. What strategies to account for nuclear clustering
2. EDF in a nutshell
3. EDF & clustering

1 Nuclear structure from a microscopic viewpoint

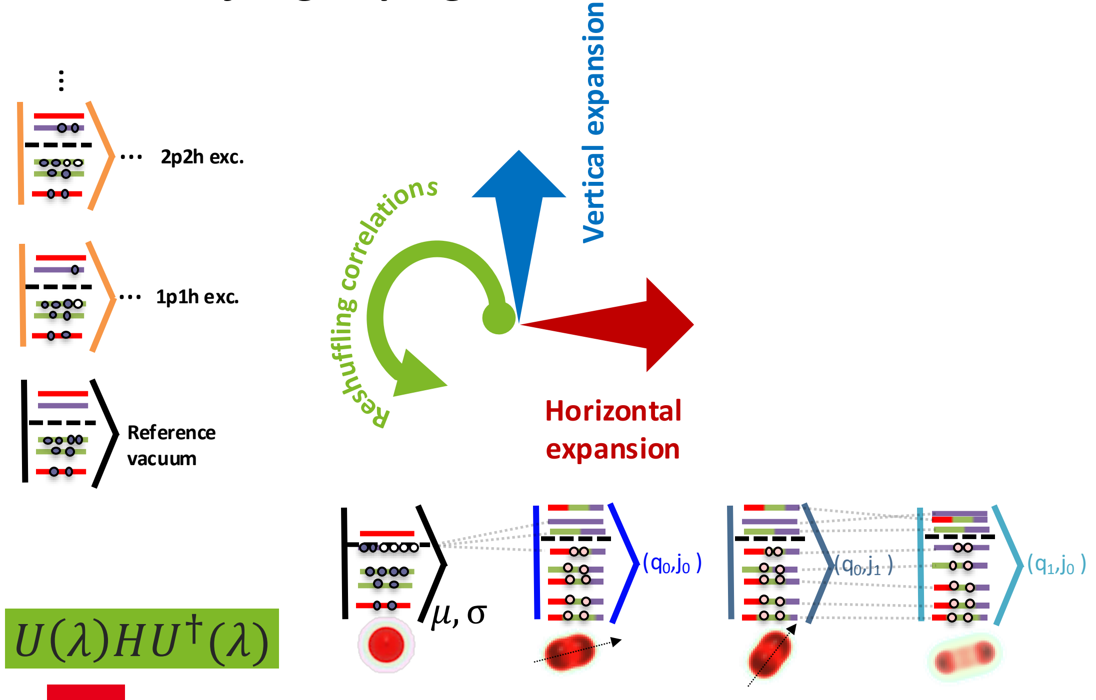
1) Nucleus: *A* interacting, structure-less nucleons
2) Structure & dynamic encoded in Hamiltonian, Functional, …
3) Solve *A*-nucleon Schrödinger/Dirac equation to desired accuracy

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

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



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

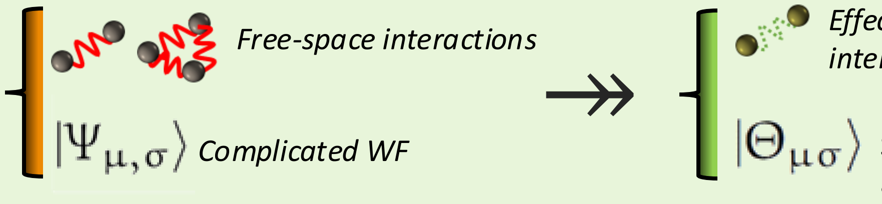
Ab initio

- **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***

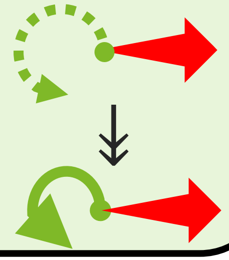
How to challenge ab initio frontiers

EDF

- **Effective pseudo-Hamiltonian**



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



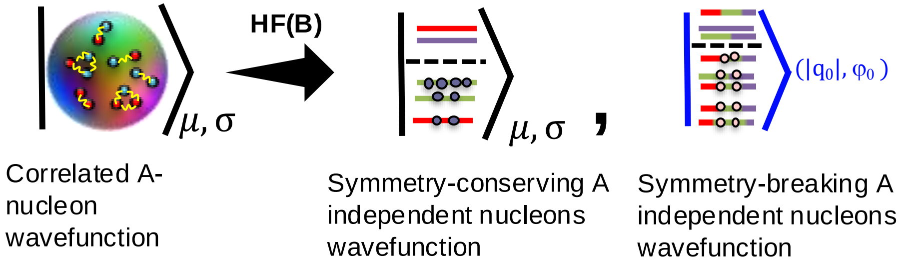
How to improve current EDFs

How to turn EDF in EFT ?

The Energy Density Functional Method

◉ HFB treatment

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



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

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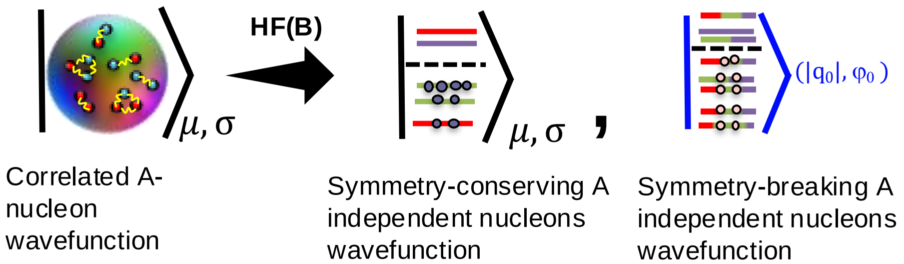

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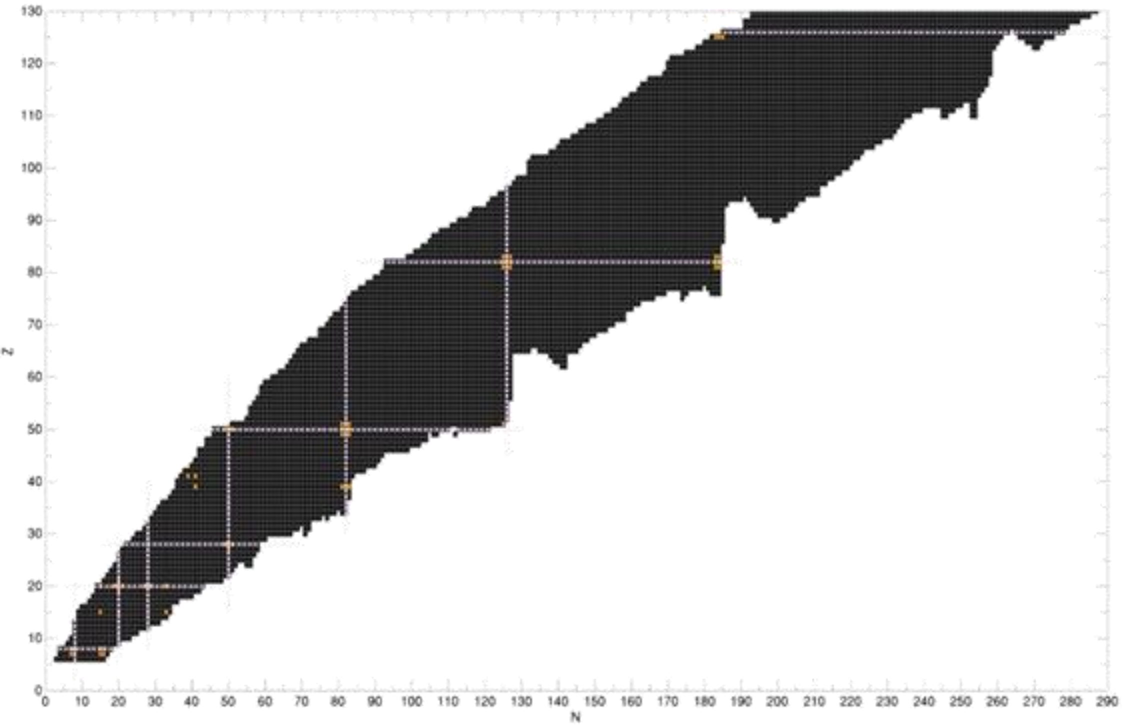
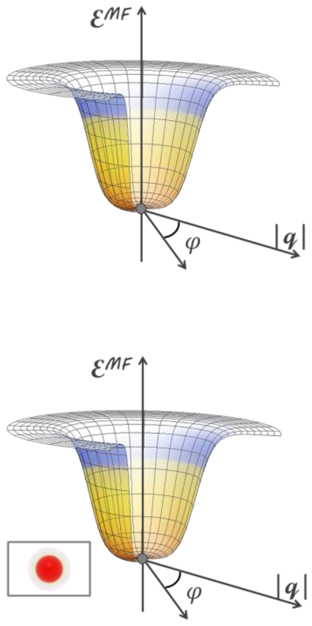


Symmetry-restriced HF : good description of GS of doubly closed-shell nuclei & neighbors (~30 nuclei)



The Energy Density Functional Method

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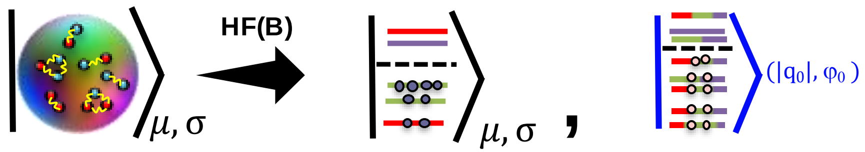
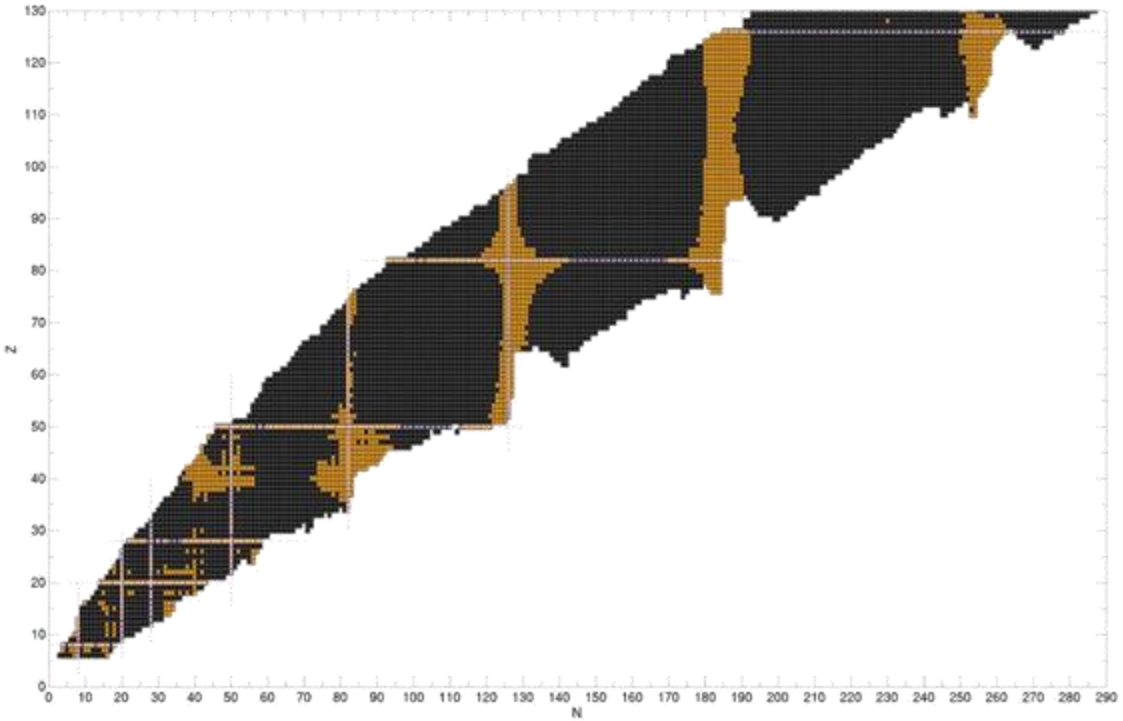


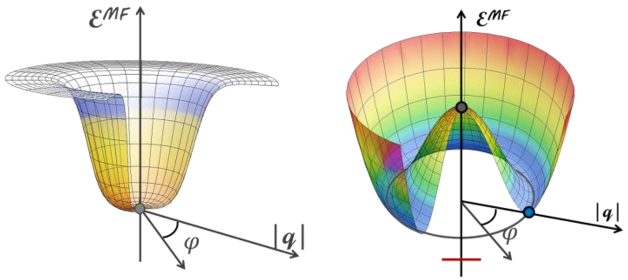
Correlated A-nucleon wavefunction

Symmetry-conserving A independent nucleons wavefunction

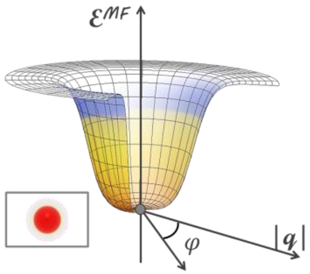
Symmetry-breaking A independent nucleons wavefunction

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





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



The Energy Density Functional Method

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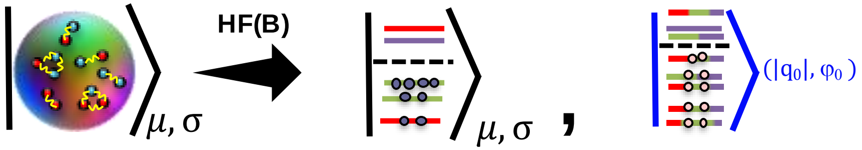

Correlated A-nucleon wavefunction

Symmetry-conserving A independent nucleons wavefunction

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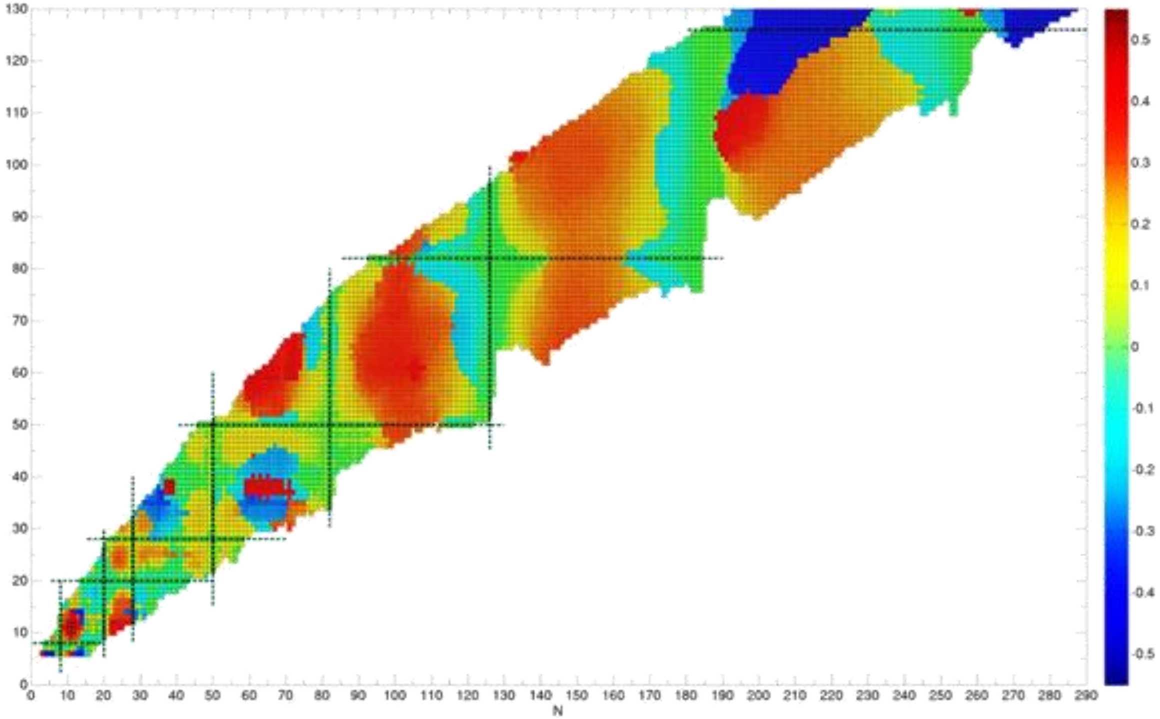
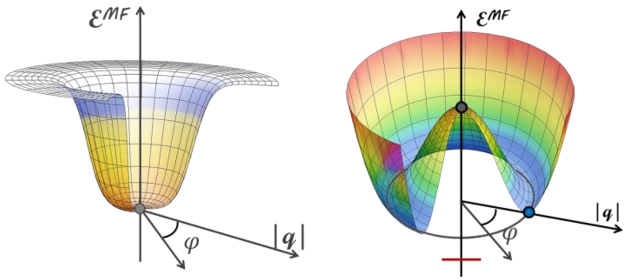
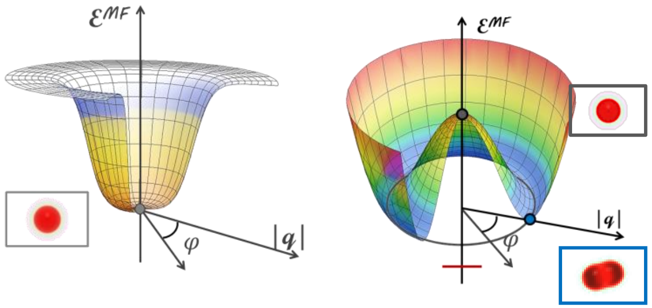




Symmetry-unrestricted HFB: good description of GS of all nuclei



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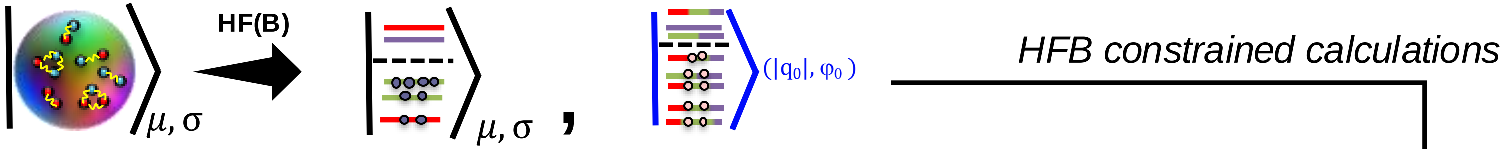
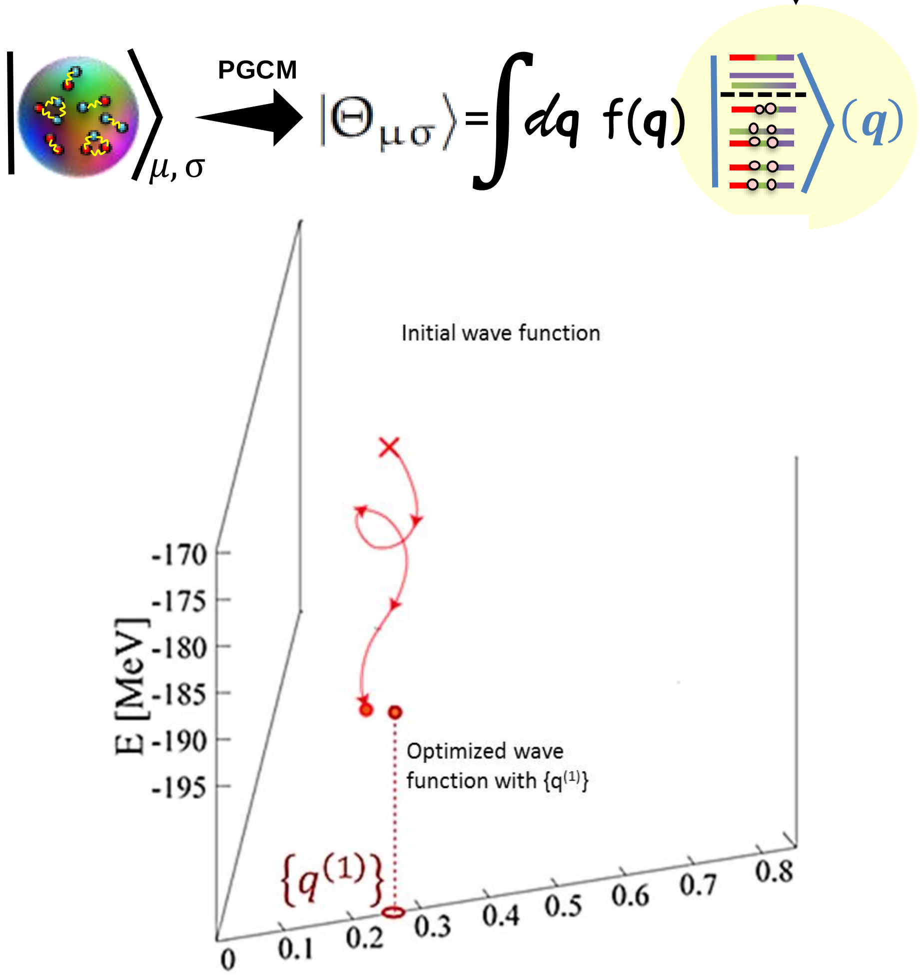


◉ Post-HFB treatment : PGCM

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



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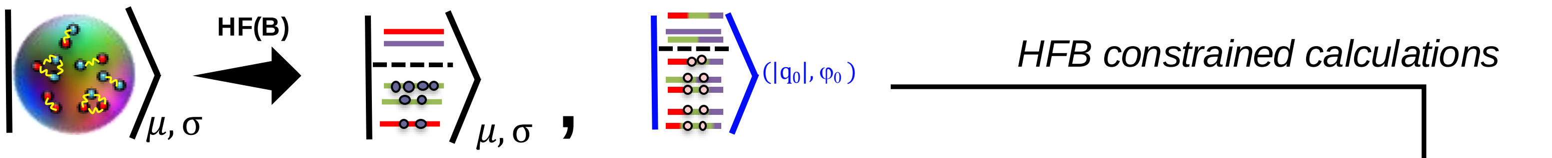

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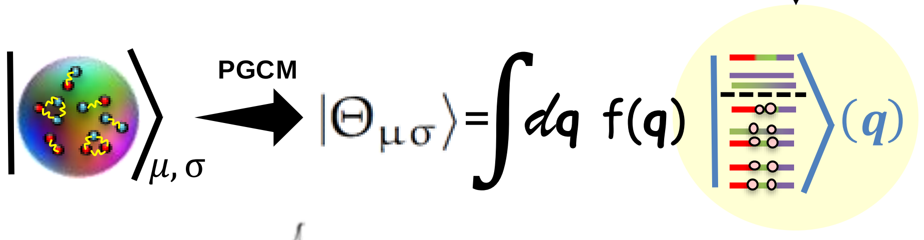

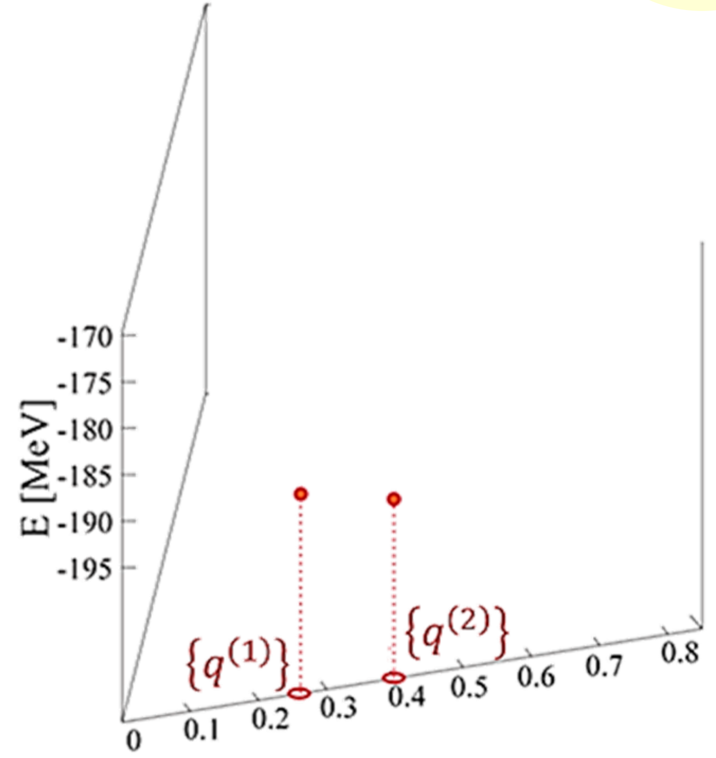

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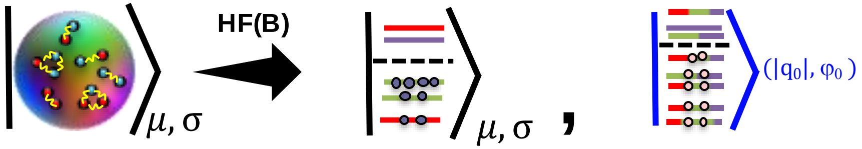

HFB constrained calculations

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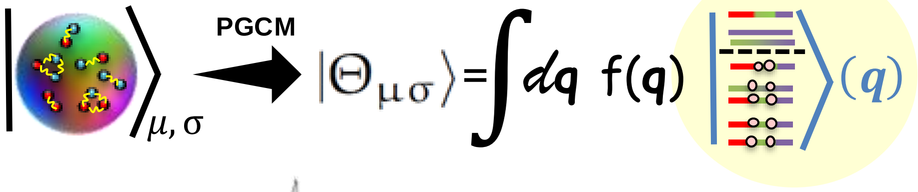

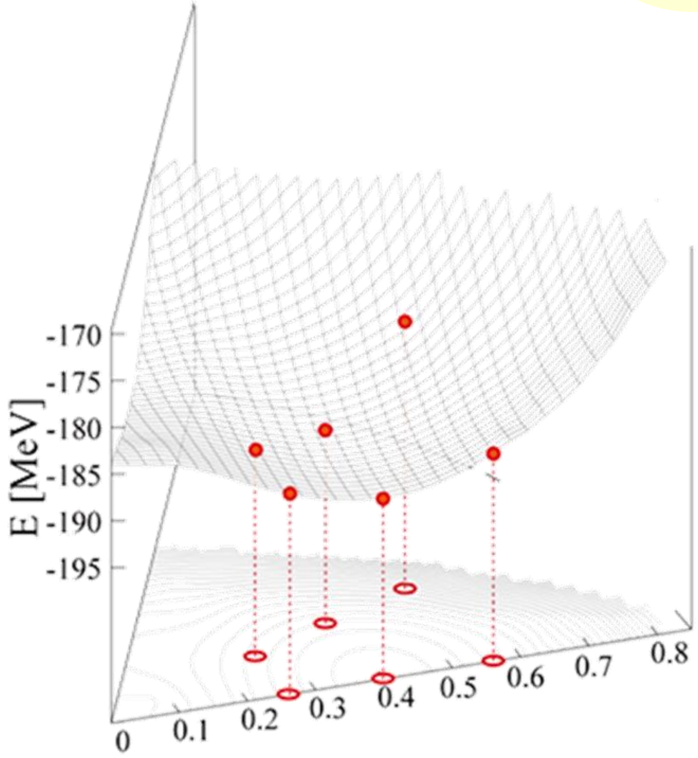

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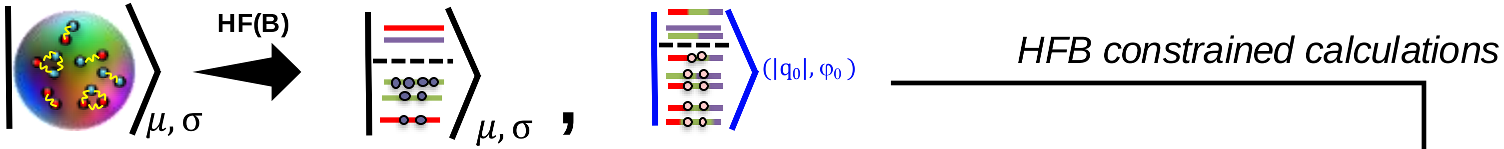
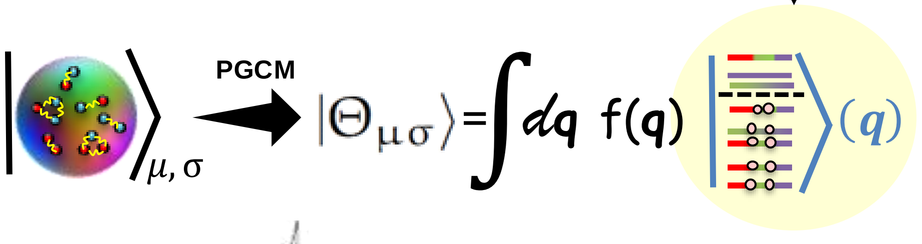
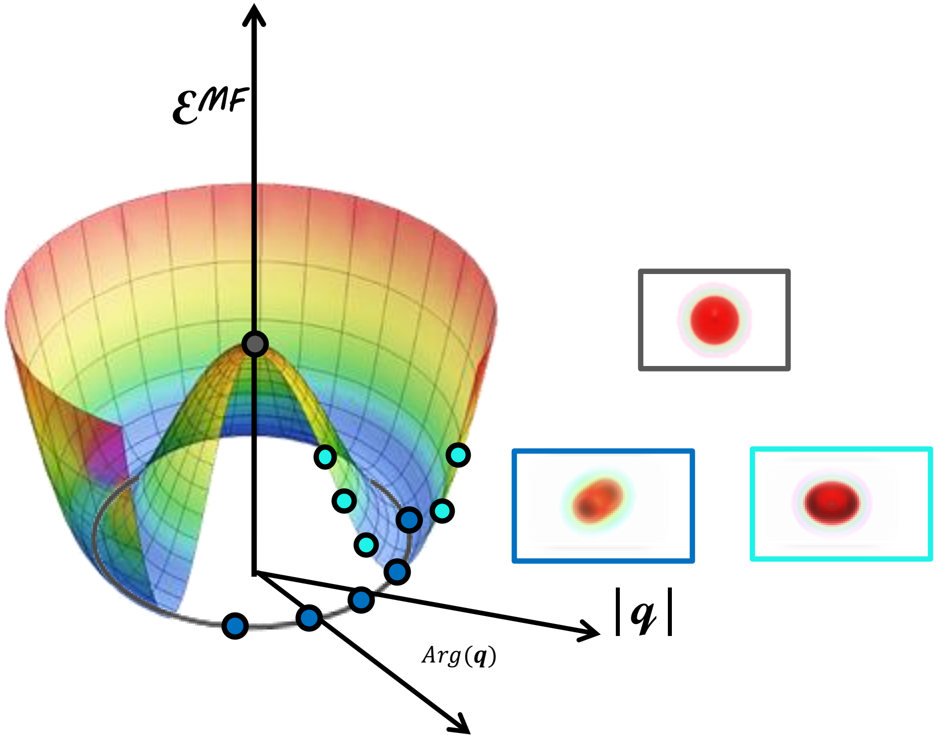
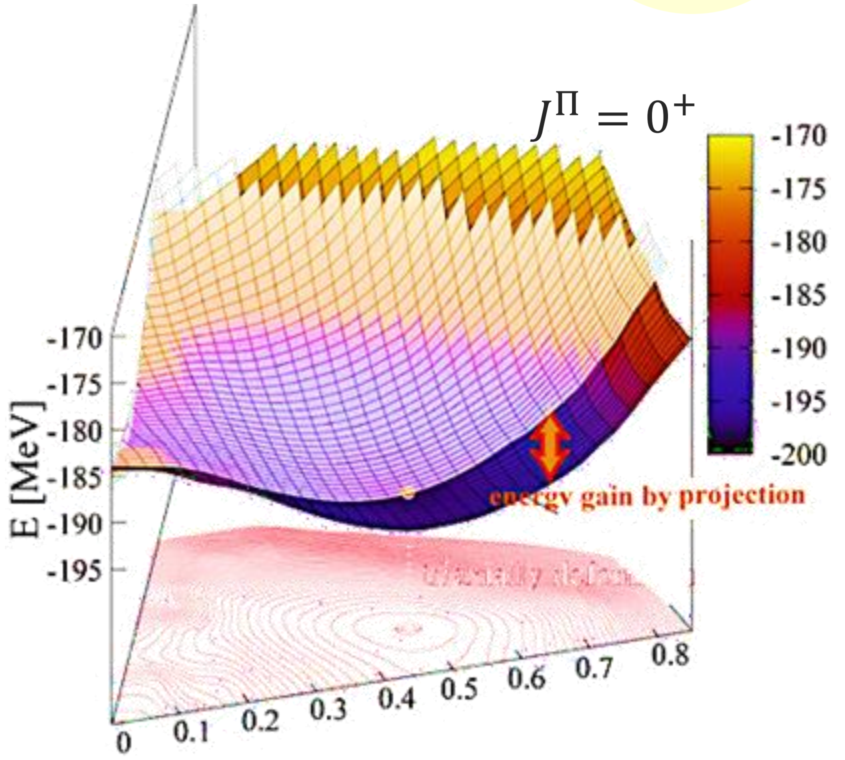


◉ Post-HFB treatment : PGCM

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



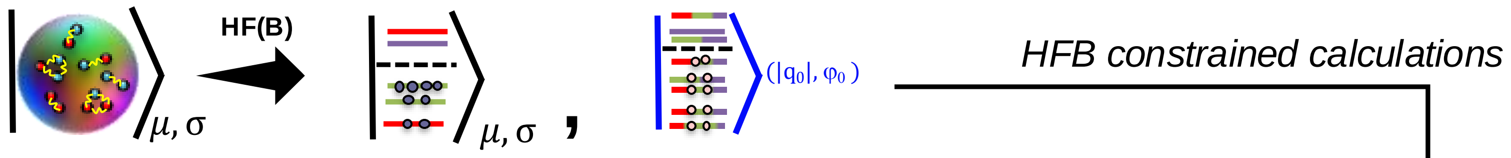




The Energy Density Functional Method

◉ HFB treatment

⇢ A-nucleon problem ⟶ A 1-nucleon problems



◉ Post-HFB treatment : PGCM

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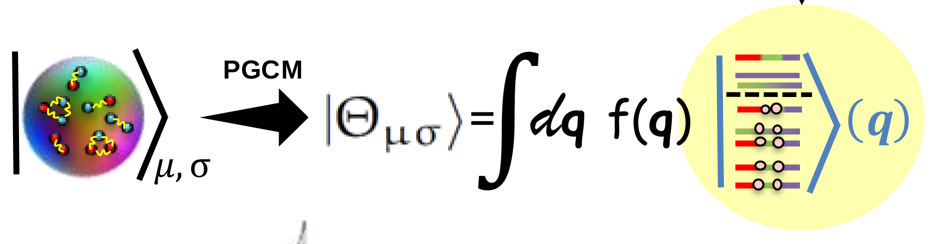
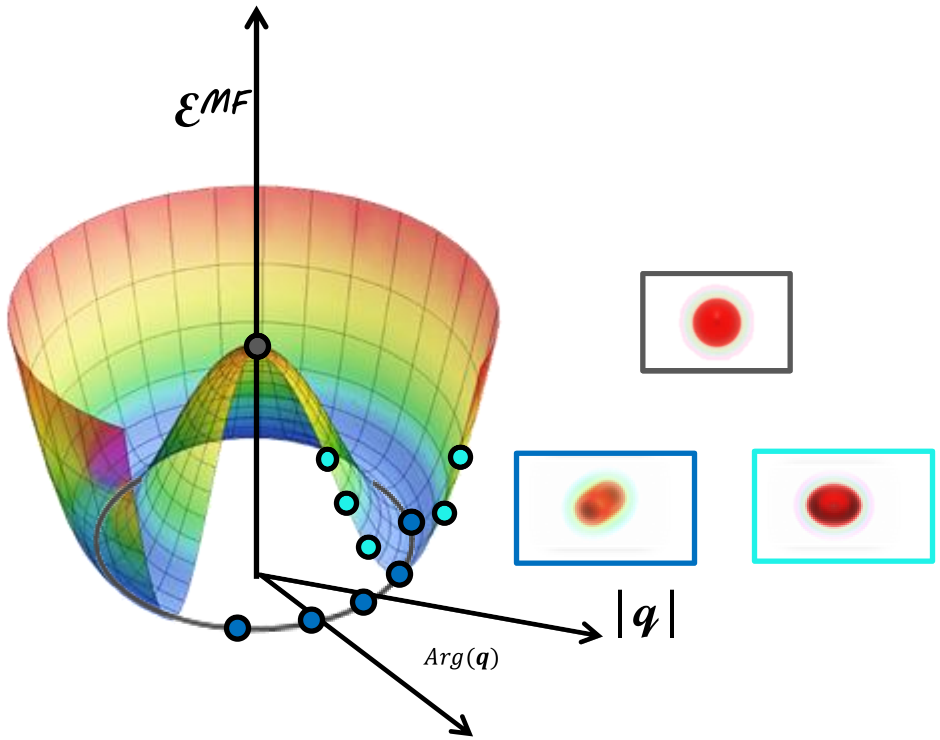
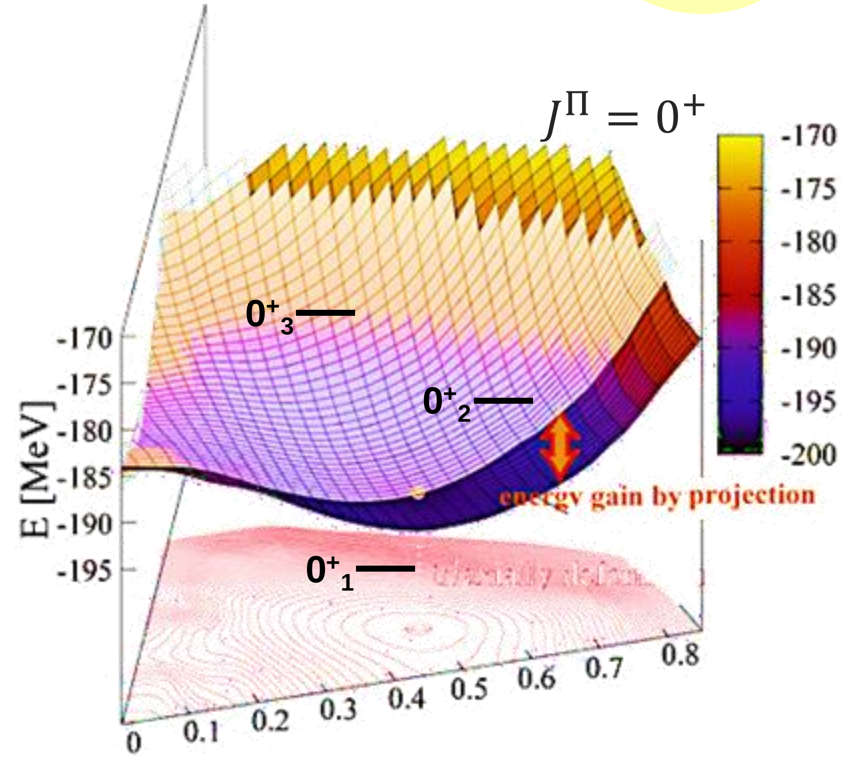


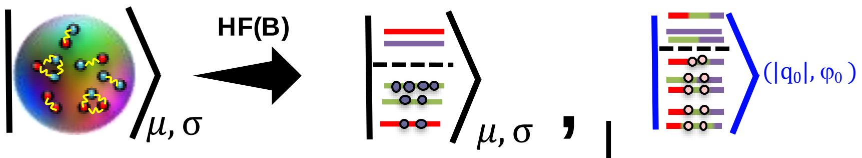




The Energy Density Functional Method

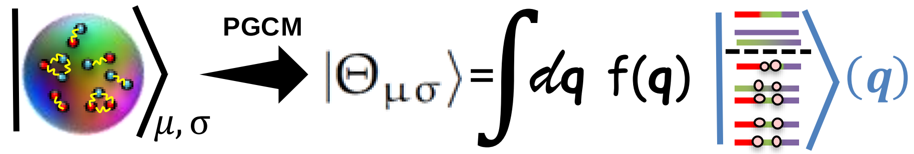
◉ HFB treatment

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



◉ Post-HFB treatment : PGCM

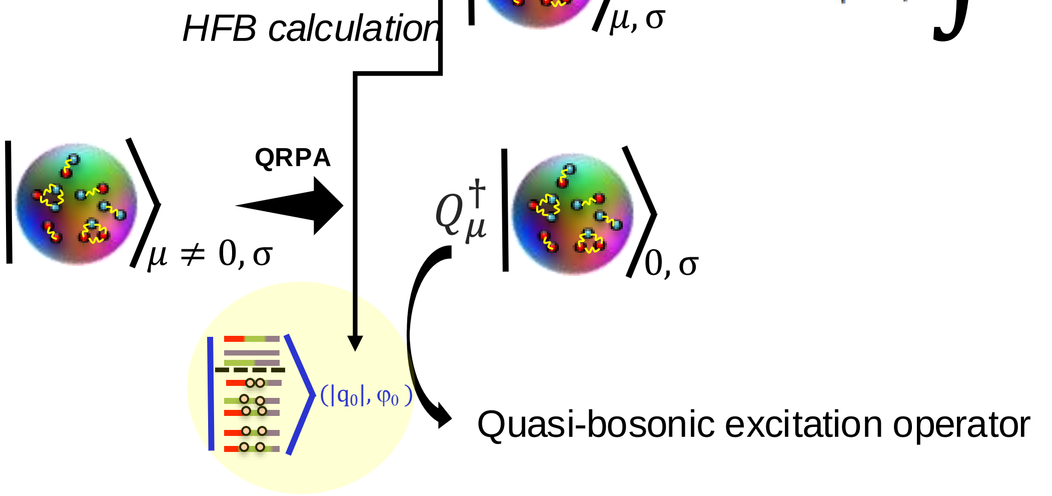
--> Symmetry-conserving (non orthogonal) mixture of symmetry-breaking HFB vacua



◉ Post-HFB : QRPA

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

--> Harmonic limit of the GCM



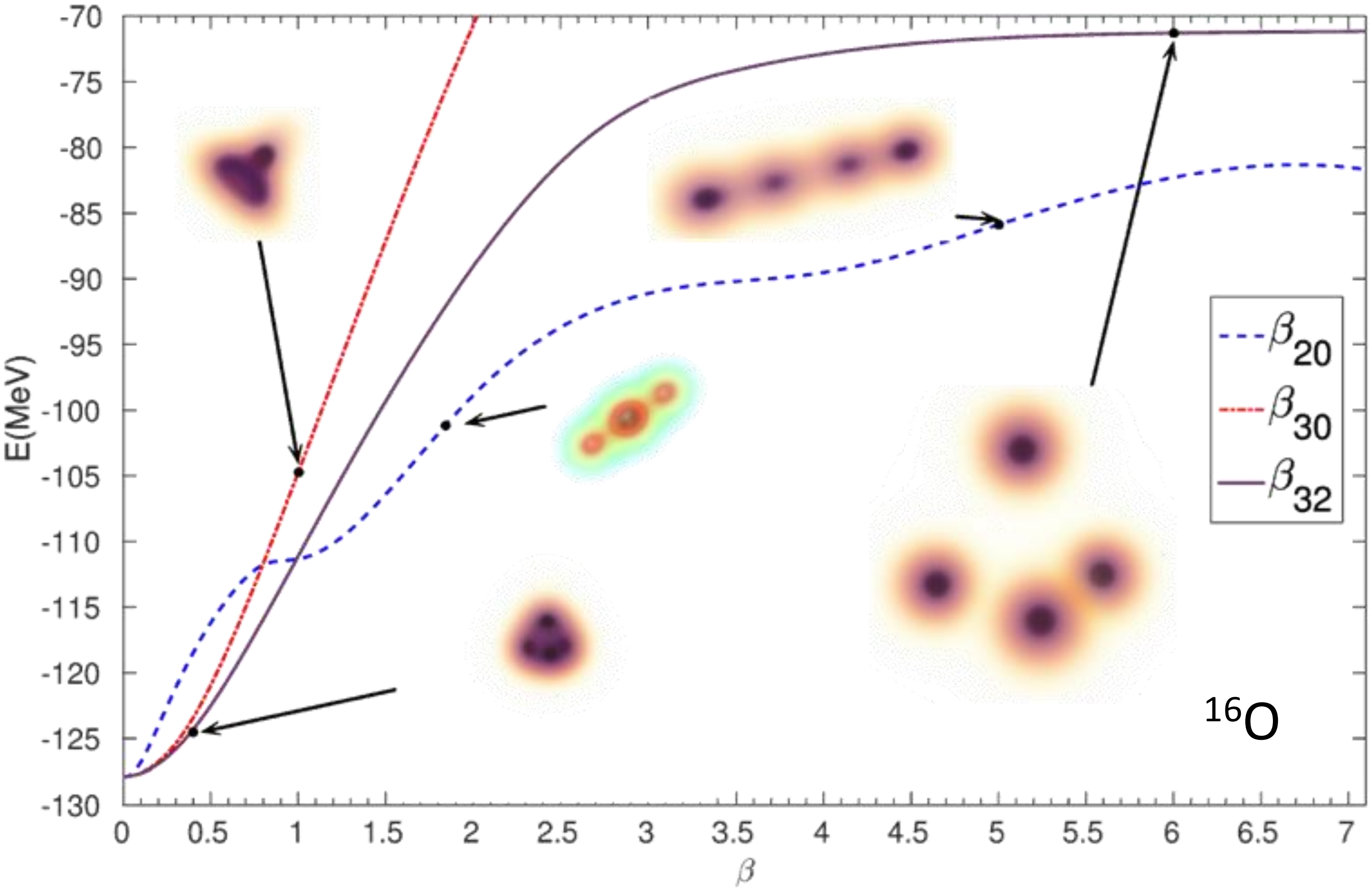
Outline

1. What strategies to account for nuclear clustering
2. EDF in a nutshell
3. EDF & clustering

EDF & Nuclear clustering

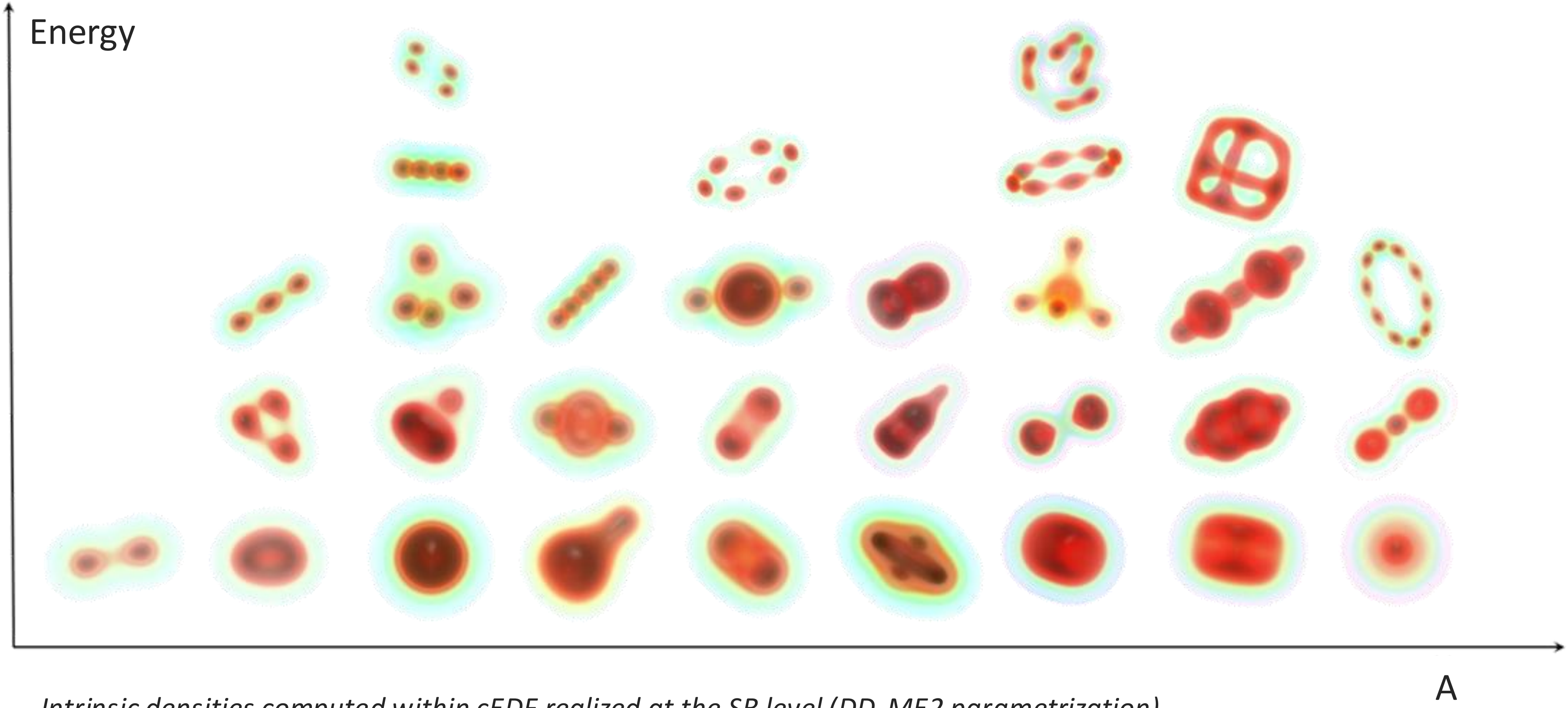
- Look for a collective field whose fluctuations cause nucleon to aggregate into α dofs

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



Nuclear clustering

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



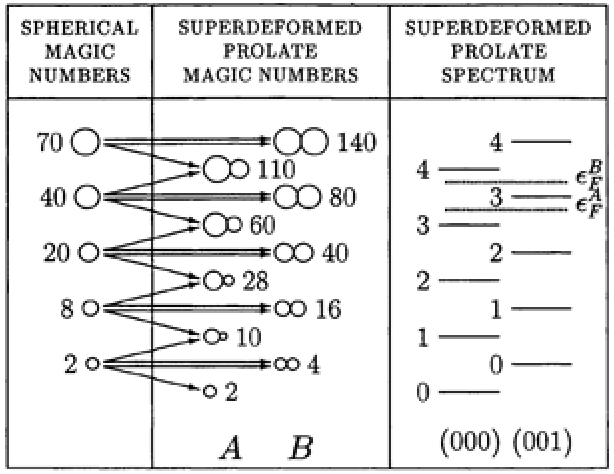
Intrinsic densities computed within cEDF realized at the SR level (DD-ME2 parametrization)

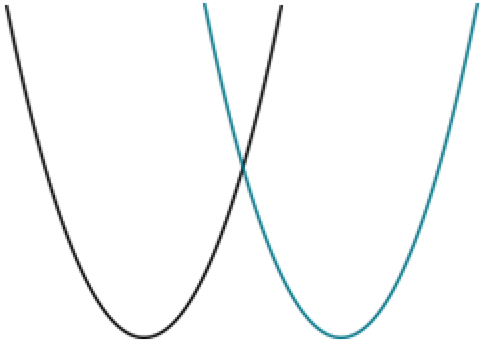
Deformation & Nuclear clustering

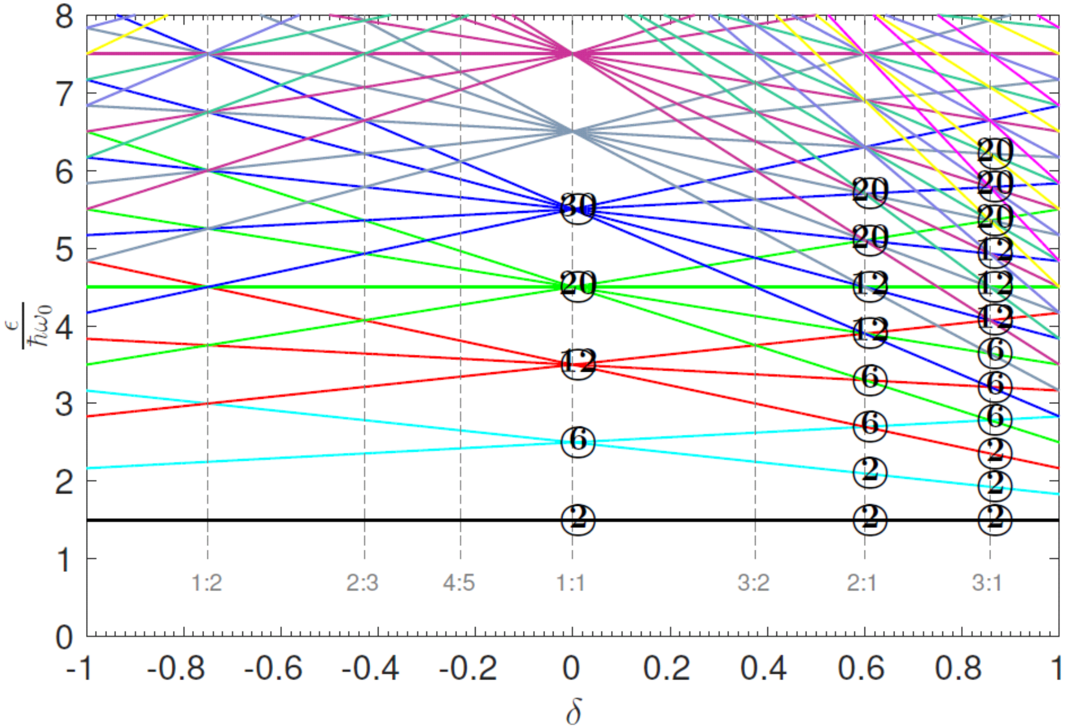
◉ Role of deformation

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

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







Nazarewicz & *Dobaczewski*, PRL 1992

Deformation = necessary condition, but not a sufficient one

Strength of correlations

- Strength of correlations measured by dimensionless ratios

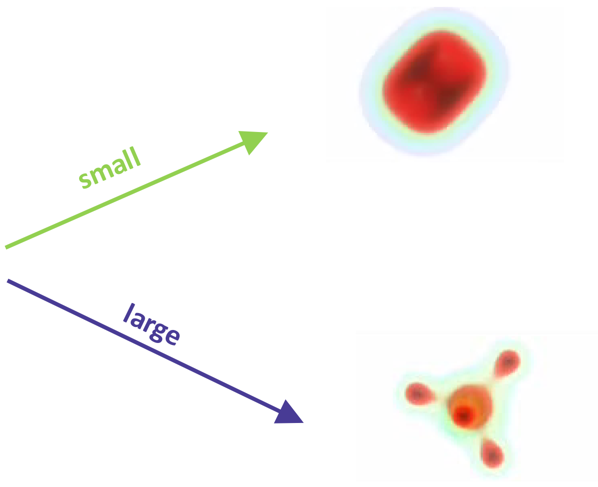
$$\sqrt{\Lambda} \equiv \sqrt{\frac{\langle V\rangle}{\langle T\rangle}} = \sqrt{2}\left(\frac{3}{4\pi}\right)^{\frac{1}{6}} (2MU)^{\frac{1}{4}} (An)^{-\frac{1}{6}} \sim \alpha_{loc}$$

Nucleon mass (M)

Number of nucleons (A)

Depth of the confining potential (U)

Mean density (n)



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

Strength of correlations

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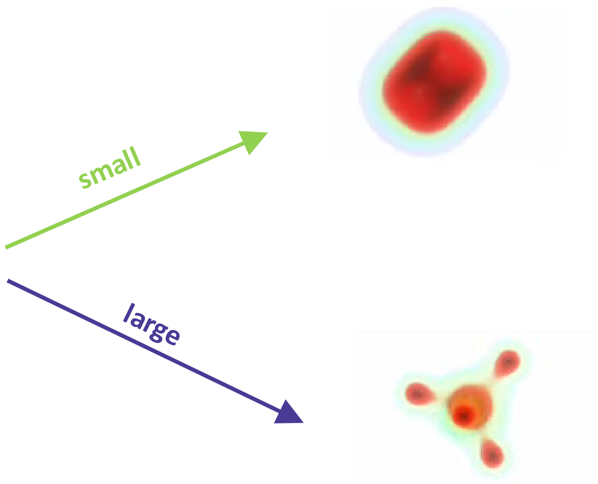
Depth of the confining potential

Mean density

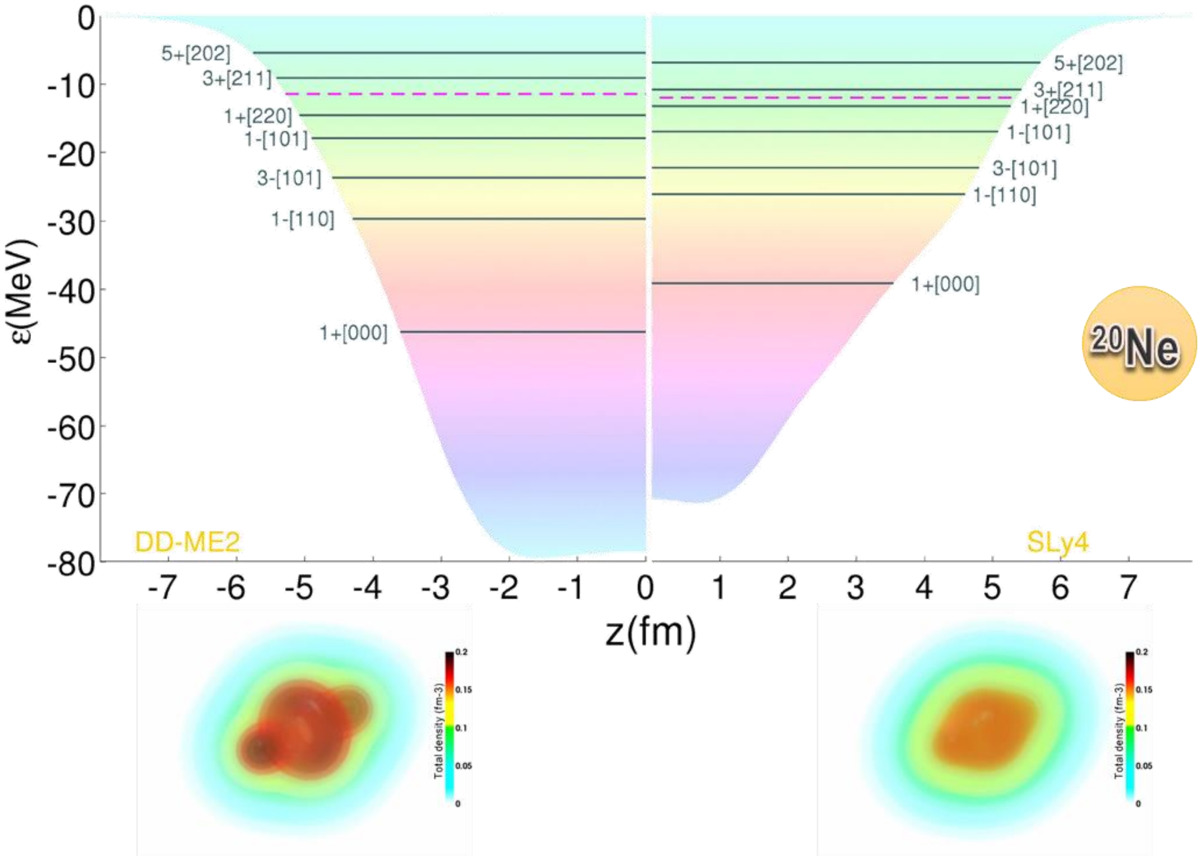


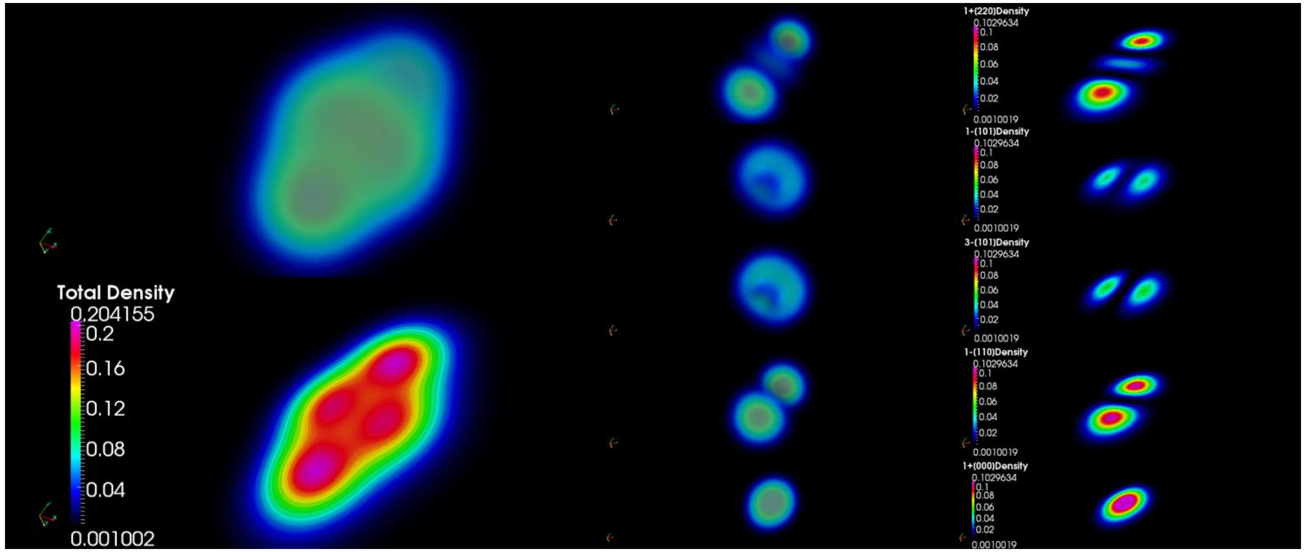
Clustering favored
⇢ For deep confining potential
⇢ For light nuclei
⇢ In regions at low-density

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

Effect of the depth of the confining potential

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





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

Strength of correlations

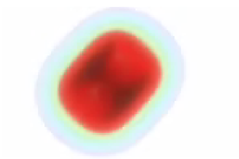
- Strength of correlations measured by dimensionless ratios

Nucleon mass — Number of nucleons

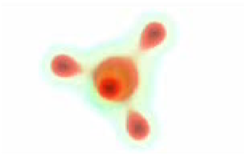
$$\sqrt{\Lambda} \equiv \sqrt{\frac{\langle V \rangle}{\langle T \rangle}} = \sqrt{2}\left(\frac{3}{4\pi}\right)^{\frac{1}{6}} (2MU)^{\frac{1}{4}} (An)^{-\frac{1}{6}} \sim \alpha_{loc}$$

Depth of the confining potential — Mean density

small



large



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

- Formation/dissolution of clusters : Mott parameter

Size of the nucleus X

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

inter-nucleon average distance

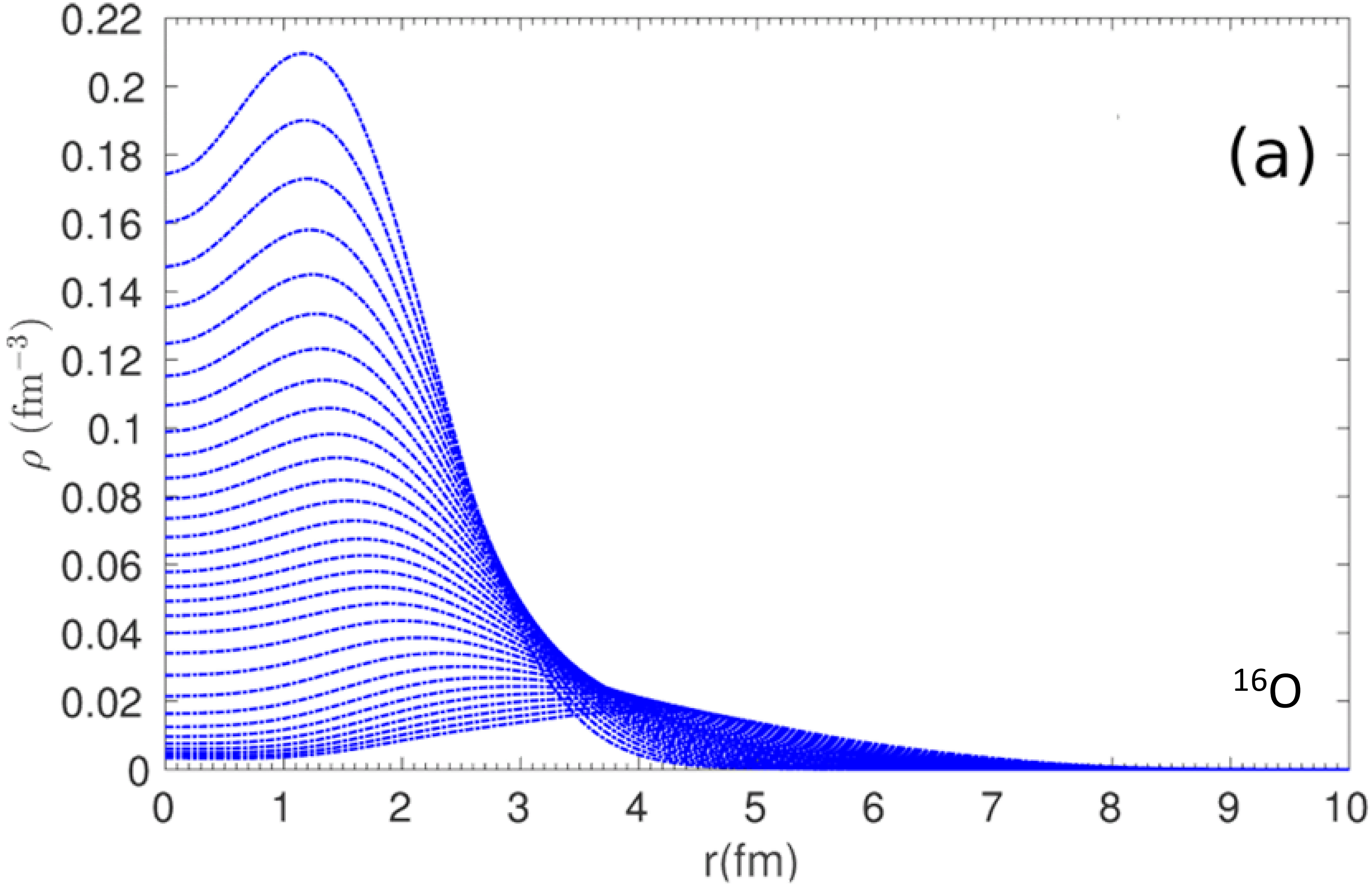
$n^{\alpha}_{Mott} \sim 0.25\rho_{sat}$ — Size of an α in free-space

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

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

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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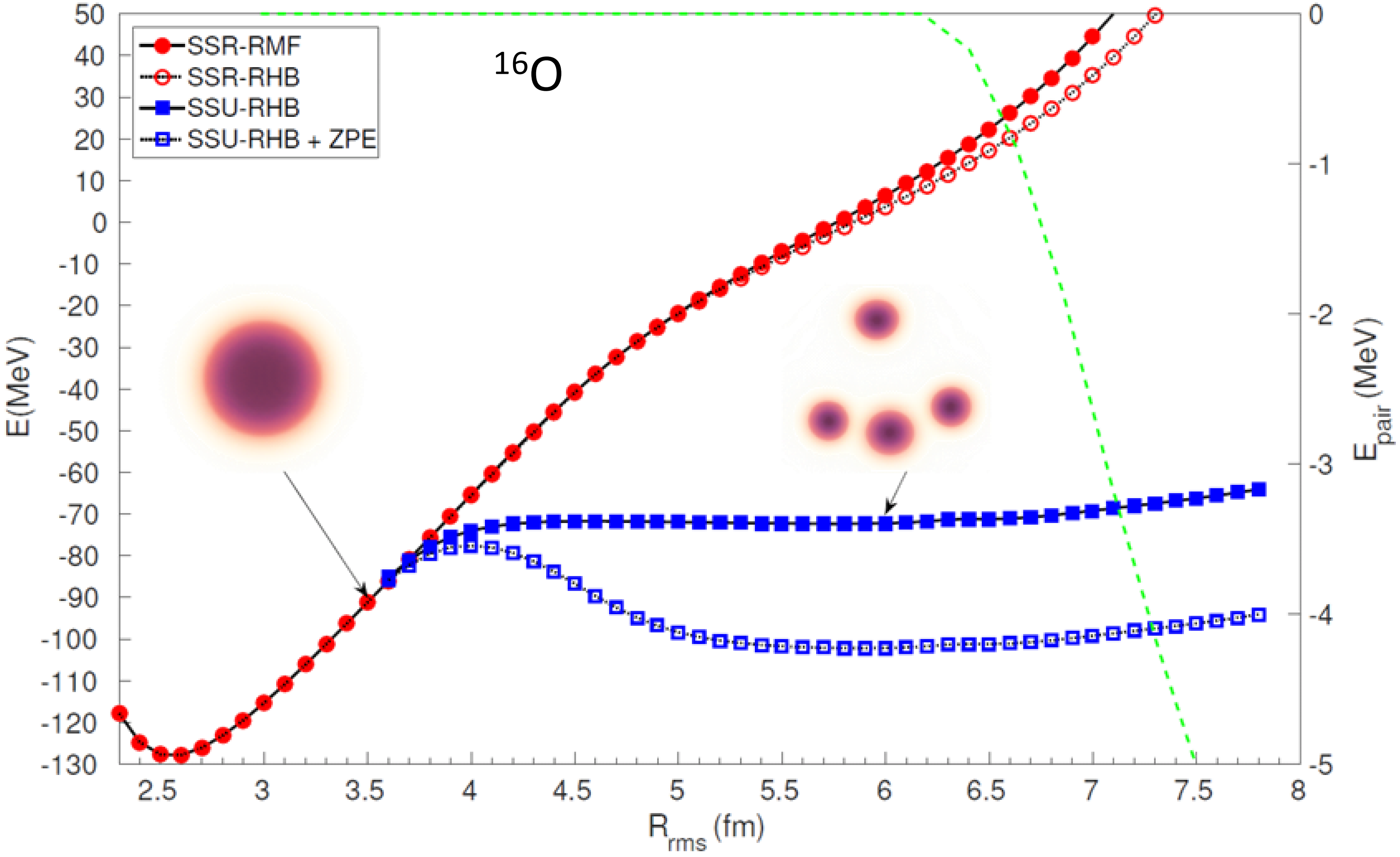

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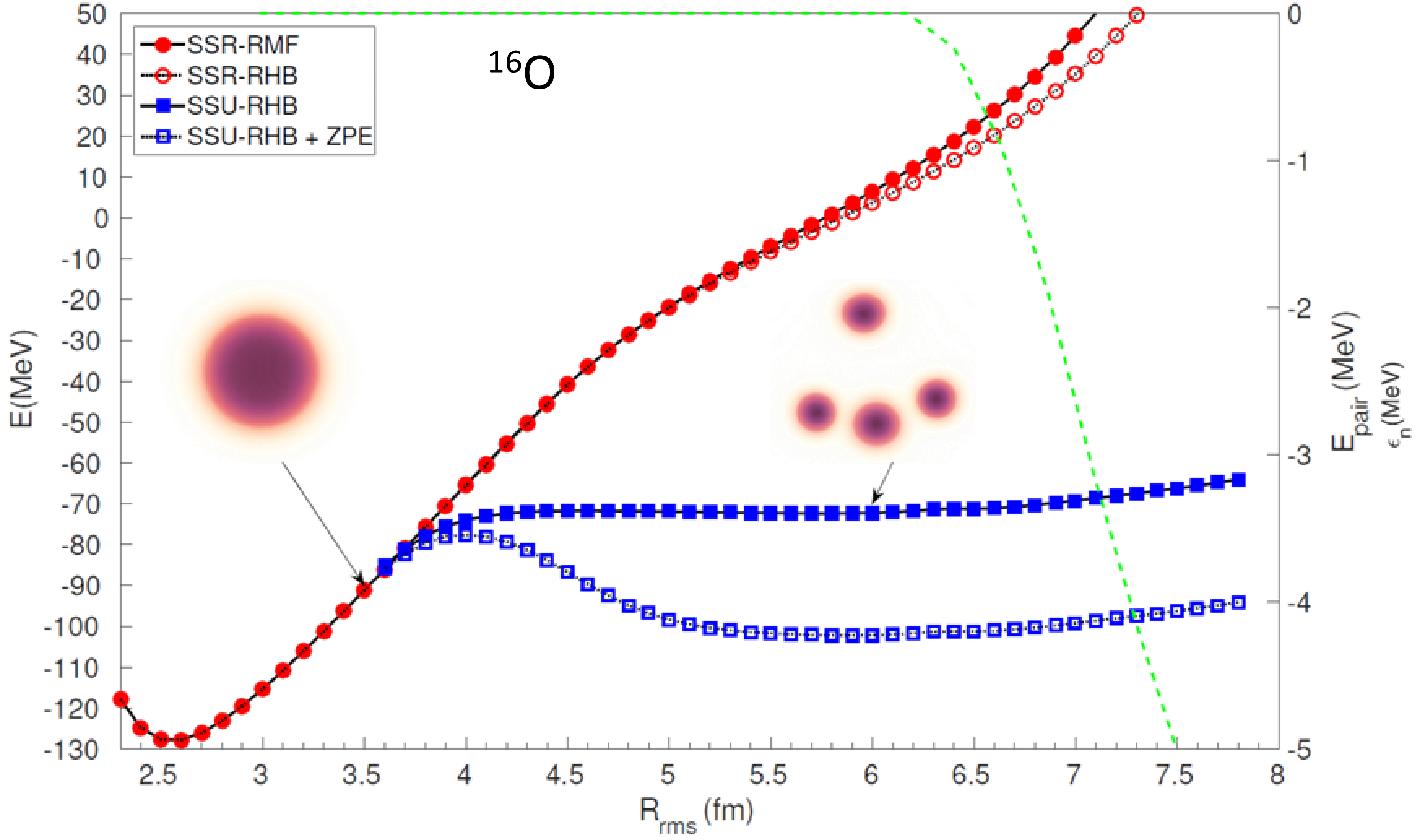

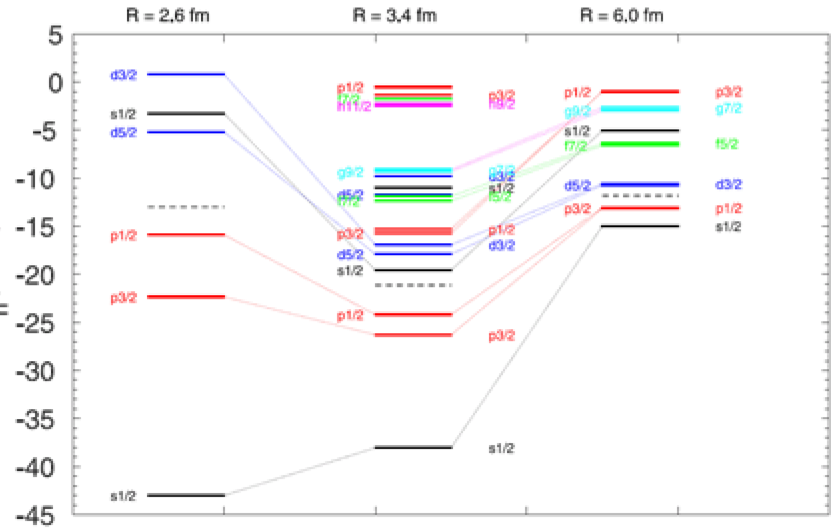

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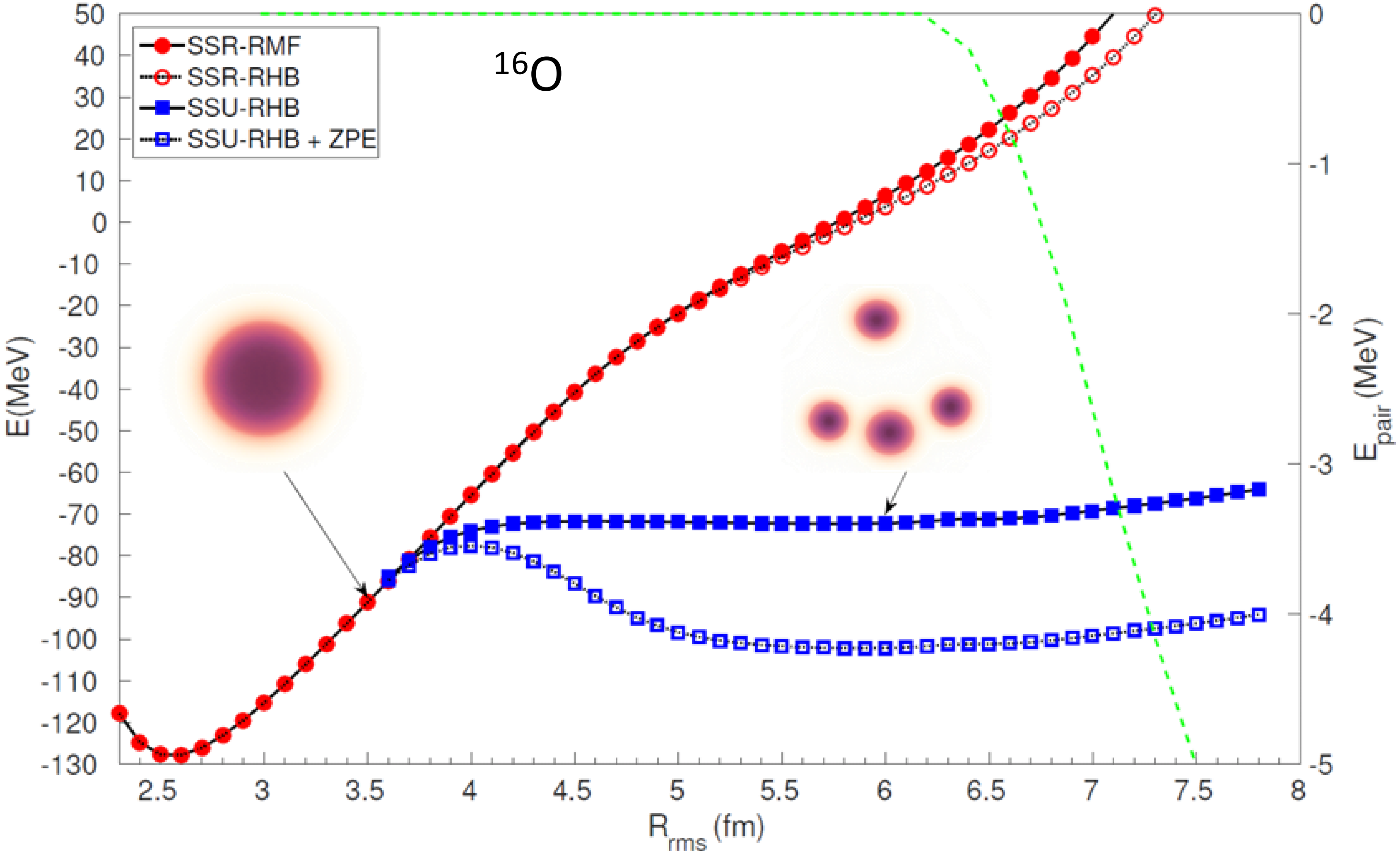

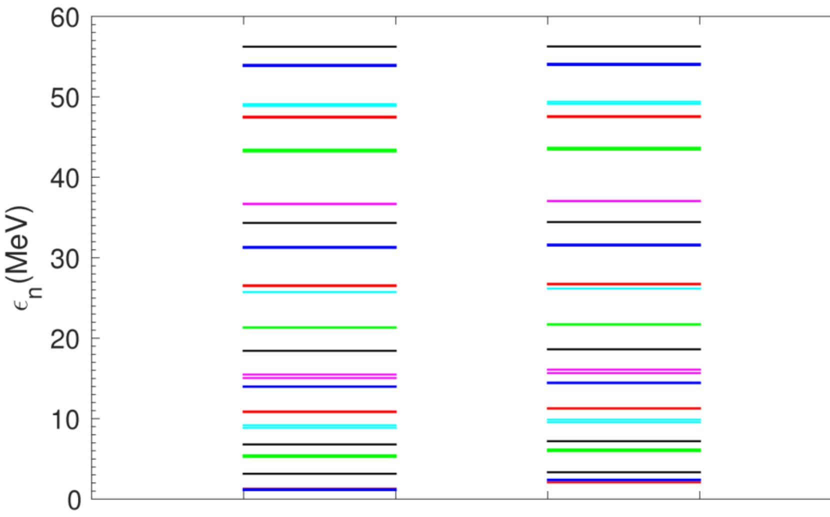

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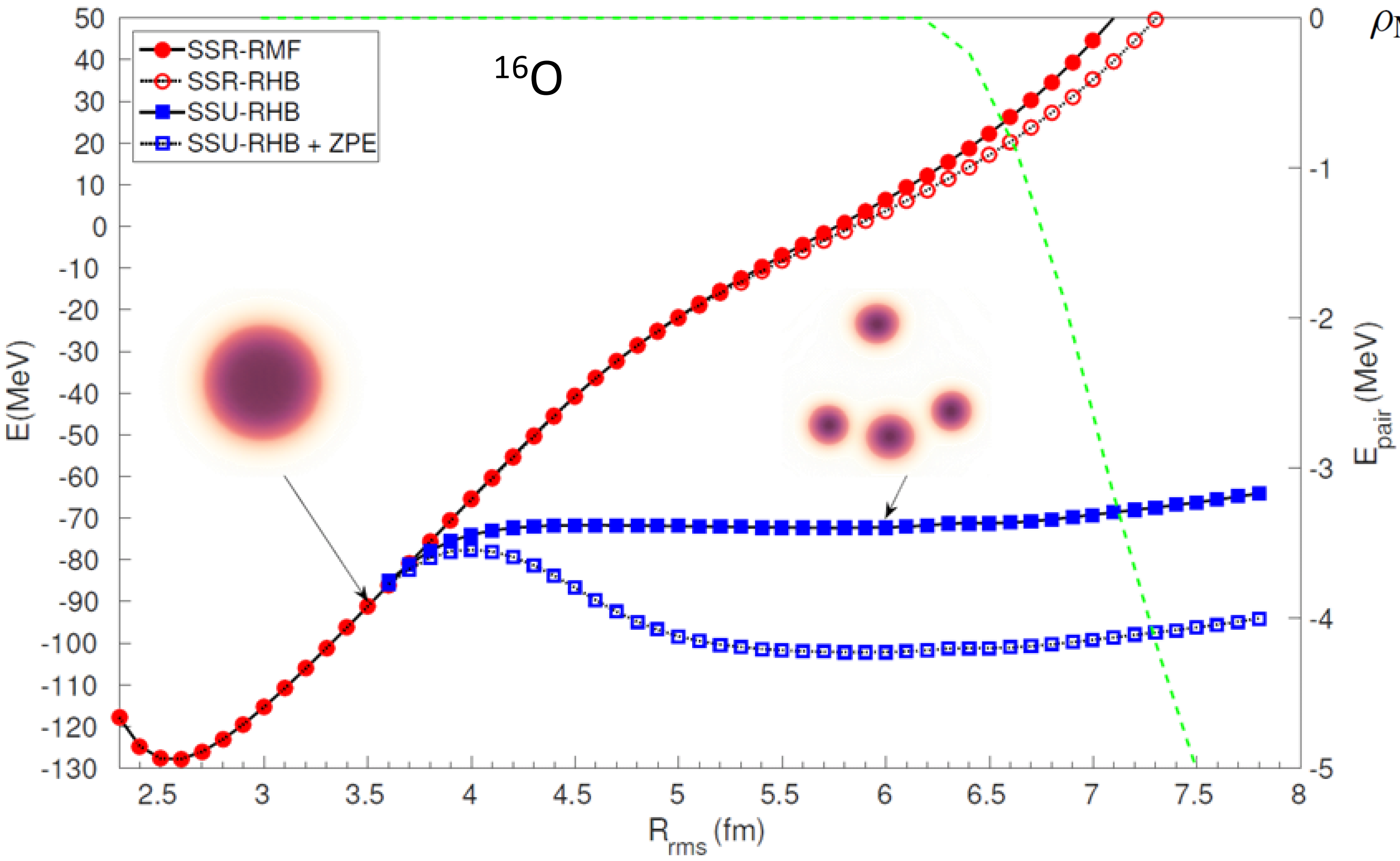
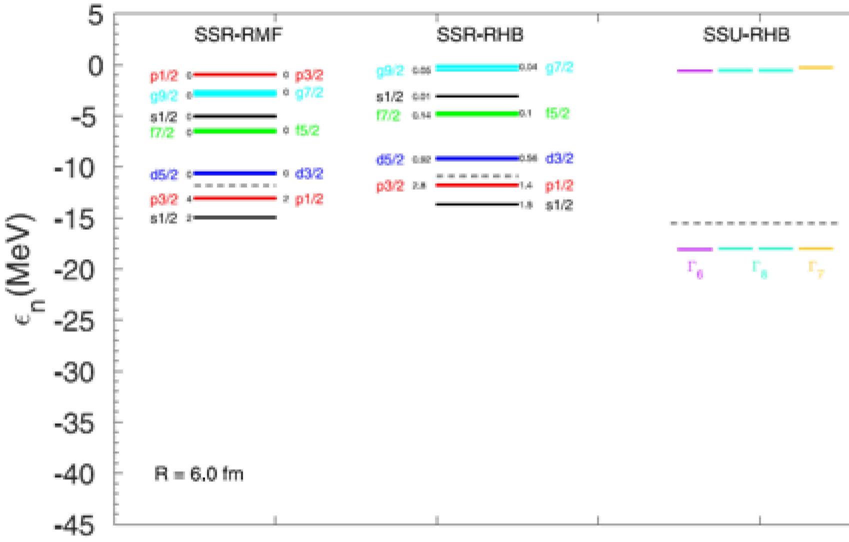
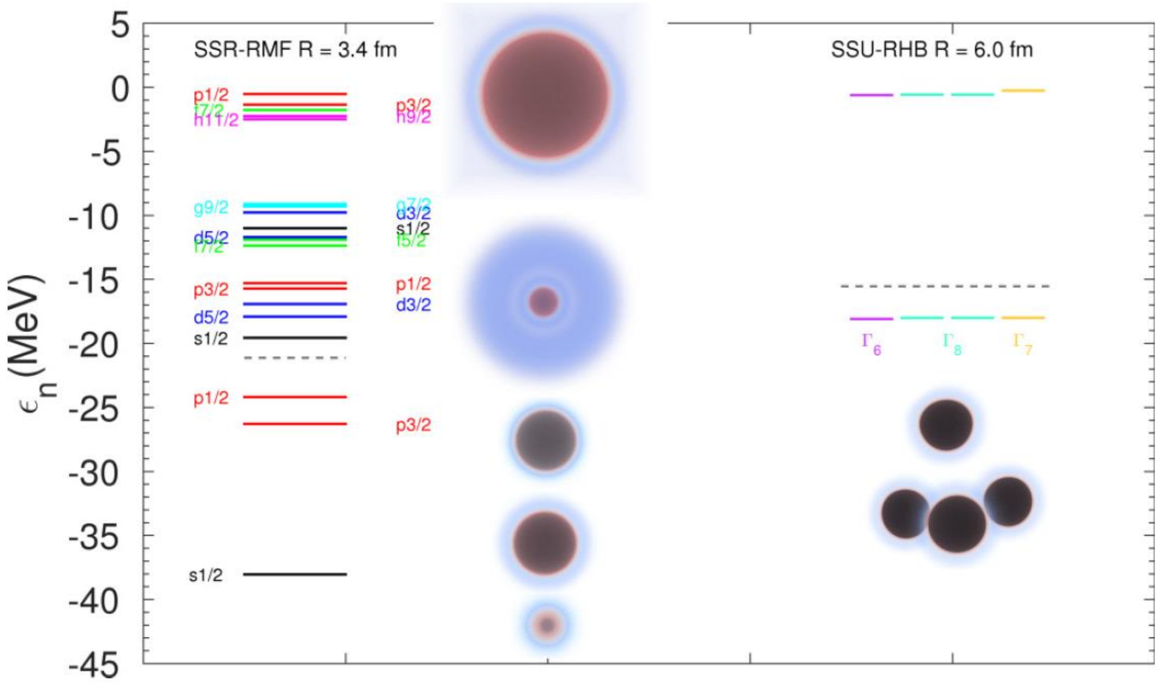


$$\rho_{\mathrm{Mott}}/\rho_0 = (R_{\mathrm{eq}}/R_c)^3 \approx \rho_0/3$$

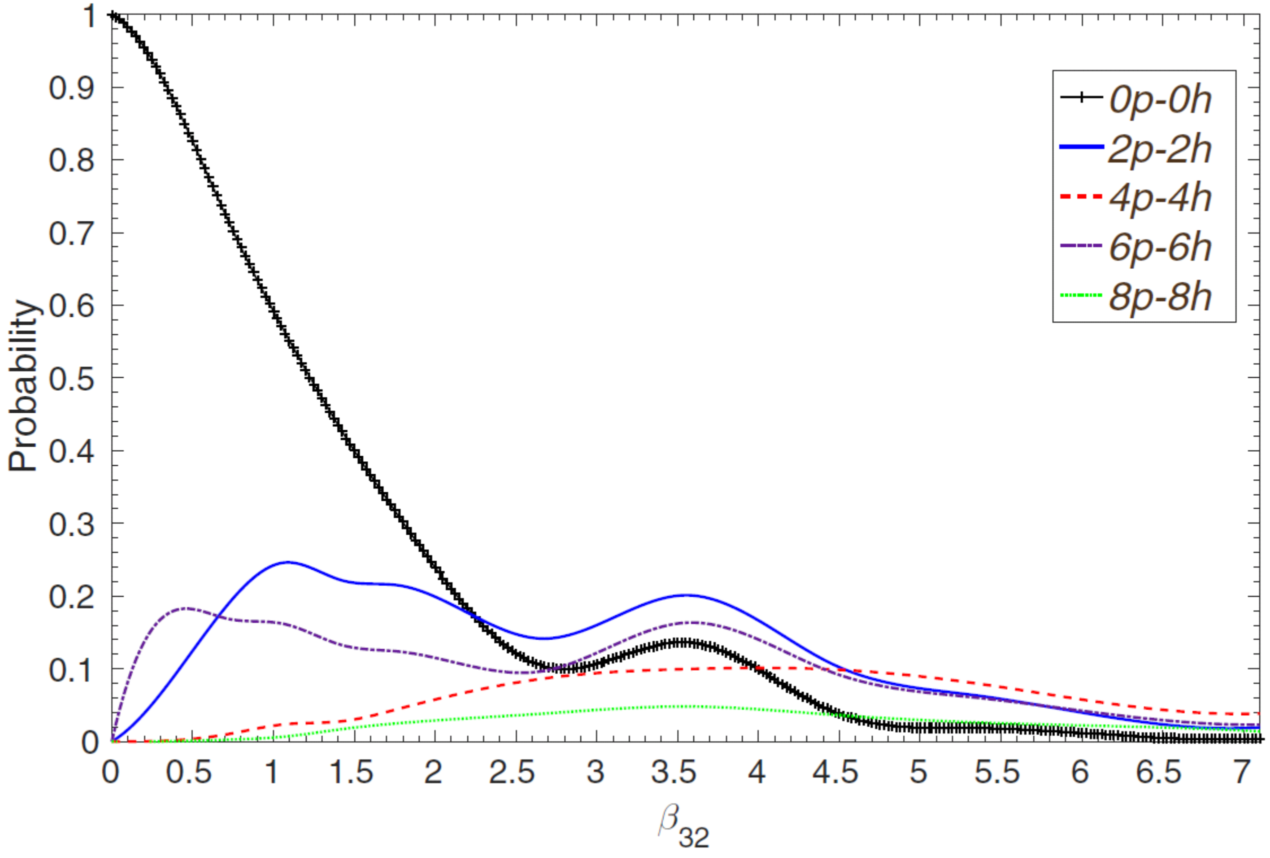


Effect of the density

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

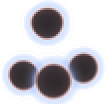


Symmetry breaking : O(3) → Td



LCAO-MO

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



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

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

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

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

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

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

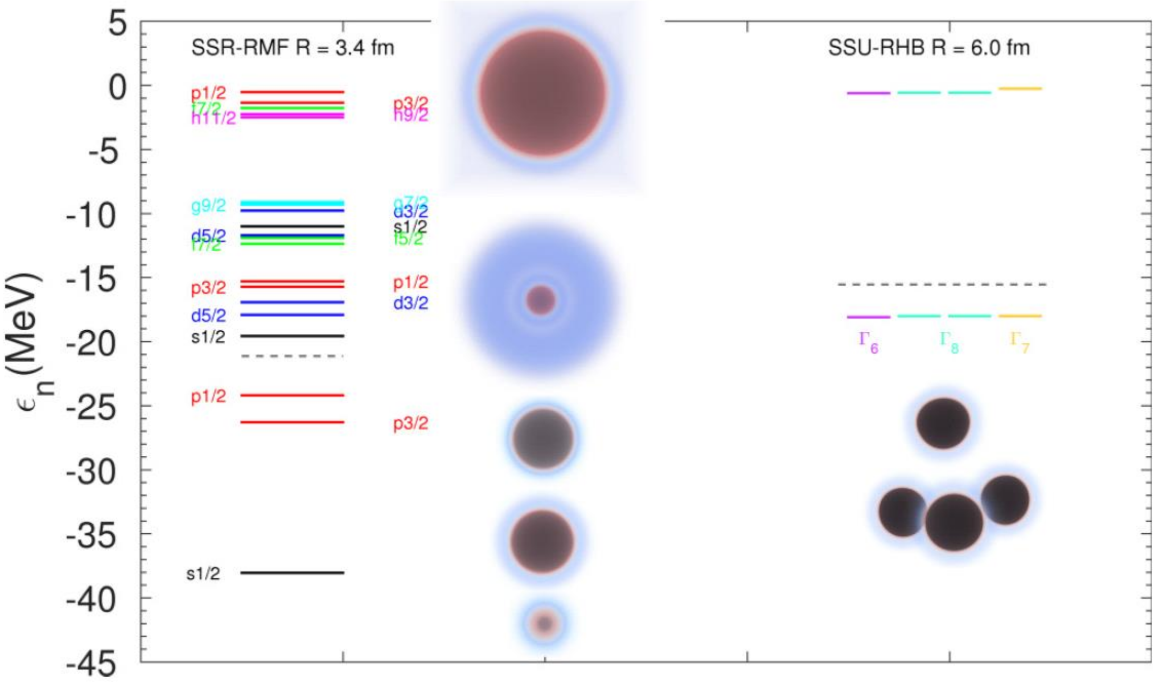
$$\psi_3 = \frac{1}{\sqrt{2}}(-\phi_1 + \phi_3) \qquad E_3 = E_2$$

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

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

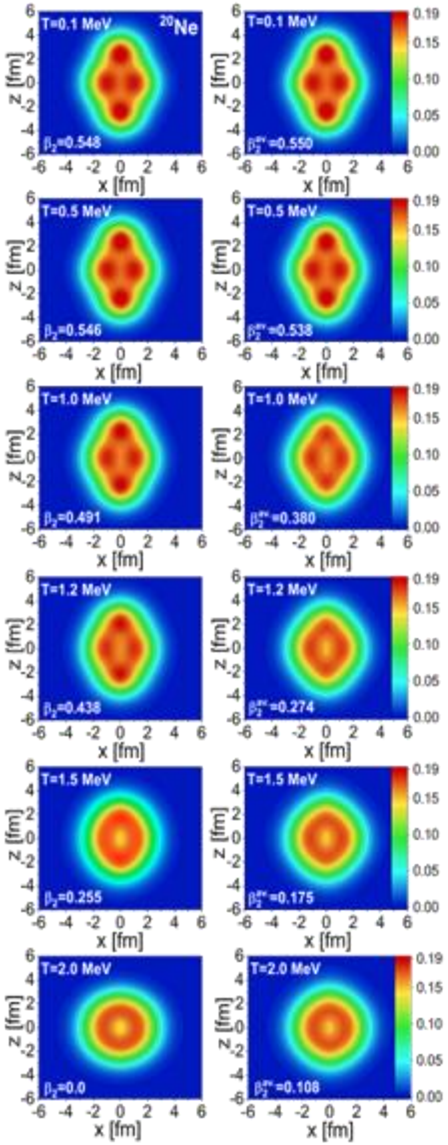
$$\psi'_3 = \frac{1}{2}(\phi_1 + \phi_2 - \phi_3 - \phi_4),$$

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

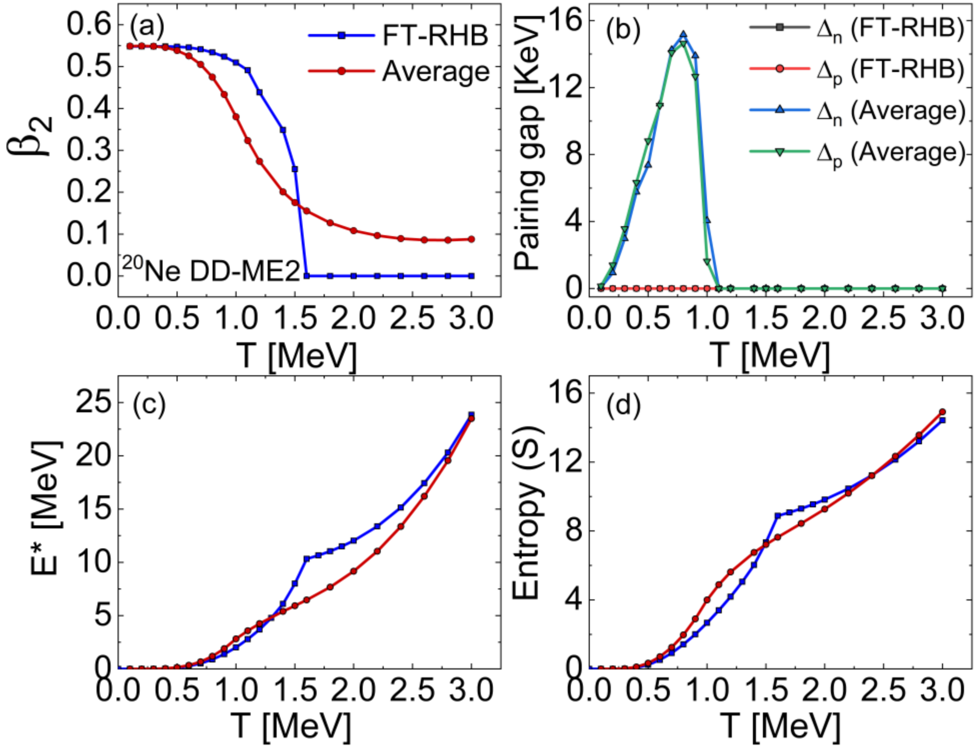


Thermal phase transition   see Elias Khan talk

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



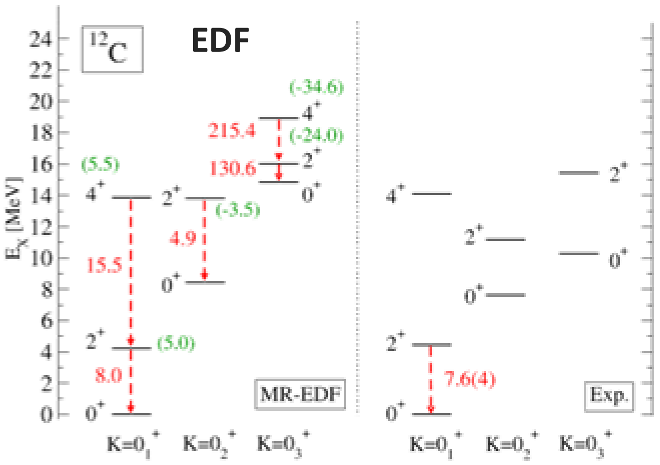
$$\overline{O} = \frac{\int d\beta_2 O(\beta_2, T) \exp(-\Delta F(\beta_2, T)/T)}{\int d\beta_2 \exp(-\Delta F(\beta_2, T)/T)}.$$



Nuclear clustering & PGCM

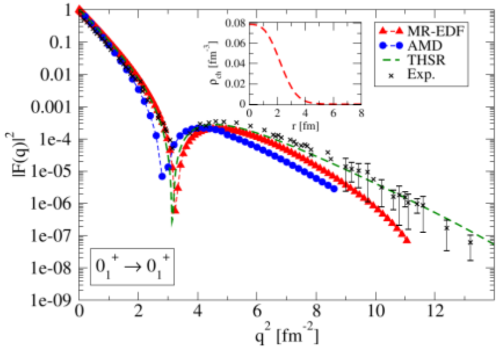
◉ Spectroscopy

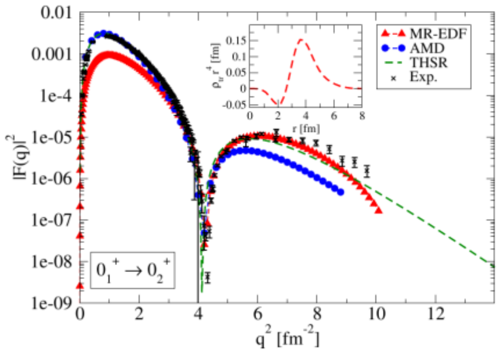
EDF



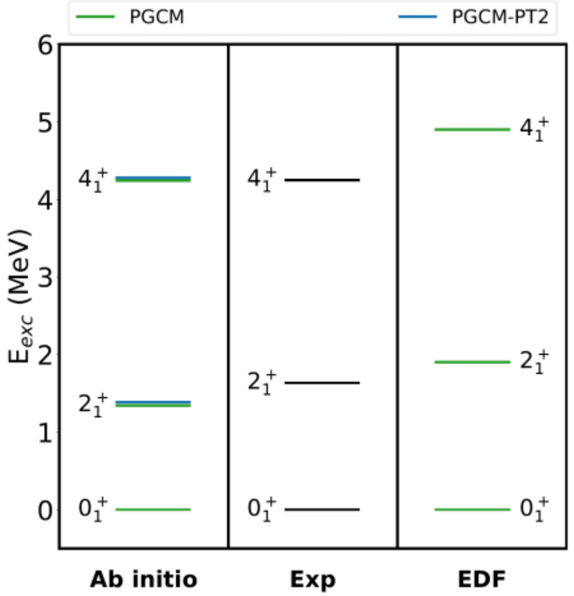
Marević, Ebran, Khan, Nikšić, and Vretenar, 2019

EDF





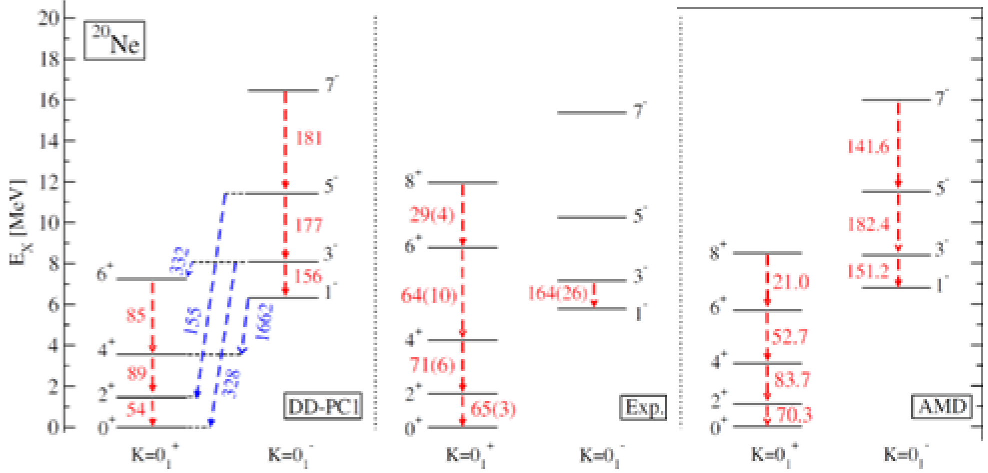
Ab initio



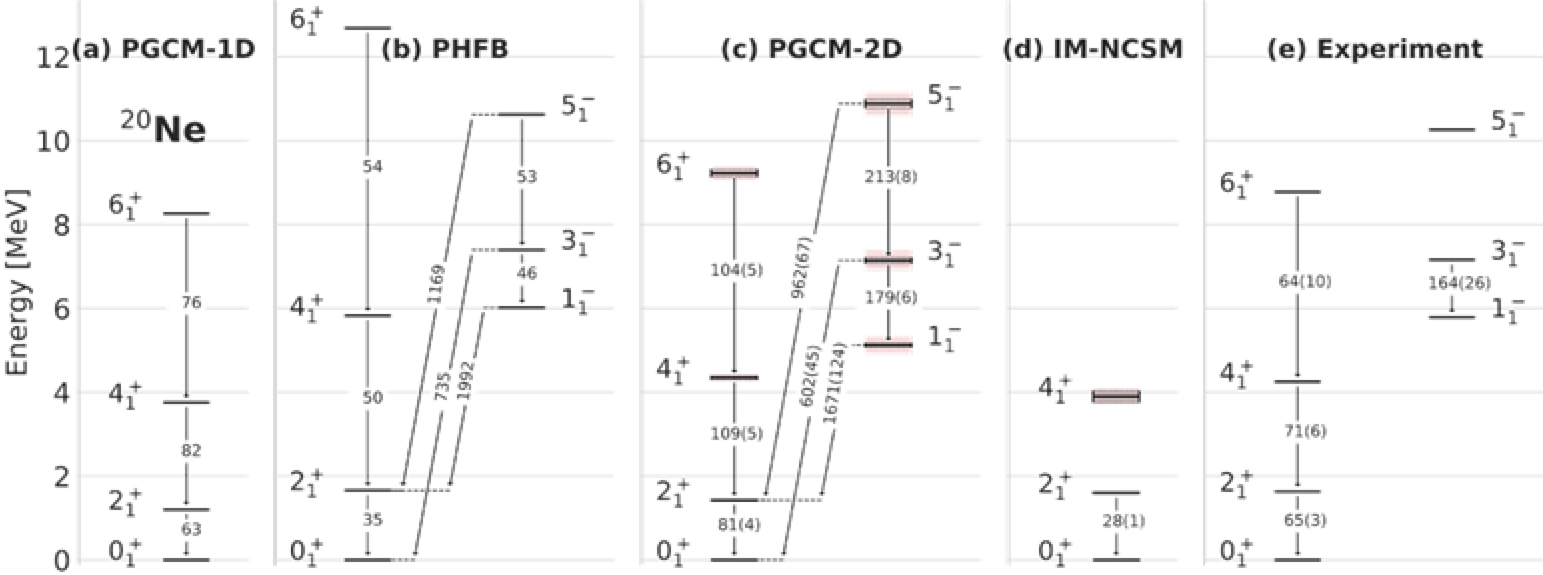
Frosini, Duguet, Ebran, Bally, Hergert, Rodriguez, Roth, Yao, Somà, EPJA 2022

EDF

Marevic, Ebran, Khan, Niksic, Vretenar, 2018



Ab initio



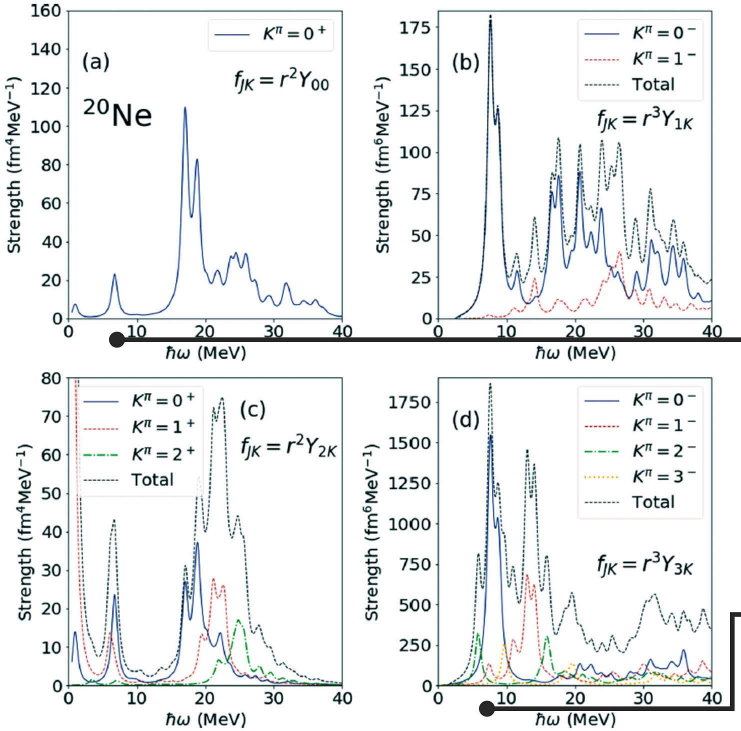
Frosini, Duguet, Ebran, Bally, Mongelli, Rodriguez, Roth, Somà, EPJA 2022

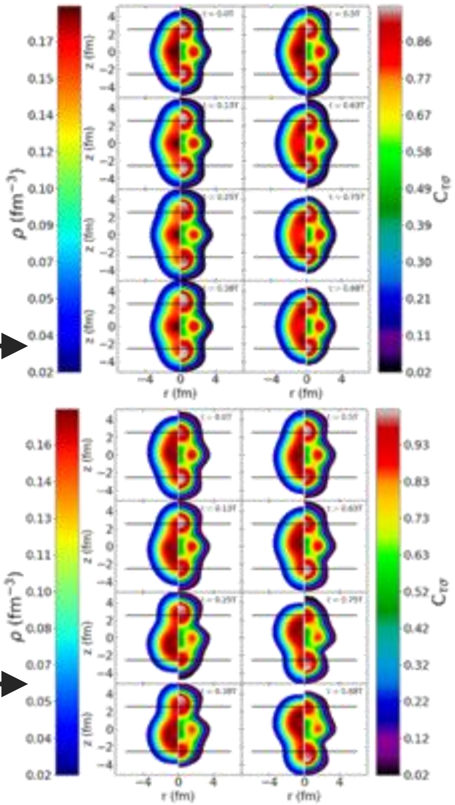
Nuclear clustering & QRPA

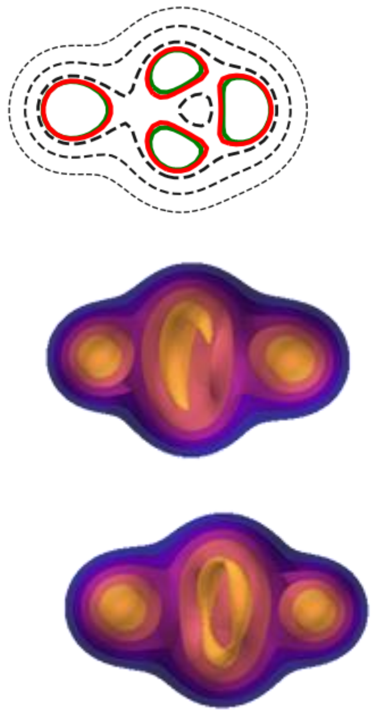
◉ Cluster vibration

Ab initio

EDF



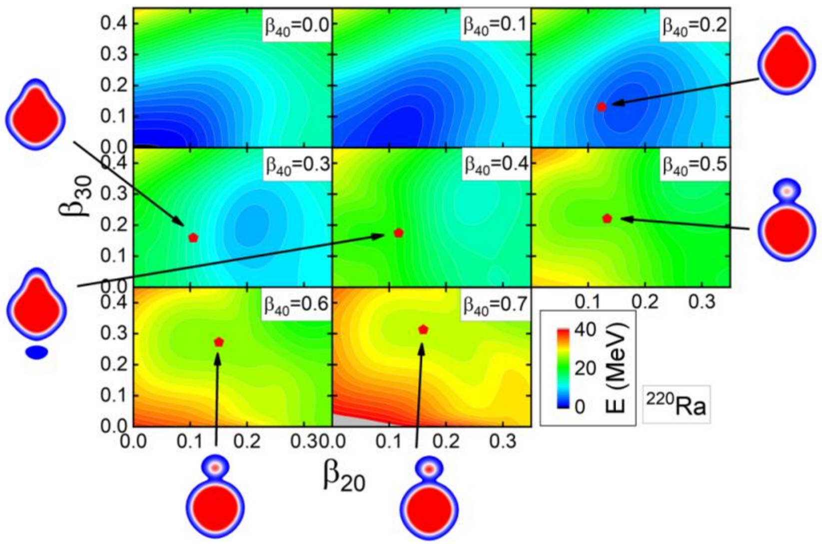


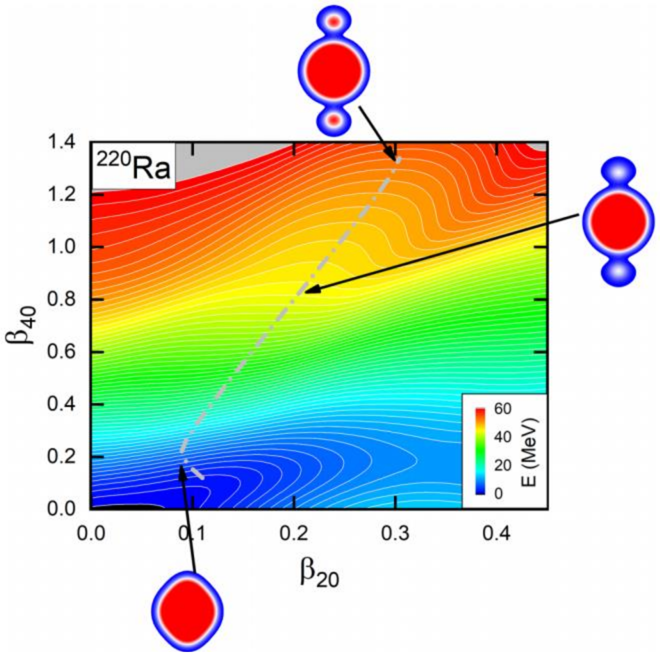


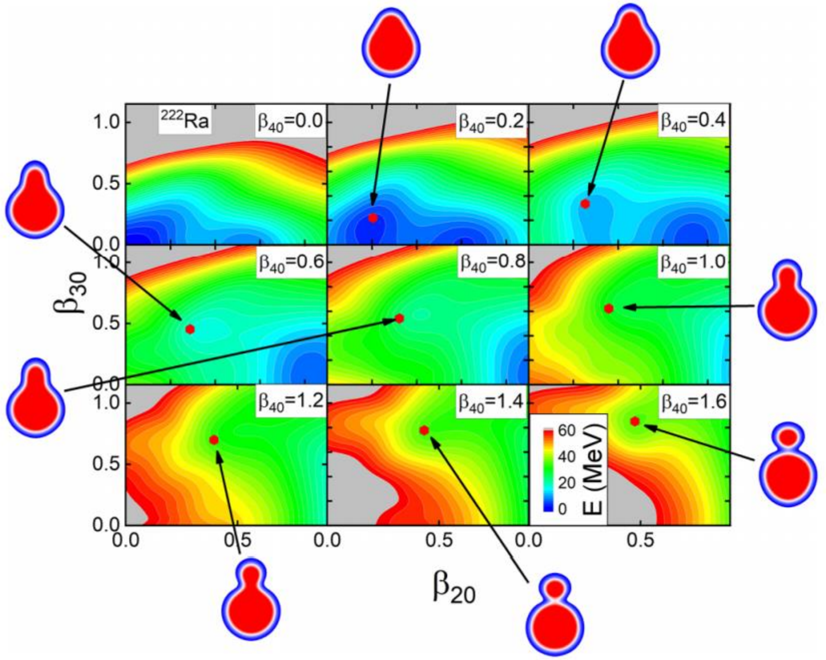
Mercier, Bjelčić, Nikšić, Ebran, Khan, Vretenar 2021
Mercier, Ebran, Khan 2022

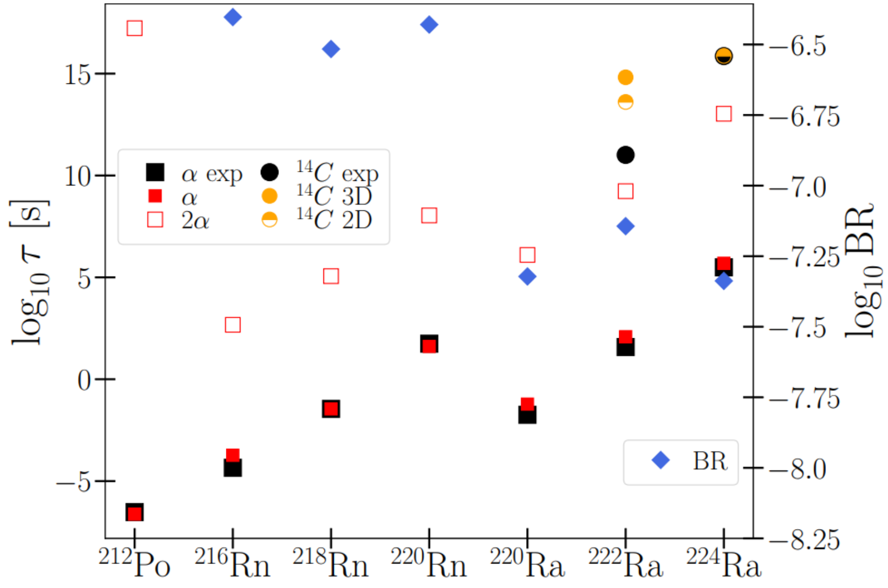
Ab initio QFAM time-dependent intrinsic density
Frosini, Ebran, Duguet, Somà, unpublished

Cluster, α and 2α radioactivities







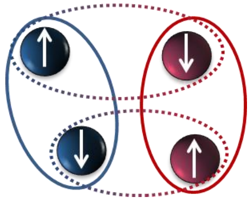


Zhao , Ebran, Heitz , Khan , Mercier, Nikšic,Vretenar (2023)

EDF & Nuclear clustering

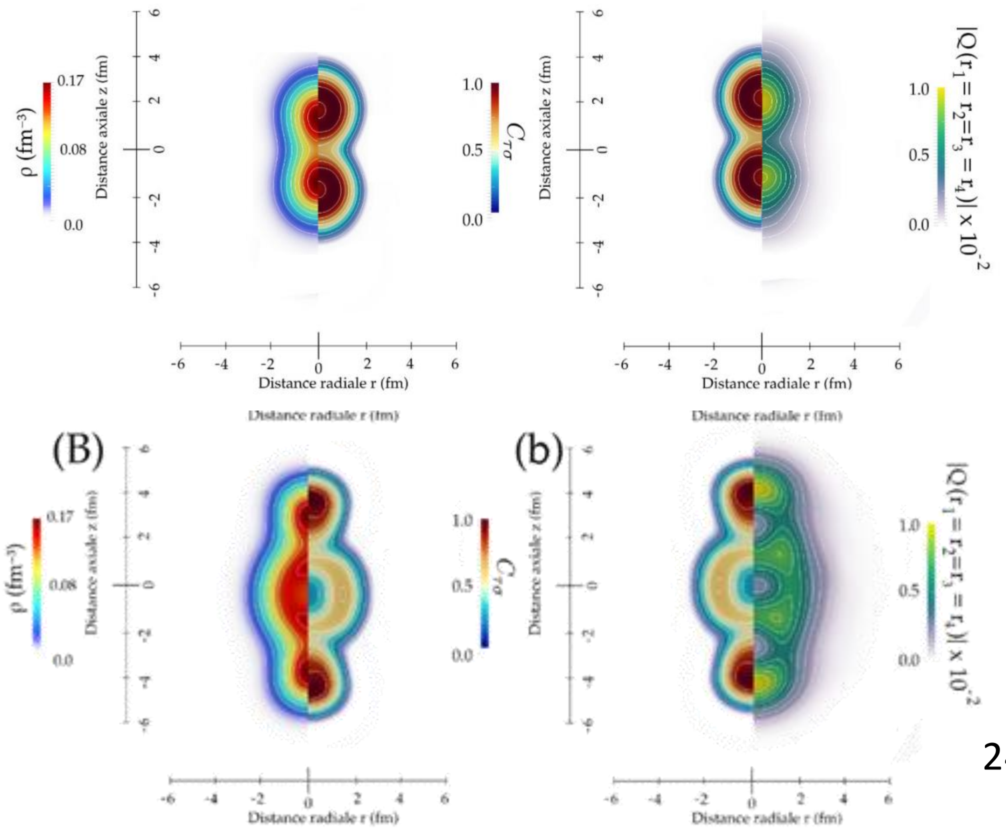
◉ How to account for correlations underpinning α-clustering ?

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



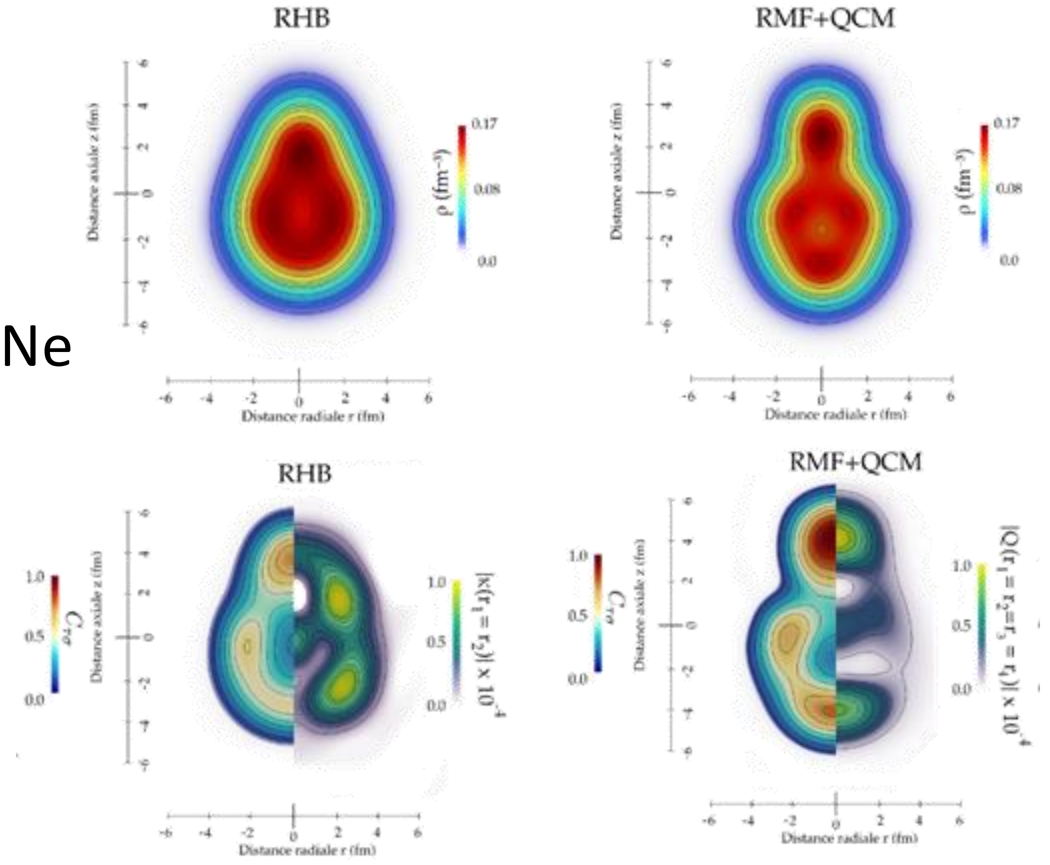
$$|\Psi\rangle = \left(\mathcal{Q}^\dagger\right)^{n_q}|0\rangle \qquad \mathcal{Q}^\dagger = 2\Gamma_1^\dagger\Gamma_{-1}^\dagger - \left(\Gamma_0^\dagger\right)^2 \qquad \Gamma_t^\dagger = \sum_k x_k P_{k,t}^\dagger$$

Lasseri, Ebran, Khan, Sandulescu



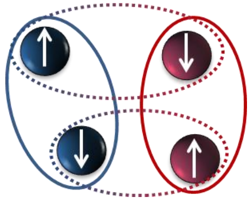
^{8}Be

^{24}Mg



^{20}Ne

Quartet BCS-like theory

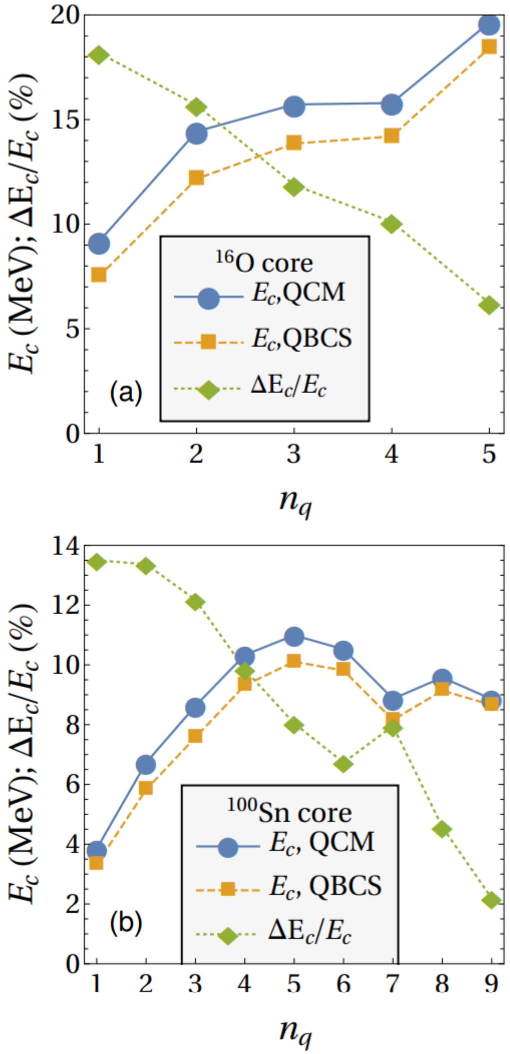


$$|\Psi\rangle = \left(Q^\dagger\right)^{n_q}|0\rangle \qquad Q^\dagger = 2\Gamma_1^\dagger\Gamma_{-1}^\dagger - \left(\Gamma_0^\dagger\right)^2 \qquad \Gamma_t^\dagger = \sum_k x_k P_{k,t}^\dagger$$

Lasseri, Ebran, Khan, Sandulescu

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

Baran, Delion, 2019



Thank you for your attention