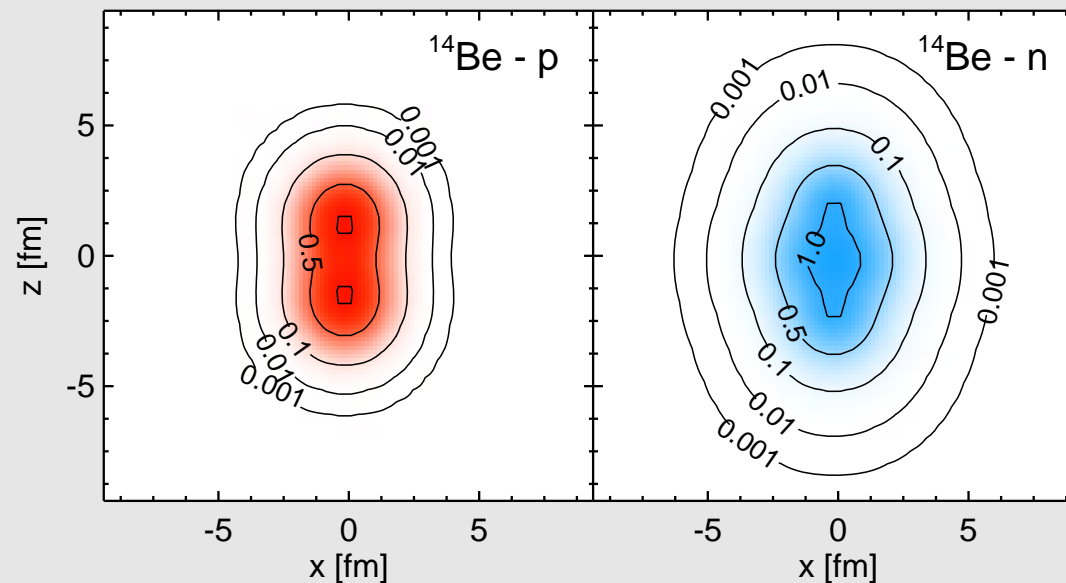


# Structure of Light Exotic Nuclei within Fermionic Molecular Dynamics

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# Nuclear Structure – ab initio

## Aim

→ describe low energy properties of nuclear many-body system

in terms of a **Hamiltonian**  
and **many-body states**

$$\tilde{H} = \tilde{T} + \tilde{V}_{NN}$$
$$|\hat{\Psi}\rangle$$

→ solve Schrödinger equation

$$\tilde{H} |\hat{\Psi}_n\rangle = E_n |\hat{\Psi}_n\rangle$$

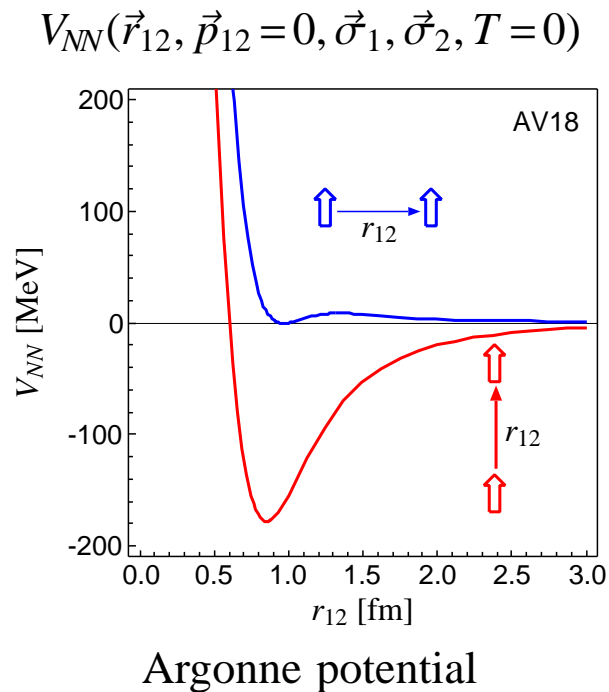
## Ingredients

$\tilde{H}$  = **Hamiltonian** with realistic  $NN$ -potential  $\tilde{V}_{NN}$   
(phase shifts, deuteron)

$|\hat{\Psi}_n\rangle \in$  **many-body Hilbert space**

$\langle \vec{r}_1 \vec{\sigma}_1 \tau_1, \vec{r}_2 \vec{\sigma}_2 \tau_2, \dots, \vec{r}_A \vec{\sigma}_A \tau_A | \hat{\Psi}_n \rangle$  is terribly complicated for realistic interaction  
main problem: short-range **repulsive** and **tensor** correlations induced by  $\tilde{V}_{NN}$

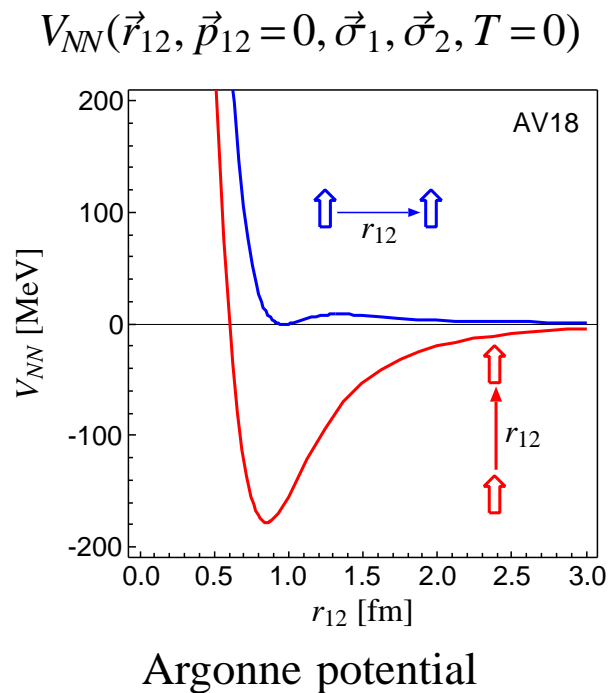
# Realistic $NN$ -potential



- $V_{NN}$  repulsive at small distances
  - ➔ strong short-range central correlations  
nucleons cannot get closer than  $\approx 0.6$  fm
- $V_{NN}$  depends strongly on orientation of  $\vec{\sigma}_1, \vec{\sigma}_2$  with respect to  $\vec{r}_{12}$ 
  - ➔ tensor correlations  
protons and neutrons want to align their spins with  $\vec{r}_{12}$

**Problem:**  
Slater determinants **cannot** describe these correlations

# Realistic $NN$ -potential



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protons and neutrons want to align their spins with  $\vec{r}_{12}$

## Problem:

Slater determinants **cannot** describe these correlations

**Solution:** include short-range correlations by unitary transformation (UCOM)

$$|\widehat{\Phi}\rangle = \underset{\sim}{C} |\Phi\rangle = \underset{\sim}{C}_{\Omega} \underset{\sim}{C}_r |\Phi\rangle$$

- $\underset{\sim}{C}_r$  central correlator shifts nucleons out of repulsive core
- $\underset{\sim}{C}_{\Omega}$  tensor correlator aligns spins along  $\vec{r}_{12}$

# Unitary Transformation

## Unitary Transformation

transform eigenvalue problem

$$\tilde{H} |\widehat{\Psi}_n\rangle = E_n |\widehat{\Psi}_n\rangle$$

with the unitary operator  $\tilde{C}$

$$|\widehat{\Psi}_n\rangle = \tilde{C} |\Psi_n\rangle, \quad \tilde{C}^{-1} = \tilde{C}^\dagger$$

into the equivalent eigenvalue problem

$$\widehat{H} |\Psi_n\rangle = (\tilde{C}^\dagger H \tilde{C}) |\Psi_n\rangle = E_n |\Psi_n\rangle$$

“pre-diagonalization”

include typical effects  
common to all states

effective Hamiltonian  $\widehat{H}$   
has same phase shifts and energies  
as realistic original  $H$  !

**Idea:** nuclear system has different scales:

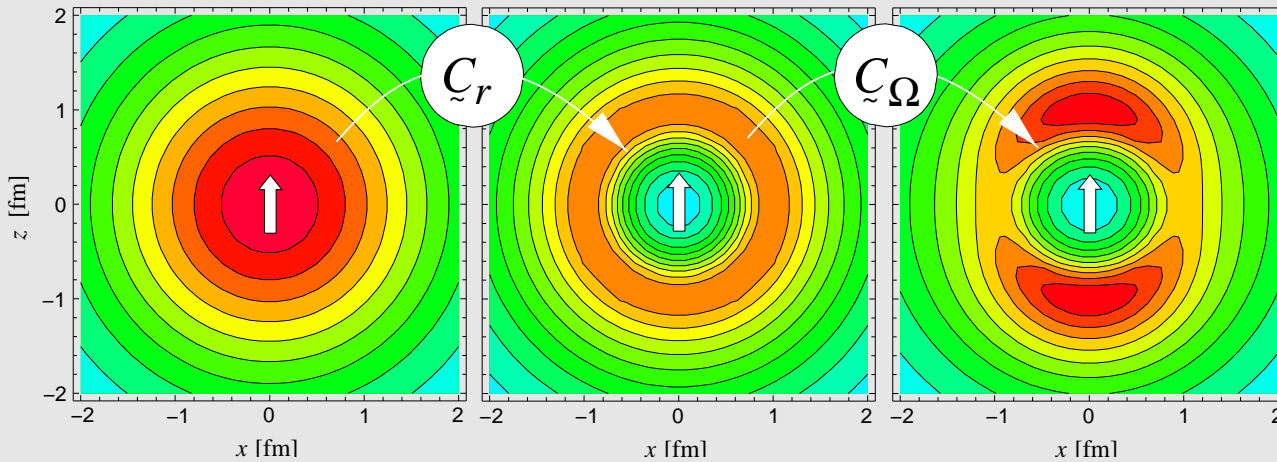
- long range (low momenta) – can be described by mean-field (Slater determinant)
- short-range (high momenta) – cannot be described by mean-field

- ➔ treat long range correlations in  $|\Psi\rangle$
- ➔ short range correlations in unitary  $\tilde{C} = \tilde{C}_\Omega \tilde{C}_r$

**Result:** many-body states  $|\widehat{\Psi}\rangle = \tilde{C} |\Psi\rangle$  contain both

# Correlations in Nuclei

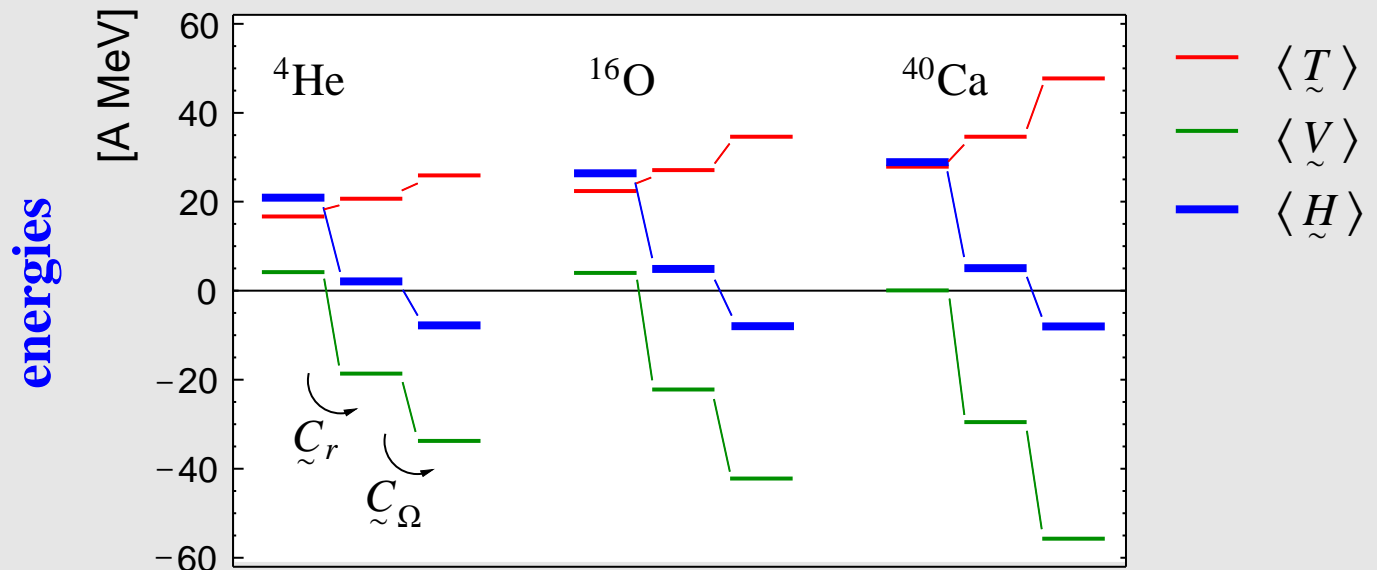
two-body densities



$$\rho_{S,T}^{(2)}(\vec{r}_1 - \vec{r}_2) \quad S = 1, M_S = 1, T = 0$$

- central correlator shifts density out of the repulsive core
- tensor correlator aligns density with spin orientation

- both, central and tensor correlations are essential for binding



# Hilbert Space: Fermionic Molecular Dynamics

## Fermionic

Slater determinant

$$|Q\rangle = \mathcal{A}\left(|q_1\rangle \otimes \cdots \otimes |q_A\rangle\right)$$

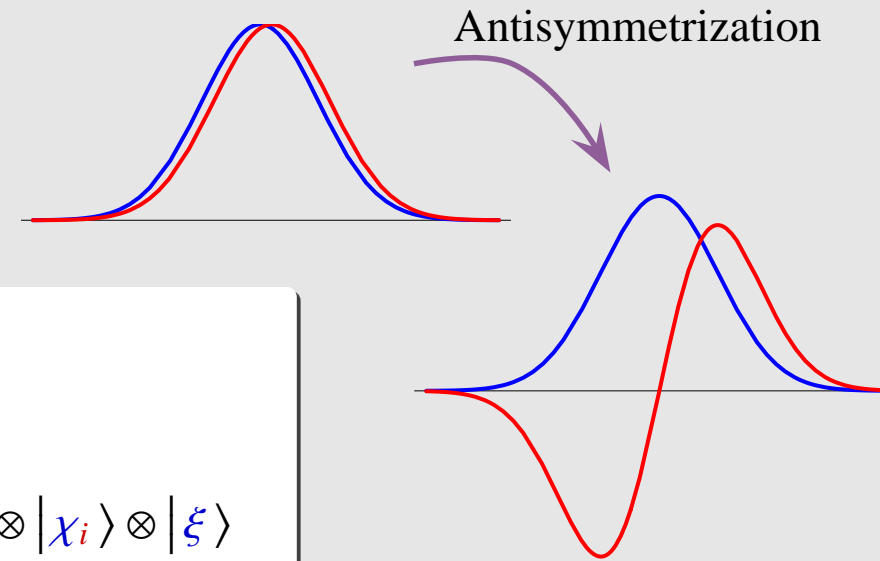
➔ antisymmetrized A-body state

## Molecular

single-particle states

$$\langle \vec{x} | q \rangle = \sum_i c_i \exp\left\{-\frac{(\vec{x} - \vec{b}_i)^2}{2a_i}\right\} \otimes |\chi_i\rangle \otimes |\xi\rangle$$

➔ Gaussian wave-packets in phase-space,  
spin is free, isospin is fixed



➔ Hilbert space contains  
shell-model, clusters, halos

## Dynamics in Hilbert space

spanned by one or several non-orthogonal  $|Q^{(a)}\rangle$

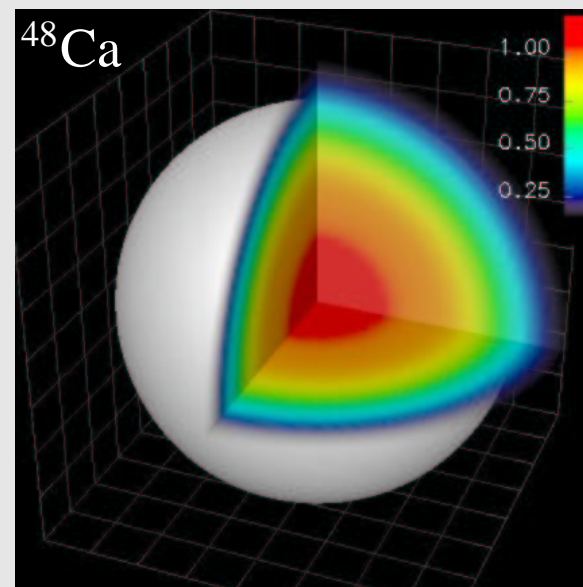
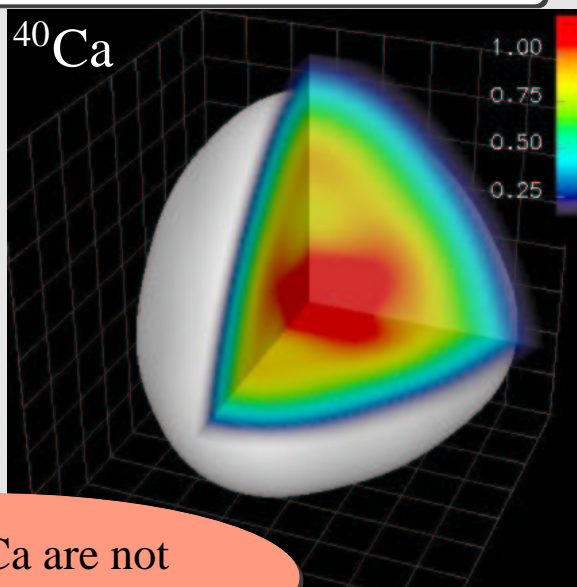
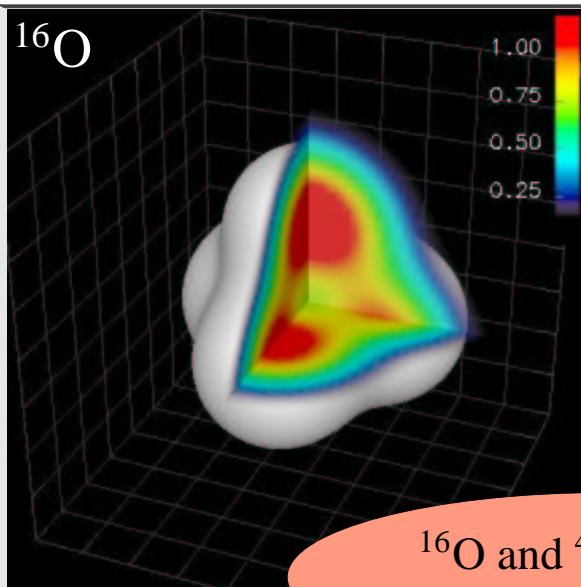
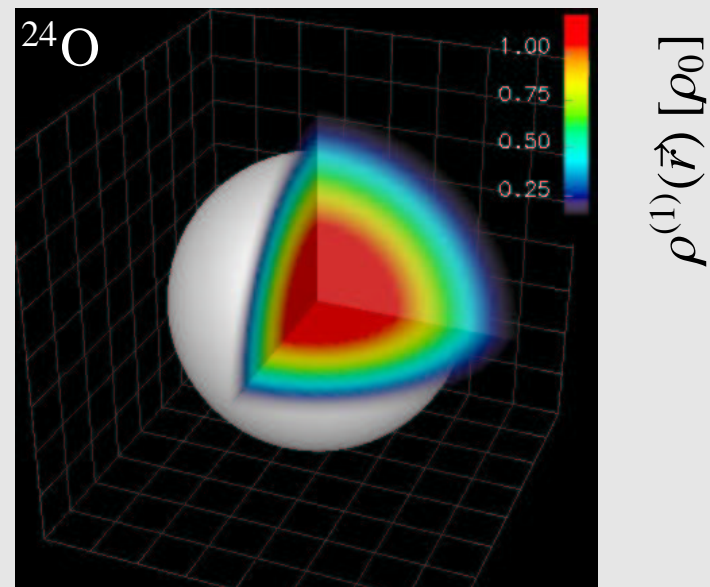
$$|\Psi\rangle = \sum_a \psi_a |Q^{(a)}\rangle$$

variational principle →  $Q^{(a)} = \{q_v^{(a)}, v=1 \cdots A\}$ ,  $\psi_a$

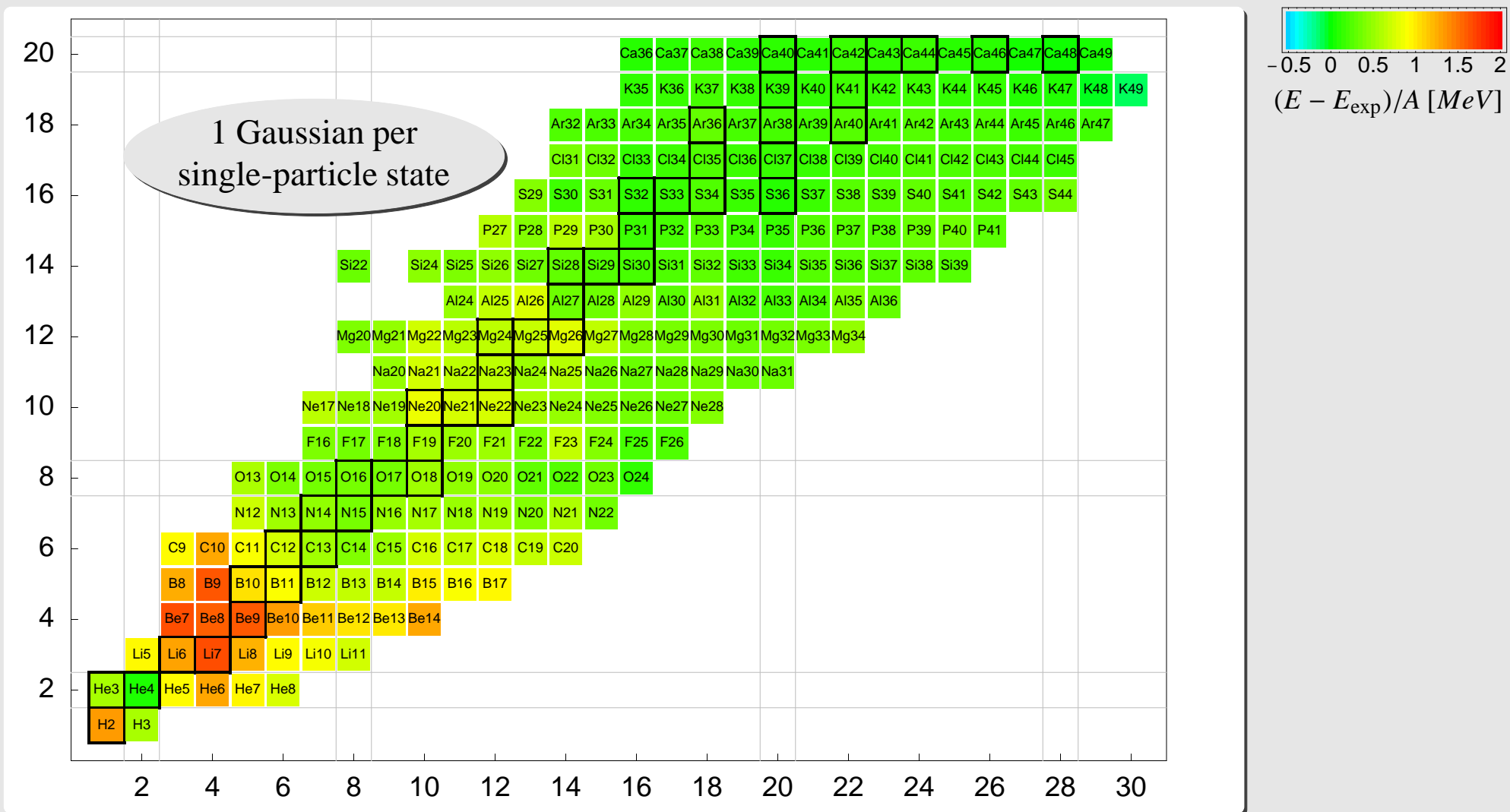
# ● Effective Correction to the Interaction

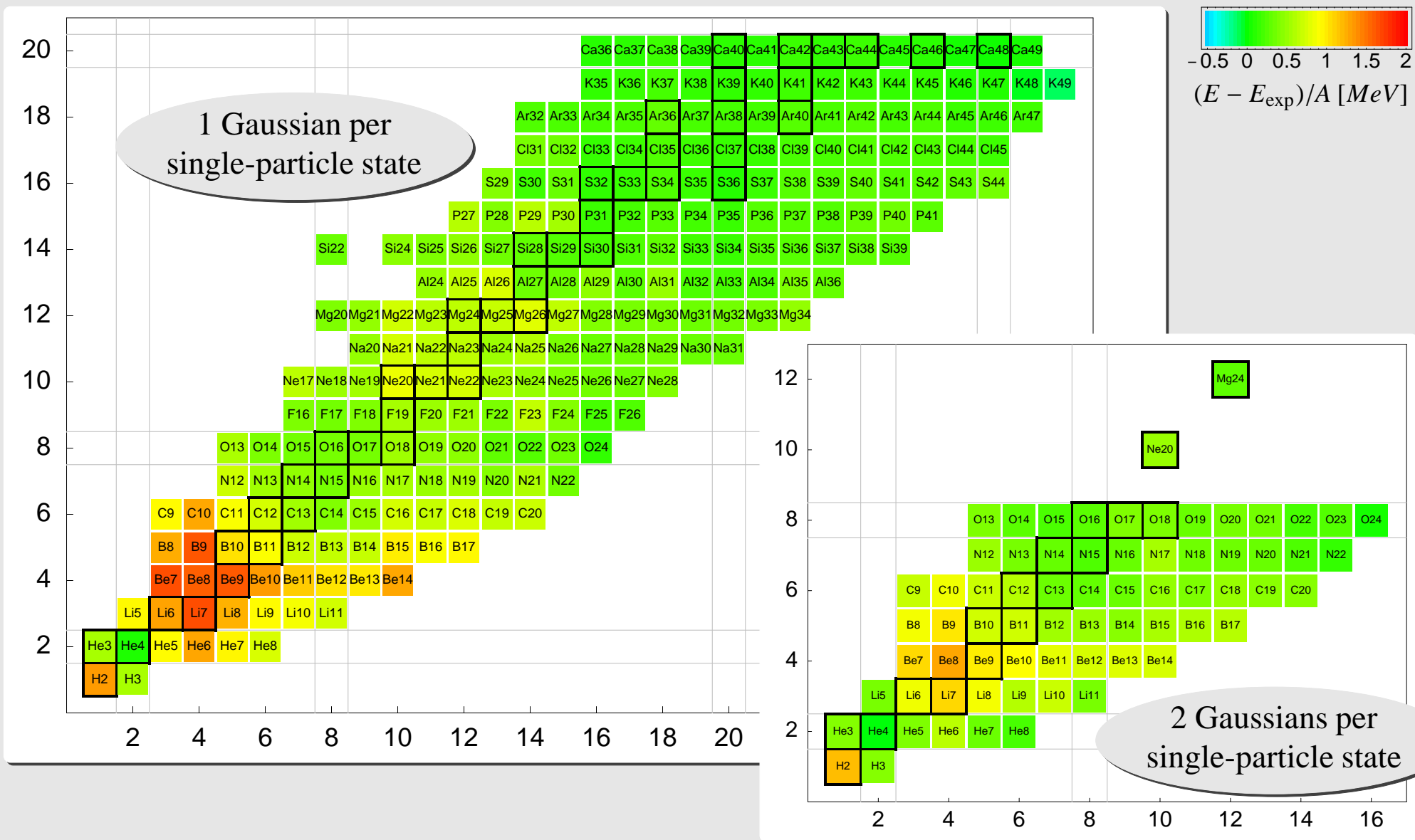
## Effective two-body interaction

- ➔ correlated two-body interaction  $\widehat{H} = \widetilde{C}^\dagger H \widetilde{C}$  is lacking three-body forces
- ➔ instead of three-body force use additional **momentum-dependent** and **spin-orbit** two-body correction term
- ➔ fit correction term to binding energies and radii of “closed-shell” nuclei
- ➔ altogether a **15%** correction to the *ab-initio* two-body potential



<sup>16</sup>O and <sup>40</sup>Ca are not “closed shell” nuclei !





# How to improve ?

## Projection After Variation (PAV)

- mean-field may break symmetries of Hamiltonian
- restore reflection and rotational symmetry by parity and angular-momentum projection  $P_{MK}^{J\pi}$

$$\sum_{K'} \langle Q | \tilde{H} P_{KK'}^{J\pi} | Q \rangle \cdot c_{K'} = E_K^{J\pi} \sum_{K'} \langle Q | \tilde{P}_{KK'}^{J\pi} | Q \rangle \cdot c_{K'}$$

## Variation After Projection (VAP)

- effect of projection can be large
- perform VAP applying **constraints** on radius, dipole moment, quadrupole moment or octupole moment and minimize the energy in the projected energy surface

## Multiconfiguration Calculations

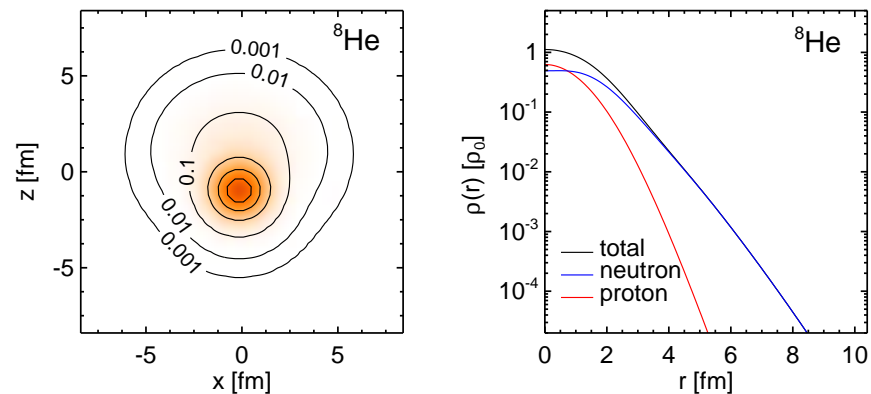
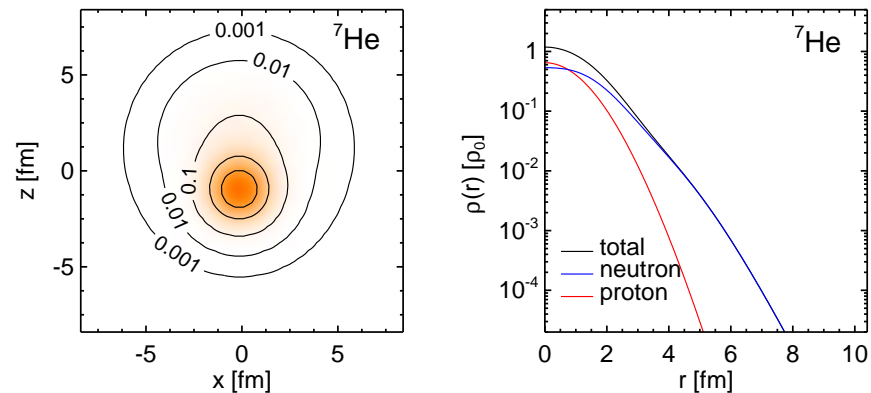
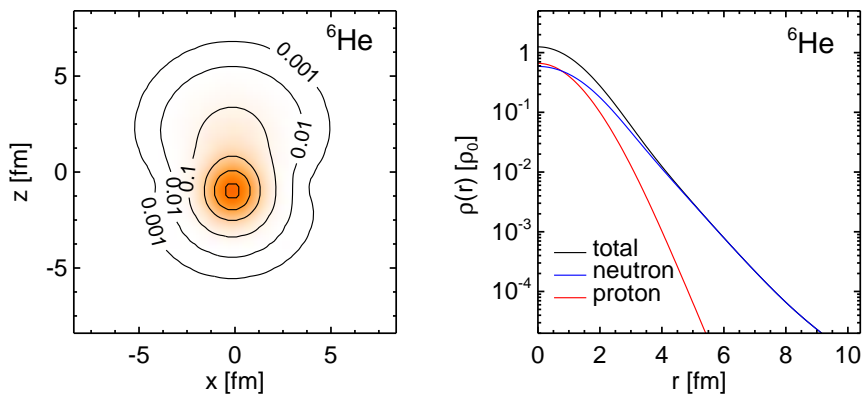
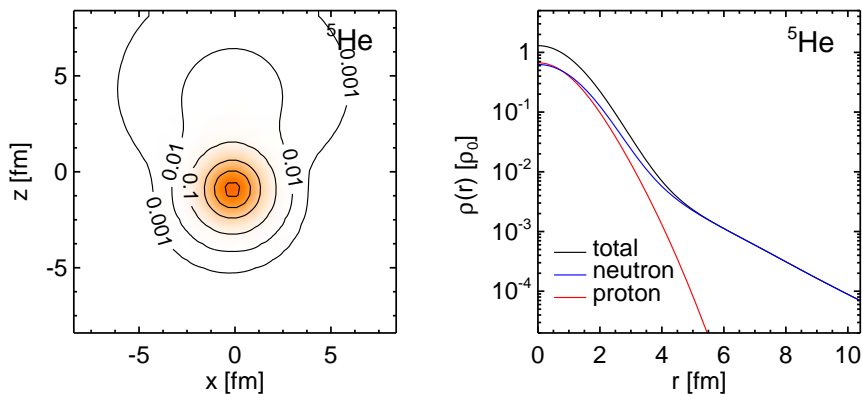
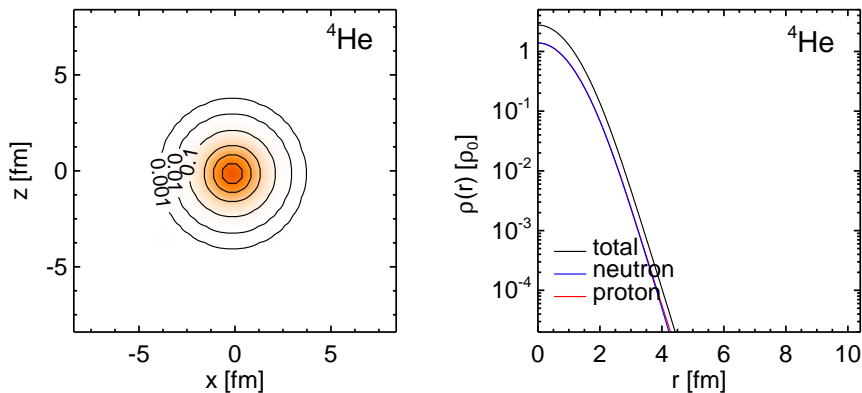
- diagonalize Hamiltonian in a set of projected intrinsic states

$$\left\{ P_{KK'}^{J\pi} | Q^{(a)} \rangle, \quad a = 1, \dots, N \right\}$$



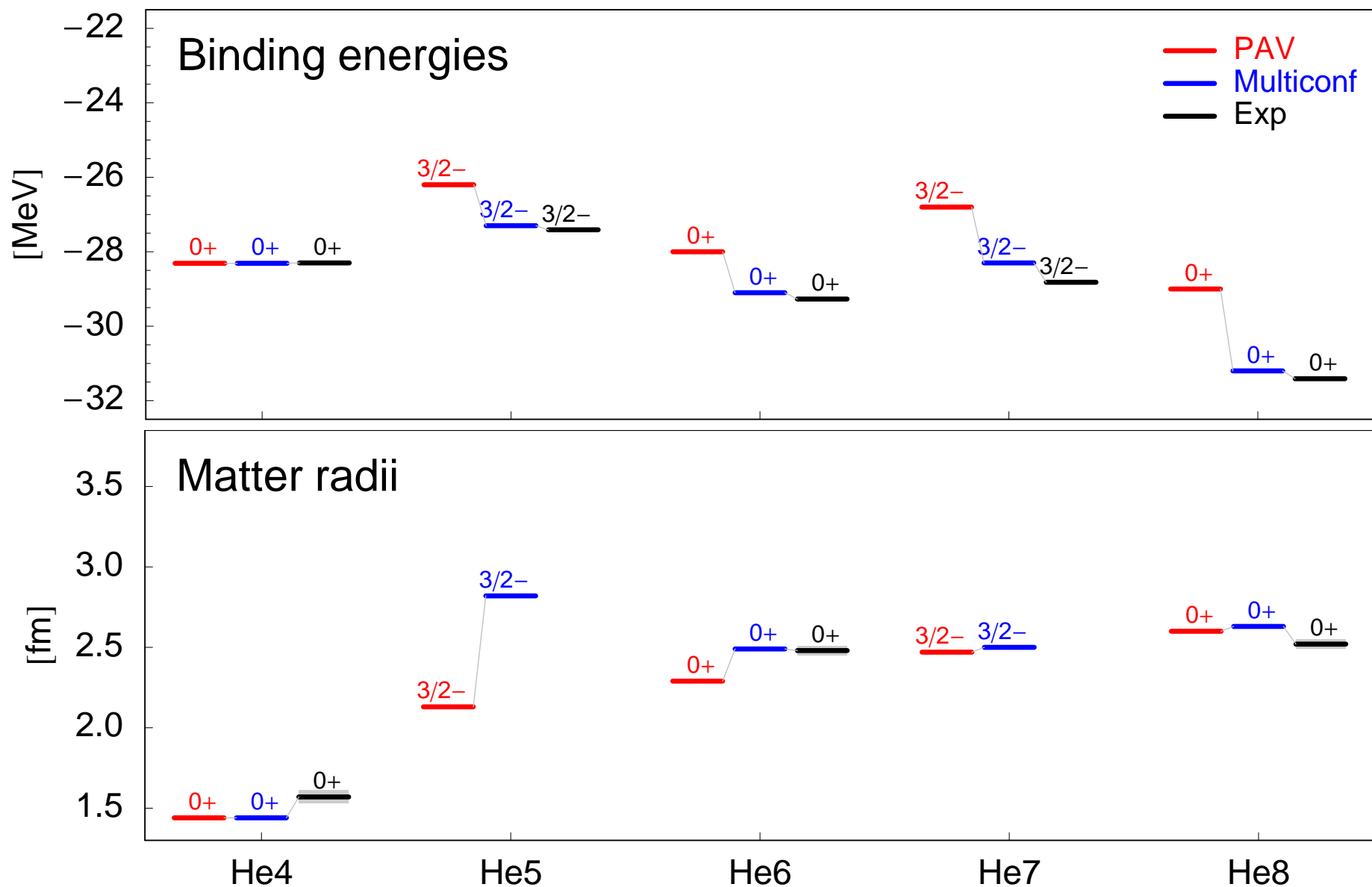


# Helium Isotopes

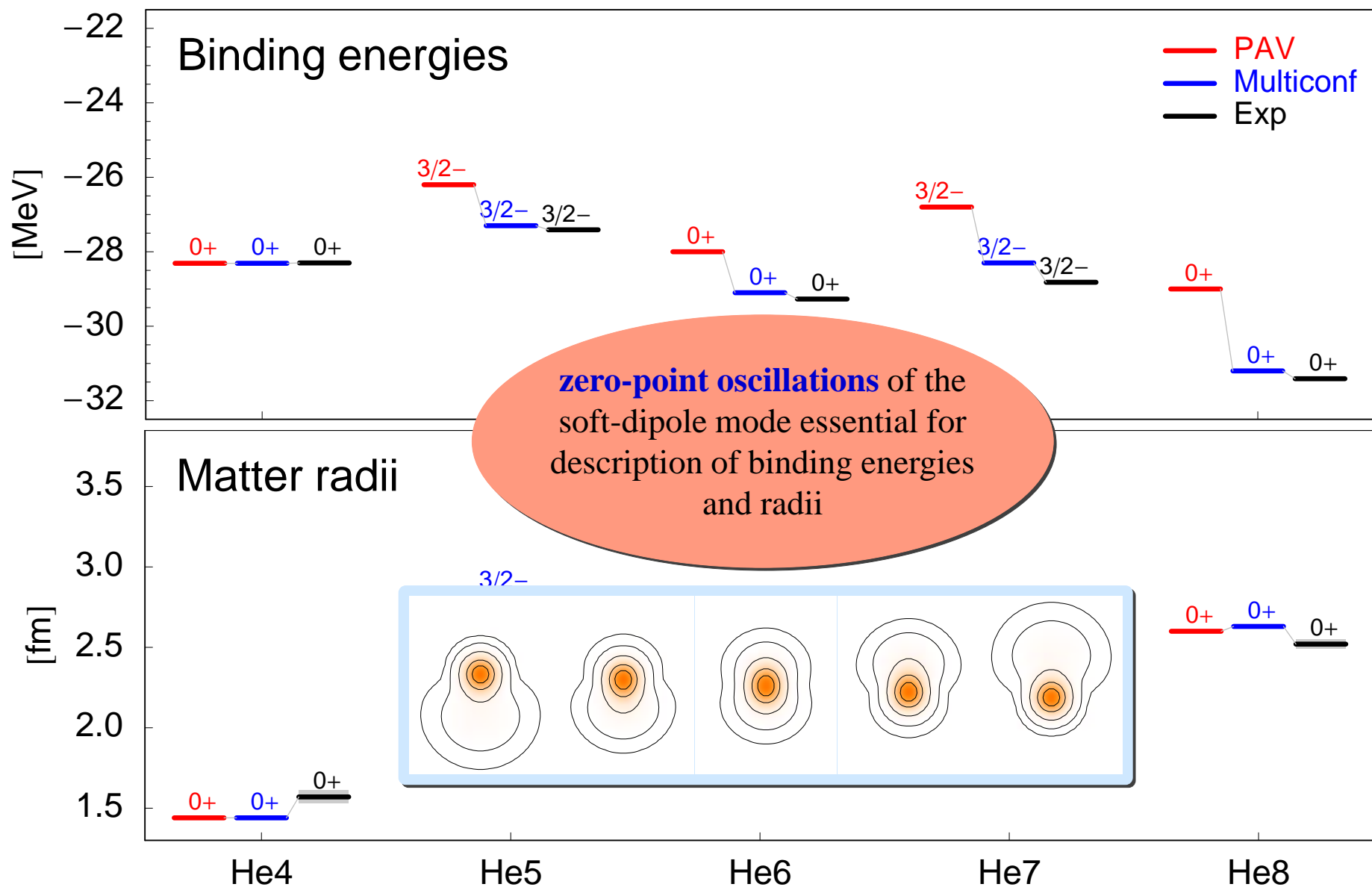


**soft-dipole mode**  
neutrons are oscillating  
against  $\alpha$ -core

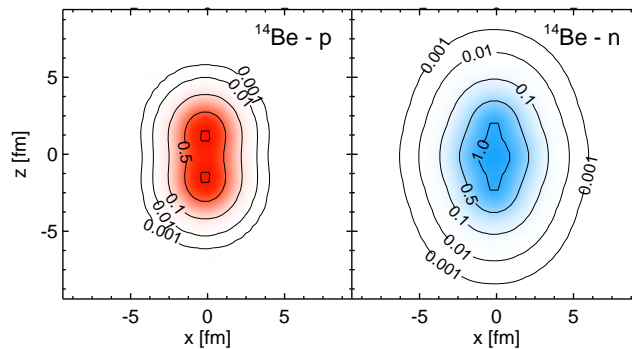
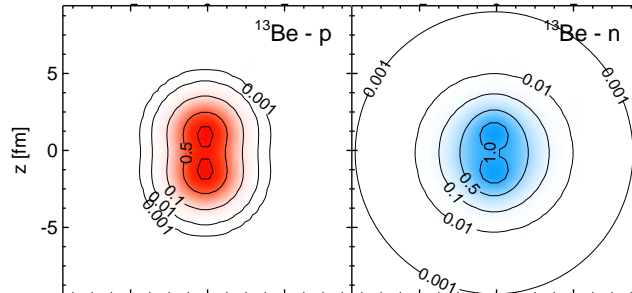
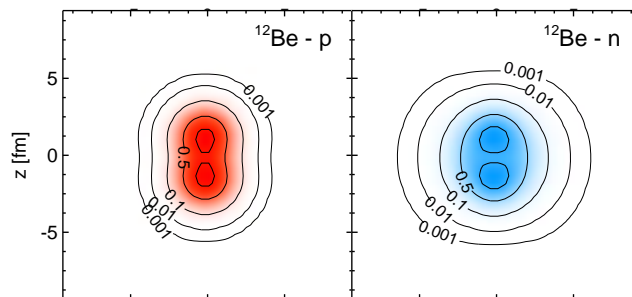
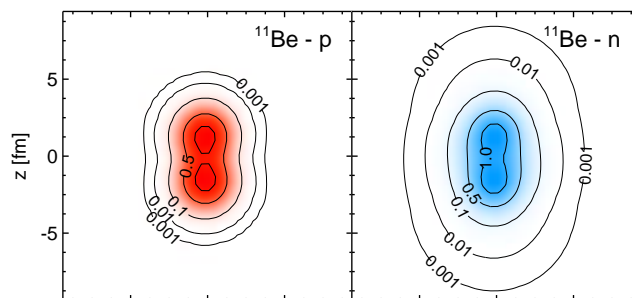
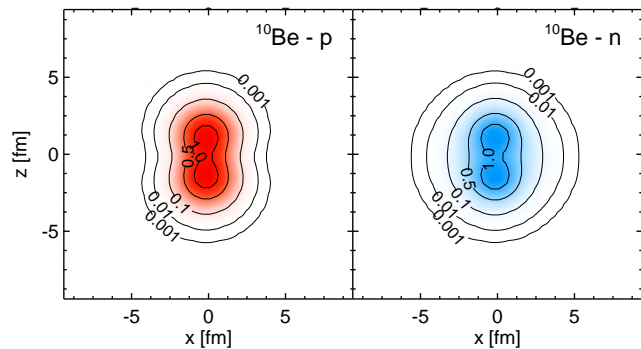
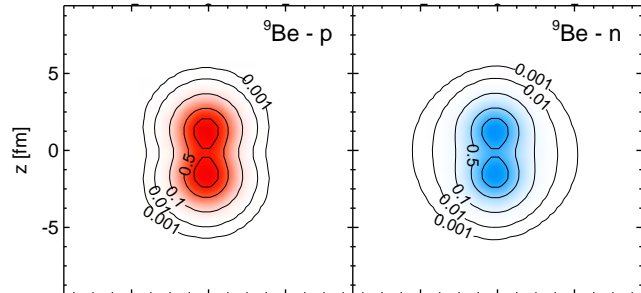
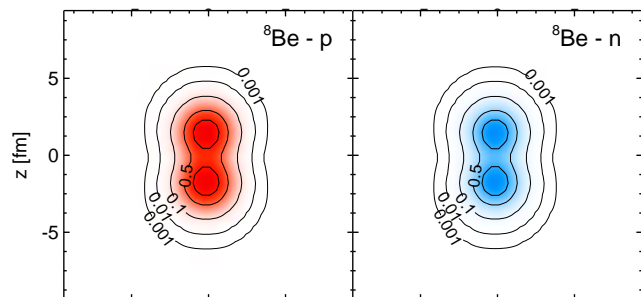
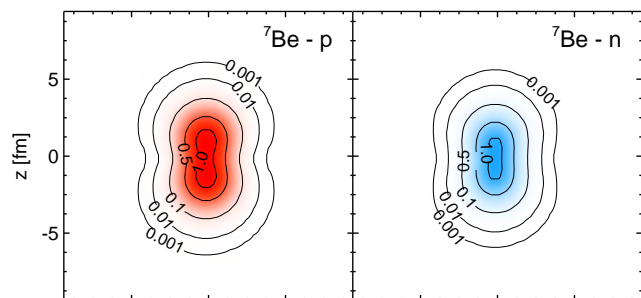
# Helium Isotopes



# Helium Isotopes

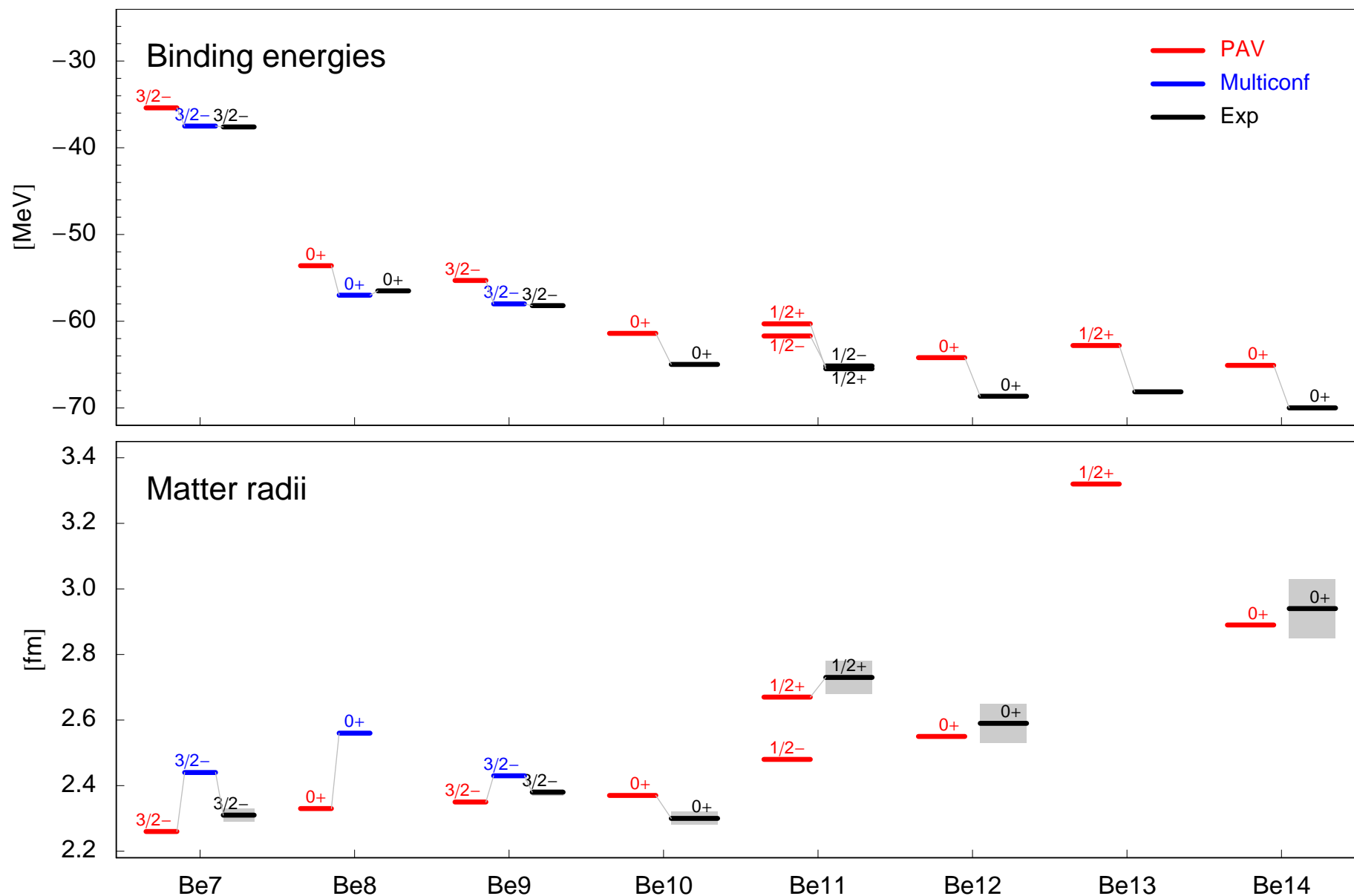


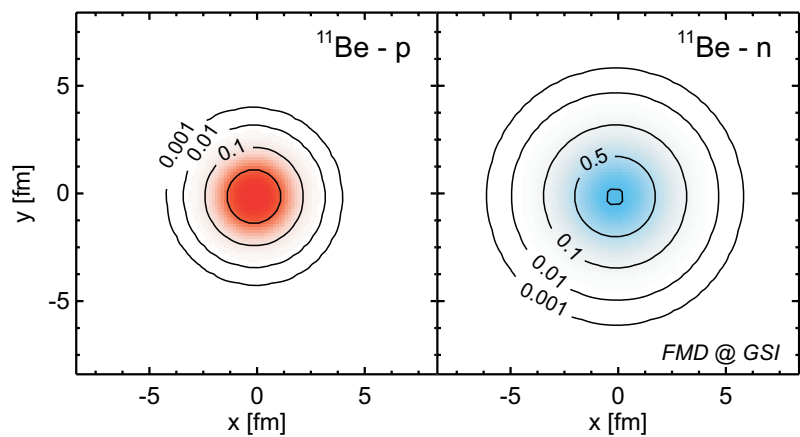
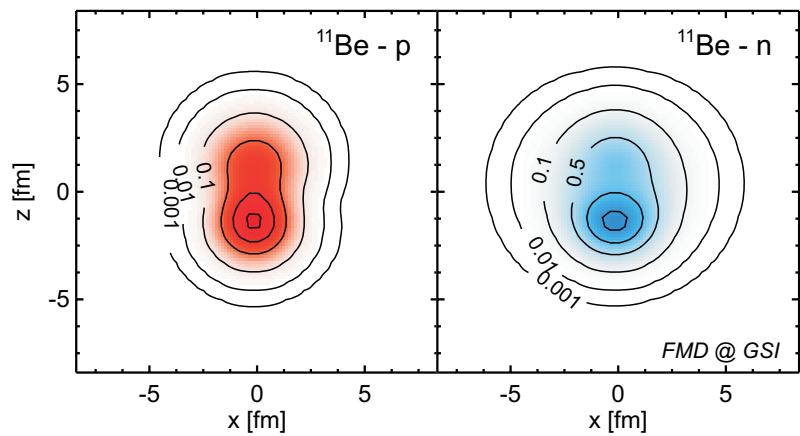
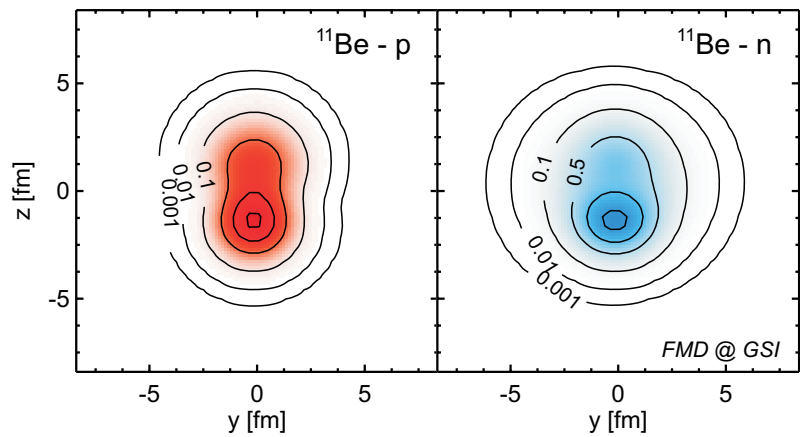
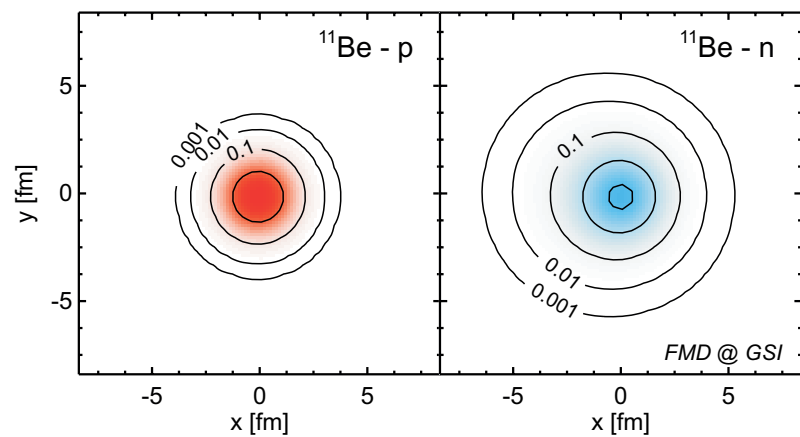
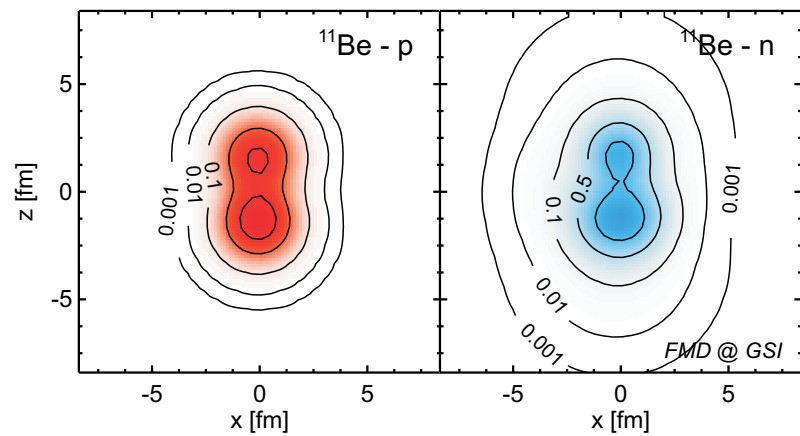
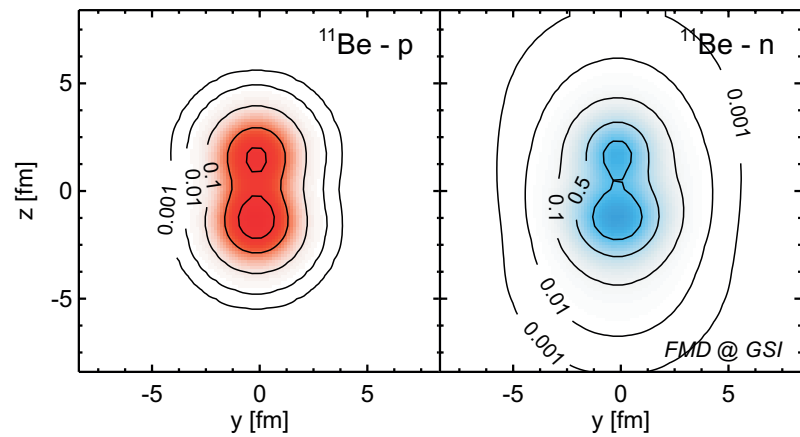
# Beryllium Isotopes



cluster structure  
changes with  
addition of neutrons

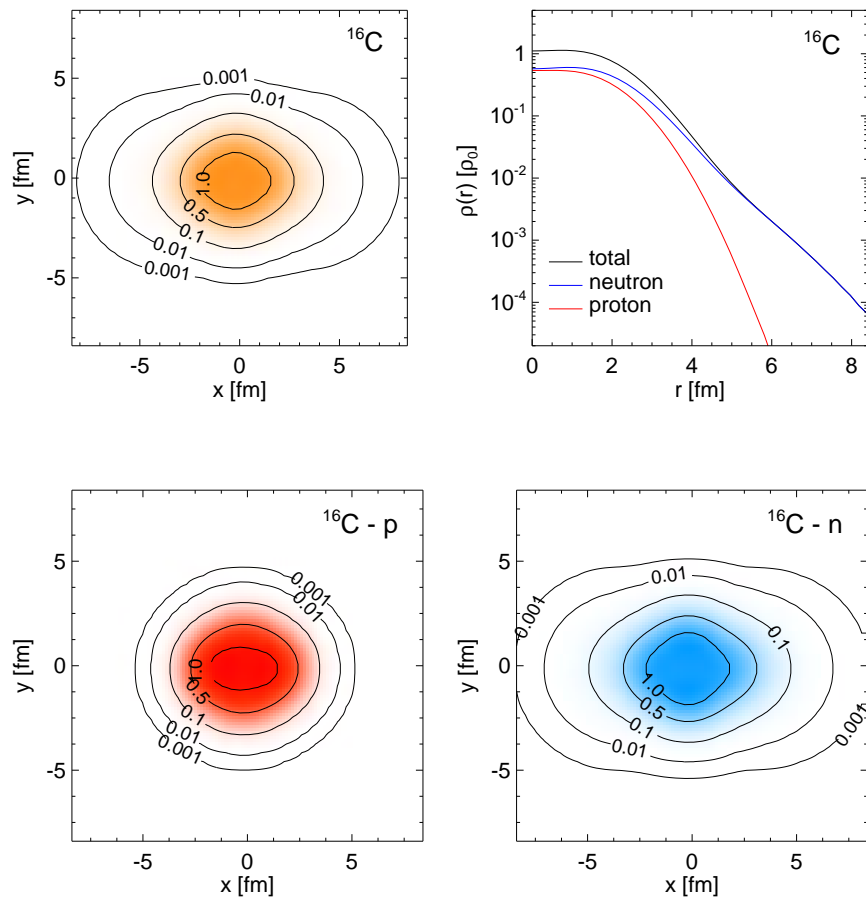
# Beryllium Isotopes



$1/2^-$  $1/2^+$ 

# $^{16}\text{C}$ PAV only

## Variation



	$E_b$ [MeV]	$r_{charge}$ [fm]	$r_{matter}$ [fm]
PAV 1g	99.1	2.52	2.88
PAV	105.0	2.49	2.60
Exp	110.8		$2.70 \pm 0.03$ $2.76 \pm 0.06$

	$E_{2^+}$ [MeV]	$B(E2)$ [ $e^2\text{fm}^4$ ]
PAV	1.29	4.6
Exp	1.77	$3.15 \pm 0.95$
Global Best Fit <sup>1</sup>	1.77	$82 \pm 14$

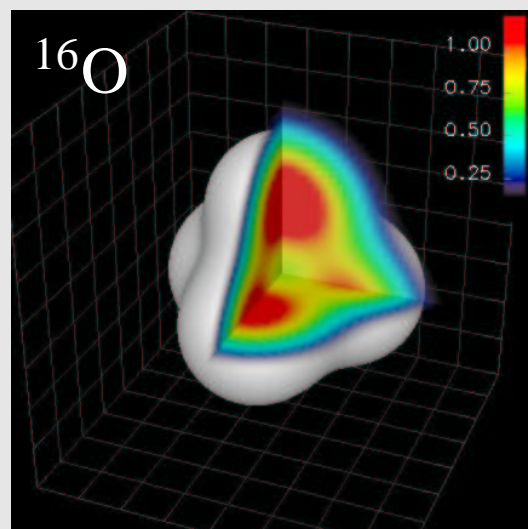
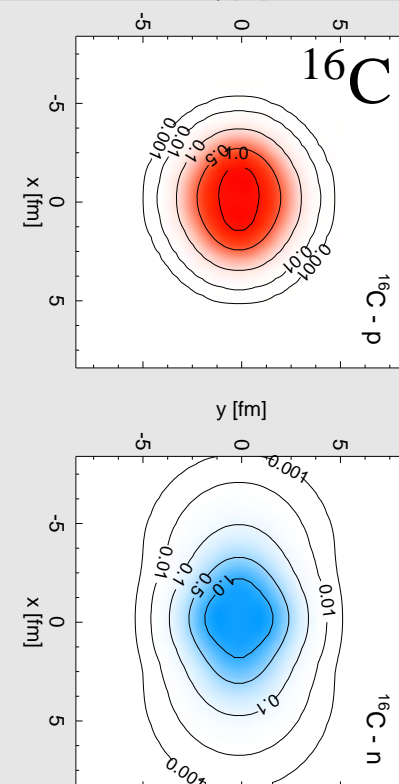
<sup>1</sup> Raman *et al*, Atomic Data and Nuclear Data Tables **78** (2001) 1

→ calculated  $B(E2)$  consistent with anomalously long lifetime of  $2^+$  state measured at RIKEN

Imai *et al*, PRL in print

# Summary and Outlook

- ➔ **Unitary Correlation Operator Method** describes short ranged central and tensor correlations
- ➔ **UCOM** provides ab-initio correlated interaction  $\widehat{H} = \underset{\sim}{C}^\dagger \underset{\sim}{H} \underset{\sim}{C}$  for many-body methods like HF, shell model, FMD
  - Feldmeier, Neff, Roth, Schnack, NP **A632** (1998) 61
  - Neff, Feldmeier, NP **A713** (2003), 311
- ➔ **FMD** Calculations with the same  $\widehat{H} + \widehat{H}^{corr}$  for  $3 \leq A \leq 60$
- ➔ Projection, configuration mixing → masses, radii, halos, spectra, transitions shell structures, pairing, ...
- ➔ No assumption about core, mean-field, core-nucleon interaction, ...



## Outlook

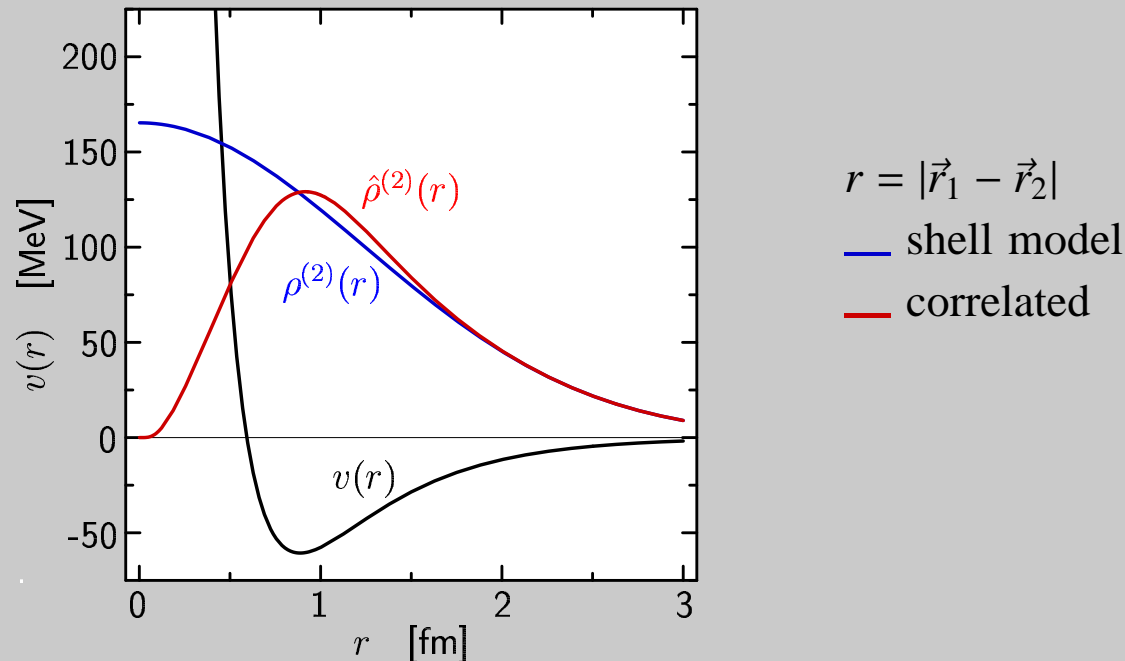
- ➔ Predictions for many exotic light nuclei (before measurement)
- ➔ Correlated transitions: M1,  $\beta$ -decay, quenching
- ➔ Resonances, width of many-body states
- ➔ Ab-initio correlated interaction in HF, RPA or similar for  $A > 60$
- ➔ Investigate long ranged tensor correlations – 3-body forces –  $\widehat{H}^{corr}$

Dr. T. Neff, A. Cribreiro, Prof. R. Roth, A. Ehrlich, H. Hergert

# Radial Correlations

**BECAUSE 1.)** realistic interactions have short-range repulsion

➔ probability density of nucleons in the repulsive core strongly suppressed



potential & two-body density of  ${}^4\text{He}$  in  $S=0$ ,  $T=1$  channel

✗ correlations in the relative distance of nucleons  
**cannot** be described by Slater determinants (product of single-particle states)

# Tensor Correlations

**BECAUSE 2)** tensor interaction is an essential component in any realistic interaction  
 → exchange of pions

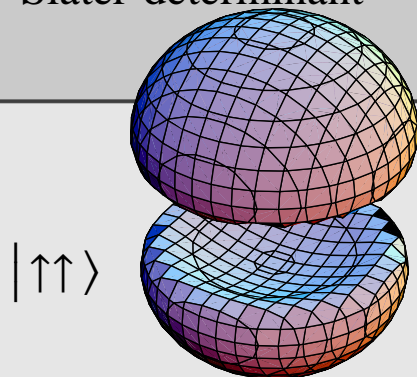
✗ without tensor force no bound nuclei !

tensor operator

$$s_{12} \left( \frac{\vec{r}}{r}, \frac{\vec{r}}{r} \right) = 3 \left( \sigma_1 \cdot \frac{\vec{r}}{r} \right) \left( \sigma_2 \cdot \frac{\vec{r}}{r} \right) - (\sigma_1 \cdot \sigma_2)$$

couples spins and the relative spatial orientation of nucleons

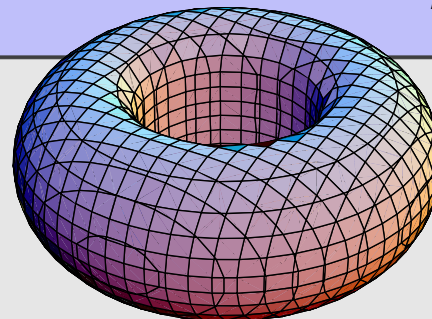
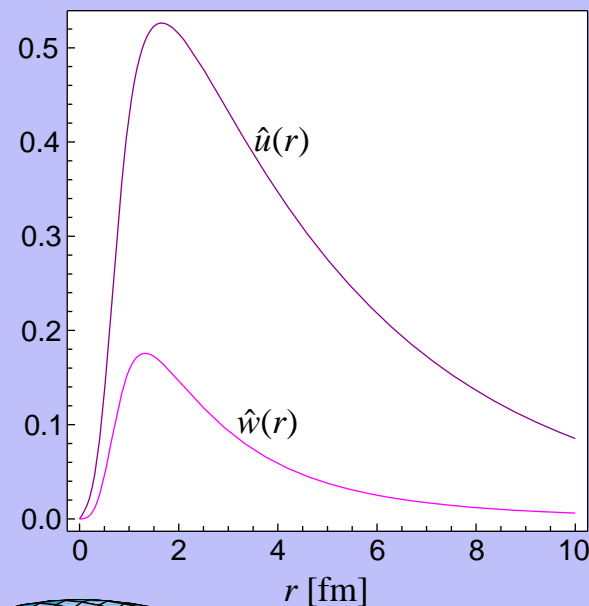
✗ correlations between the orientation of the spins and the relative orientation of nucleons **cannot** be described by Slater determinant



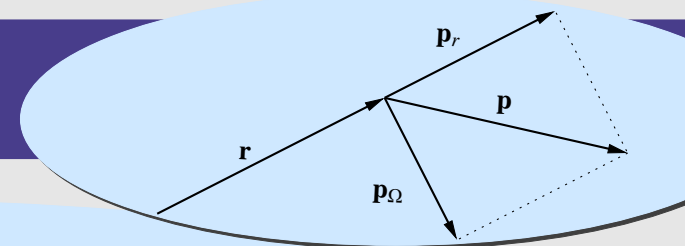
## Deuteron $S = 1, T = 0$

deuteron has  $L = 2$  admixture due to tensor force

$$\langle r | \widehat{d} \rangle = \frac{\widehat{u}(r)}{r} |L = 0\rangle + \frac{\widehat{w}(r)}{r} |L = 2\rangle$$



# Radial and Tensor Correlations



$$\tilde{C} = \tilde{C}_\Omega \tilde{C}_r$$

$$= e^{-i\tilde{G}_\Omega} e^{-i\tilde{G}_r}$$

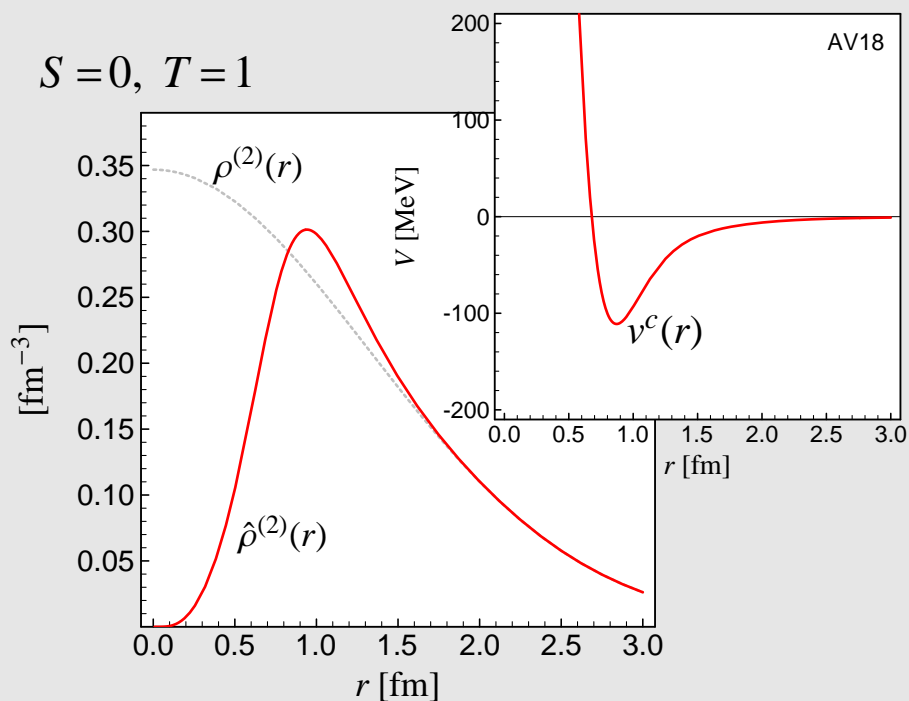
$$\vec{p} = \vec{p}_r + \vec{p}_\Omega$$

$$\vec{p}_r = \frac{1}{2} \left\{ \frac{\vec{r}}{r} \left( \frac{\vec{r}}{r} \vec{p} \right) + \left( \vec{p} \frac{\vec{r}}{r} \right) \frac{\vec{r}}{r} \right\}, \quad \vec{p}_\Omega = \frac{1}{2r} \left\{ \vec{l} \times \frac{\vec{r}}{r} - \frac{\vec{r}}{r} \times \vec{l} \right\}$$

## Radial Correlator

$$g_r = \frac{1}{2} \{ p_r s(r) + s(r) p_r \}$$

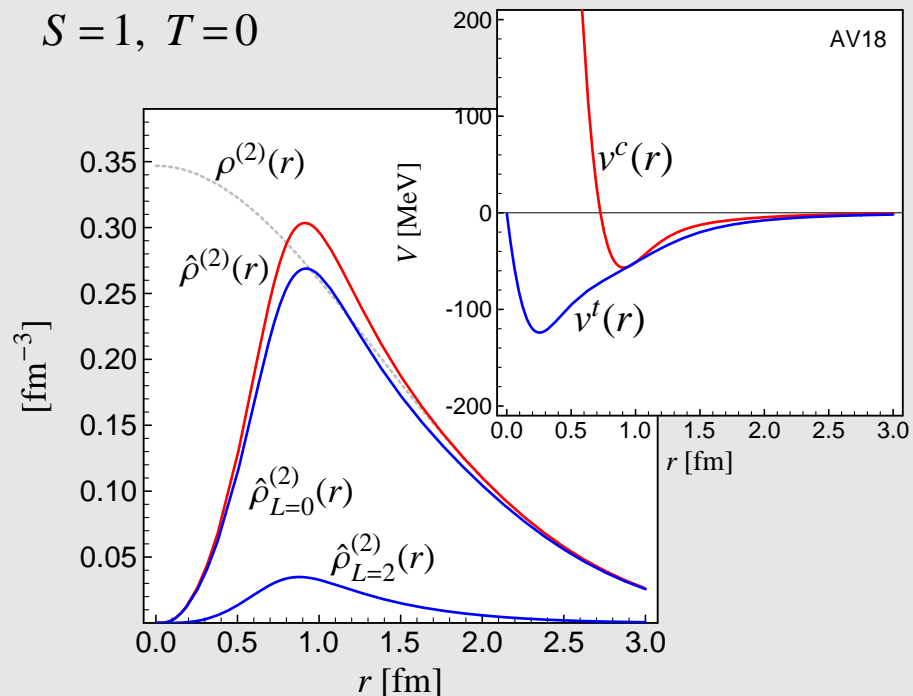
➔ probability density shifted out of the repulsive core



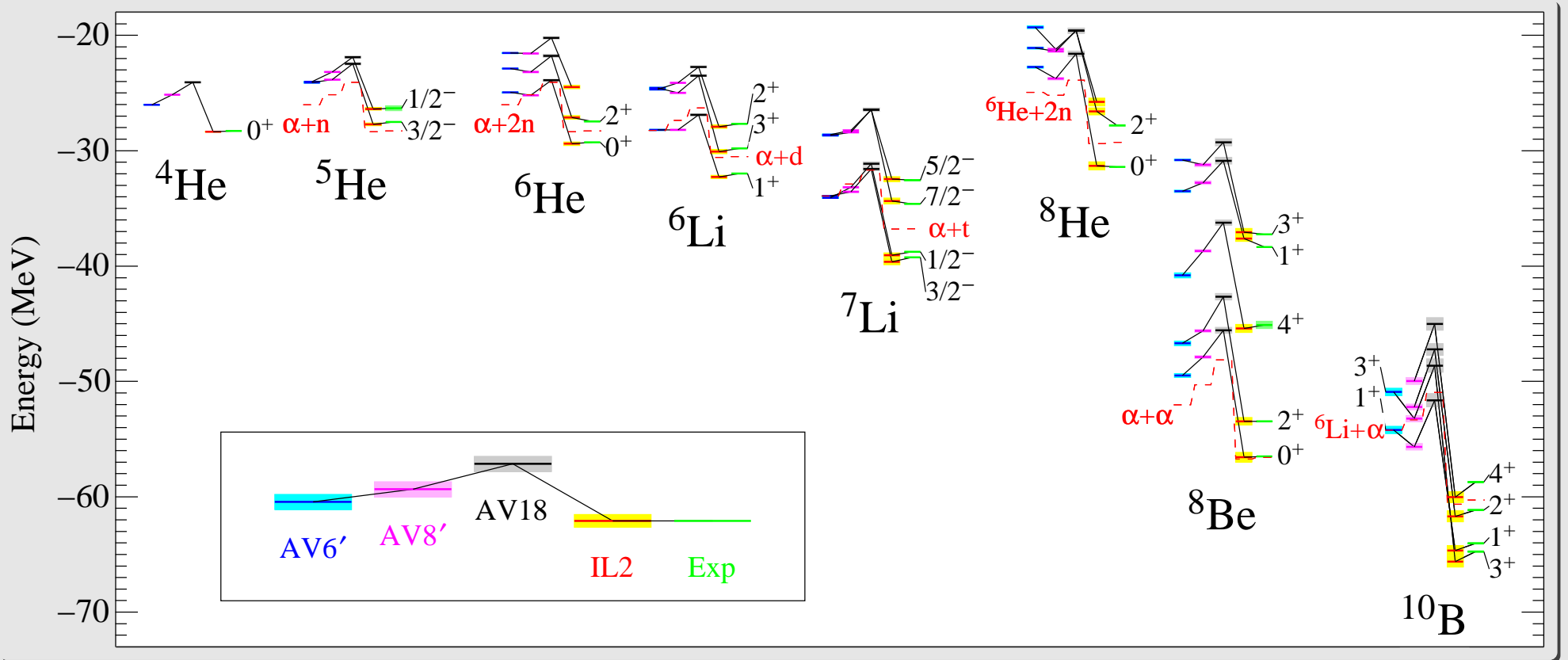
## Tensor Correlations

$$g_\Omega = \vartheta(r) \frac{3}{2} \{ (\tilde{\sigma}_1 \cdot \vec{p}_\Omega) (\tilde{\sigma}_2 \cdot \vec{r}) + (\tilde{\sigma}_1 \cdot \vec{r}) (\tilde{\sigma}_2 \cdot \vec{p}_\Omega) \}$$

➔ tensor force admixes other angular momenta



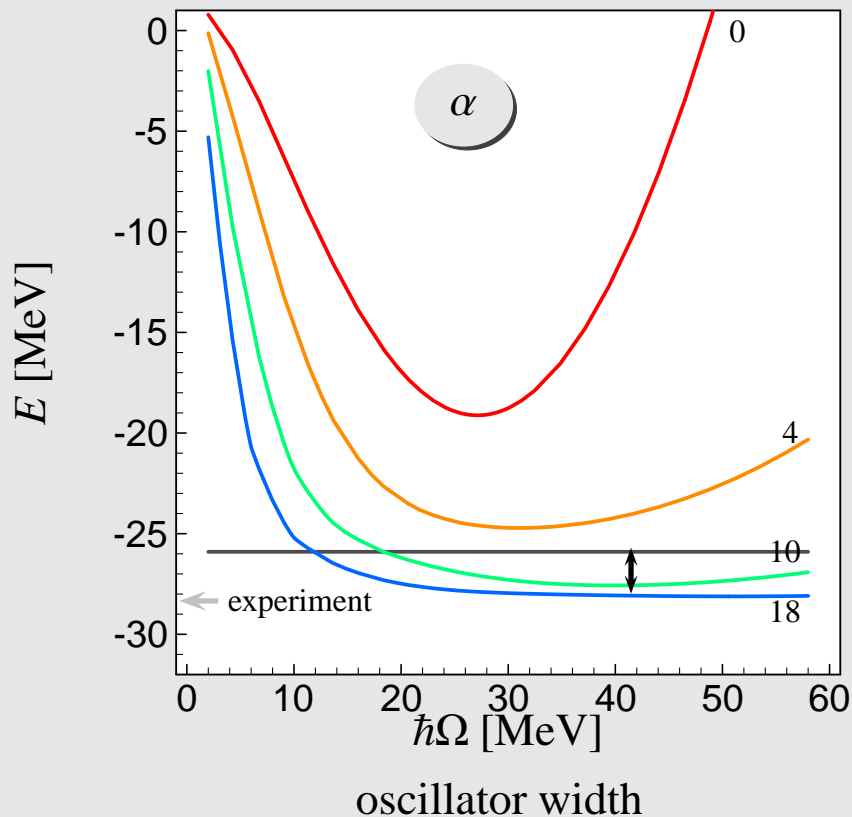
# GFMC calculations



Wiringa, Pieper, PRL **89** (2002) 182501

genuine three-body forces (IL2)  
needed for description of real  
nuclei

$^4\text{He}$



test of two-body approximation

Quasi-exact calculations for light nuclei possible

exact result from PRC64 (2001) 044001

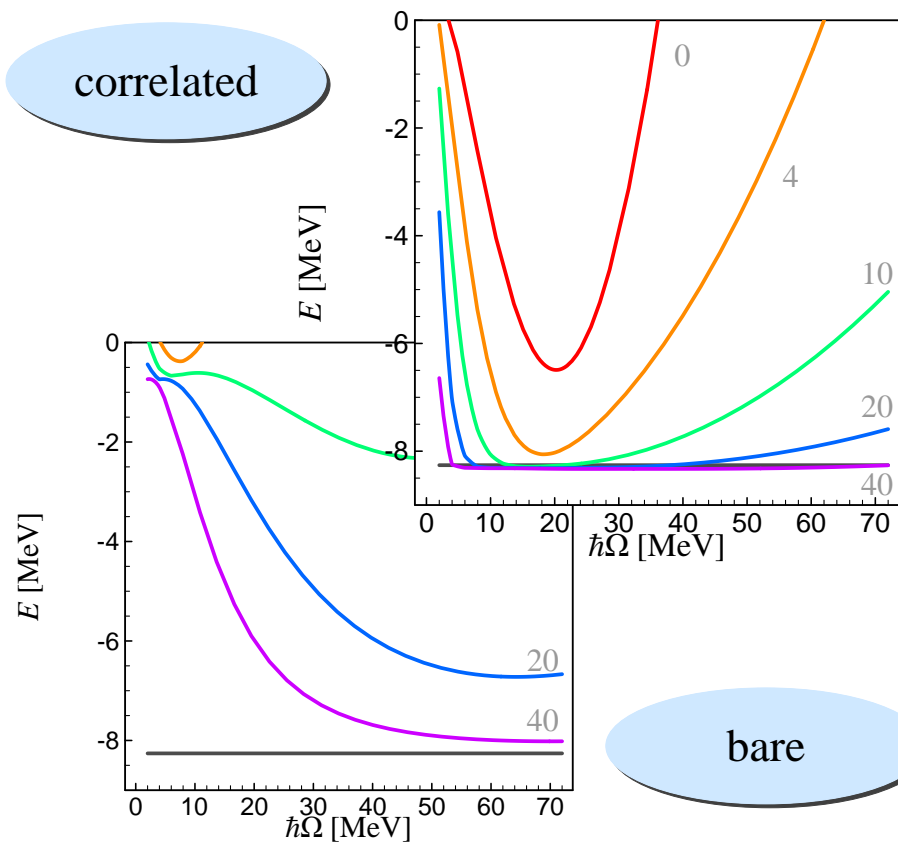
- use no-core shell model code from Petr Navratil (LLNL)

- neglected 3-body correlated terms same order as genuine 3N interactions
- more investigations needed

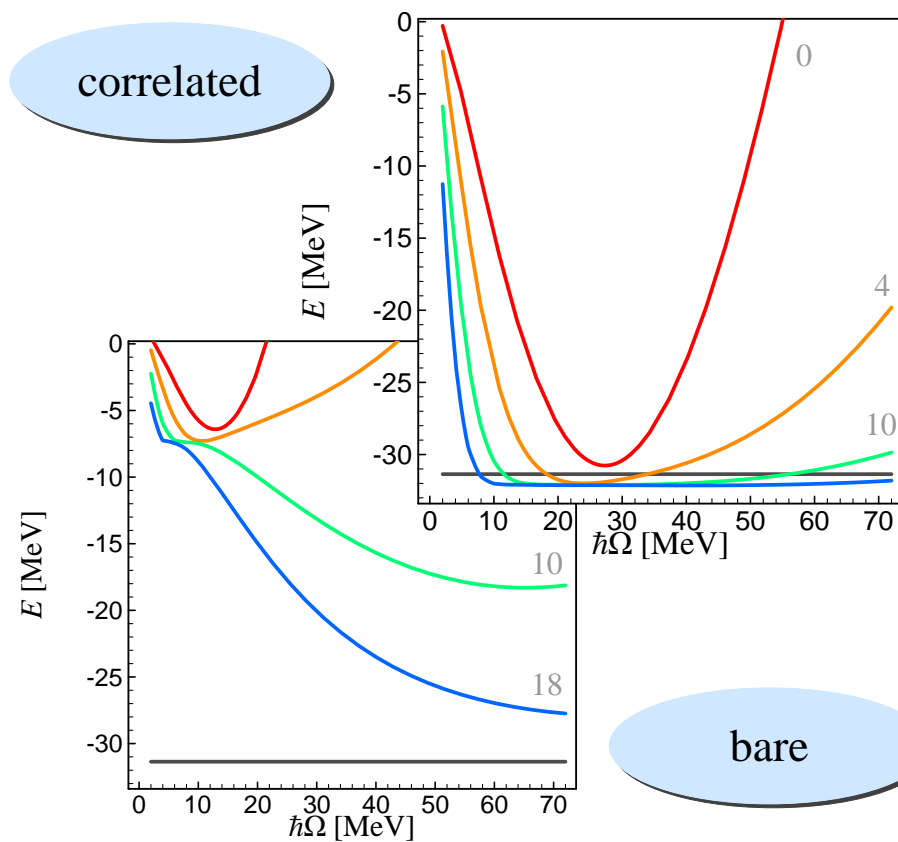
# MTV Interaction

# No-Core Shell Model Calculations

$^3\text{He}$



$^4\text{He}$



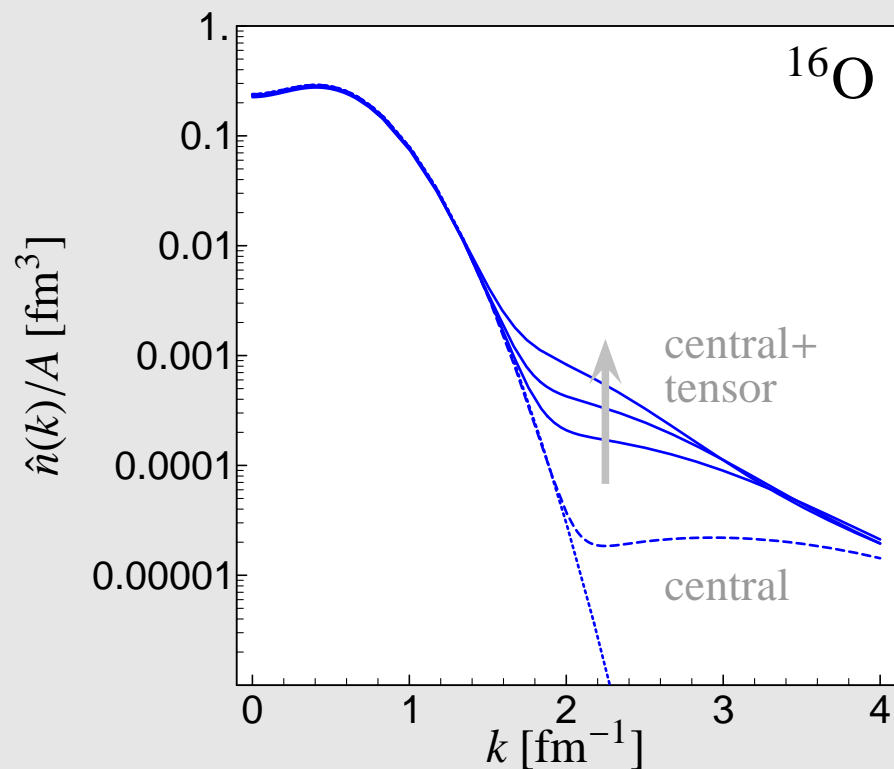
exact results from PRC52 (1995) 2885

only radial correlations

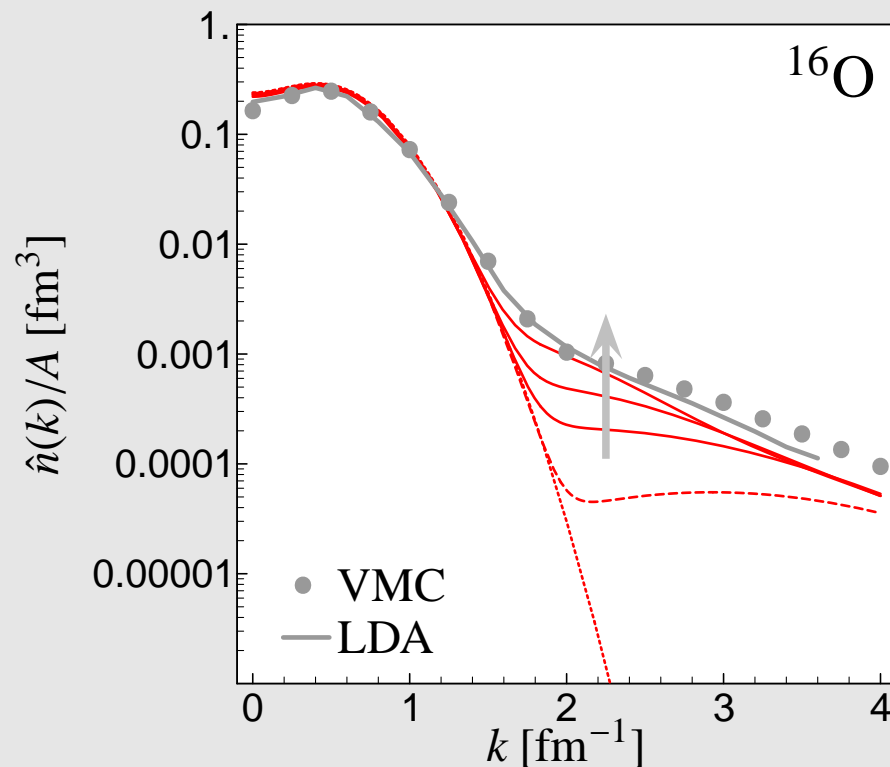
- use no-core shell model code from P  tr Navratil (LLNL)

# Nucleon Momentum Distributions

## Bonn-A



## Argonne V18

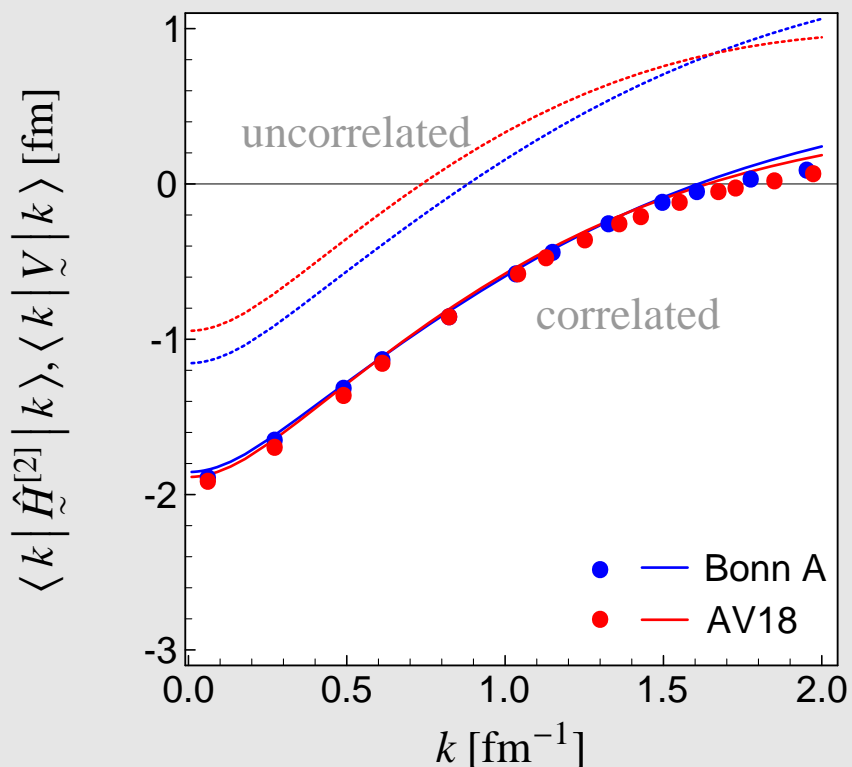


- correlations induce high-momentum components
- contributions of tensor correlations very big
- different correlator ranges relevant especially at the fermi surface

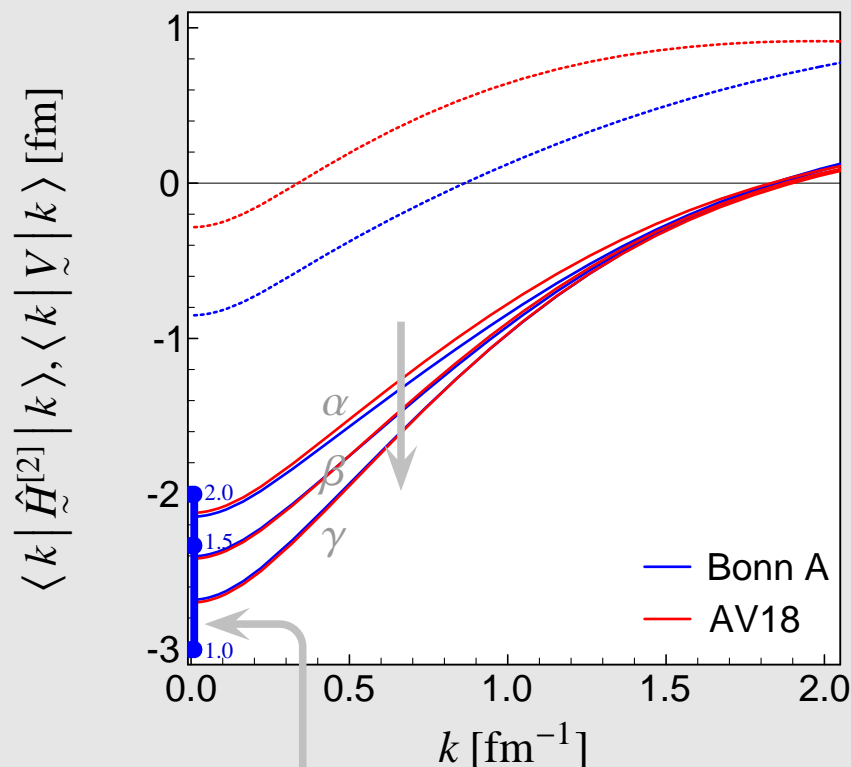
# Interaction in Momentum Space

$$\langle klm | \widehat{H}^{[2]} | k'l'm' \rangle = i^{l'-l} M \int d^3x Y_{lm}^*(\hat{x}) j_l(kx) \langle \vec{x} | \widehat{H}^{[2]} | \vec{x} \rangle j_{l'}(k'x) Y_{l'm'}(\hat{x})$$

$^1S_0$  channel



$^3S_1$  channel

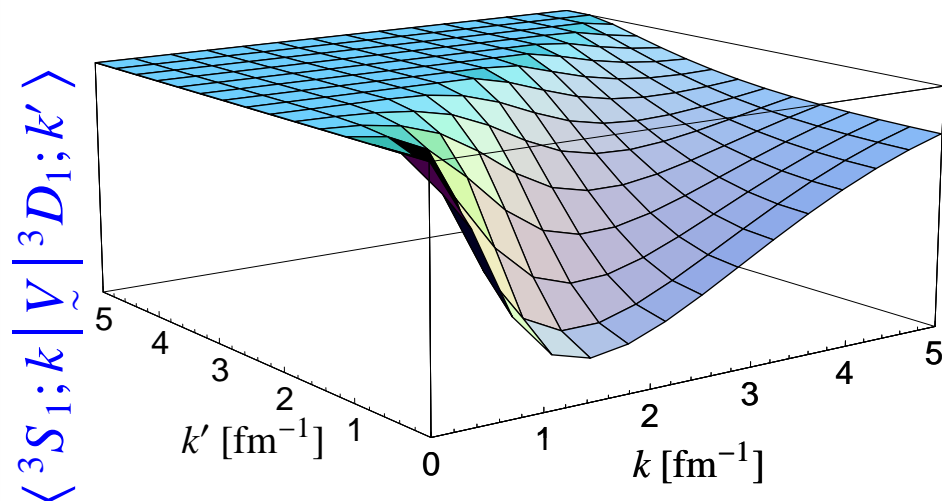
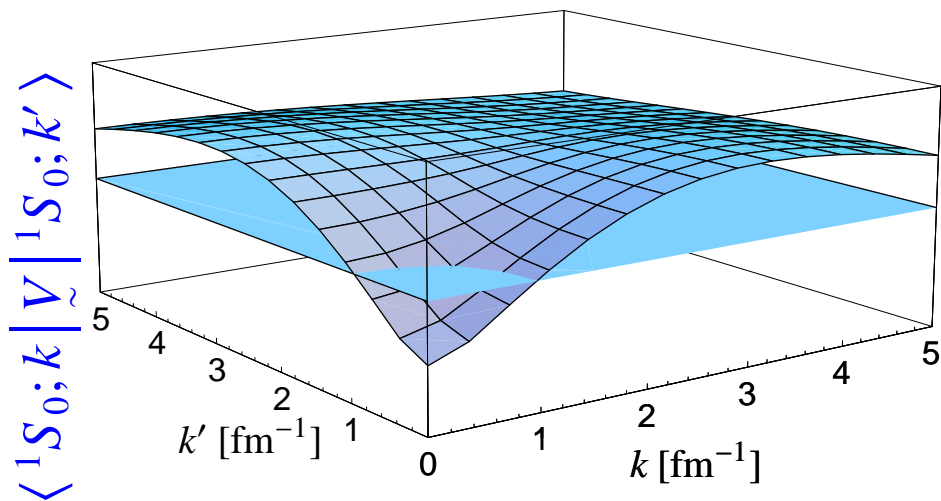


→ unique effective potential – identical to  $V_{\text{lowk}}$

Kuo, Schwenk, nucl-th/0108041

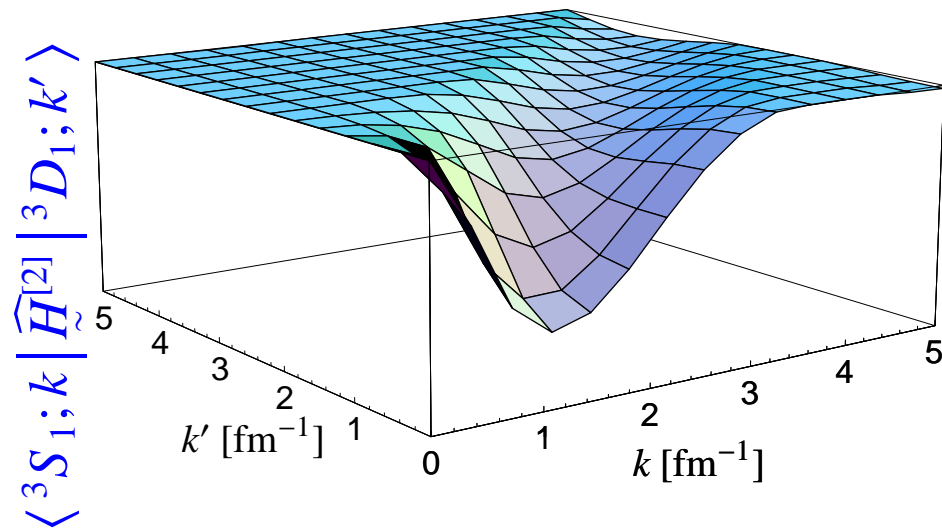
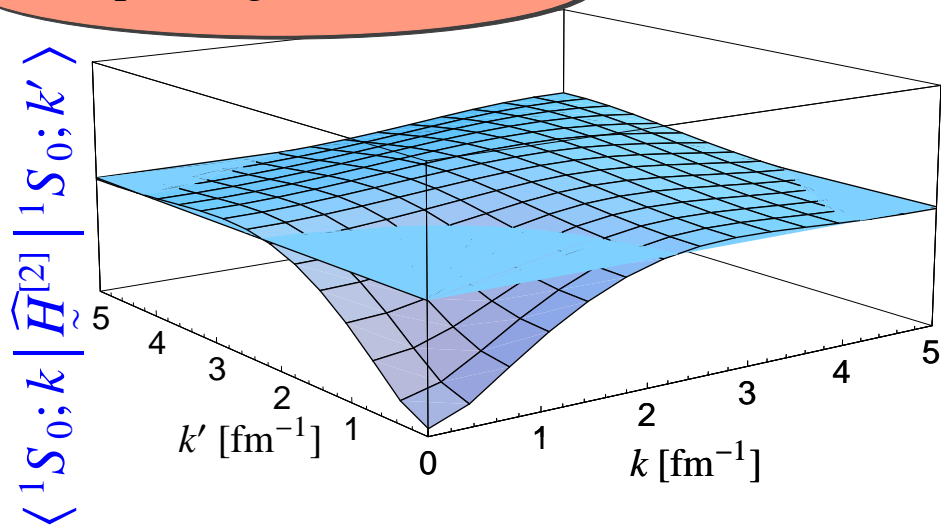
→  $V_{\text{lowk}}$  Cutoff  $\Lambda = 1.0 - 2.0 \text{ fm}^{-1}$

# Off-diagonal Matrix Elements



bare potential

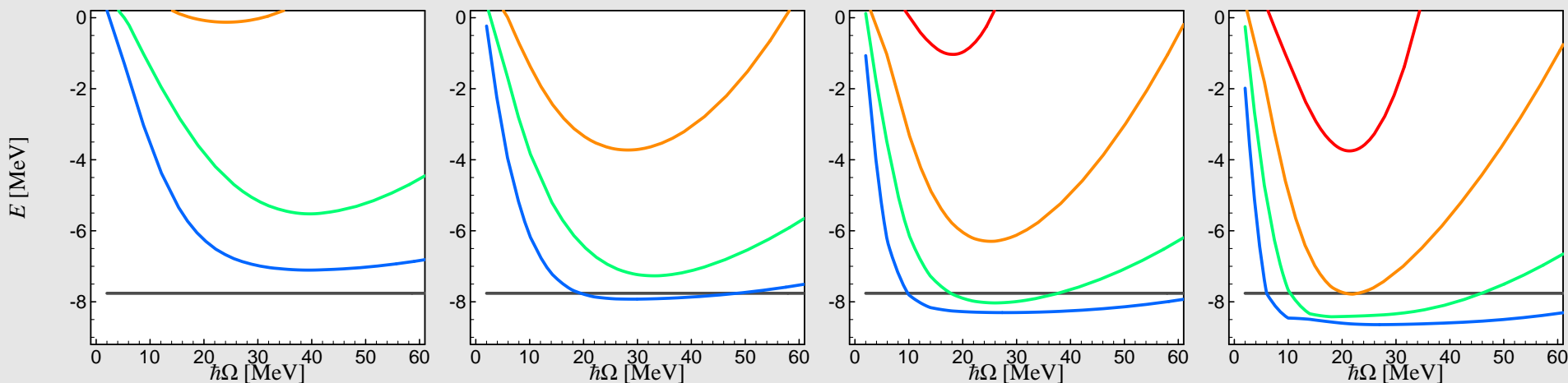
→ “pre-diagonalization”



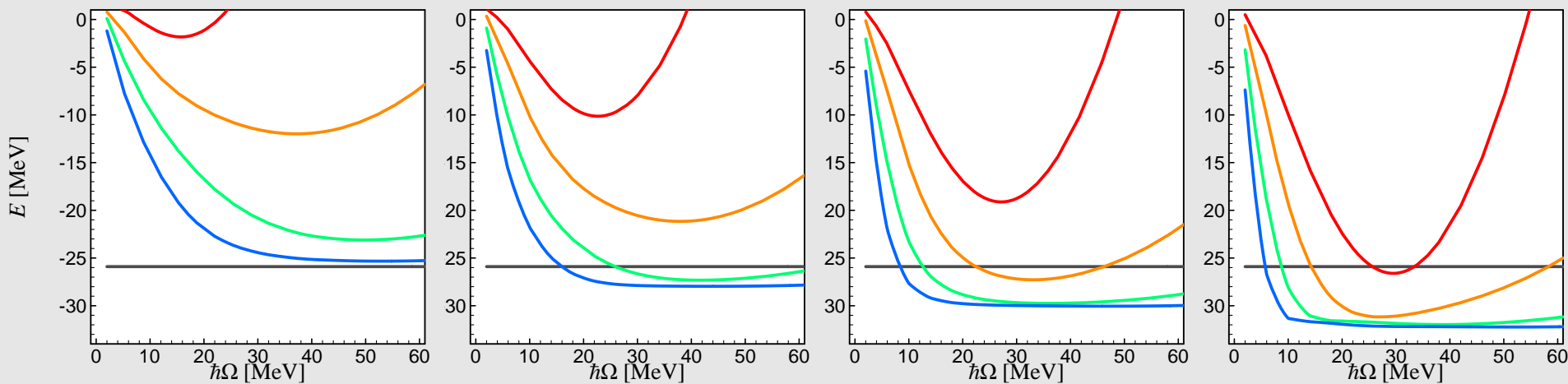
correlated interaction

Increasing range of tensor correlator

$^3\text{He}$

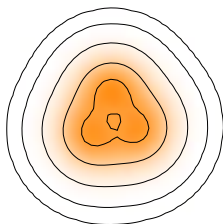


$^4\text{He}$



# $^{11}\text{B} (^3\text{He}, t) ^{11}\text{C}$ – Gamov-Teller transitions

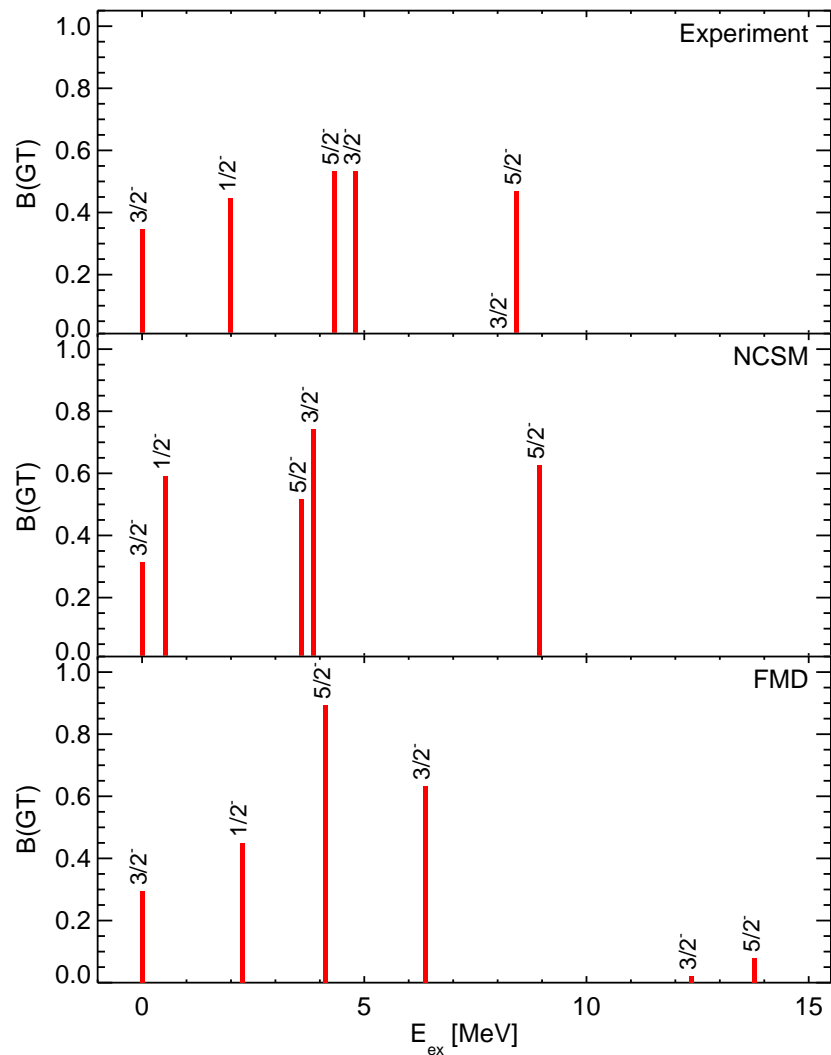
$^{11}\text{B}$



transition:  $\sigma \cdot \tau_+$

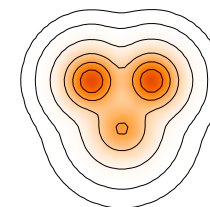
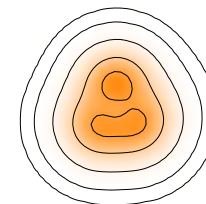
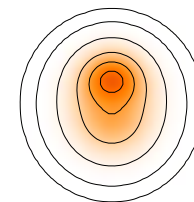
NCSM: Navrátil, Ormand  
no core shell model with 3-body  
force, PRC 68(2003)  
third  $3/2^-$  missing

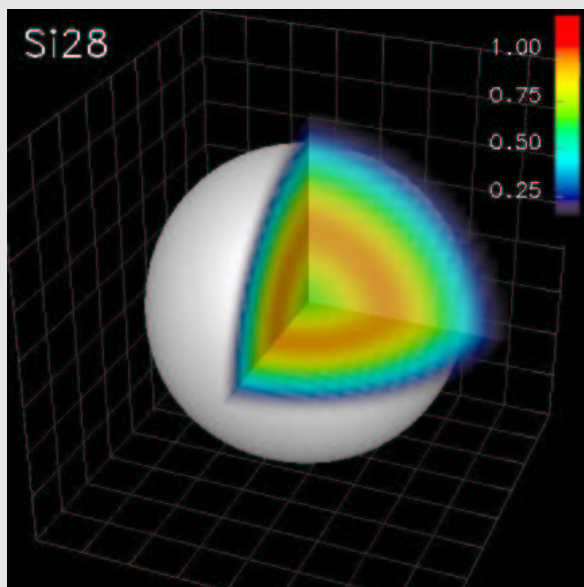
FMD with configuration mixing



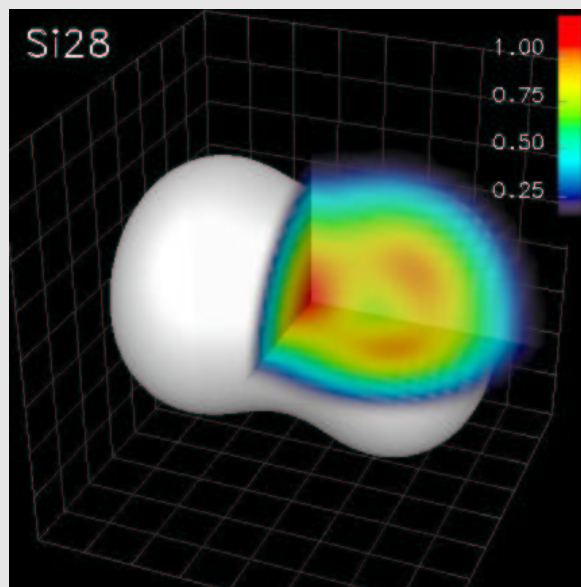
Exp.: Y. Fujita, P. von Bretano et al. to be published

$^{11}\text{C}$

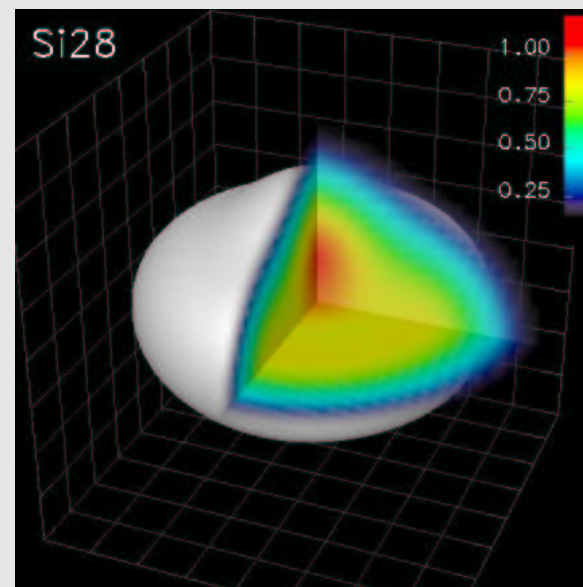




Variation → rund



Erdnuss  
lokales Minimum  
vor Projektion ca. 5 MeV  
höher als rund



Ufo  
vor Projektion ca. 10 MeV  
höher als rund

$$\rho^{(1)}(\vec{r}) [\rho_0]$$