Cluster Structures, Halos, Skins, and S-Factors

within Fermionic Molecular Dynamics

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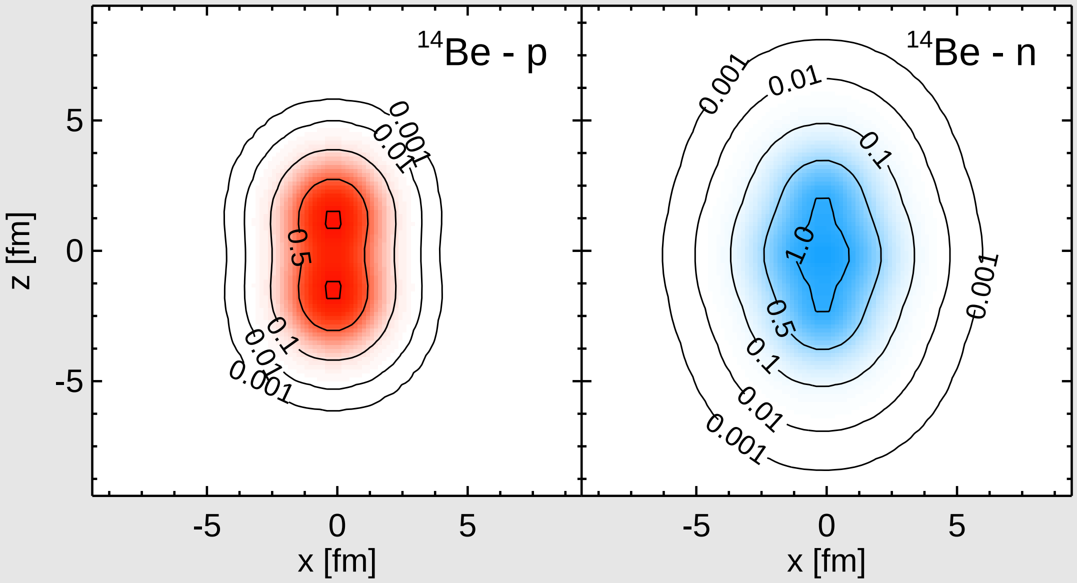


Nuclear Structure – ab initio

Aim

- describe low energy properties of nuclear many-body system

  in terms of a Hamiltonian $H = T + V_{NN}$

  and many-body states $|\hat{\Psi}\rangle$

- solve Schrödinger equation $H|\widehat{\Psi}_n\rangle = E_n|\widehat{\Psi}_n\rangle$

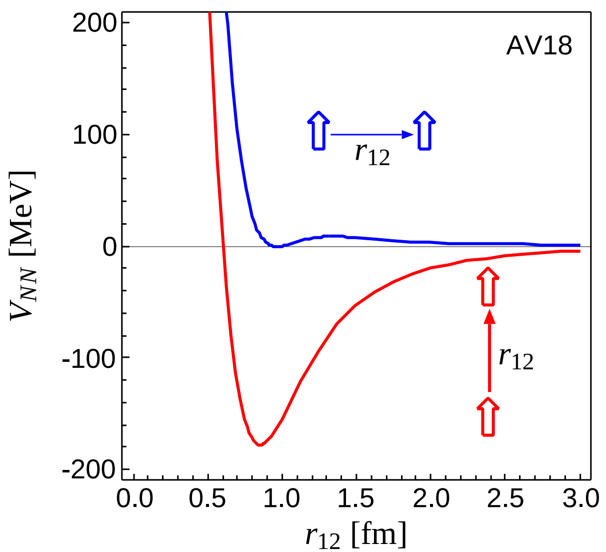
Ingredients

H = Hamiltonian with realistic NN-potential V_{NN}
(phase shifts, deuteron)

$|\widehat{\Psi}_n\rangle$ ϵ many-body Hilbert space
$\langle \vec{r}_1\vec{\sigma}_1\tau_1, \vec{r}_2\vec{\sigma}_2\tau_2, \cdots, \vec{r}_A\vec{\sigma}_A\tau_A | \widehat{\Psi}_n\rangle$ is terribly complicated for realistic interaction
main problem: short-range repulsive and tensor correlations induced by V_{NN}

Realistic NN-potential

$V_{NN}(\vec{r}_{12}, \vec{p}_{12} = 0, \vec{\sigma}_1, \vec{\sigma}_2, T = 0)$



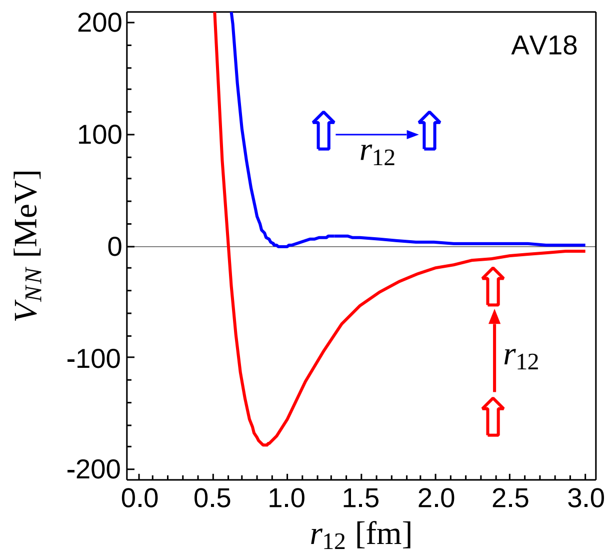
Argonne potential

- V_{NN} repulsive at small distances
  - ➨ strong short-range central correlations
    nucleons cannot get closer than ≈ 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

$V_{NN}(\vec{r}_{12}, \vec{p}_{12}=0, \vec{\sigma}_1, \vec{\sigma}_2, T=0)$



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

$$\left|\widehat{\Psi}\right\rangle = C\left|\Psi\right\rangle = C_\Omega\, C_r \left|\Psi\right\rangle$$

- C_r central correlator shifts nucleons out of repulsive core
- C_Ω tensor correlator aligns spins along $\vec{r}_{12}$

Unitary Transformation

Unitary Transformation

transform eigenvalue problem

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

with the unitary operator C

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

into the equivalent eigenvalue problem

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

"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

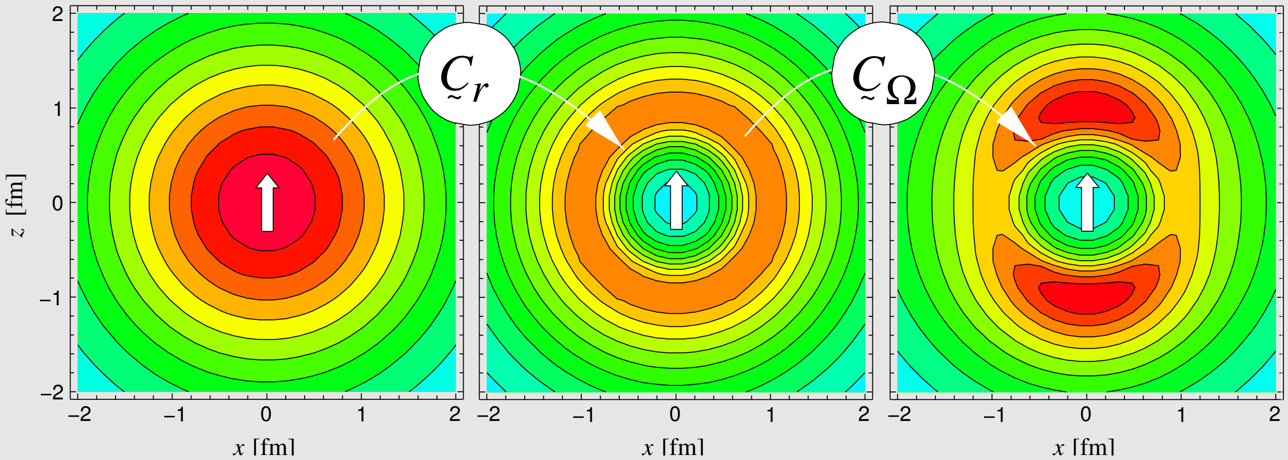
➨ treat long range correlations in $\left| \Psi \right\rangle$

➨ short range correlations in unitary $C = C_\Omega C_r$

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

Correlations in Nuclei

two-body densities

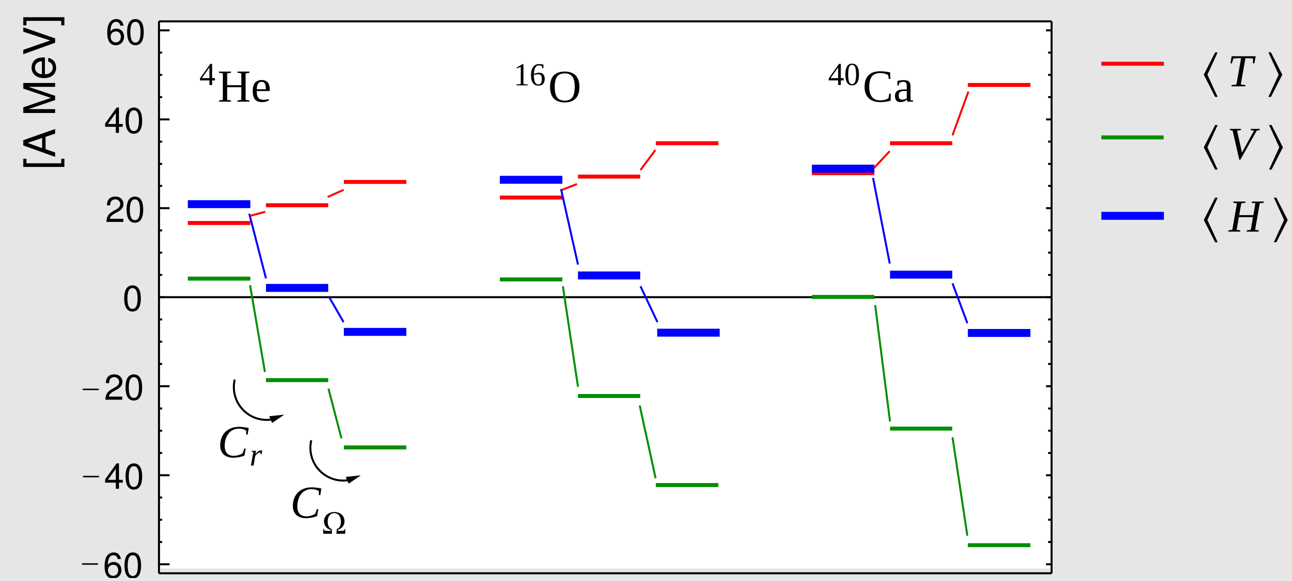


$\rho^{(2)}_{S,T}(\vec{r}_1 - \vec{r}_2) \quad S = 1, M_S = 1, T = 0$

- 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

energies



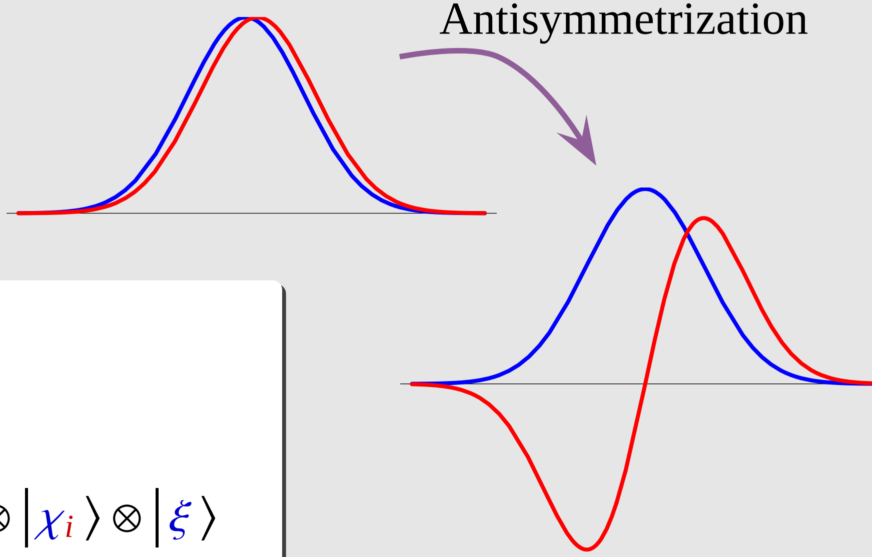
Hilbert Space: Fermionic Molecular Dynamics

Fermionic

Slater determinant

$$\big|\, Q \,\big\rangle = \mathcal{A}\Big(\big|\, q_1 \,\big\rangle \otimes \cdots \otimes \big|\, q_A \,\big\rangle\Big)$$

➨ antisymmetrized *A*-body state



Molecular

single-particle states

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

➨ 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 $\big|\, Q^{(a)} \,\big\rangle$

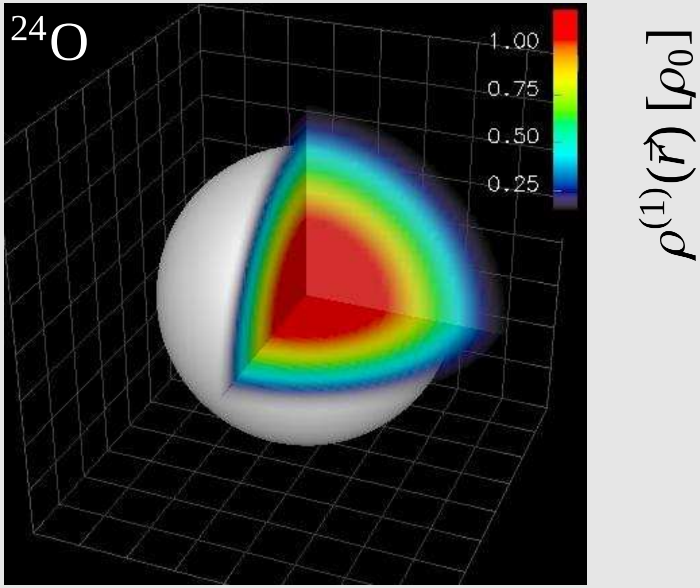
$$\big|\, \Psi \,\big\rangle = \sum_a \psi_a \,\big|\, Q^{(a)} \,\big\rangle$$

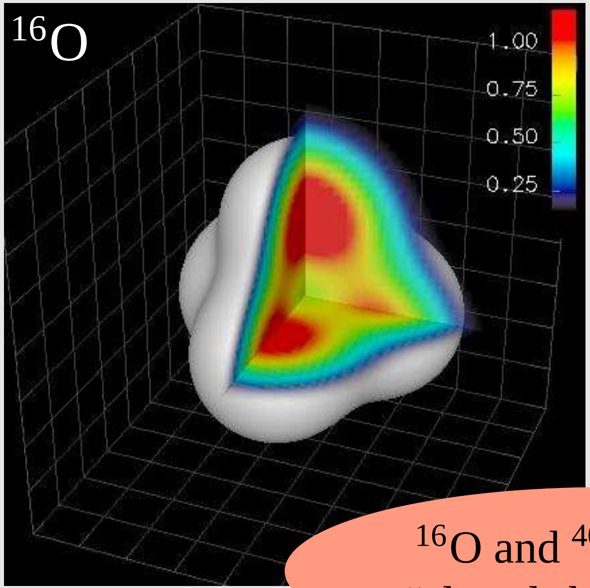
variational principle $\rightarrow$ $Q^{(a)} = \{\, q_\nu^{(a)},\, \nu = 1 \cdots A \,\},\ \psi_a$

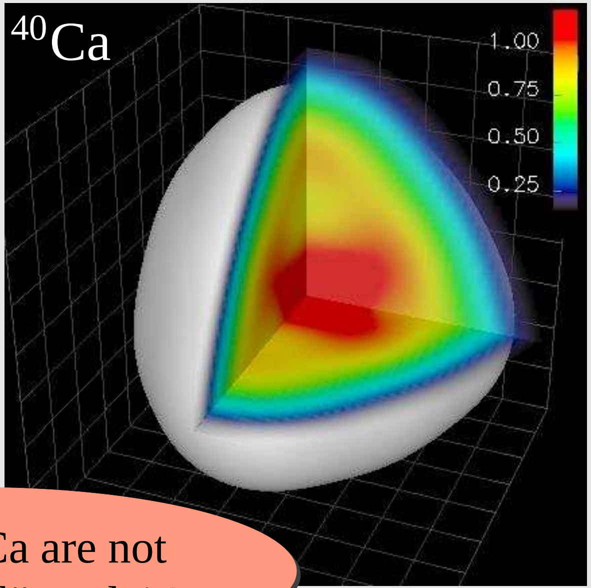
Effective Correction to the Interaction

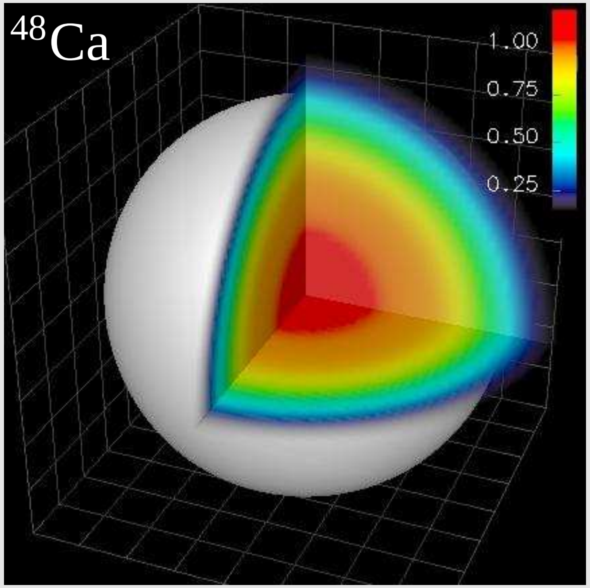
Effective two-body interaction

- correlated two-body interaction $\widehat{H} = C^\dagger H\, C$ 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









^{16}O and ^{40}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 $P^{J\pi}_{MK}$

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

Variation After Projection (VAP)

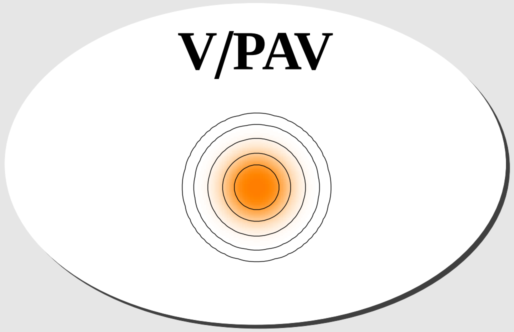
- effect of projection can be large
- perform VAP applying **constraints** on radius, dipole moment, quadrupole moment or octupole moment and minimize the energy in the projected energy surface

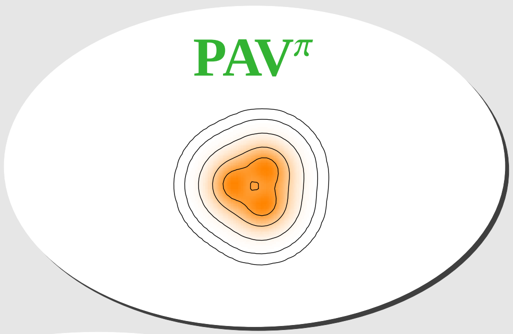
Multiconfiguration Calculations

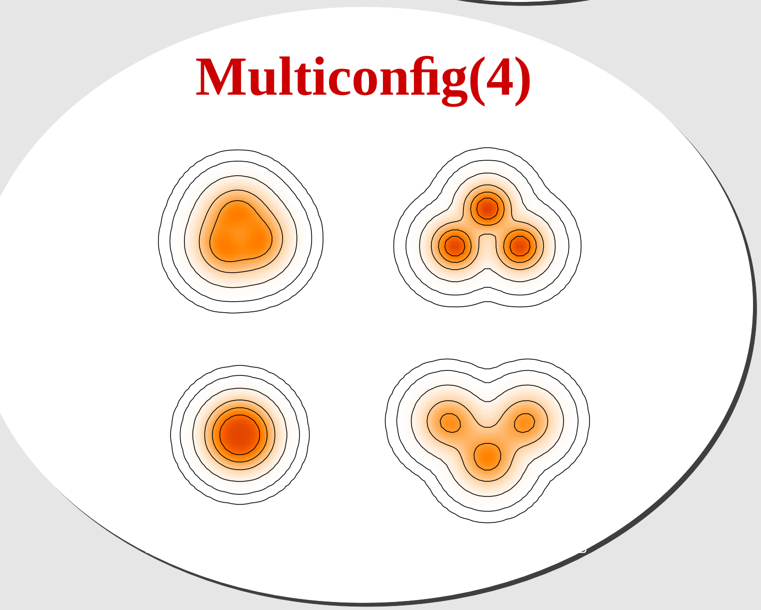
- diagonalize Hamiltonian in a set of projected intrinsic states

$$\left\{ P^{J\pi}_{KK'} \middle| Q^{(a)} \right\rangle , \quad a = 1, \cdots , N \right\}$$

FMD - Variation, PAV$^\pi$, Multiconfig.

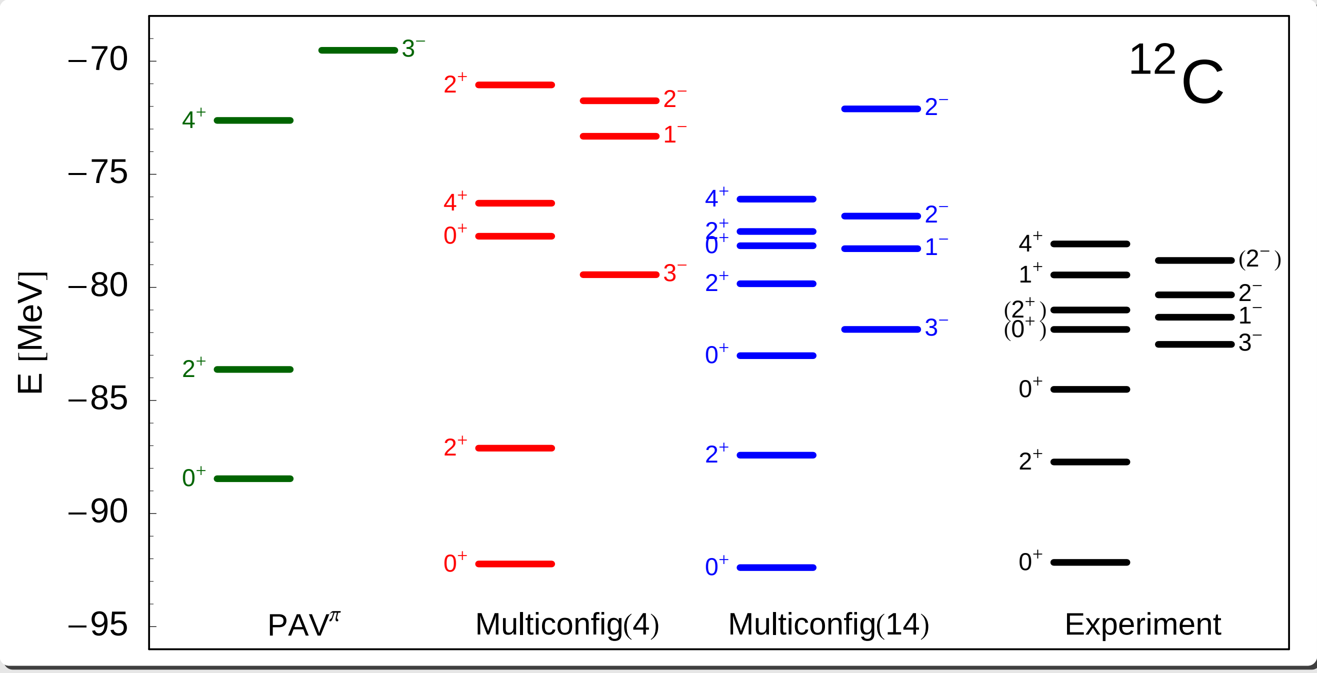






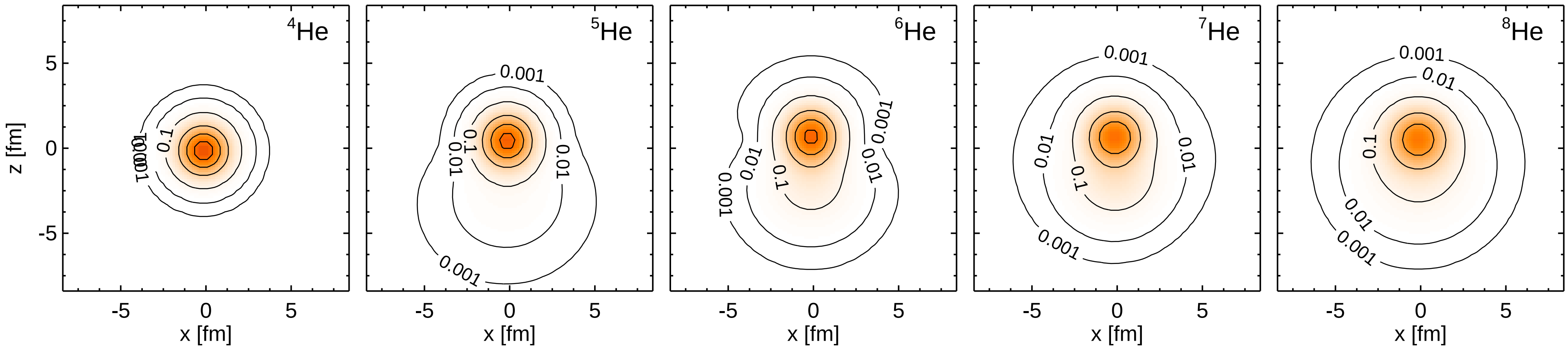
^{12}C

	E [MeV]	r_{charge} [fm]	$B(E2)$ [e^2fm^4]
V/PAV	-81.4	2.36	-
PAV$^\pi$	-88.5	2.51	36.3
Multiconfig(4)	-92.2	2.52	42.8
Multiconfig(14)	-92.4	2.52	42.9
Exp	-92.2	2.47	39.7 ± 3.3

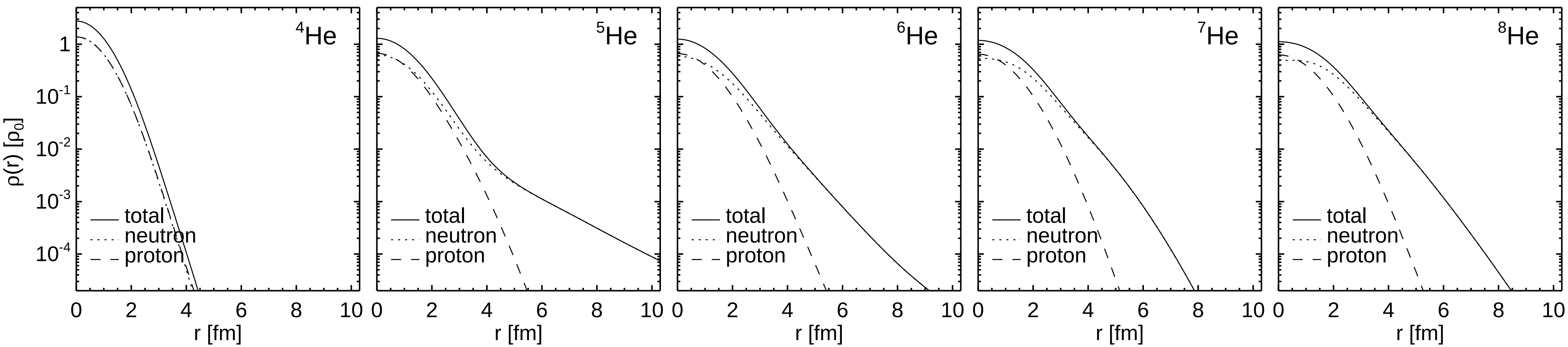


He Isotopes - Variation After Parity Projection

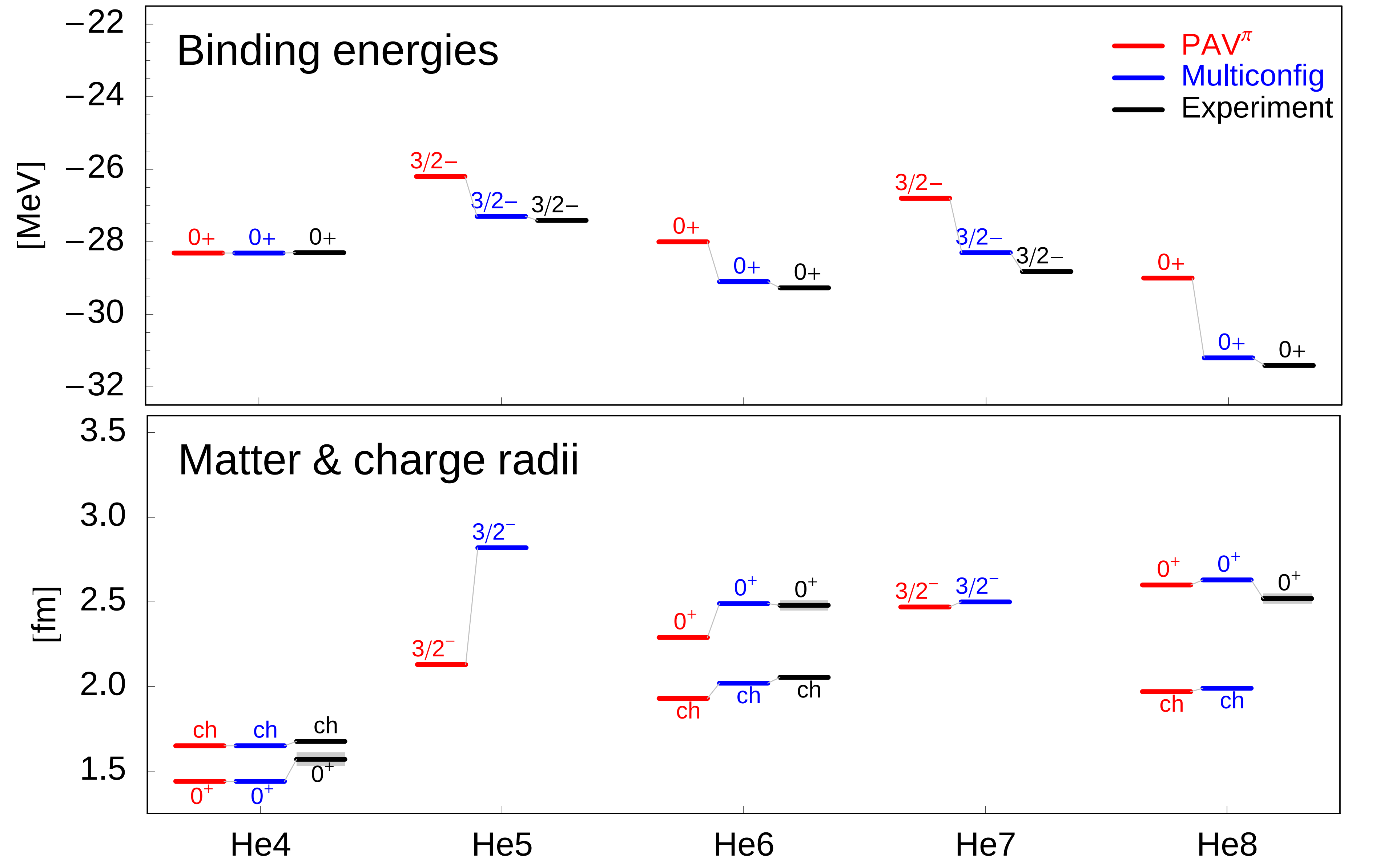
intrinsic densities $\langle\, Q \,|\, \hat{\rho}(\vec{r}) \,|\, Q \,\rangle$ $\qquad$ $|\, Q^\pi \,\rangle = |\, Q \,\rangle + (-1)^\pi\, \hat{\Pi}\, |\, Q \,\rangle$



radial densities of J^π-projected states (PAV$^\pi$) $\qquad$ $|\, J^\pi M \,\rangle = \hat{P}^J_M \,|\, Q^\pi \,\rangle$

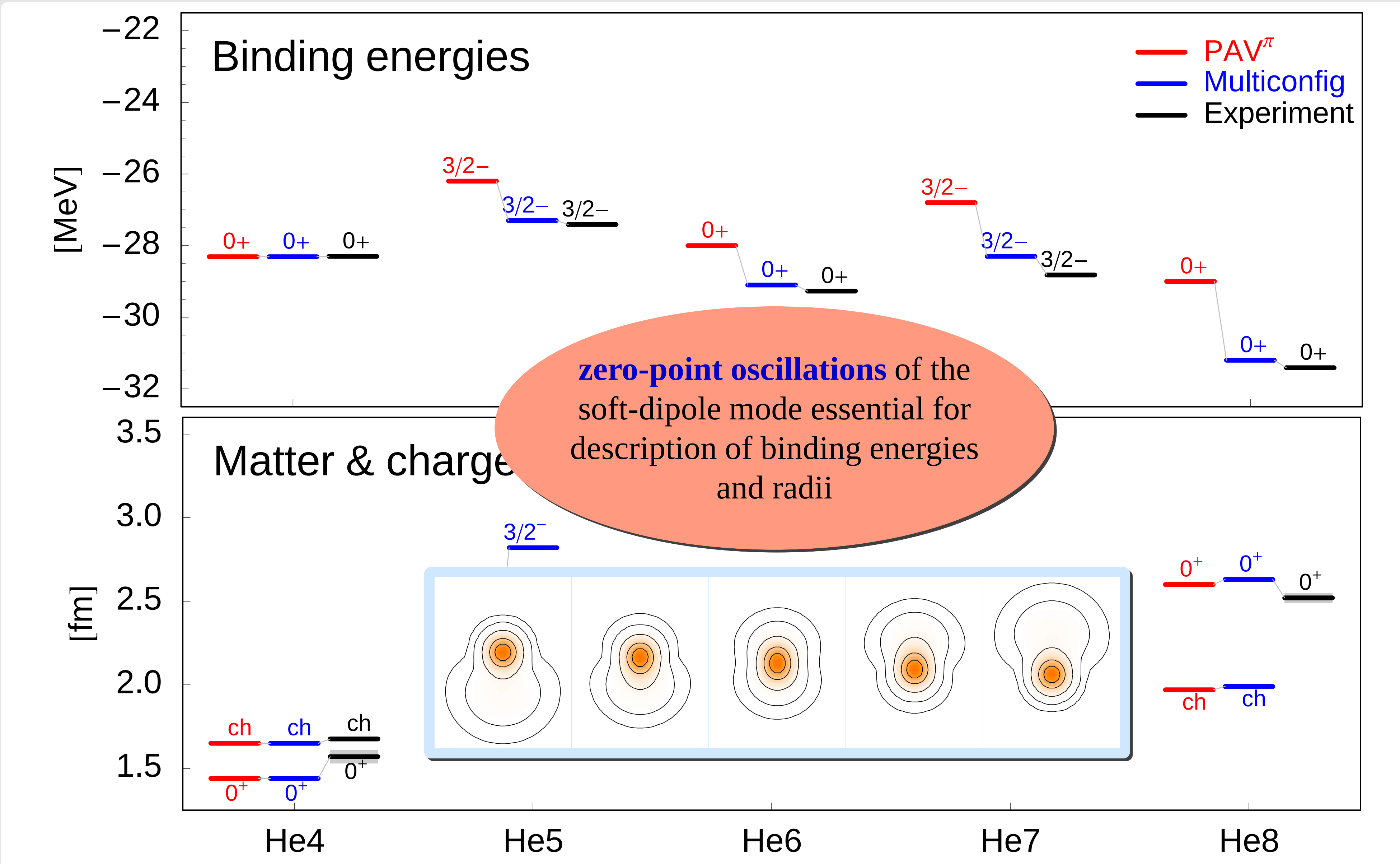


Helium Isotopes



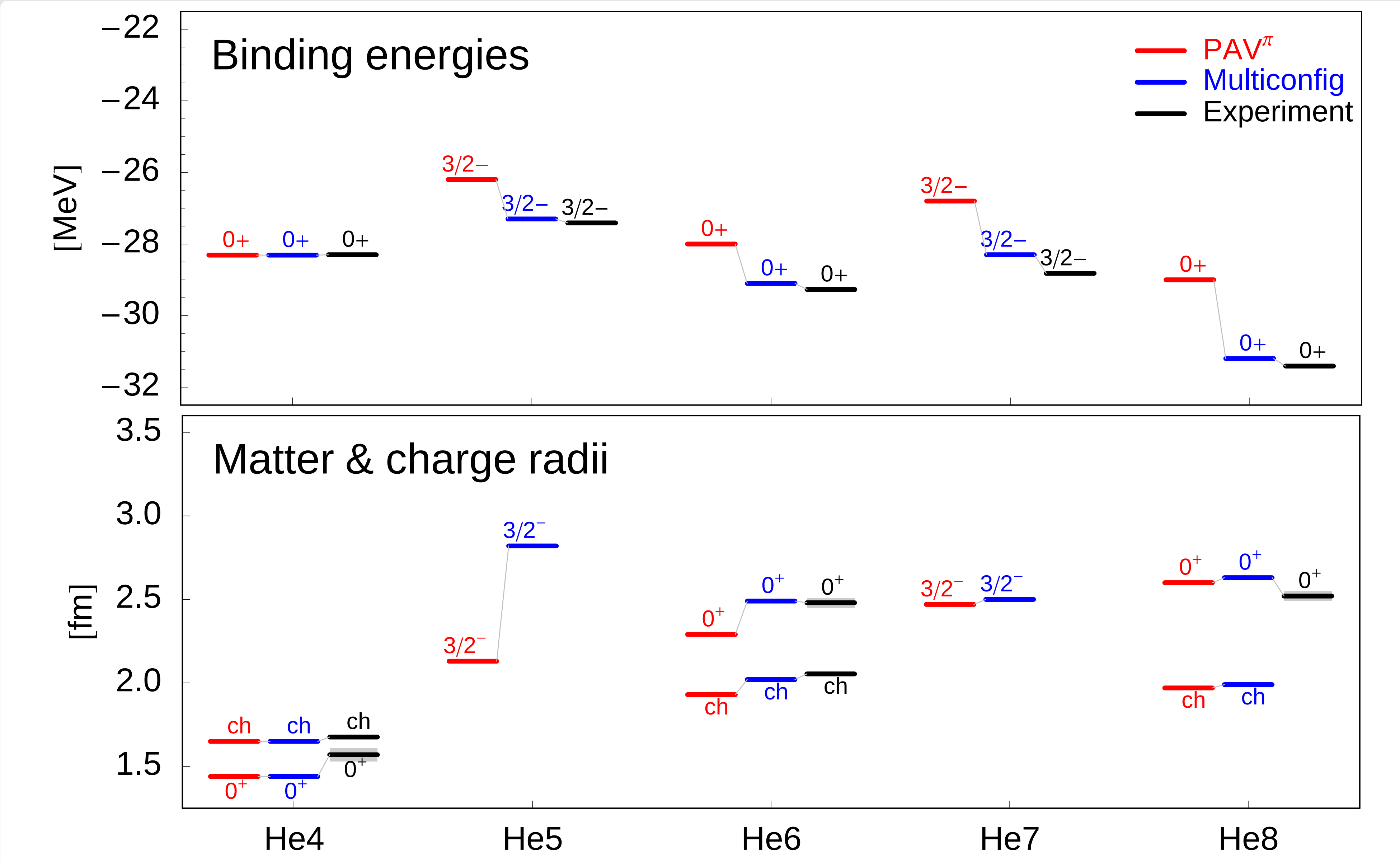
Exp: Ozawa,Suzuki,Tanihata, NP**A693**(2001)32; Raman,Nestor,Tikkanen, Atomic Data and Nucl. Data Tables **78**(2001)1

Helium Isotopes - Multi-Configuration Mixing



Exp: Ozawa,Suzuki,Tanihata, NP**A693**(2001)32; Raman,Nestor,Tikkanen, Atomic Data and Nucl. Data Tables **78**(2001)1

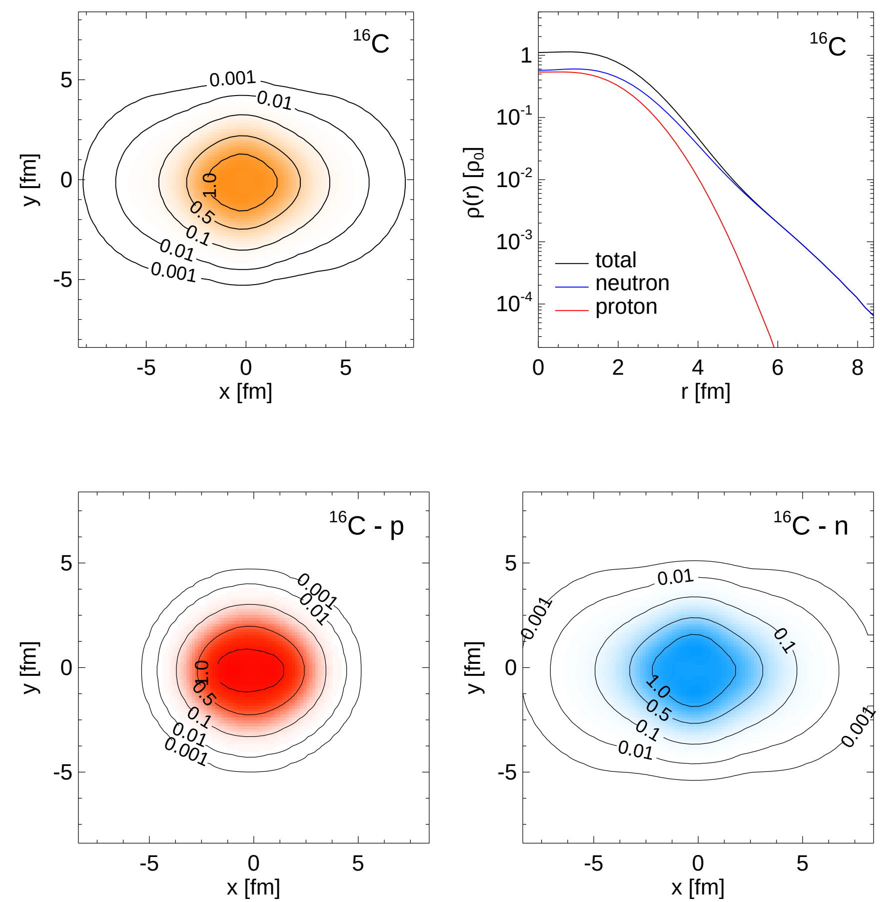
Helium Isotopes



Exp: Ozawa,Suzuki,Tanihata, NP**A693**(2001)32; Raman,Nestor,Tikkanen, Atomic Data and Nucl. Data Tables **78**(2001)1

^{16}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 ± 0.03
			2.76 ± 0.06

	E_{2^+} [MeV]	$B(E2)$ [e^2fm^4]
PAV	1.29	4.6
Exp	1.77	3.15 ± 0.95
Global Best Fit[1]	1.77	82 ± 14

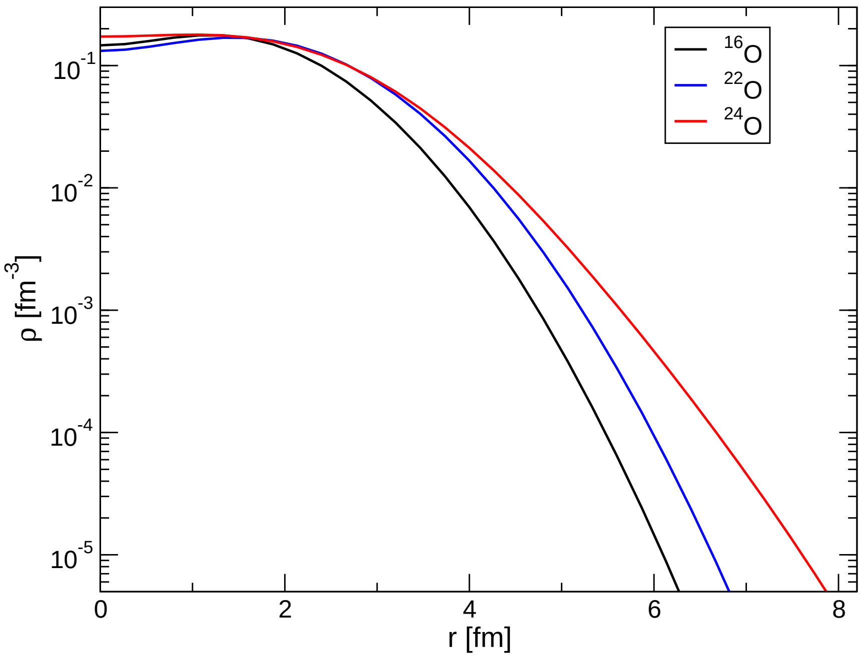
[1] Raman *et al*, Atomic Data and Nuclear Data Tables **78** (2001) 1

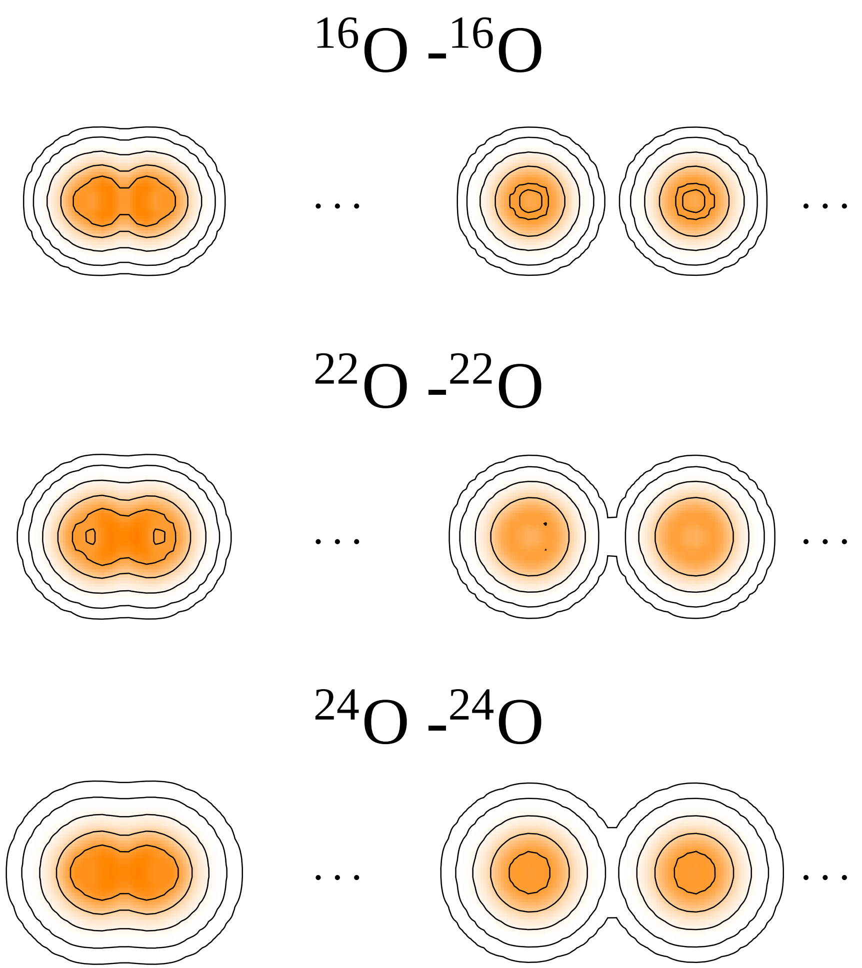
- calculated B(E2) consistent with anomalously long lifetime of 2^+ state measured at RIKEN

  Imai *et al*, PRL in print

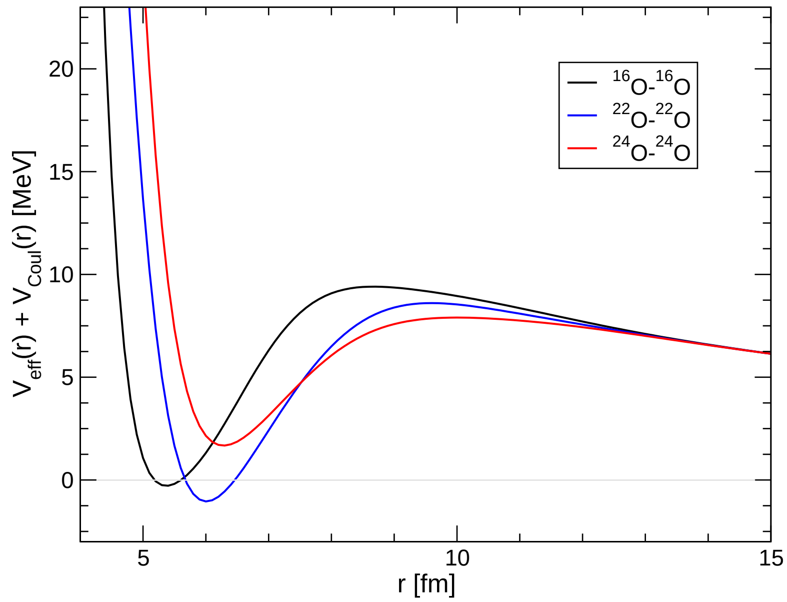
Microscopic Nucleus-Nucleus Interactions

- Fermionic Molecular Dynamics (FMD) many-body states
- Effective nucleon-nucleon interaction derived from realistic Argonne V18 interaction





S-Factors

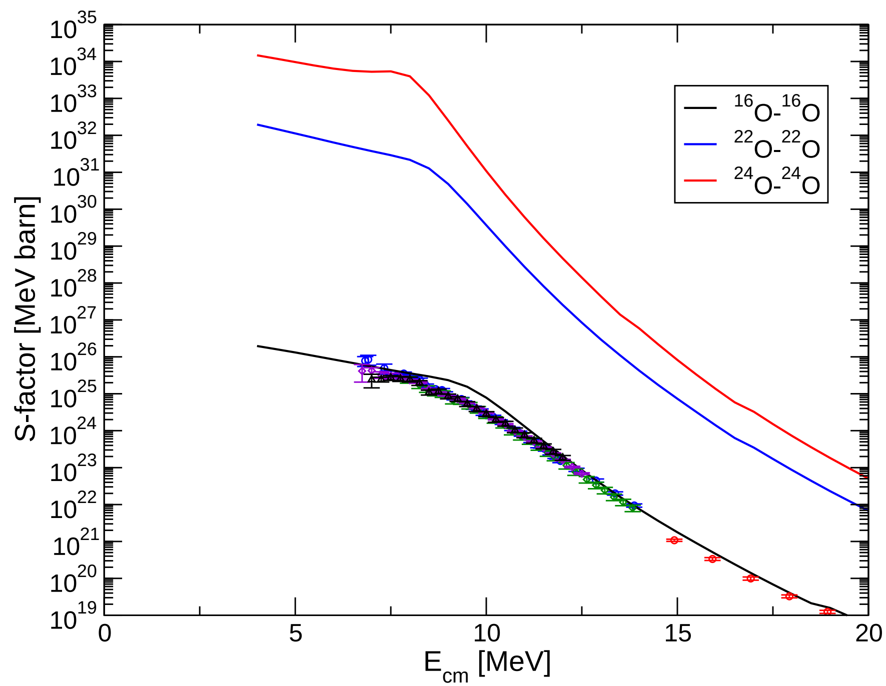


Microscopically derived
Nucleus-Nucleus potentials

Astrophysical S-factor

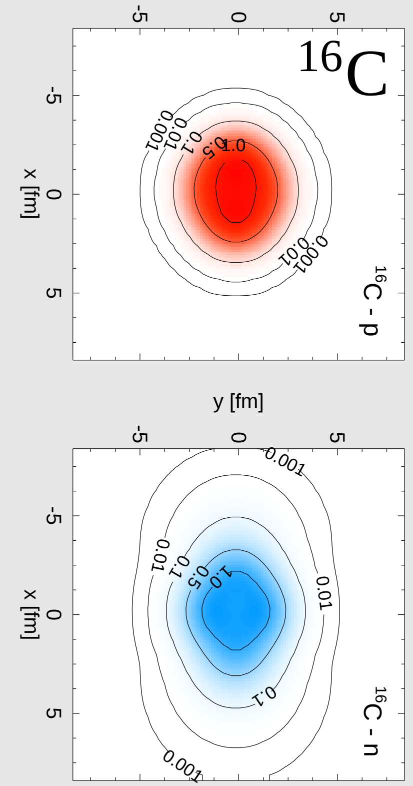
$$S(E) = \sigma(E)\,E\,e^{2\pi\eta}$$

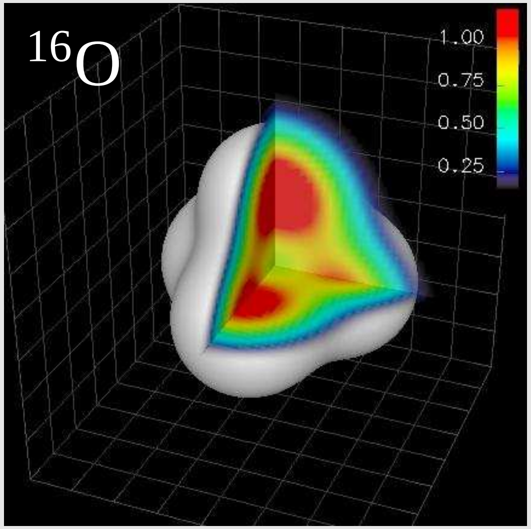
$$\eta = \frac{Z_1 Z_2 e^2}{\hbar^2 v}$$



Summary and Outlook

- **Unitary Correlation Operator Method**
  describes short ranged central and tensor correlations
- UCOM provides ab-initio correlated interaction $\widehat{H} = C^{\dagger} H\, C$
  for many-body methods like HF, shell model, FMD
- 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,
  nucleus-nucleus scattering, S-factor ...
- No assumption about core, mean-field, core-nucleon interaction, ...



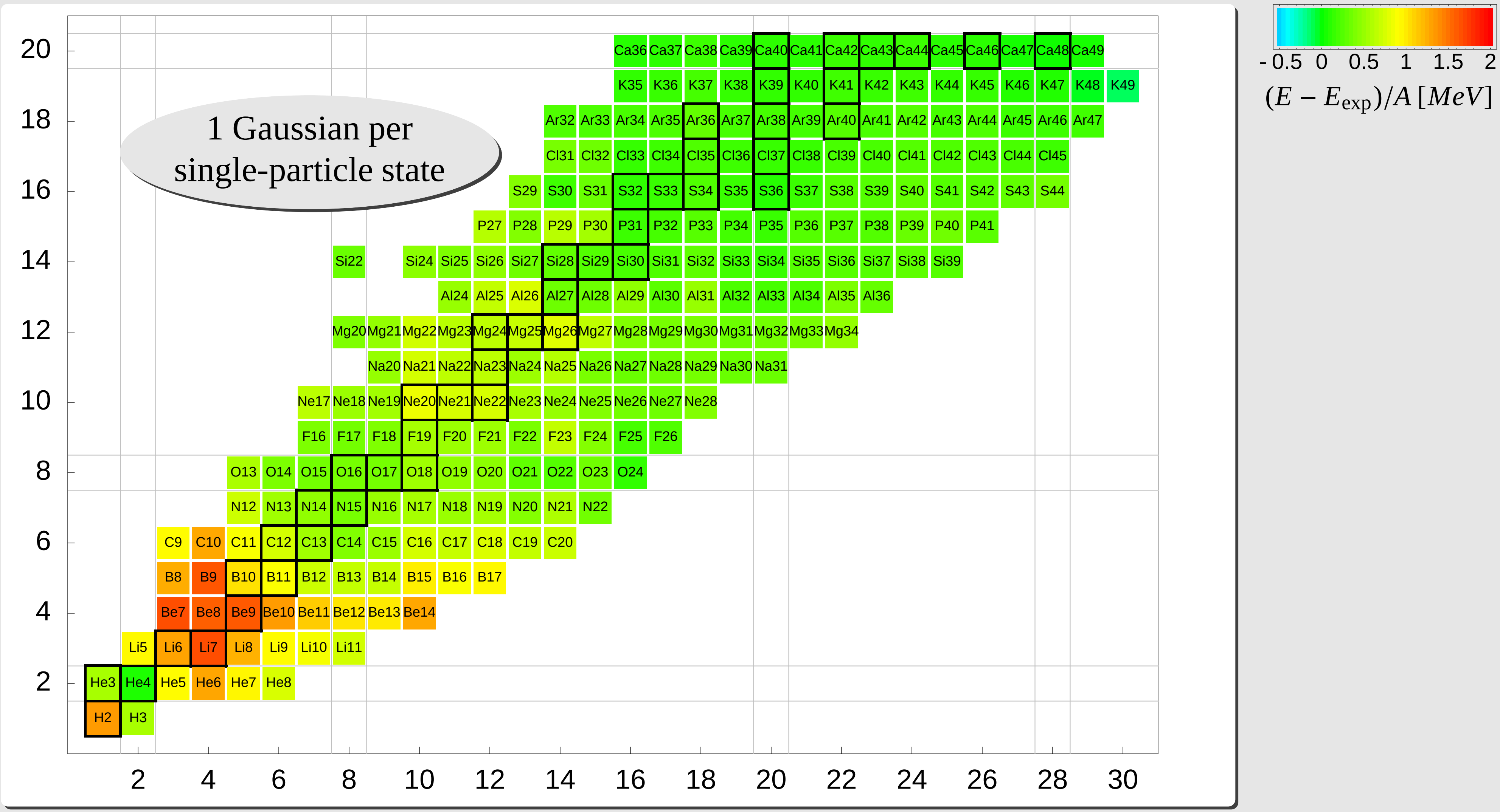


Outlook

- Predictions for many exotic light nuclei (before measurement)
- More applications in low energy nuclear astrophysics
- Ab-initio correlated interaction in HF, RPA or large scale shell model
  H. Hergert, Panagiota Papakonstantinou, N. Paar, R. Roth
  TU Darmstadt
- Investigate long ranged tensor correlations – 3-body forces – $\widehat{H}^{corr}$

Nuclear Chart

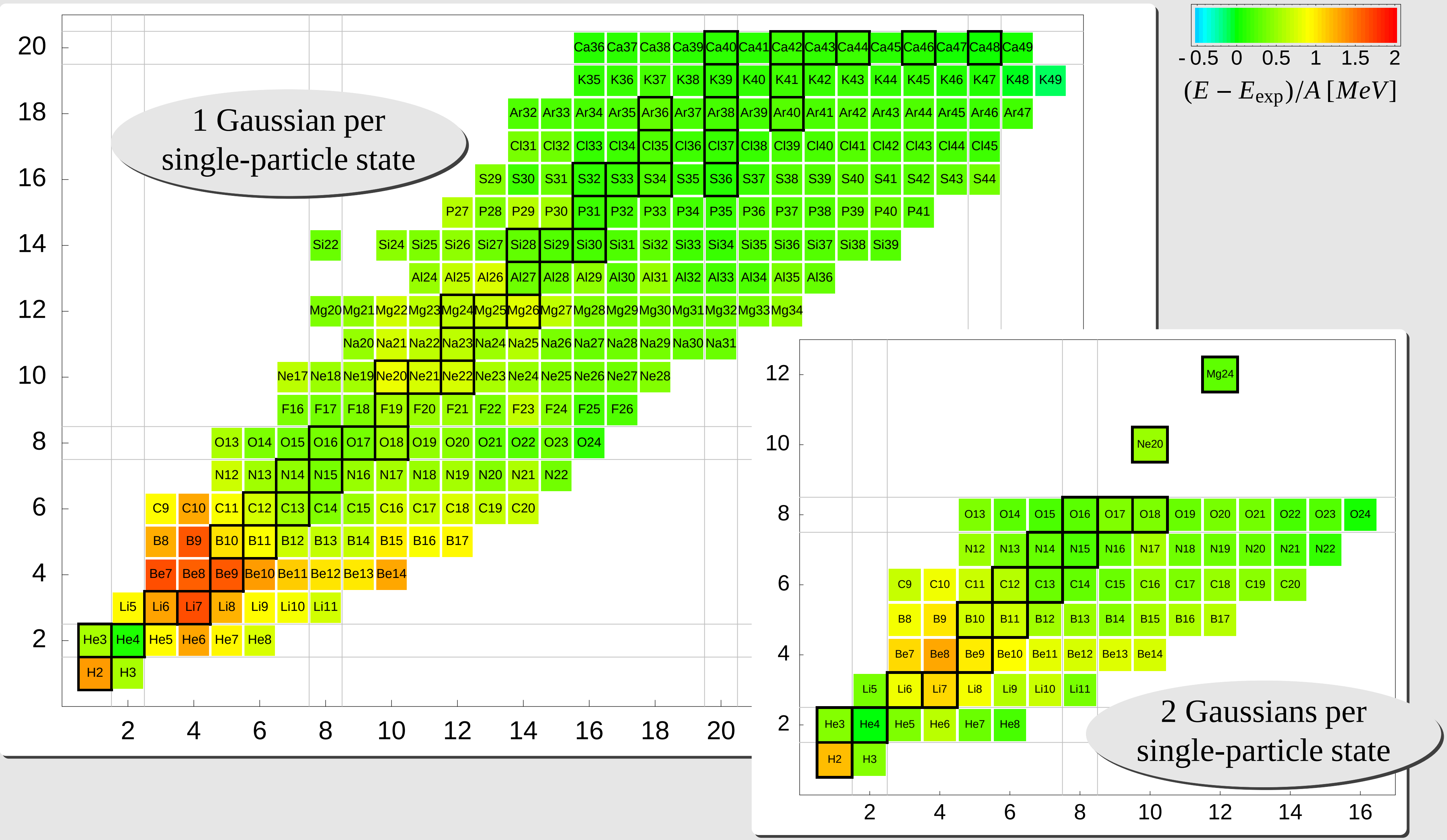
Variation of single determinant



FMD

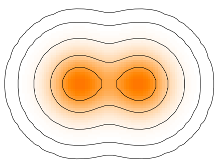
Nuclear Chart

Variation of single determinant

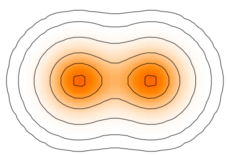


FMD - Projection, Variation after Proj., Multiconfiguration

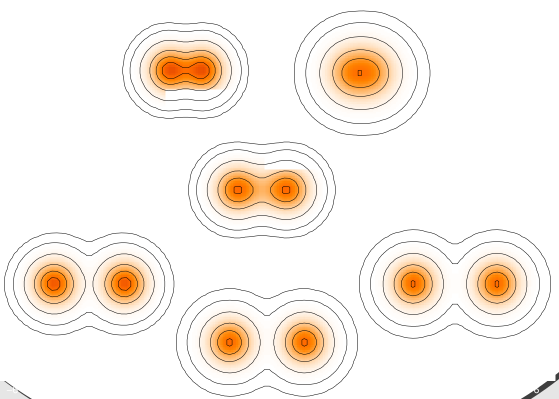
PAV



VAP

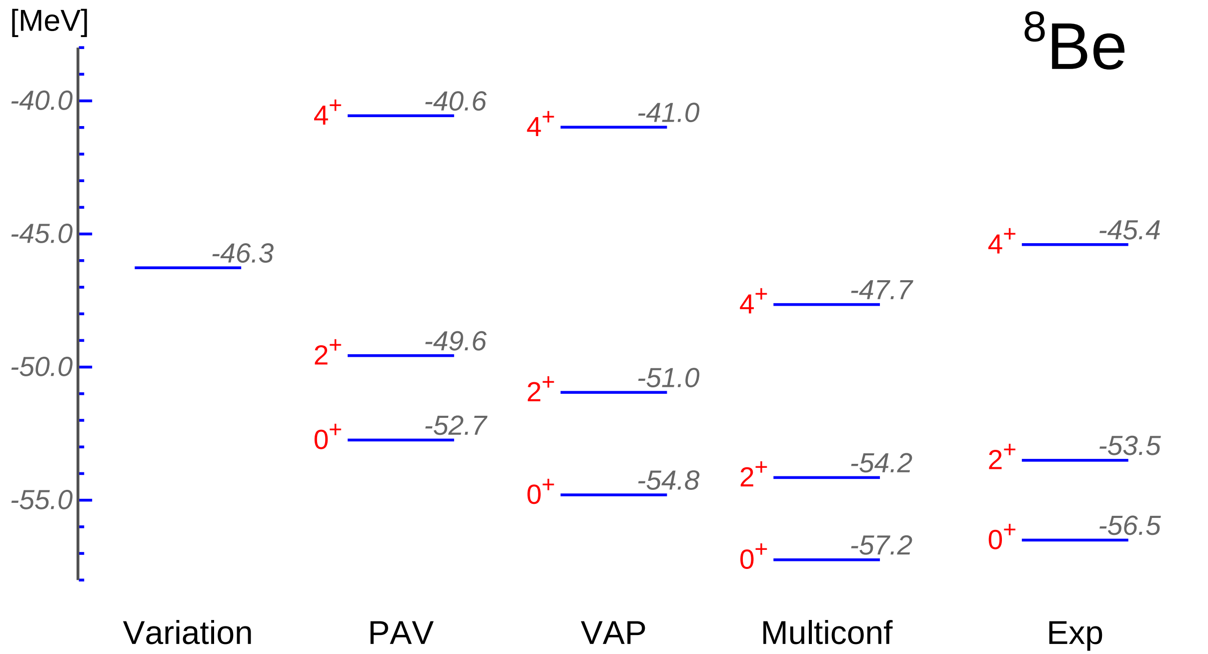


Multiconfig

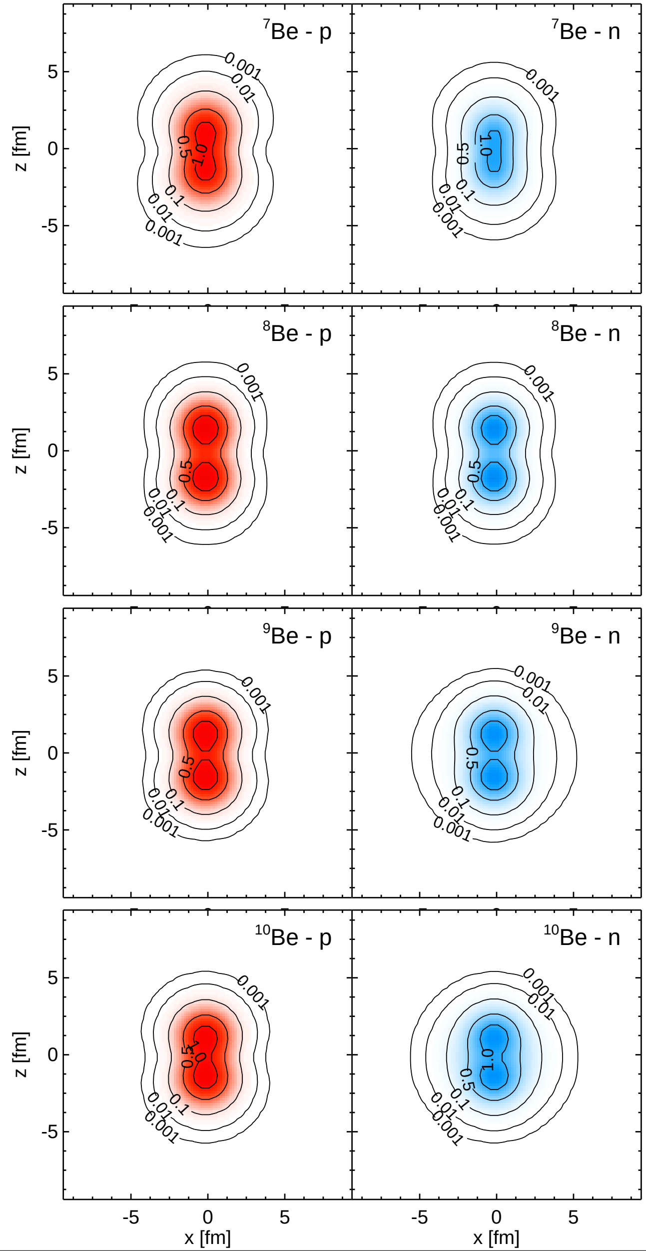


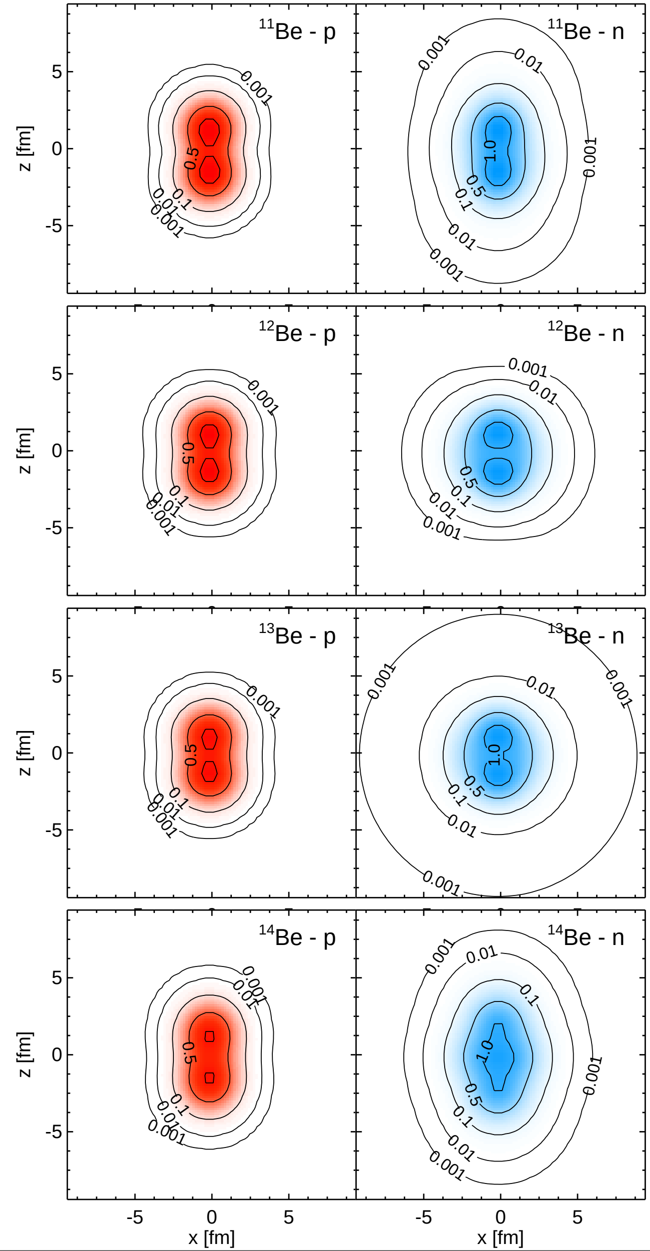
Radius and Quadrupole Moment as Generator Coordinates

	r_{charge} [fm]	Q [fm^2]	$B(E2)$ [e^2fm^4]
PAV	2.39	-6.25	9.31
VAP	2.49	-8.02	15.36
Multiconfig	2.74	-11.88	30.39



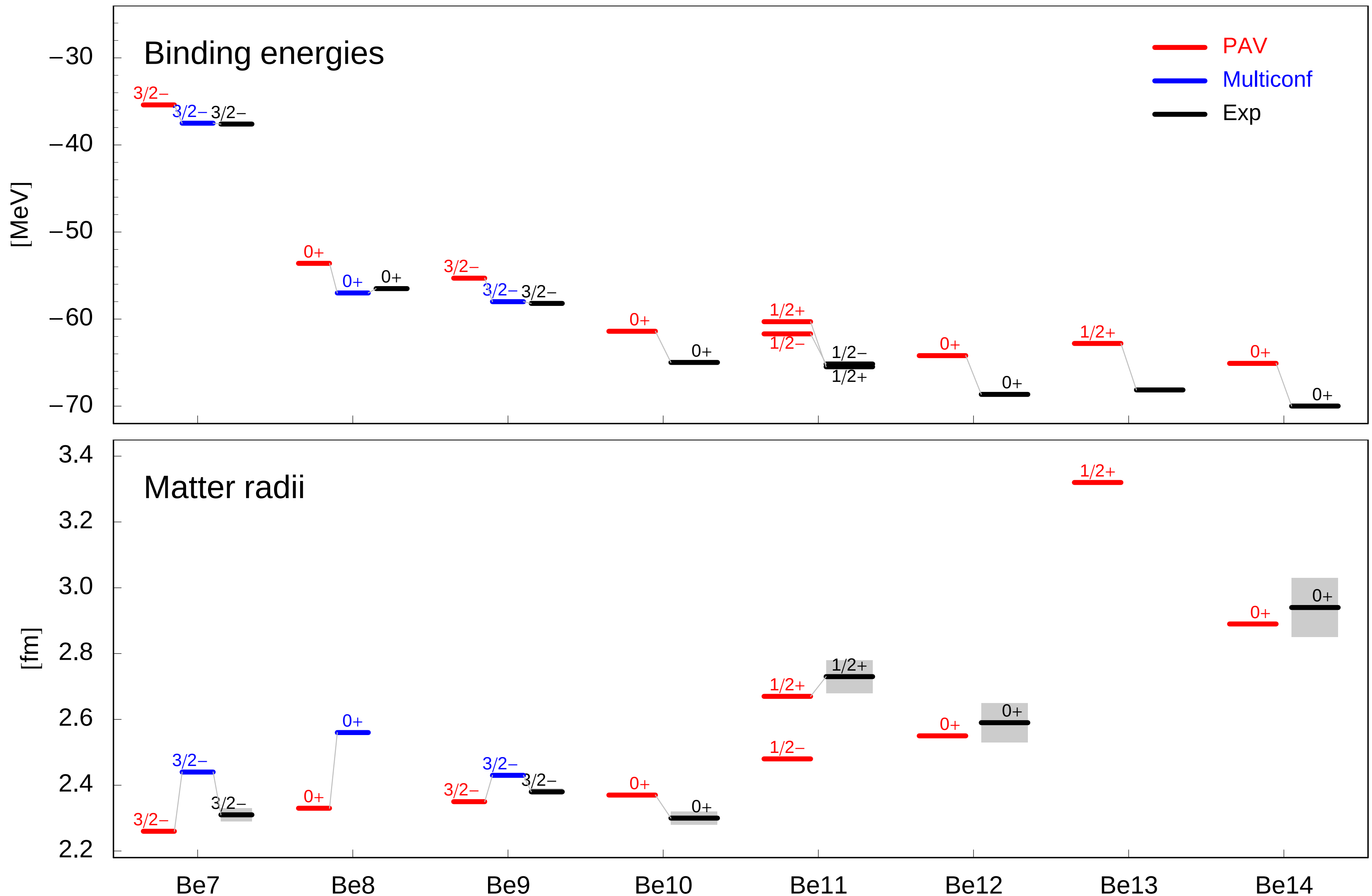
Beryllium Isotopes





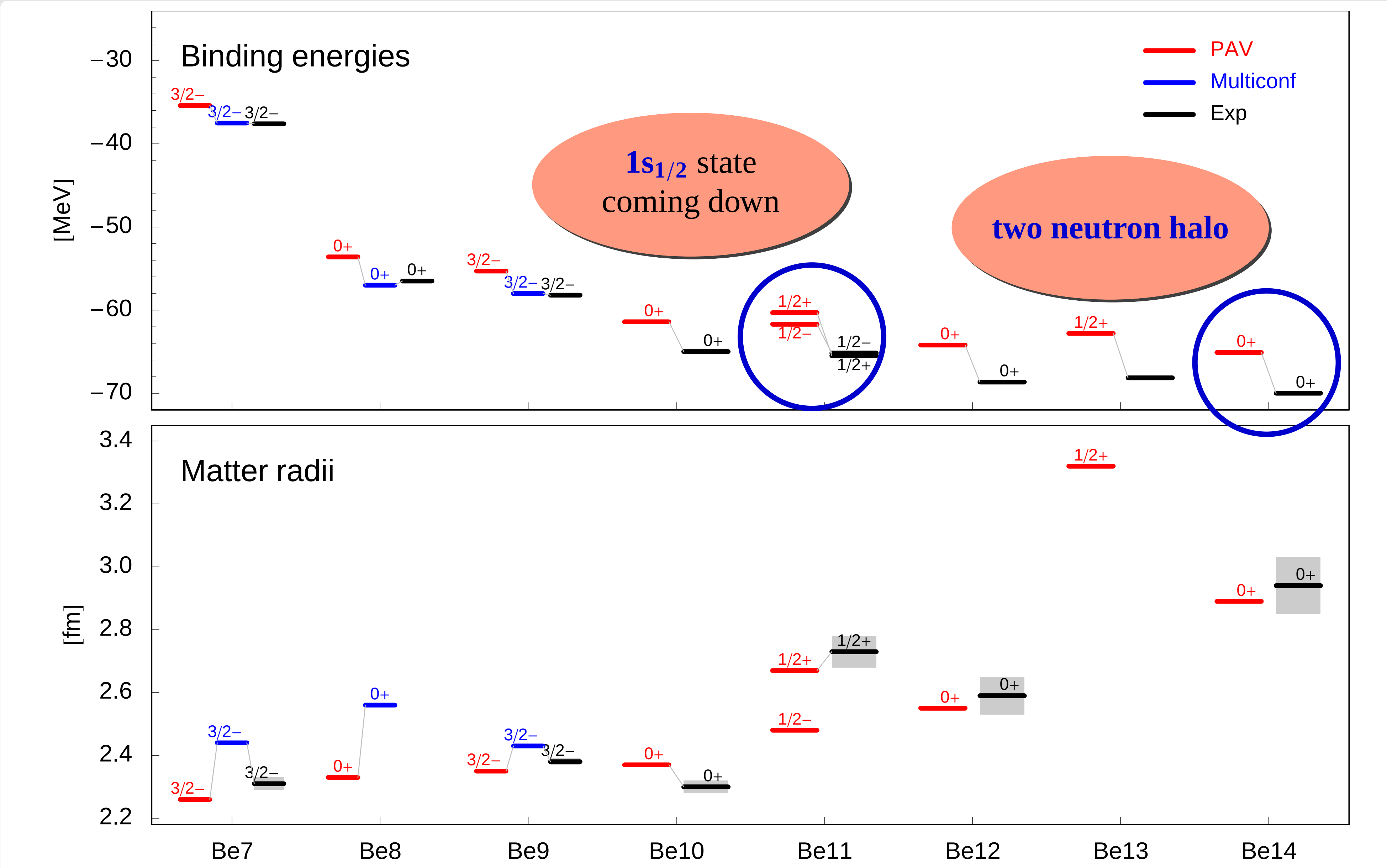
cluster structure changes with addition of neutrons

Beryllium Isotopes



Exp: Ozawa,Suzuki,Tanihata, NP**A693**(2001)32; Raman,Nestor,Tikkanen, Atomic Data and Nucl. Data Tables **78**(2001)1

Beryllium Isotopes



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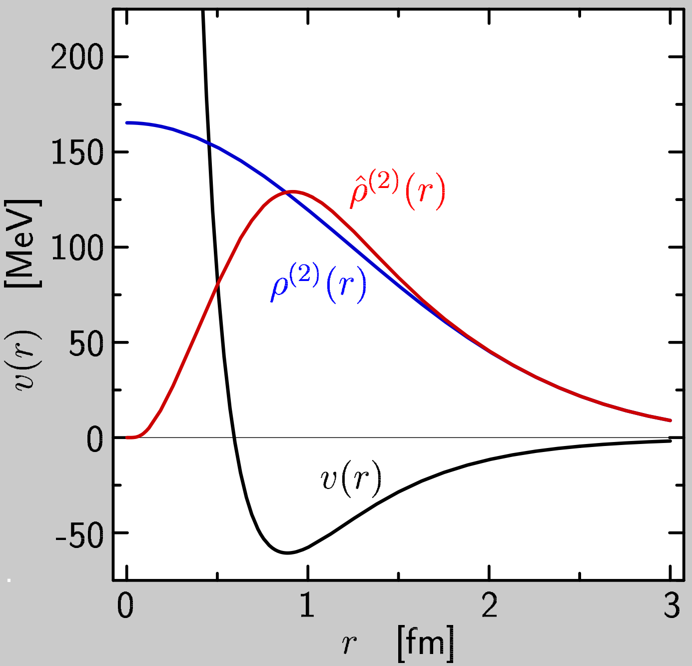
Radial Correlations

BECAUSE 1.) realistic interactions have short-range repulsion

➨ probability density of nucleons in the repulsive core strongly suppressed



$r = |\vec{r}_1 - \vec{r}_2|$

shell model

correlated

potential & two-body density of ^{4}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

$$s_{12}\left(\frac{\vec{r}}{r},\frac{\vec{r}}{r}\right) = 3\left(\boldsymbol{\sigma}_1\cdot\frac{\vec{r}}{r}\right)\left(\boldsymbol{\sigma}_2\cdot\frac{\vec{r}}{r}\right) - (\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)$$

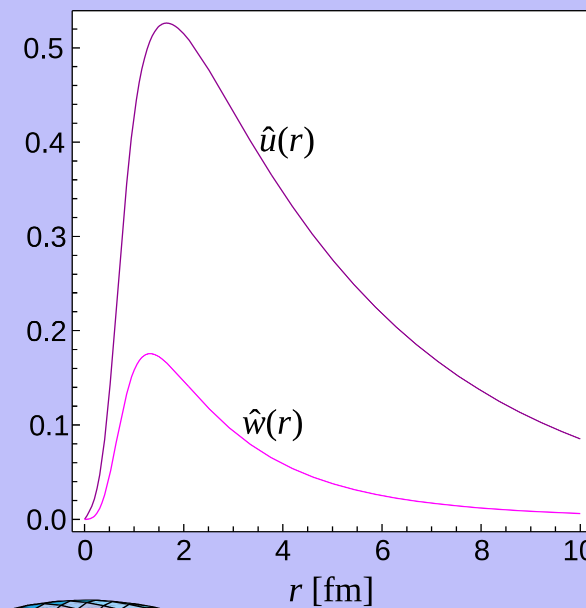
couples spins and the relative spatial orientation of nucleons

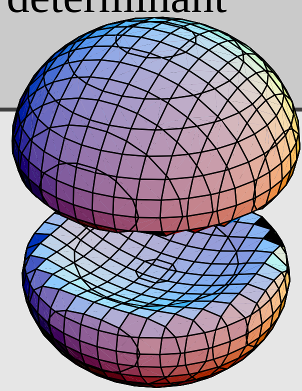
✘ correlations between the orientation of the spins and the relative orientation of nucleons cannot be described by Slater determinant

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

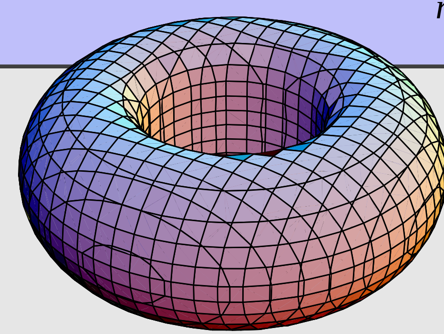
deuteron has $L=2$ admixture due to tensor force

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



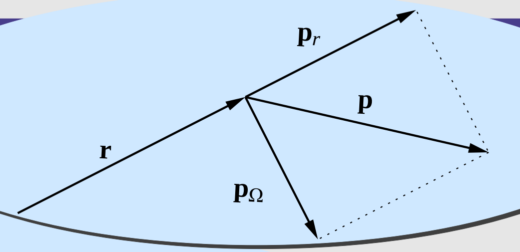


$|\uparrow\uparrow\rangle$



$\frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right)$

Radial and Tensor Correlations



$$C = C_\Omega C_r = e^{-iG_\Omega} e^{-iG_r}$$

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

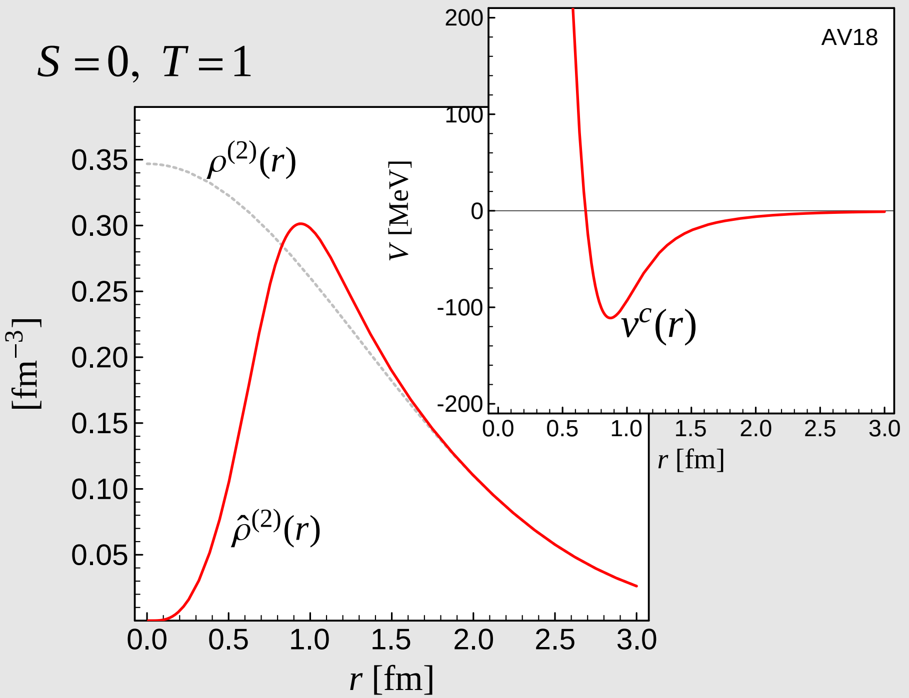
$$\vec{p}_r = \frac{1}{2}\left\{\frac{\vec{r}}{r}\left(\frac{\vec{r}}{r}\vec{p}\right) + \left(\vec{p}\frac{\vec{r}}{r}\right)\frac{\vec{r}}{r}\right\}, \qquad \vec{p}_\Omega = \frac{1}{2r}\left\{\vec{l}\times\frac{\vec{r}}{r} - \frac{\vec{r}}{r}\times\vec{l}\right\}$$

Radial Correlator

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

- probability density shifted out of the repulsive core

$S=0,\ T=1$



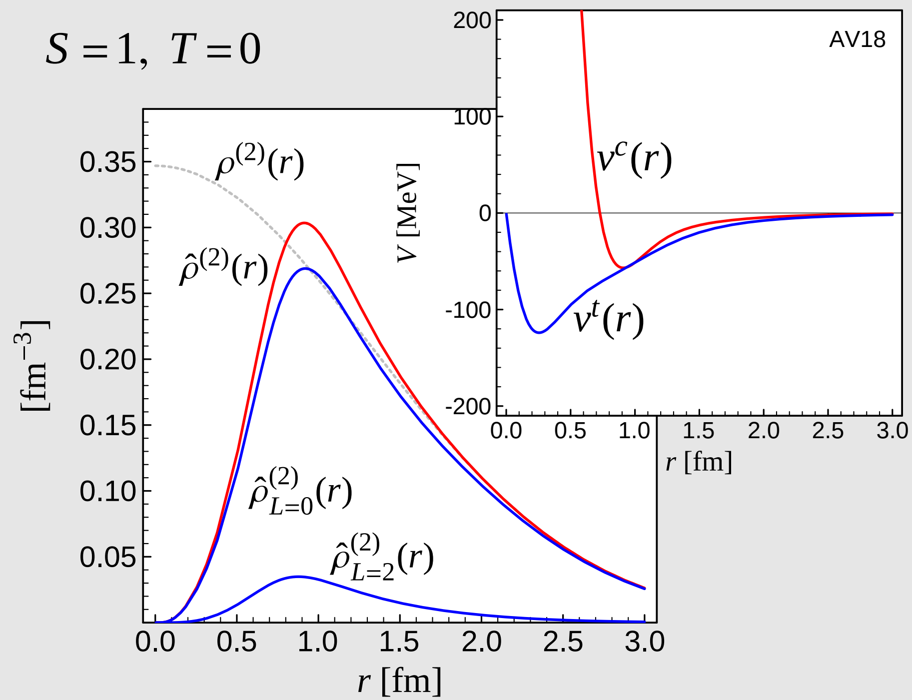
Manfred Ristig Z.Physik **199** (1967) 325

Tensor Correlations

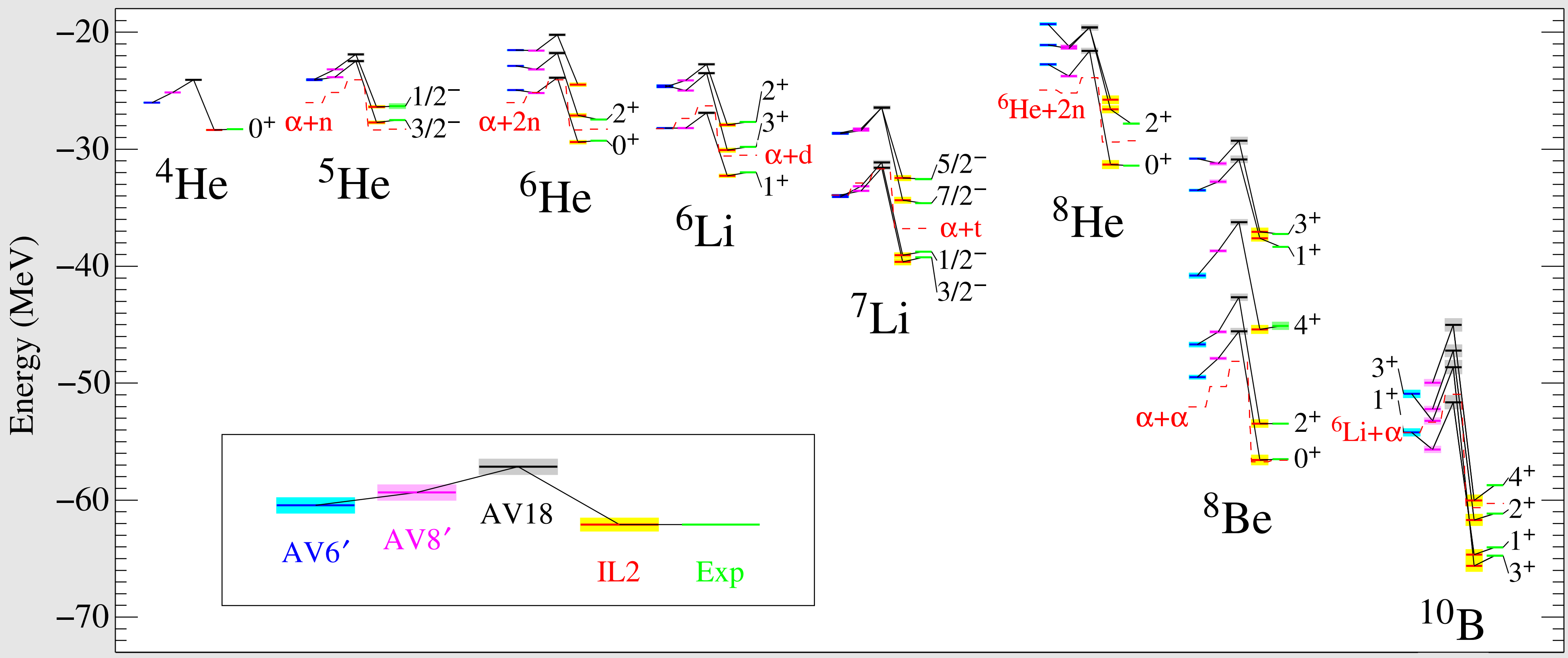
$$G_\Omega = \vartheta(r)\frac{3}{2}\left\{(\boldsymbol{\sigma}_1\cdot\vec{p}_\Omega)(\boldsymbol{\sigma}_2\cdot\vec{r}) + (\boldsymbol{\sigma}_1\cdot\vec{r})(\boldsymbol{\sigma}_2\cdot\vec{p}_\Omega)\right\}$$

- tensor force admixes other angular momenta

$S=1,\ T=0$



GFMC calculations



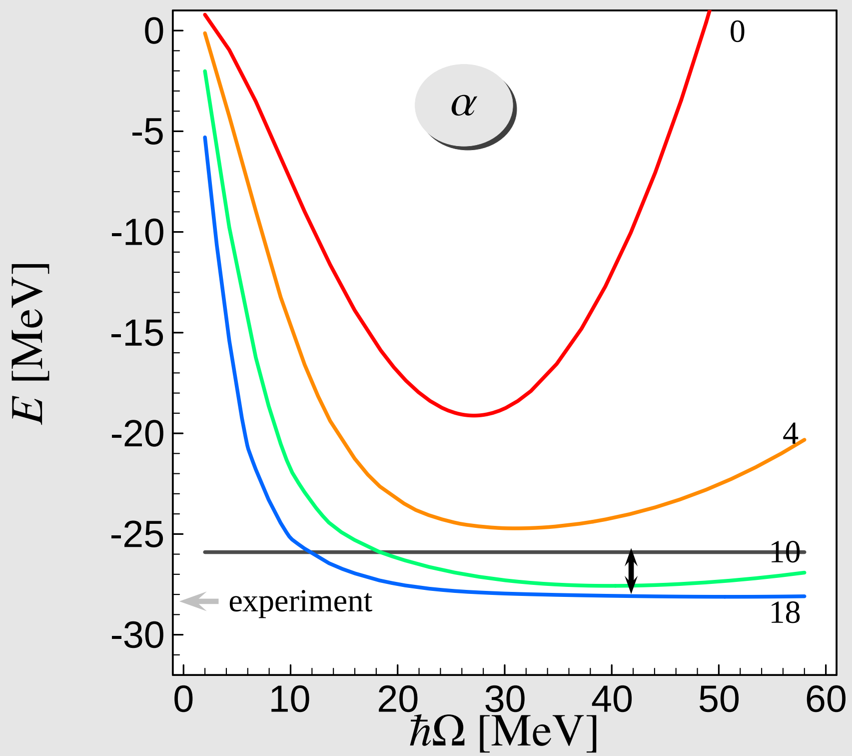
Wiringa, Pieper, PRL **89** (2002) 182501

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

No-Core Shell Model Calculations

preliminary

^{4}He



oscillator width

test of two-body approximation

Quasi-exact calculations for light nuclei possible

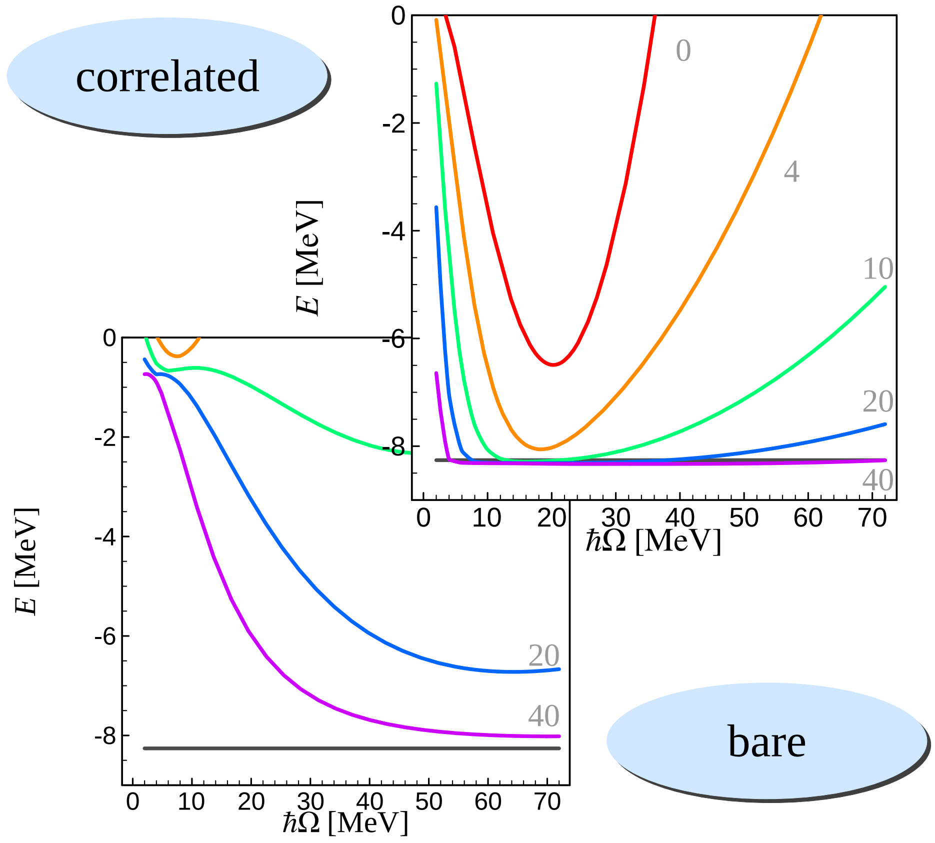
exact result from PR**C64** (2001) 044001

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

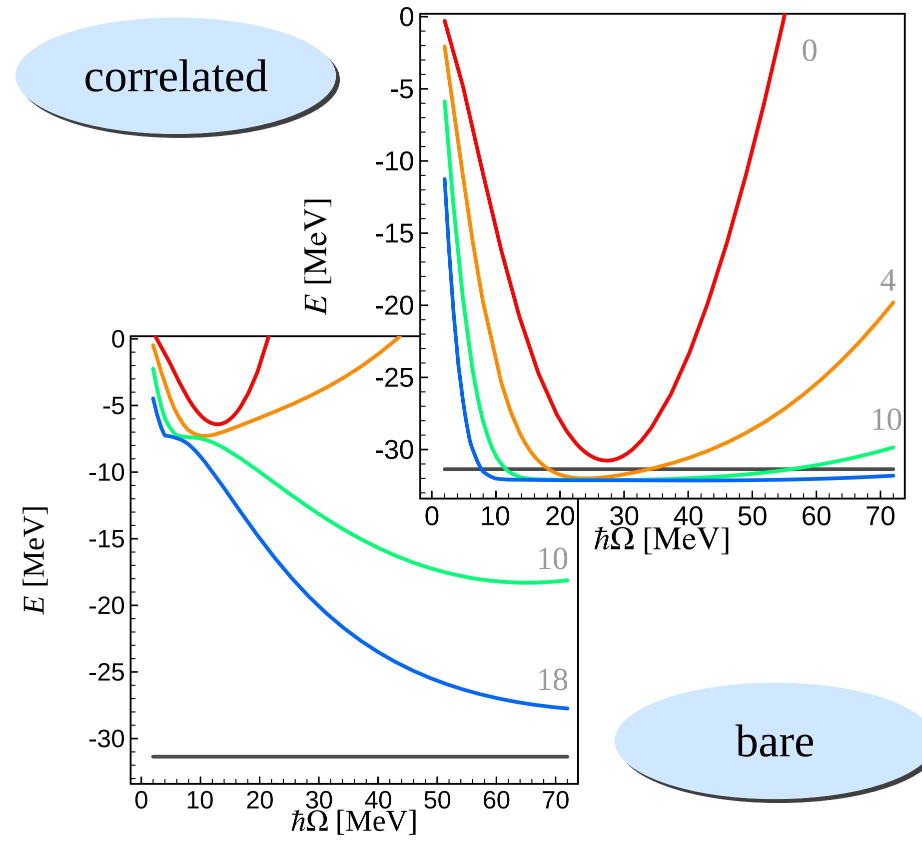
- neglected 3-body correlated terms same order as genuine 3N interactions
- more investigations needed

No-Core Shell Model Calculations

^{3}He



^{4}He



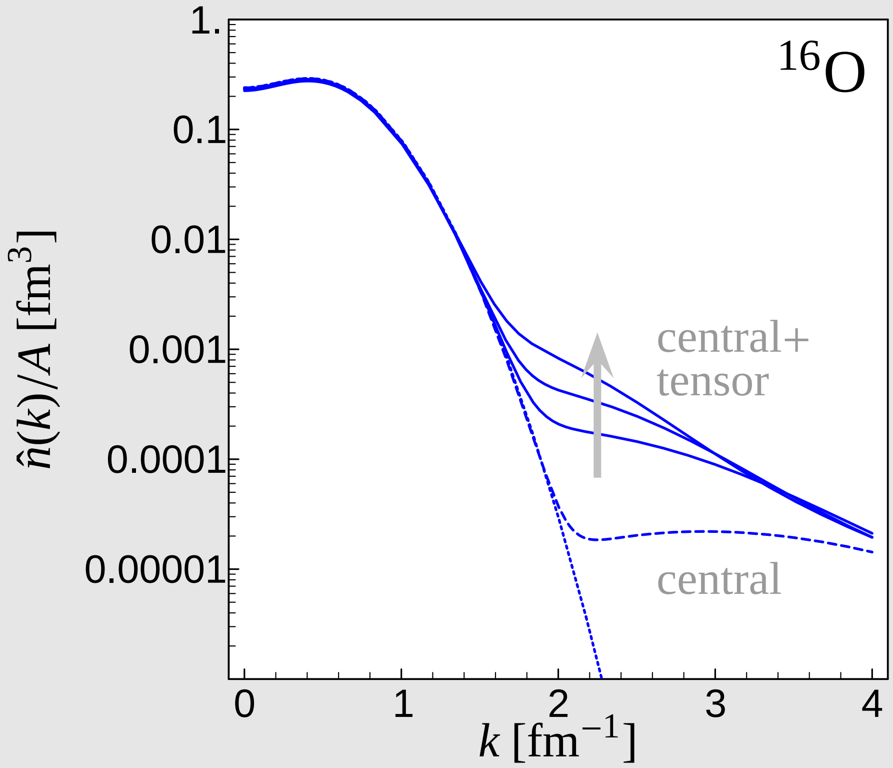
exact results from PR**C52** (1995) 2885

only radial correlations

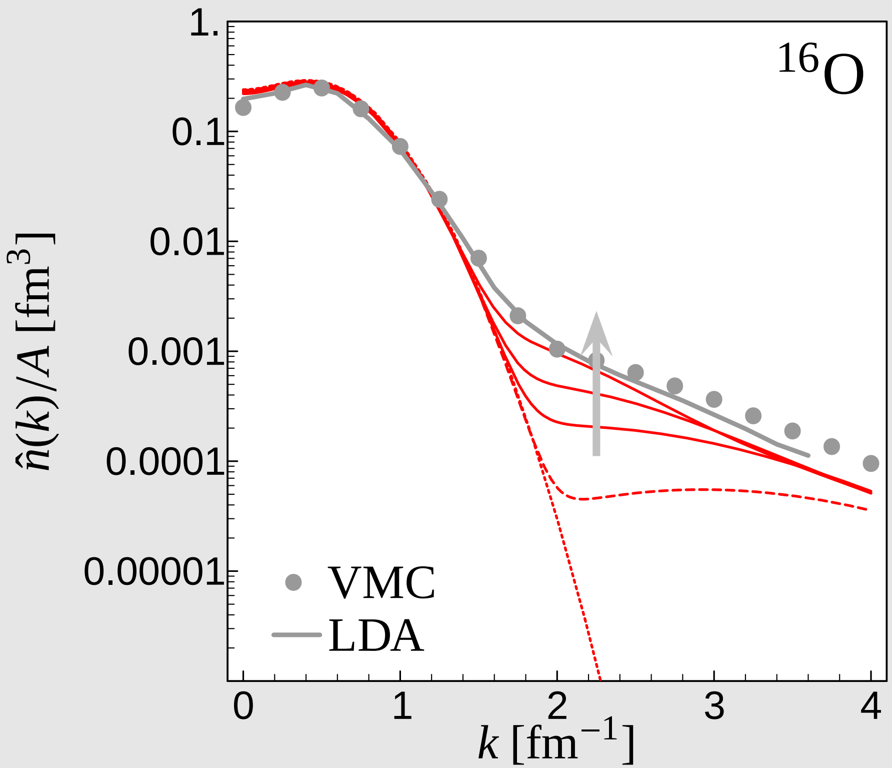
- use no-core shell model code from Pétr Navratil (LLNL)

Nucleon Momentum Distributions

Bonn-A



Argonne V18

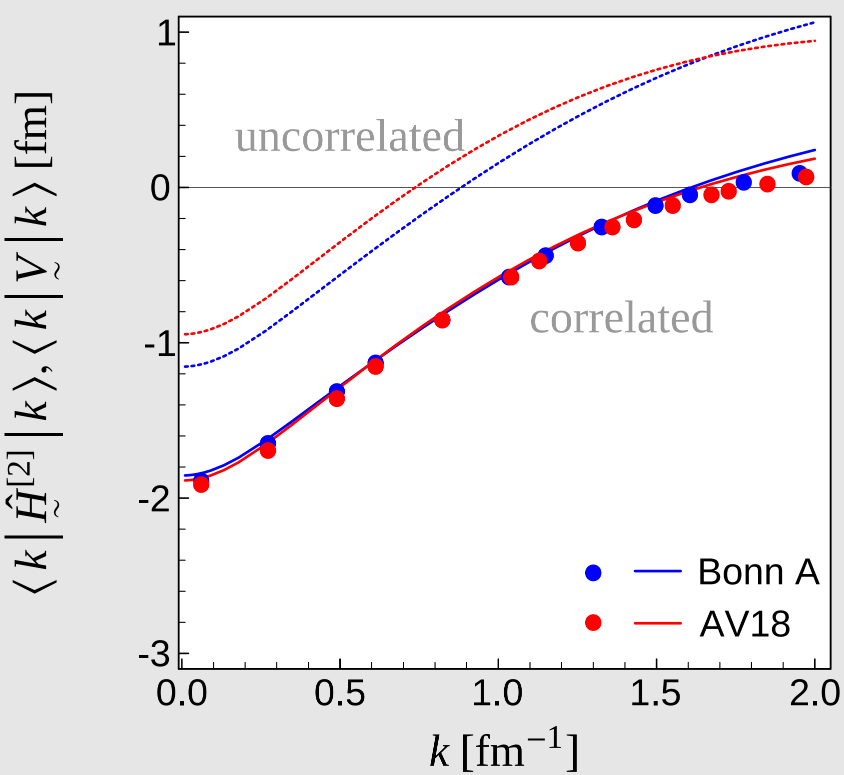


- correlations induce high-momentum components
- contributions of tensor correlations very big
- different correlator ranges relevant especially at the fermi surface

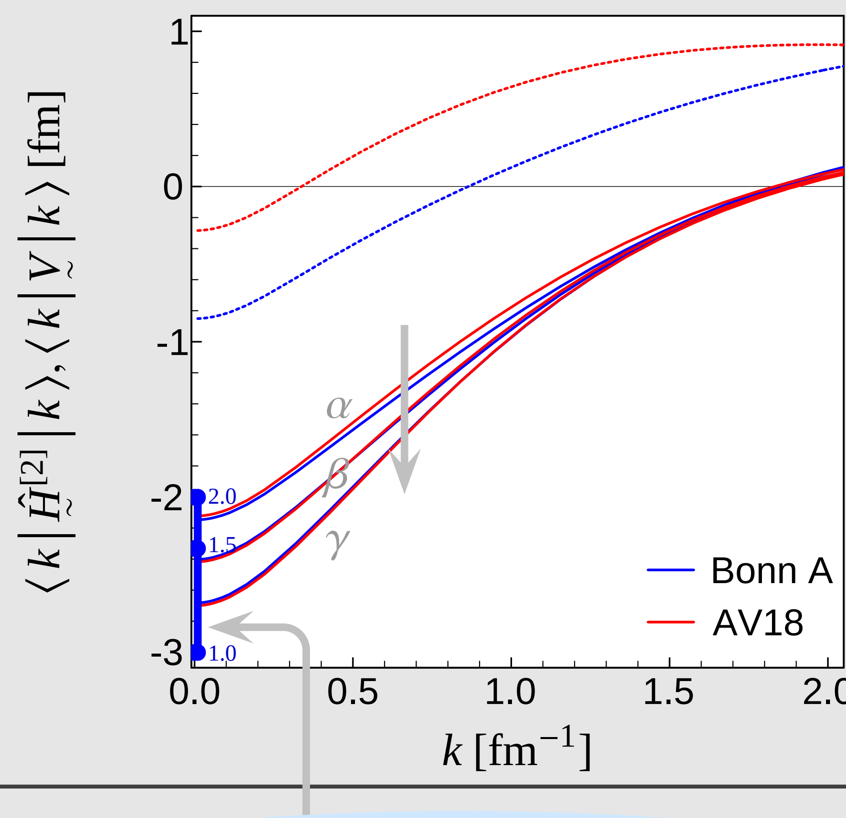
Interaction in Momentum Space

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

${}^1S_0$ channel



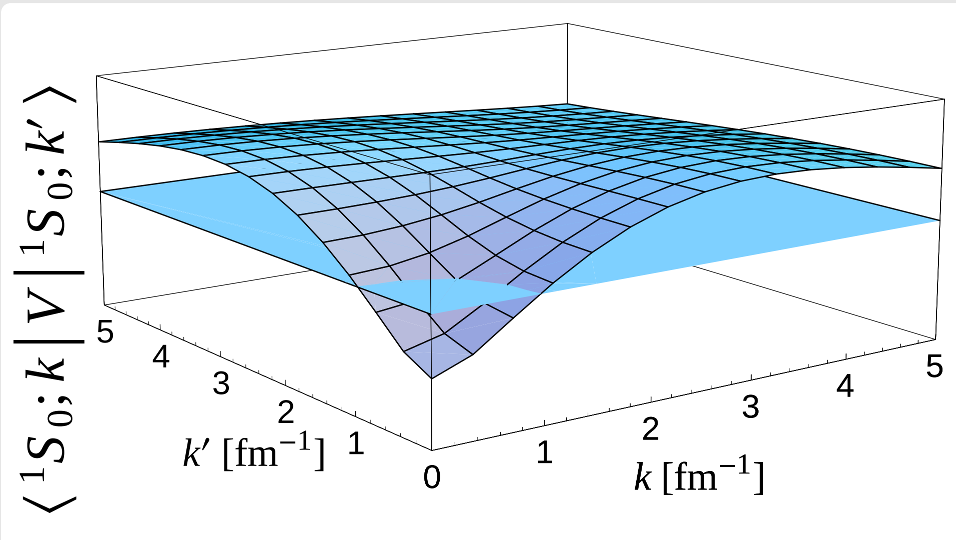
${}^3S_1$ channel

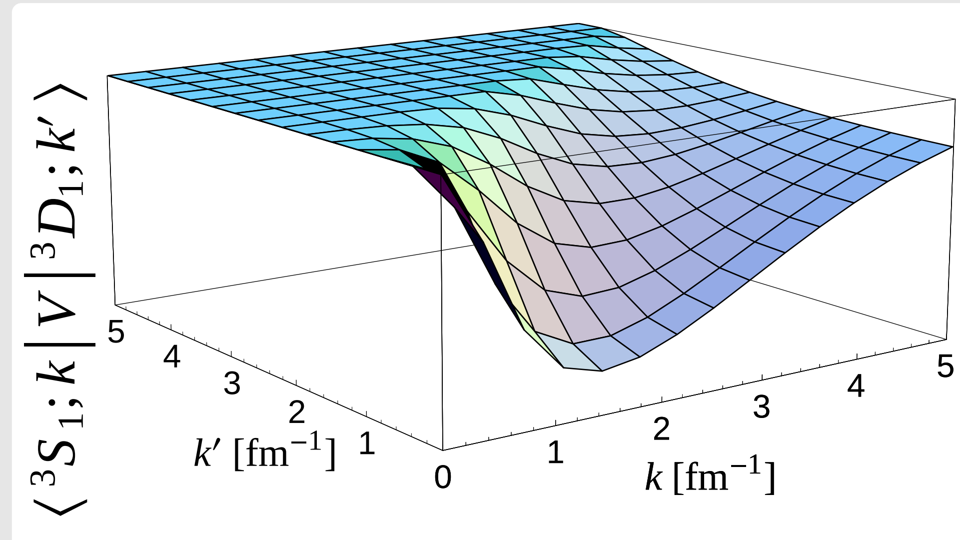


- unique effective potential – identical to V_{lowk}
  Kuo, Schwenk, nucl-th/0108041

- V_{lowk} Cutoff $\Lambda = 1.0 - 2.0\,\mathrm{fm}^{-1}$

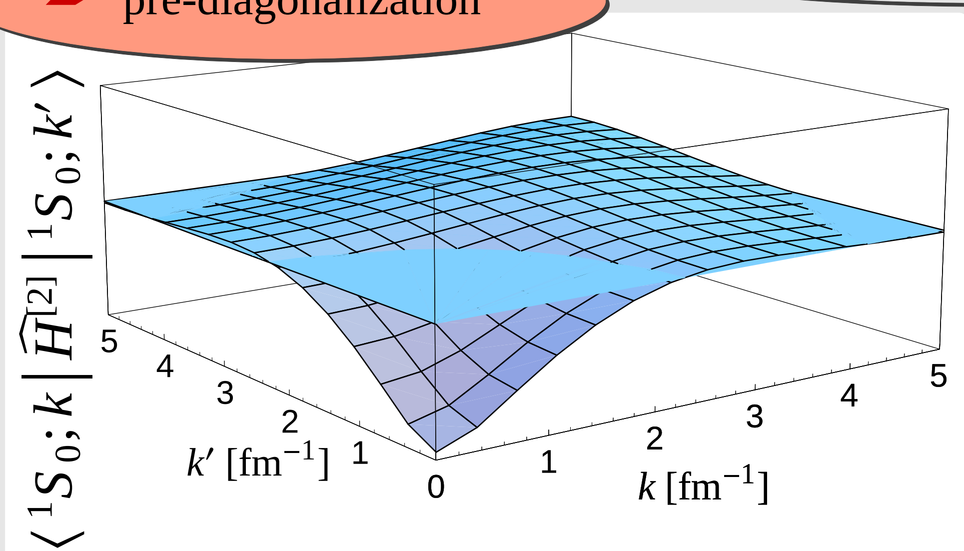
Off-diagonal Matrix Elements

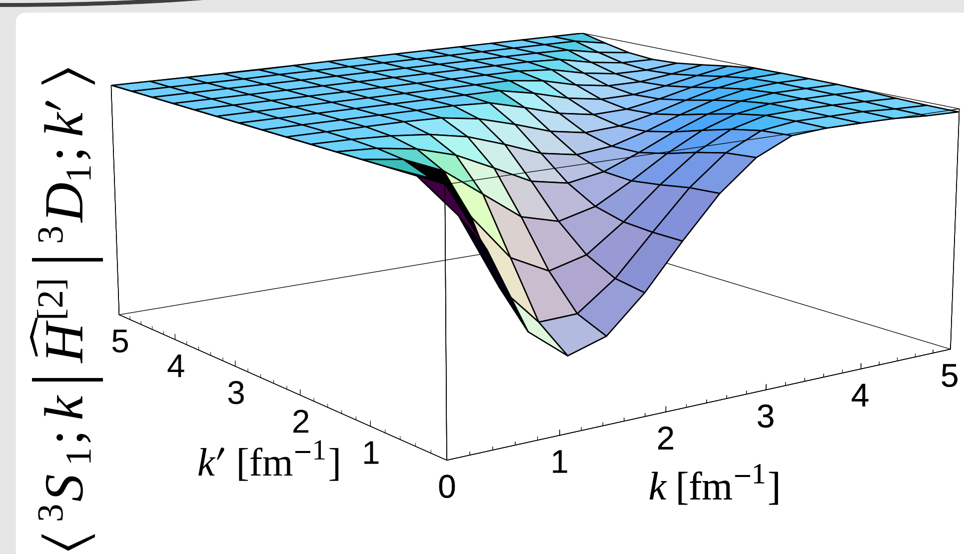




bare potential

➨ "pre-diagonalization"





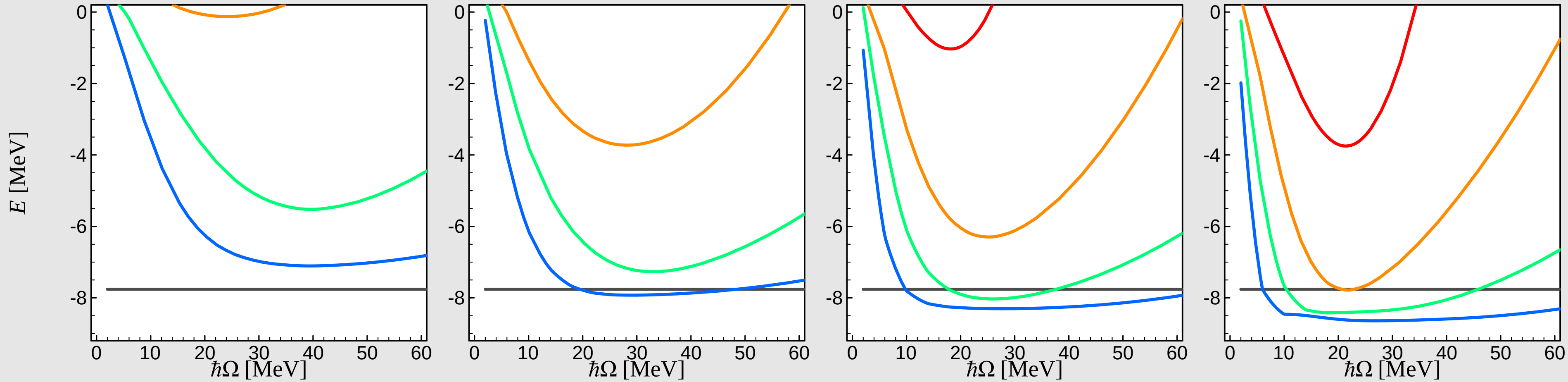
correlated interaction

No-Core Shell Model Calculations

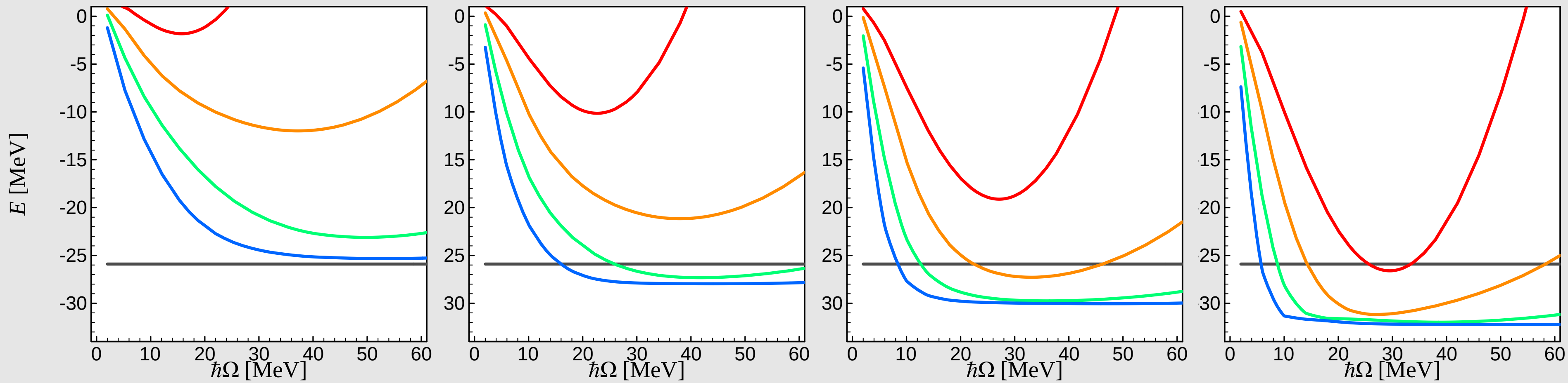
preliminary

Increasing range of tensor correlator

^{3}He

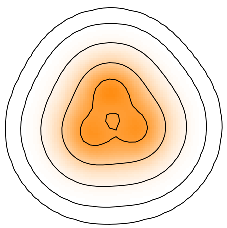


^{4}He



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

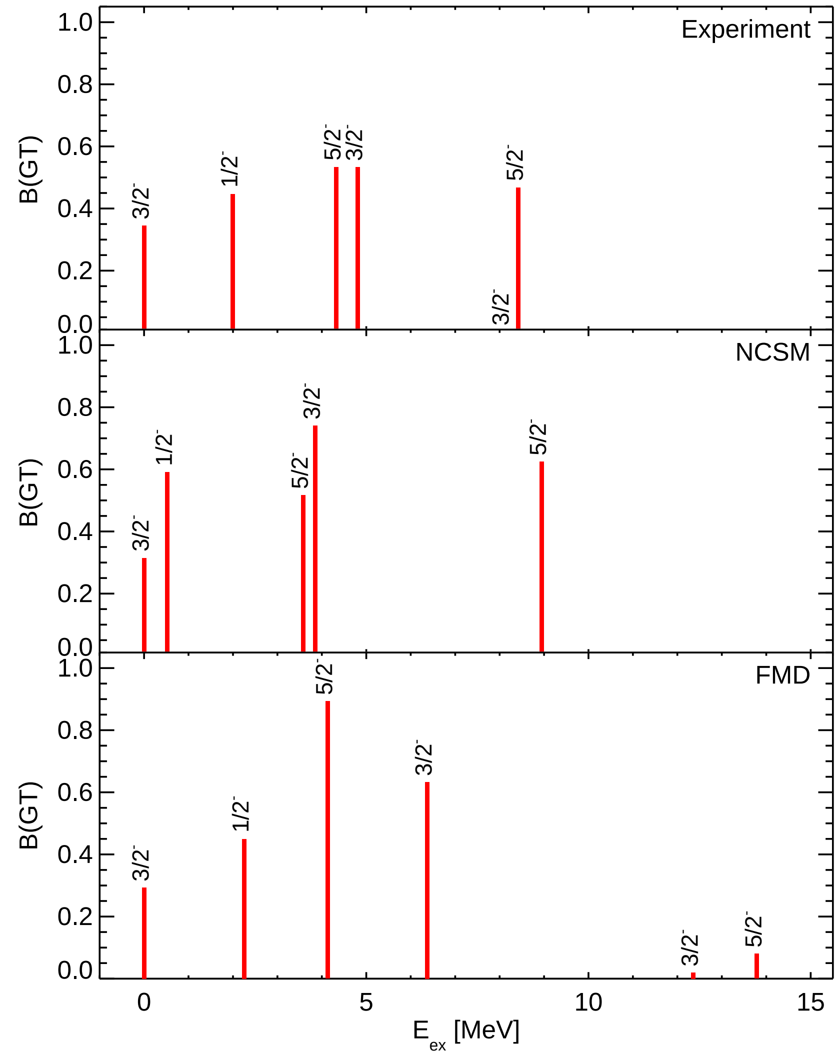
^{11}B



transition: $\sigma \cdot \tau_{+}$

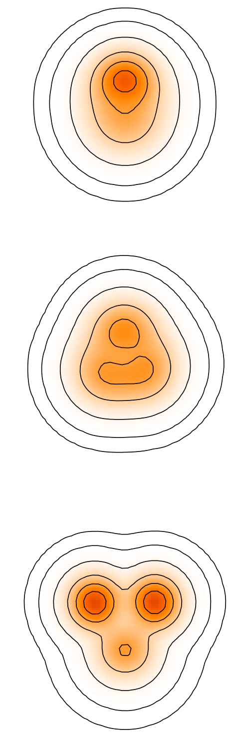
NCSM: Navrátil, Ormand
no core shell model with 3-body force, PRC 68(2003)
third $3/2^{-}$ missing

FMD with configuration mixing

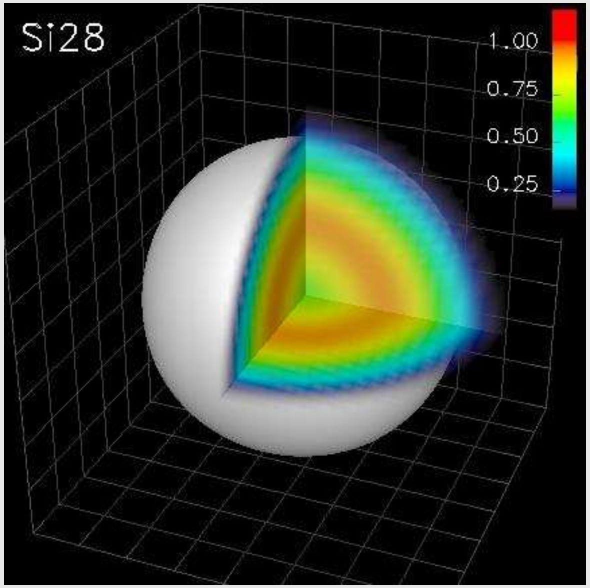


Exp.: Y. Fujita, P. von Bretano et al. to be published

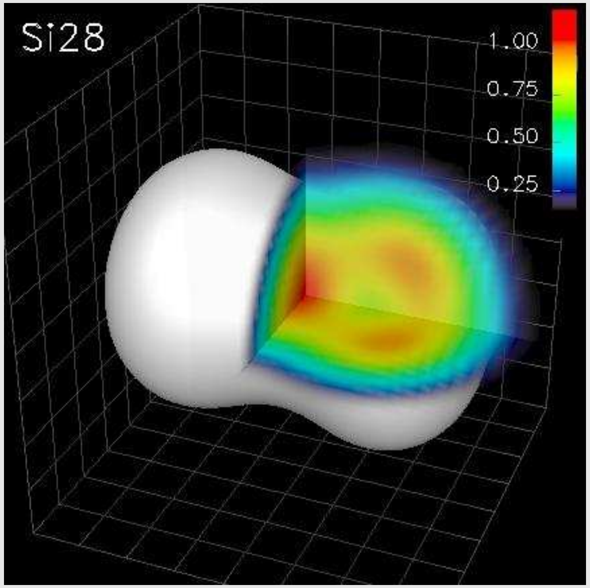
^{11}C



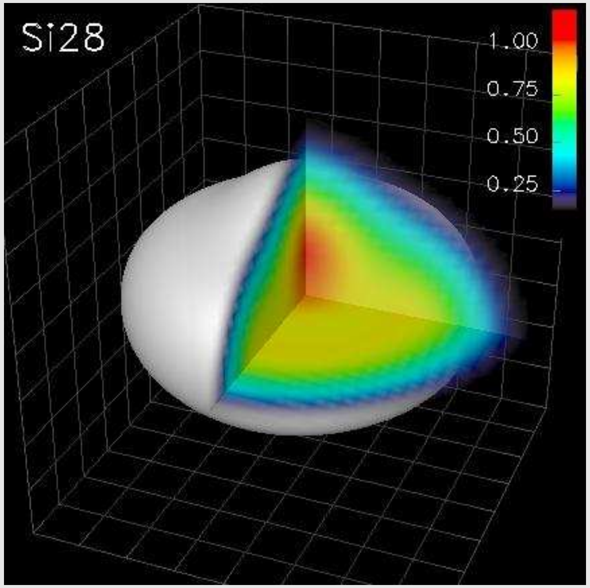
Silizium - Einteilchendichte des intrinsischen Zustands



Variation → rund



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



Ufo
vor Projektion ca. 10 MeV
höher als rund

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