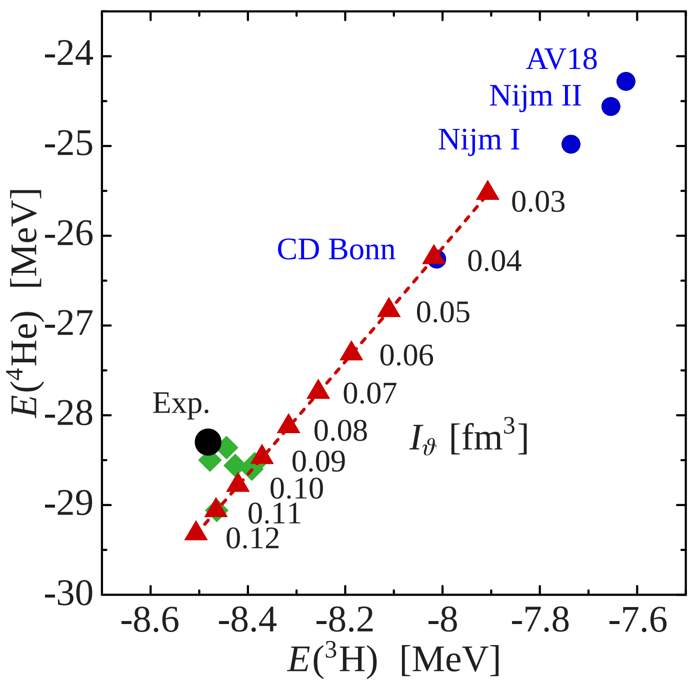
Nuclear Structure with the Unitary Correlation Operator Method



Thomas Neff

3rd ANL/MSU/INT/JINA RIA Theory Meeting
Argonne National Laboratory, USA
April 4-7, 2006

Overview

Unitary Correlation Operator Method

- Central and Tensor correlations
- Correlated Interaction
- *ab initio* calculations

Fermionic Molecular Dynamics

- PAV, VAP and Multiconfiguration
- Helium, Beryllium, Carbon isotopes, ^{12}C
- Resonances and Scattering States

Realistic and Effective Nucleon-Nucleon Interactions

Realistic Interactions

- reproduce scattering data and deuteron properties
- meson-exchange (Bonn), phenomenological (AV18), χ-PT (Idaho)
- **repulsive core** and **tensor force** induce **strong short-range correlations**

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Effective Interactions

- phenomenological effective interactions describe many properties of nuclear systems like energies, radii, spectra successfully using simple many-body wave functions (HF, shell model, microscopic cluster models)
- No-Core Shell Model uses Lee-Suzuki transformation in oscillator basis
- G-matrix and V_{lowk} derive effective interaction in momentum space

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Our approach

- derive **effective interaction** from **realistic interaction** by explicitly including correlations with **unitary correlation operator** $\underset{\sim}{C}$ formulated in **coordinate space**
- correlated (effective) interaction

$$\underset{\sim}{\hat{H}} = \underset{\sim}{C}^{\dagger} \underset{\sim}{H} \underset{\sim}{C}$$

Unitary Correlation Operator Method

Correlation Operator

- induce short-range (two-body) central and tensor correlations into the many-body state

$$\underset{\sim}{C} = \underset{\sim}{C}_{\Omega}\underset{\sim}{C}_{r} = \exp\Big[-i\sum_{i<j}\underset{\sim}{g}_{\Omega,ij}\Big]\exp\Big[-i\sum_{i<j}\underset{\sim}{g}_{r,ij}\Big] \quad , \quad \underset{\sim}{C}^{\dagger}\underset{\sim}{C} = \underset{\sim}{1}$$

- correlation operator should conserve the symmetries of the Hamiltonian and should be of finite-range, **phase shift equivalent** to bare interaction by construction

Correlated Operators

- correlated operators will have contributions in higher cluster orders

$$\underset{\sim}{C}^{\dagger}\underset{\sim}{O}\underset{\sim}{C} = \underset{\sim}{\hat{O}}^{[1]} + \underset{\sim}{\hat{O}}^{[2]} + \underset{\sim}{\hat{O}}^{[3]} + \dots$$

- two-body approximation: correlation range should be small compared to mean particle distance

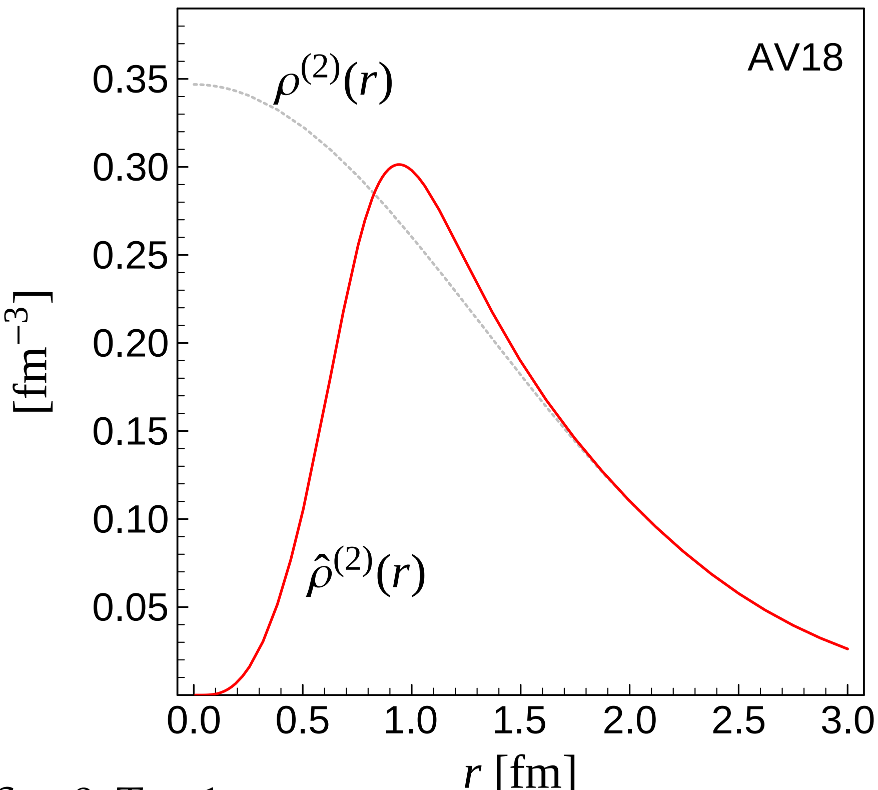
Correlated Interaction

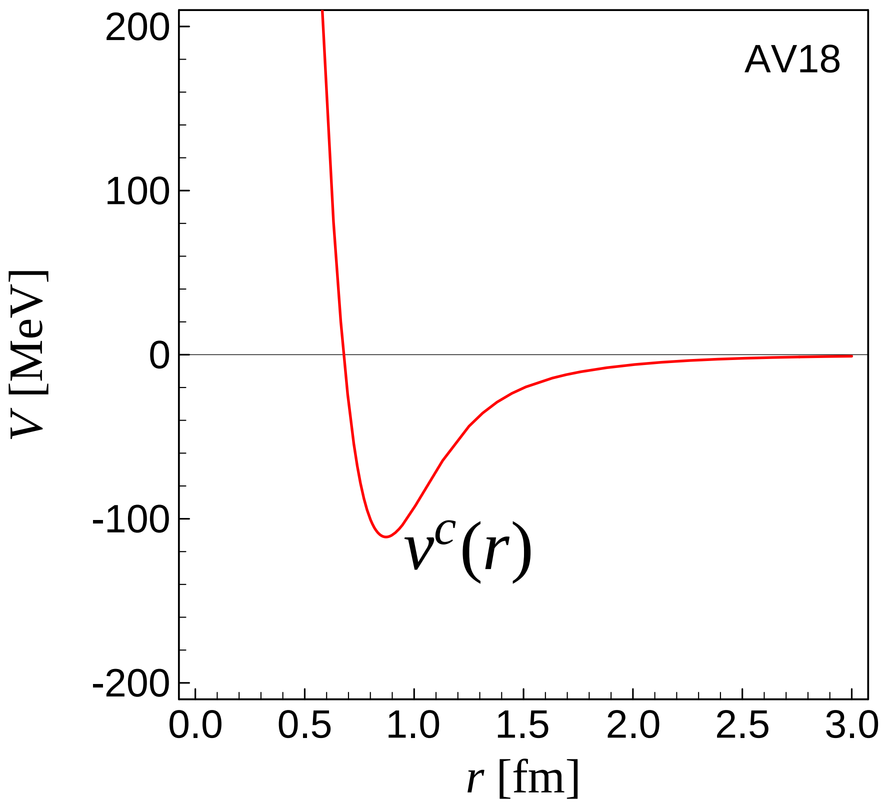
$$\underset{\sim}{C}^{\dagger}\,(\underset{\sim}{T} + \underset{\sim}{V})\,\underset{\sim}{C} = \underset{\sim}{T} + \underset{\sim}{V}_{\text{UCOM}} + \underset{\sim}{V}^{[3]}_{\text{UCOM}} + \dots$$

Central Correlations

- radial distance-dependent **shift in the relative coordinate** of each nucleon pair

$$g_r = \frac{1}{2}\Big[p_r\, s(r) + s(r)\, p_r\Big] \quad , \quad p_r = \frac{1}{2}[\mathbf{p}\cdot\mathbf{r} + \mathbf{r}\cdot\mathbf{p}]$$





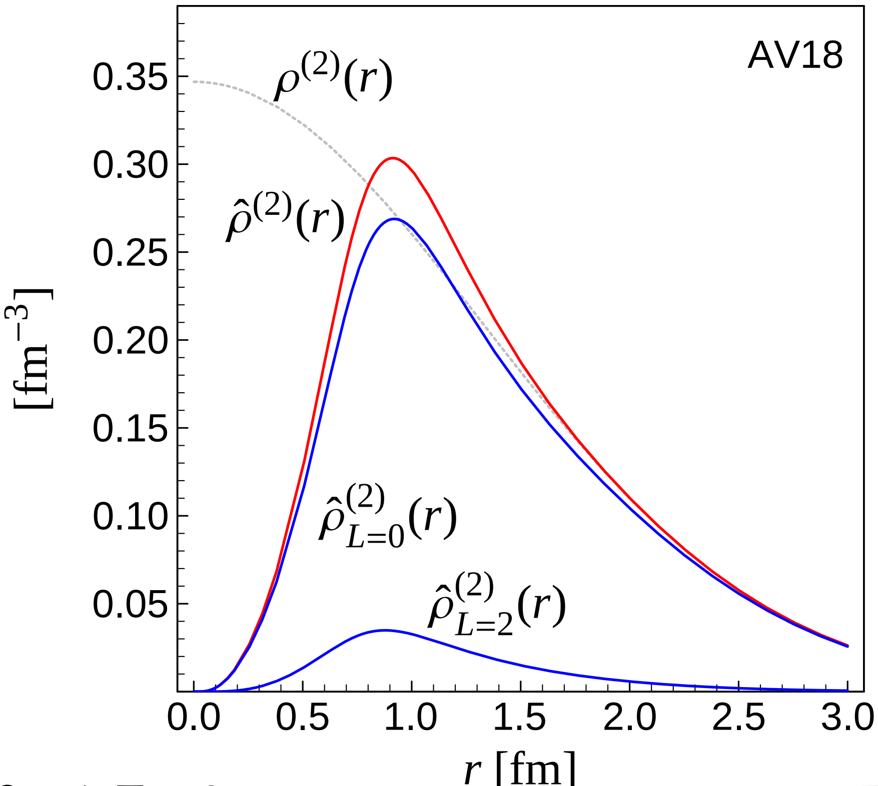
$S = 0, T = 1$

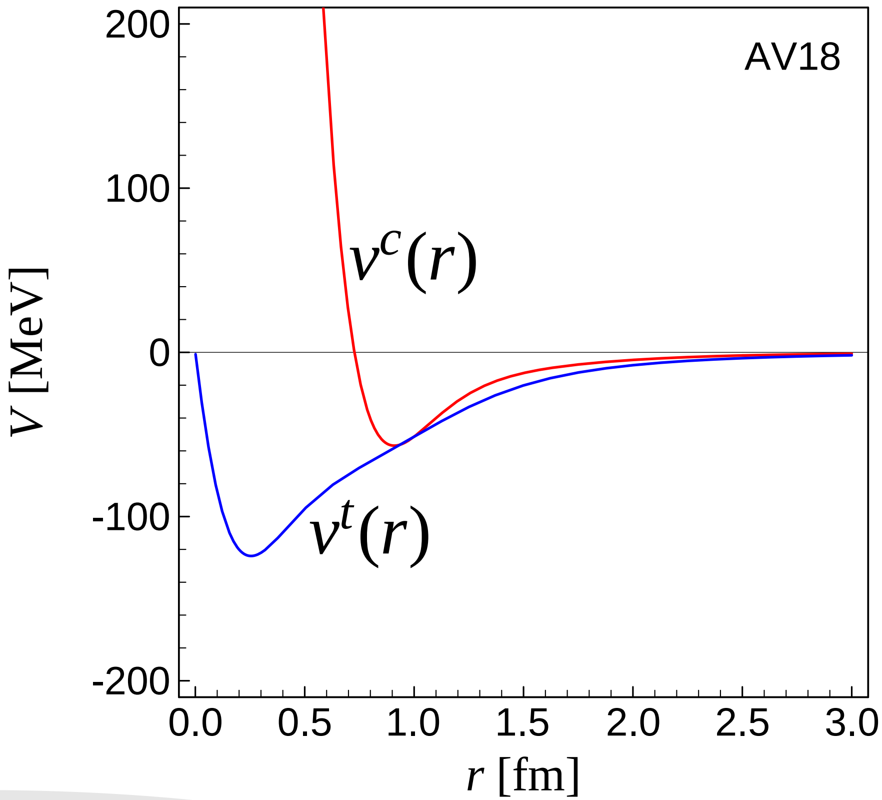
nucleons shifted out of repulsive core

Tensor Correlations

- **angular shift in the relative coordinate** of each nucleon pair depending on the orientation of the spins

$$g_\Omega = \vartheta(r)\Big[\tfrac{3}{2}(\boldsymbol{\sigma}_1\cdot\mathbf{p}_\Omega)(\boldsymbol{\sigma}_2\cdot\mathbf{r}) + \tfrac{3}{2}(\boldsymbol{\sigma}_1\cdot\mathbf{r})(\boldsymbol{\sigma}_2\cdot\mathbf{p}_\Omega)\Big] \quad , \quad \mathbf{p}_\Omega = \mathbf{p} - \mathbf{r}\, p_r$$



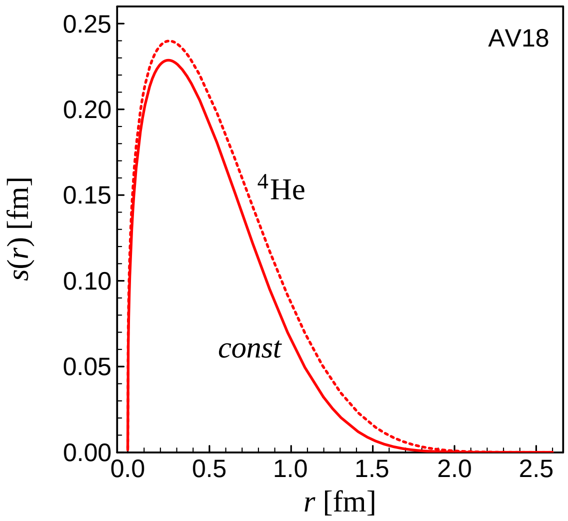


$S = 1, T = 0$

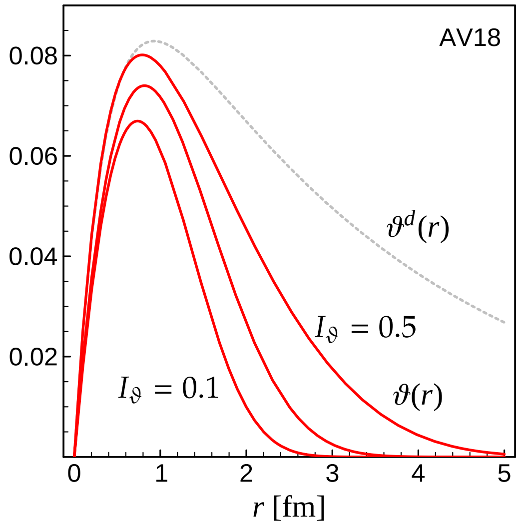
nucleons aligned with total spin of nucleon pair

Determine Correlation Functions

Central Correlations



Tensor Correlations



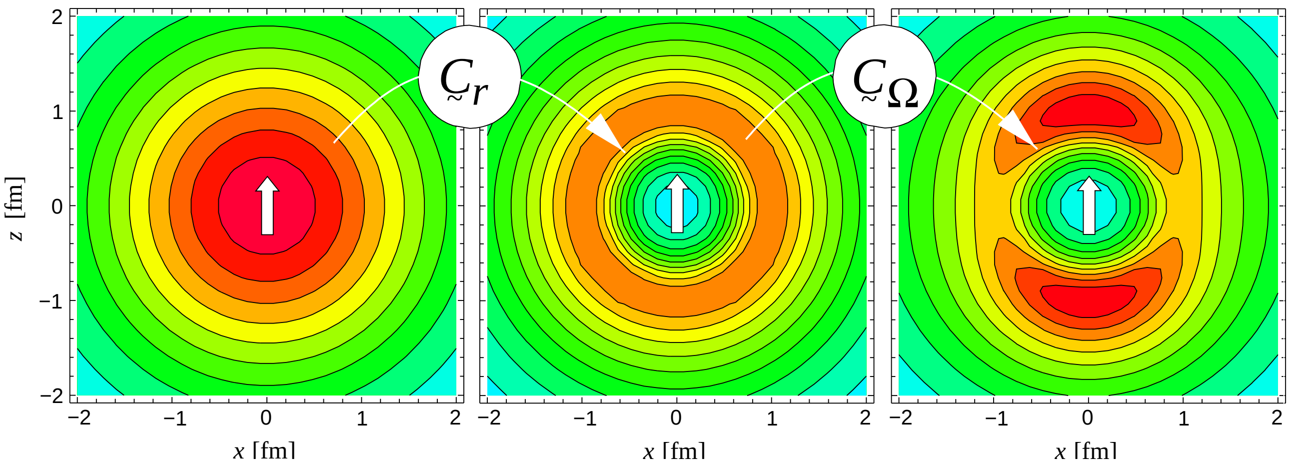
- determine $s(r)$ und $\vartheta(r)$ in each spin-isospin channel by minimizing the energy in the two-body system

$$\min_{s(r),\vartheta(r)} \left\langle \phi_{trial}^{ST} \middle| \underset{\sim}{C}_r^\dagger \underset{\sim}{C}_\Omega^\dagger \underset{\sim}{H} \underset{\sim}{C}_\Omega \underset{\sim}{C}_r \middle| \phi_{trial}^{ST} \right\rangle$$

- correlation functions depend only weakly on the trial wave function
- restrict the range of the tensor correlations in the $S = 1, T = 0$ channel (parameter I_ϑ)

Correlated Two-Body Densities and Energies

two-body densities



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

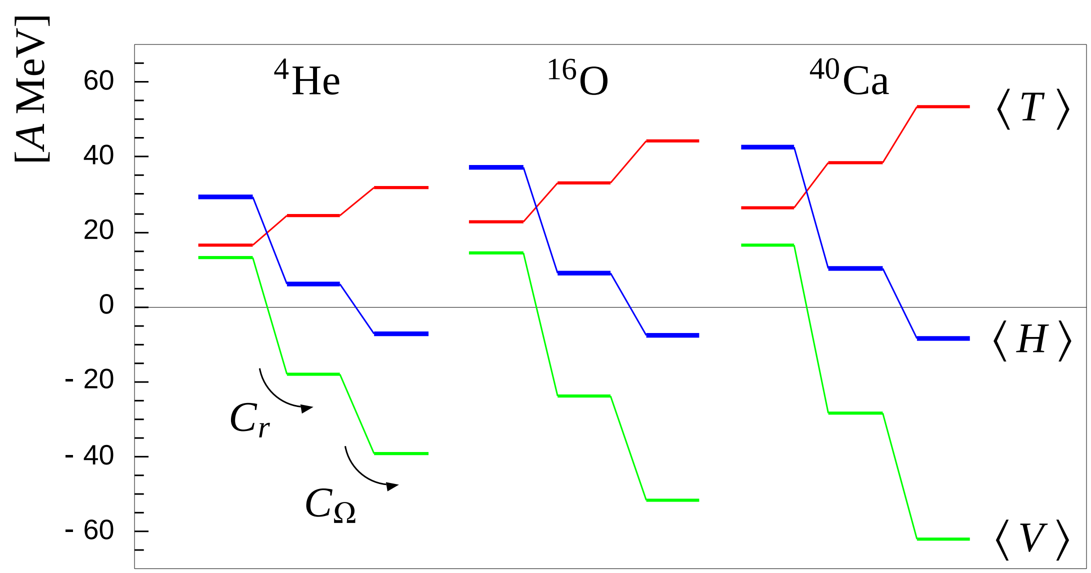
central correlator $\underset{\sim}{C}_{\mathbf{r}}$
shifts density out of the repulsive core

tensor correlator $\underset{\sim}{C}_{\mathbf{\Omega}}$
aligns density with spin orientation

both central and tensor correlations are essential for binding

energies

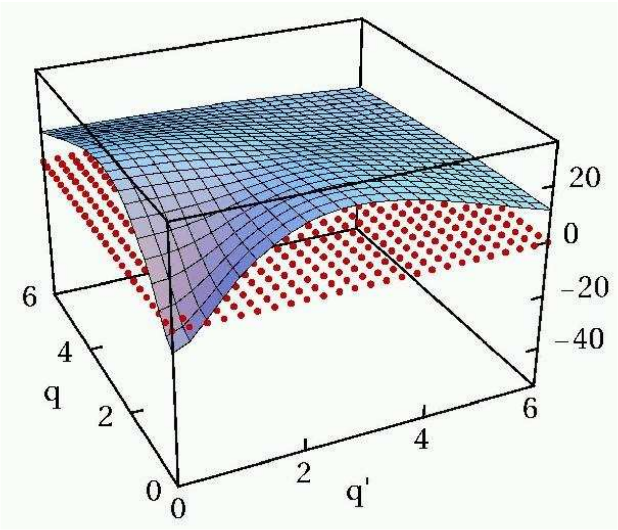
$0\hbar\omega$ Harmonic Oscillator



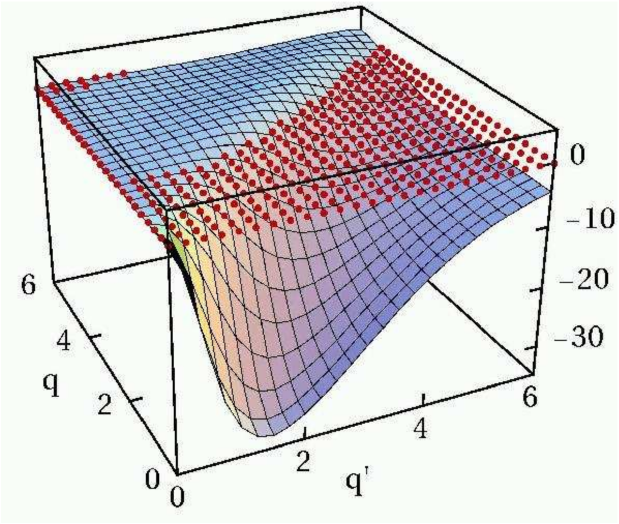
Nucl. Phys. **A713** (2003) 311

Correlated Interaction in Momentum Space

$^3S_1$ bare

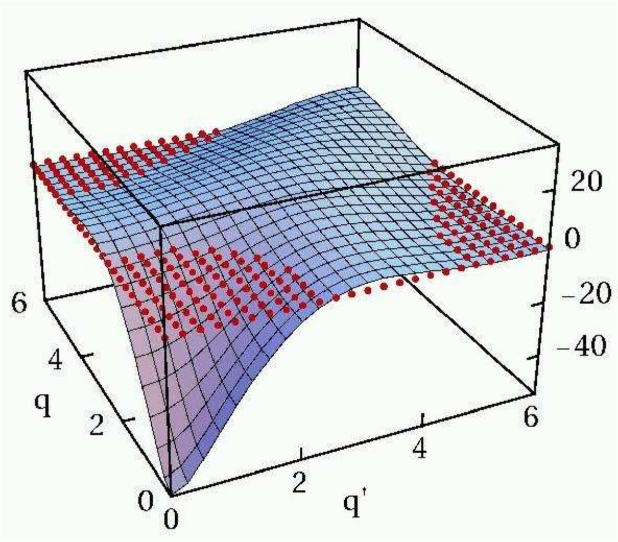


$^3S_1$ - $^3D_1$ bare

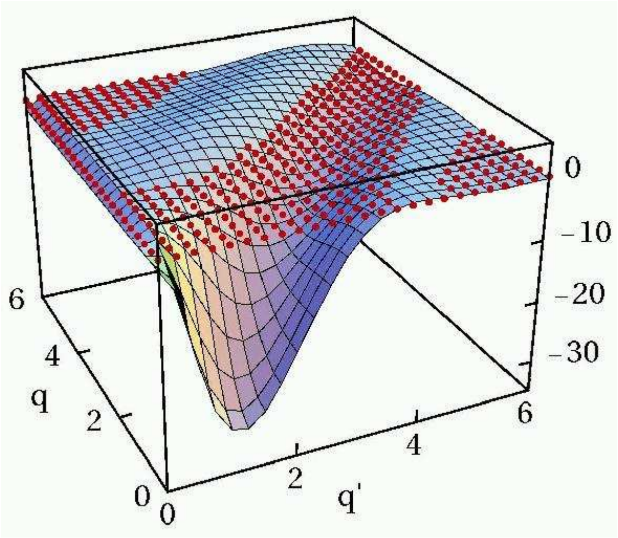


correlated interaction is **more attractive** at low momenta

$^3S_1$ correlated



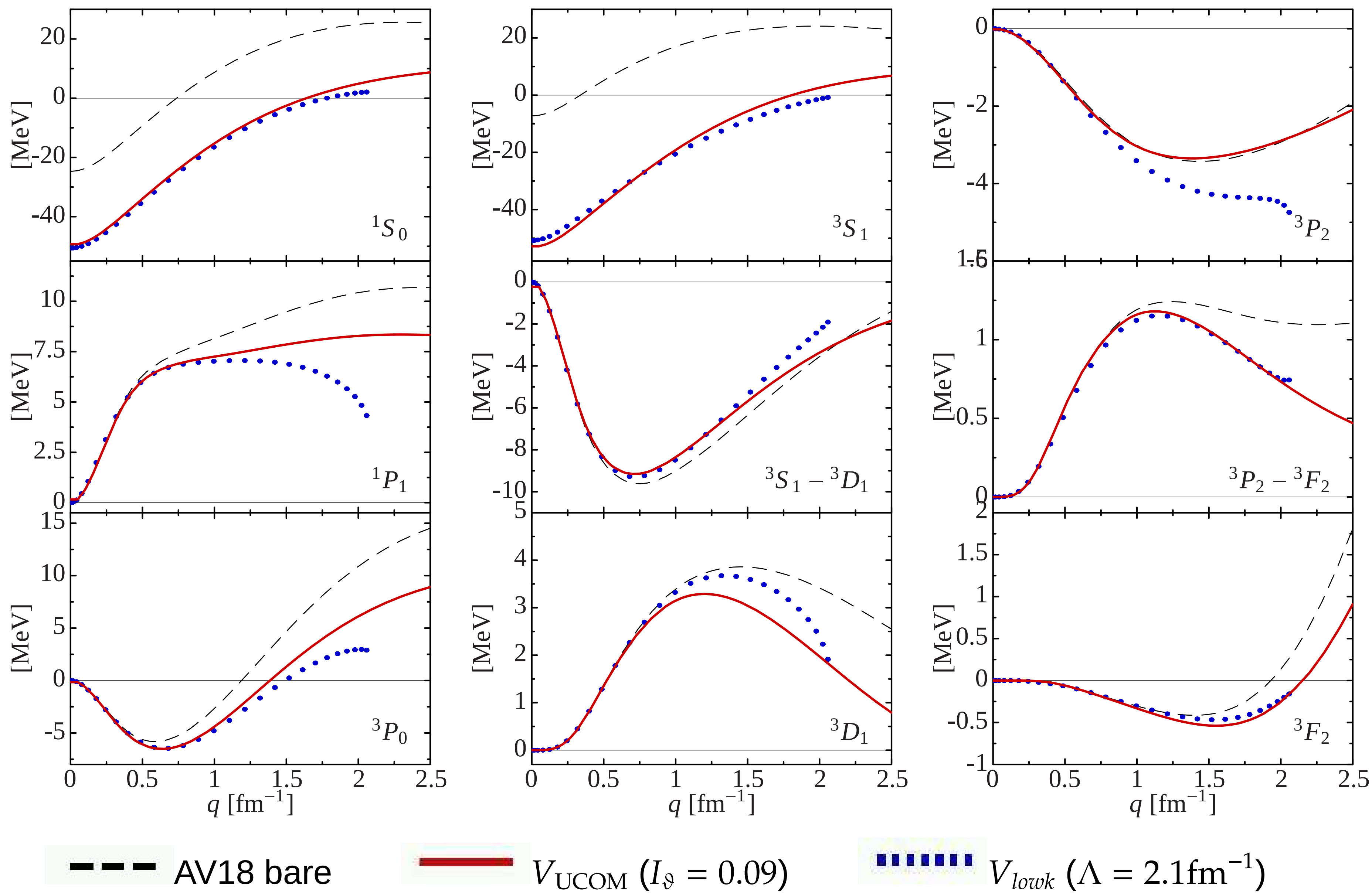
$^3S_1$ - $^3D_1$ correlated



off-diagonal matrix elements connecting low- and high-momentum states are **strongly reduced**

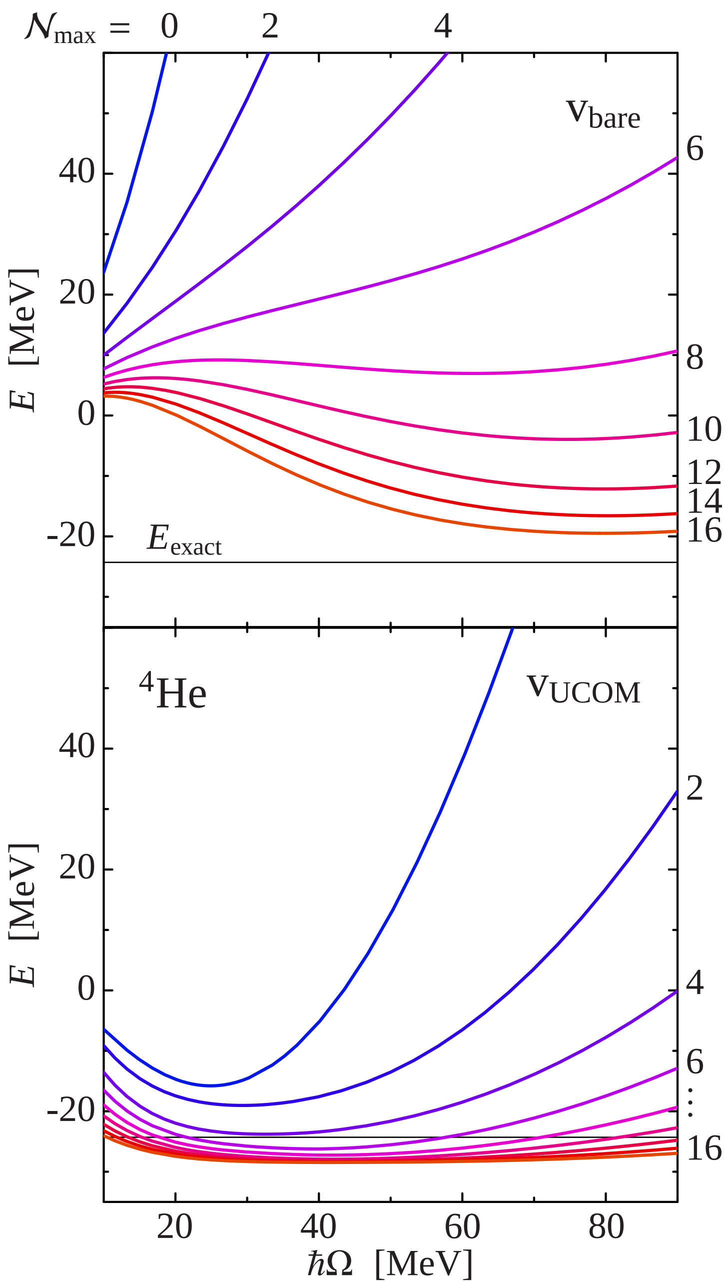
Phys. Rev. **C72** (2005) 034002

Correlated AV18 Interaction in Momentum Space



Bogner, Kuo, Schwenk, Phys. Rept. **386** (2003) 1

No-Core Shell Model Calculations

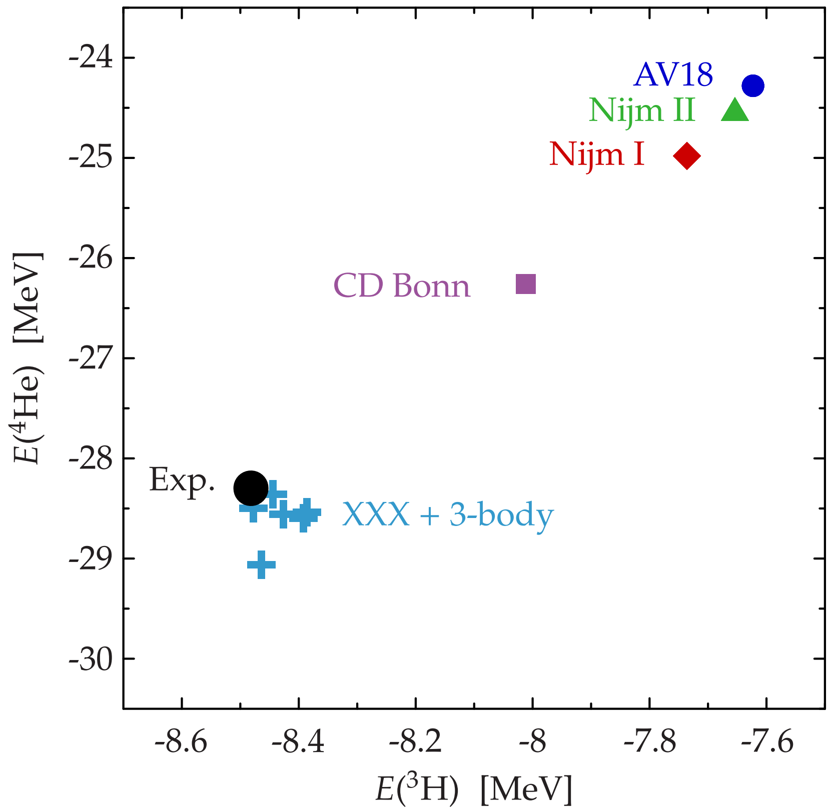


- use Jacobi-coordinate NCSM code by Petr Navrátil, LLNL for ^{3}He and ^{4}He (don't use Lee-Suzuki transformation)

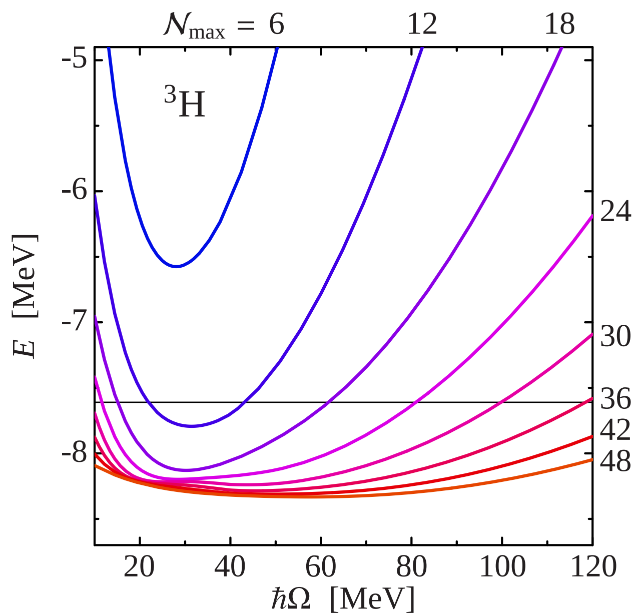
- dramatically **improved convergence** compared to bare interaction
- **does not converge to exact result for bare interaction** due to omitted higher order terms $V_{UCOM}^{[3]}, \ldots$
- study the effect of higher order contributions as a function of tensor correlation range I_ϑ.

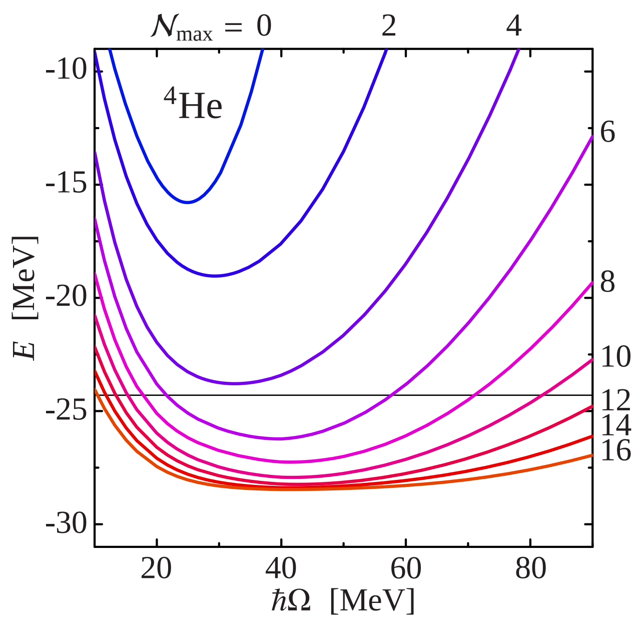
No-Core Shell Model Calculations

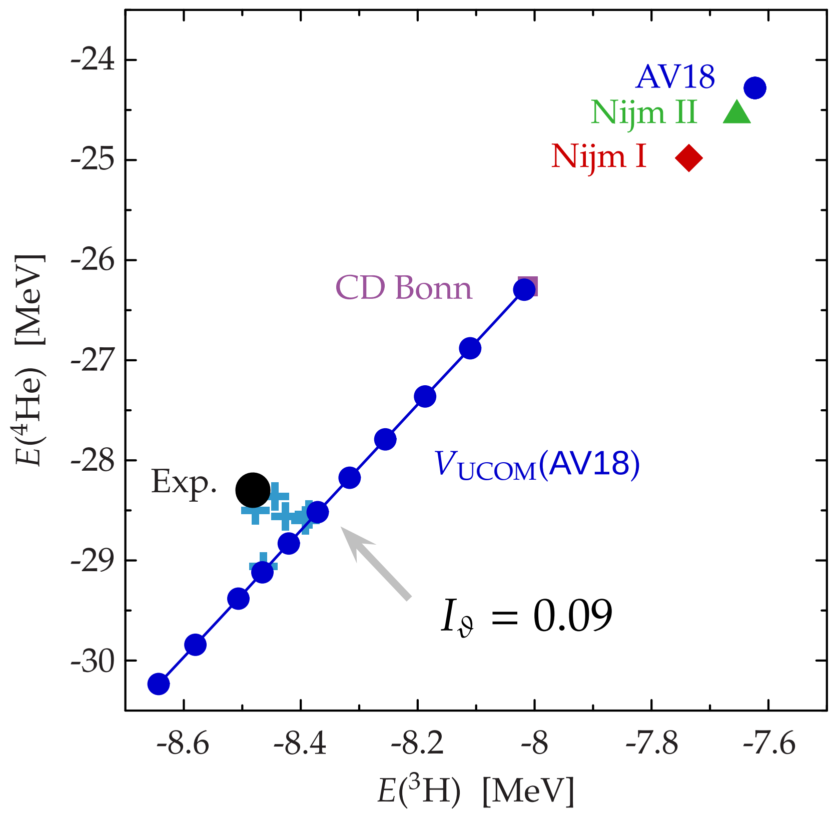
Tjon Line



No-Core Shell Model Calculations
Tjon Line



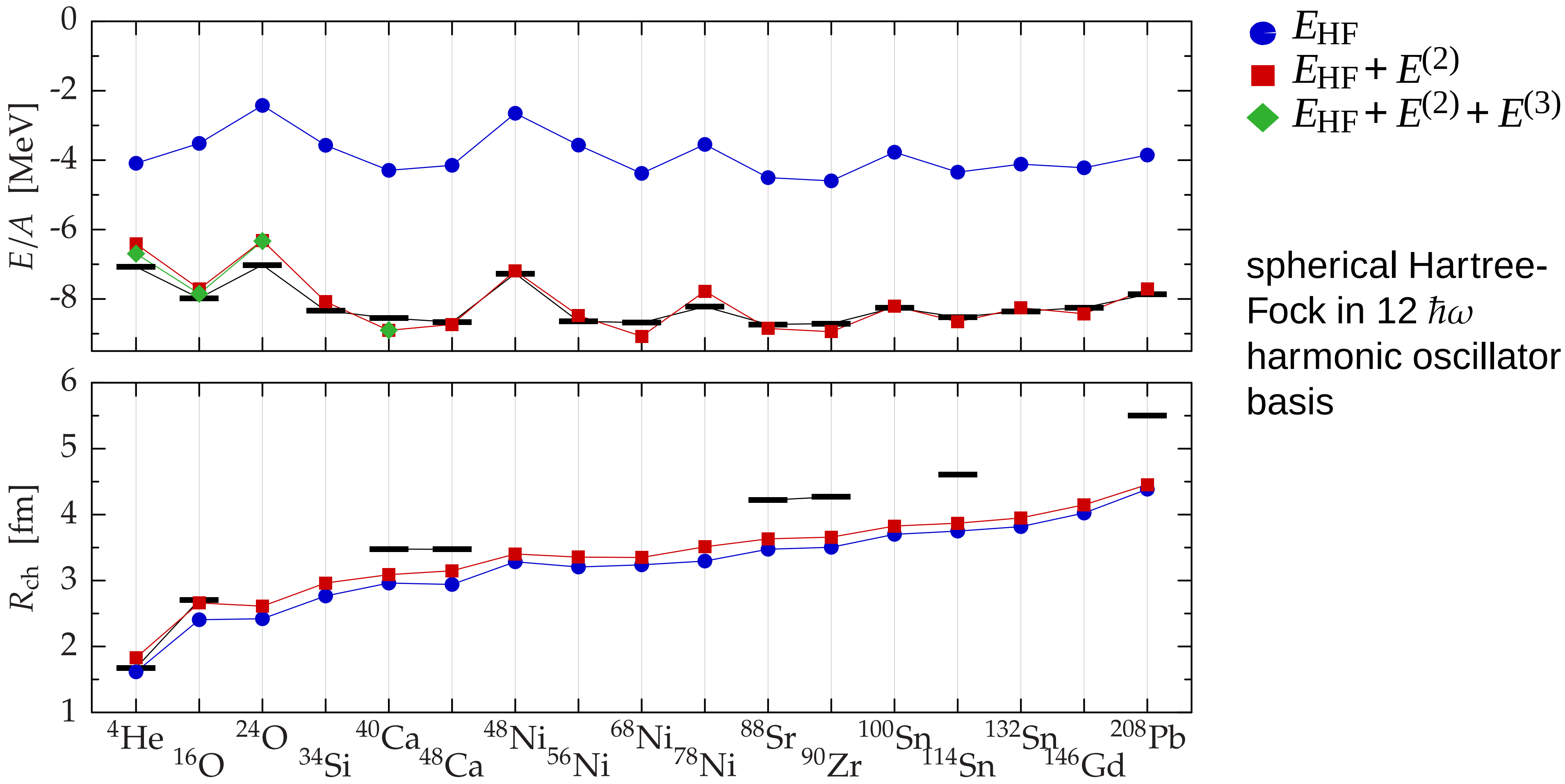




- choose tensor correlation range $I_\vartheta = 0.09$ such that **need for three-body forces is minimized**

➨ **different perspective**: don't try to reproduce the results of the bare interaction but consider **V_{UCOM} as a realistic potential** to describe experiment

HF and MBPT calculations



spherical Hartree-Fock in 12 $\hbar\omega$ harmonic oscillator basis

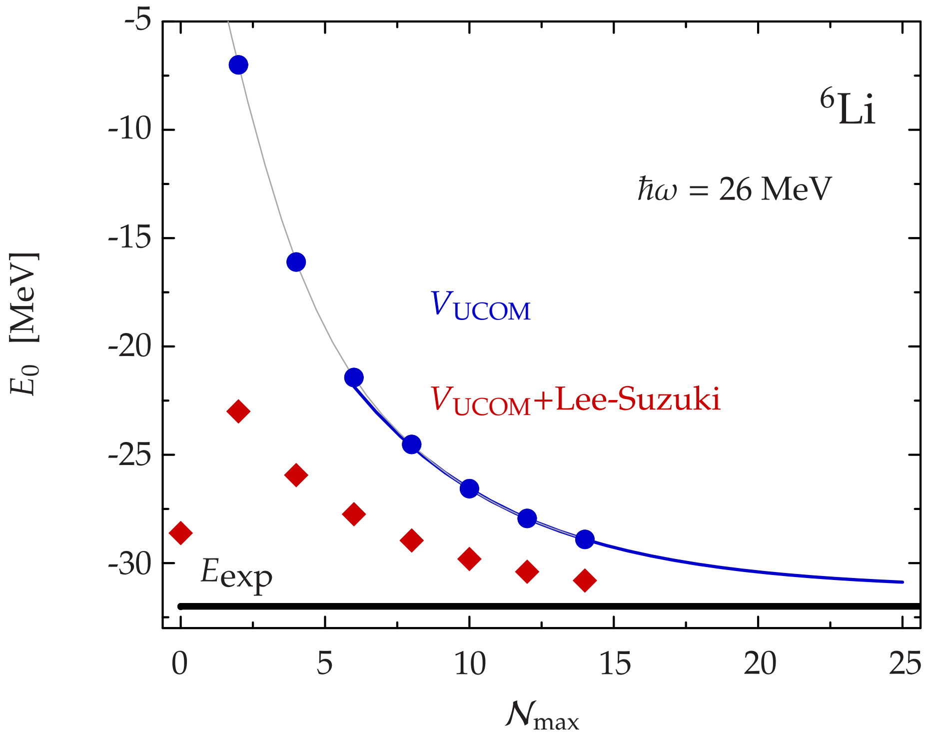
additional binding mainly due to **medium to long range tensor forces**

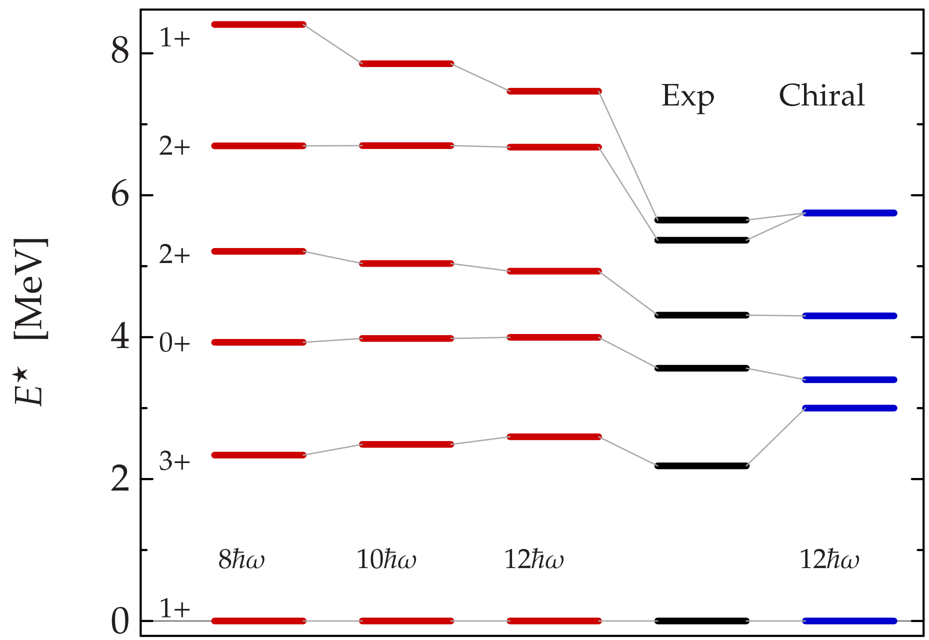
long-range correlations appear to be perturbative

problems with saturation indicate need for **three-body forces**

No-Core Shell Model
^{6}Li

preliminary



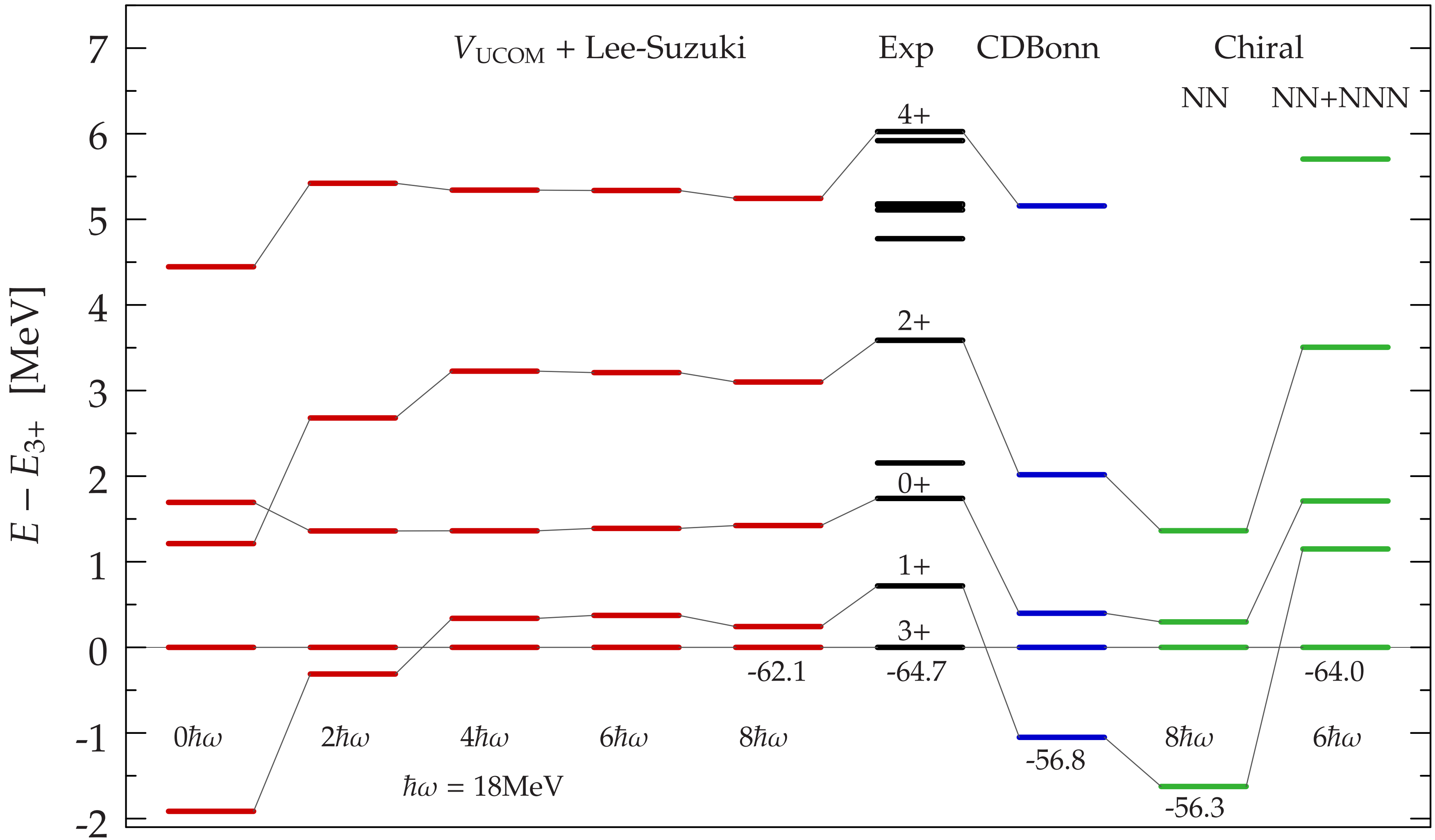


calculations by Petr Navrátil, LLNL

- NCSM calculations with “bare” V_{UCOM} and Lee-Suzuki effective interaction derived from V_{UCOM} show consistent convergence pattern
- Binding energy close to experiment
- Spectra with V_{UCOM} are of similar quality than with other modern NN forces

No-Core Shell Model
^{10}B

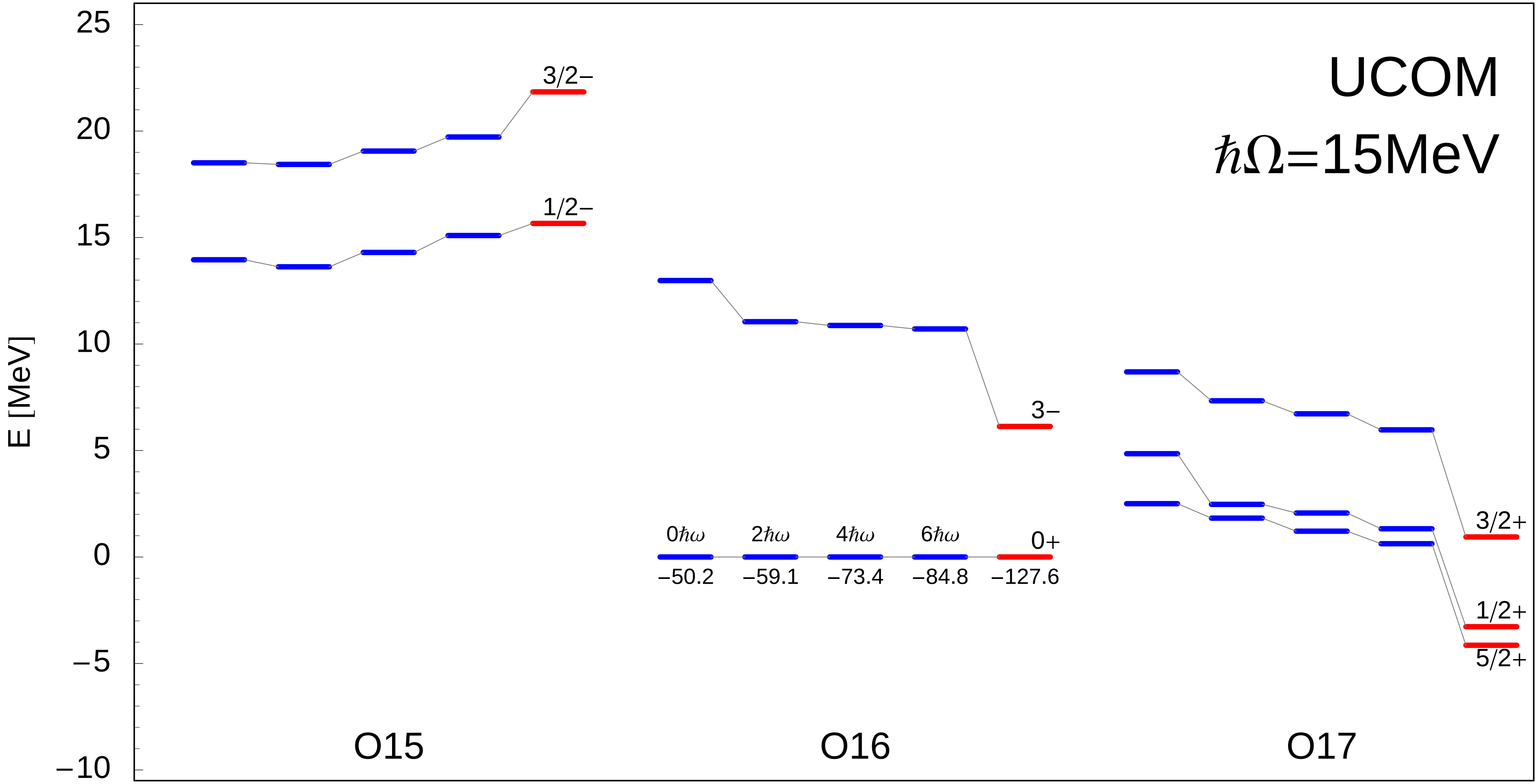
preliminary



calculations by Petr Navrátil, LLNL

- correct level ordering without three-body forces
- binding energy close to experiment

No-Core Shell Model
^{15}O - ^{16}O - ^{17}O



binding energy with bare $V_{\rm UCOM}$ not converged, spectra appear to be quite stable

spin-orbit splittings about right but 3^- in ^{16}O and ^{17}O separation energy off

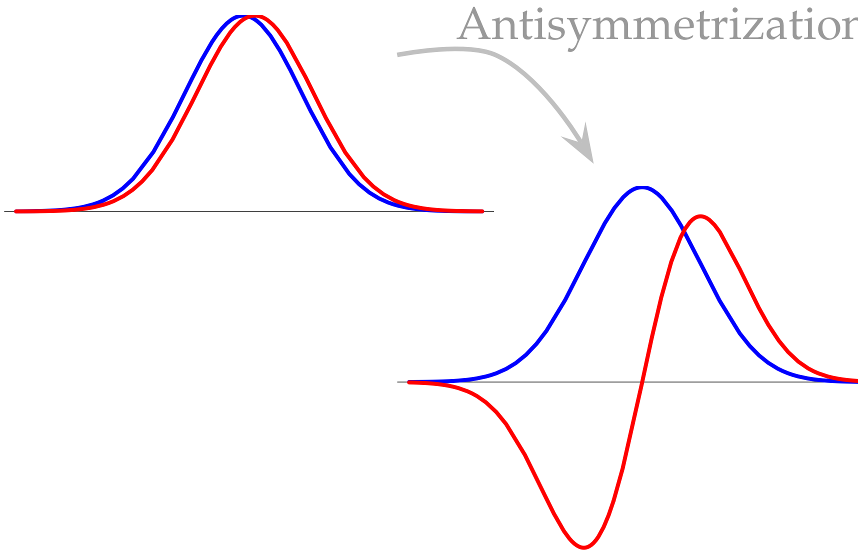
Fermionic Molecular Dynamics

Fermionic

Slater determinant

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

- antisymmetrized A-body state



Molecular

single-particle states

$$\left\langle \mathbf{x} \middle| q \right\rangle = \sum_i c_i \exp\left\{ -\frac{(\mathbf{x}-\mathbf{b}_i)^2}{2a_i} \right\} \otimes \left| \chi^{\uparrow}_i, \chi^{\downarrow}_i \right\rangle \otimes \left| \xi \right\rangle$$

- Gaussian wave-packets in phase-space (complex parameter $\mathbf{b}_i$ encodes mean position and mean momentum), spin is free, isospin is fixed
- width a_i is an independent variational parameter for each wave packet
- superposition of two wave packets for each single particle state

Rev. Mod. Phys. **72** (2000) 655

Nucl. Phys. **A745** (2004) 3

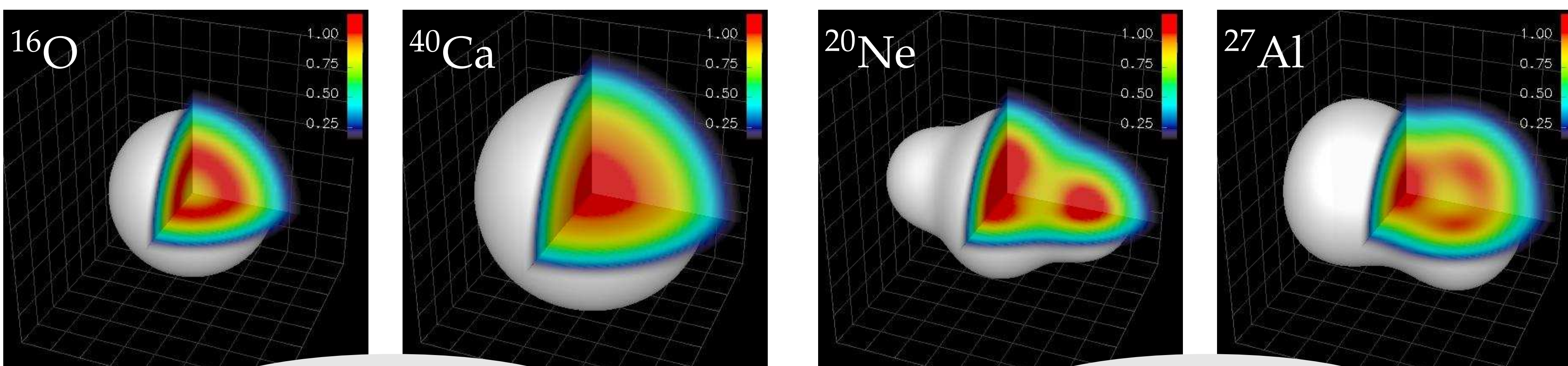
Perform Variation

Minimization

- minimize Hamiltonian expectation value with respect to all single-particle parameters q_k

$$\min_{\{q_k\}} \frac{\left\langle Q \middle| \underset{\sim}{\hat{H}} - \underset{\sim}{T}_{cm} \middle| Q \right\rangle}{\left\langle Q \middle| Q \right\rangle}$$

- this is a Hartree-Fock calculation in our particular single-particle basis
- the mean-field may break the symmetries of the Hamiltonian



spherical nuclei

intrinsically deformed nuclei

Operator Representation of V_{UCOM}

$$\underset{\sim}{C}^\dagger(\underset{\sim}{T} + \underset{\sim}{V})\underset{\sim}{C} \quad = \quad \underset{\sim}{T}$$

one-body kinetic energy

$$+ \sum_{ST} \hat{V}_c^{ST}(r) + \frac{1}{2}\Big(\underset{\sim}{p_r}^2\, \hat{V}_{p^2}^{ST}(r) + \hat{V}_{p^2}^{ST}(r)\, \underset{\sim}{p_r}^2\Big) + \hat{V}_{l^2}^{ST}(r)\, \underset{\sim}{\mathbf{l}}^2$$

central potentials

$$+ \sum_{T} \hat{V}_{ls}^{T}(r)\, \underset{\sim}{\mathbf{l}} \cdot \underset{\sim}{\mathbf{s}} + \hat{V}_{l^2ls}^{T}(r)\, \underset{\sim}{\mathbf{l}}^2 \underset{\sim}{\mathbf{l}} \cdot \underset{\sim}{\mathbf{s}}$$

spin-orbit potentials

$$+ \sum_{T} \hat{V}_{t}^{T}(r)\, \underset{\sim}{S}_{12}(\mathbf{r},\mathbf{r}) + \hat{V}_{trp_\Omega}^{T}(r)\, \underset{\sim}{p_r}\, \underset{\sim}{S}_{12}(\mathbf{r},\mathbf{p}_\Omega) + \hat{V}_{tll}^{T}(r)\, \underset{\sim}{S}_{12}(\mathbf{l},\mathbf{l}) +$$

$$\hat{V}_{tp_\Omega p_\Omega}^{T}(r)\, \underset{\sim}{S}_{12}(\mathbf{p}_\Omega,\mathbf{p}_\Omega) + \hat{V}_{l^2tp_\Omega p_\Omega}^{T}(r)\, \underset{\sim}{\mathbf{l}}^2 \underset{\sim}{S}_{12}(\mathbf{p}_\Omega,\mathbf{p}_\Omega)$$

tensor potentials

bulk of tensor force mapped onto central part of correlated interaction

tensor correlations also change the spin-orbit part of the interaction

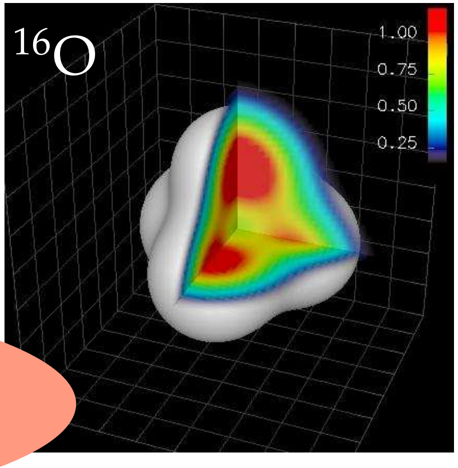
Nucl. Phys. **A745** (2004) 3

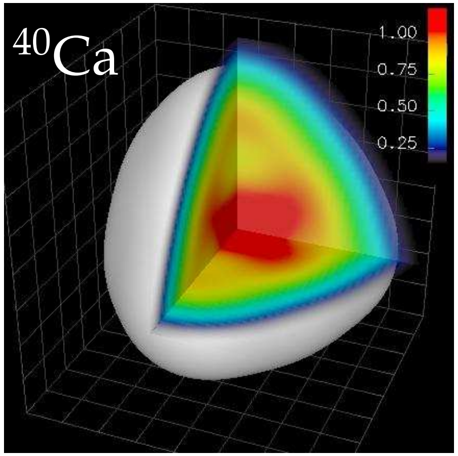
Phenomenological Correction to V_{UCOM}

Effective two-body interaction

- FMD model space can't describe correlations induced by residual medium-long ranged tensor forces
- use **longer ranged tensor correlator** to partly account for that
- add phenomenological two-body correction term with a **momentum-dependend** central and (isospin-dependend) **spin-orbit** part
- fit correction term to binding energies and radii of "closed-shell" nuclei (^{4}He, ^{16}O, ^{40}Ca), (^{24}O, ^{34}Si, ^{48}Ca)

➨ develop a new correction term that is checked against (small scale) No-Core Shell Model calculations

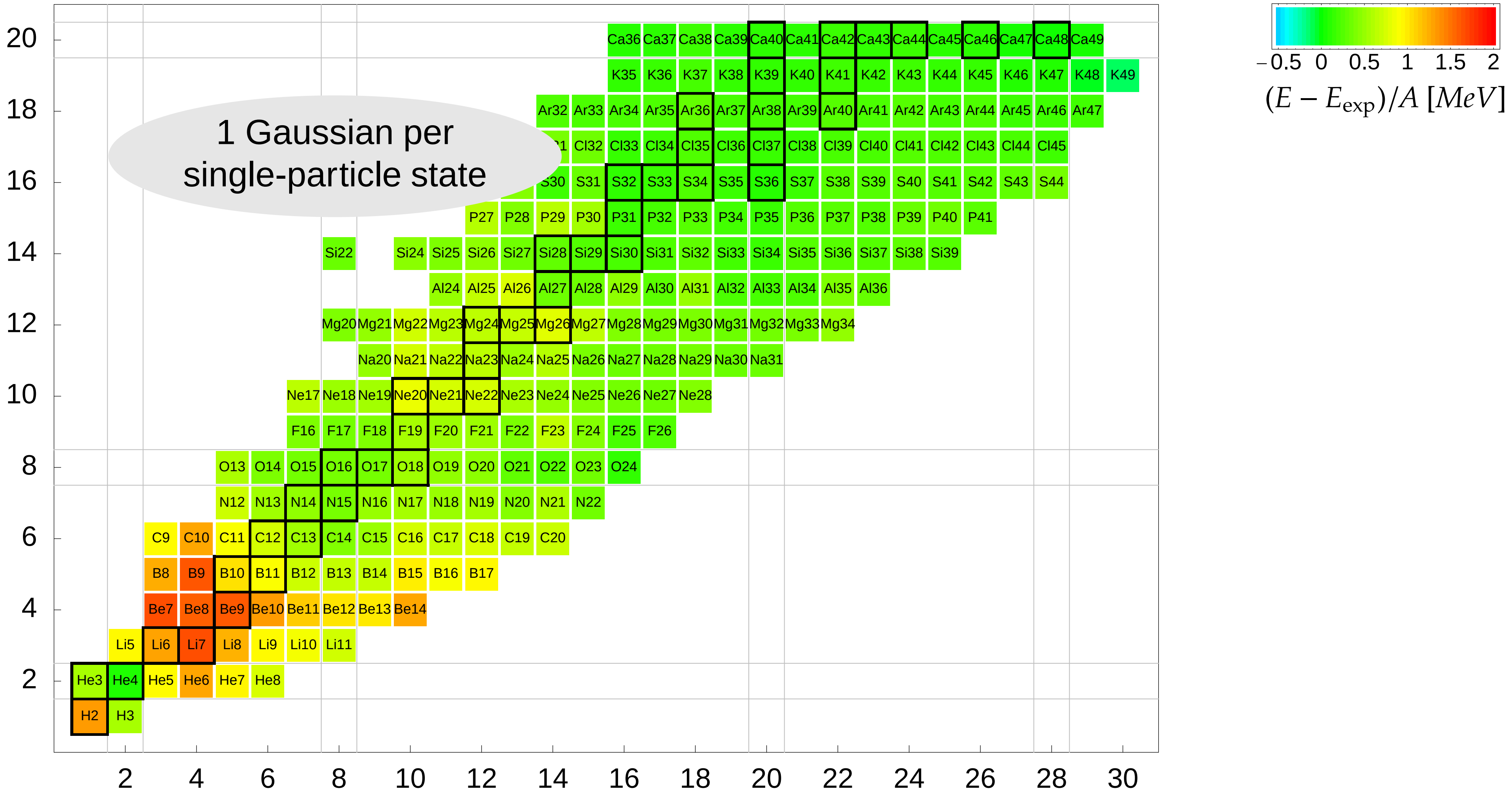




projected tetrahedral configurations are about 6 MeV lower in energy than "closed-shell" configurations

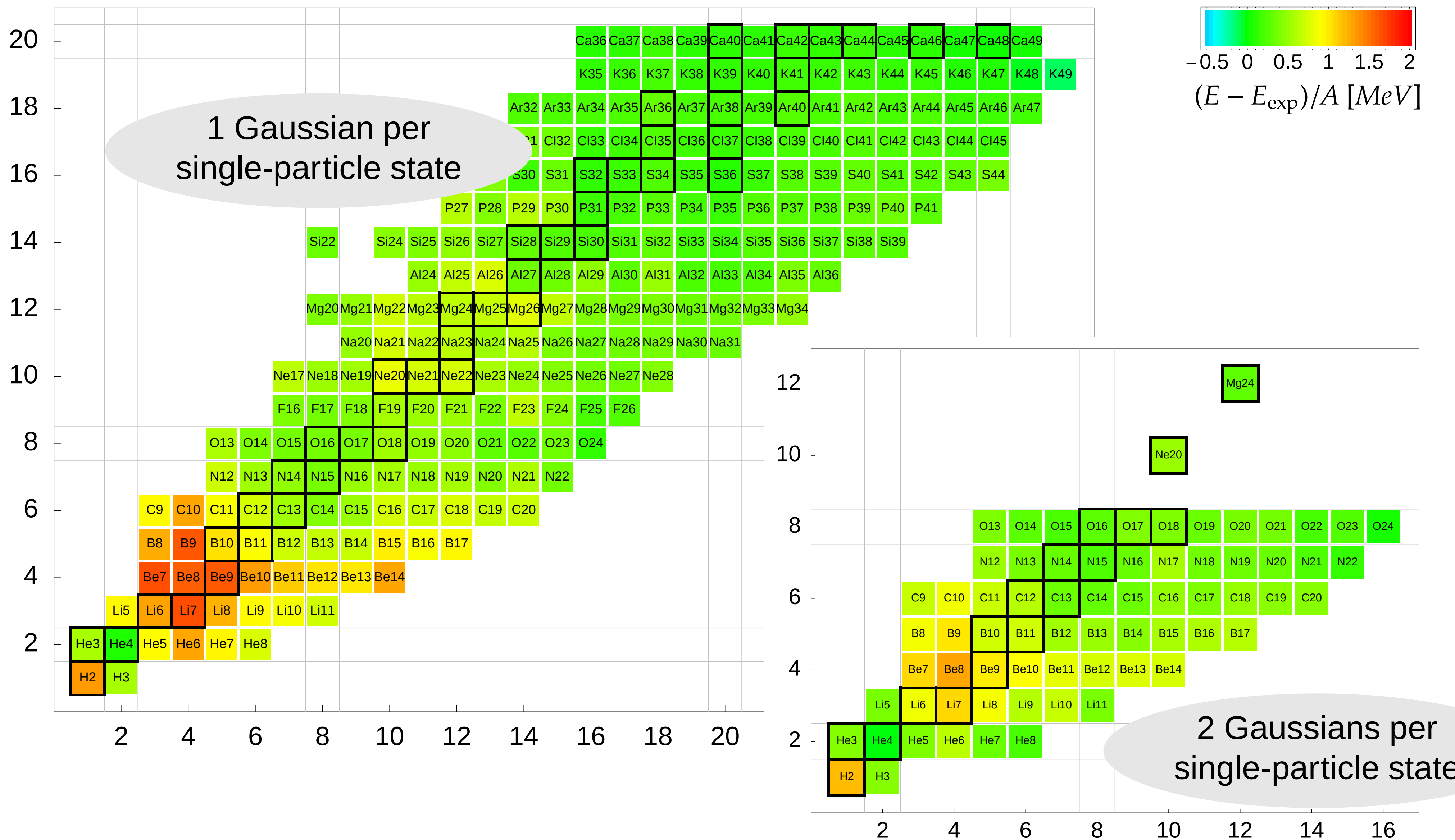
Nuclear Chart

Variation



Nuclear Chart

Variation



PAV, VAP and Multiconfiguration

Projection After Variation (PAV)

- mean-field may break symmetries of Hamiltonian
- restore inversion, translational and rotational symmetry by projection on parity, linear and angular momentum

$$\underset{\sim}{P}^{\mathbf{P}} = \frac{1}{(2\pi)^3} \int d^3X \; \exp\{-i(\underset{\sim}{\mathbf{P}} - \mathbf{P}) \cdot \mathbf{X}\}$$

$$\underset{\sim}{P}^{J}_{MK} = \frac{2J+1}{8\pi^2} \int d^3\Omega \; D^{J\,\star}_{MK}(\Omega) \; \underset{\sim}{R}(\Omega)$$

Variation After Projection (VAP)

- effect of projection can be large
- perform Variation after Parity Projection VAP$^{\pi}$
- perform VAP in GCM sense by applying **constraints** on radius, dipole moment, quadrupole moment or octupole moment and minimize the energy in the projected energy surface

➨ investigate “real” VAP

Multiconfiguration Calculations

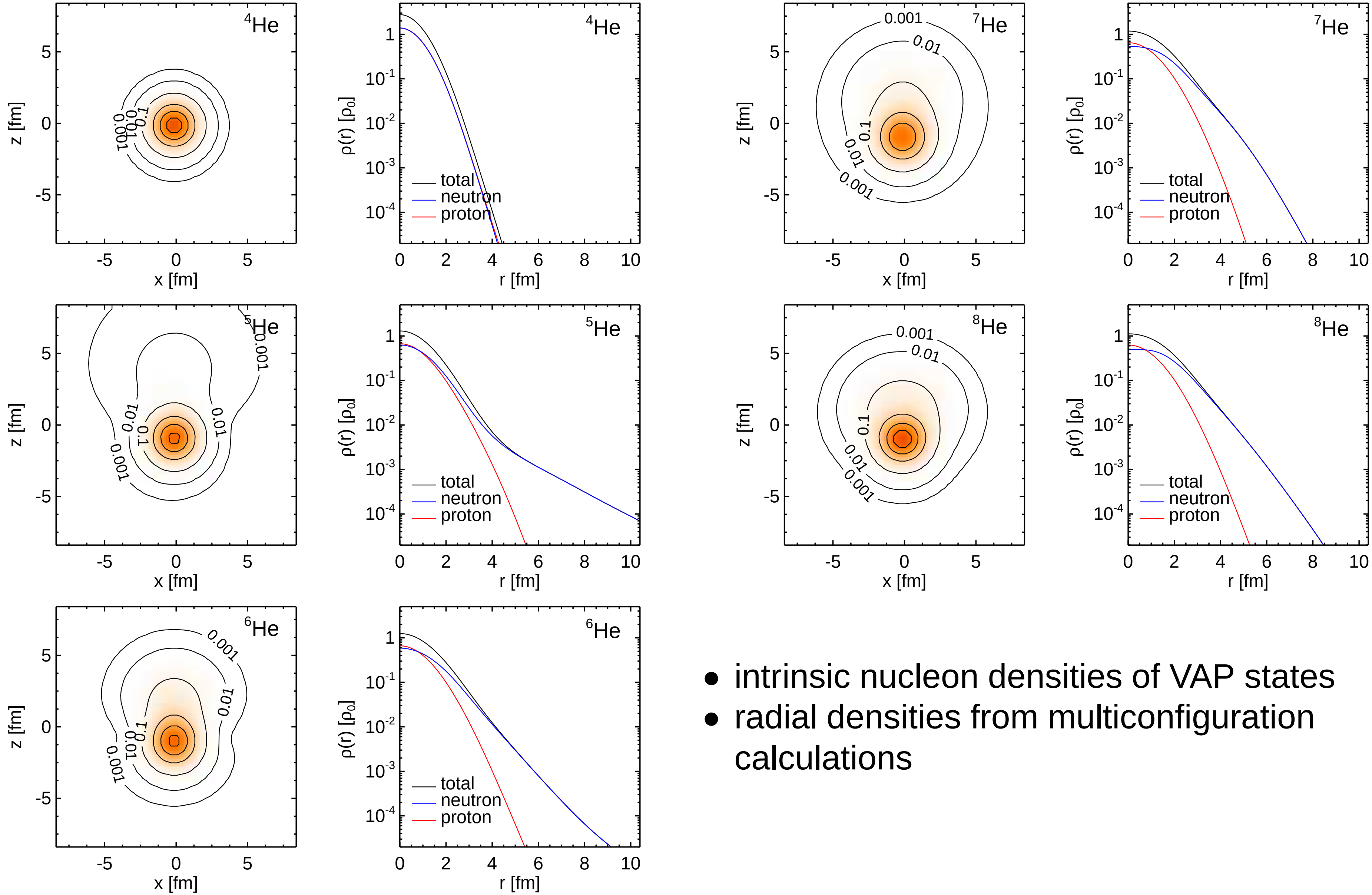
- **diagonalize** Hamiltonian in a set of projected intrinsic states

$$\left\{ \left| Q^{(a)} \right\rangle, \quad a = 1, \ldots, N \right\}$$

$$\sum_{K'b} \left\langle Q^{(a)} \right| \underset{\sim}{H} \underset{\sim}{P}^{J^\pi}_{KK'} \underset{\sim}{P}^{\mathbf{P}=0} \left| Q^{(b)} \right\rangle \cdot c^{(i)}_{K'b} = E^{J^\pi (i)} \sum_{K'b} \left\langle Q^{(a)} \right| \underset{\sim}{P}^{J^\pi}_{KK'} \underset{\sim}{P}^{\mathbf{P}=0} \left| Q^{(b)} \right\rangle \cdot c^{(i)}_{K'b}$$

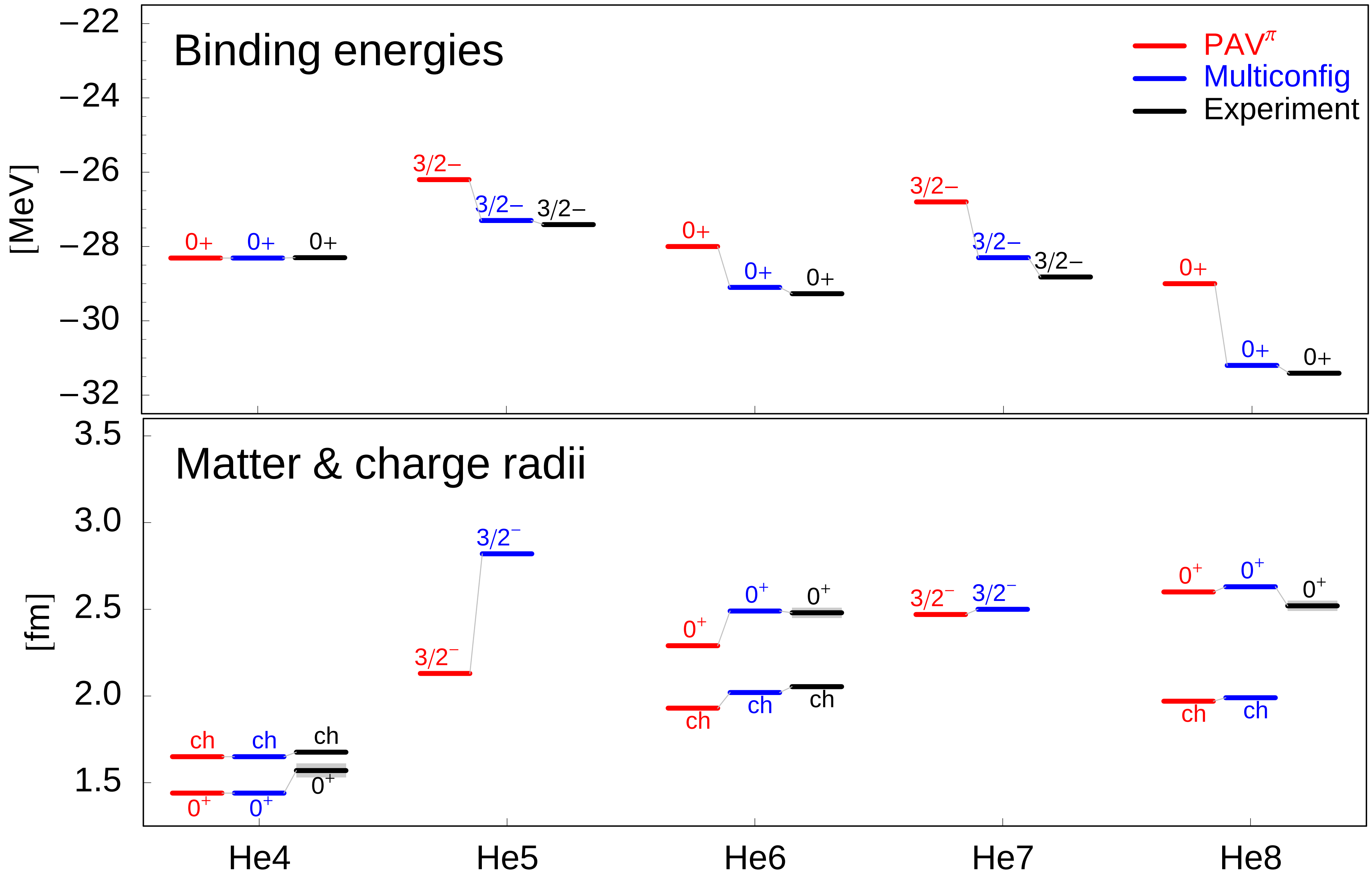
Helium Isotopes

dipole and quadrupole constraints



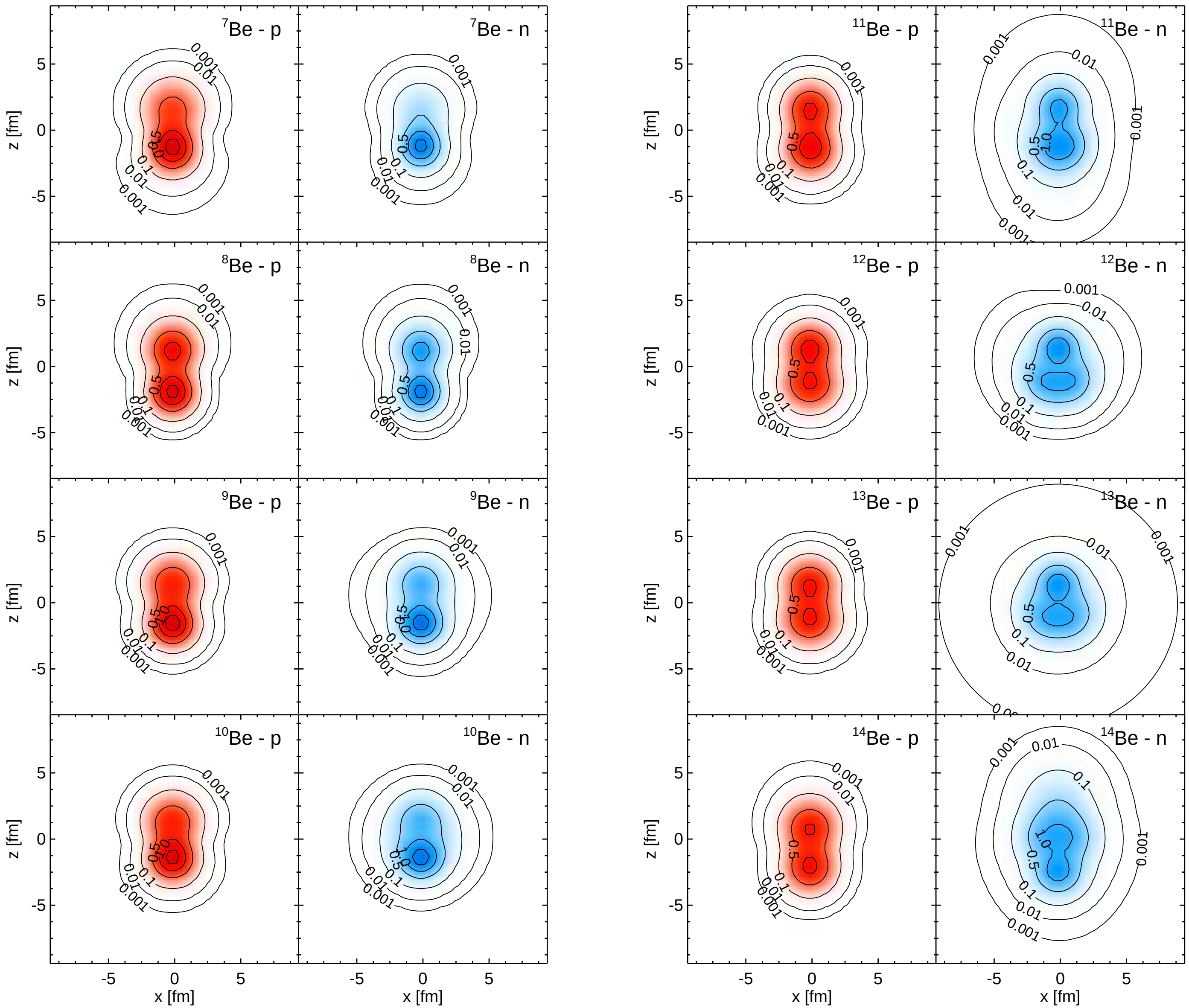
- intrinsic nucleon densities of VAP states
- radial densities from multiconfiguration calculations

Helium Isotopes



^{6}He charge radius: L.-B. Wang et al, Phys. Rev. Lett. **94** (2004) 142501

Beryllium Isotopes

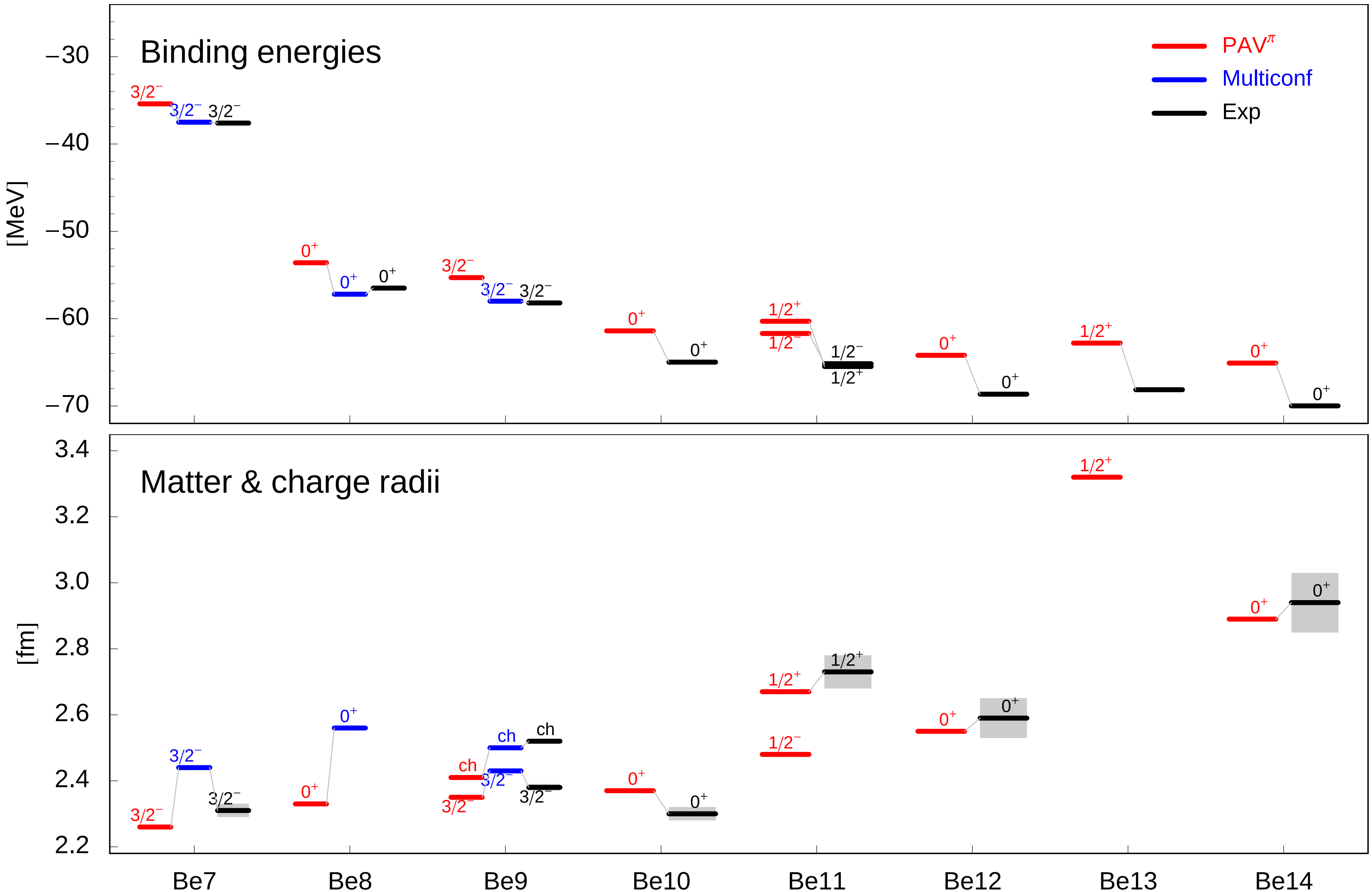


- intrinsic densities of V^{π} states

cluster structure evolves with addition of neutrons

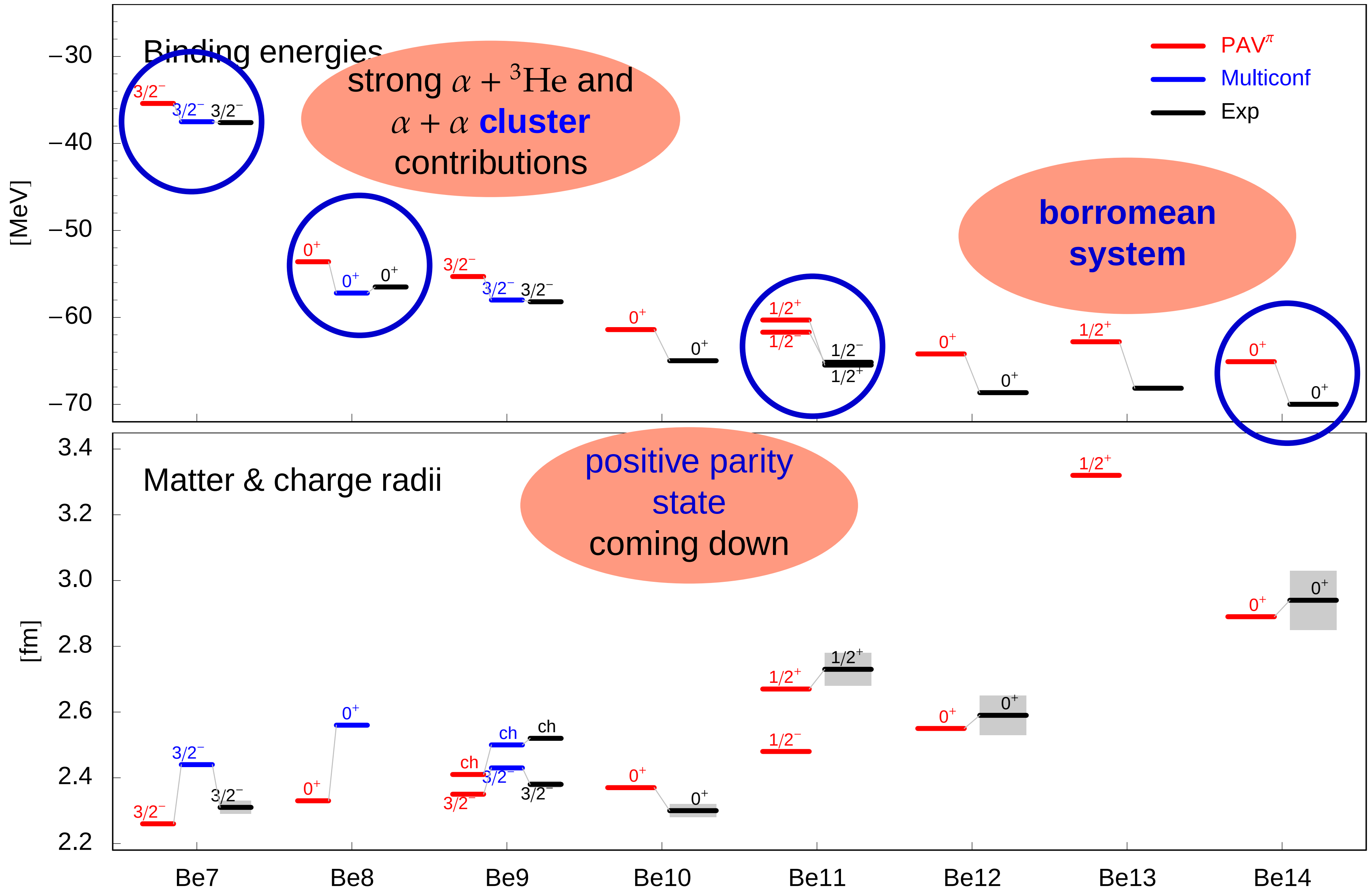
Beryllium Isotopes

quadrupole constraints

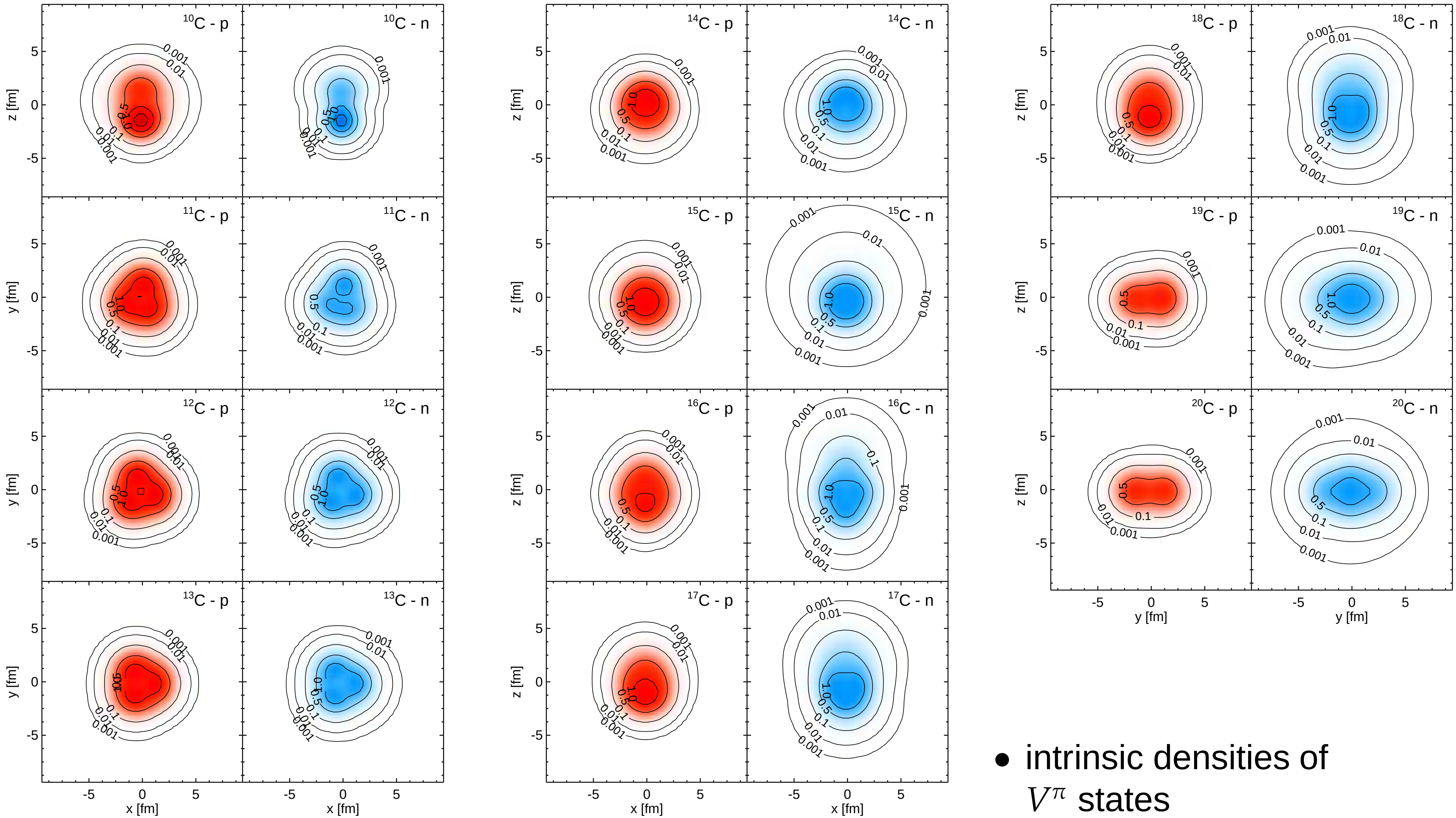


Beryllium Isotopes

quadrupole constraints



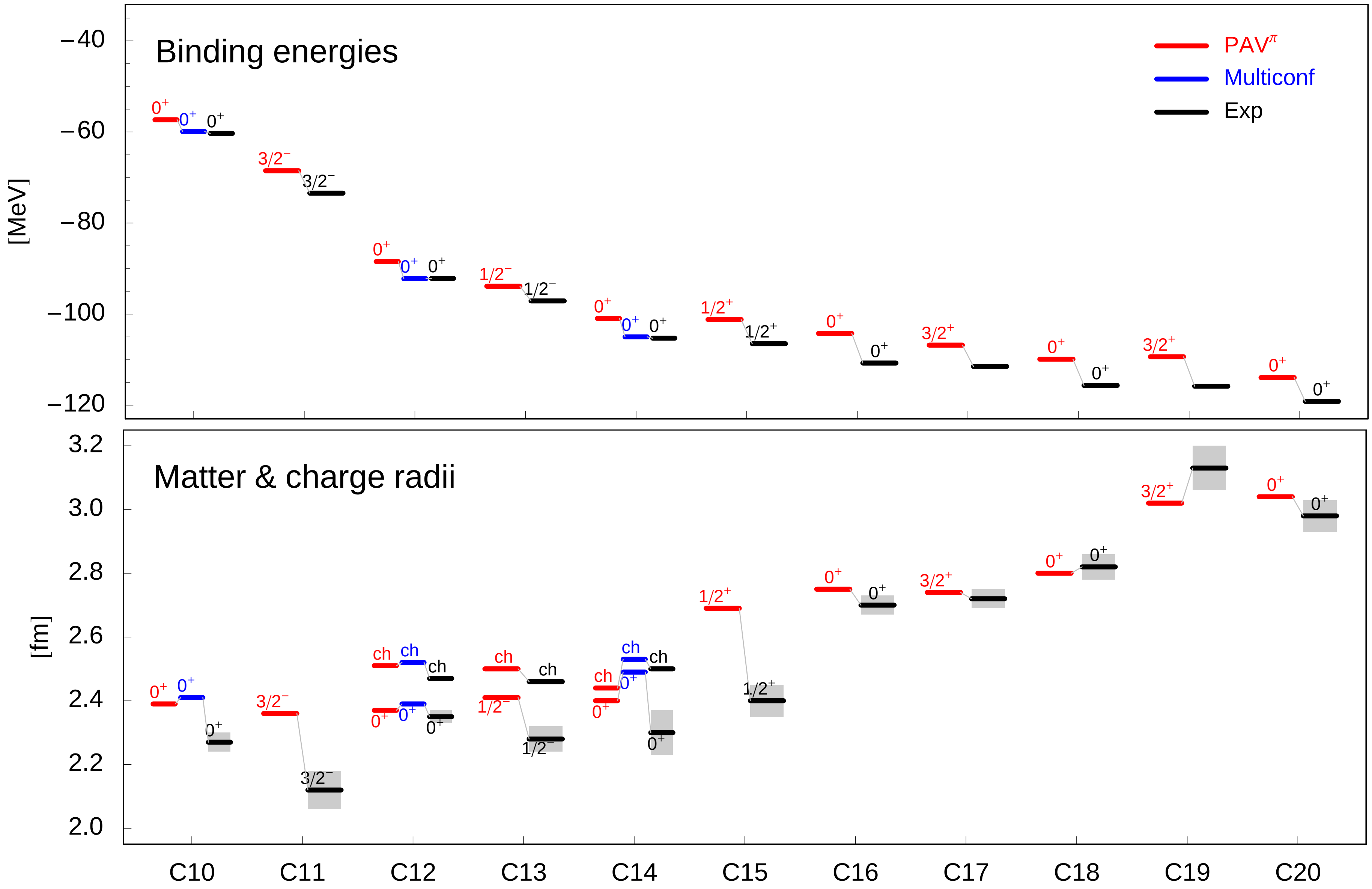
Carbon Isotopes



- intrinsic densities of V^{π} states

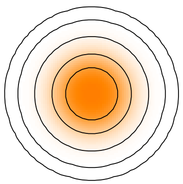
Carbon Isotopes

quadrupole constraints

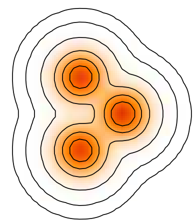


radius and octupole constraints

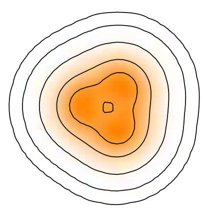
V/PAV



VAP α

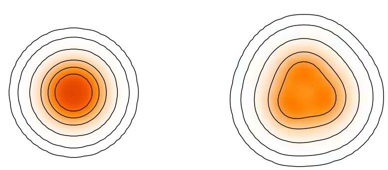


V^{π}/PAV^{π}

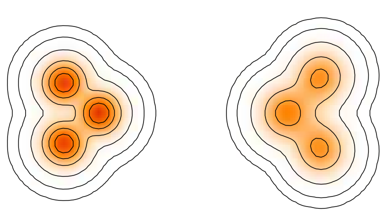


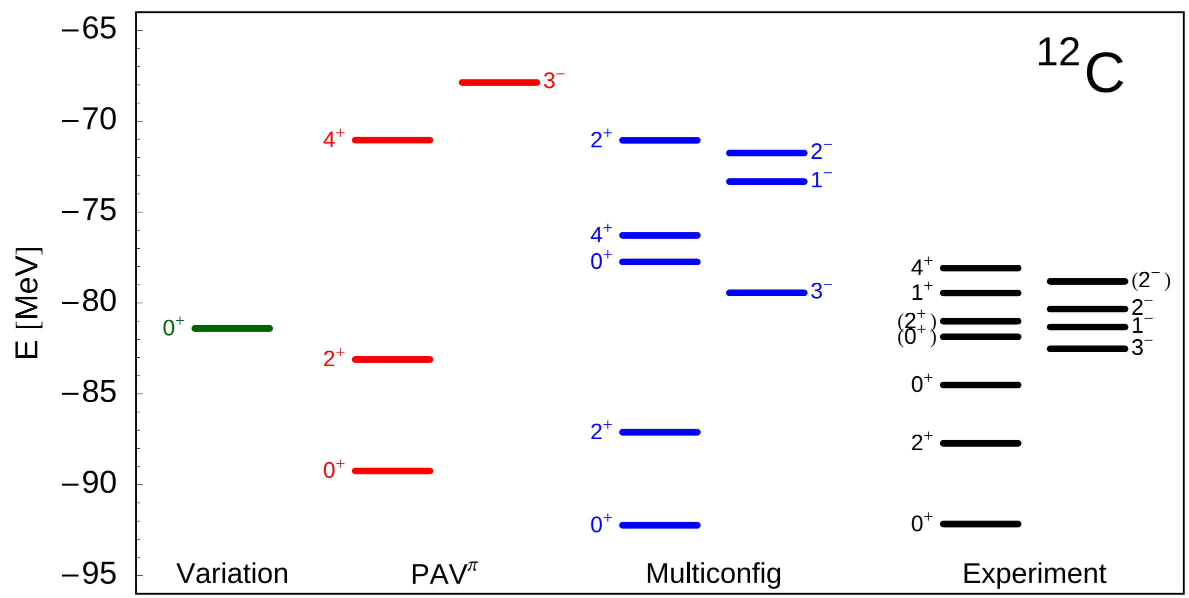
	E_b [MeV]	r_{charge} [fm]	$B(E2)$ [e^2fm^4]
V/PAV	81.4	2.36	-
VAP α-cluster	79.1	2.70	76.9
PAV$^{\pi}$	88.5	2.51	36.3
VAP	89.2	2.42	26.8
Multiconfig	92.2	2.52	42.8
Experiment	92.2	2.47	39.7 ± 3.3

Multiconfig



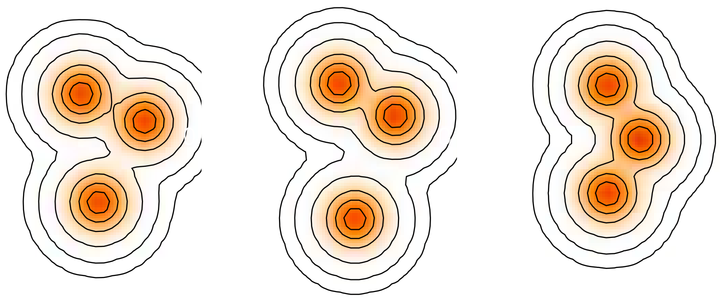
VAP





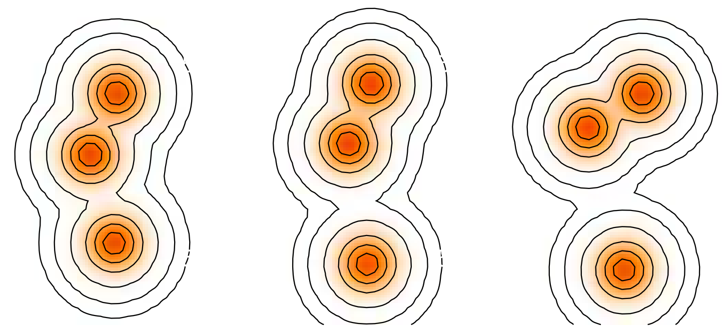
quadrupole and octupole constraints

0_2^+ state



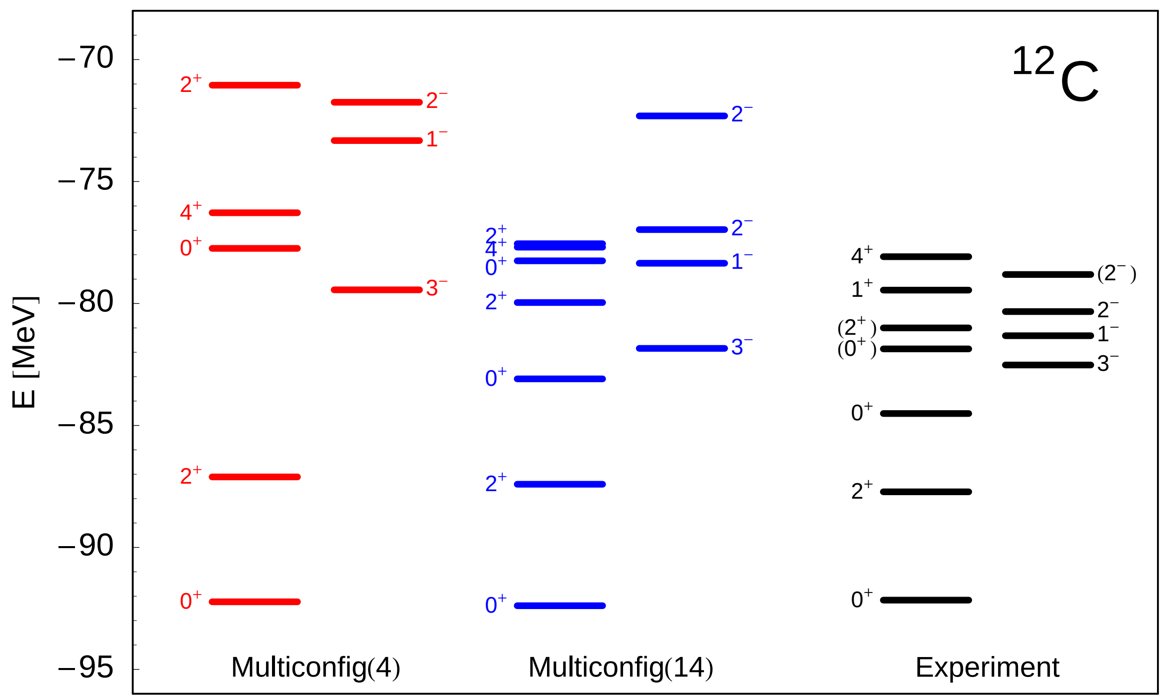
$|\langle \cdot | 0_2^+ \rangle| = 0.76$ $|\langle \cdot | 0_2^+ \rangle| = 0.71$ $|\langle \cdot | 0_2^+ \rangle| = 0.50$

0_3^+ state



$|\langle \cdot | 0_3^+ \rangle| = 0.69$ $|\langle \cdot | 0_3^+ \rangle| = 0.65$ $|\langle \cdot | 0_3^+ \rangle| = 0.44$

	Multiconfig	Experiment
E_b [MeV]	92.4	92.2
r_{charge}[fm]	2.52	2.47
$B(E2)(0_1^+ \rightarrow 2_1^+)$ [e^2fm^4]	42.9	39.7 ± 3.3
$M(E0)(0_1^+ \rightarrow 0_2^+)$[fm^2]	5.67	5.5 ± 0.2
$r_{rms}(0_1^+)$[fm]	2.38	
$r_{rms}(0_2^+)$[fm]	3.42	
$r_{rms}(0_3^+)$[fm]	3.85	
$r_{rms}(2_1^+)$[fm]	2.44	
$r_{rms}(2_2^+)$[fm]	3.64	
$r_{rms}(2_3^+)$[fm]	3.63	
$Q(2_1^+)[e$fm$^2]$	5.85	
$Q(2_2^+)[e$fm$^2]$	-23.65	
$Q(2_3^+)[e$fm$^2]$	5.89	



Resonances and Scattering States

Aim: Microscopic description of ${}^{3}\mathrm{He}(\alpha,\gamma)^{7}\mathrm{Be}$

- GCM states with FMD states for ${}^{3}\mathrm{He}$ and ${}^{4}\mathrm{He}$ like in a microscopic cluster model for the description of the asymptotic behaviour
- use FMD states for ${}^{7}\mathrm{Be}$ in the interaction region

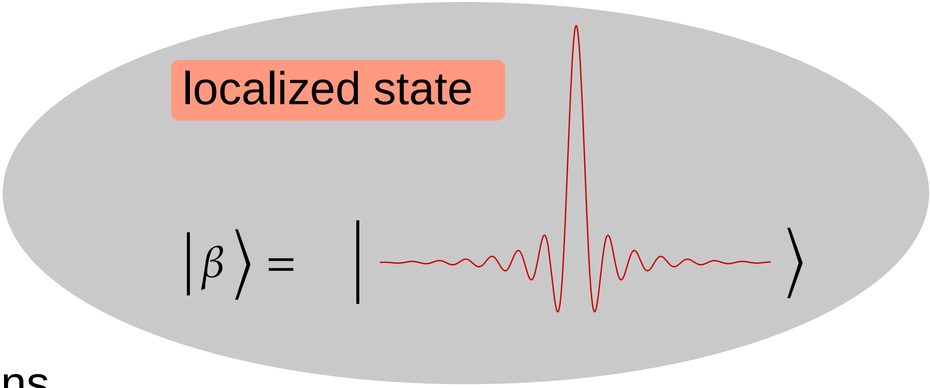
Matching to the asymptotic solution

- for scattering and resonance states we have to implement **boundary conditions** by matching to the Coulomb solution of two point-like nuclei
- in the GCM Slater determinants the relative motion of the clusters, the internal wave functions of the clusters and the center-of-mass wave function are entangled
- if the widths of all Gaussians are equal the relative motion of the two nuclei and the center of mass wave function can be given analytically
- in the FMD we use a **projection on total linear momentum** to get rid of the center of mass problem and introduce a **collective variable representation** to access the relative wave function

Resonances and Scattering States

Collective Coordinate Representation

Size measure



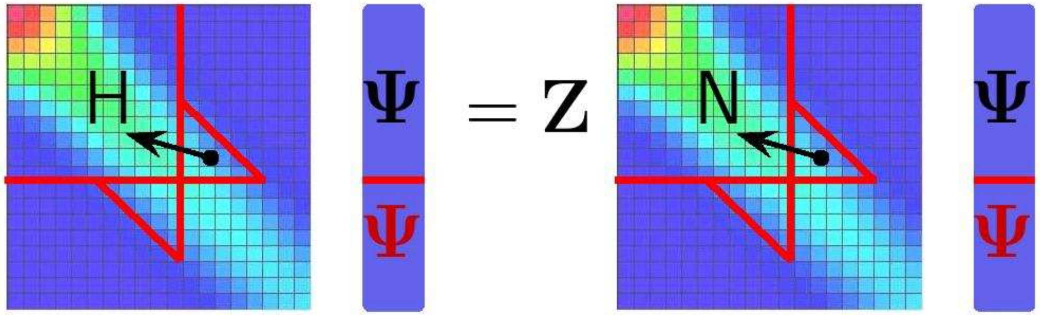
- Operator $\underset{\sim}{B}$ measures the size of the system

$$\underset{\sim}{B} = \frac{1}{A^2}\sum_{i<j}\left(\underset{\sim}{x}(i) - \underset{\sim}{x}(j)\right)^2$$

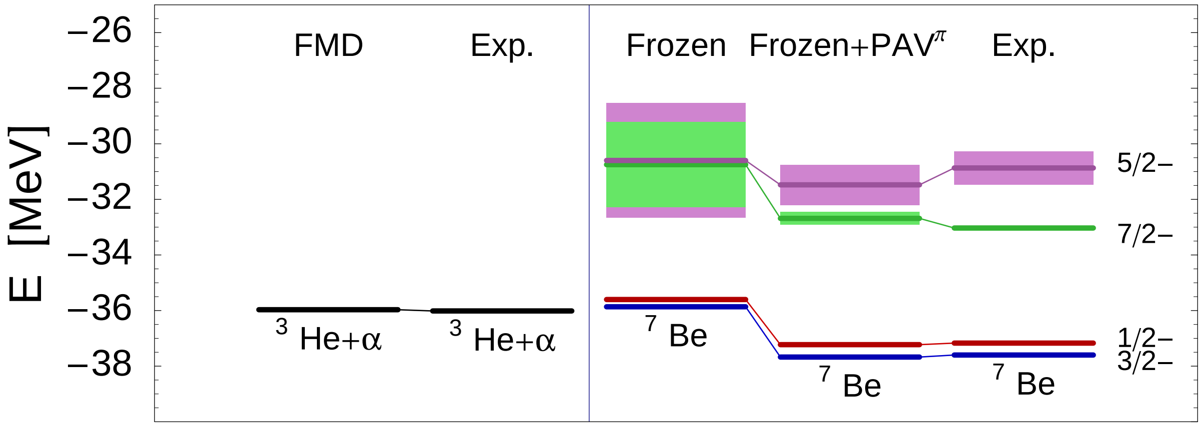
- diagonalize in the space of the cluster configurations, eigenvalues relate to relative distance in the asymptotic region

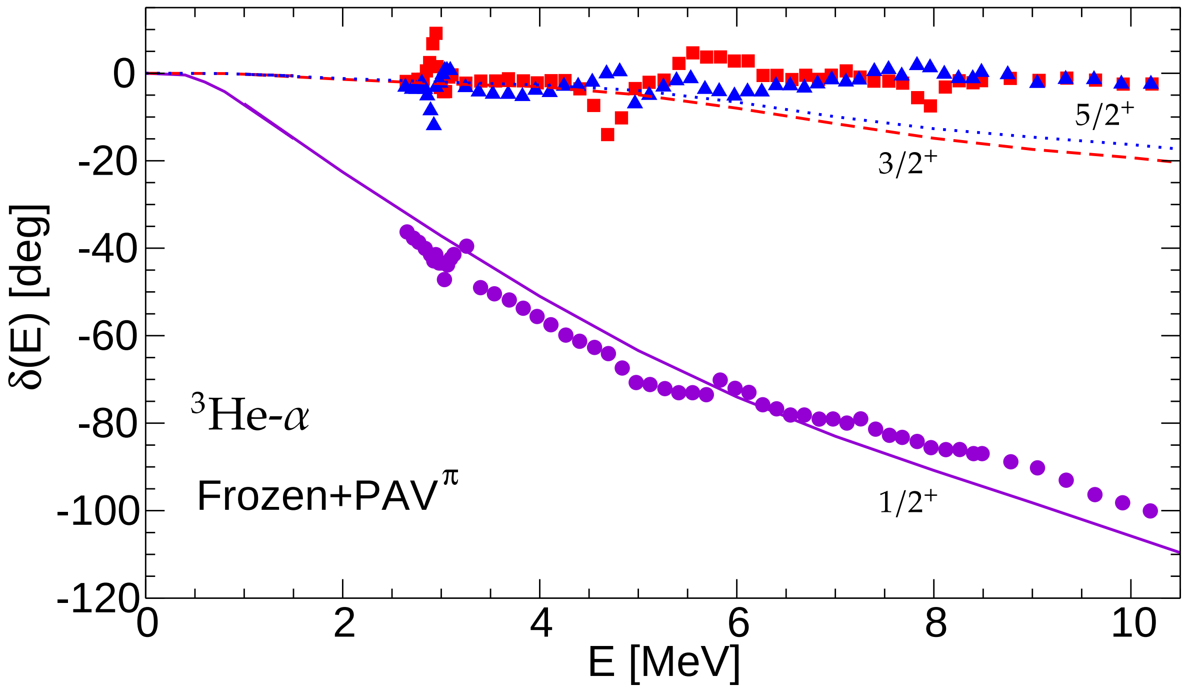
$$\underset{\sim}{B}\left|\beta\right\rangle = \beta\left|\beta\right\rangle \quad \Rightarrow \quad \beta = \frac{1}{A}\left\{\mu\left\langle\rho^2\right\rangle + A_1\left\langle r_1^2\right\rangle + A_2\left\langle r_2^2\right\rangle\right\}$$

- evaluate $\left\langle\beta\left|[\underset{\sim}{H},\underset{\sim}{B}]^s\right|\Psi\right\rangle$ in many-body and two-body world to get boundary conditions
- match to outgoing Coulomb (Resonances) or Coulomb scattering solutions and solve non-linear eigenvalue problem



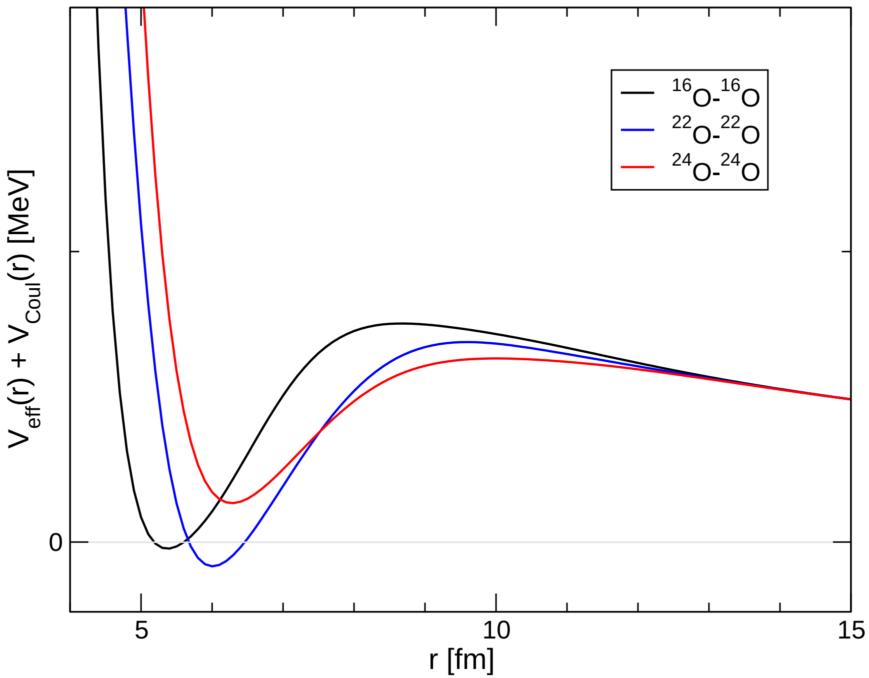
Resonances and Scattering States





first steps towards microscopic and consistent description of **structure and reactions**

Microscopic Nucleus-Nucleus Potentials



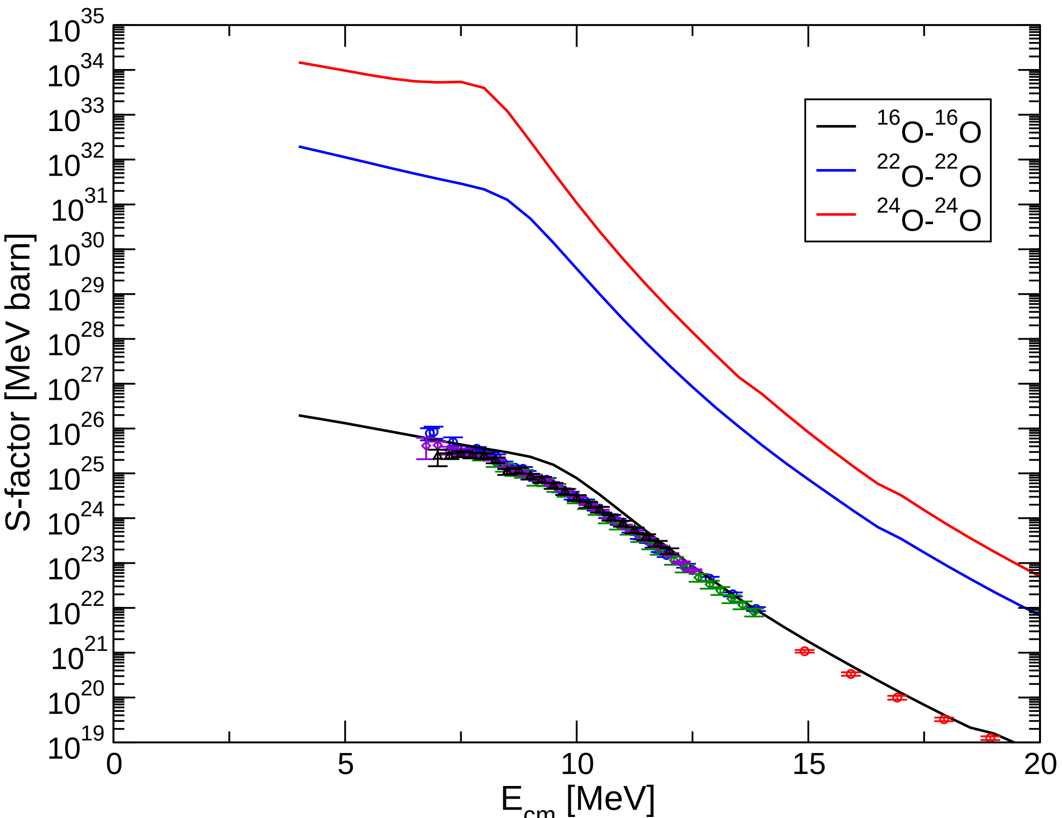
- use GCM wave function

$$\left| \Psi^J_M(\mathbf{R}) \right\rangle = \underset{\sim}{P}^J_{M0} \mathcal{A} \left\{ \left| {}^x\mathrm{O}; \tfrac{1}{2}\mathbf{R} \right\rangle \left| {}^x\mathrm{O}; -\tfrac{1}{2}\mathbf{R} \right\rangle \right\}$$

- transform into RGM wave function to get rid of center-of-mass
- fit a local equivalent potential to the RGM potential surface (diagonalize the RGM norm kernel)
- solve two-body Schrödinger equation for all l with Incoming Wave Boundary Condition
- calculate and sum the penetration probabilities to calculate the fusion cross section

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

➨ **pycnonuclear reactions** in the crust of neutron stars



Summary

Unitary Correlation Operator Method

- explicit description of short-range central and tensor correlations
- phase-shift equivalent correlated interaction V_{UCOM}
- V_{UCOM} used in HF+MBPT and first NCSM calculations

Fermionic Molecular Dynamics

- Structure of light nuclei
- Halos and clustering
- First steps in calculating resonances, scattering states and reactions

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