Fermionic Molecular Dynamics

FMD Wave Functions

Nucleon-Nucleon Interaction

Mean-Field Calculations

Projection After Variation and Variation After Projection

Wave Functions

Fermionic

Slater determinant

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

- 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

Gaussian Wave Packets

- Wave Packet

$$\left\langle \mathbf{x} \middle| a, \mathbf{b} \right\rangle = \exp\left\{ -\frac{(\mathbf{x}-\mathbf{b})^2}{2a} \right\}$$

- Norm

$$\left\langle a, \mathbf{b} \middle| a, \mathbf{b} \right\rangle = \left(2\pi \frac{a^\star a}{a^\star + a} \right)^{3/2} \exp\left\{ -\frac{(\mathbf{b}^\star - \mathbf{b})^2}{2(a^\star + a)} \right\}$$

- Mean Position, Mean Momentum

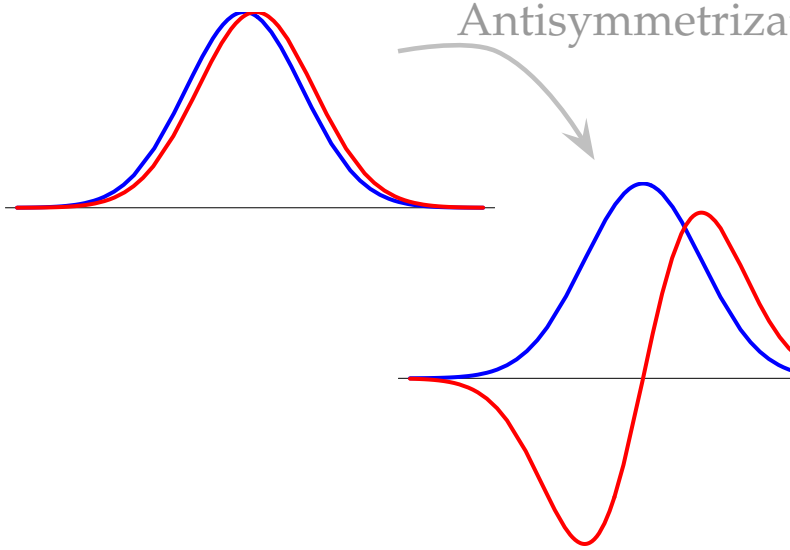
$$\frac{\left\langle a, \mathbf{b} \middle| \underset{\sim}{x} \middle| a, \mathbf{b} \right\rangle}{\left\langle a, \mathbf{b} \middle| a, \mathbf{b} \right\rangle} = \frac{a^\star \mathbf{b} + a \mathbf{b}^\star}{a^\star + a}, \qquad \frac{\left\langle a, \mathbf{b} \middle| \underset{\sim}{k} \middle| a, \mathbf{b} \right\rangle}{\left\langle a, \mathbf{b} \middle| a, \mathbf{b} \right\rangle} = i \frac{\mathbf{b}^\star - \mathbf{b}}{a^\star + a}$$

- Variance of Position and Momentum

$$\frac{\left\langle a, \mathbf{b} \middle| \left(\underset{\sim}{x} - \left\langle \underset{\sim}{x} \right\rangle \right)^2 \middle| a, \mathbf{b} \right\rangle}{\left\langle a, \mathbf{b} \middle| a, \mathbf{b} \right\rangle} = 3 \frac{a^\star a}{a^\star + a} \qquad \frac{\left\langle a, \mathbf{b} \middle| \left(\underset{\sim}{k} - \left\langle \underset{\sim}{k} \right\rangle \right)^2 \middle| a, \mathbf{b} \right\rangle}{\left\langle a, \mathbf{b} \middle| a, \mathbf{b} \right\rangle} = 3 \frac{1}{a^\star + a}$$

Gaussian Wave Packets and Harmonic Oscillator

- Slater determinant invariant under linear transformation of single-particle states
- Harmonic Oscillator wave functions can be obtained by linear combinations of Gaussians



- Create s- and p-wave Harmonic Oscillator wave functions with two slightly shifted Gaussians

$$\lim_{\Delta\to 0}\frac{1}{2}\left(\left\langle x\middle|a,+\Delta\right\rangle+\left\langle x\middle|a,-\Delta\right\rangle\right)=\left\langle x\middle|a,0\right\rangle$$

$$\lim_{\Delta\to 0}\frac{1}{2\Delta}\left(\left\langle x\middle|a,+\Delta\right\rangle-\left\langle x\middle|a,-\Delta\right\rangle\right)=x\left\langle x\middle|a,0\right\rangle$$

Dynamics

Time-dependent

Time-dependent variational principle

$$\delta \int dt \frac{\left\langle Q \left| i\frac{d}{dt} - \underset{\sim}{\hat{H}} \right| Q \right\rangle}{\left\langle Q \middle| Q \right\rangle} = 0$$

➨ describe heavy-ion reactions

Time-independent

Ritz variational principle

$$\delta \frac{\left\langle Q \left| \underset{\sim}{\hat{H}} - \underset{\sim}{\hat{T}}_{\rm cm} \right| Q \right\rangle}{\left\langle Q \middle| Q \right\rangle} = 0$$

➨ minimize expectation value with respect to all the parameters $q_k = \{c_k, a_k, \mathbf{b}_k, \chi_k\}$, $k = 1 \ldots A$

➨ need analytical gradients

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

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

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

Non-Orthogonal Basis

- Slater determinant is the antisymmetrized product state

$$\begin{aligned}\left|\, Q \,\right\rangle &= \underset{\sim}{\mathcal{A}}\left(\left|\, q_1 \,\right\rangle \otimes \cdots \otimes \left|\, q_A \,\right\rangle\right) \\ &= \frac{1}{A!}\sum_{\mathcal{P}} (-1)^{\mathcal{P}}\left(\left|\, q_{\mathcal{P}(1)} \,\right\rangle \otimes \cdots \otimes \left|\, q_{\mathcal{P}(A)} \,\right\rangle\right)\end{aligned}$$

- Antisymmetrization operator is a projection operator

$$\underset{\sim}{\mathcal{A}}\underset{\sim}{\mathcal{A}} = \underset{\sim}{\mathcal{A}}$$

- Many-Body Overlap

$$\begin{aligned}\left\langle\, Q \,\middle|\, Q \,\right\rangle &= \left(\left\langle\, q_1 \,\right| \otimes \cdots \otimes \left\langle\, q_A \,\right|\right) \underset{\sim}{\mathcal{A}}^{\dagger}\underset{\sim}{\mathcal{A}}\left(\left|\, q_1 \,\right\rangle \otimes \cdots \otimes \left|\, q_A \,\right\rangle\right) \\ &= \left(\left\langle\, q_1 \,\right| \otimes \cdots \otimes \left\langle\, q_A \,\right|\right) \underset{\sim}{\mathcal{A}}\left(\left|\, q_1 \,\right\rangle \otimes \cdots \otimes \left|\, q_A \,\right\rangle\right) \\ &= \left(\left\langle\, q_1 \,\right| \otimes \cdots \otimes \left\langle\, q_A \,\right|\right) \frac{1}{A!}\sum_{\mathcal{P}} (-1)^{\mathcal{P}}\left(\left|\, q_{\mathcal{P}(1)} \,\right\rangle \otimes \cdots \otimes \left|\, q_{\mathcal{P}(A)} \,\right\rangle\right) \\ &= \det\left(\left\langle\, q_k \,\middle|\, q_l \,\right\rangle\right)\end{aligned}$$

Evaluation of Matrix Elements

- non-orthogonal basis, use inverse overlap matrix

One-Body Matrix Elements

$$\frac{\left\langle Q \left| \underset{\sim}{O}^{[1]} \right| Q \right\rangle}{\left\langle Q \middle| Q \right\rangle} = \sum_{k,l}^{A} \left\langle q_k \left| \underset{\sim}{O}^{[1]} \right| q_l \right\rangle o_{lk}$$

Two-body operators

$$\frac{\left\langle Q \left| \underset{\sim}{O}^{[2]} \right| Q \right\rangle}{\left\langle Q \middle| Q \right\rangle} = \frac{1}{2} \sum_{k,l,m,n}^{A} \left\langle q_k, q_l \left| \underset{\sim}{O}^{[2]} \right| q_m, q_n \right\rangle (o_{mk} o_{nl} - o_{ml} o_{nk})$$

$$o = n^{-1} = \left(\left\langle q_i \middle| q_j \right\rangle \right)^{-1}$$

Interaction Matrix Elements

(One-body) Kinetic Energy

$$\left\langle q_k \left| \underset{\sim}{T} \right| q_l \right\rangle = \left\langle a_k \mathbf{b}_k \left| \underset{\sim}{T} \right| a_l \mathbf{b}_l \right\rangle \left\langle \chi_k \middle| \chi_l \right\rangle \left\langle \xi_k \middle| \xi_l \right\rangle$$

$$\left\langle a_k \mathbf{b}_k \left| T \right| a_l \mathbf{b}_l \right\rangle = \frac{1}{2m} \left(\frac{3}{a_k^\star + a_l} - \frac{(\mathbf{b}_k^\star - \mathbf{b}_l)^2}{(a_k^\star + a_l)^2} \right) R_{kl}$$

(Two-body) Potential

- fit radial dependencies by (a sum of) Gaussians

$$G(\mathbf{x}_1 - \mathbf{x}_2) = \exp\left\{ -\frac{(\mathbf{x}_1 - \mathbf{x}_2)^2}{2\kappa} \right\}$$

- perform Gaussian integrals

$$\left\langle a_k \mathbf{b}_k, a_l \mathbf{b}_l \left| \underset{\sim}{G} \right| a_m \mathbf{b}_m, a_n \mathbf{b}_n \right\rangle = R_{km} R_{ln} \left(\frac{\kappa}{\alpha_{klmn} + \kappa} \right)^{3/2} \exp\left\{ -\frac{\rho_{klmn}^2}{2(\alpha_{klmn} + \kappa)} \right\}$$

- analytical formulas for matrix elements

$$\alpha_{klmn} = \frac{a_k{}^\star a_m}{a_k{}^\star + a_m} + \frac{a_l{}^\star a_n}{a_l{}^\star + a_n}$$

$$\rho_{klmn} = \frac{a_m \mathbf{b}_k{}^\star + a_k{}^\star \mathbf{b}_m}{a_k{}^\star + a_m} - \frac{a_n \mathbf{b}_l{}^\star + a_l{}^\star \mathbf{b}_n}{a_l{}^\star + a_n}$$

$$R_{km} = \left\langle a_k \mathbf{b}_k \middle| a_m \mathbf{b}_m \right\rangle$$

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

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

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

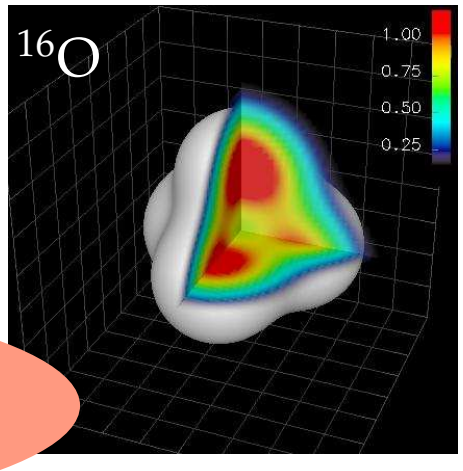
Nucl. Phys. **A745** (2004) 3

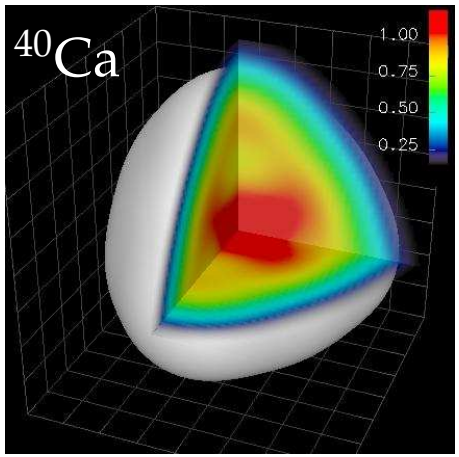
Phenomenological Correction to V_{UCOM}

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

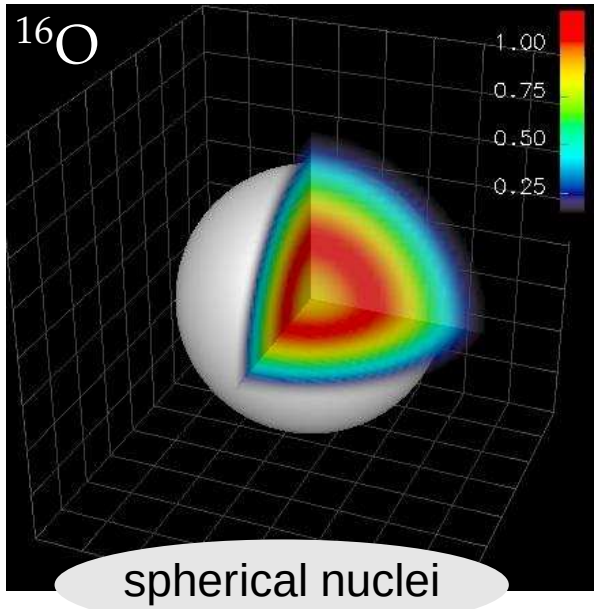
Perform Variation

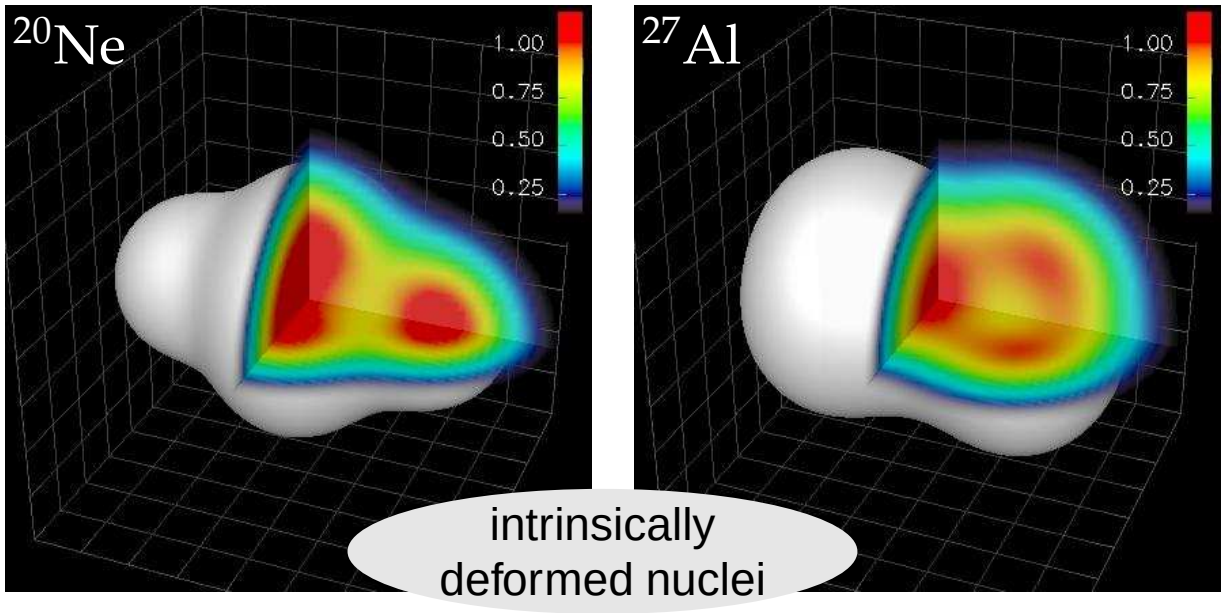
Minimization

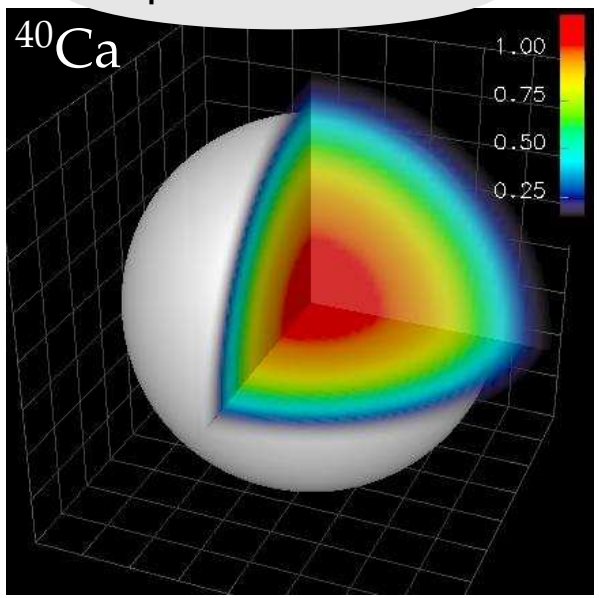
- minimize Hamiltonian with respect to all single-particle parameters q_k

$$\min_{\{q_k\}} \frac{\left\langle Q \left| \hat{H} - T_{cm} \right| Q \right\rangle}{\left\langle Q \middle| Q \right\rangle}$$

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



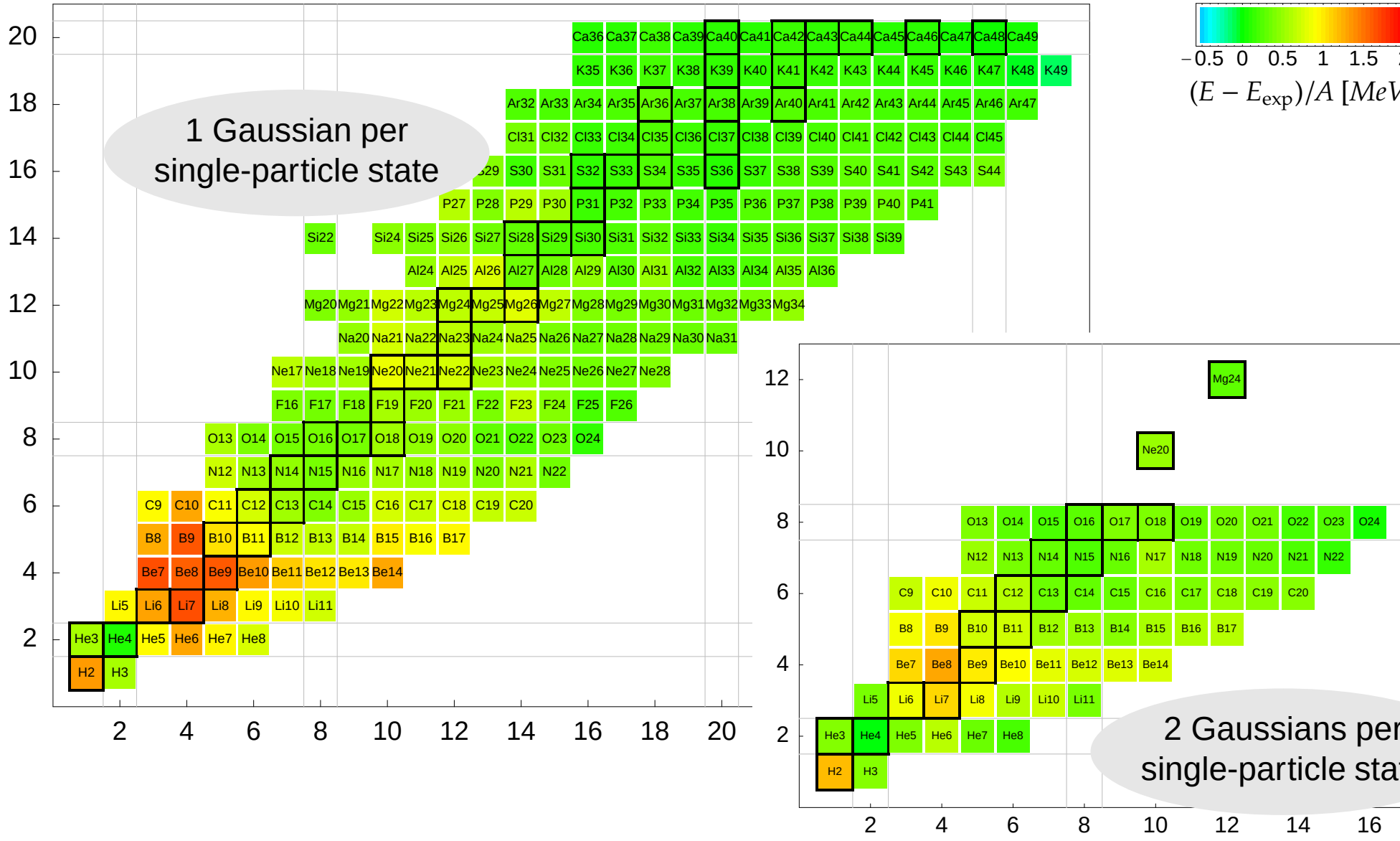




$\rho^{(1)}(\mathbf{r})\,[\rho_0]$

Mean field

Variation



Beyond Mean-Field

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

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

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

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

➨ "real" VAP is possible for p-shell nuclei

Multiconfiguration Calculations

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

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

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

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

Angular Momentum Projection

Intrinsic State

- the intrinsic state is in general not an angular momentum eigenstate
- it is a superposition of angular momentum eigenstates

$$\left|\underset{\sim}{Q}\right\rangle = \sum_{JM\alpha} \left|\underset{\sim}{Q}; JM\alpha\right\rangle c_{JM\alpha}, \qquad \underset{\sim}{\mathbf{J}}^2 \left|\underset{\sim}{Q}; JM\alpha\right\rangle = J(J+1)\left|\underset{\sim}{Q}; JM\alpha\right\rangle, \qquad \underset{\sim}{J_z}\left|\underset{\sim}{Q}; JM\alpha\right\rangle = M\left|\underset{\sim}{Q}; JM\alpha\right\rangle$$

Angular Momentum Projection Operator

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

- Rotation Operator $\underset{\sim}{R}(\Omega)$ rotates the wave function with the Euler angles $\Omega = (\alpha, \beta, \gamma)$
- Wigner D-matrix

$$D^J_{MK}(\Omega) = \left\langle JM\left|\underset{\sim}{R}(\Omega)\right|JK\right\rangle = \left\langle JM\left|e^{\underset{\sim}{iJ_z}\alpha} e^{\underset{\sim}{iJ_y}\beta} e^{\underset{\sim}{iJ_z}\gamma}\right|JK\right\rangle = \exp\{-iM\alpha\}\, d^J_{MK}(\beta)\, \exp\{iM\gamma\}$$

- not a true projection operator

$$(\underset{\sim}{P}^J_{MK})^\dagger \underset{\sim}{P}^{J'}_{M'K'} = \delta_{JJ'}\delta_{MM'}\underset{\sim}{P}^J_{KK'}$$

Angular Momentum Projection

K-mixing

- angular momentum eigenstates are linear combinations of projected states with different K

$$\left| Q; JM\alpha \right\rangle = \sum_K \underset{\sim}{P}^J_{MK} \left| Q \right\rangle c^{J\alpha}_K$$

- solve the generalized eigenvalue problem to get the eigenstates

$$\sum_{K'} \left\langle Q \right| (\underset{\sim}{P}^J_{MK})^\dagger \underset{\sim}{H} \underset{\sim}{P}^J_{MK'} \left| Q \right\rangle c^{J\alpha}_{K'} = E^{J\alpha} \sum_{K'} \left\langle Q \right| (\underset{\sim}{P}^J_{MK})^\dagger \underset{\sim}{P}^J_{MK'} \left| Q \right\rangle c^{J\alpha}_{K'}$$

- as the Hamiltonian commutes with rotations this simplifies to

$$\sum_{K'} \left\langle Q \right| \underset{\sim}{H} \underset{\sim}{P}^J_{KK'} \left| Q \right\rangle c^{J\alpha}_{K'} = E^{J\alpha} \sum_{K'} \left\langle Q \right| \underset{\sim}{P}^J_{KK'} \left| Q \right\rangle c^{J\alpha}_{K'}$$

Axial Symmetry

- if $\left| Q \right\rangle$ is an eigenstate of $\underset{\sim}{J}_z$ the integrations over α and γ become trivial and only the β integration remains

Center-Of-Mass Problem

- Hamiltonian does not couple internal and center-of-mass motion

$$\underset{\sim}{H} = \underset{\sim}{H}_{\text{internal}} + \underset{\sim}{T}_{\text{cm}}$$

- in product states (Slater determinants) the internal motion is entangled with the center-of-mass motion

➨ zero-th order correction: always use internal operators $\underset{\sim}{H}_{\text{internal}} = \underset{\sim}{H} - \underset{\sim}{T}_{\text{cm}}, \ldots$

➨ in the special case where all widths a are equal the wave function factorizes in the internal wave function and the center-of-mass wave function

$$\left\langle \mathbf{x}_1, \ldots, \mathbf{x}_A \middle| Q \right\rangle = \Phi_{\text{internal}}(\xi_1, \ldots, \xi_A)\Phi^a_{\text{cm}}(\mathbf{X})$$

with coordinates $\xi_i = \mathbf{x}_i - \mathbf{X}$ and $\mathbf{X} = \frac{1}{A}\sum_i \mathbf{x}_i$

➨ in the general case we project the wave function on total momentum $\mathbf{P} = 0$ with the projection operator

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

The projected wave function is then given as

$$\left\langle \mathbf{x}_1, \ldots, \mathbf{x}_A \middle| \underset{\sim}{P}^{\mathbf{P}} \middle| Q \right\rangle = \frac{1}{(2\pi)^3}\int \mathrm{d}^3X \, e^{i\mathbf{P}\cdot\mathbf{X}} \left\langle \mathbf{x}_1 - \mathbf{X}, \ldots, \mathbf{x}_A - \mathbf{X} \middle| Q \right\rangle$$

Center-Of-Mass Problem

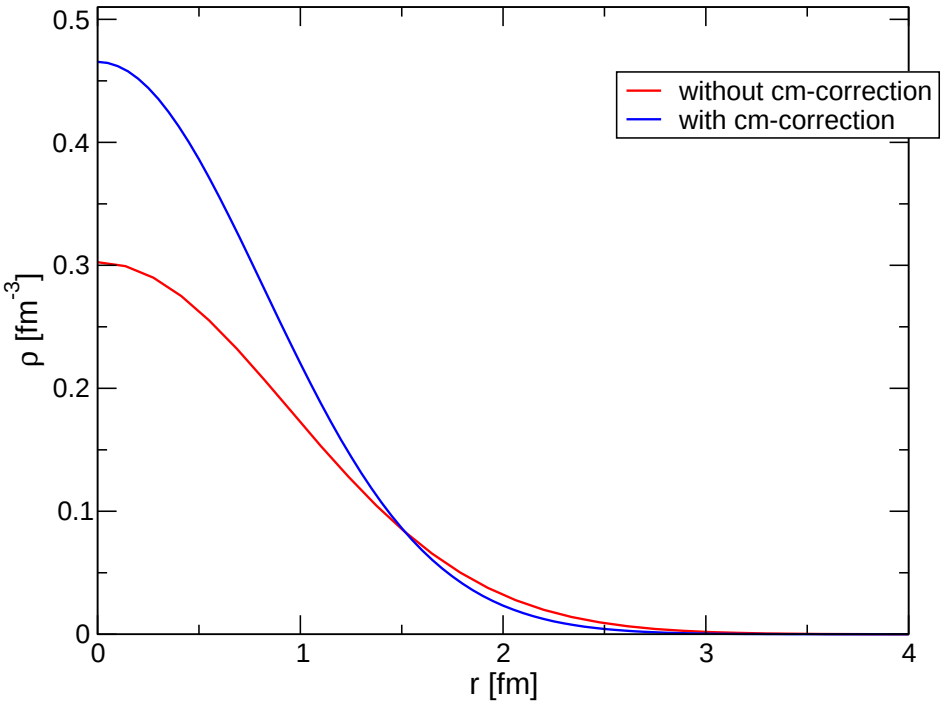
- one-body density calculated with Slater determinant

$$\rho^{(1)}(\mathbf{r}) = \left\langle \Psi \left| \sum_i \delta(\underset{\sim}{\mathbf{r}}_i - \mathbf{r}) \right| \Psi \right\rangle$$

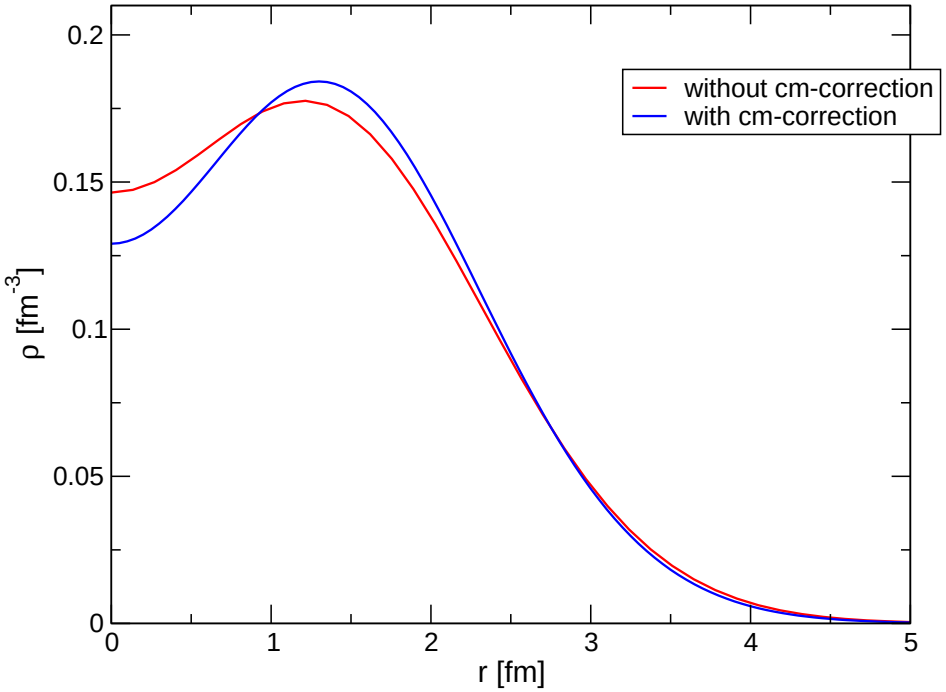
- density of internal wave function

$$\rho^{(1)}_{\text{internal}}(\mathbf{r}) = \left\langle \Psi \left| \sum_i \delta(\underset{\sim}{\mathbf{r}}_i - \underset{\sim}{\mathbf{R}} - \mathbf{r}) \right| \Psi \right\rangle$$

^{4}He

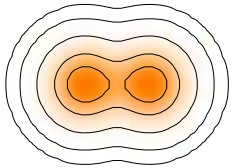


^{16}O

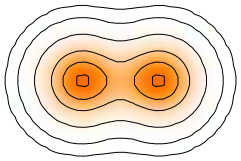


radius and quadrupole constrain

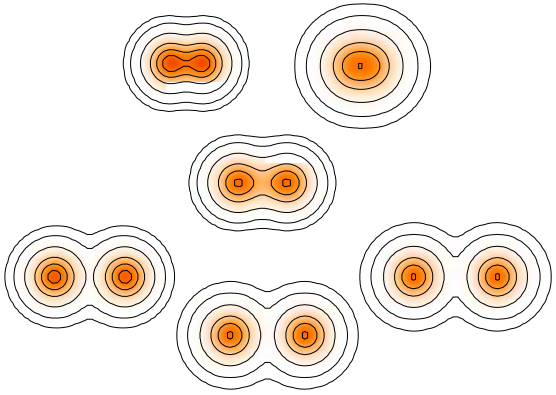
V/PAV



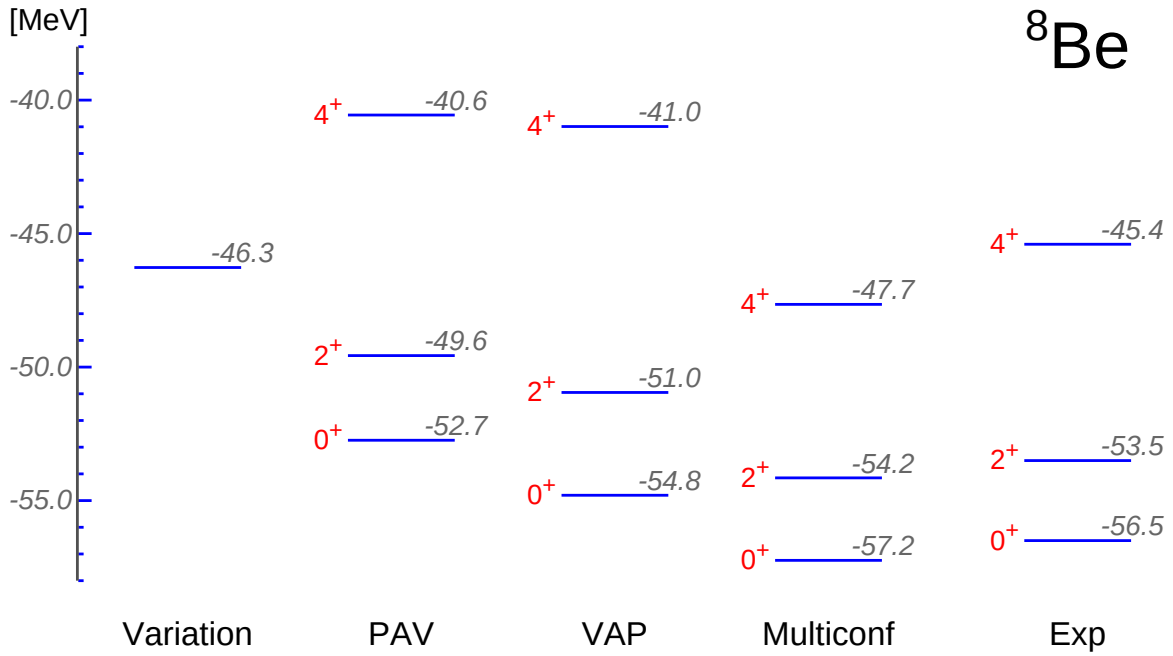
VAP



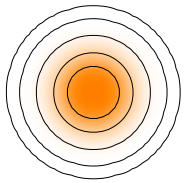
Multiconfig



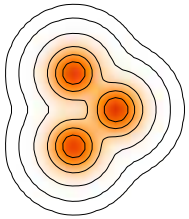
	E_b [MeV]	r_{charge} [fm]	$B(E2)$ [e^2fm^4]
PAV	52.7	2.39	9.31
VAP	54.8	2.49	15.36
Multiconfig	57.2	2.74	30.39
Exp	56.5		



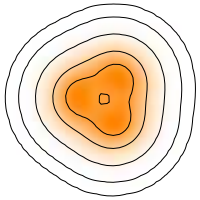
V/PAV



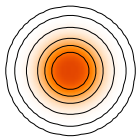
VAP α

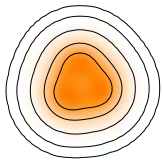


V$^{\pi}$/PAV$^{\pi}$

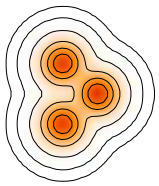


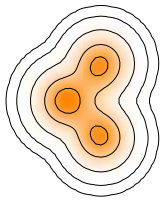
Multiconfig



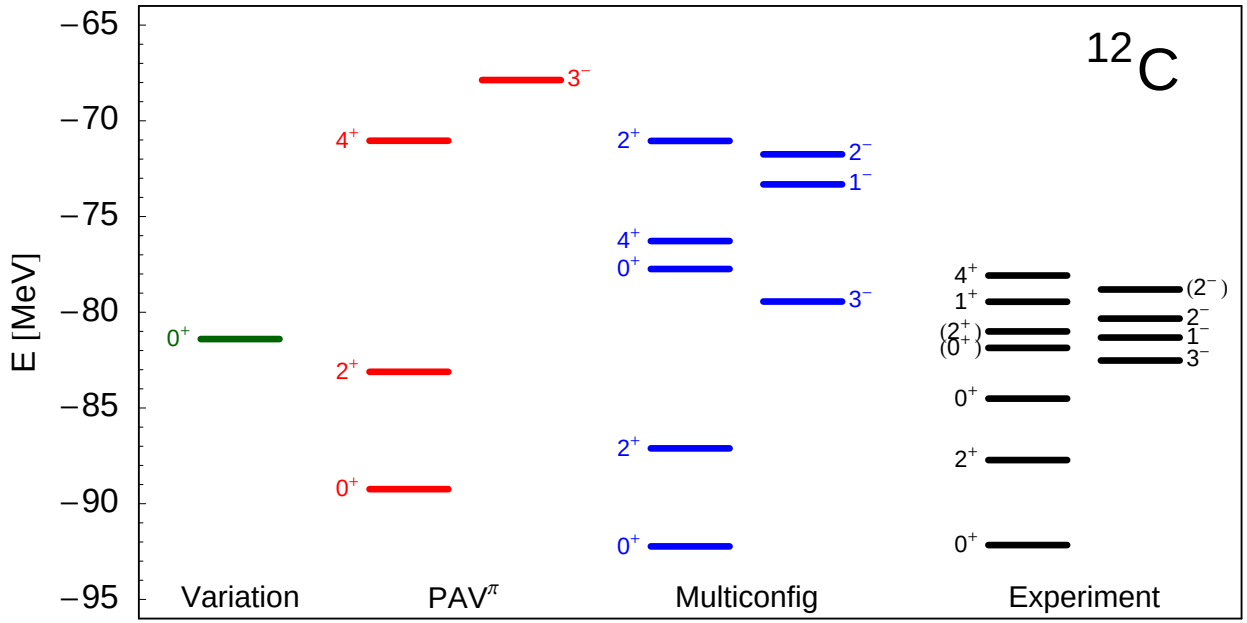


VAP

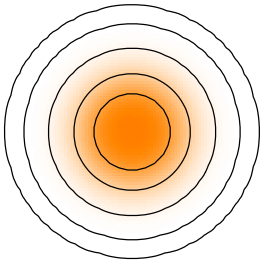
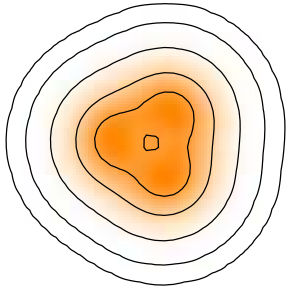
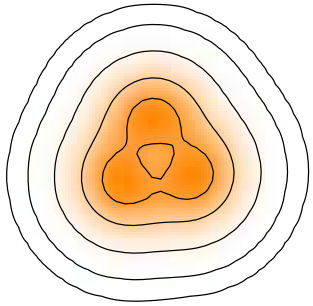
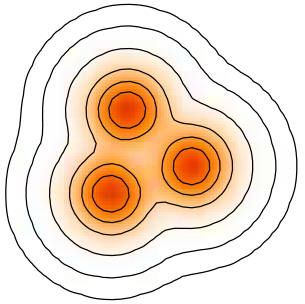




	E_b [MeV]	r_{charge} [fm]	$B(E2)$ [e^2fm^4]
V/PAV	81.4	2.36	-
VAP α-cluster	79.1	2.70	76.9
PAV$^{\pi}$	88.5	2.51	36.3
VAP	89.2	2.42	26.8
Multiconfig	92.2	2.52	42.8
Experiment	92.2	2.47	39.7 ± 3.3



Shell-structure versus Cluster states in ^{12}C

	intrinsic	projected	intrinsic	projected	intrinsic	projected	intrinsic	projected
$\langle \underset{\sim}{H} \rangle$	-81.4	-81.5	-77.0	-88.5	-74.1	-85.5	-57.0	-75.9
$\langle \underset{\sim}{T} \rangle$	212.1	212.1	189.2	186.1	182.8	179.0	213.9	201.4
$\langle \underset{\sim}{V}_{ls} \rangle$	-39.8	-40.2	-12.0	-17.1	-5.8	-8.0	-	-
$\sqrt{\langle \underset{\sim}{r^2} \rangle}$	2.22	2.22	2.40	2.37	2.45	2.42	2.44	2.42

spin-orbit force “breaks” clusters

cluster states strongly “feel” projection

Applications

Helium Isotopes

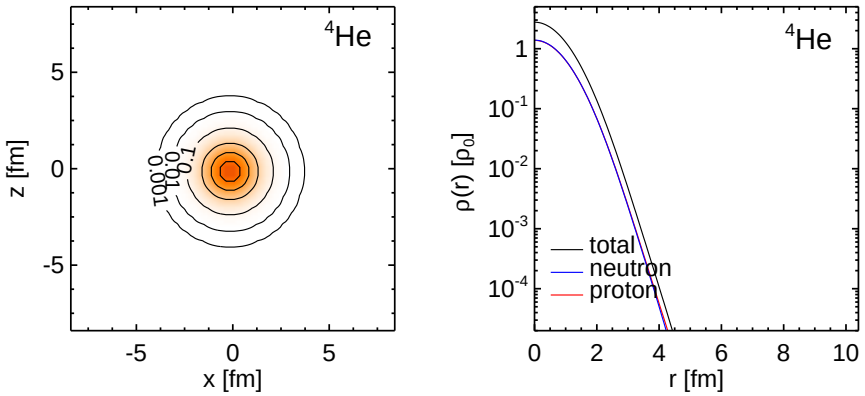
Lithium Isotopes

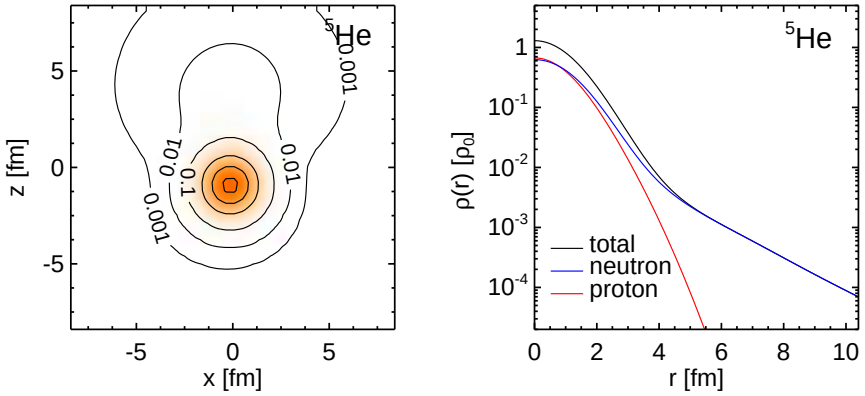
Beryllium Isotopes

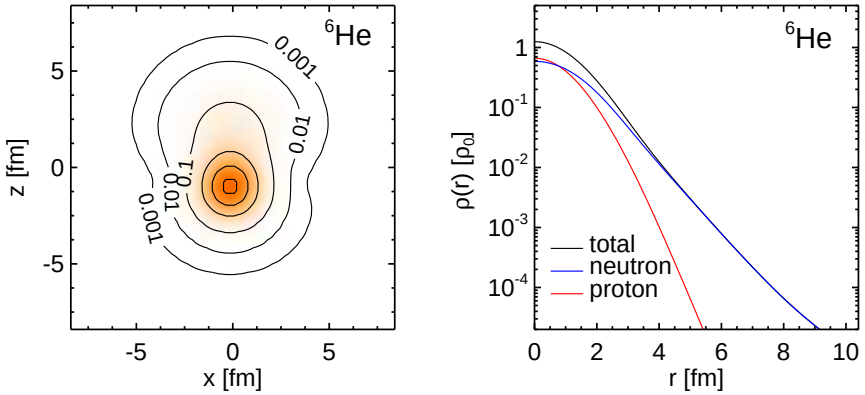
Carbon Isotopes

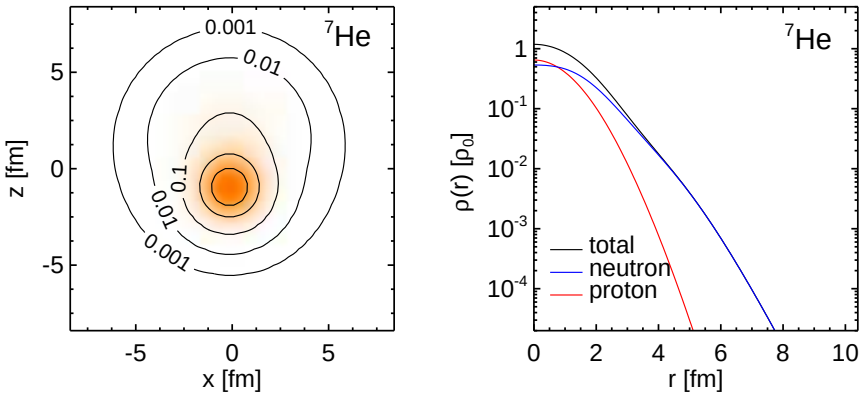
Helium Isotopes

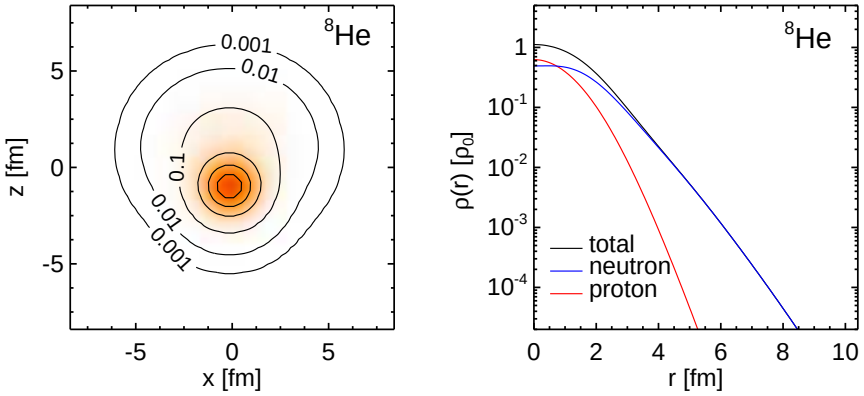
dipole and quadrupole constrai





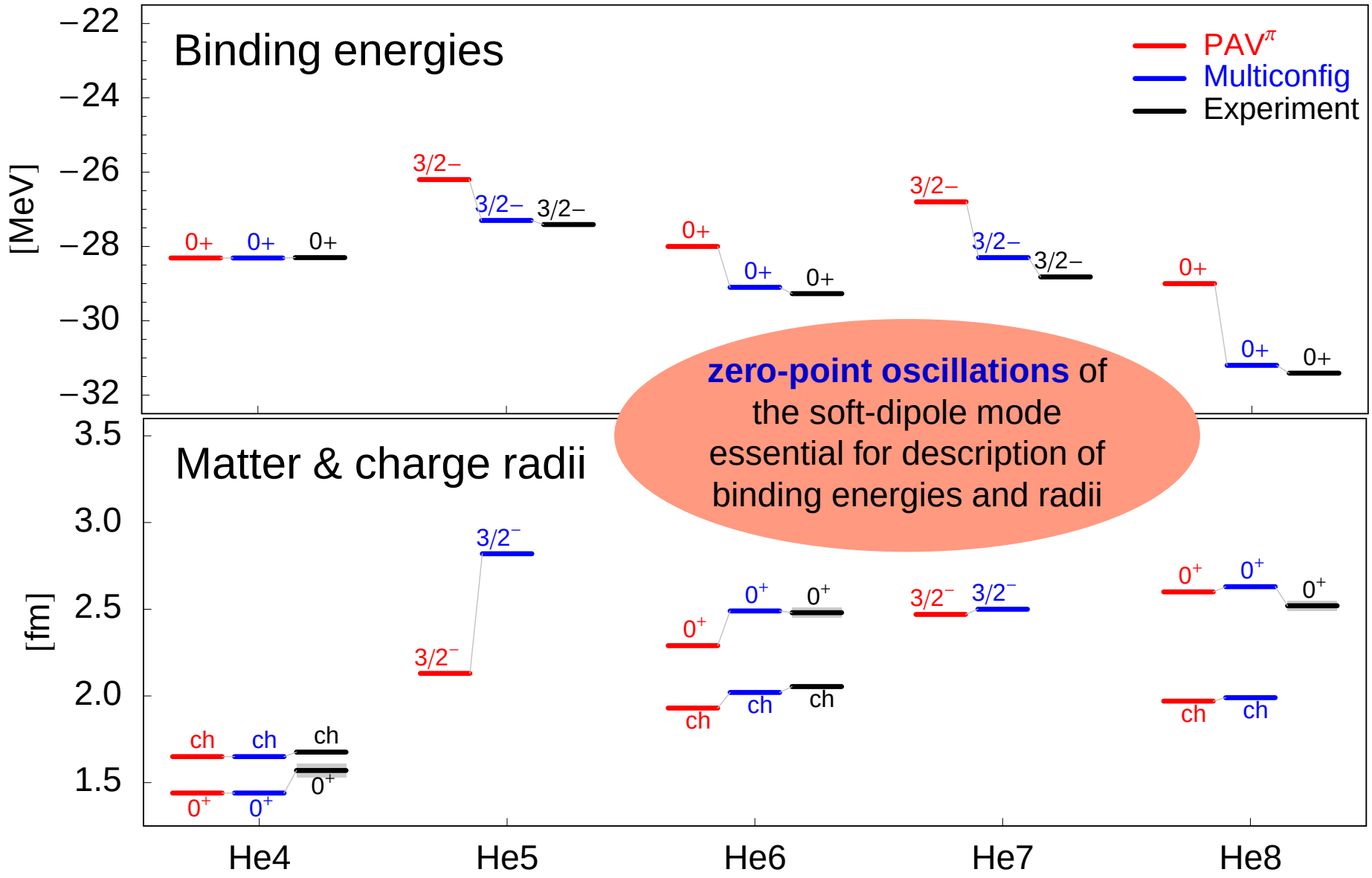






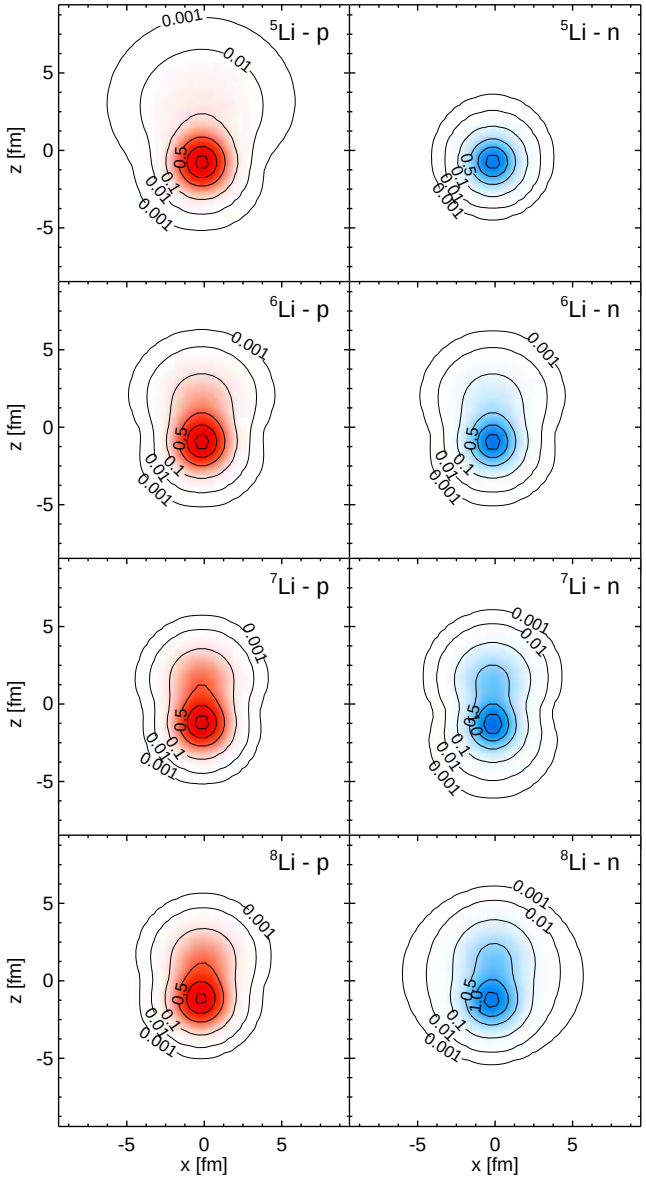
- intrinsic nucleon densities of VAP states
- radial densities from multiconfiguration calculations

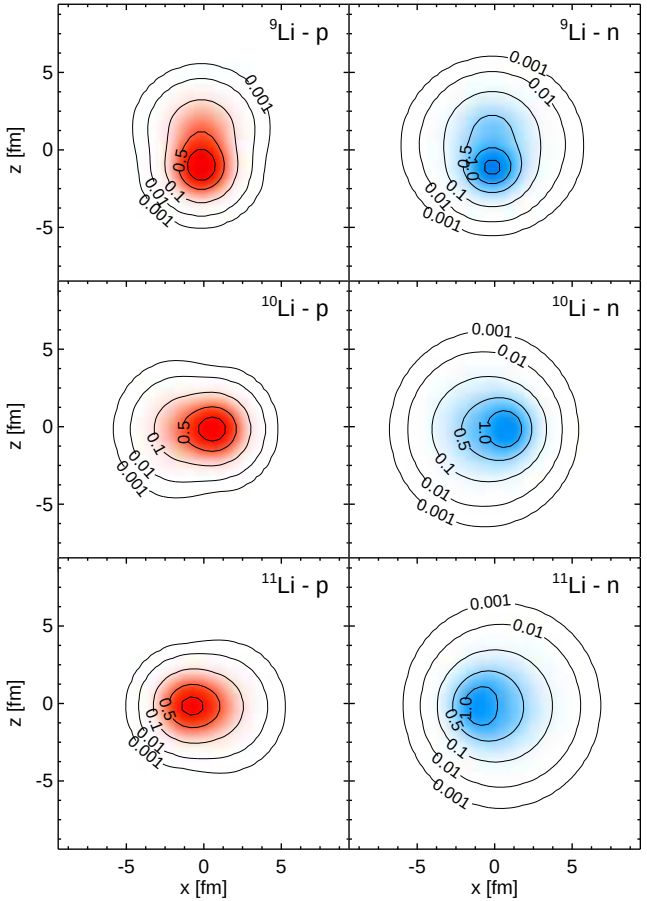
Helium Isotopes



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

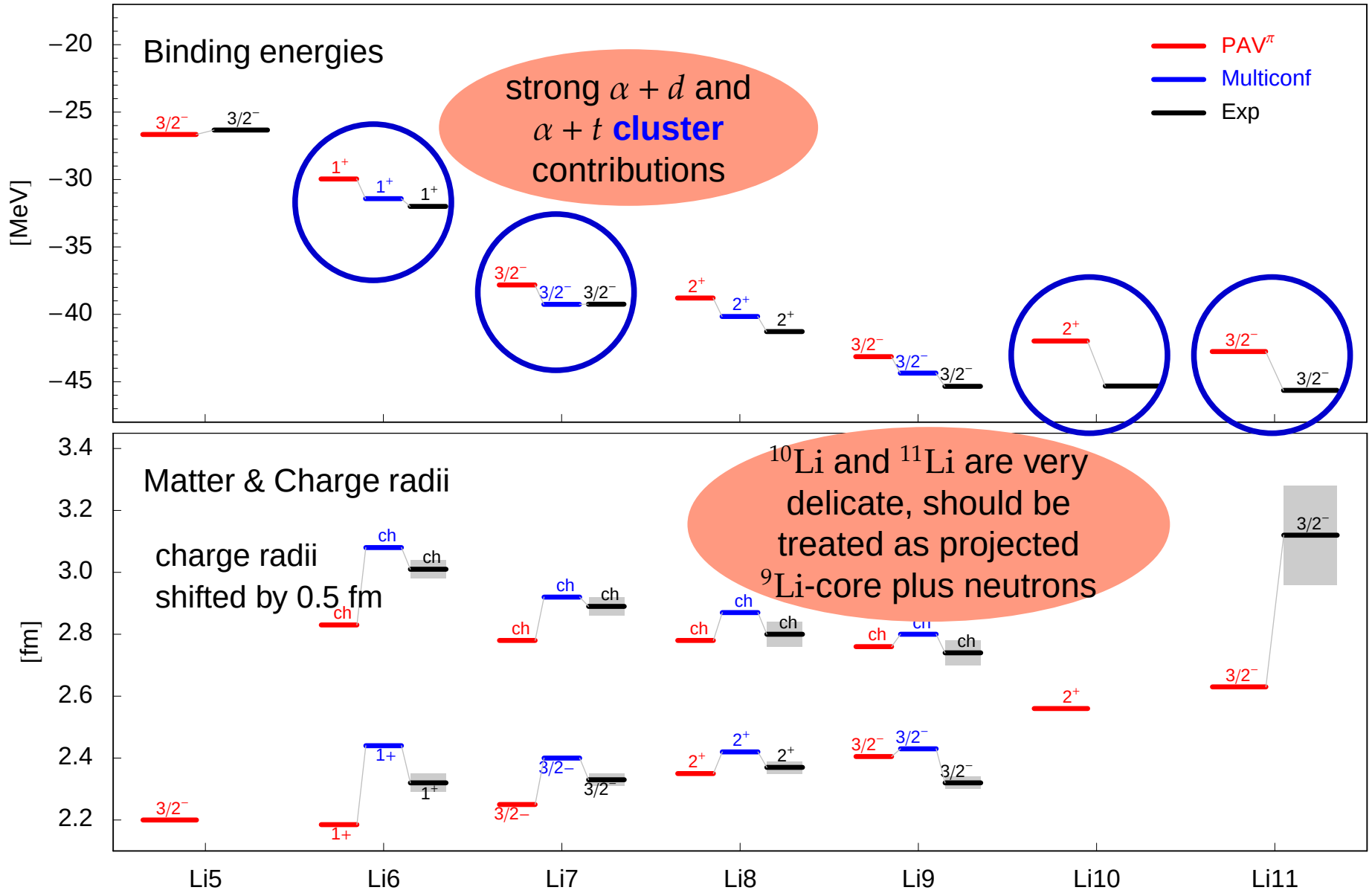
Lithium Isotopes





- intrinsic densities of V^{π} states

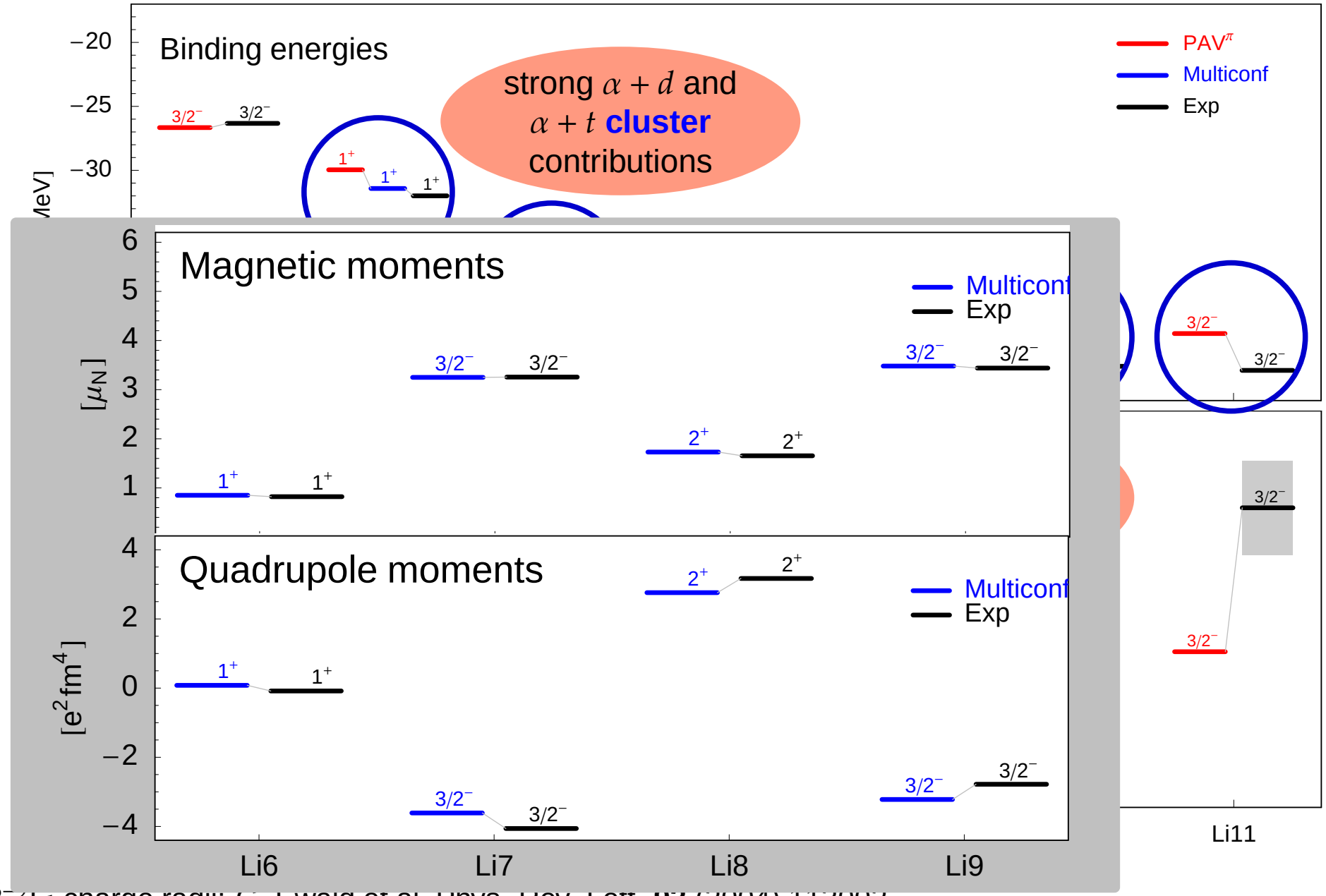
Lithium Isotopes



$^{6-9}$Li charge radii: G. Ewald et al, Phys. Rev. Lett. **93** (2004) 113002

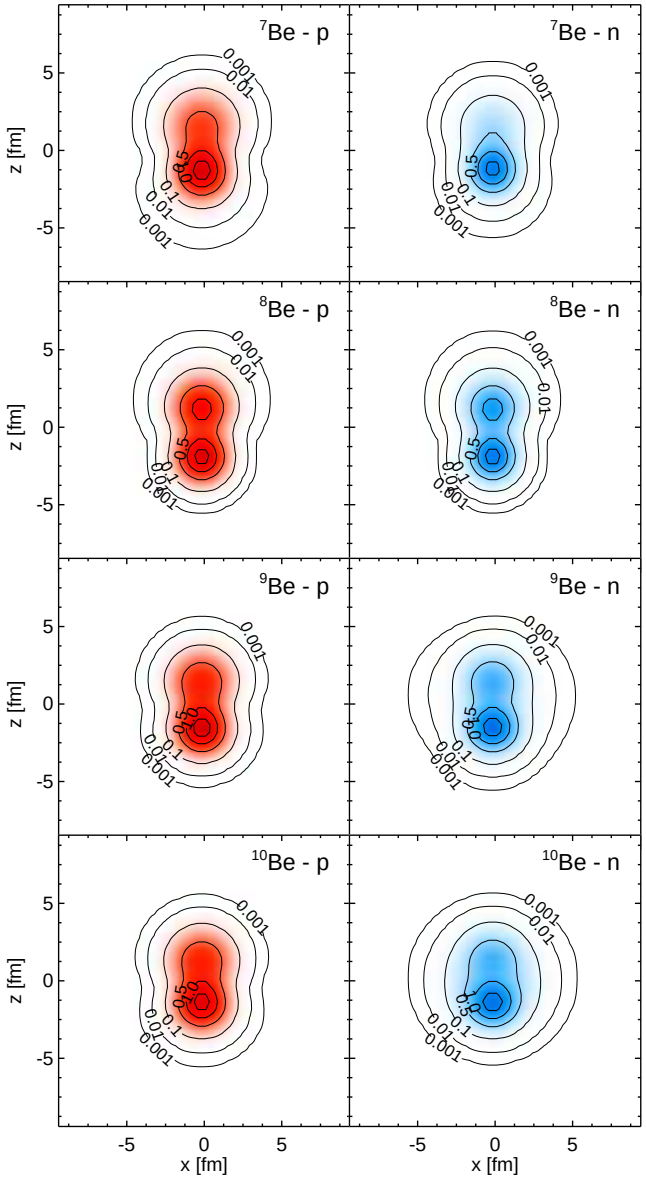
Lithium Isotopes

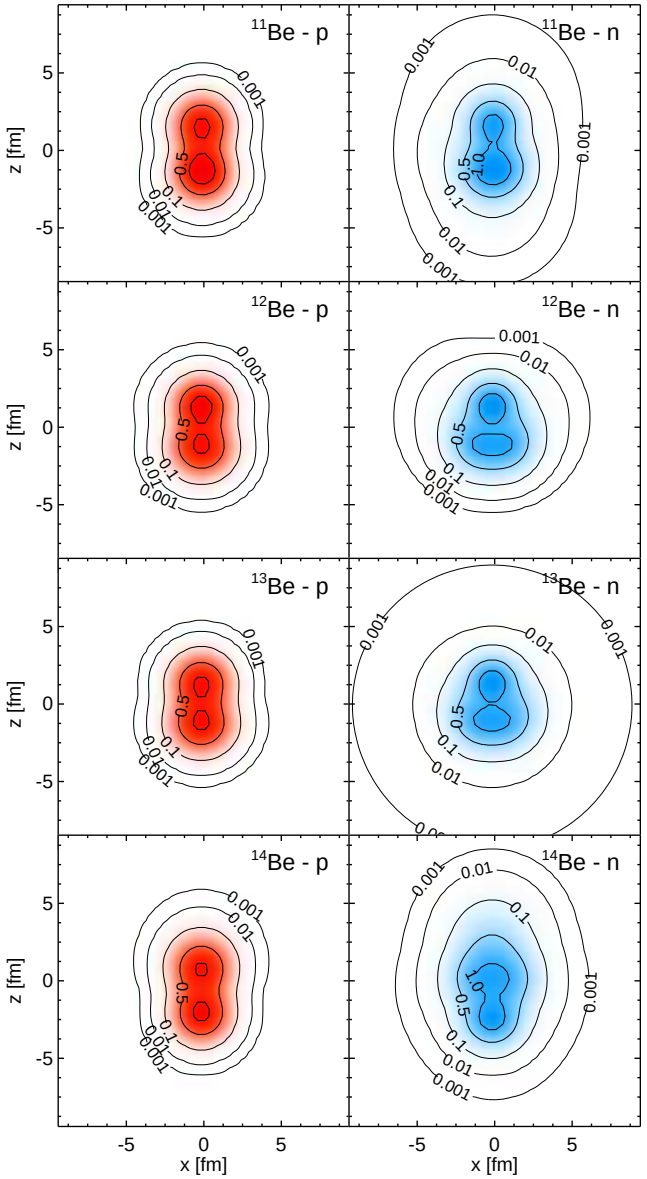
with cm-project



6–9Li charge radii: G. Ewald et al, Phys. Rev. Lett. **93** (2004) 113002

Beryllium Isotopes

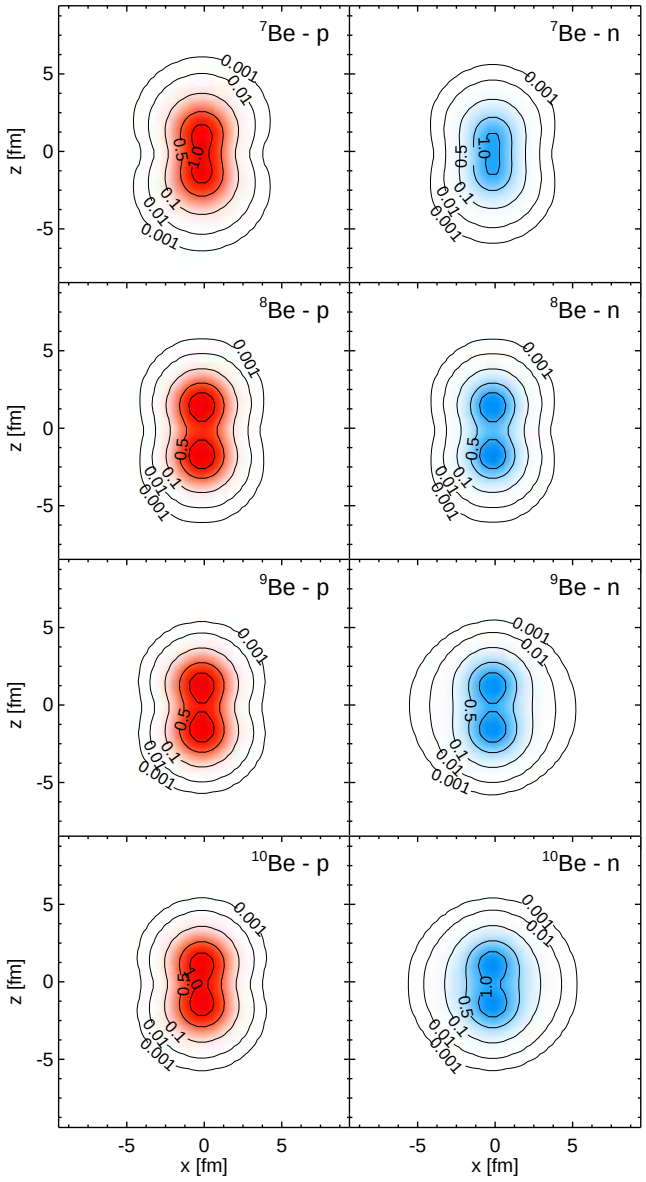


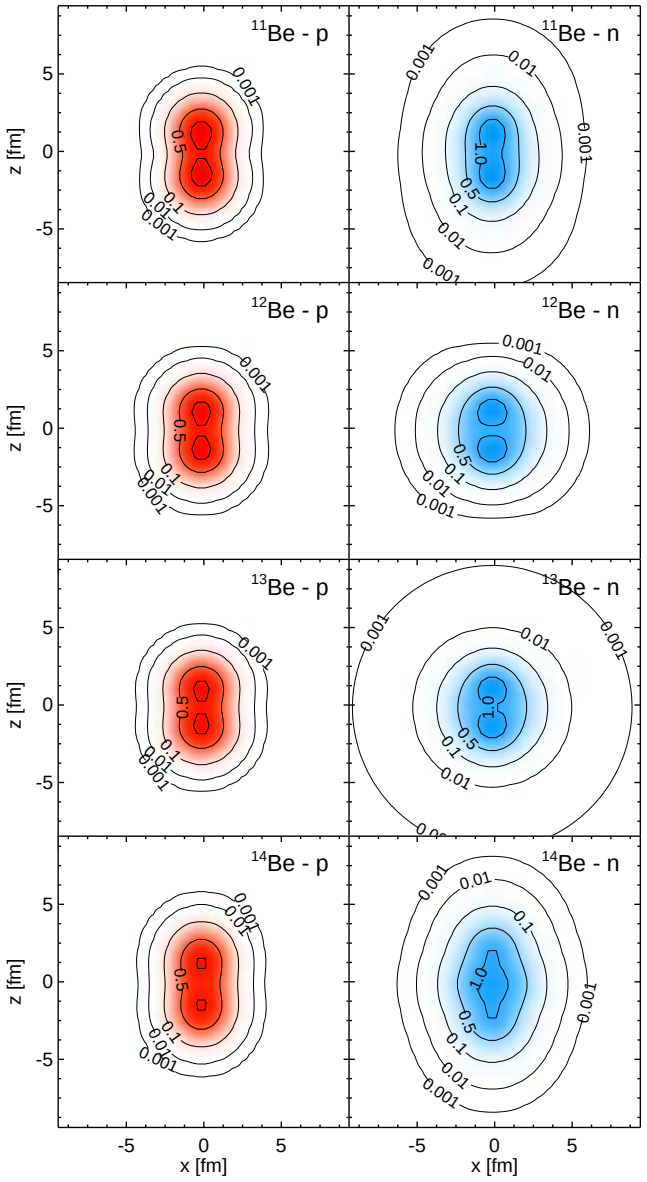


- intrinsic densities of V^{π} states

cluster structure evolves with addition of neutrons

Beryllium Isotopes

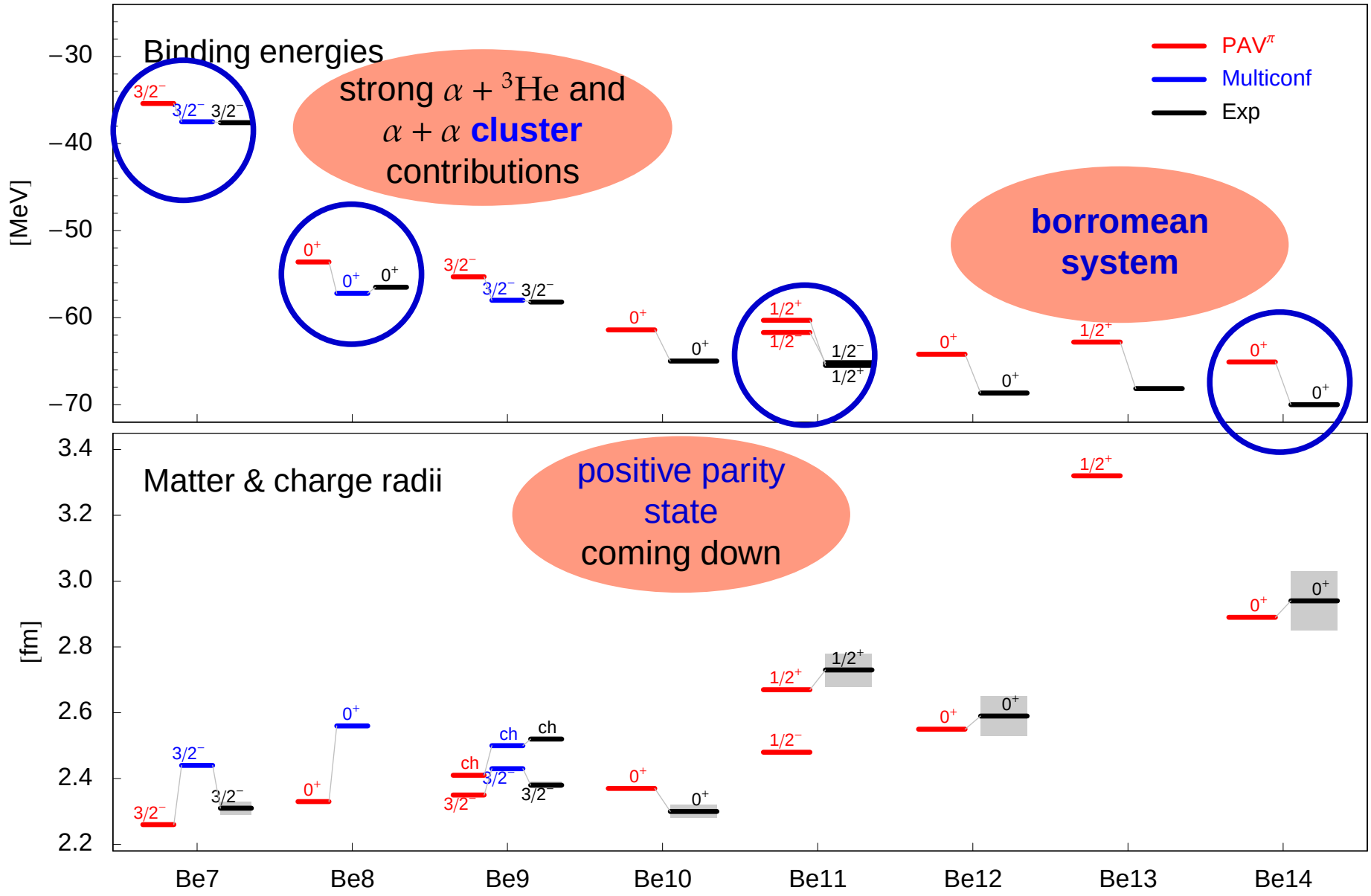




- intrinsic densities of parity projected V^{π} states

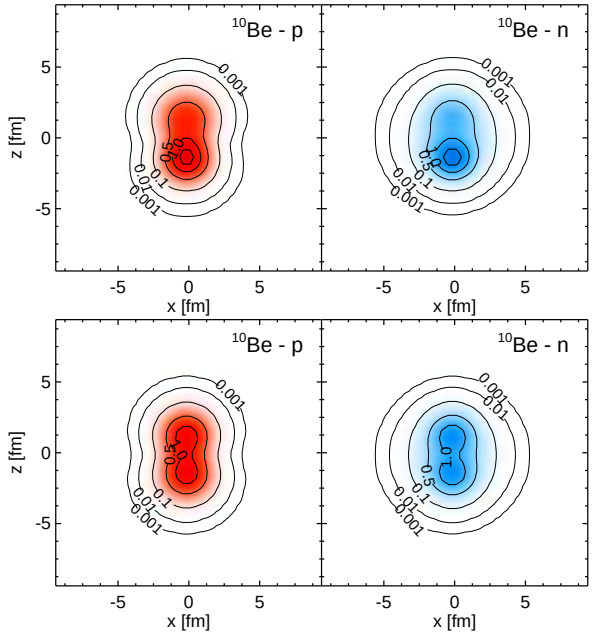
cluster structure evolves with addition of neutrons

Beryllium Isotopes

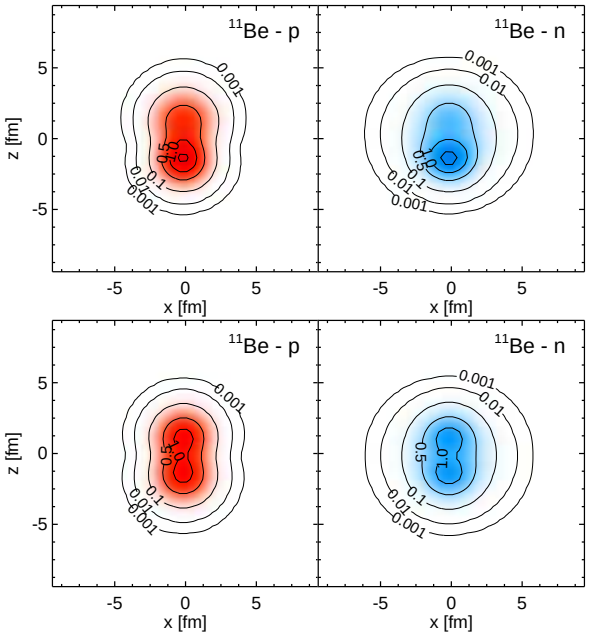


^{11}Be positive parity intruder

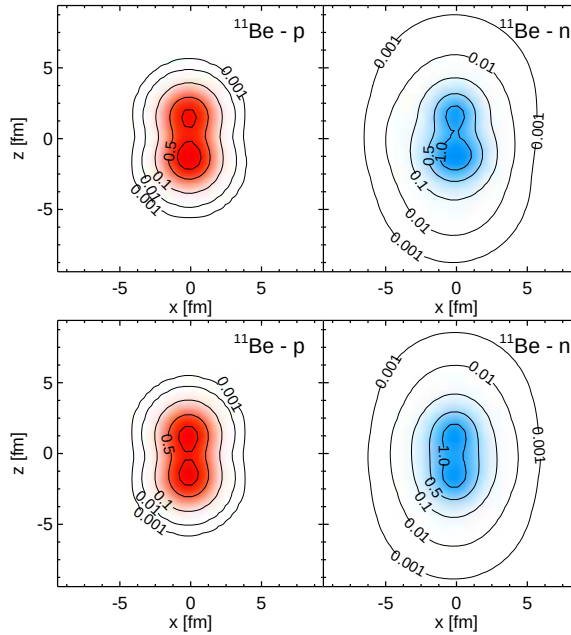
^{10}Be

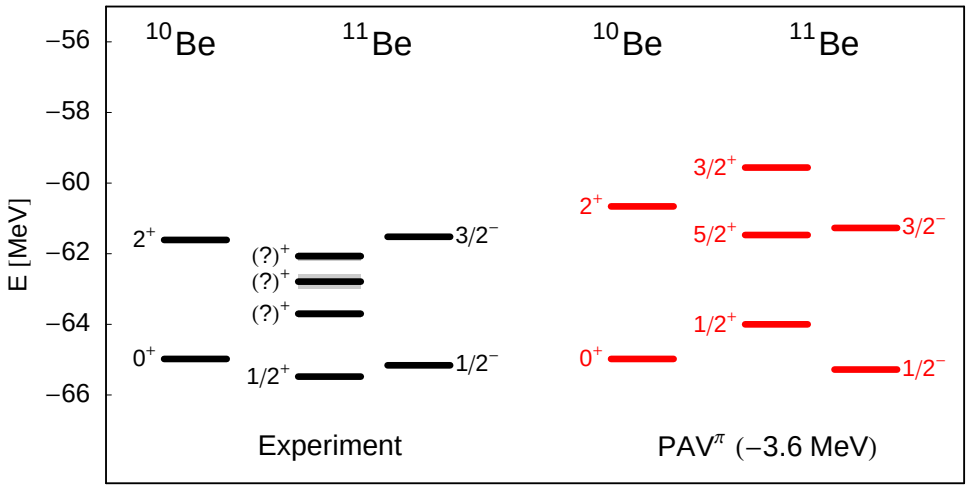


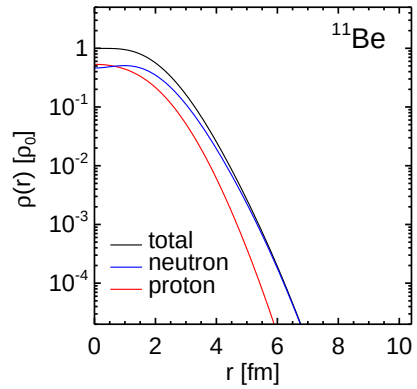
^{11}Be negative parity

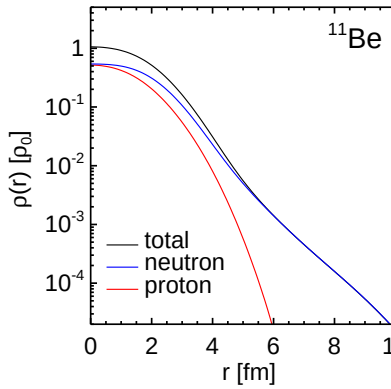


^{11}Be positive parity



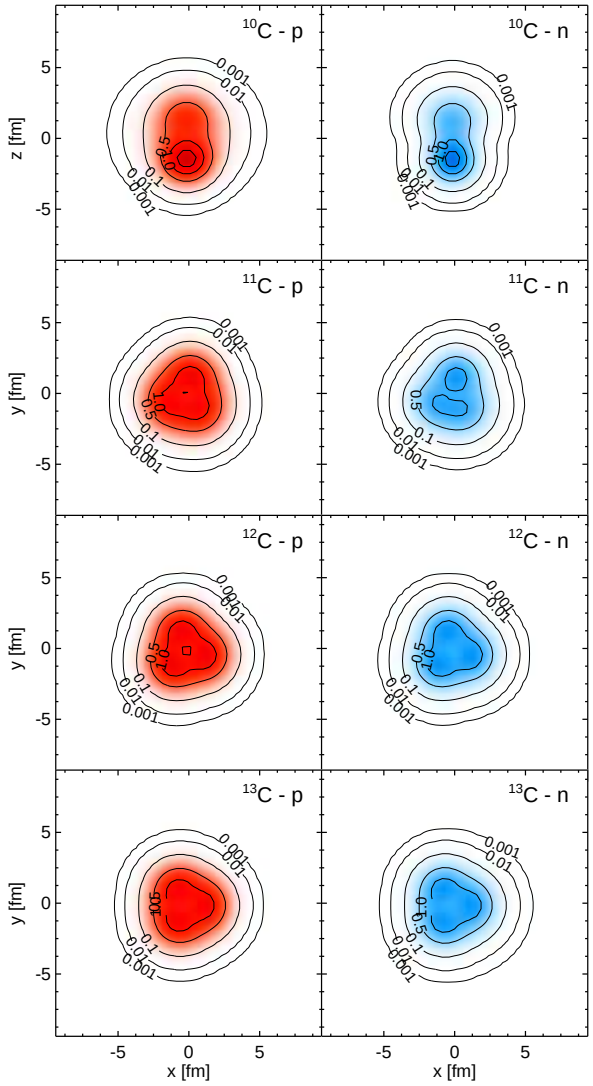


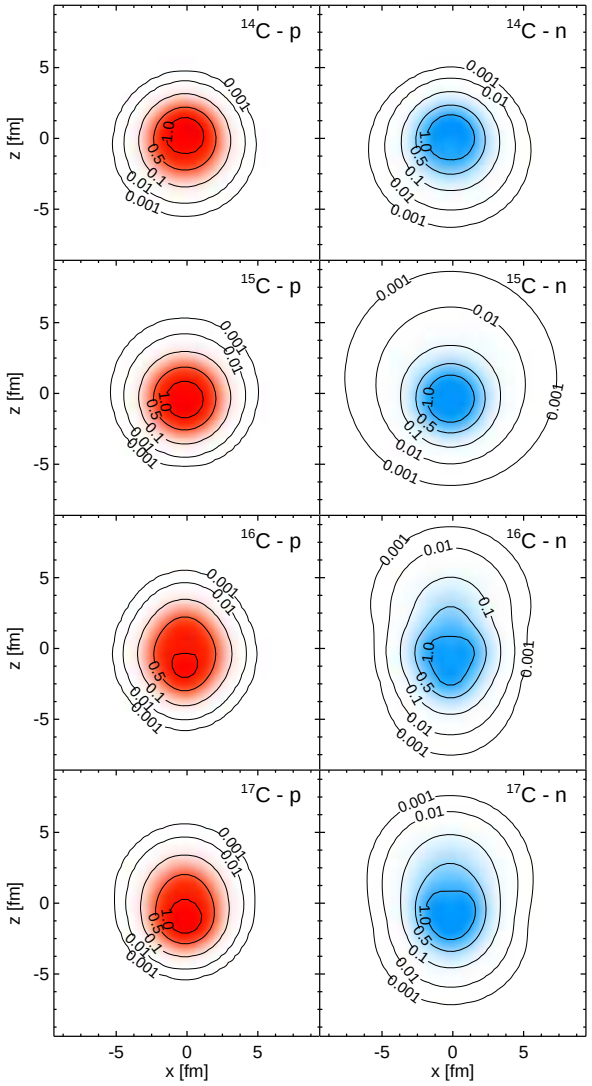


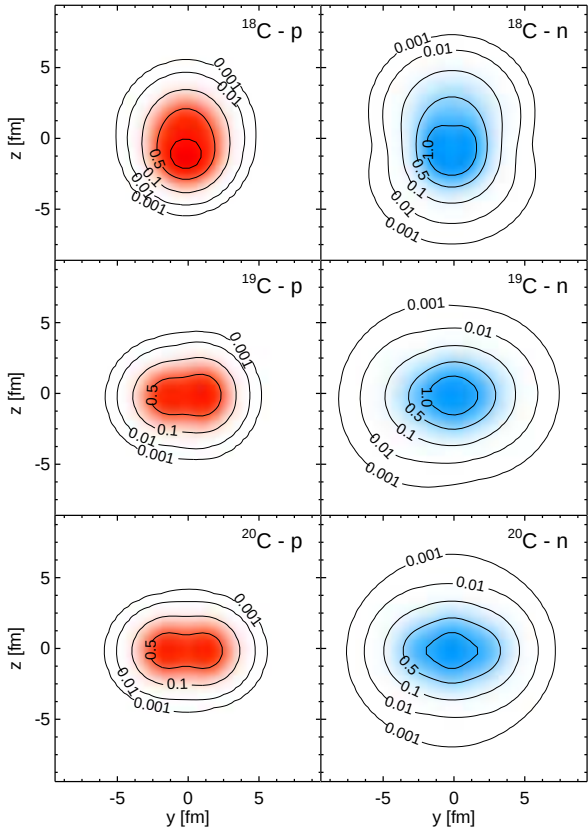


➨ $1/2^+$ state has a neutron halo

Carbon Isotopes

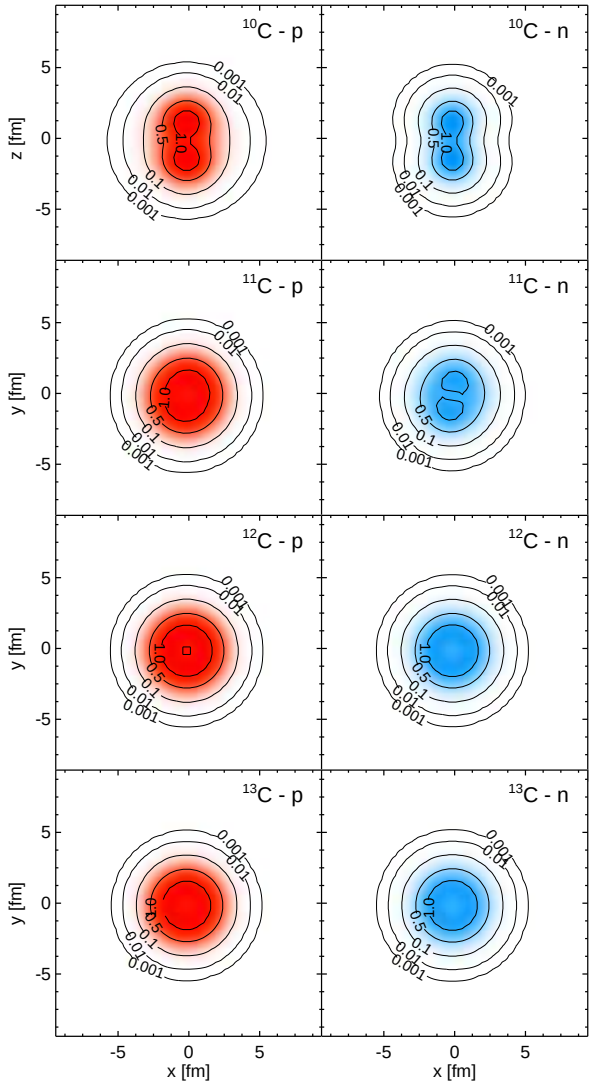


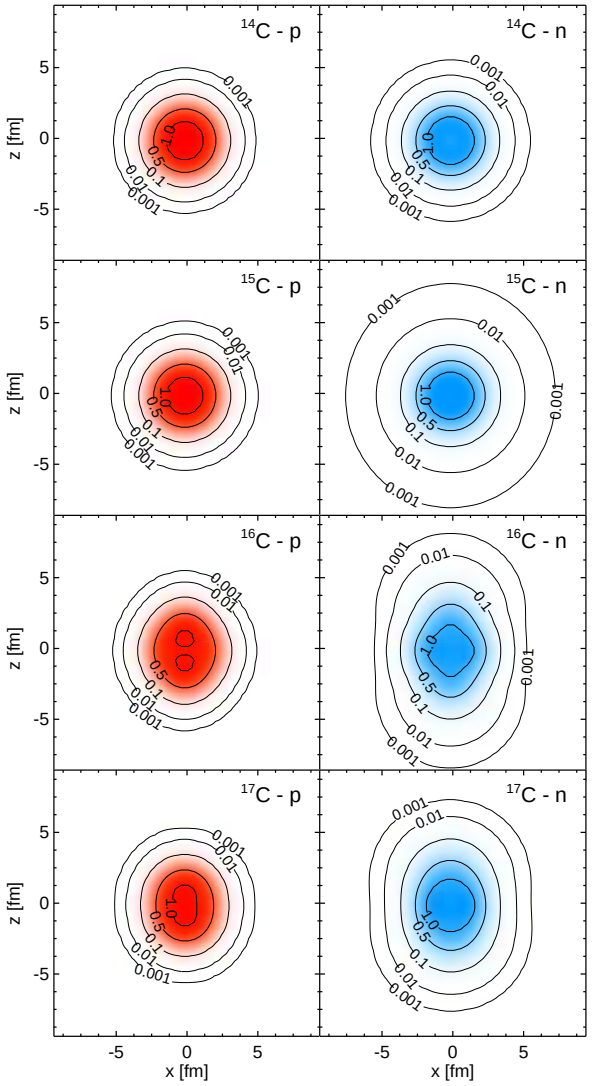


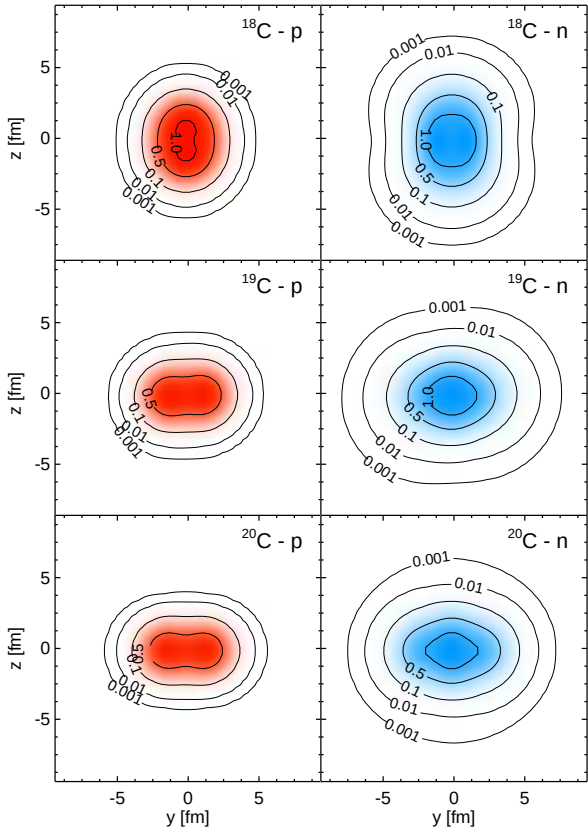


- intrinsic densities of V^{π} states

Carbon Isotopes

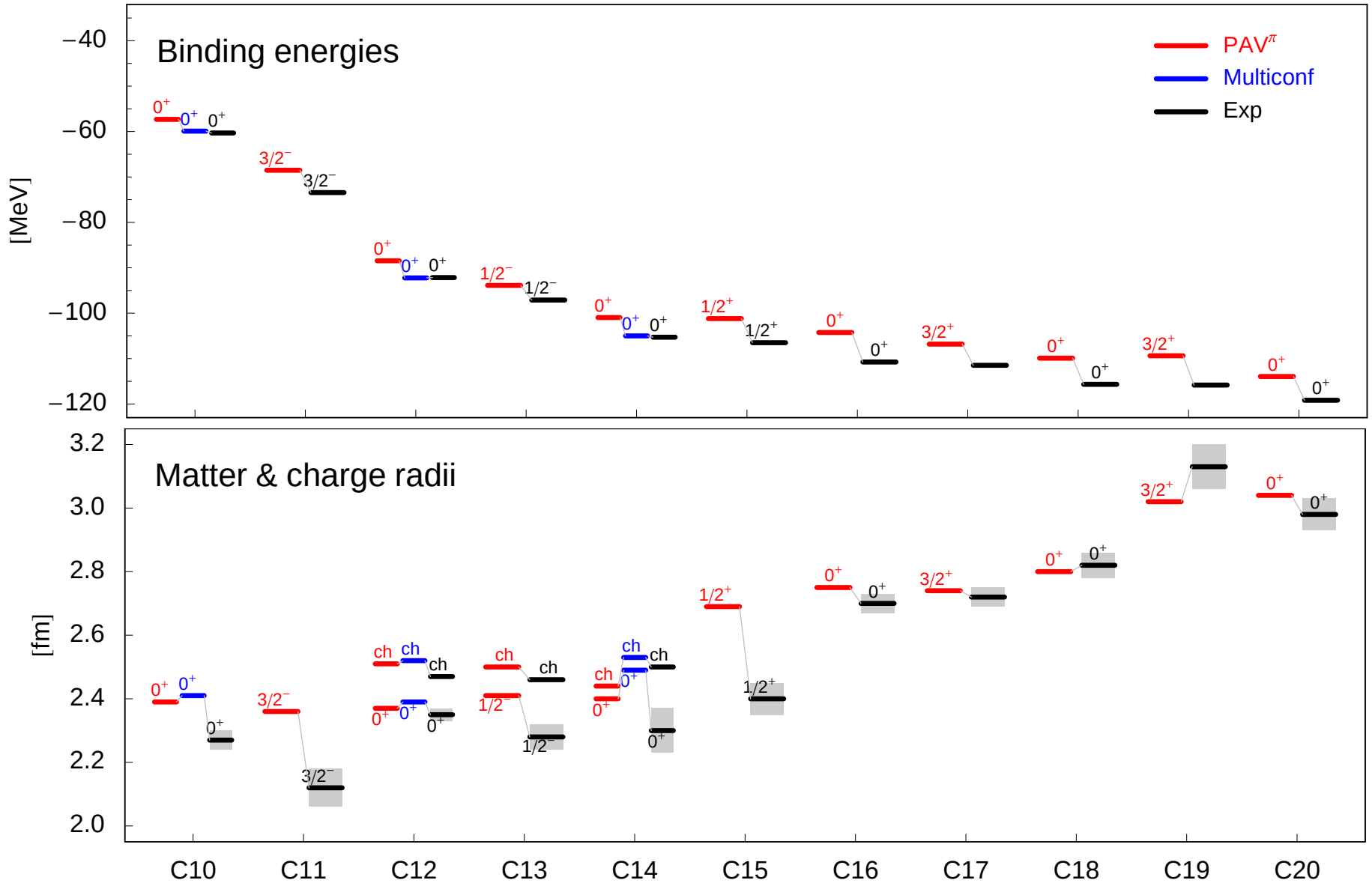






- intrinsic densities of parity projected V^{π} states

Carbon Isotopes



Hoyle State in ^{12}C

Astrophysical Motivation

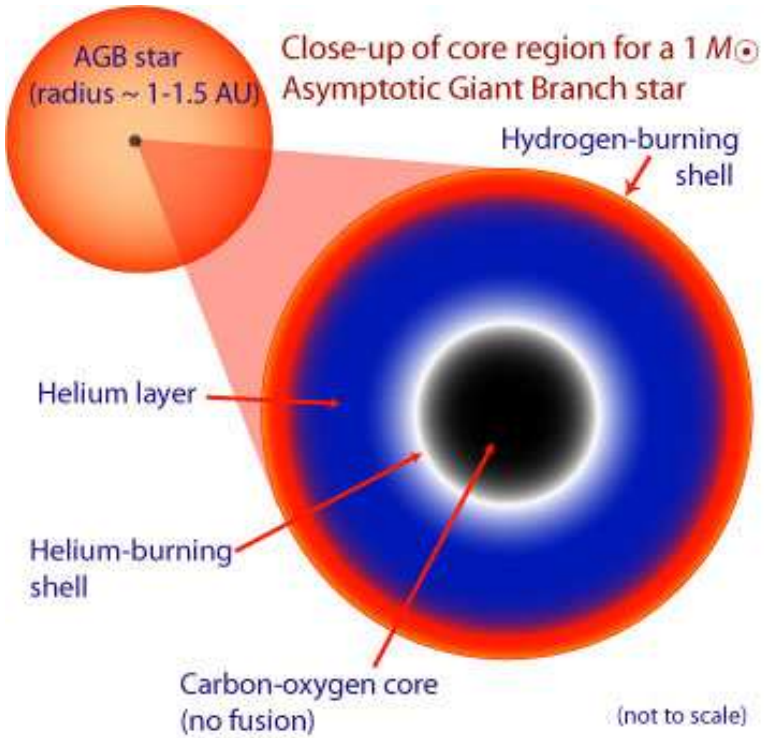
Nuclear Structure

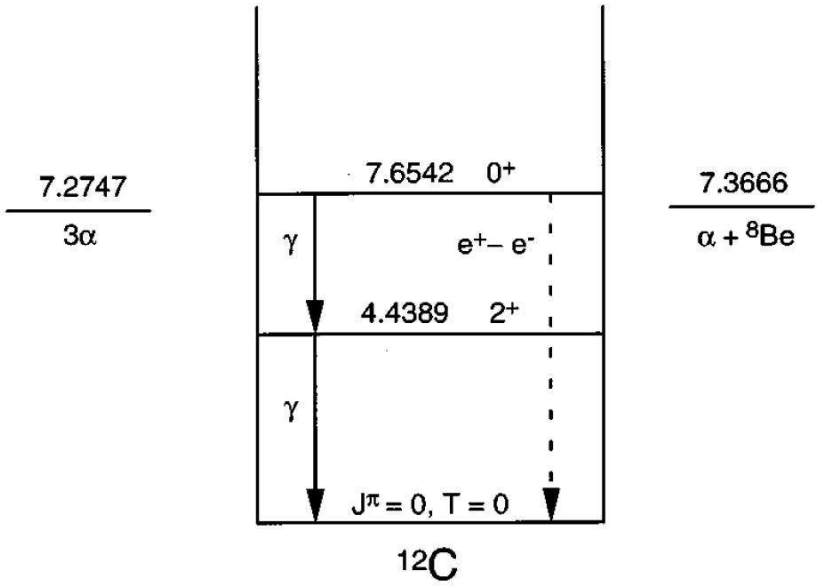
- **What is the structure of the Hoyle state ?**
- **higher lying 0^+ and 2^+ states**

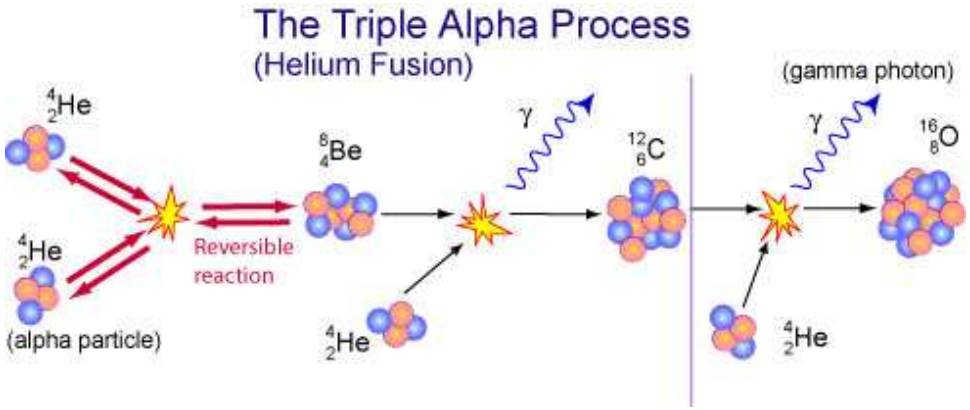
➨ **Compare to α-cluster model**

Phys. Rev. Lett. 98, 032501 (2007)

Triple α Reaction

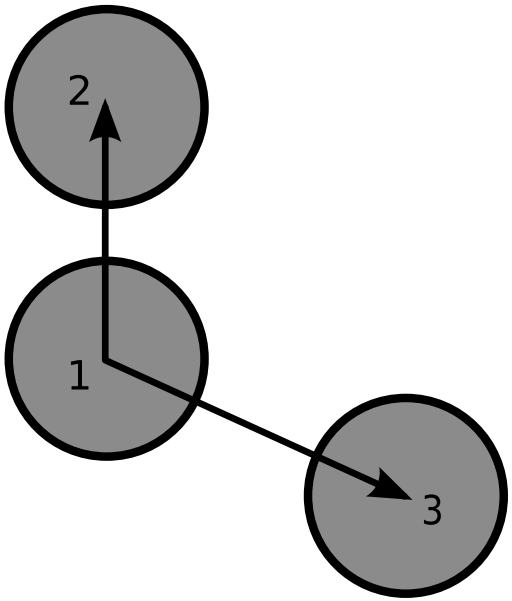






http://outreach.atnf.csiro.au/education/senior/astrophysics/stellarevolution_postmain.html

Microscopic α-Cluster Model



$$R_{12} = (2, 4, \ldots, 10)\ \text{fm}$$
$$R_{13} = (2, 4, \ldots, 10)\ \text{fm}$$
$$\cos(\vartheta) = (1.0, 0.8, \ldots, -1.0)$$

alltogether 165 configurations

Basis States

- describe Hoyle State as a system of 3 ^{4}He nuclei

$$\left| \Psi_{3\alpha}(\mathbf{R}_1, \mathbf{R}_2, \mathbf{R}_3); JMK\pi \right\rangle = P^J_{MK} P^\pi \mathcal{A} \left\{ \left| \psi_\alpha(\mathbf{R}_1) \right\rangle \otimes \left| \psi_\alpha(\mathbf{R}_2) \right\rangle \otimes \left| \psi_\alpha(\mathbf{R}_3) \right\rangle \right\}$$

Volkov Interaction

- simple central interaction
- parameters adjusted to reproduce α binding energy and radius, $\alpha - \alpha$ scattering data and Hoyle State ground state energy

✘ only reasonable for ^{4}He, ^{8}Be and ^{12}C nuclei

Kamimura, Nuc. Phys. **A351**, 456 (1981)

FMD

Basis States

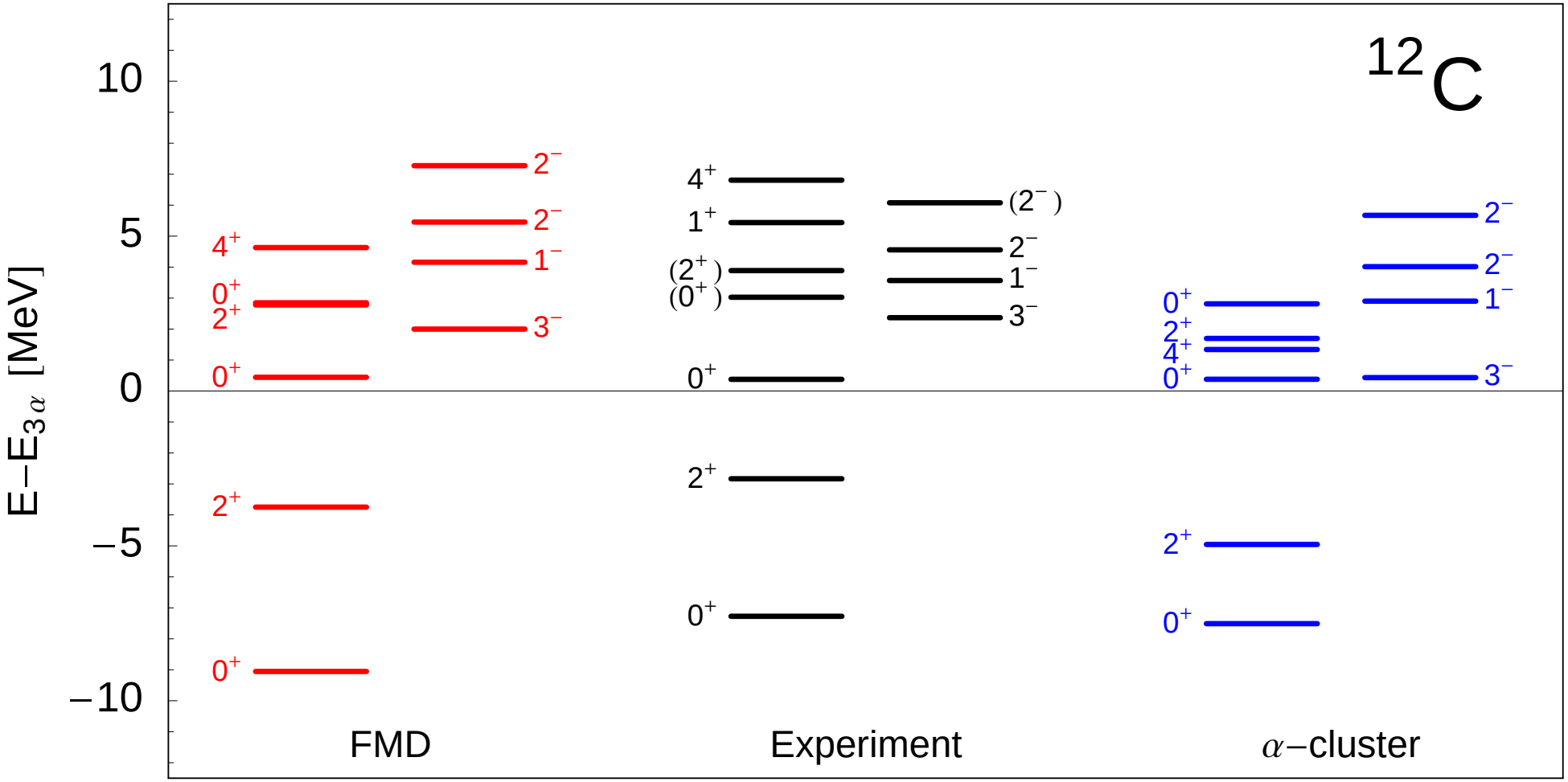
- 20 FMD states obtained in Variation after Projection on 0^+ and 2^+ with constraints on the radius
- 42 FMD states obtained in Variation after Projection on parity with constraints on radius and quadrupole deformation
- 165 α-cluster configurations

➨ projected on angular momentum and linear momentum

Interaction

- FMD interaction based on UCOM interaction with phenomenological two-body correction term fitted to energies and radii of doubly-magic nuclei
- not explicitly tuned for α-α scattering or Hoyle State properties

Hoyle State
Comparison



Hoyle State
Comparison

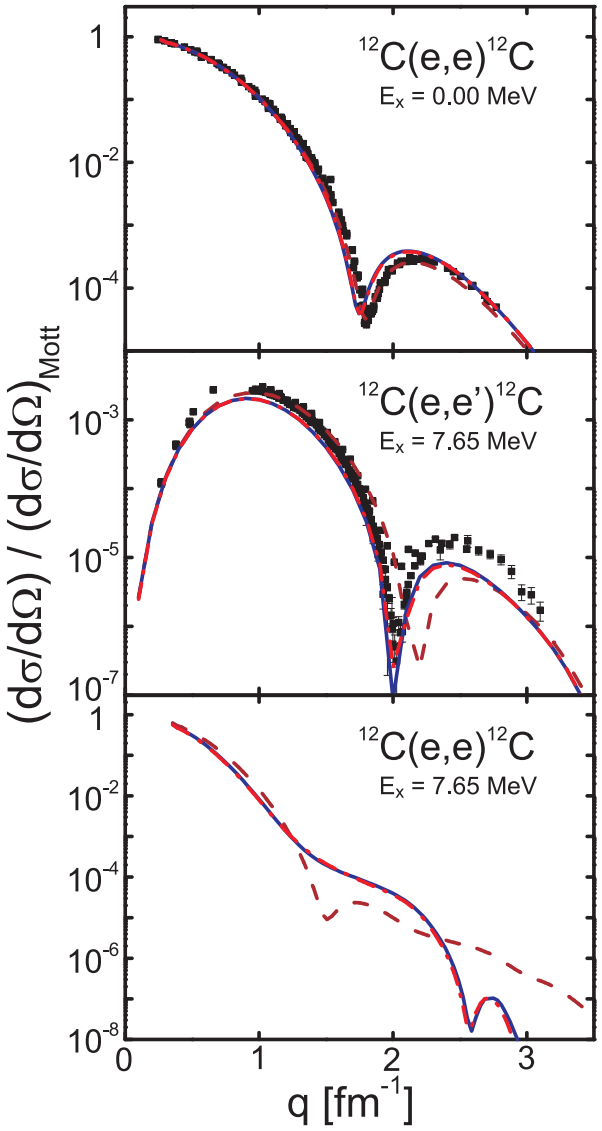
	Exp[1]	Exp[2]	Exp[3]	FMD	α-cluster	'BEC'[4]
$E(0_1^+)$	-92.16			-92.64	-89.56	-89.52
$E^*(2_1^+)$	4.44			5.31	2.56	2.81
$E(3\alpha)$	-84.89			-83.59	-82.05	-82.05
$E(0_2^+) - E(3\alpha)$	0.38			0.43	0.38	0.26
$E(0_3^+) - E(3\alpha)$	(3.0)	2.7(3)	3.96(5)	2.84	2.81	
$E(2_2^+) - E(3\alpha)$	(3.89)	2.6(3)	6.63(3)	2.77	1.70	
$r_{\text{charge}}(0_1^+)$	2.47(2)			2.53	2.54	
$r(0_1^+)$				2.39	2.40	2.40
$r(0_2^+)$				3.38	3.71	3.83
$r(0_3^+)$				4.62	4.75	
$r(2_1^+)$				2.50	2.37	2.38
$r(2_2^+)$				4.43	4.02	
$M(E0, 0_1^+ \to 0_2^+)$	5.4(2)			6.53	6.52	6.45
$B(E2, 2_1^+ \to 0_1^+)$	7.6(4)			8.69	9.16	
$B(E2, 2_1^+ \to 0_2^+)$	2.6(4)			3.83	0.84	

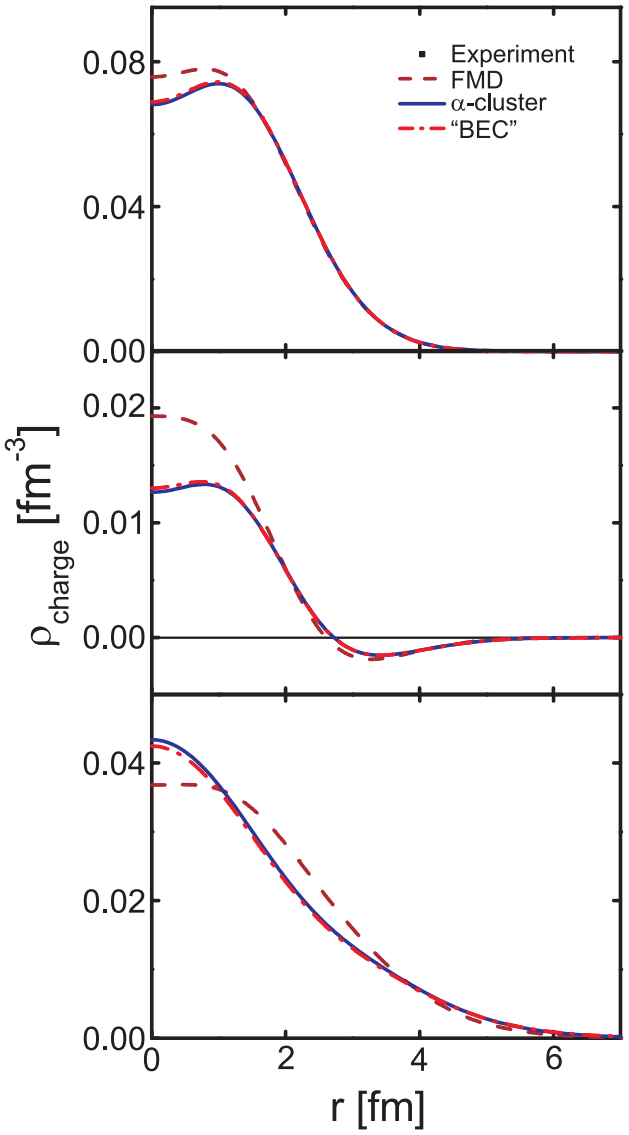
experimental situa
for 0_3^+ and 2_2^+ sta
still unsettled

2_2^+ resonance a
1.8 MeV abov
treshold included
NACRE compilat

[1] Ajzenberg-Selove, Nuc. Phys. **A506**, 1 (1990)
[2] Itoh et al., Nuc. Phys. **A738**, 268 (2004)
[3] Fynbo et al., Nature **433**, 137 (2005). Diget et al., Nuc. Phys. **A738**, 760 (2005)
[4] Funaki et al., Phys. Rev. C **67**, 051306(R) (2003)

Form factors and Densities





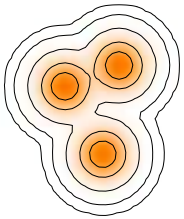
- compare with electron scattering data in Distorted Wave Born Approximation
- elastic form factor described very well by FMD
- transition form factor in first maximum better described by FMD, position of minimum and second maximum better described by cluster model

use intrinsic density

$$\rho(\mathbf{x}) = \sum_{k=1}^{A} \left\langle \Psi \left| \delta(\mathbf{x}_k - \mathbf{X} - \mathbf{x}) \right| \right.$$

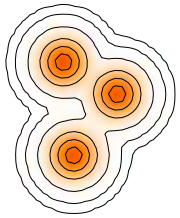
Important Configurations

- Calculate the overlap with FMD basis states to find the most important contributions to the Hoyle state



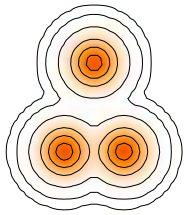
$\left|\left\langle \cdot \mid 0_1^+ \right\rangle\right| = 0.30$

$\left|\left\langle \cdot \mid 0_2^+ \right\rangle\right| = 0.72$



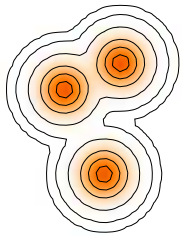
$\left|\left\langle \cdot \mid 0_1^+ \right\rangle\right| = 0.25$

$\left|\left\langle \cdot \mid 0_2^+ \right\rangle\right| = 0.71$



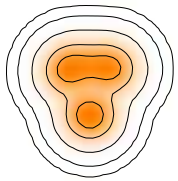
$\left|\left\langle \cdot \mid 0_1^+ \right\rangle\right| = 0.15$

$\left|\left\langle \cdot \mid 0_2^+ \right\rangle\right| = 0.61$



$\left|\left\langle \cdot \mid 0_1^+ \right\rangle\right| = 0.08$

$\left|\left\langle \cdot \mid 0_2^+ \right\rangle\right| = 0.61$



$\left|\left\langle \cdot \mid 0_1^+ \right\rangle\right| = 0.94$

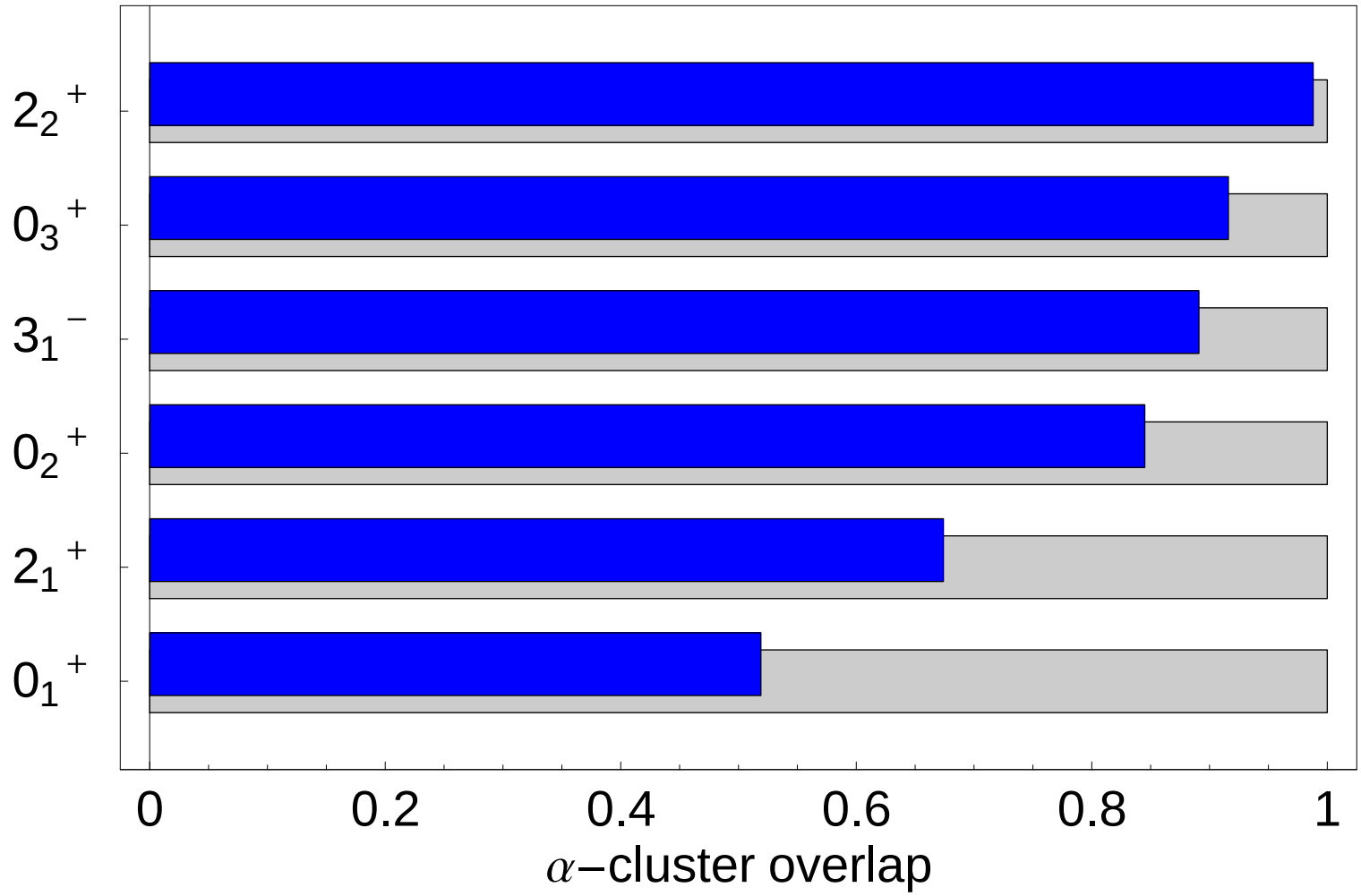
$\left|\left\langle \cdot \mid 0_2^+ \right\rangle\right| = 0.04$

FMD basis states are not orthogonal!

Overlap with Cluster Model Space

Calculate the overlap of FMD wave functions with pure α-cluster model space

$$N_\alpha = \left\langle \Psi \left| P_{3\alpha} \right| \Psi \right\rangle$$

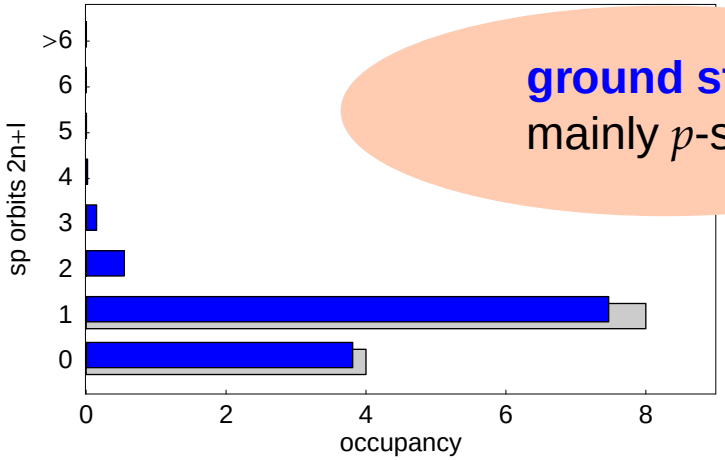


Harmonic Oscillator Occupation Numbers

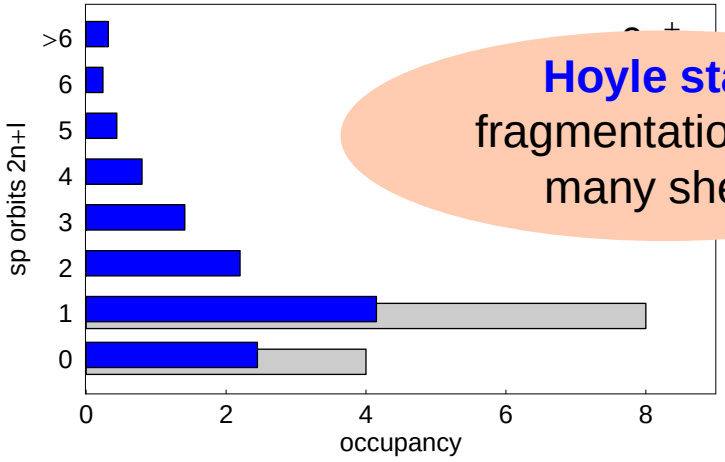
calculate one-body density in harmonic oscillator basis

$$n_{nlj} = \sum_m \left\langle \Psi \left| a^\dagger_{nljm} a_{nljm} \right| \Psi \right\rangle$$

FMD

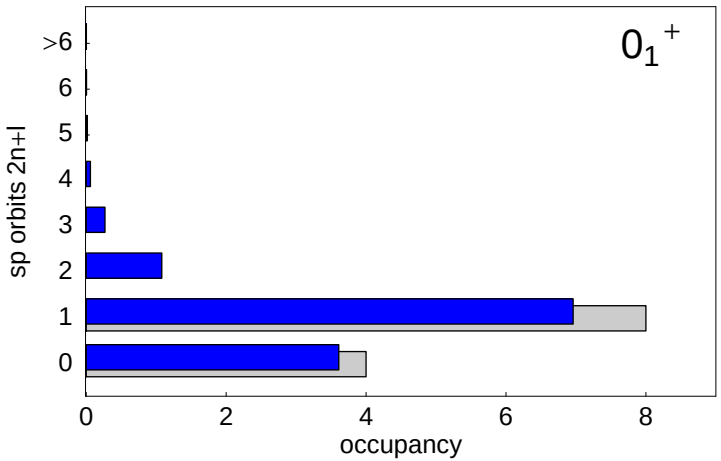


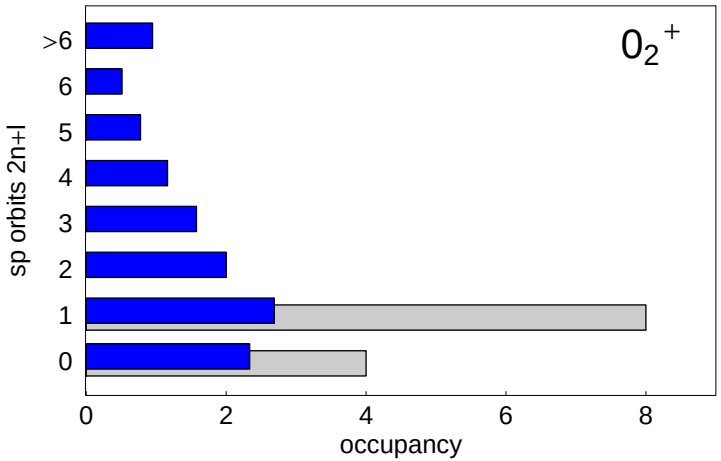
ground state
mainly p-shell



Hoyle state
fragmentation over many shells

α-cluster



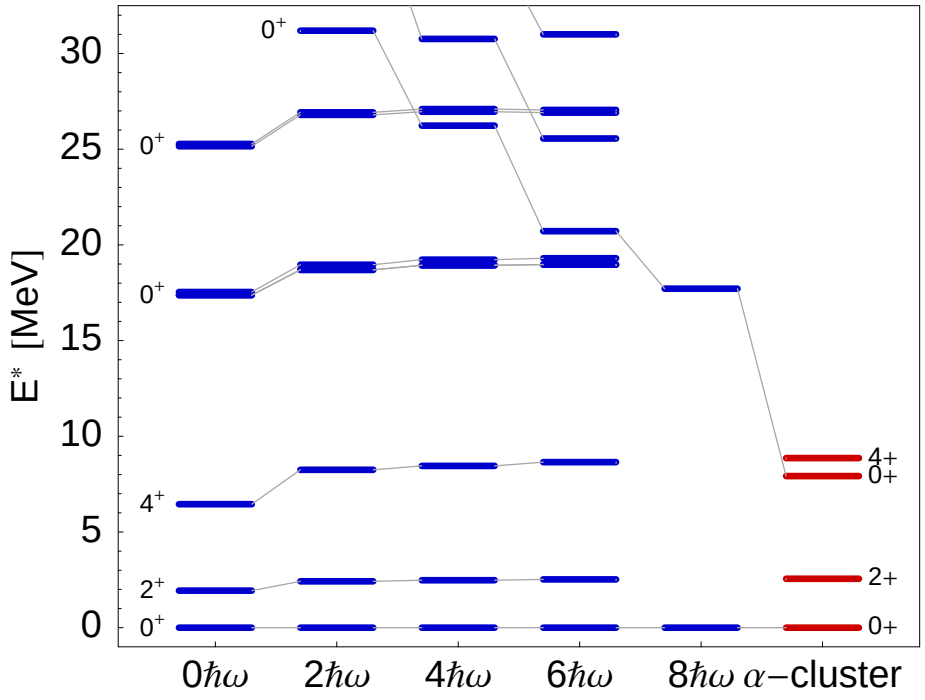


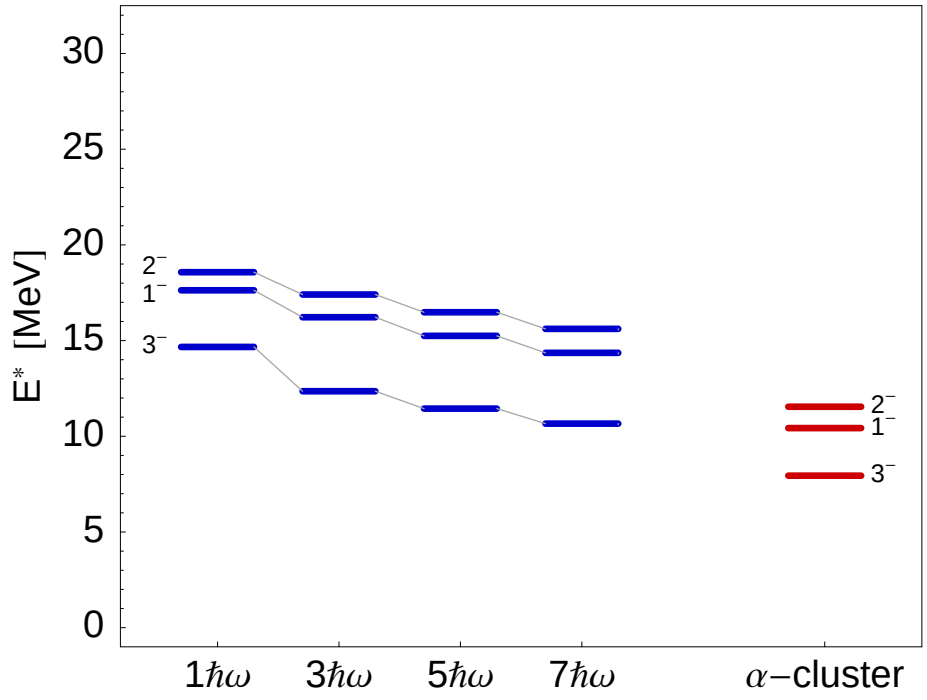
α-cluster states in the No-Core Shell Model

- compare spectra in NCSM and α-cluster model using the Volkov interaction
- bare interaction used in NCSM calculations

➨ good agreement for ground state band (0^+_1, 2^+_1, 4^+_1)

➨ very slow convergence for cluster states





Fusion Cross Sections for Oxygen Isotopes

Astrophysical Motivation

Nuclear Structure

- Nucleus-Nucleus Interaction
- Map onto two-body problem
- Fusion Cross-Section

nucl-th/0703030

Pynconuclear Reactions

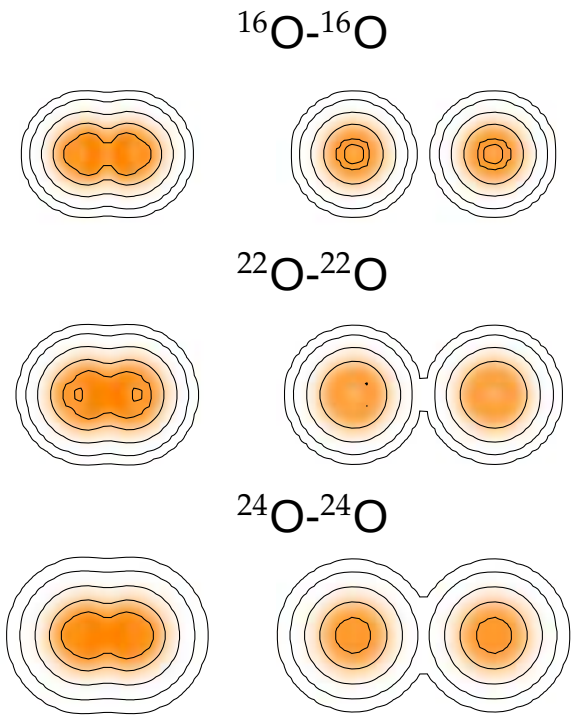
- **pycnonuclear reactions** between neutron-rich isotopes are of importance for nucleosynthesis at high density in the deeper layers of accreting white dwarfs and neutron star envelopes
- at these high densities (*pyknos* means compact, dense) the nuclei are positioned on a grid and the fusion cross section is enhanced because of electron screening effects

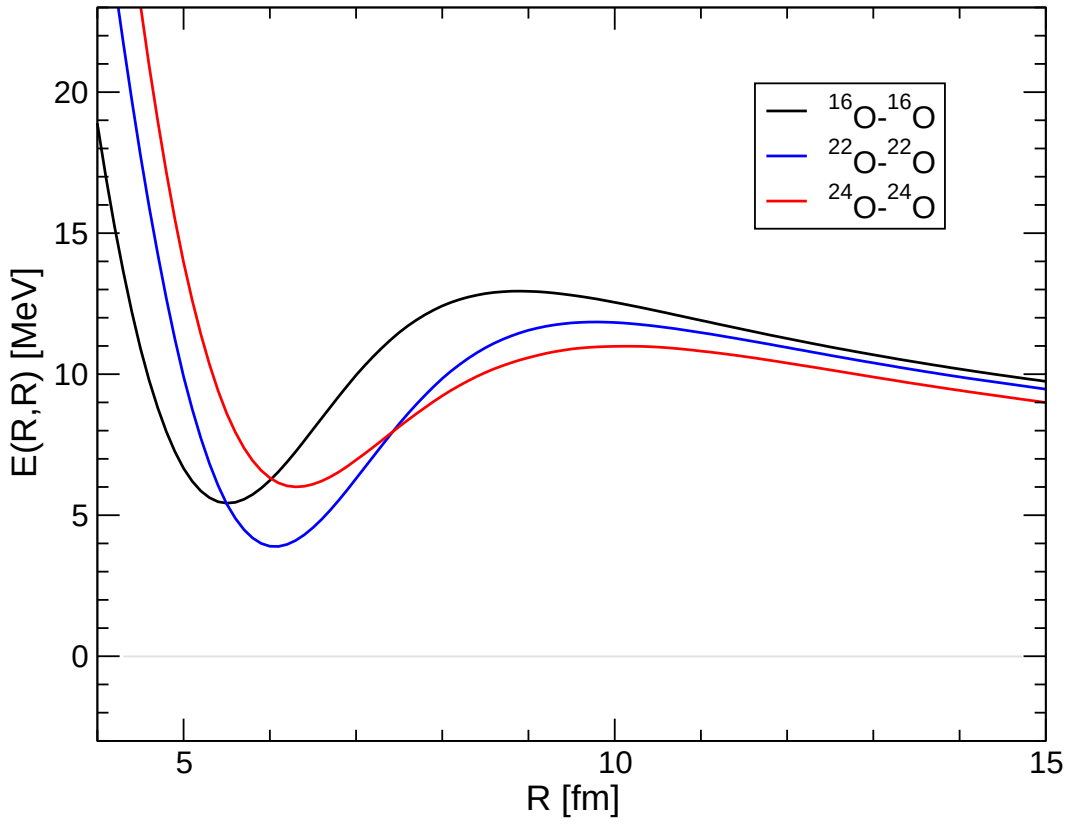
➨ FMD calculations provide an independent test for the cross-sections calculated with a Folding model

Michael Wiescher, Leandro R. Gasques

Nucleus-Nucleus Energy Surface

- calculate FMD ground states
- use GCM wave function $\left|\Psi(\mathbf{R})\right\rangle = \mathcal{A}\left\{\left|{}^{x}\mathrm{O};\tfrac{1}{2}\mathbf{R}\right\rangle\left|{}^{x}\mathrm{O};-\tfrac{1}{2}\mathbf{R}\right\rangle\right\}$
- calculate GCM energy surface $E^{L}(R) = \dfrac{\left\langle\Psi(R\mathbf{e_z})\right|(H-T_{\mathrm{cm}})P^{L}_{00}\left|\Psi(R\mathbf{e_z})\right\rangle}{\left\langle\Psi(R\mathbf{e_z})\right|P^{L}_{00}\left|\Psi(R\mathbf{e_z})\right\rangle}$





Map onto two-body system

- relative position of two clusters is smeared out in Slater determinant
- transform into RGM basis states
  $\phi(\xi)$ is internal wave function of oxygen nucleus

$$\left\langle \boldsymbol{\rho}, \xi_1, \xi_2 \middle| \Phi(\mathbf{r}) \right\rangle = \mathcal{A}\left\{\delta(\mathbf{r}-\boldsymbol{\rho})\,\phi(\xi_1)\,\phi(\xi_2)\right\}$$

- if the same Gaussian width parameter a is used for all single-particle states is used, we can express the GCM state with the RGM basis states

$$\left|\Psi(\mathbf{R})\right\rangle = \int d^3r\, \Gamma(\mathbf{R}-\mathbf{r}) \left|\Phi(\mathbf{r})\right\rangle \otimes \left|\Phi_{\text{cm}}\right\rangle$$

with

$$\Gamma(\mathbf{R}-\mathbf{r}) = \left(\frac{\mu}{\pi a}\right)^{3/4} \exp\left(-\mu\frac{(\mathbf{R}-\mathbf{r})^2}{2a}\right), \quad \mu = \frac{A_1 A_2}{A_1+A_2}$$

and the center-of-mass wave function

$$\left\langle \mathbf{X} \middle| \Phi_{\text{cm}} \right\rangle = \left(\frac{A_1+A_2}{\pi a}\right)^{3/4} \exp\left(-(A_1+A_2)\frac{\mathbf{X}^2}{2a}\right)$$

Map onto two-body system

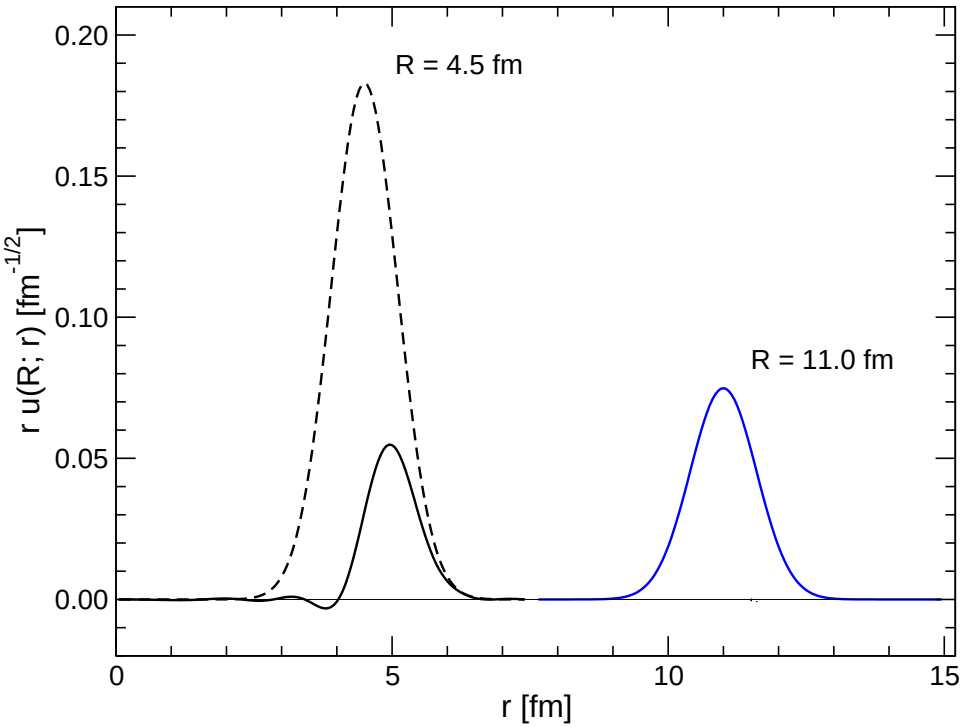
The RGM norm kernel is diagonal asymptotically

$$\left\langle \Phi(\mathbf{r}) \middle| \Phi(\mathbf{r}') \right\rangle = n(\mathbf{r},\mathbf{r}') \overset{r,r'\to\infty}{=} [1+\delta_{ab}(-1)^L]\delta(\mathbf{r}-\mathbf{r}')$$

- in order to map onto two-body system transform basis states diagonalize RGM norm kernel

$$\left|\tilde{\Phi}(\mathbf{r})\right\rangle = \int d^3r' \left|\Phi(\mathbf{r}')\right\rangle n^{-1/2}(\mathbf{r}',\mathbf{r}), \qquad \left\langle \tilde{\Phi}(\mathbf{r}) \middle| \tilde{\Phi}(\mathbf{r}') \right\rangle = [1+\delta_{ab}(-1)^L]\delta(\mathbf{r}-\mathbf{r}')$$

➨ this procedure takes care of the **Pauli forbidden** states



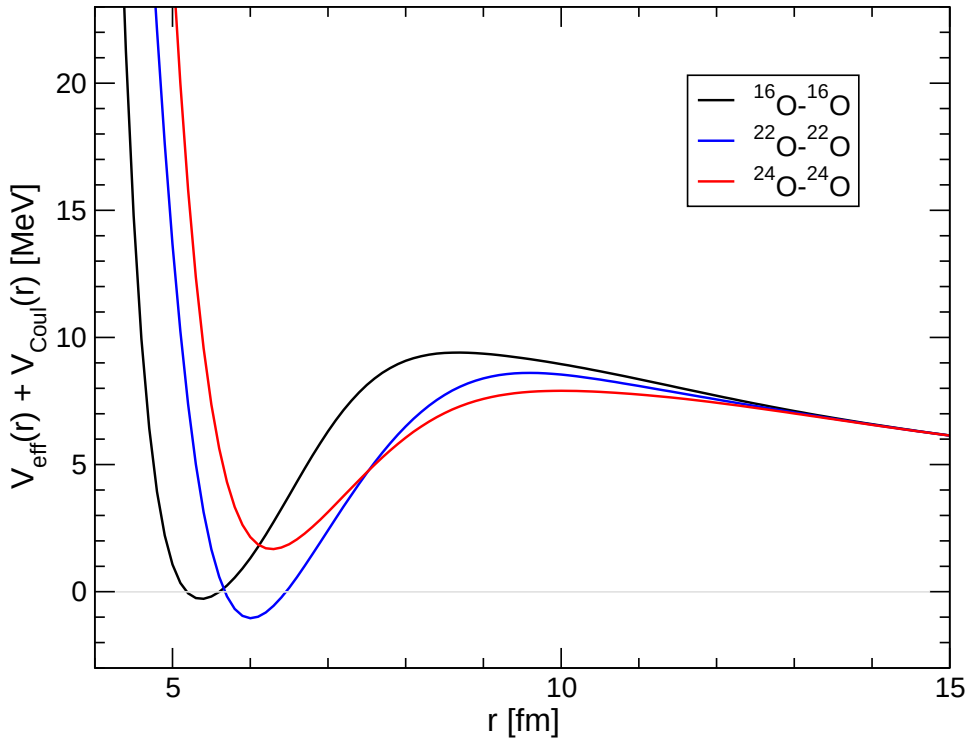
Nucleus-Nucleus Potential

- Now fit a local effective potential to the GCM matrix elements

$$\left\langle \Psi(R_i \mathbf{e_z}) \left| P^L_{00} \right| \Psi(R_i \mathbf{e_z}) \right\rangle \stackrel{!}{=} \int dr\, r^2\, \tilde{\Gamma}_L(R_i; r) \tilde{\Gamma}_L(R_i; r)$$

with

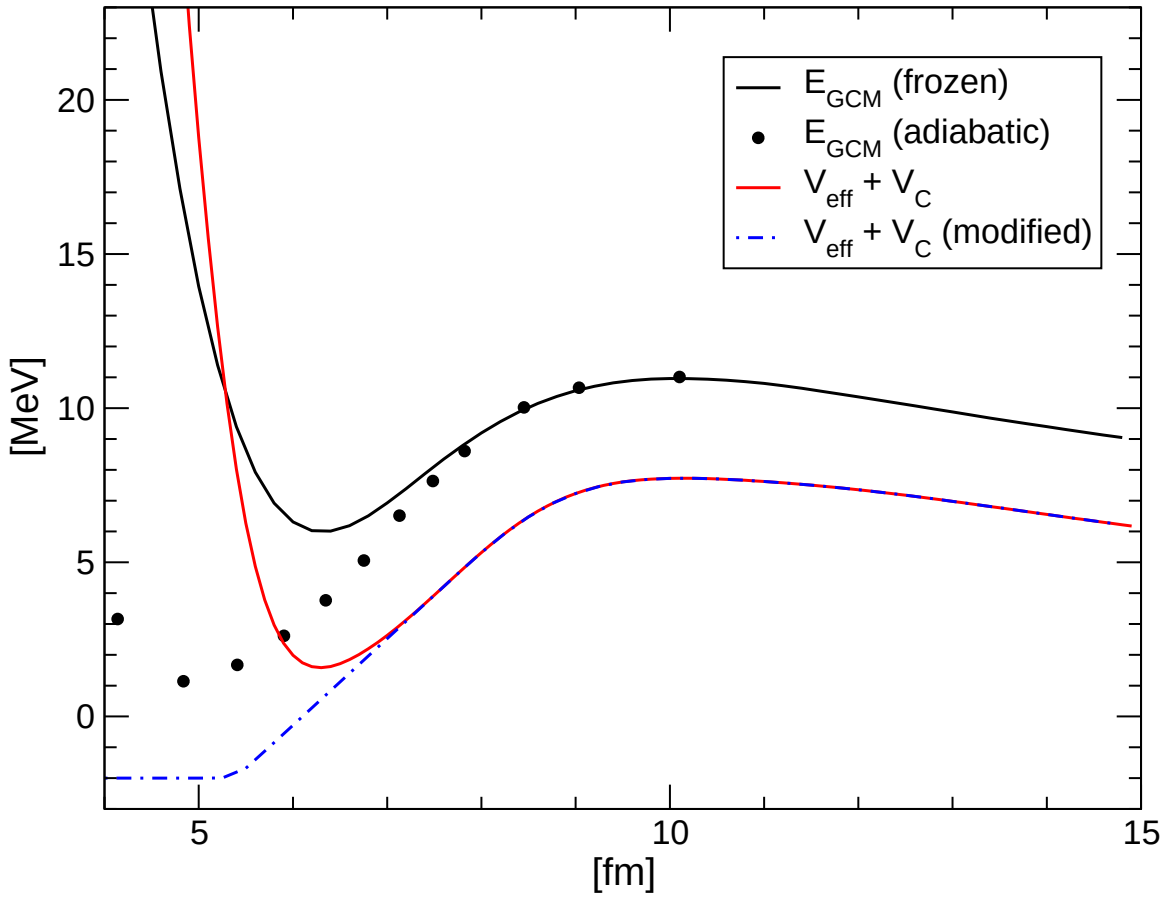
$$H^L_{\text{eff}}(r) = \frac{1}{2\mu m_N} p^2_{\text{rel}} + \frac{L(L+1)}{2\mu m_N r^2} + V^L_{\text{eff}}(r) + V_C(r) + E_1 + E_2$$



fit turns out to be independent of L

Adiabatic Effects

- estimate effects beyond the single-channel approximation
- adiabatic energy surface by constraining **quadrupole deformation** of system
- modify effective potential V_{eff} accordingly



Calculate Fusion Cross-Section

- solve two-body Schrödinger equation for all L with **Incoming Wave Boundary Condition** (assume that nuclei will fuse when the minimum of the potential is reached)

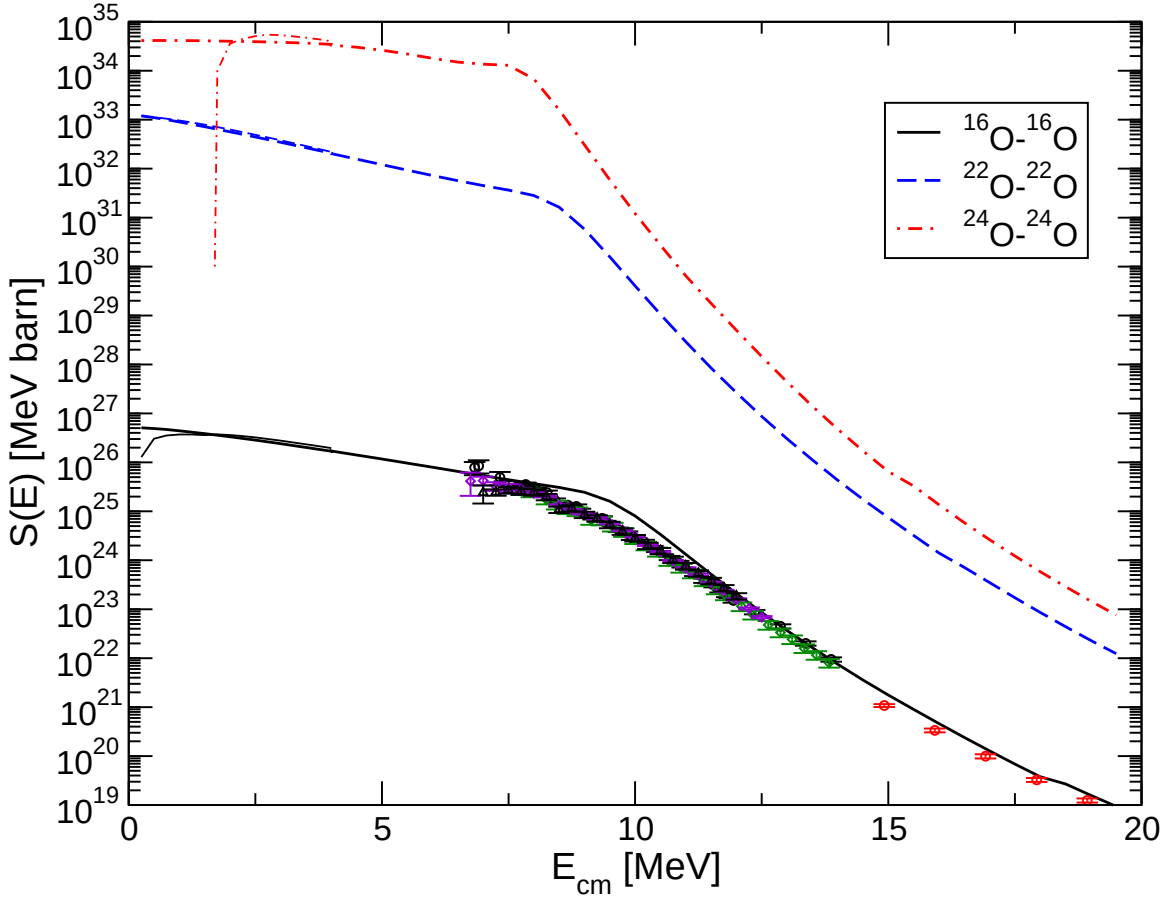
➨ therefore only real part of nucleus-nucleus potential is needed

- calculate and sum the penetration probabilities to calculate the fusion cross section

$$\sigma(E) = \frac{\pi}{k^2} \sum_{L=0}^{L_{crit}} [1+\delta_{12}(-1)^L](2L+1)P_L(E)$$

- convert into S-factor

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



Radiative Capture

^{3}He(α,γ)^{7}Be reaction

- cluster model wave functions with FMD ground states
- improve description in the interaction region with FMD states for ^{7}Be

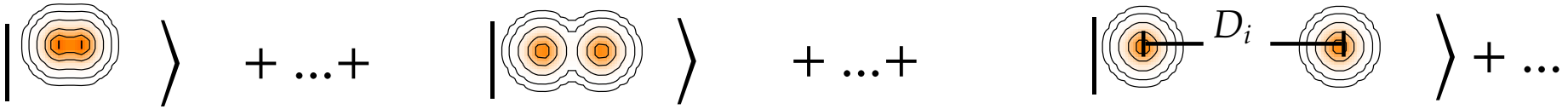
Program

- Implement boundary conditions
- Bound states, resonances and scattering states
- Capture cross section

Wave Functions

$^3\mathrm{He} + {}^4\mathrm{He} \longrightarrow {}^7\mathrm{Be} + \gamma$

- asymptotic states like in a cluster model with FMD states for ^{3}He and ^{3}He
- FMD states for ^{7}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
- if the widths of all Gaussians are equal the relative motion of the two nuclei and the center of mass wave function is 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

Alberto Cribeiro (GSI),
PhD thesis

Collective-Coordinate Representation

Size Measure

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

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

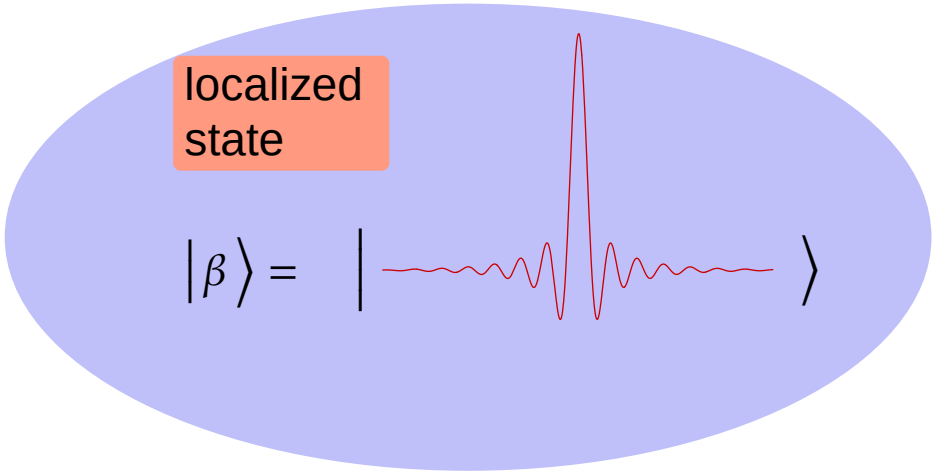
Asymptotic Interpretation

- Eigenvalues relate to relative distance r

$$\underset{\sim}{B}\left|\beta\right\rangle = \beta\left|\beta\right\rangle \Rightarrow \beta(r) = \frac{A_1 A_2}{A^2}r^2 + \beta_1 + \beta_2$$

- Eigenvectors localize in r (localized states)

$$\left\langle\beta\left|\underset{\sim}{B}^2\right|\beta\right\rangle = \left\langle\beta\left|\underset{\sim}{B}\right|\beta\right\rangle^2$$



- Identify Collective Wave Function

$$\Psi(r(\beta)) := \frac{1}{\sqrt{\Delta}}\left\langle\beta\left|\Psi\right\rangle\right.$$

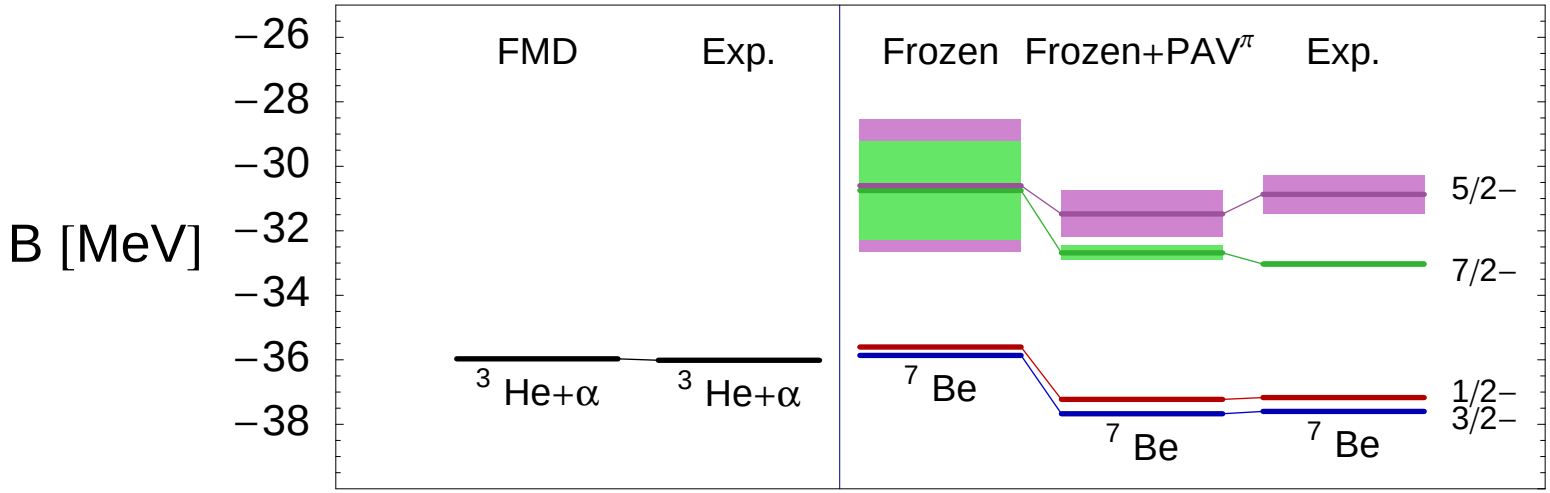
^{7}Be Bound states and Resonances

- calculate bound states by matching RGM wave function to Whittaker function

$$u_L(r) \propto W_{-\eta, L+\frac{1}{2}}(2kr)/(kr), \qquad k = \sqrt{-2\mu E}, \eta = (\mu Z_1 Z_2 e^2)/k$$

- calculate resonances by matching to purely outgoing Coulomb solution (Gamow boundary conditions), complex eigenvalue $E_{\rm res} + \frac{i}{2}\Gamma$

$$u_L(r) \propto [G_L(\eta, kr) + iF_L(\eta, kr)], \qquad k = \sqrt{2\mu E}$$

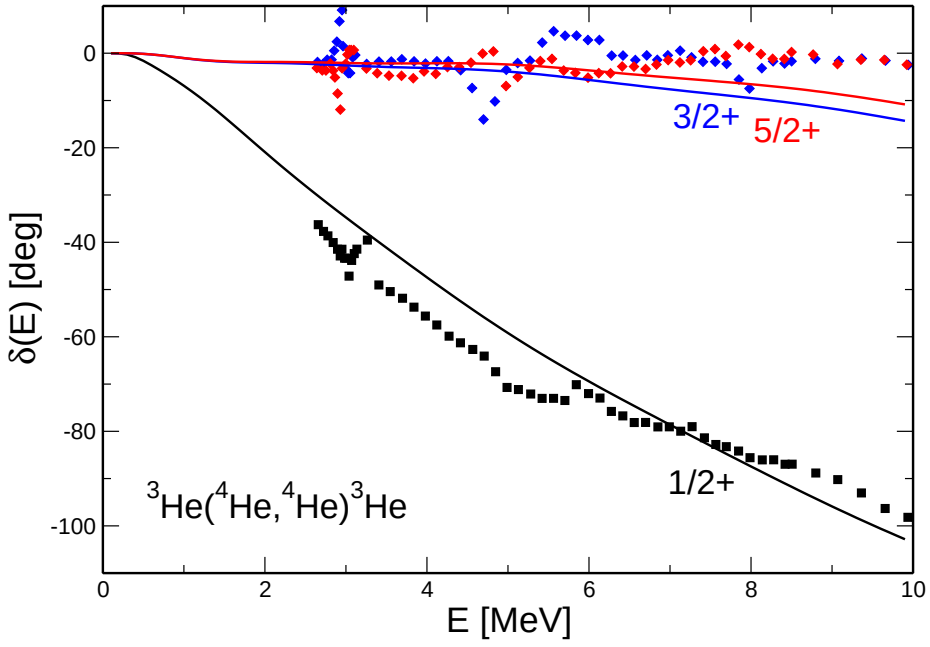


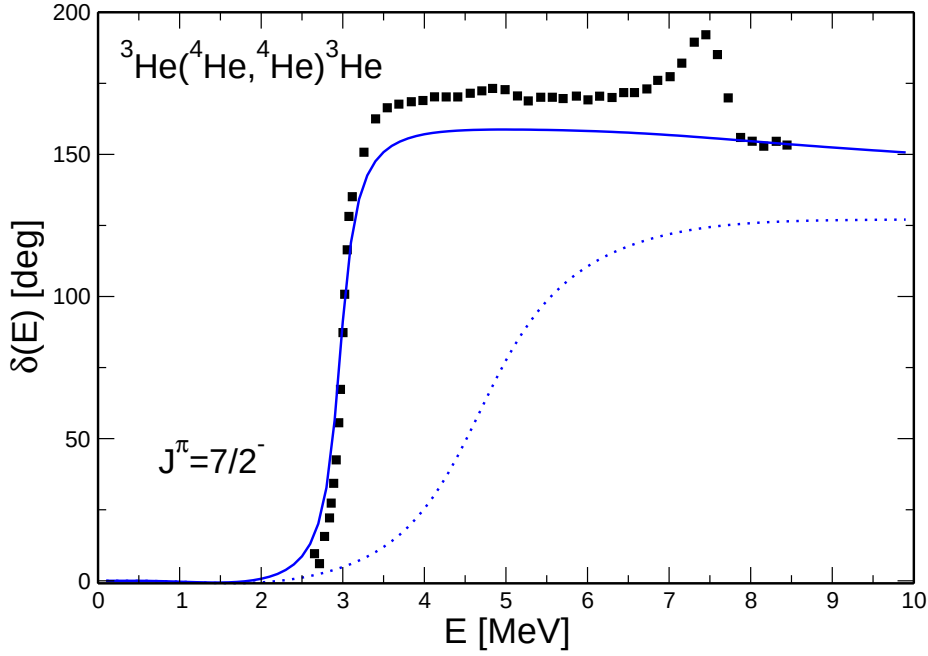
^{3}He-^{4}He Phaseshifts

- determine scattering solutions by matching to Coulomb solutions

unit flux scattering wave function

$$\left\langle \mathbf{r} \middle| \Psi \right\rangle = \frac{1}{\sqrt{v}} \sum_L \sqrt{4\pi}\,\sqrt{2L+1} i^L e^{i\sigma_L} \left[F_L(\eta, kr) + \tan(\delta) G_L(\eta, kr)\right] Y_{L0}(\hat{r})/(kr)$$

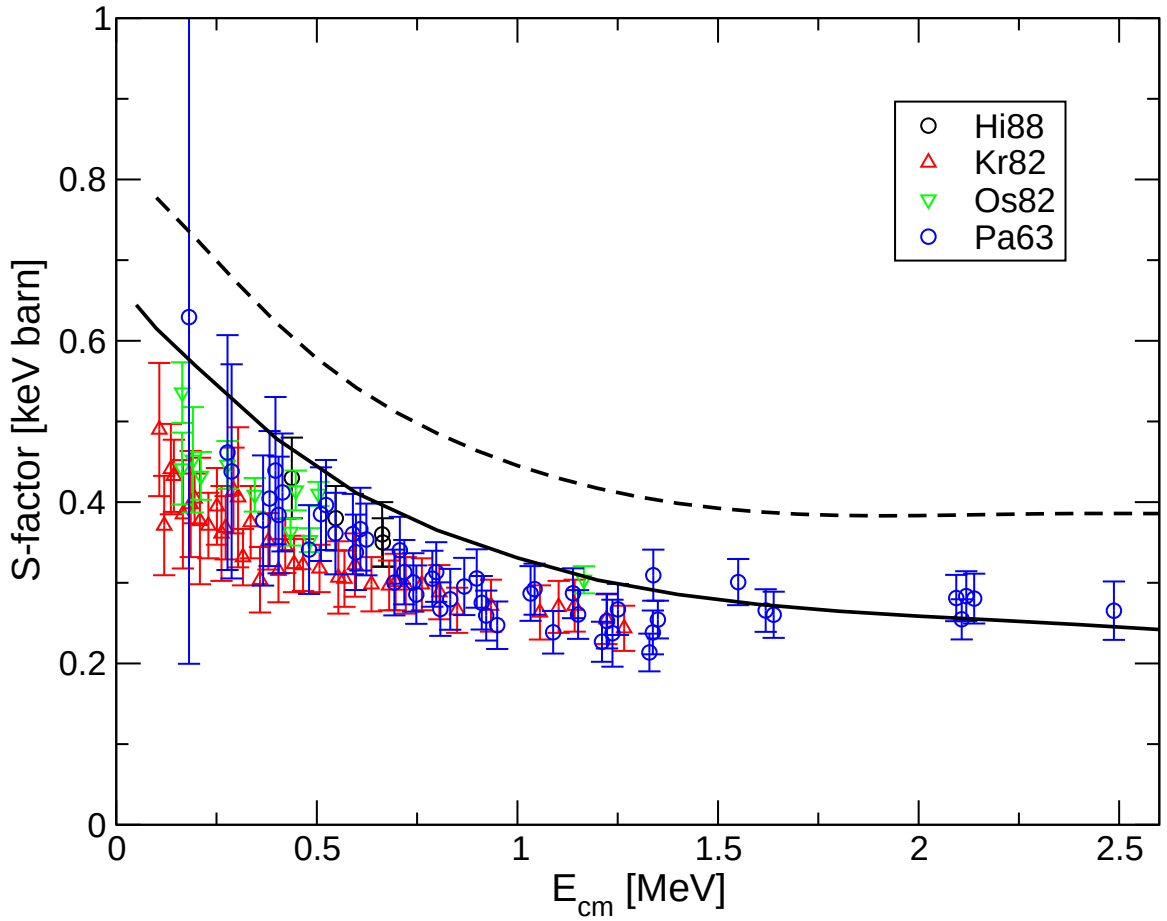




S-Factor

preliminary

- Capture from $1/2^+$, $3/2^+$ and $5/2^+$ scattering states into $3/2^-$ and $1/2^-$ bound states
- S-Factor for ^{7}Be described in the interaction region by single PAV$^\pi$ configuration (dashed line) or VAP configurations for $3/2^-$ and $1/2^-$ (solid line)



Summary

Unitary Correlation Operator Method

- explicit description of short-range central and tensor correlations
- phase-shift equivalent correlated interaction V_{UCOM}

Fermionic Molecular Dynamics

- Structure of light nuclei
- Halos and clustering

Cluster Degrees of Freedom

- GCM cluster states naturally described in FMD
- RGM wave function needed to implement boundary conditions for scattering or resonance states
- use for fusion and radiative capture reactions

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