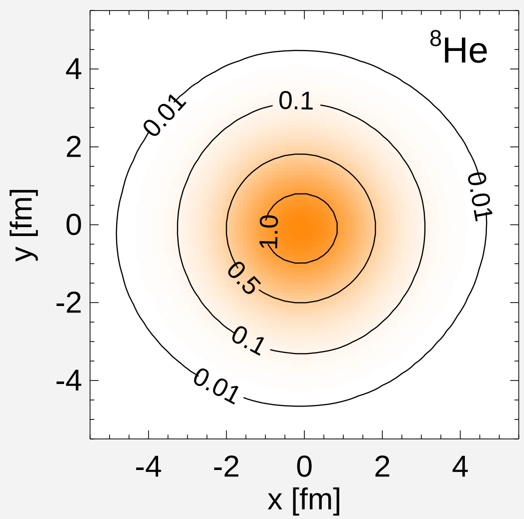
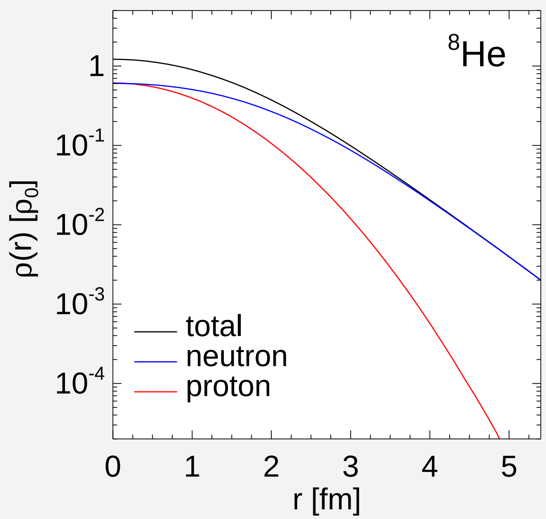




Multiconfiguration Calculations

in

Fermionic Molecular Dynamics

Rauischholzhausen XII @ Burg Rieneck, June 19-21, 2000

Thomas Neff, Robert Roth, Hans Feldmeier

FMD attributes

Fermionic

$$\left| \hat{Q} \right\rangle = \underset{\sim}{C}\,\underset{\sim}{\mathscr{A}} \left(\left| q_1 \right\rangle \otimes \cdots \otimes \left| q_A \right\rangle \right)$$

- Unitary Correlator $\underset{\sim}{C}$
- antisymmetrized A-particle state

Molecular

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

Dynamics

Variational Principle

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

Equations of motion

$$i \sum_\nu \mathscr{C}_{\mu\nu} \dot{q}_\nu = \frac{\partial \mathscr{H}}{\partial q_\mu^\star}$$

$$\mathscr{C}_{\mu\nu} = \frac{\partial}{\partial q_\mu^\star} \frac{\partial}{\partial q_\nu} \ln \left\langle \hat{Q} \middle| \hat{Q} \right\rangle$$

$$\mathscr{H} = \frac{\left\langle \hat{Q} \middle| \underset{\sim}{H} \middle| \hat{Q} \right\rangle}{\left\langle \hat{Q} \middle| \hat{Q} \right\rangle}$$

Evaluation of Matrix-Elements

One-Body Matrix-Elements

$$\mathcal{O} = \left(\langle\, q_i \,|\, q_j \,\rangle \right)^{-1}$$

$$\frac{\langle\, \hat{Q} \,|\, \underset{\sim}{O}^{[1]} \,|\, \hat{Q} \,\rangle}{\langle\, \hat{Q} \,|\, \hat{Q} \,\rangle} = \sum_{k,l} \langle\, q_k \,|\, \underset{\sim}{O}^{[1]} \,|\, q_l \,\rangle \mathcal{O}_{lk}$$

Two-Body Matrix-Elements

$$\frac{\langle\, \hat{Q} \,|\, \underset{\sim}{O}^{[2]} \,|\, \hat{Q} \,\rangle}{\langle\, \hat{Q} \,|\, \hat{Q} \,\rangle} = \frac{1}{2} \sum_{k,l,m,n} {}_a\langle\, q_k, q_l \,|\, \underset{\sim}{O}^{[2]} \,|\, q_m, q_n \,\rangle_a \mathcal{O}_{mk} \mathcal{O}_{nl}$$

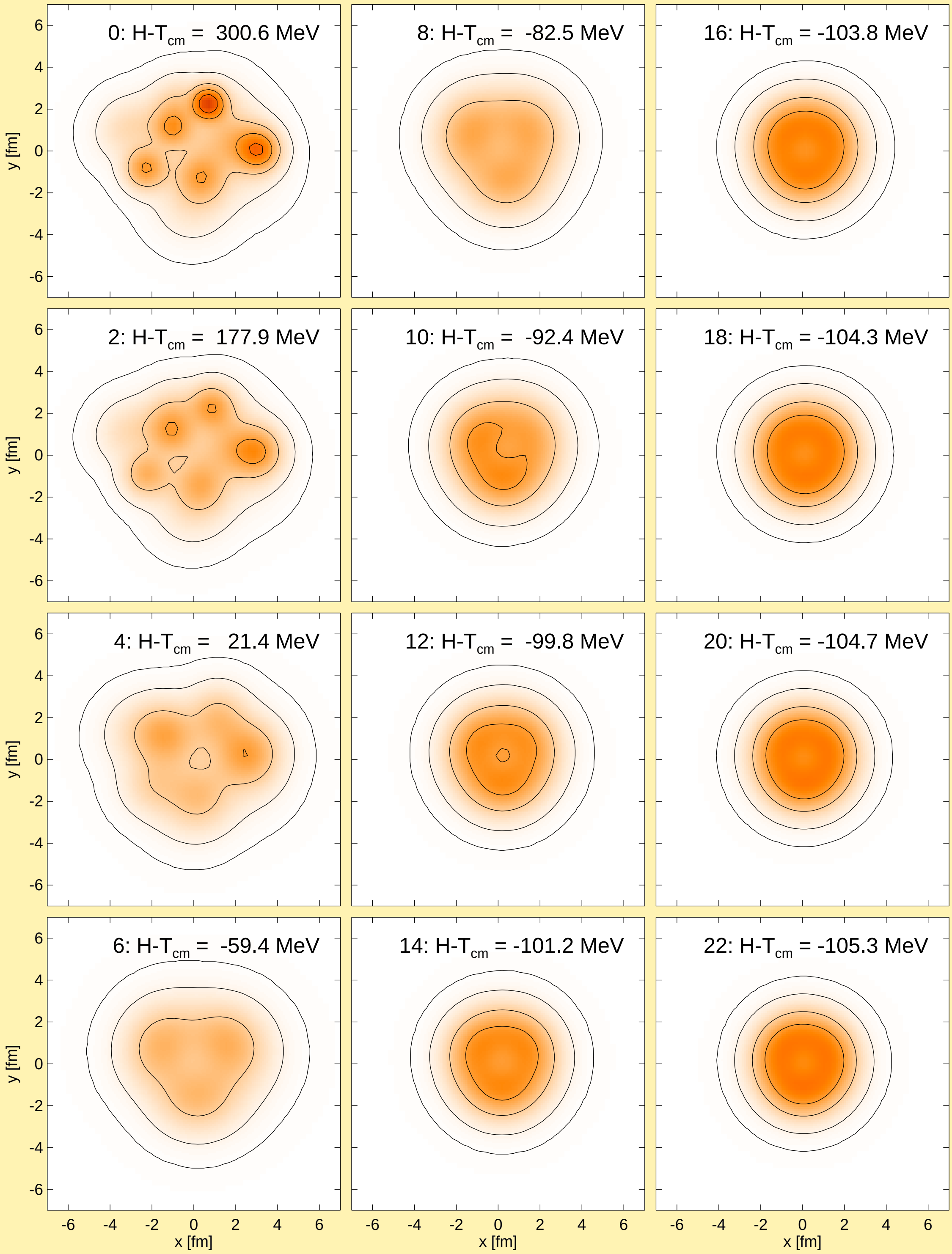
Gaussian Integrals

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

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

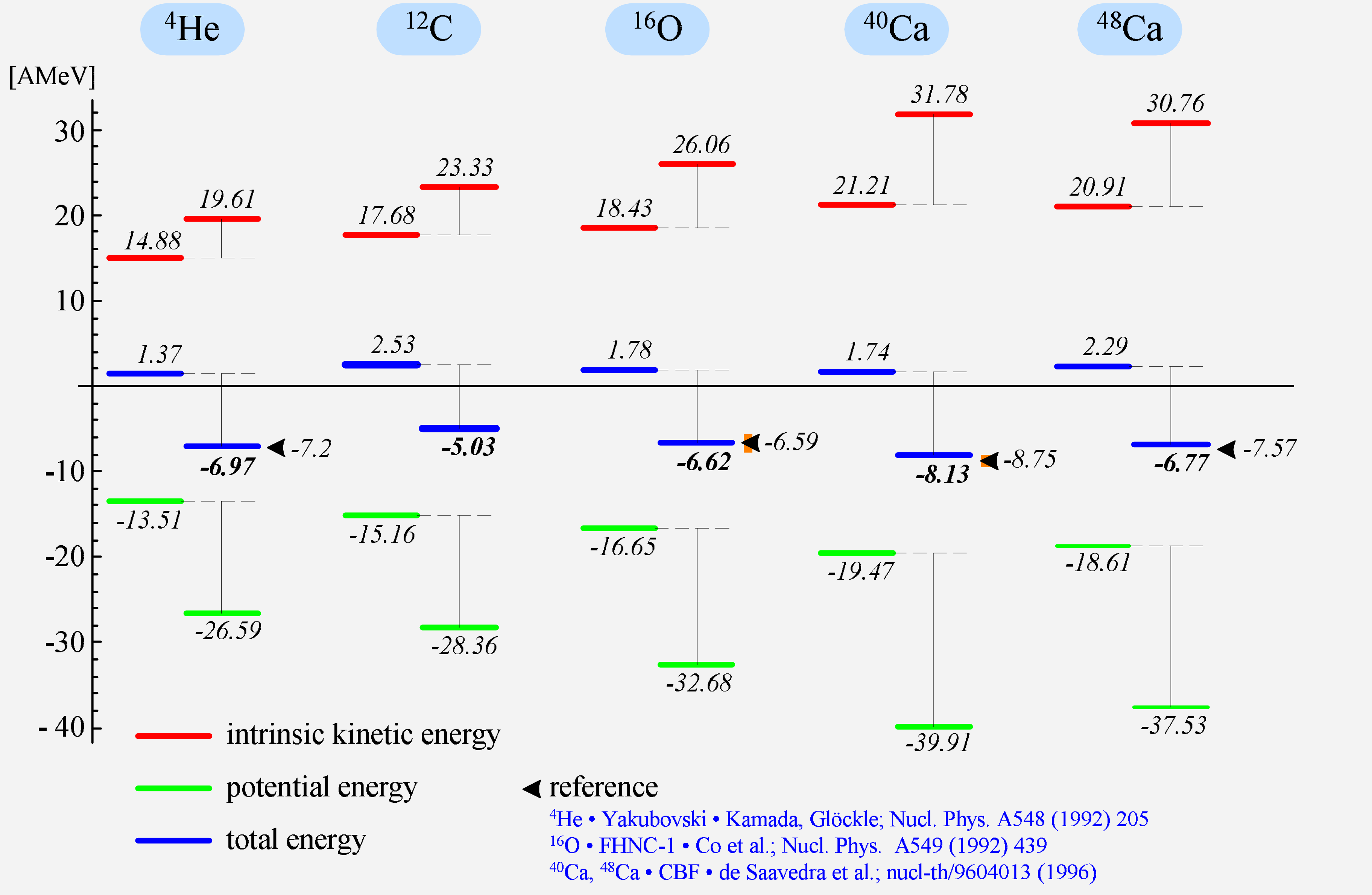
$$\alpha_{klmn} = \frac{a_k^\star a_m}{a_k^\star + a_m} + \frac{a_l^\star a_n}{a_l^\star + a_n}, \qquad \vec{\rho}_{klmn} = \frac{a_m \vec{b}_k^\star + a_k^\star \vec{b}_m}{a_k^\star + a_m} - \frac{a_n \vec{b}_l^\star + a_l^\star \vec{b}_n}{a_l^\star + a_n}, \qquad R_{km} = \langle\, a_k \vec{b}_k \,|\, a_m \vec{b}_m \,\rangle$$

searching the ^{16}O ground state

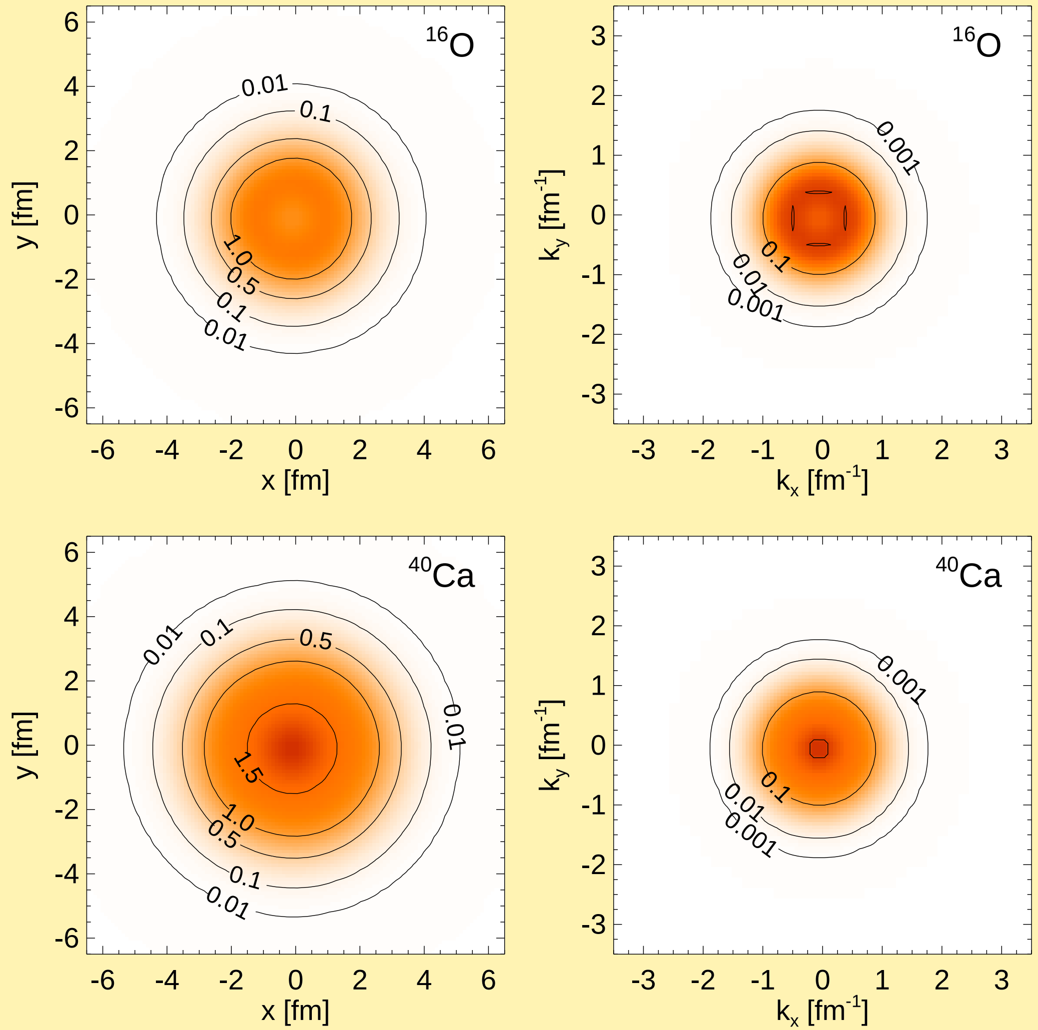


- Minimization of ground state energy with quasi-Newton-method

Afnan-Tang S3M results



shell-model-states



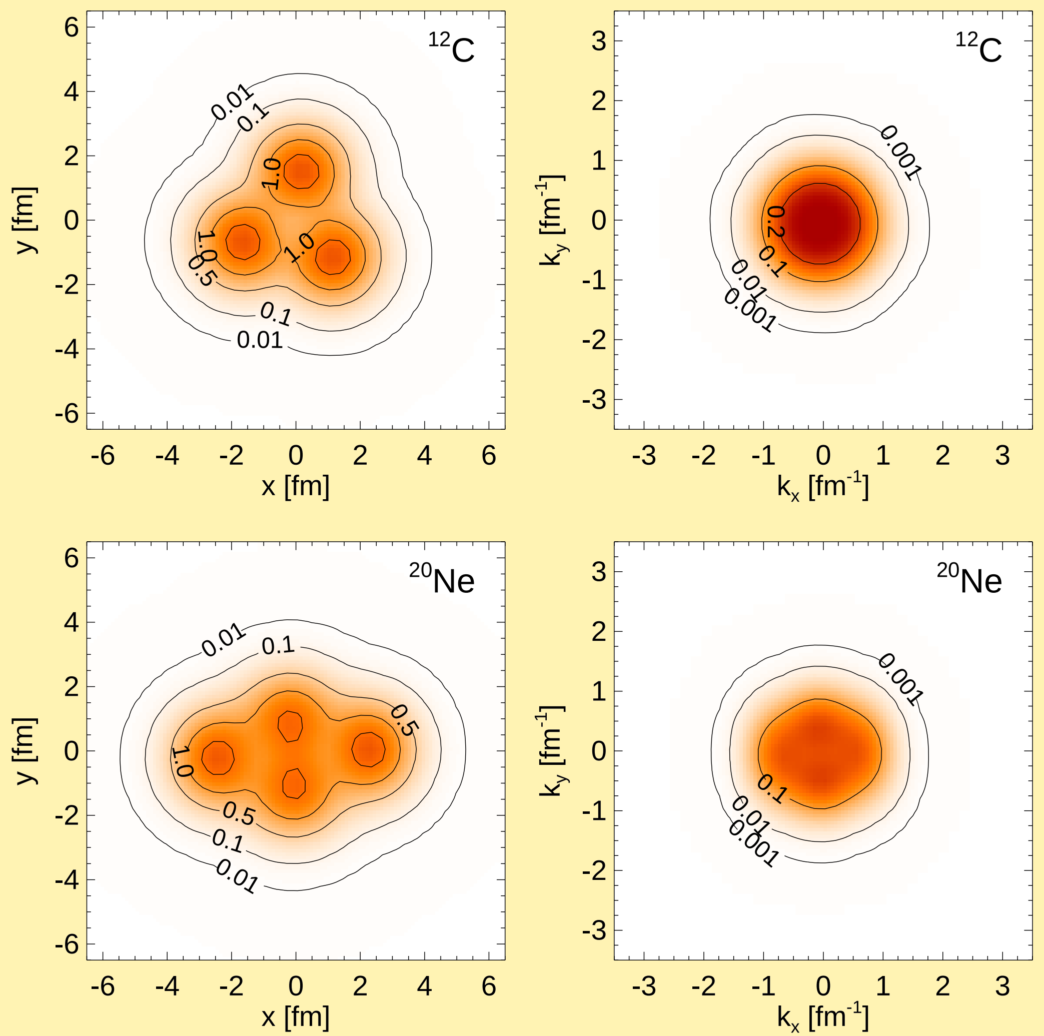
- Afnan-Tang S3M Interaction

✔ gaussian-basis generates perfect shell-model states

✔ linear combinations of slightly shifted gaussians result in harmonic oscillator *p*- and *d*-states – these linear combinations are a result of the antisymmetrization – the slater-determinant is invariant under unitary transformations of the single-particle states

✔ these states are the result of a unconstrained minimization of all $(A \cdot 8)$ Parameters

intrinsically-deformed-states



- Afnan-Tang S3M Interaction

✔ FMD can also describe intrinsically deformed nuclei

✔ this is very difficult to do in other calculations

✔ in FMD this is just the result of the unconstrained minimization in the parameter space

✘ intrinsically deformed ground states have not the rotational symmetry of the Hamiltonian

Multiconfiguration Calculations

Improve FMD description

- long-range correlations beyond the meanfield
- address intrinsically deformed ground states
- discuss contributions of different configurations

Multiconfiguration FMD

diagonalize Hamiltonian in a set

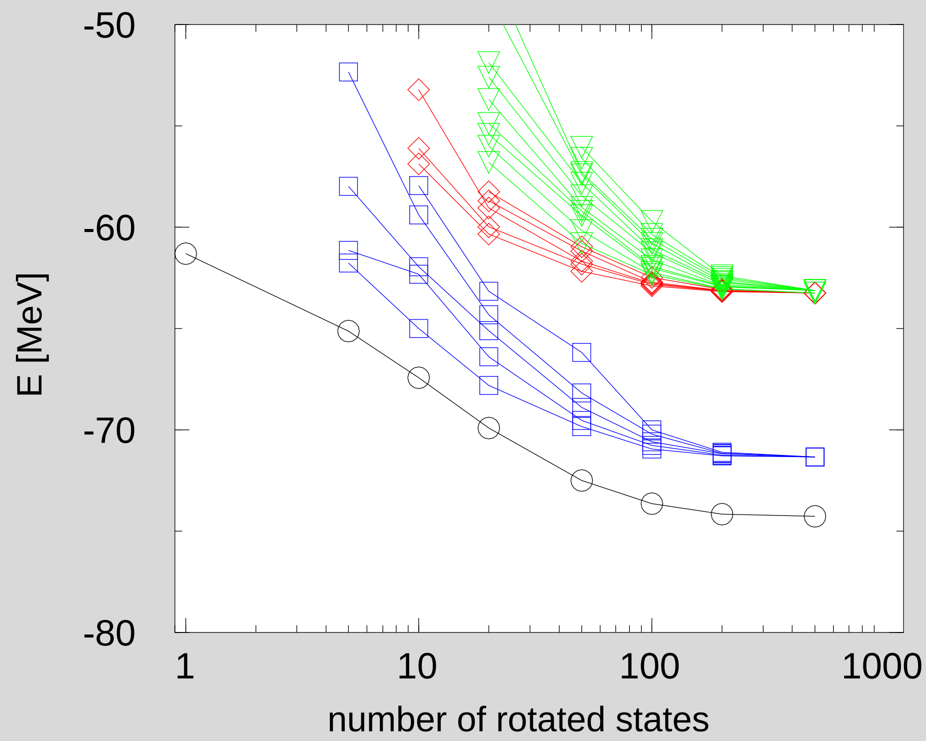
$$\{ | \hat{Q}^i \rangle \}$$

of (nonorthogonal) FMD states, leads to generalized eigenvalue problem

$$\sum_j \langle \hat{Q}^i | \underset{\sim}{H} | \hat{Q}^j \rangle c_j^\alpha = E^\alpha \sum_j \langle \hat{Q}^i | \hat{Q}^j \rangle c_j^\alpha$$

^{12}C

diagonalization in a set of randomly rotated states

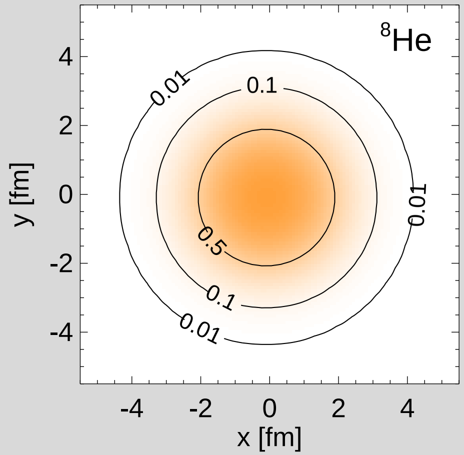


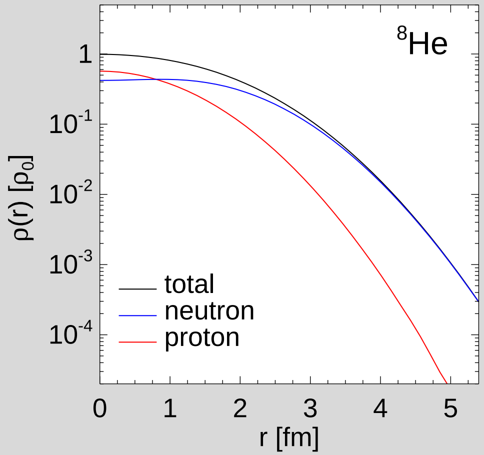
- ✔ big increase in binding energy
- ✔ eigenstates of angular momentum and parity
- ✔ spectrum of rotational excitations

Halo Nuclei

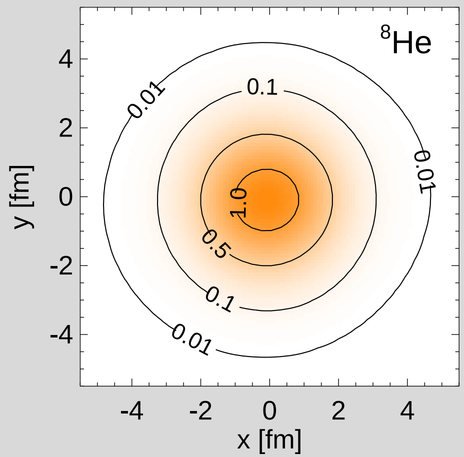
^{8}He

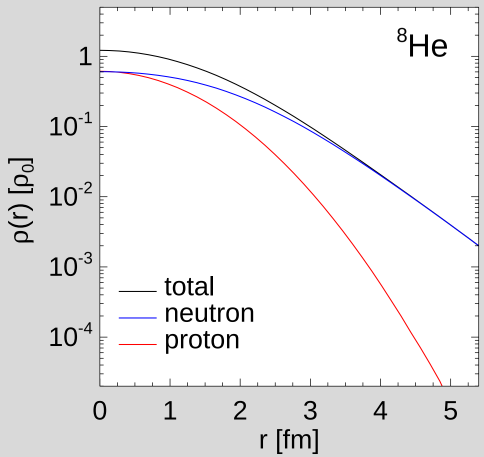
One gaussian per one-particle state





Two gaussians per one-particle state





^{8}He

	FMD		*AVRGM*
	1g	2g	
E_B	-21.67	-24.86	-24.22
R_m	2.27	2.38	2.73
R_p	1.79	1.70	2.08
R_n	2.41	2.55	2.91

diagonalization in rotated states

	2g	2g/2c	2g/25c
E_B	-24.86	-25.49	-26.70

AVRGM
three-cluster microscopic model
`nucl-th/0006001`

Summary & Outlook

FMD

- ✔ FMD works well for nuclei in the valley of stability
- ✔ FMD seems to work also quite fine for halo-nuclei

Halo Nuclei

- study the importance of different configurations
- study spectrum and other properties of nuclei

Choice of Interaction

- ✔ effective and (semi-) realistic interactions can be used
- ✔ Unitary Correlator works well for the hard-core of realistic interactions
- ✘ correlator for tensor- and spin-orbit interactions necessary ?