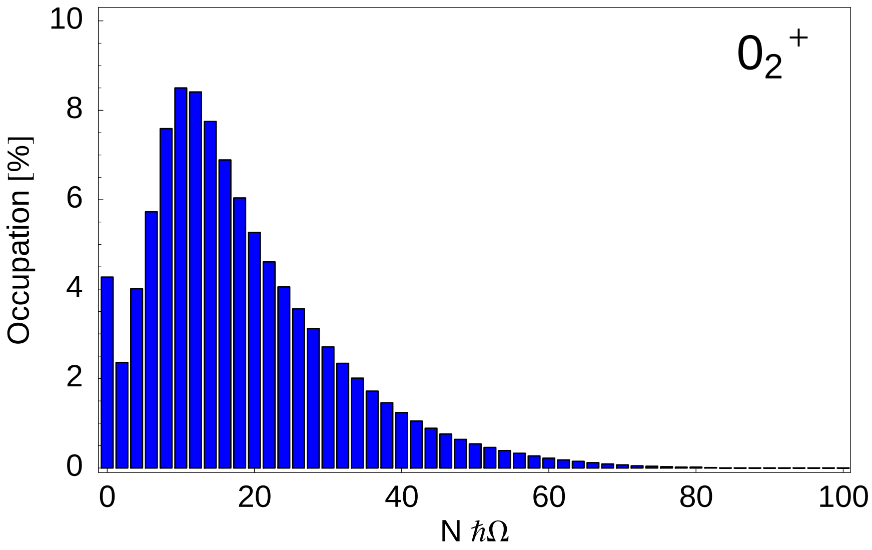
Microscopic Description of Few-Body Systems in the Fermionic Molecular Dynamics Approach



Thomas Neff

Critical Stability
Ettore Majorana Centre for Scientific Culture, Erice
October 16, 2008

Overview

Unitary Correlation Operator Method

Fermionic Molecular Dynamics

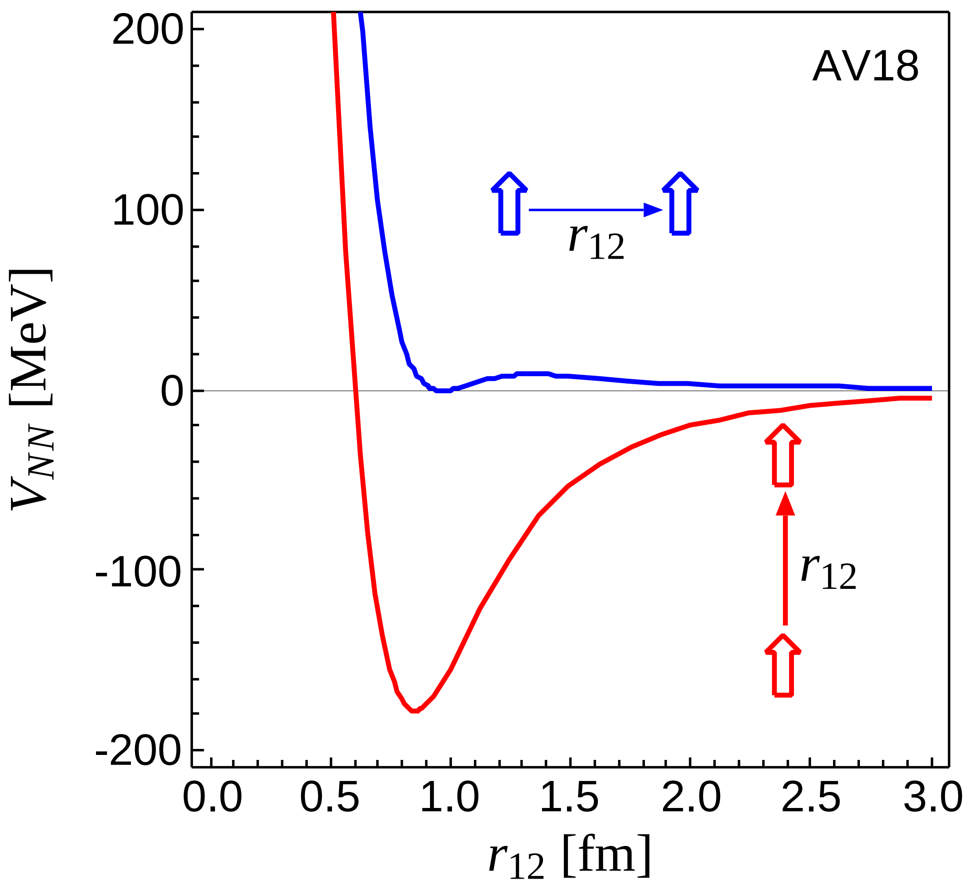
Hoyle State in ^{12}C

Neon Isotopes, ^{17}Ne

Nuclear Force

Argonne V18 (T=0)

spins aligned parallel or perpendicular to the relative distance vector



- strong repulsive core: nucleons can not get closer than ≈ 0.5 fm

➨ **central correlations**

- strong dependence on the orientation of the spins due to the tensor force

➨ **tensor correlations**

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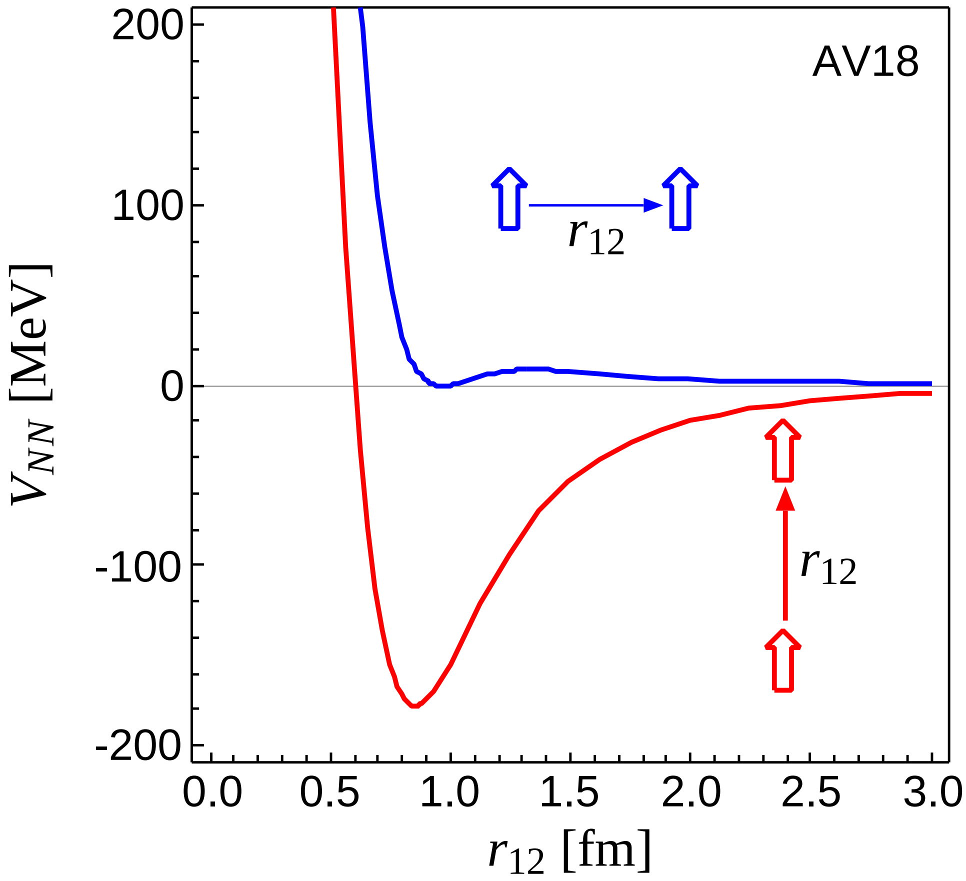

- strong repulsive core: nucleons can not get closer than ≈ 0.5 fm

➨ **central correlations**

- strong dependence on the orientation of the spins due to the tensor force

➨ **tensor correlations**

the nuclear force will induce **strong short-range correlations** in the nuclear wave function

Central and Tensor Correlations

$$\underset{\sim}{C} = \underset{\sim}{C}_\Omega \underset{\sim}{C}_r$$

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

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

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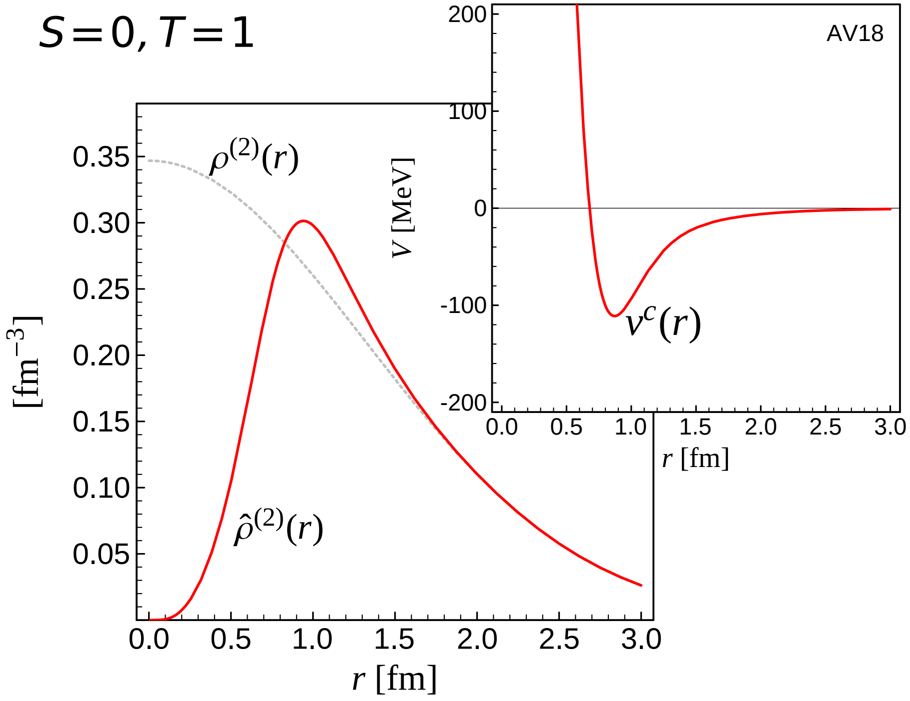
Central Correlations

$$\underset{\sim}{c}_r = \exp\left\{-\frac{i}{2}\{p_r s(r) + s(r) p_r\}\right\}$$

- probability density shifted out of the repulsive core

$S=0, T=1$



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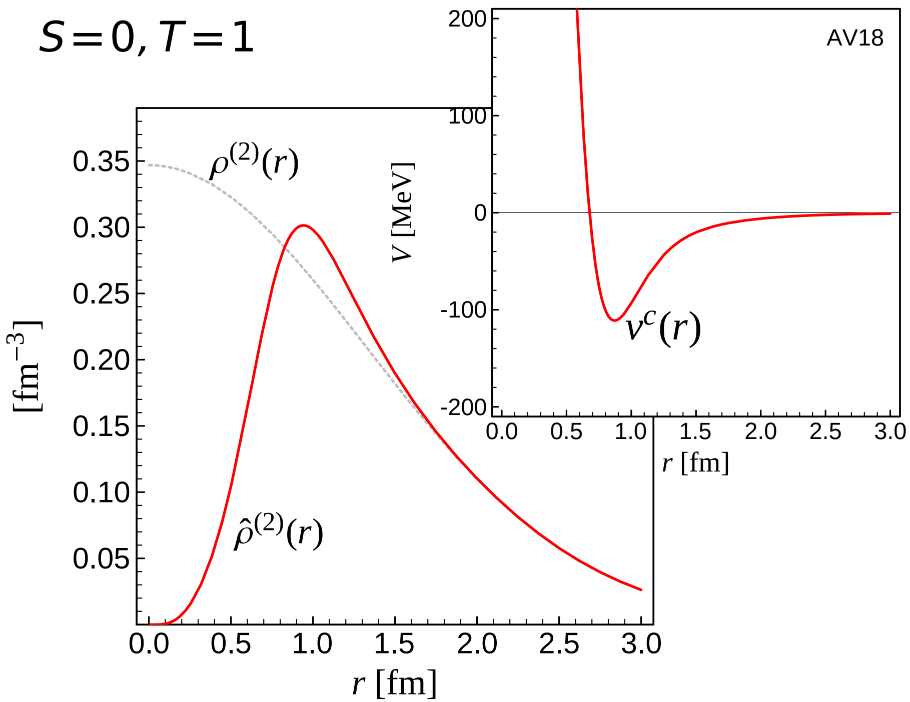
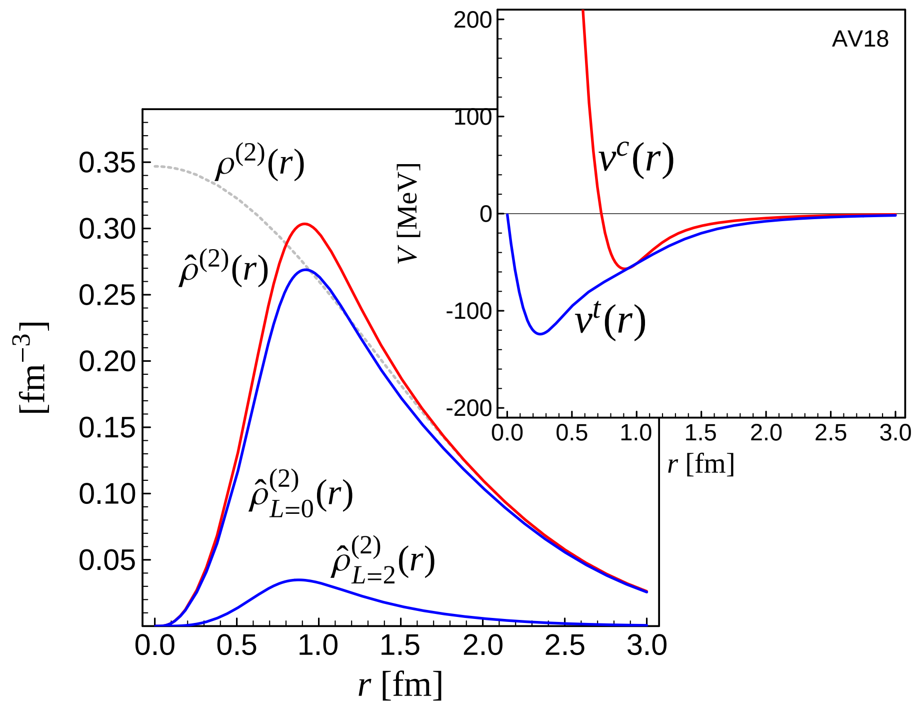


Tensor Correlations

$$\underset{\sim}{c}_\Omega = \exp\left\{-i\vartheta(r)\left\{\frac{3}{2}(\boldsymbol{\sigma}_1\cdot\mathbf{p}_\Omega)(\boldsymbol{\sigma}_2\cdot\mathbf{r}) + \frac{3}{2}(\boldsymbol{\sigma}_1\cdot\mathbf{r})(\boldsymbol{\sigma}_2\cdot\mathbf{p}_\Omega\right.\right.$$

- tensor force admixes other angular momenta



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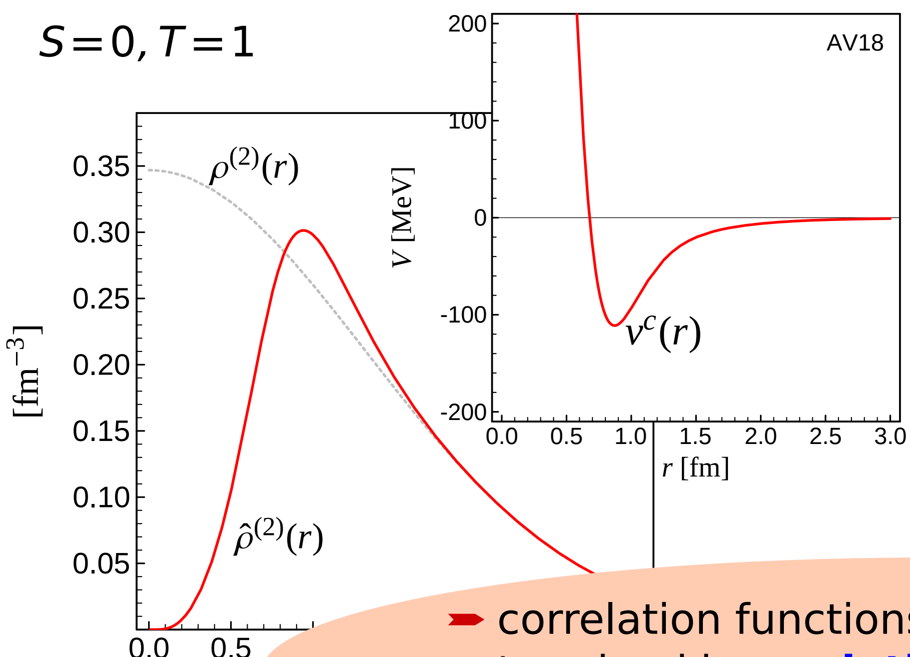

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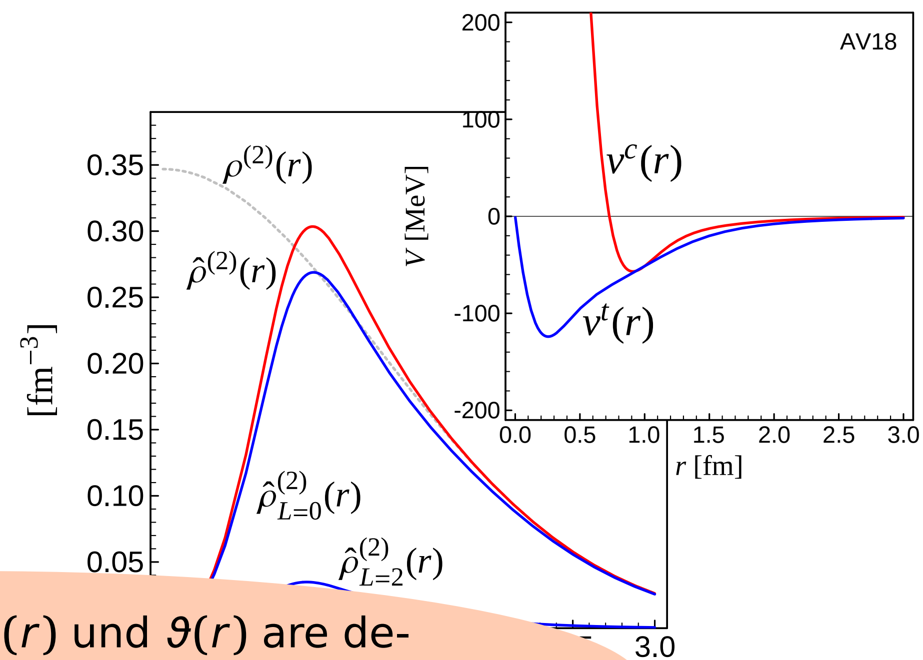
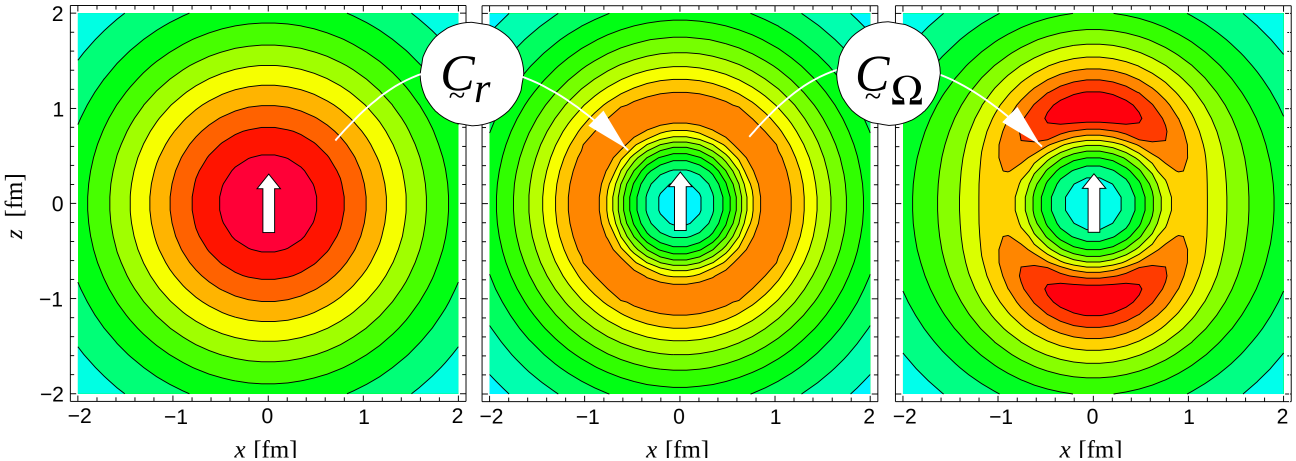


- correlation functions $s(r)$ und $\vartheta(r)$ are determined by **variation** of the energy in the **two-body system** for each S, T channel

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

T. Neff and H. Feldmeier, Nucl. Phys. **A713** (2003) 311

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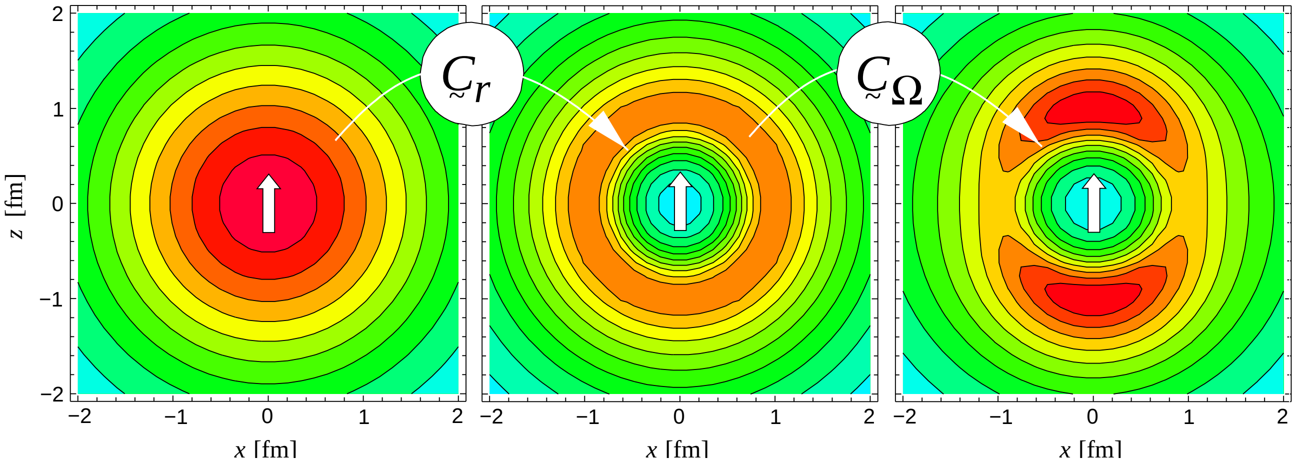

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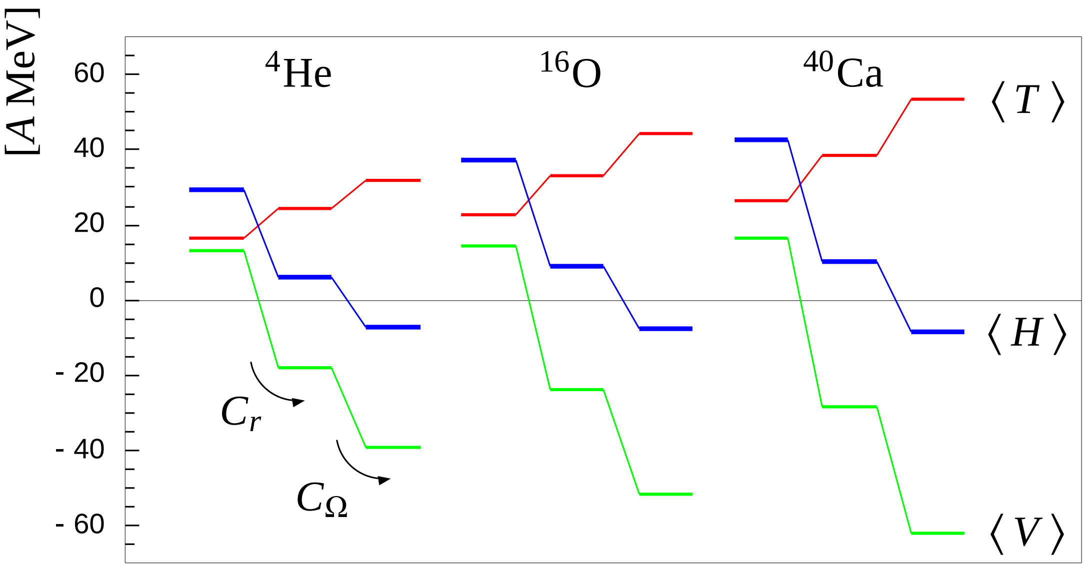
energies

$0\hbar\omega$ Harmonic Oscillator

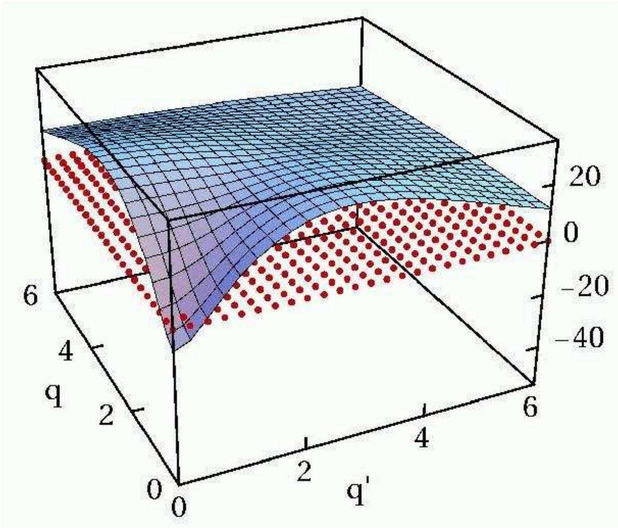


both central and tensor correlations are essential for binding

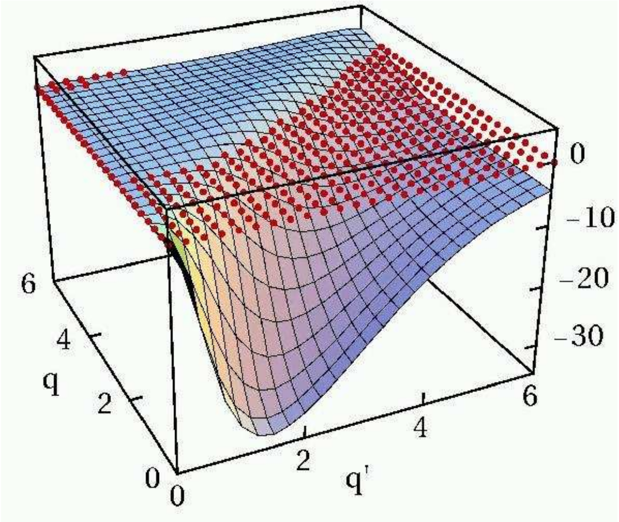
T. Neff and H. Feldmeier, Nucl. Phys. **A713** (2003) 311

Correlated Interaction in Momentum Space

$^3S_1$ bare



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



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

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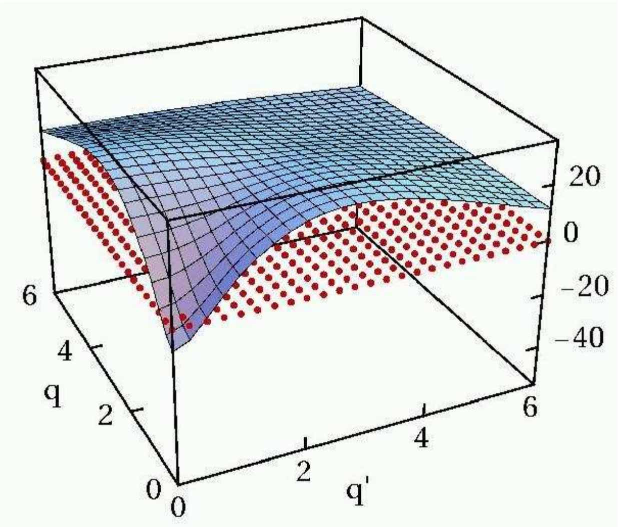

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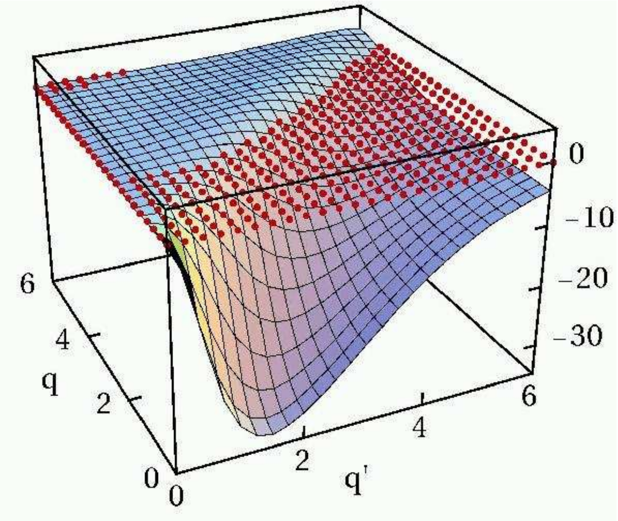
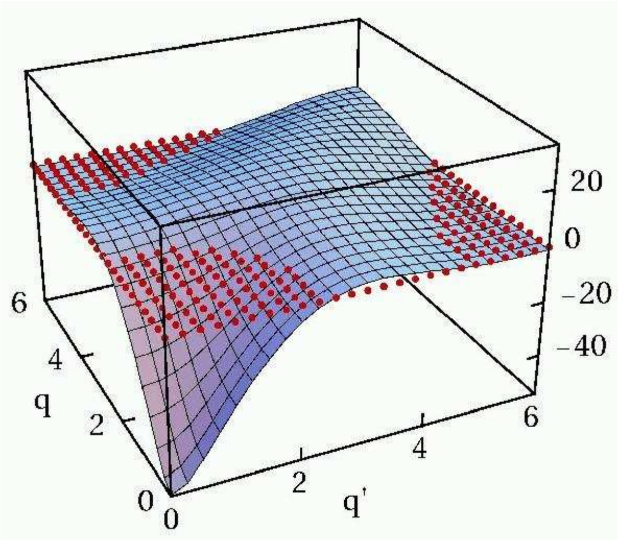


correlated interaction is **more attractive** at low momenta

$^3S_1$ correlated



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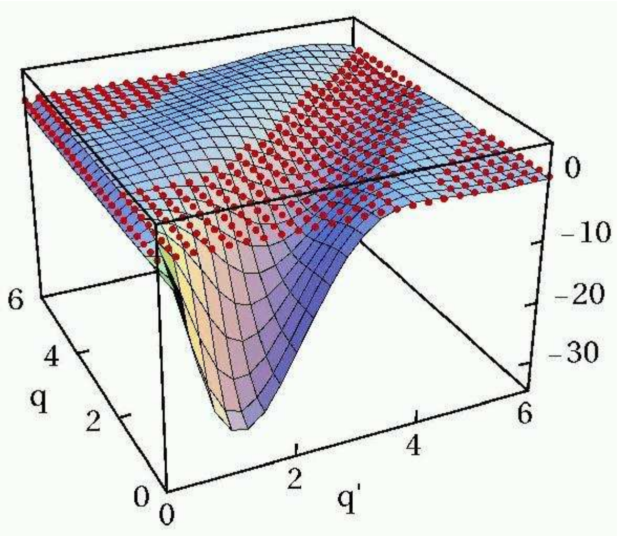

off-diagonal matrix elements connecting low- and high- momentum states are **strongly reduced**

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

Fermionic Molecular Dynamics

FMD Wave Functions

Nucleon-Nucleon Interaction

Mean-Field Calculations

Projection After Variation,
Variation After Projection
and Multiconfiguration

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

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

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

Fermionic Molecular Dynamics

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Molecular

single-particle states

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

- 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

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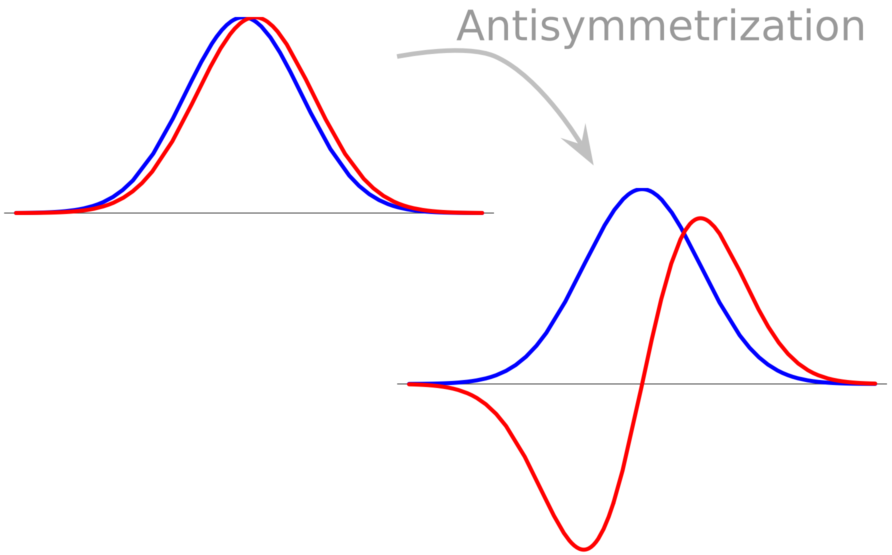

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Interaction Matrix Elements

(One-body) Kinetic Energy

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

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

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

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

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

(Two-body) Potential

- fit radial dependencies by (a sum of) Gaussians

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

- Gaussian integrals

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

- analytical formulas for matrix elements

Operator Representation of V_{UCOM}

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

one-body kinetic energy

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

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

- no three-body forces, saturation with UCOM force not correct

➨ add phenomenological two-body correction term with a **momentum-dependend** central and (isospin-dependend) **spin-orbit** part (about 15% contribution to potential)

➨ fit correction term to binding energies and radii of "closed-shell" nuclei (^{4}He, ^{16}O, ^{40}Cα), (^{24}O, ^{34}Si, ^{48}Cα)

➨ **Todo:**
use **three-body** or **density dependent two-body force** instead of two-body correction term

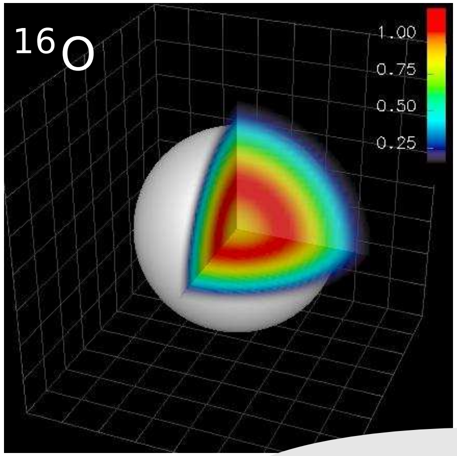
Perform Variation

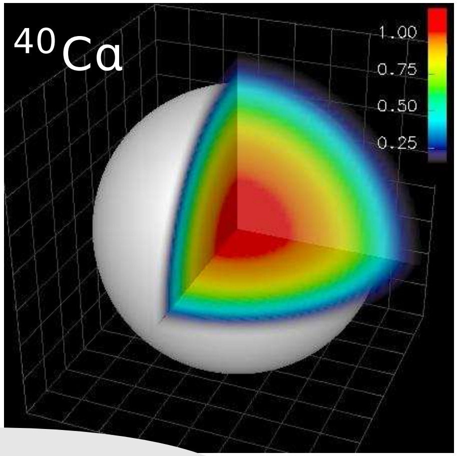
Minimization

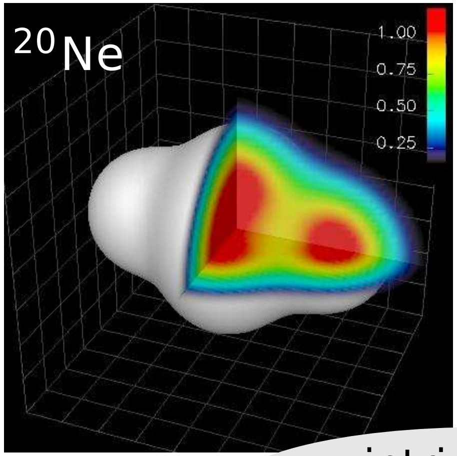
- minimize Hamiltonian expectation value with respect to all single-particle parameters q_k

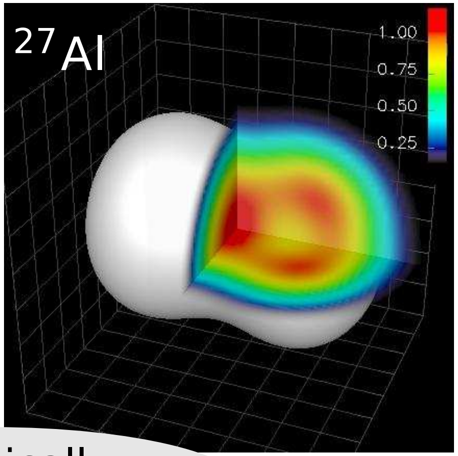
$$\min_{\{q_k\}} \frac{\left\langle Q \middle| \underset{\sim}{H} - \underset{\sim}{T}_{cm} \middle| Q \right\rangle}{\left\langle Q \middle| Q \right\rangle}$$

- 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

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

$$\underset{\sim}{P}^{\pi} = \frac{1}{2}(1 + \pi \underset{\sim}{\Pi})$$

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

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

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Variation After Projection (VAP)

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- effect of projection can be large
- perform Variation after Parity Projection PAV^{π}
- full Variation after Angular Momentum Projection (VAP)
- perform VAP in GCM sense by applying **constraints** on radius, dipole moment, quadrupole moment or octupole moment and minimizing the energy in the projected energy surface

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Multiconfiguration Calculations

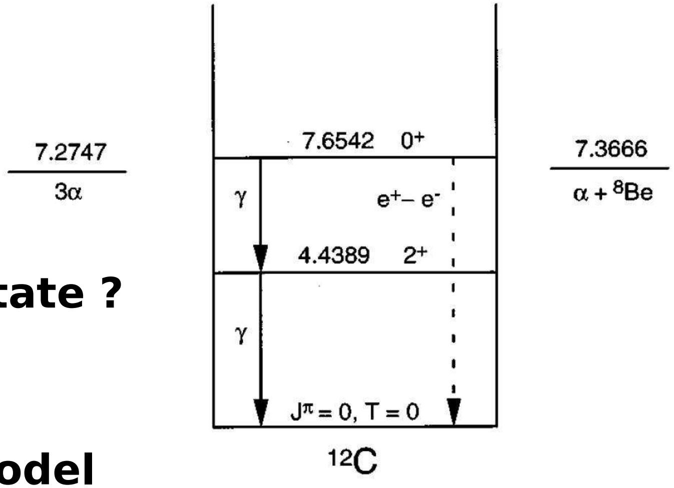
- **diagonalize** Hamiltonian in a set of projected intrinsic states

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

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

Cluster States in ^{12}C

Astrophysical Motivation



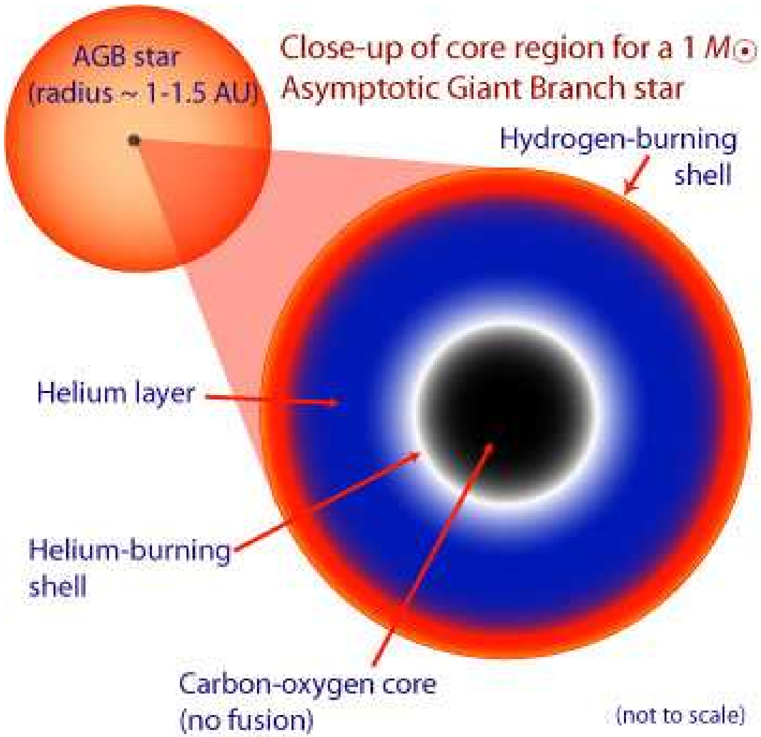
Structure

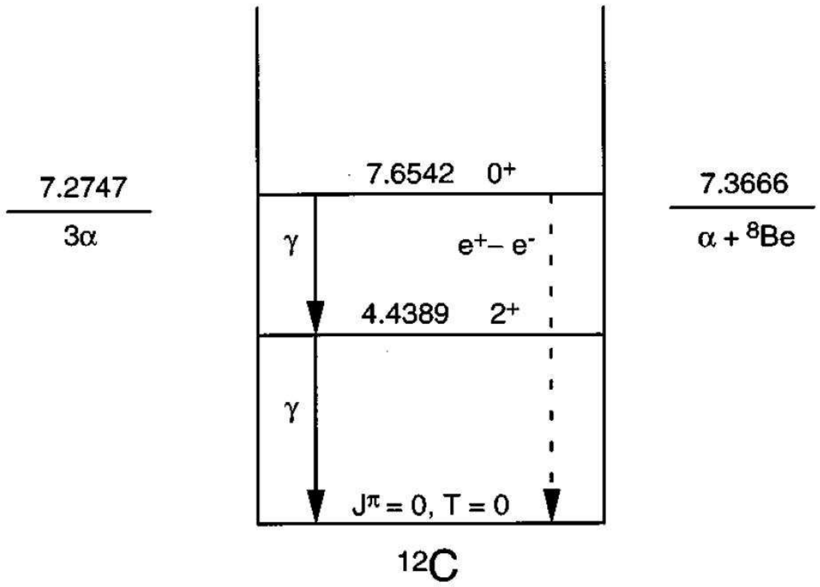
- **Is the Hoyle state a pure α-cluster state ?**
- **Other excited 0^+ and 2^+ states**

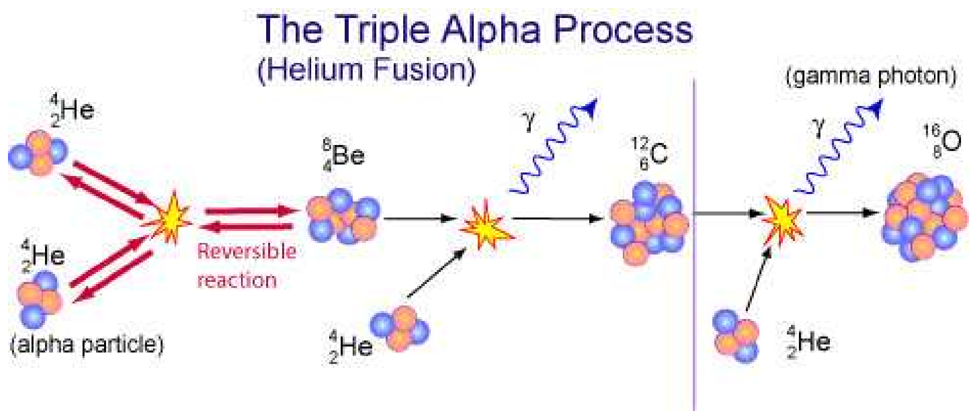
➨ **Compare FMD results to α-cluster model**
➨ **Analyze wave functions in harmonic oscillator basis**

➨ **No-Core Shell Model Calculations ?**

Triple α Reaction

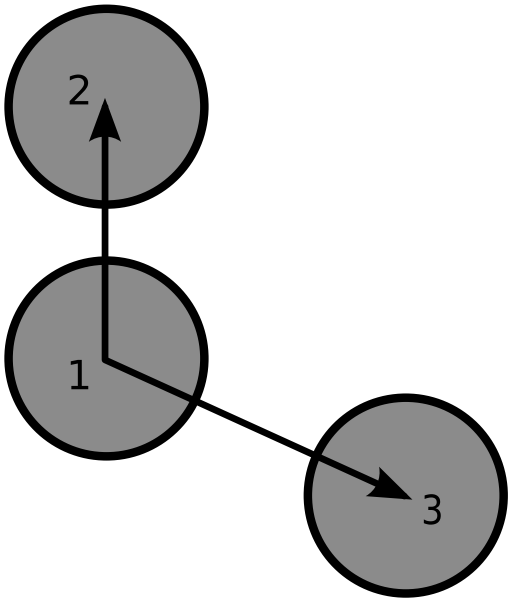






http://outreach.atnf.csiro.au/education/senior/astrophysics/stellarevolution_postmain.html

Microscopic α-Cluster Model



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

alltogether 165 configurations

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

Funaki et al., Phys. Rev. C **67** (2003) 051306(R)

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 C12 ground state energy

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

'BEC' wave functions

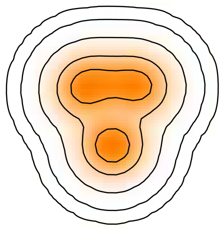
- same interaction and α-cluster parameters used by Funaki et al.

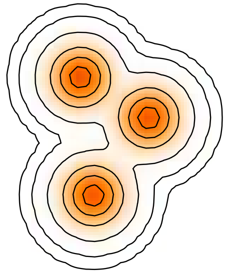
Cluster States in ^{12}C
FMD

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



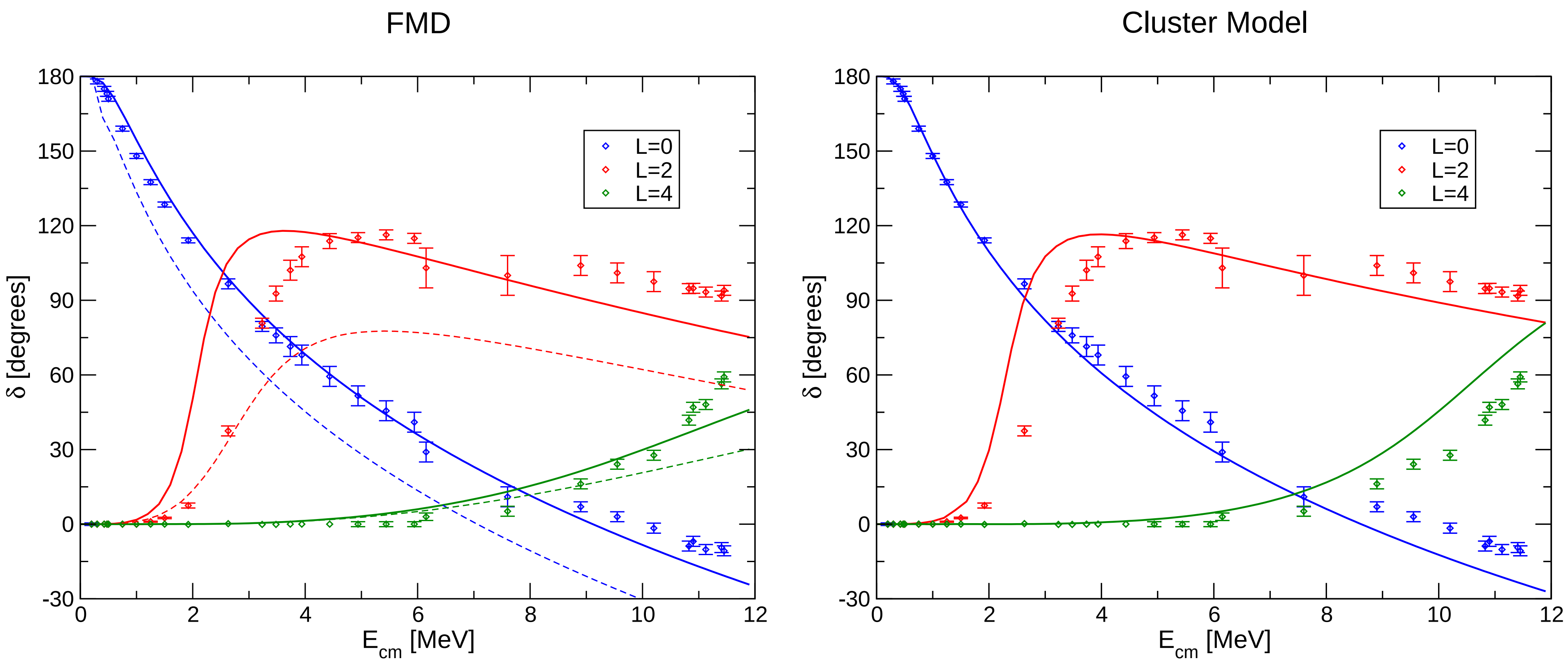


Interaction

- not tuned for α-α scattering or ^{12}C properties

Cluster States in ^{12}C

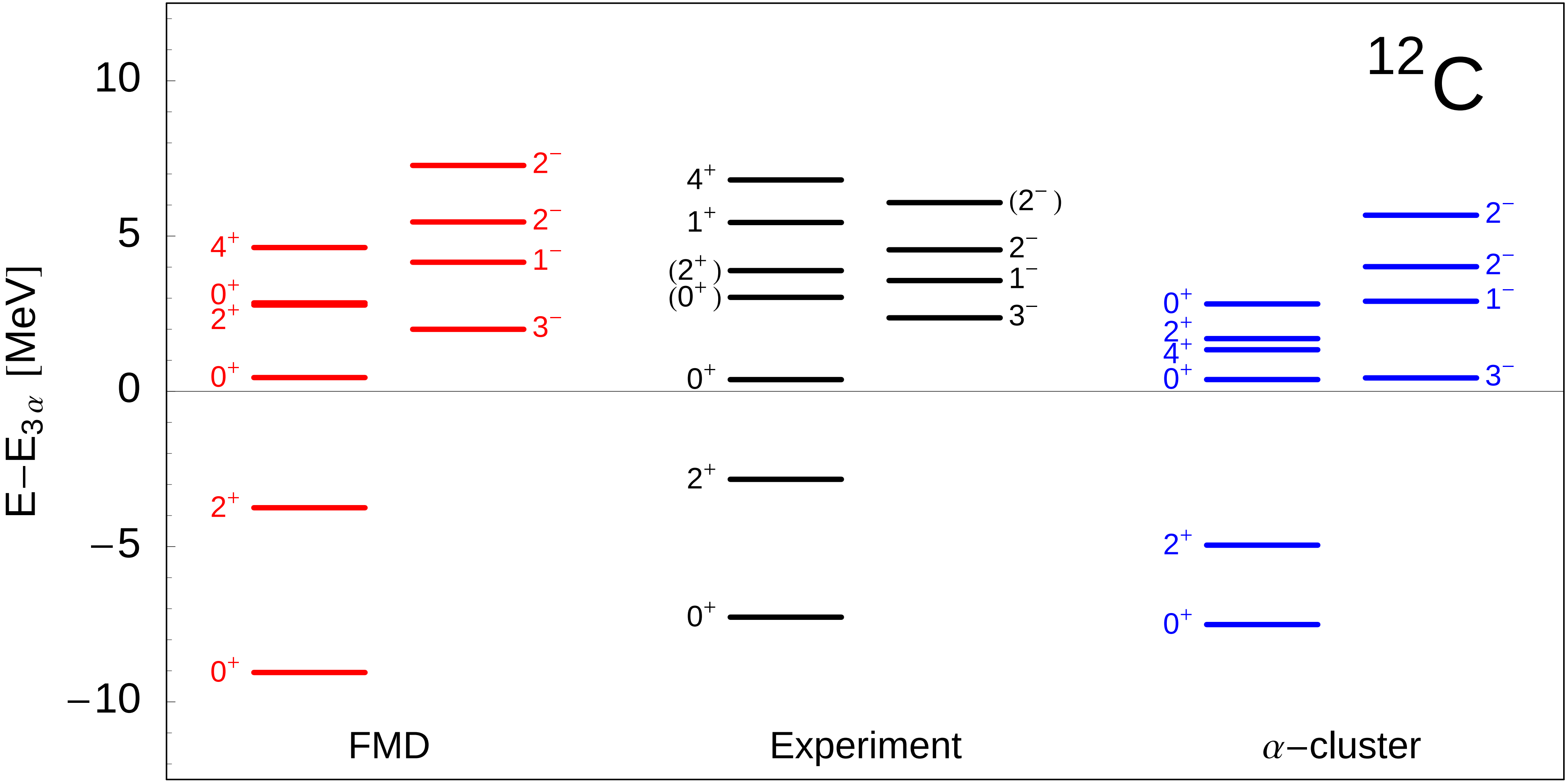
α-α Phaseshifts



- Phaseshifts calculated with cluster configurations only (dashed lines)
- Phaseshifts calculated with additional FMD VAP configurations in the interaction region (solid lines)
- only cluster configurations included

➨ similar quality for description of α-α-scattering

Comparison


^{12}C
E−E$_{3\alpha}$ [MeV]
10
5
0
−5
−10
FMD
Experiment
α−cluster
2⁻
2⁻
1⁻
3⁻
4⁺
0⁺
2⁺
0⁺
2⁺
0⁺
4⁺
1⁺
(2⁺)
(0⁺)
0⁺
2⁺
0⁺
(2⁻)
2⁻
1⁻
3⁻
0⁺
2⁺
4⁺
0⁺
2⁺
0⁺
2⁻
2⁻
1⁻
3⁻

Comparison

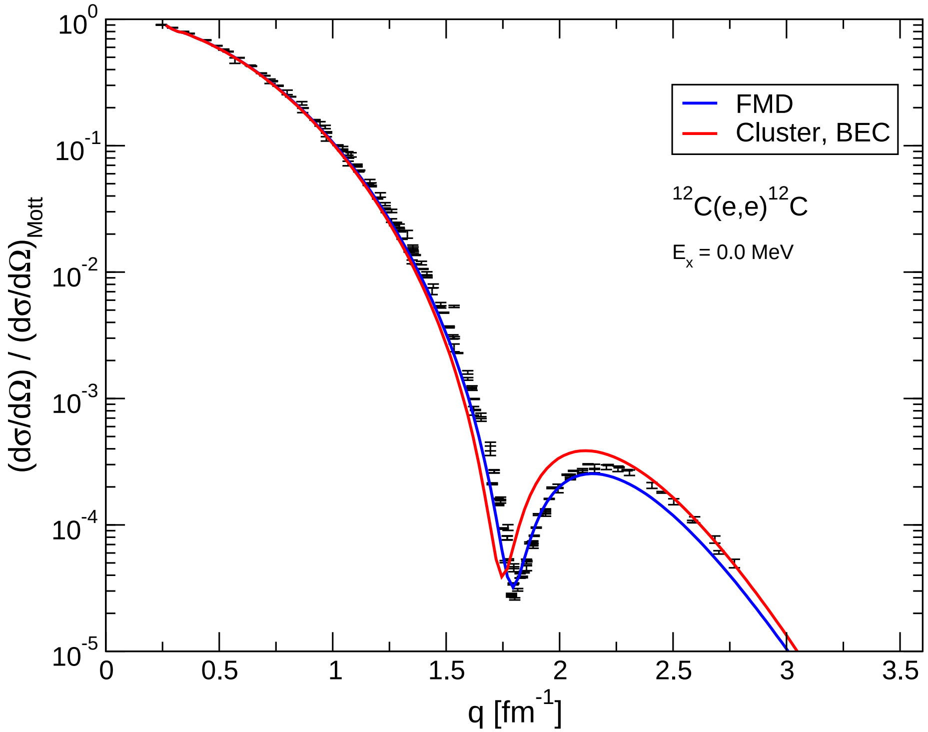
	Exp[1]	Exp[2]	Exp[3]	FMD	α-cluster	'BEC'[4]
$E(0_1^+)$	-92.16			-92.64	-89.56	-89.52
$E^*(2_1^+)$	4.44			5.31	2.56	2.81
$E(3\alpha)$	-84.89			-83.59	-82.05	-82.05
$E(0_2^+)-E(3\alpha)$	0.38			0.43	0.38	0.26
$E(0_3^+)-E(3\alpha)$	(3.0)	2.7(3)	3.96(5)	2.84	2.81	
$E(2_2^+)-E(3\alpha)$	(3.89)	2.6(3)	6.63(3)	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	
$M(E0, 0_1^+ \rightarrow 0_2^+)$	5.4(2)			6.53	6.52	6.45
$B(E2, 2_1^+ \rightarrow 0_1^+)$	7.6(4)			8.69	9.16	
$B(E2, 2_1^+ \rightarrow 0_2^+)$	2.6(4)			3.83	0.84	

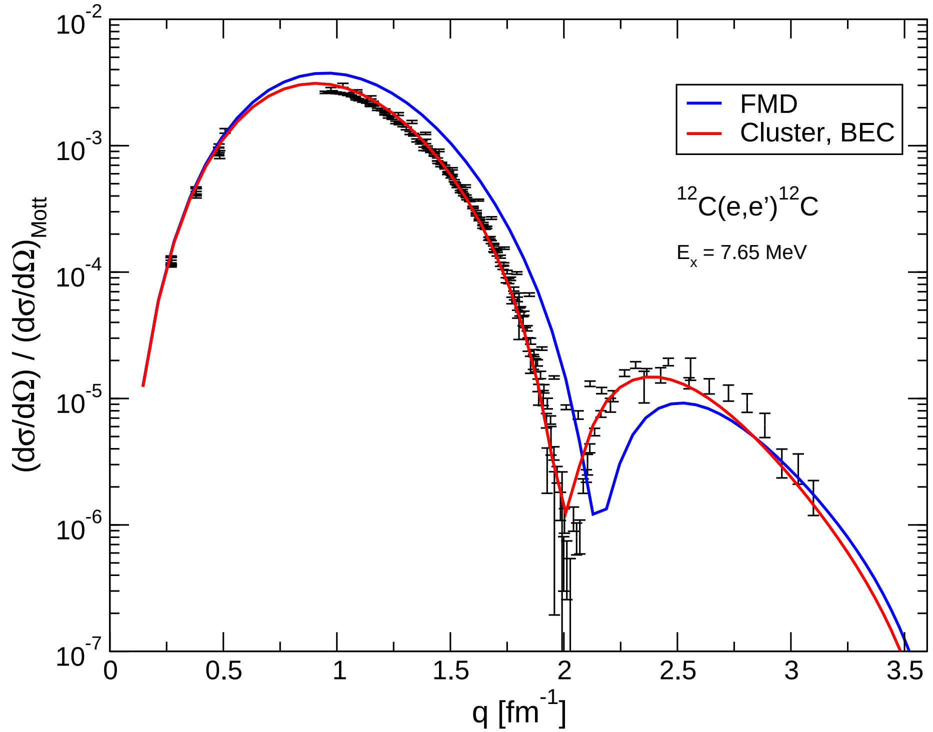
experimental situation for 0_3^+ and 2_2^+ states still unsettled

2_2^+ resonance at 1.8 MeV above treshold included in NACRE compilation

[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)

Electron Scattering Data





- compare with precise electron scattering data up to high momenta in Distorted Wave Born Approximation
- use intrinsic density

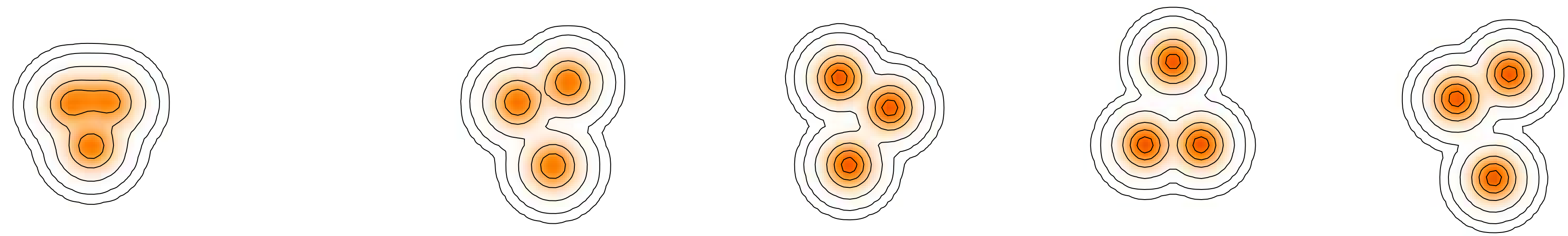
$$\rho(\mathbf{x}) = \sum_{k=1}^{A} \left\langle \Psi \middle| \delta(\underset{\sim}{\mathbf{x}}_k - \underset{\sim}{\mathbf{X}} - \mathbf{x}) \middle| \Psi \right\rangle$$

- ➨ elastic form factor described very well by FMD
- ➨ transition form factor better described by cluster model

M. Chernykh, H. Feldmeier, T. Neff, P. von Neumann-Cosel, and A. Richter, Phys. Rev. Lett. **98** (2007) 032501

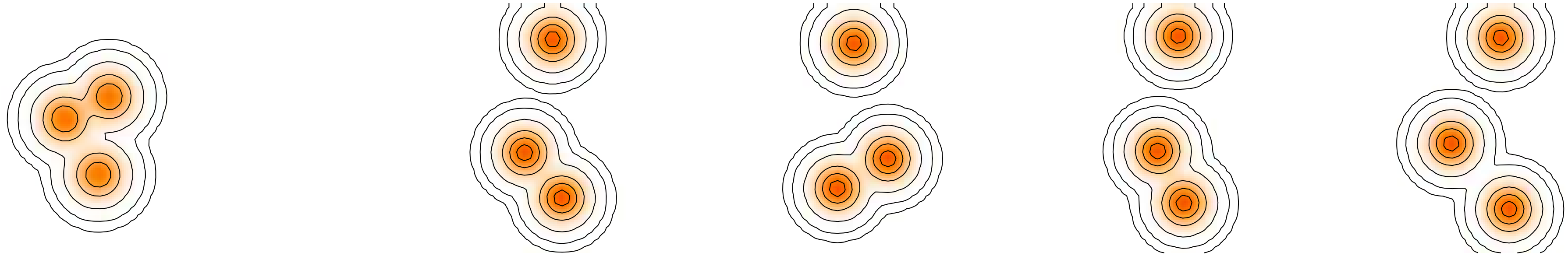
Important Configurations

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



$\left|\left\langle \cdot \mid 0_1^+ \right\rangle\right| = 0.94$
$\left|\left\langle \cdot \mid 2_1^+ \right\rangle\right| = 0.93$

$\left|\left\langle \cdot \mid 0_2^+ \right\rangle\right| = 0.72$ $\left|\left\langle \cdot \mid 0_2^+ \right\rangle\right| = 0.71$ $\left|\left\langle \cdot \mid 0_2^+ \right\rangle\right| = 0.61$ $\left|\left\langle \cdot \mid 0_2^+ \right\rangle\right| = 0.61$



$\left|\left\langle \cdot \mid 3_1^- \right\rangle\right| = 0.83$

$\left|\left\langle \cdot \mid 0_3^+ \right\rangle\right| = 0.50$ $\left|\left\langle \cdot \mid 0_3^+ \right\rangle\right| = 0.49$ $\left|\left\langle \cdot \mid 0_3^+ \right\rangle\right| = 0.44$ $\left|\left\langle \cdot \mid 0_3^+ \right\rangle\right| = 0.41$

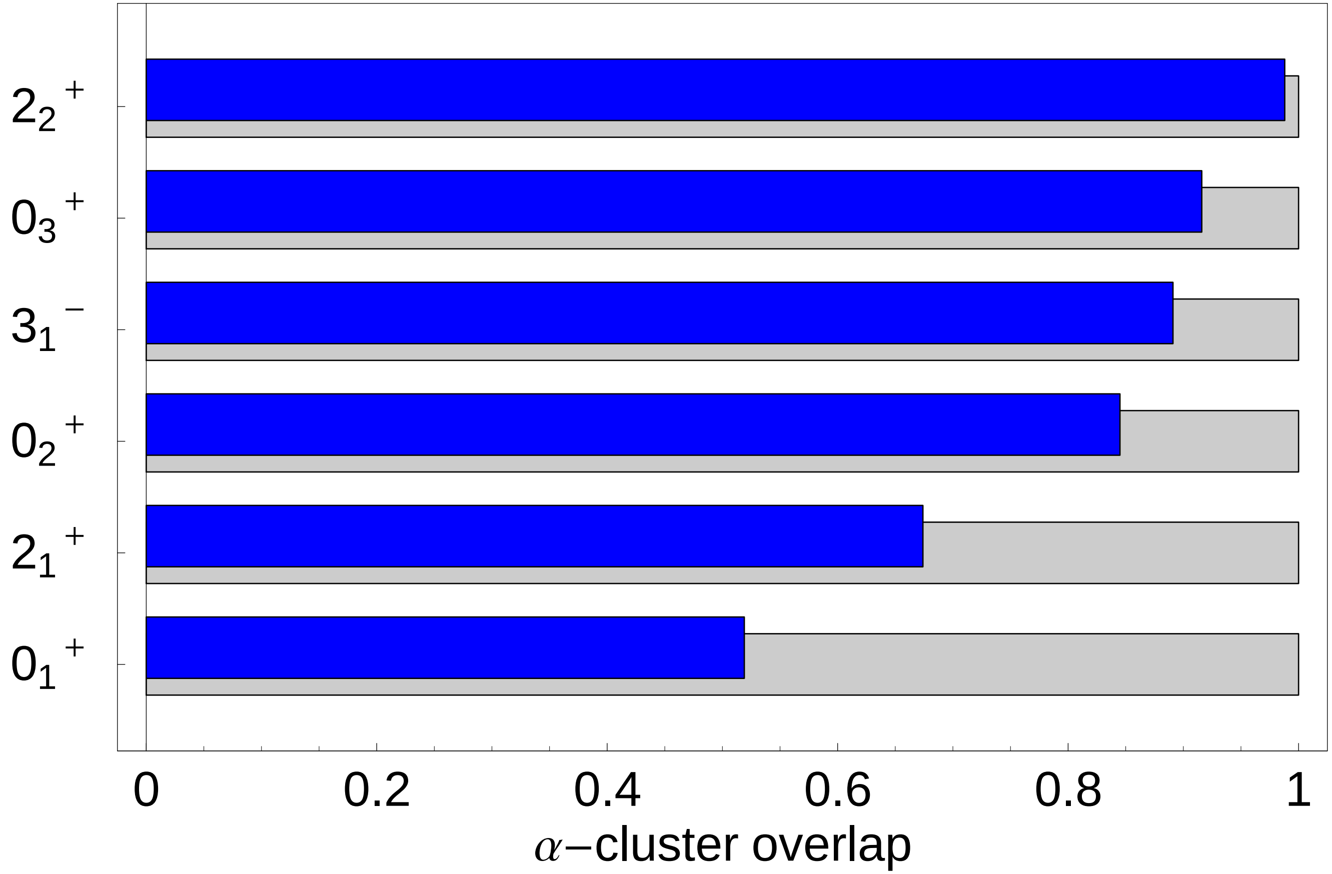
FMD basis states are not orthogonal!

loosely bound, gas-like states

Overlap with Cluster Model Space

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

$$N_\alpha = \langle \Psi \,|\, \underset{\sim}{P}_{3\alpha} \,|\, \Psi \rangle$$



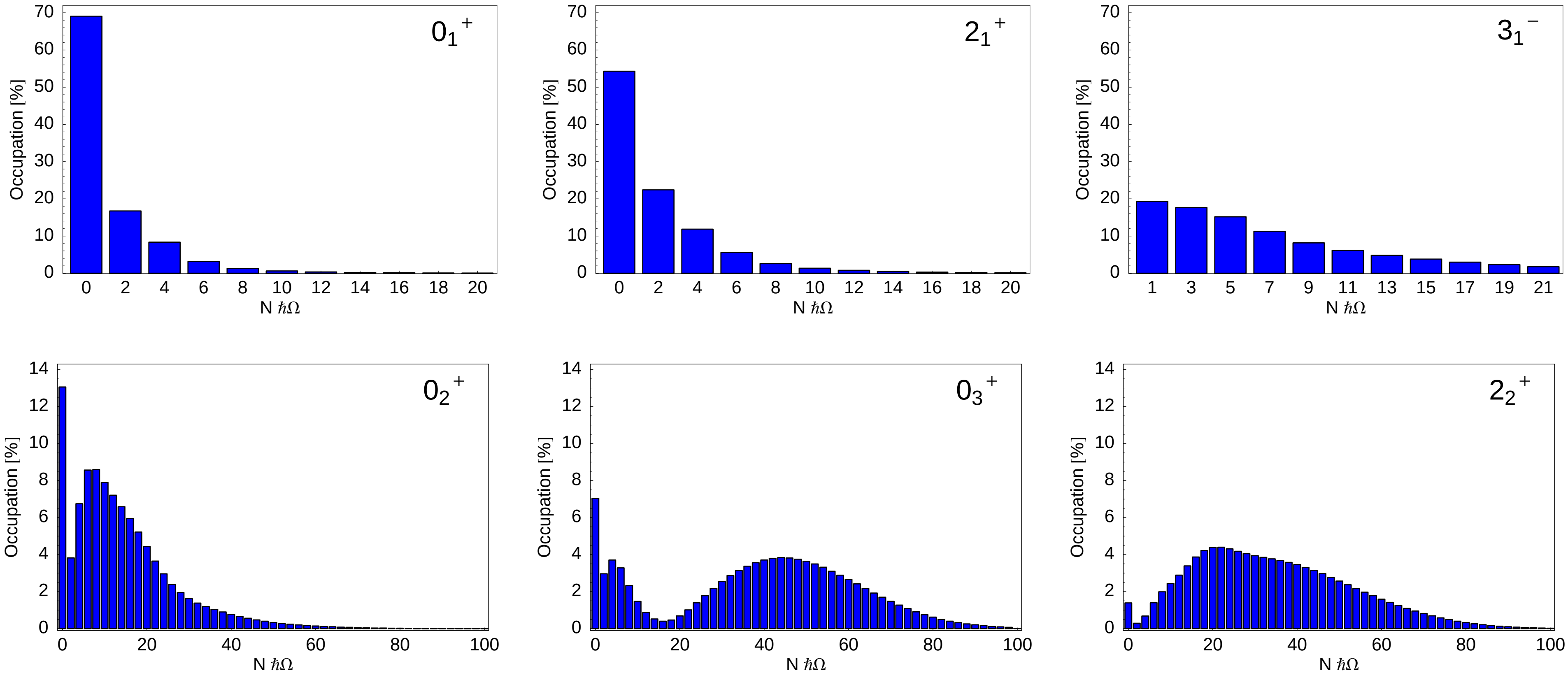
Hoyle state has 15% non-alpha admixtures

Cluster States in ^{12}C
Harmonic Oscillator $N\hbar\Omega$ Excitations

Y. Suzuki et al., Phys. Rev. C **54** (1996) 2073

$$N_Q = \langle\, \Psi \,|\, \delta \left(\textstyle\sum_i (\underset{\sim}{H}_i^{HO}/\hbar\Omega - 3/2) - Q \right) |\, \Psi \,\rangle$$

FMD



α-cluster states in the No-Core Shell Model ?

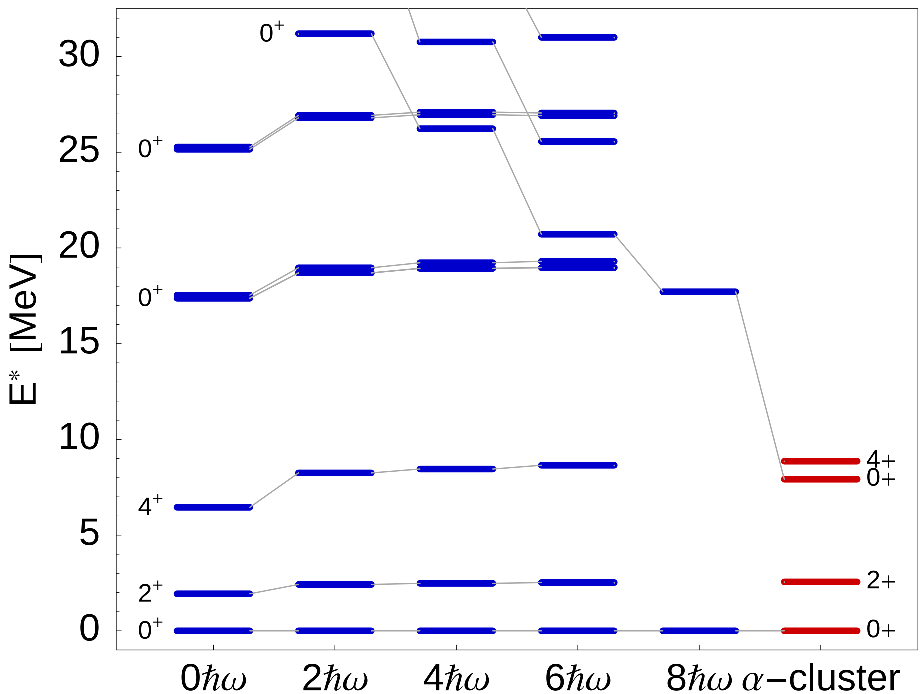
- compare spectra in NCSM and α-cluster model using the Volkov interaction
- bare interaction used in NCSM calculations

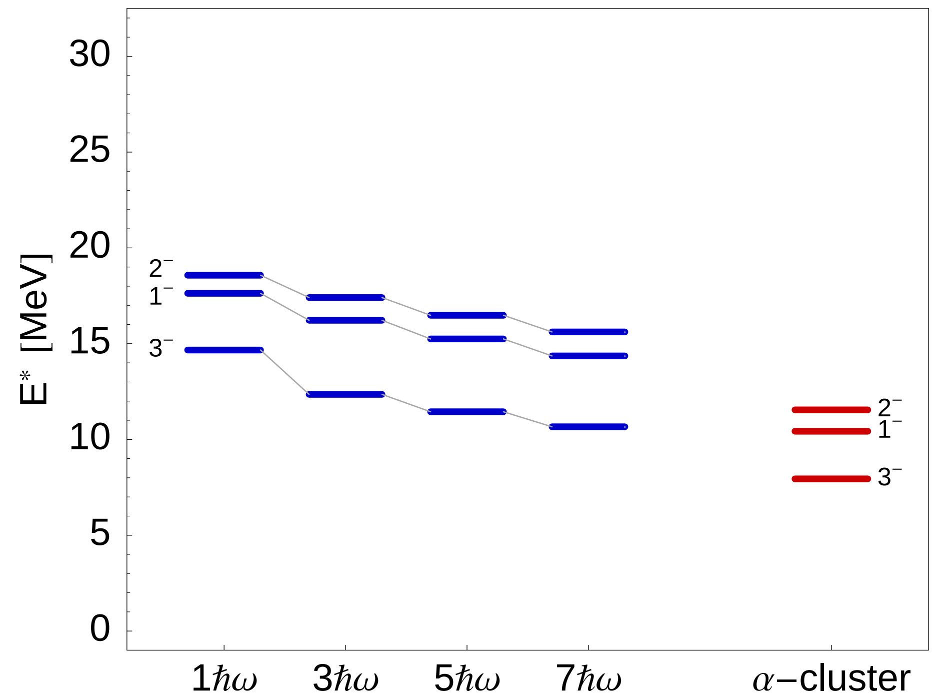
➨ good agreement for ground state band (0^+_1, 2^+_1, 4^+_1)

➨ very slow convergence for cluster states

Binding energies

	^{4}He	^{12}C
Cluster	-27.3 MeV	-89.6 MeV
NCSM	-28.3 MeV	-95.4 MeV





Neon Isotopes ^{17}Ne-^{22}Ne

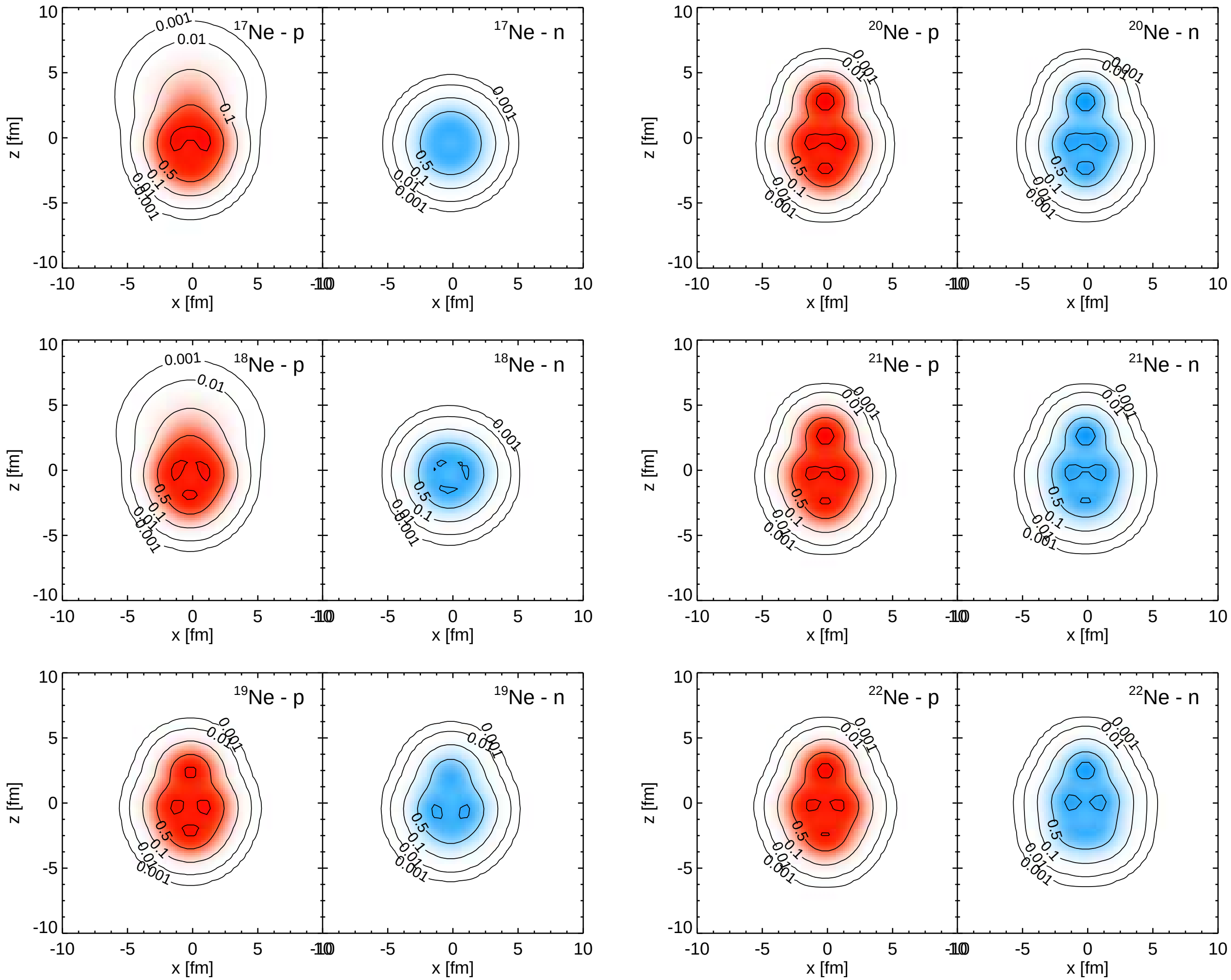
Structure

- s^2/d^2 **occupation in** ^{17}Ne **and** ^{18}Ne
- ^{3}He **and** ^{4}He **cluster admixtures**

Observables

- **Charge Radii**
- **Matter Radii**
- **Is** ^{17}Ne **a Halo nucleus ?**

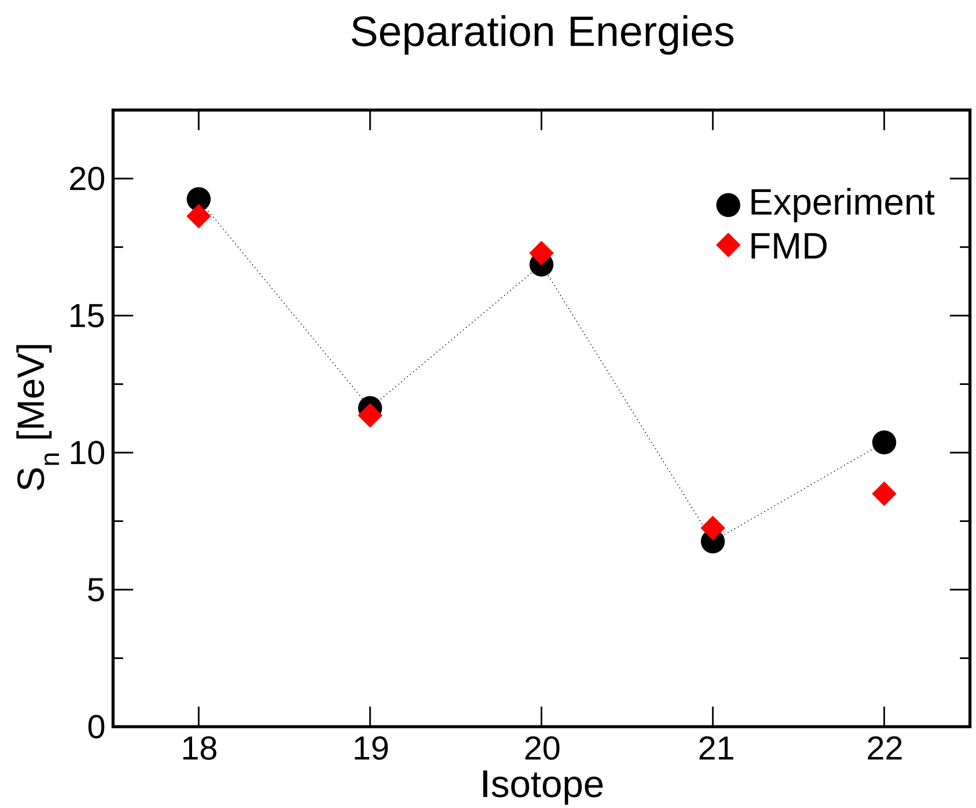
Calculation



- Variation after parity projection on positive and negative parity
- Crank strength of spin-orbit force, changes properties of single-particle orbits and their occupations
- "s^2" and "d^2" minima in ^{17,18}Ne
- explicit cluster configurations:
  - ^{17}Ne: ^{14}O-^{3}He
  - ^{18}Ne: ^{14}O-^{4}He
  - ^{19}Ne: ^{16}O-^{3}He and ^{15}O-^{4}He
  - ^{20}Ne: ^{16}O-^{4}He
  - ^{21}Ne: "^{17}O"-^{4}He
  - ^{22}Ne: "^{18}O"-^{4}He

Intrinsic proton/neutron densities of dominant FMD state

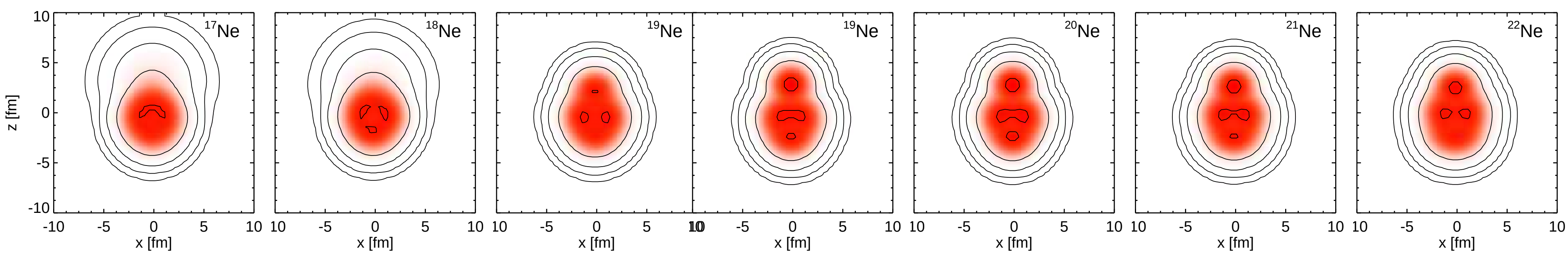
Separation energies



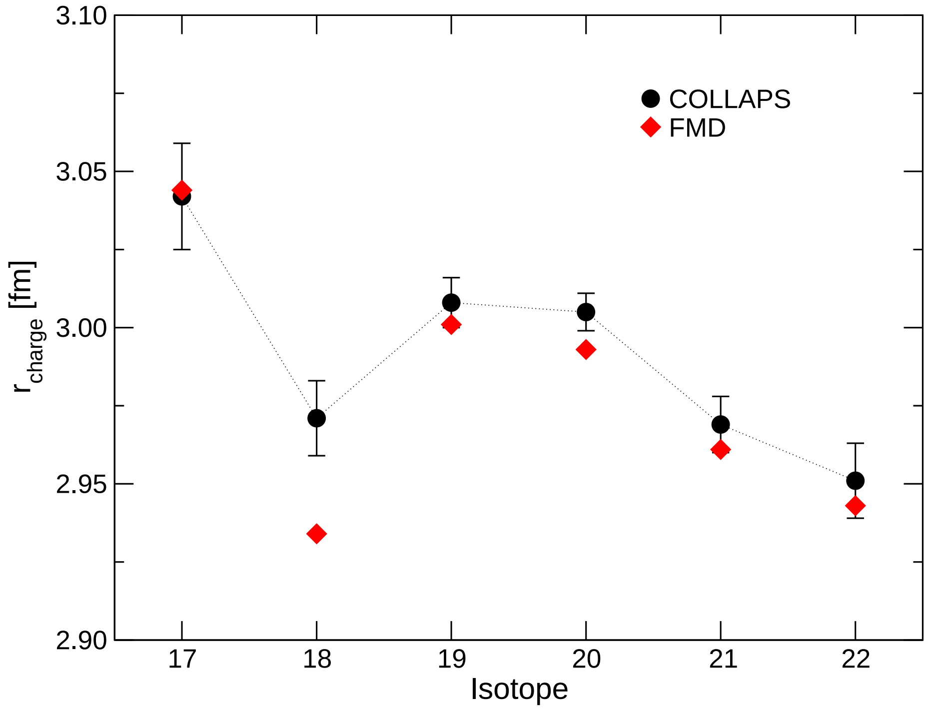
^{17,18}Ne: s^2/d^2 admixture

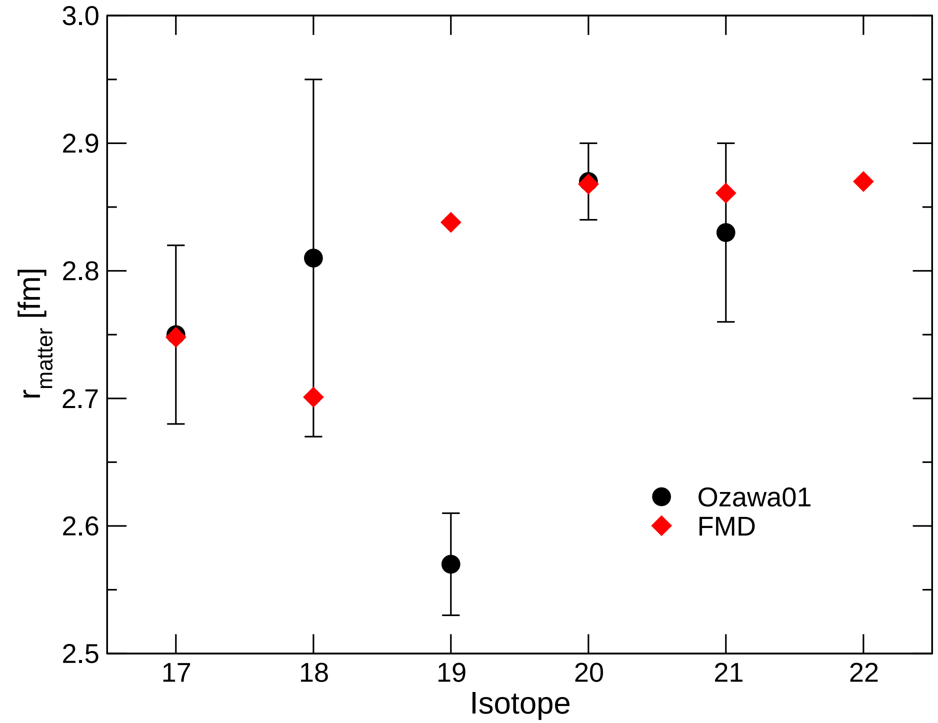
^{19}Ne: ^{3}He, α clustering

$^{20-22}$Ne: α clustering



Charge and Matter Radii





- charge radii of ^{17,18}Ne depend strongly on s^2/d^2 occupations
- cluster admixtures responsible for large charge radii in $^{19-22}$Ne
- measurements of charge radii by COLLAPS@ISOLDE

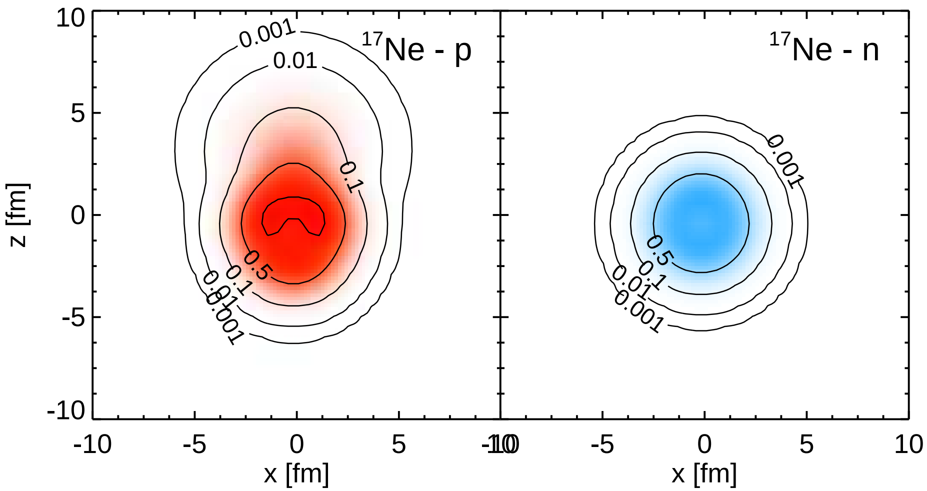
- matter radii from interaction cross sections

  A. Ozawa et al., Nuc. Phys. **A693** (2001) 32

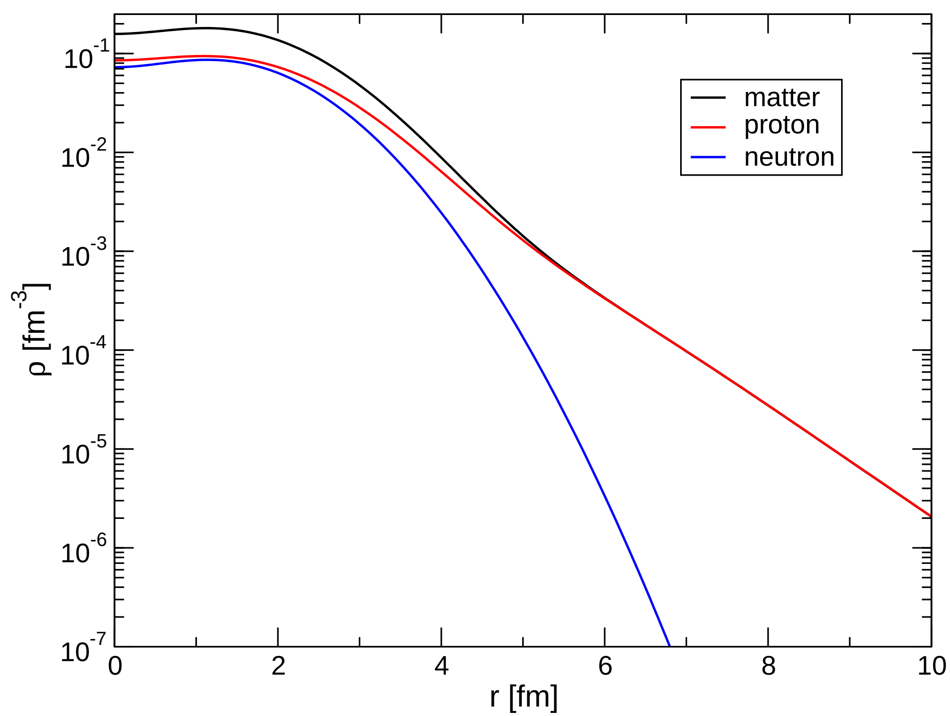
- good agreement with expection of ^{19}Ne

W. Geithner, T. Neff, *et al.*, submitted to Phys. Rev. Lett.

Neon Isotopes
^{17}Ne **Halo ?**



	FMD	Experiment
r_{ch}[fm]	3.03	3.042(17)
r_{mat}[fm]	2.75	2.75(7)
$B(E2;\frac{1}{2}^- \rightarrow \frac{3}{2}^-)[e^2\text{fm}^4]$	76.7	66^{+18}_{-25}
$B(E2;\frac{1}{2}^- \rightarrow \frac{5}{2}^-)[e^2\text{fm}^4]$	119.8	124(18)
occupancy s^2	40%	
occupancy d^2	55%	



- proton skin $r_p - r_n = 0.45$ fm
- 40% probability to find a proton at $r > 5$ fm

Summary

Unitary Correlation Operator Method

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

Fermionic Molecular Dynamics

- Microscopic many-body approach using Gaussian wave-packets
- Consistent description of well bound states with shell structure and loosely bound states of cluster or halo nature
- ^{12}C spectrum, Hoyle state and other high-lying 0^+ and 2^+ states, monopole transition form factor, analysis of FMD wave functions in harmonic oscillator basis, comparison with no-core shell model calculations
- Neon isotopes, separation energies, charge and matter radii, halo structure in ^{17}Ne, importance of cluster admixtures in $^{19-22}$Ne ground states

Thanks

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