Exotic Nuclear Structures and Reactions in Fermionic Molecular Dynamics

Hans Feldmeier, GSI, Darmstadt
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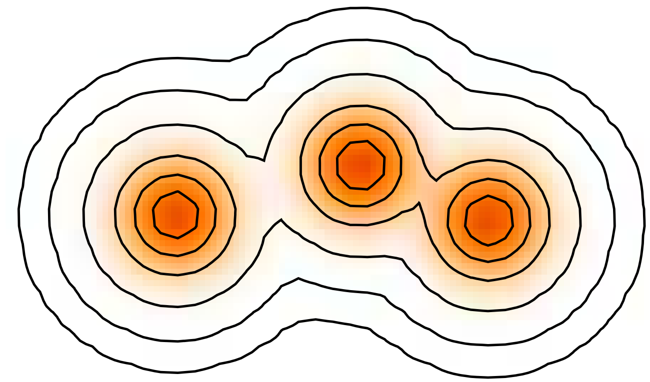


Overview

Fermionic Molecular Dynamics

Hoyle State in ^{12}C

Helium Isotopes

Neon Isotopes, ^{17}Ne **2 Proton Halo**

Scattering ^{3}He **–** ^{4}He **and**
Radiative Capture $^{3}He(\alpha,\gamma)^{7}Be$

Fermionic Molecular Dynamics (FMD)

Nucleon-Nucleon Interaction

FMD Wave Functions

Projection After Variation,
Variation After Projection
Multiconfiguration

Microscopic Approach

Aim

- degrees of freedom: nucleons
- describe low energy properties of nuclear many-body system

  in terms of a Hamiltonian $\underset{\sim}{H} = \underset{\sim}{T} + \underset{\sim}{V}_{NN} + \underset{\sim}{V}_{NNN}$

  and many-body states $\left| \widehat{\Psi} \right\rangle$

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

Ingredients

$\underset{\sim}{H}$ = Hamiltonian with realistic NN-potential $\underset{\sim}{V}_{NN}$ and corresponding 3-body force $\underset{\sim}{V}_{NNN}$ (phase shifts, deuteron, 3 and 4 nucleon systems)

$\left| \widehat{\Psi}_n \right\rangle \in$ many-body Hilbert space

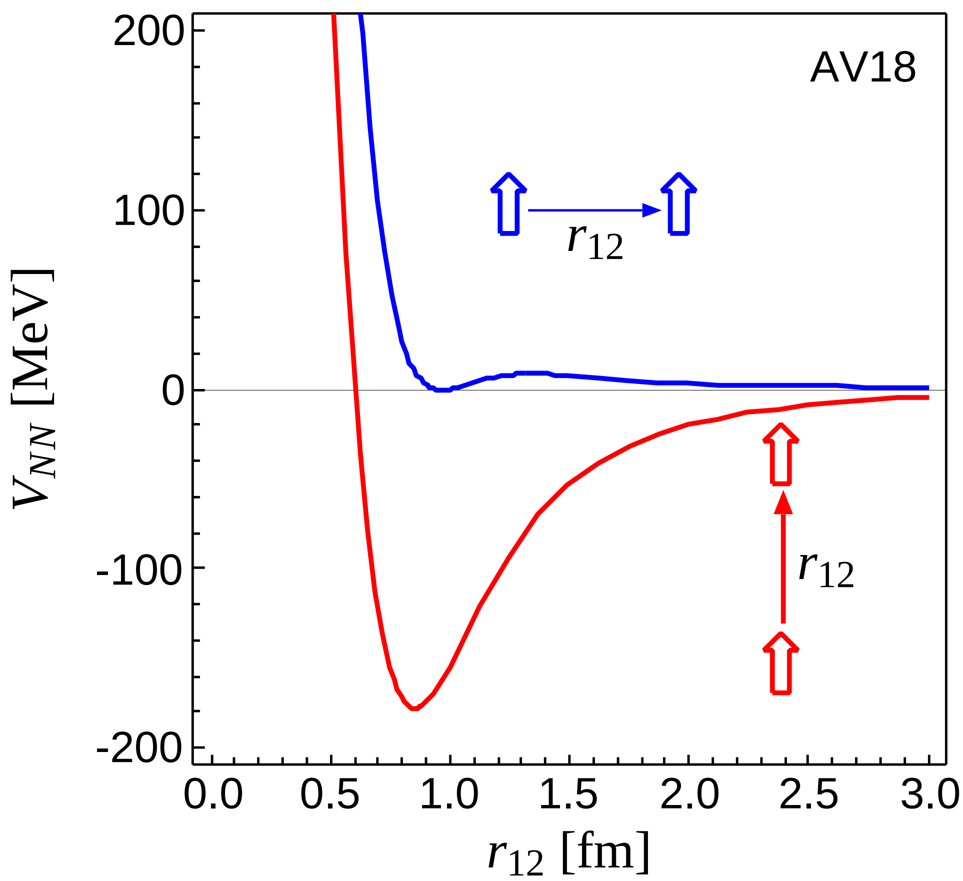
$\left\langle \mathbf{r}_1\sigma_1\tau_1, \mathbf{r}_2\sigma_2\tau_2, \cdots, \mathbf{r}_A\sigma_A\tau_A \middle| \widehat{\Psi}_n \right\rangle$ is terribly complicated for realistic interaction

main problem: short-range repulsive and tensor correlations induced by $\underset{\sim}{V}_{NN}$

Realistic Nuclear Force

Argonne V18 **(** $S = 1,\ T = 0$ **)**

spins 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**

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

Effective Interaction for FMD

Effective two-body interaction

- short range repulsive and tensor correlations treated by **UCOM**

$$\underset{\sim}{H} \implies \underset{\sim}{C}^{-1}\underset{\sim}{H}\,\underset{\sim}{C} = \underset{\sim}{T} + \underset{\sim}{V}_{\mathrm{UCOM}} + \ldots$$

- to account for medium-long ranged correlations missing in FMD Hilbert space add phenomenological two-body term $\delta\underset{\sim}{V}$ with central and spin-orbit part

- fit correction $\delta\underset{\sim}{V}$ to energies and radii of "closed-shell" nuclei (^{4}He, ^{16}O, ^{40}Ca, ^{24}O, ^{34}Si, ^{48}Ca)
$\langle\, \delta\underset{\sim}{V}\,\rangle \approx 15\% \,\langle\, \underset{\sim}{V}_{\mathrm{UCOM}}\,\rangle$

➨ Same Hamiltonian $\underset{\sim}{H} = \underset{\sim}{T} + \underset{\sim}{V}_{\mathrm{UCOM}} + \delta\underset{\sim}{V}$ for all nuclei

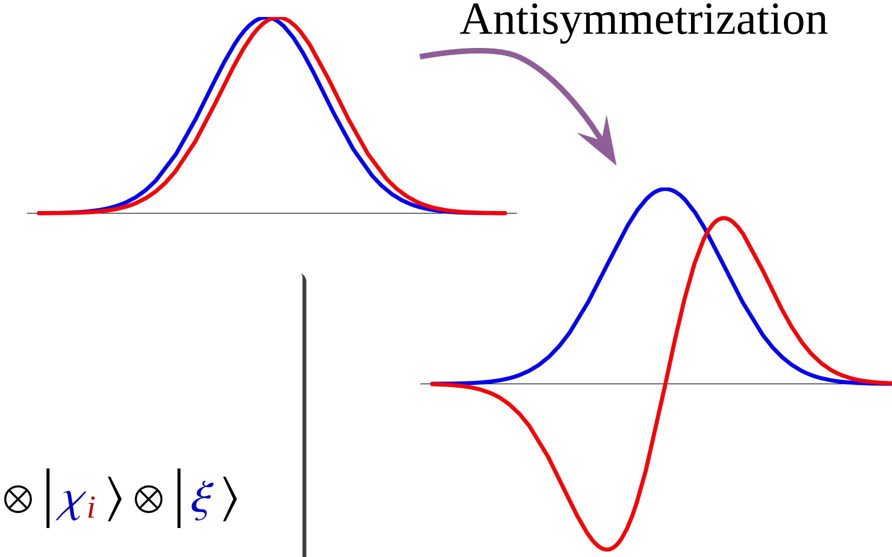
FMD Many-Body Hilbert Space

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

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

- Gaussian wave-packets in phase-space, spin is free, isospin is fixed

Dynamics in Hilbert space

spanned by one or several non-orthogonal $\left| Q^{(a)} \right\rangle$

$$\left| \Psi; J^\pi M \right\rangle = \sum_{aK} \Psi_{aK} \underset{\sim}{P}^{J^\pi}_{MK} \underset{\sim}{P}^{\mathbf{P}=0} \left| Q^{(a)} \right\rangle$$

variational principle $\Rightarrow Q^{(a)} = \{ q_\nu^{(a)}, \nu = 1 \cdots A \},\ \Psi_{aK}$

- Hilbert space contains shell-model, clusters, halos, scattering states

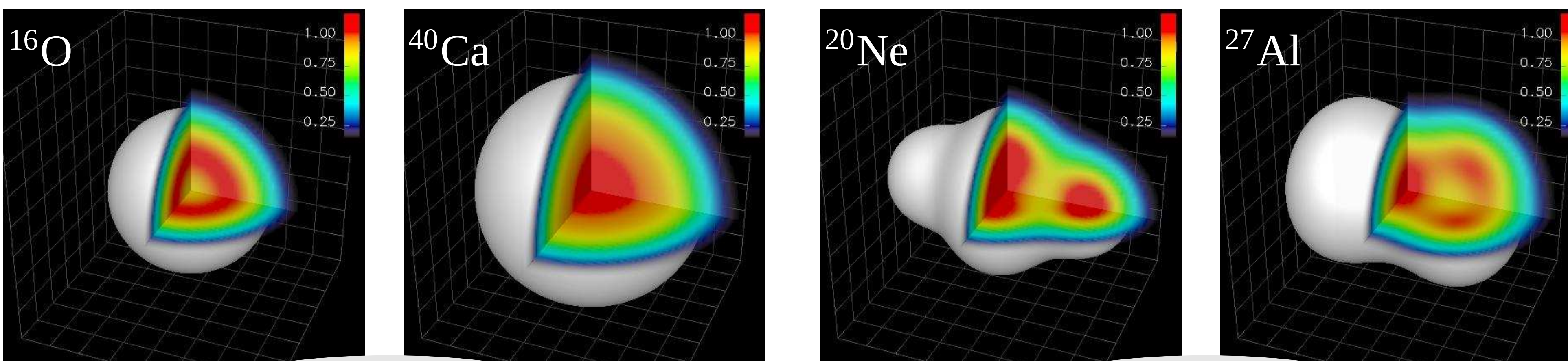
Perform Variation

Minimization

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

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

- 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

Projection to restore Symmetries

Projection After Variation (PAV)

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

$$\underset{\sim}{P}^{\pm} = \tfrac{1}{2}\left(1 \pm \underset{\sim}{\Pi}\right)$$

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

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

$$\left| Q \, ; J^{\pi} M, K \right\rangle = \underset{\sim}{P}^{\pm} \, \underset{\sim}{P}^{J}_{MK} \, \underset{\sim}{P}^{\mathbf{P}=0} \left| Q \right\rangle$$

Variation After Projection (VAP)

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

$$\left| Q^{\pm} \right\rangle = \tfrac{1}{2}\left(1 \pm \underset{\sim}{\Pi}\right) \left| Q \right\rangle$$

Multi-Configuration Mixing

- most general projected state for multi-configuration calculations

$$\left|\Psi; J^\pi M\right\rangle = \sum_{aK} \Psi_{aK}\, \underset{\sim}{P}^\pi \underset{\sim}{P}^J_{MK} \underset{\sim}{P}^{\mathbf{P}=0} \left| Q^{(a)} \right\rangle$$

- task: find a set of intrinsic states $\left\{ \left| Q^{(a)} \right\rangle, a = 1, \ldots, N \right\}$ that describe the physical situation well

Multi-configuration calculations

$$\underset{\sim}{H} \left| J^\pi M, n \right\rangle = E_n^{J^\pi} \left| J^\pi M, n \right\rangle$$

- **diagonalize** Hamiltonian in this set of non-orthogonal projected intrinsic states

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

- energy levels $E_n^{J^\pi}$ and eigenstates $\left| J^\pi M, n \right\rangle$ describing nuclear many-body system

$$\left| J^\pi M, n \right\rangle = \sum_{bK'} c^n_{bK'}\, \underset{\sim}{P}^\pi \underset{\sim}{P}^J_{MK'} \underset{\sim}{P}^{\mathbf{P}=0} \left| Q^{(b)} \right\rangle$$

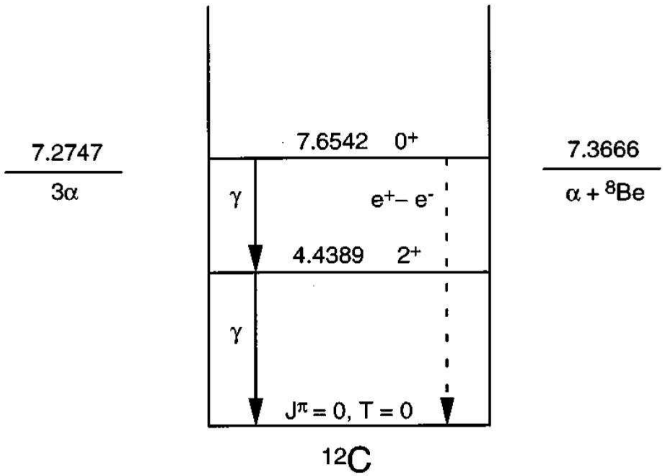
Cluster States in ^{12}C

Astrophysical Motivation

Structure

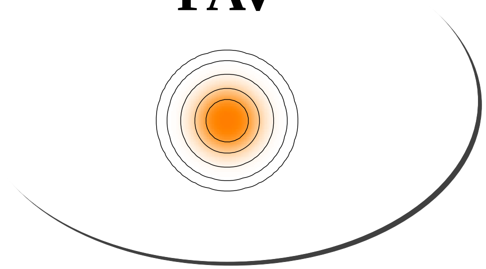
- Is the Hoyle state a α-cluster state ?
- Other excited 0^+ and 2^+ states

➨ Analyze wave functions in harmonic oscillator basis



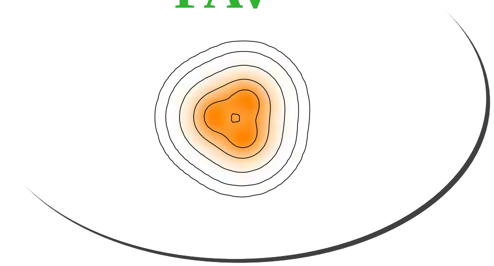
FMD - Variation, PAV$^{\pi}$, Multiconfig.

PAV

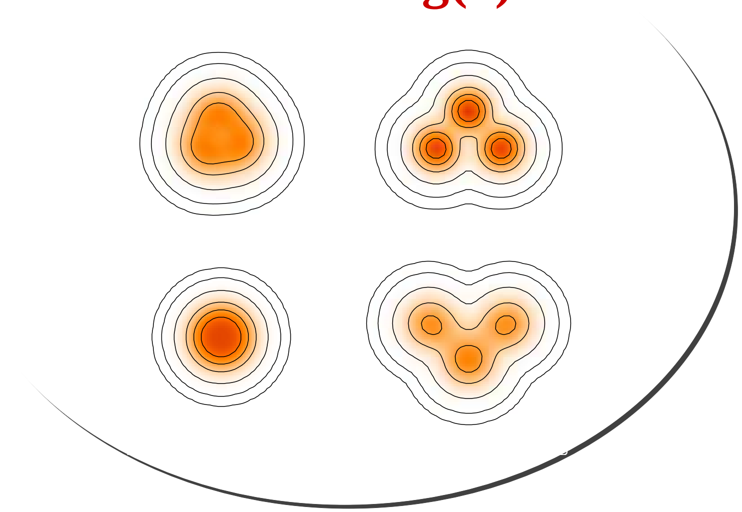


^{12}C

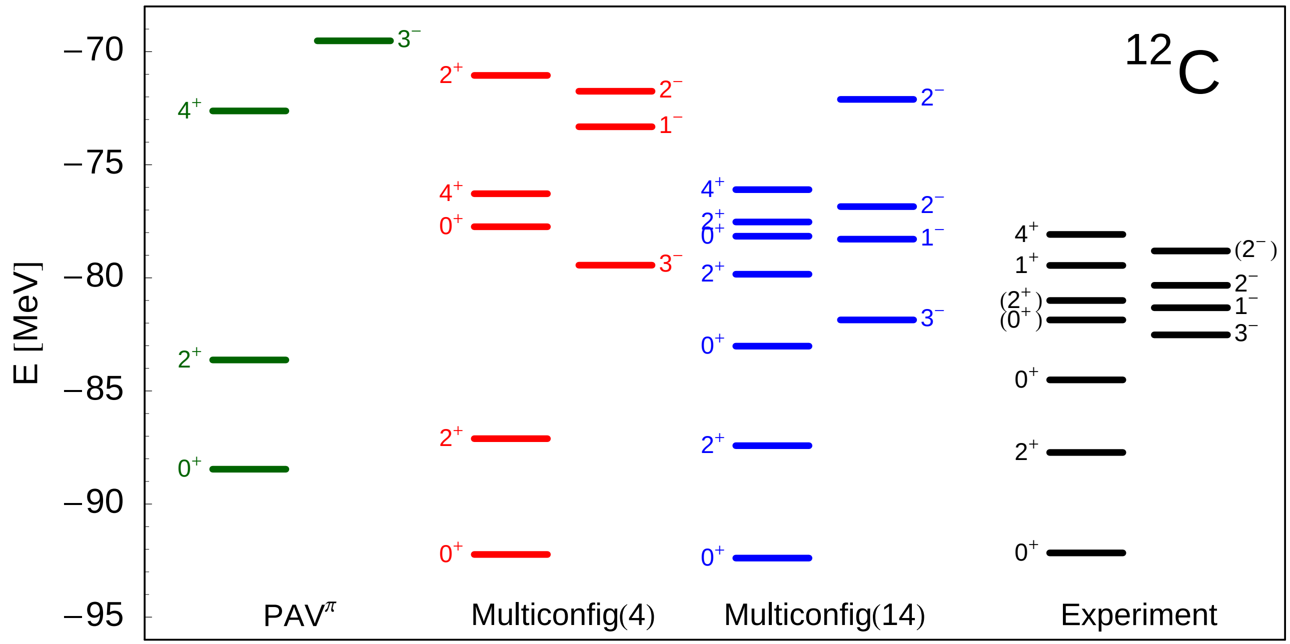
PAV$^{\pi}$



Multiconfig(4)

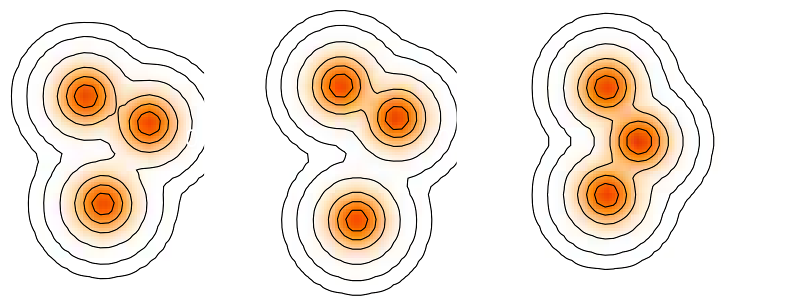


	E [MeV]	r_{charge} [fm]	$B(E2)$ [e^2fm^4]
PAV	-81.4	2.36	-
PAV$^{\pi}$	-88.5	2.51	36.3
Multiconfig(4)	-92.2	2.52	42.8
Multiconfig(14)	-92.4	2.52	42.9
Exp	-92.2	2.47	39.7 ± 3.3



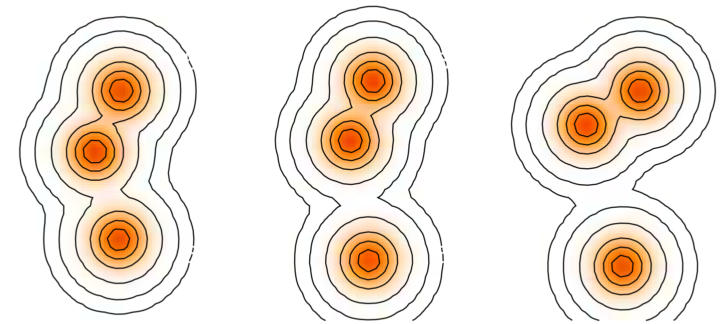
^{12}C excited 0^+ and 2^+ states

0_2^+ state



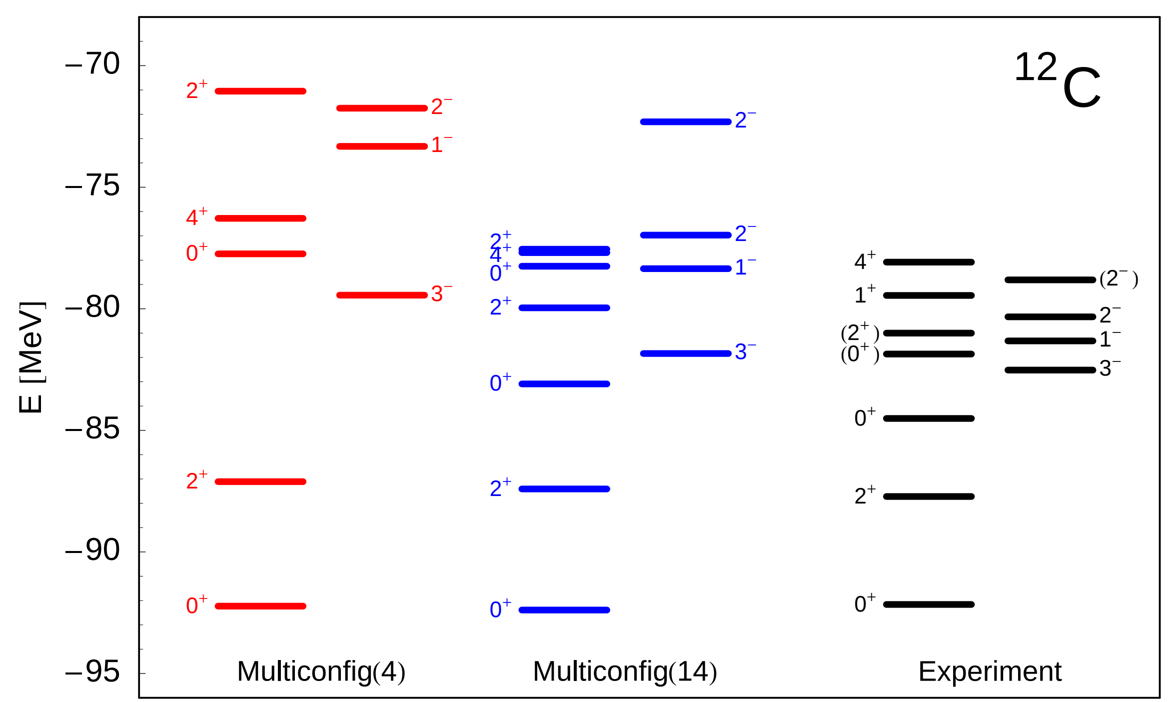
$|\langle \cdot | 0_2^+ \rangle| = 0.76$ $|\langle \cdot | 0_2^+ \rangle| = 0.71$ $|\langle \cdot | 0_2^+ \rangle| = 0.50$

0_3^+ state

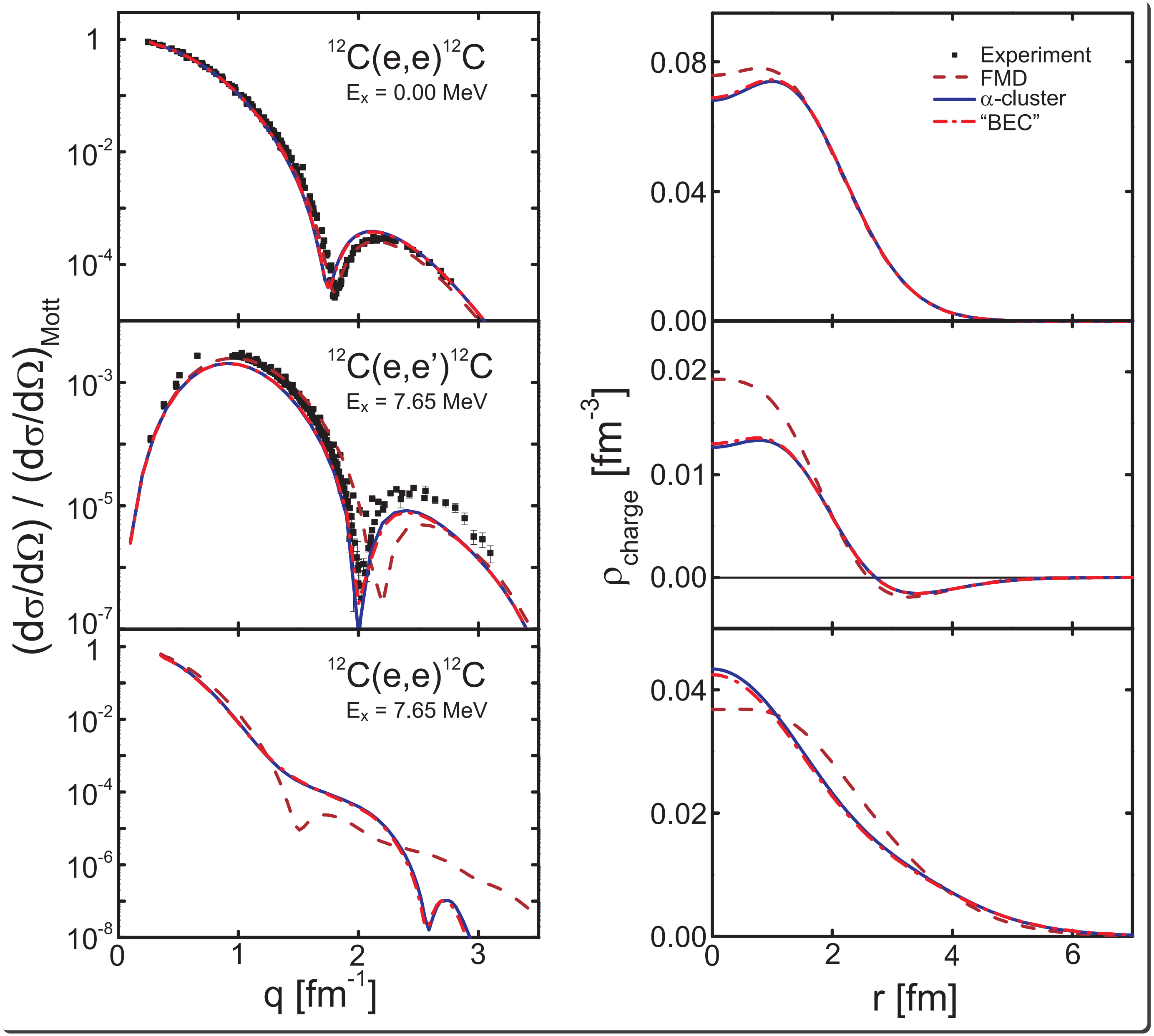


$|\langle \cdot | 0_3^+ \rangle| = 0.69$ $|\langle \cdot | 0_3^+ \rangle| = 0.65$ $|\langle \cdot | 0_3^+ \rangle| = 0.44$

	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	
$Q(2_1^+)$[efm^2]	5.85	
$Q(2_2^+)$[efm^2]	-23.65	
$Q(2_3^+)$[efm^2]	5.89	



^{12}C Hoyle State in Electron Scattering



- calculate formfactors, center-of-mass treated properly, formfactor is a *A*-body operator

$$F(\mathbf{q}) = \sum_i \langle \Psi_a \,|\, e^{i\mathbf{q}\cdot(\underset{\sim}{\mathbf{x}}_i - \underset{\sim}{\mathbf{X}})} \,|\, \Psi_b \rangle$$

- compare to experiment in Distorted Wave Born Approximation
- α-cluster and "BEC" calculated with mod. Volkov interation

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

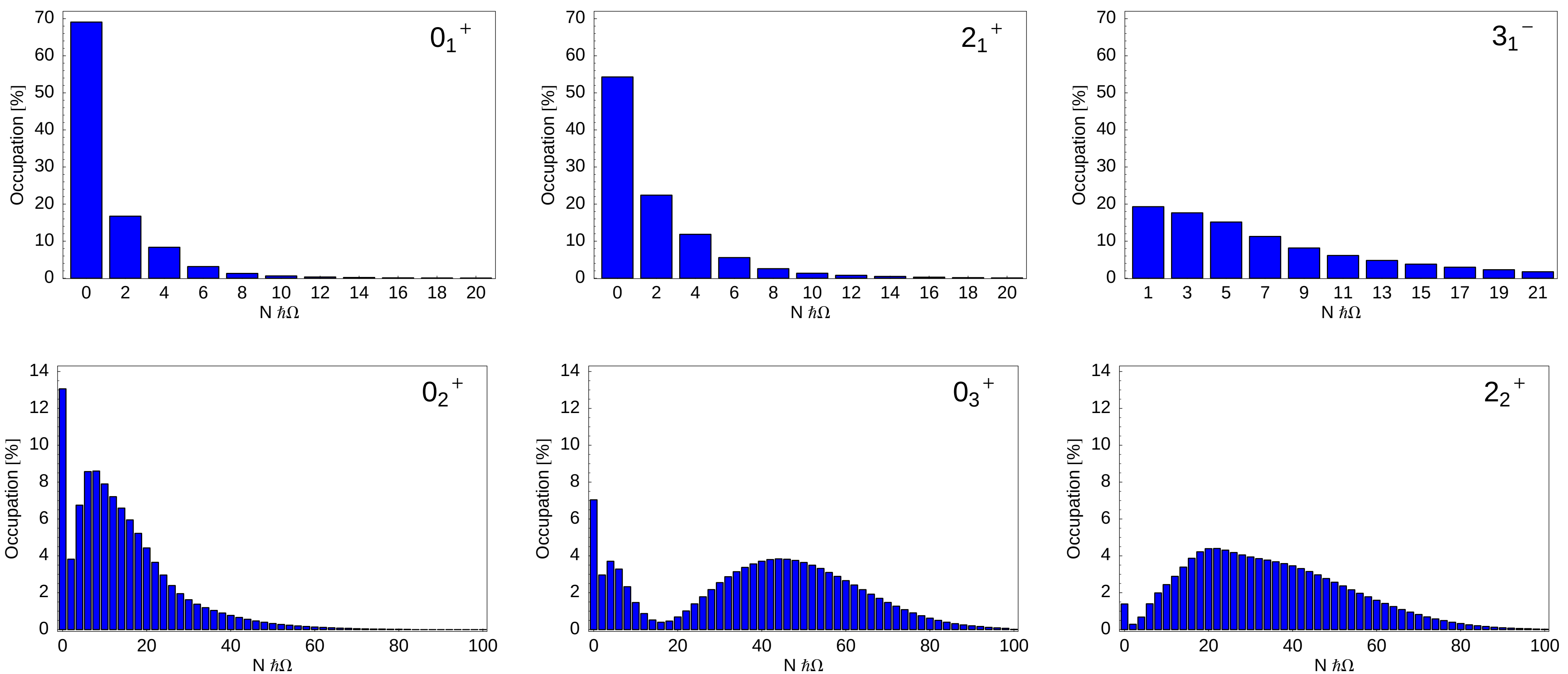
"BEC" formfactors: Y. Funaki et al. EPJA 28(2006)259 and private communication

Harmonic Oscillator $N\,\hbar\Omega$ Excitations

Occupation probabilities of spaces with N harmonic oscillator quanta

$$\mathrm{Occ}(N) = \langle \Psi \,|\, \delta\Big(\textstyle\sum_{i=1}^{A}\big(\underset{\sim}{H}^{HO}(i)/\hbar\Omega - 3/2\big) - N\Big) \,|\, \Psi \rangle$$

FMD



Helium Isotopes ^{4}He – ^{8}He

Structure

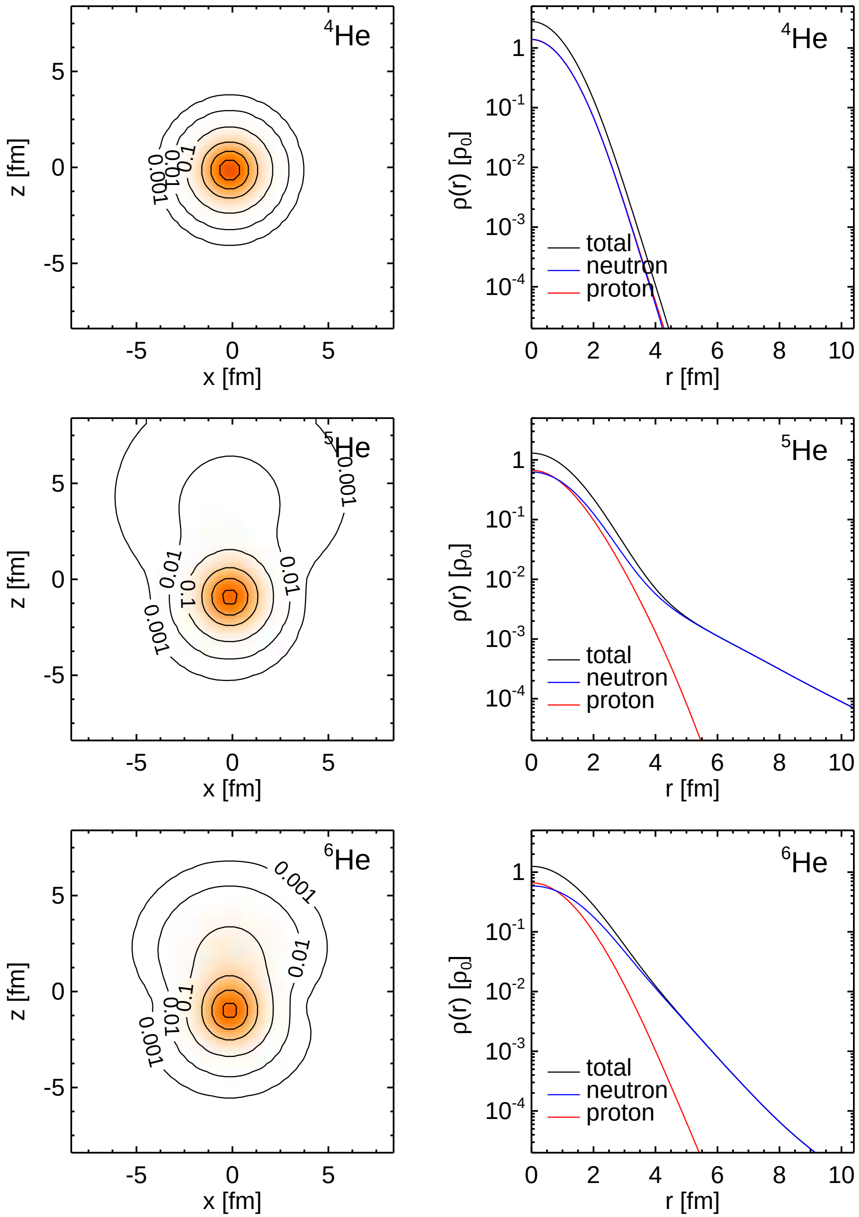
- Borromean behaviour
- Zero-point oscillation of soft dipole mode

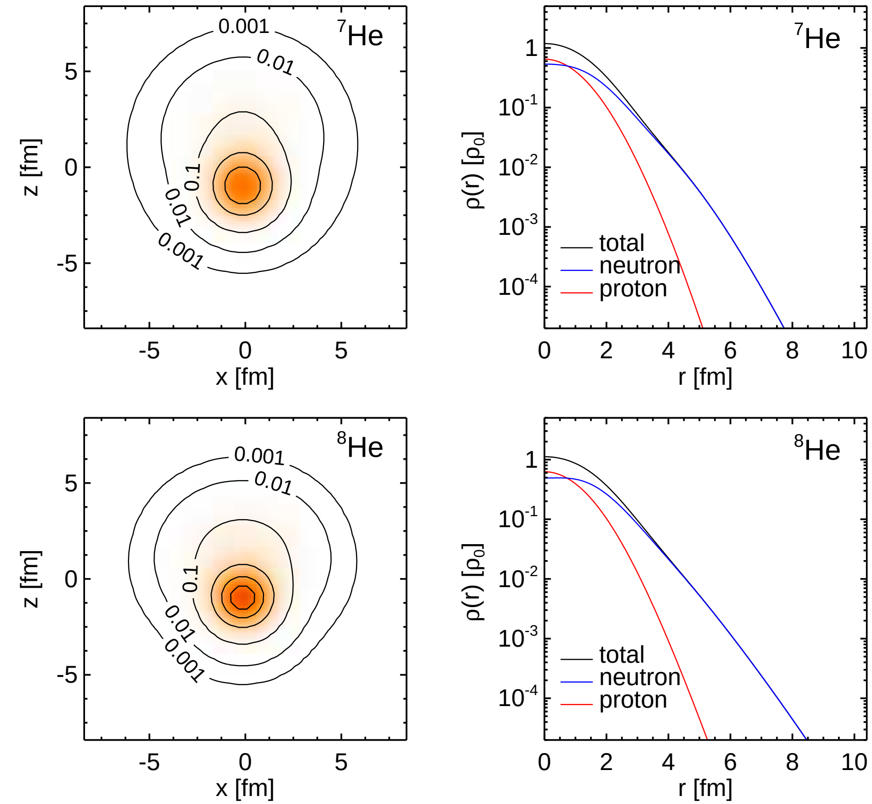
Observables

- Charge radii
- Matter radii
- Proton, neutron densities

Helium Isotopes

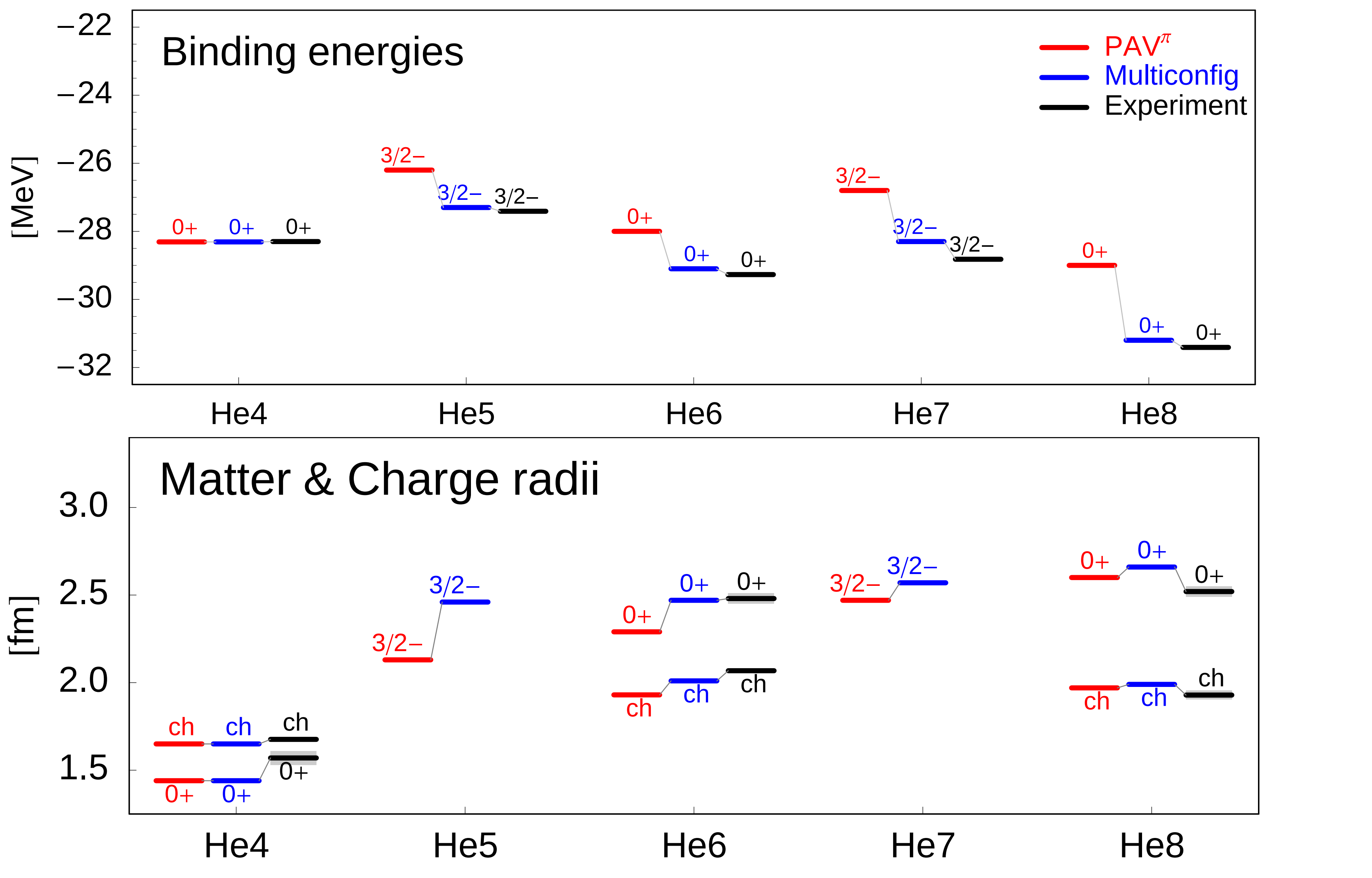
dipole and quadrupole constraints





- intrinsic densities of VAP$^\pi$ states
  $\left| Q^{\pm} \right\rangle = \frac{1}{2}\left(1 \pm \underset{\sim}{\Pi}\right) \left| Q \right\rangle$
- radial densities from multiconfiguration calculations

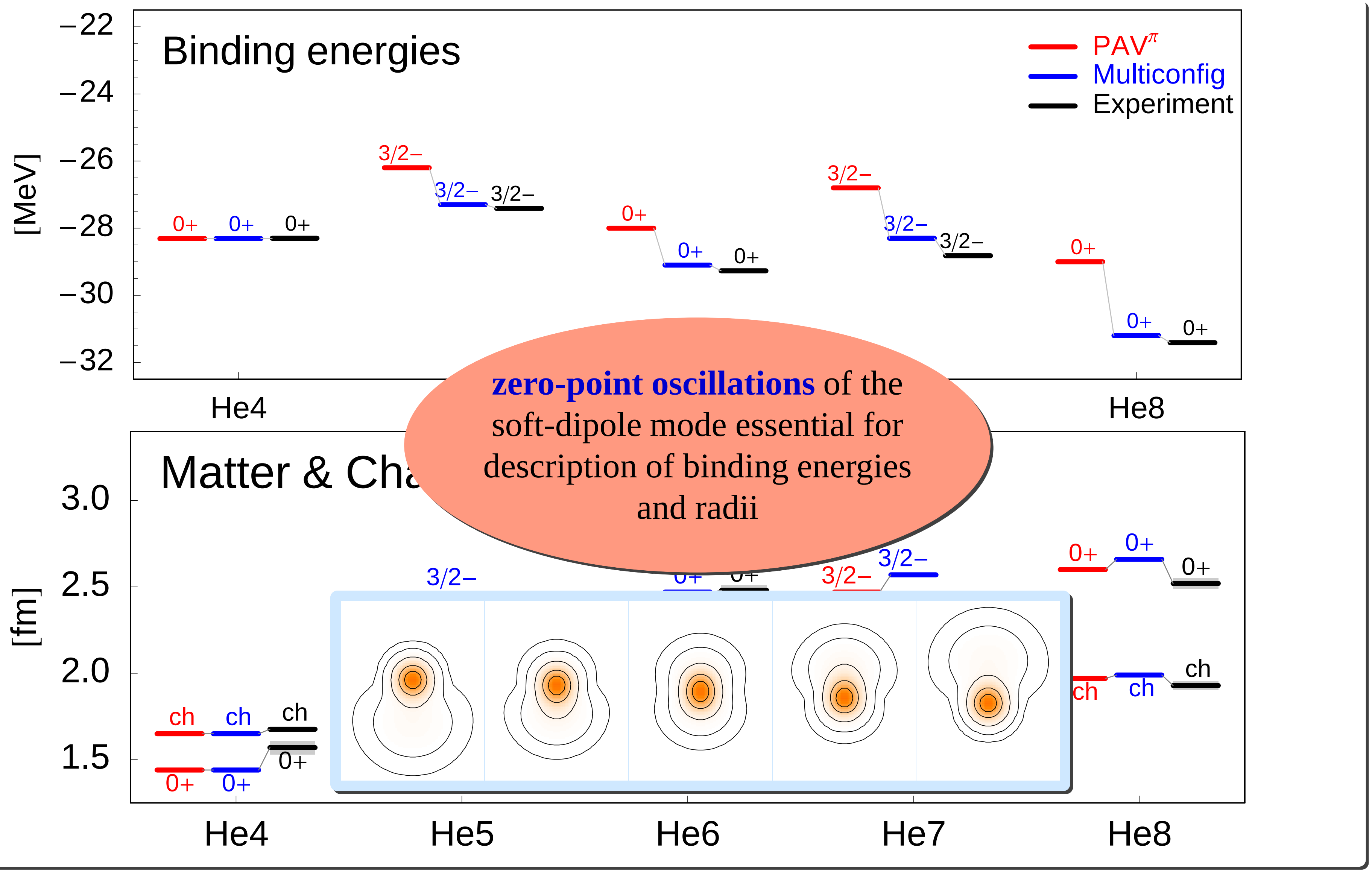
Helium Isotopes



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

^{6}He and ^{8}He charge radius: P. Mueller et al, Phys. Rev. Lett. **99** (2007) 252501

Helium Isotopes



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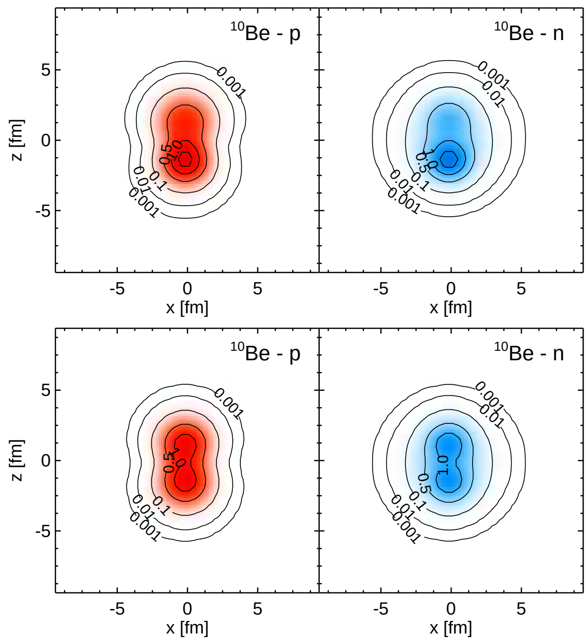
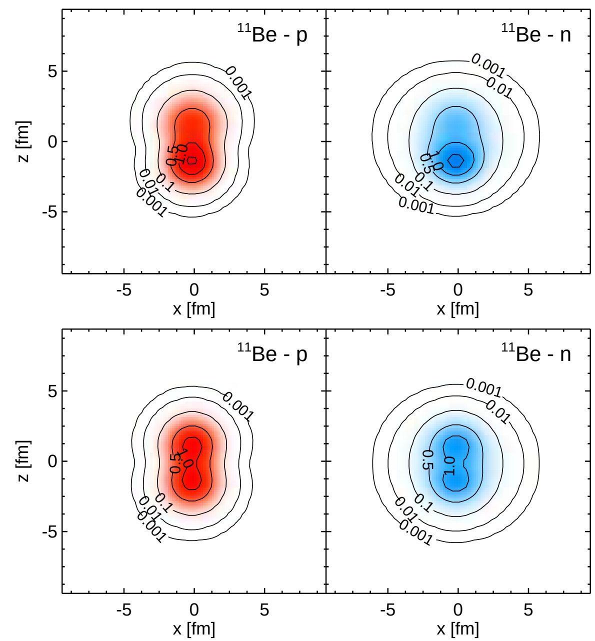
^{11}Be positive parity intruder

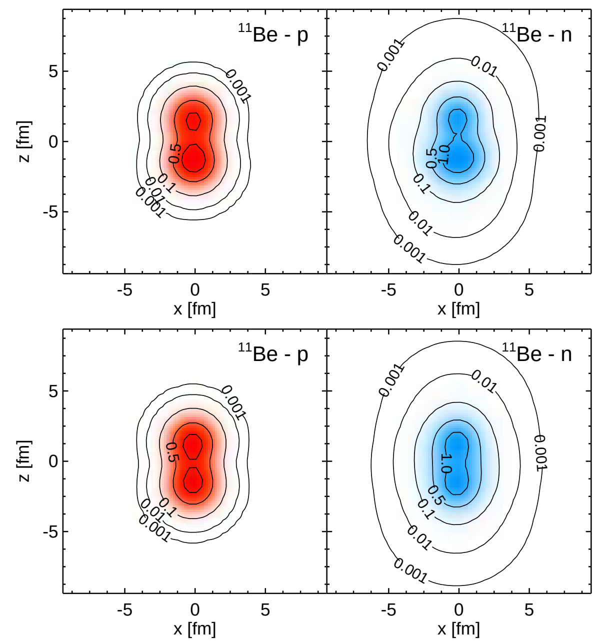
^{10}Be

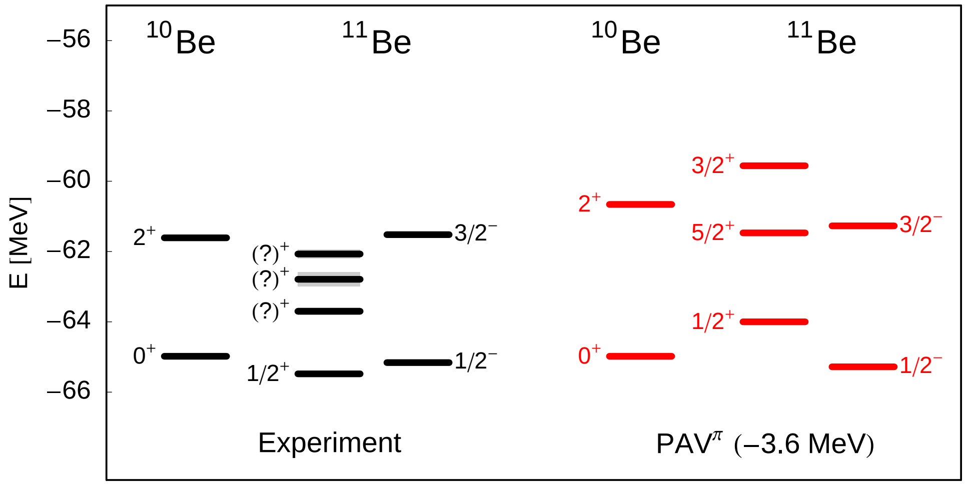


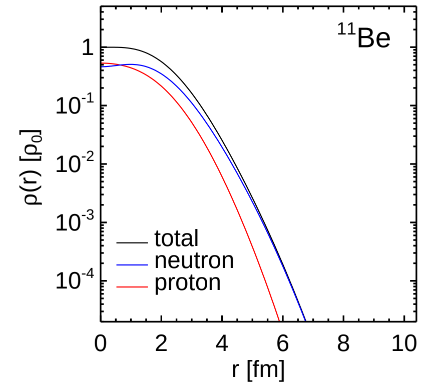
^{11}Be **negative parity**

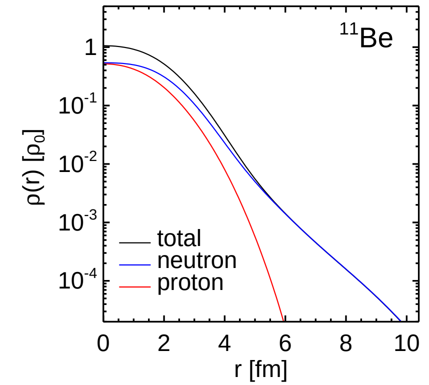


^{11}Be **positive parity**









➨ $1/2^+$ state has a neutron halo

Neon Isotopes ^{17}Ne – ^{22}Ne

Structure

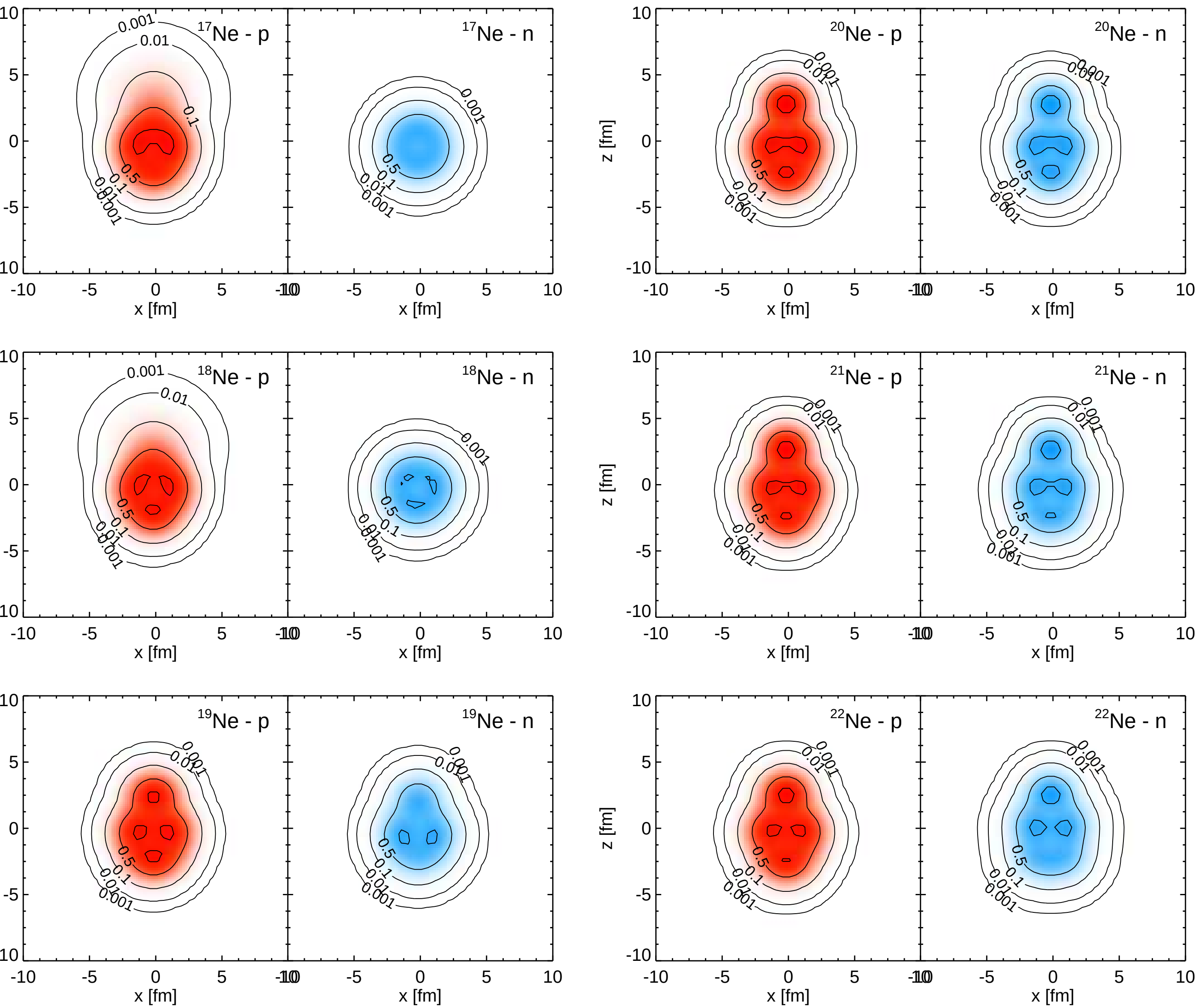
- s^2/d^2 **occupation in** ^{17}Ne **and** ^{18}Ne
- ^{3}He **and** ^{4}He **cluster admixtures**

Observables

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

Neon Isotopes

Variation after Parity Projection VAP$^{\pi}$



Intrinsic proton/neutron densities of dominant FMD state

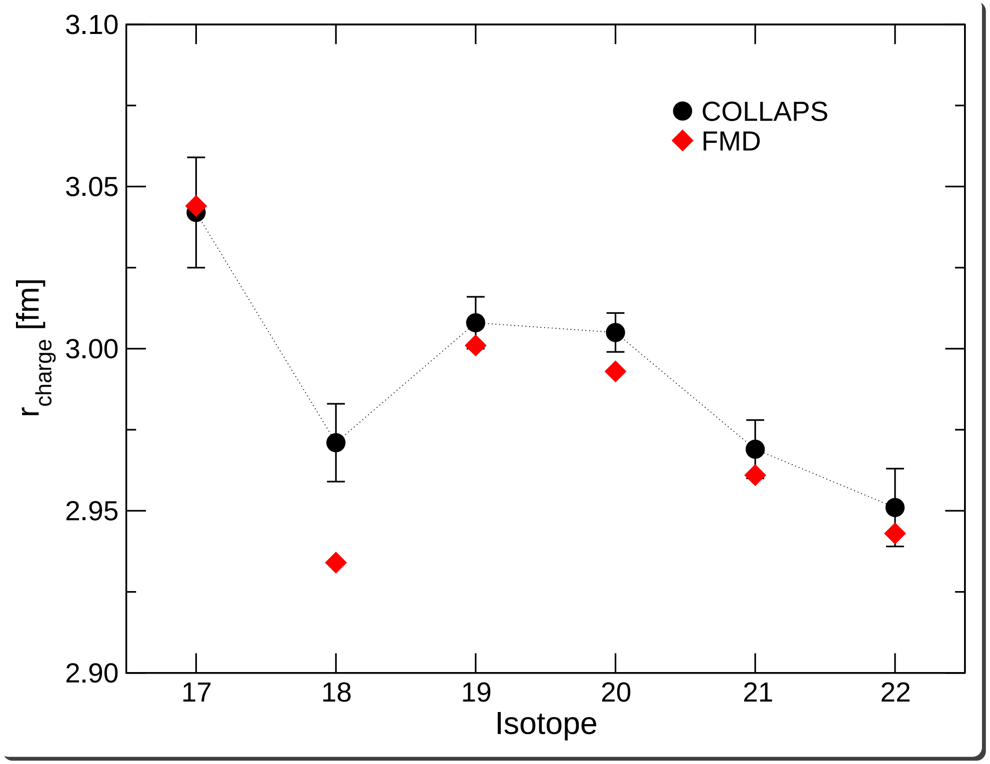
- Variation after parity projection on positive and negative parity
- Crank strength of spin-orbit force, changes properties of single-particle orbits and their occupations
- "s^2" and "d^2" minima in ^{17,18}Ne
- explicit cluster configurations:

^{17}Ne: ^{14}O-^{3}He
^{18}Ne: ^{14}O-^{4}He
^{19}Ne: ^{16}O-^{3}He, ^{15}O-^{4}He

^{20}Ne: ^{16}O-^{4}He
^{21}Ne: "^{17}O"-^{4}He
^{22}Ne: "^{18}O"-^{4}He

$\left| Q^{\pm} \right\rangle$ minima

Charge Radii



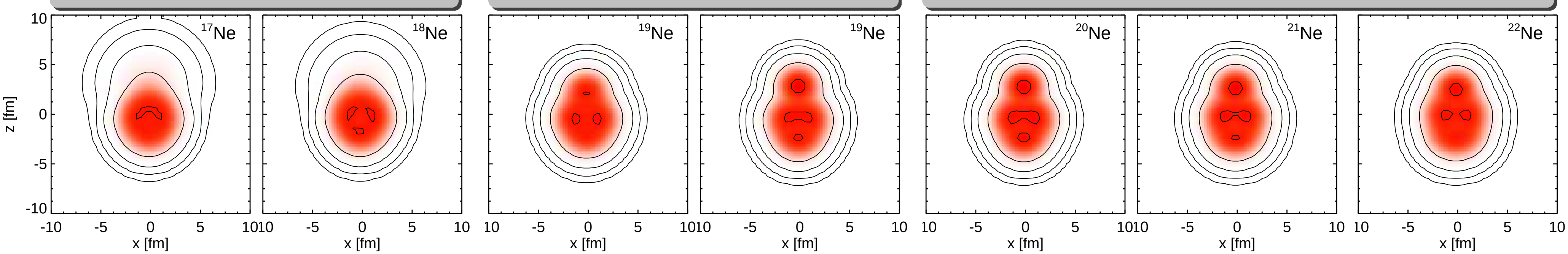
- charge radii of ^{17,18}Ne depend strongly on s^2/d^2 occupations
- cluster admixtures responsible for large charge radii in $^{19-22}$Ne
- measurements of charge radii by COLLAPS@ISOLDE

W. Geithner, T. Neff, *et al.*, submitted to PRL

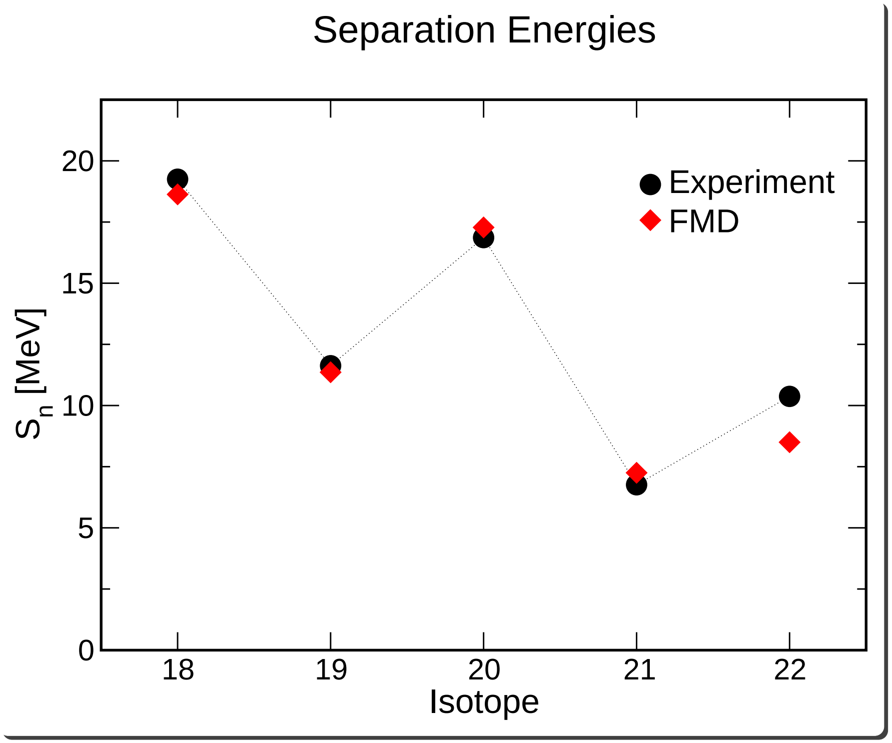
^{17,18}Ne: s^2/d^2 admixture

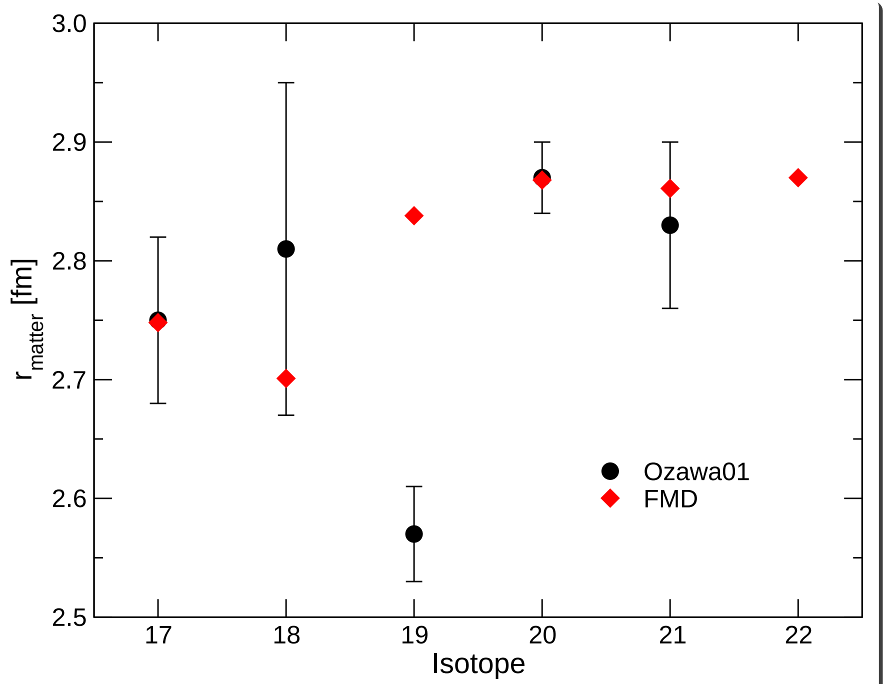
^{19}Ne: ^{3}He, α clustering

$^{20-22}$Ne: α clustering



Separation Energies and Matter Radii



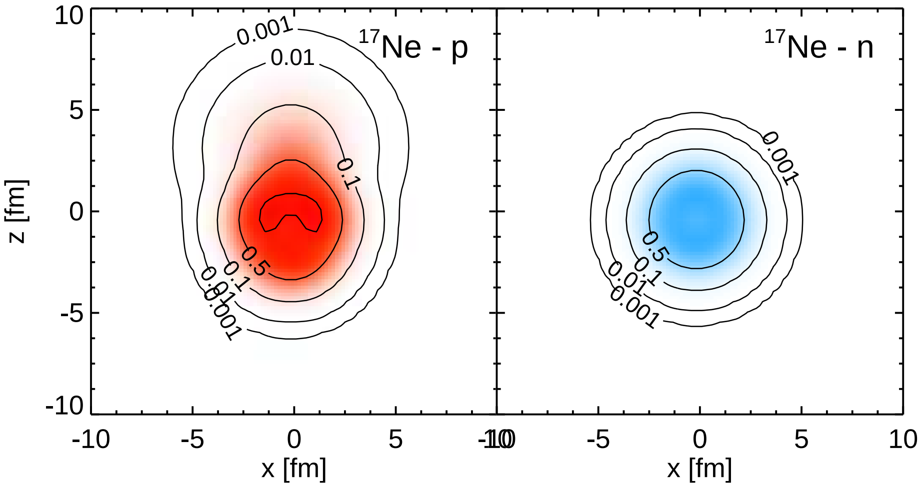


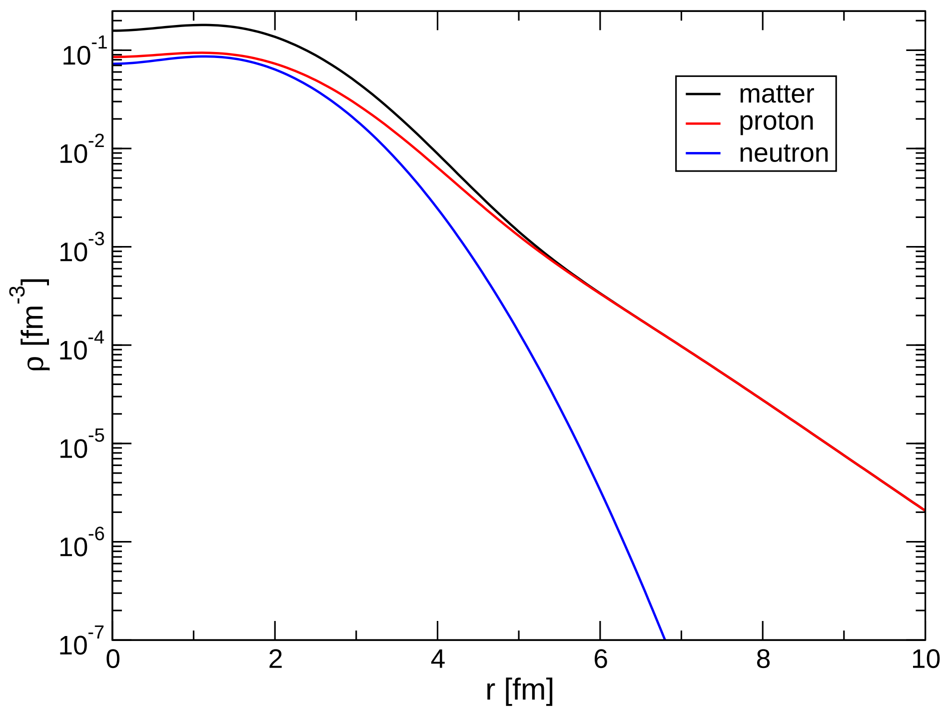
- matter radii from interaction cross sections

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

- good agreement with exception of ^{19}Ne

^{17}Ne Halo ?





	FMD	Experiment
r_{ch}[fm]	3.03	3.042(17)
r_{mat}[fm]	2.75	2.75(7)
$B(E2; \frac{1}{2}^- \to \frac{3}{2}^-)[e^2\mathrm{fm}^4]$	76.7	66^{+18}_{-25}
$B(E2; \frac{1}{2}^- \to \frac{5}{2}^-)[e^2\mathrm{fm}^4]$	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

Reactions

Program

- **FMD Hilbert space should contain besides bound states, also resonances and scattering states**
- **Implement boundary conditions**
- **Phase shifts, capture cross section**

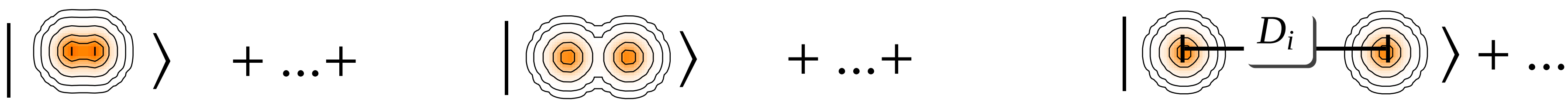
^{3}He(α,γ)^{7}Be **reaction**

Many-Body Hilbert Space for Scattering

Localized FMD states can represent many-body scattering states

- asymptotic states product of "frozen" FMD states $\left(\mathcal{A} \left| {}^3\mathrm{He}, -D_i/2 \right\rangle \otimes \left| {}^4\mathrm{He}, +D_i/2 \right\rangle \right)$
- FMD states for compound system in the interaction region $\left(\left| {}^7\mathrm{Be} \right\rangle, \left| {}^7\mathrm{Be}^* \right\rangle \ \ldots \right)$

scattering state:



interaction region

asymptotic

Boundary conditions

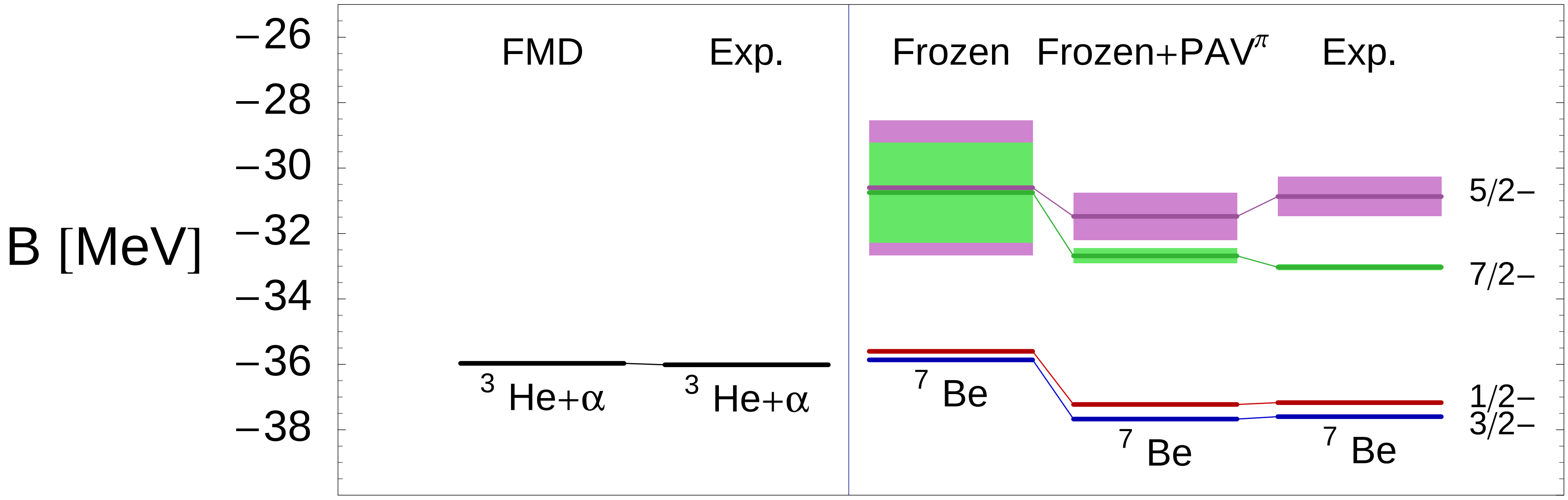
- matching to the Coulomb solution of two point-like nuclei
- phase shifts for scattering or widths of resonances

^{7}Be Levels Bound and in Continuum

- boundary condition outgoing wave only, **Gamov** state

$$\langle\, r \,\big|\, \Psi, [\ell \tfrac{1}{2}] J^{\pi} \,\rangle \;\xrightarrow{r\to\infty}\; iF_{\ell}(kr) + G_{\ell}(kr), \qquad k = +\sqrt{2\mu Z}$$

➨ complex eigenvalue $Z = E - i\,\Gamma/2$



interaction slightly adjusted
to give correct threshold

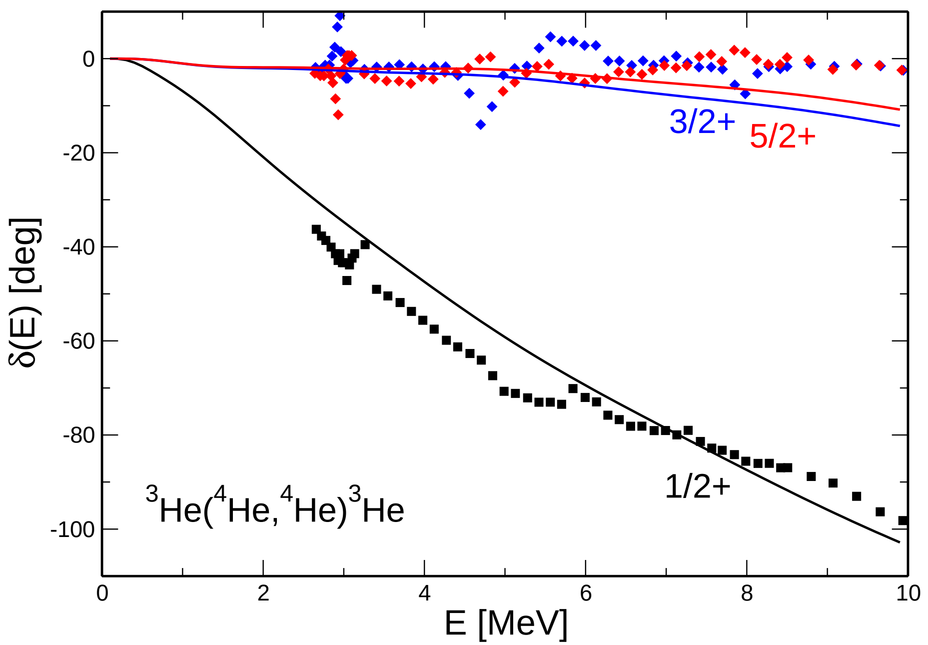
^{3}He – ^{4}He phase shifts

- boundary condition Coulomb scattering solutions

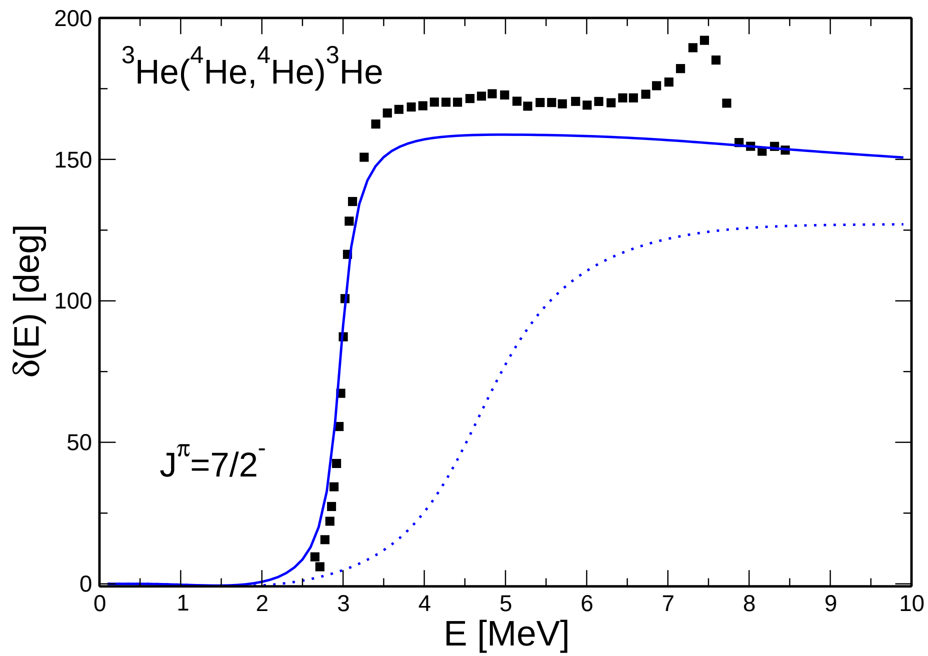
$$\langle r \,|\, \Psi, [\ell \tfrac{1}{2}] J^\pi \rangle \xrightarrow{r\to\infty} F_\ell(kr) + \tan(\delta_\ell(k))\, G_\ell(kr), \quad k = +\sqrt{2\mu E}$$

➨ phase shift $\delta(E)$

non-resonant



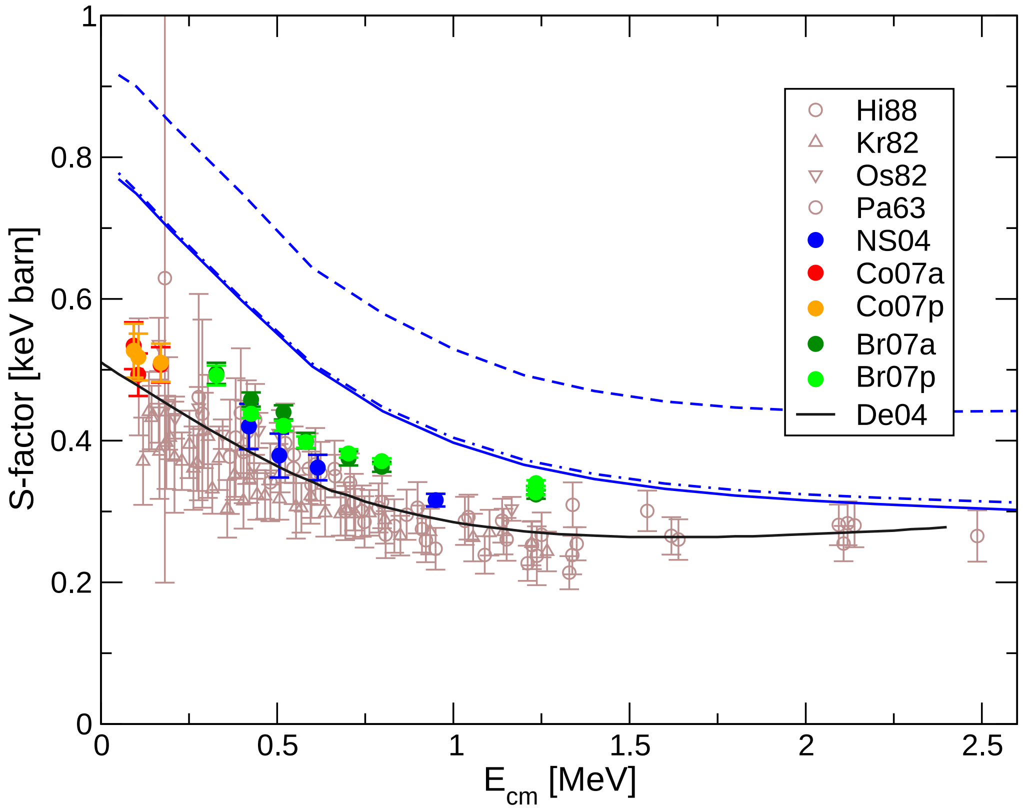
resonant



······ frozen states only

S-Factor of Radiative Capture *preliminary*

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



interaction slightly adjusted to give correct threshold

New data
(LUNA, Seattle and Weizmann)

R-matrix fit to old data (—)
Descouvement et al. (2004)

Summary

Fermionic Molecular Dynamics, $V_{\mathrm{UCOM}} + \delta V$

- Structure of light nuclei
- Halos and clustering, Hoyle state, borromean He isotopes, 2 proton halo
  energies, formfactors, radii, el. magn. & weak transitions, spectroscopic factors, ...
- Resonances, scattering states, reactions
  phase shifts, cross sections, S-factors

Microscopic unified approach for nuclear structure and reactions

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