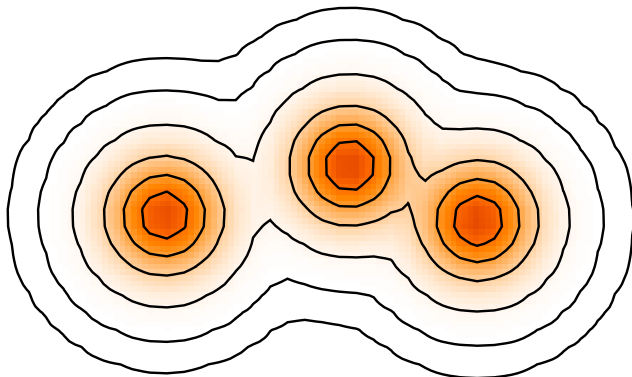


# Exotic Nuclear Structures and Reactions from an Ab Initio Perspective



**Hans Feldmeier**

**GSI Darmstadt**



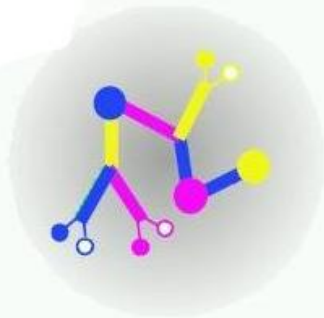
# Nuclear Degrees of Freedom

cm-coordinates and spins of nucleons

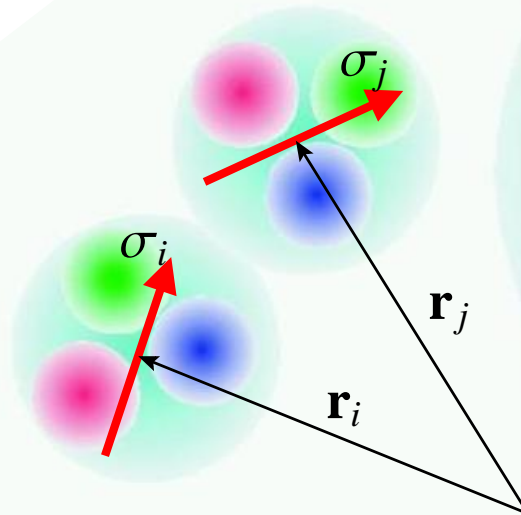
many-body-systems

few-body systems

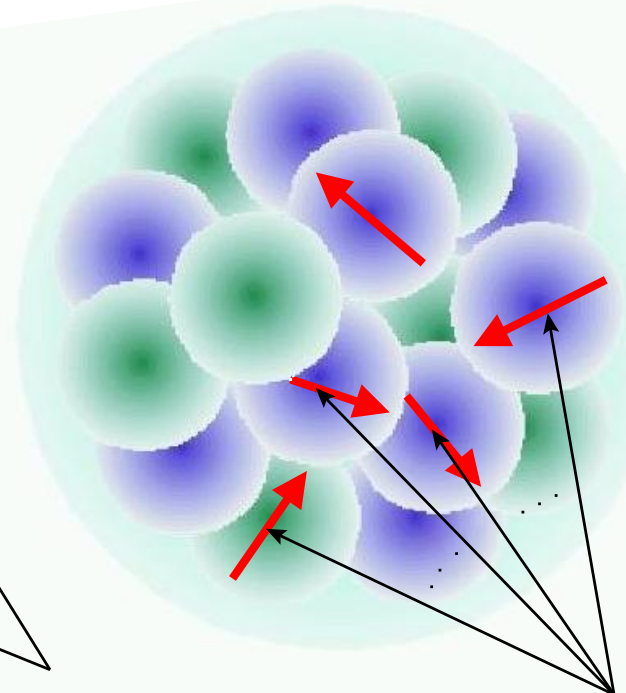
nucleon



QCD



NN force



NN+NNN+ ... force

# Modern Nuclear Structure – Ab Initio

**Ab Initio** : from the beginning, without additional assumptions or special models

”beginning”

- c.m. positions and spins of nucleons  $(\mathbf{r}_i, \sigma_i, \tau_i)$  as degrees of freedom  
 $\implies$  many-body state  $|\widehat{\Psi}\rangle \in \mathcal{H}$  Hilbert space
- interactions among nucleons approximated by potentials  $\implies V_{NN} + V_{NNN}$   
”realistic”  $V_{NN}$  describes NN phase shifts and deuteron

# Realistic NN-Potentials

## QCD motivated

- symmetries, meson-exchange picture
- chiral effective field theory

## short-range phenomenology

- short-range parametrisation or “contact” terms

## experimental two-body data

- scattering phase-shifts & deuteron properties reproduced with high precision

## supplementary three-nucleon force

- adjusted to spectra of light nuclei

Argonne V18

CD Bonn

Nijmegen I/II

Chiral N3LO

Argonne V18 +  
Illinois 2

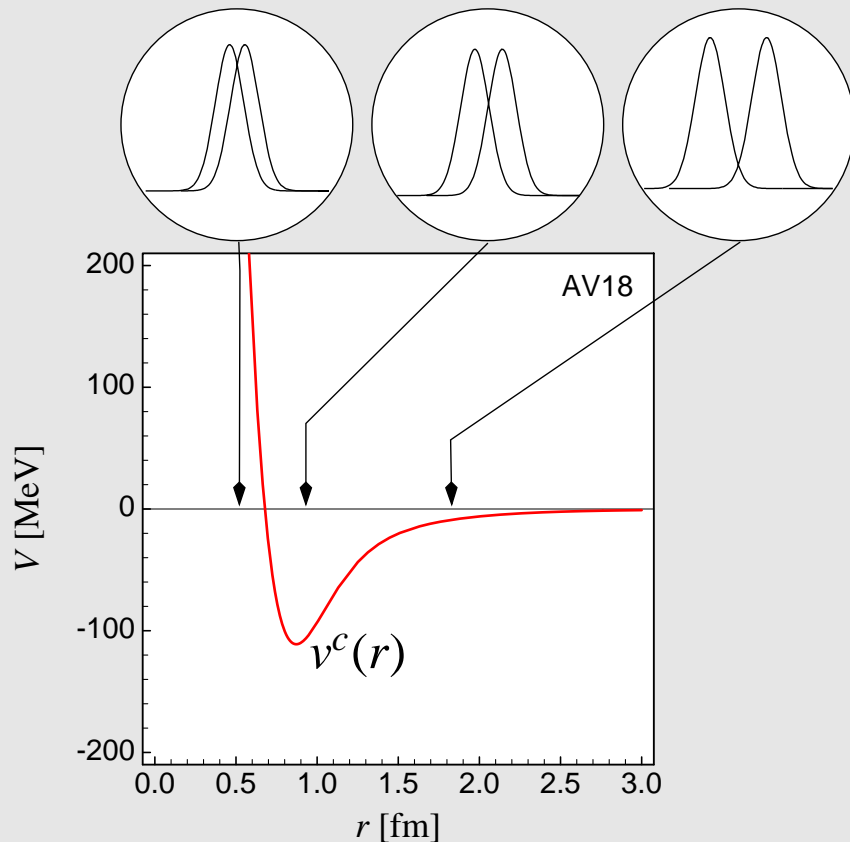
Chiral N3LO +  
N2LO

# Potential and Nucleon Size

Nucleons are not pointlike !

Proton charge radius  $\sqrt{\langle r^2 \rangle_e} = 0.86 \text{ fm}$

## Proton charge distribution and $S=0, T=1$ Potential



- proton size not small compared to interaction range
- half-density overlap at max attraction, average NN-distance  
 $1.8 \text{ fm} \approx 2 \sqrt{\langle r^2 \rangle_e}$
- $V_{NN}$  not elementary  
more like atom-atom potential
- expect three-body forces

# Modern Nuclear Structure – Ab Initio

## Ab initio treatment: solve many-body quantum problem

- $\tilde{H} |\widehat{\Psi}_n\rangle = E_n |\widehat{\Psi}_n\rangle$  with  $\tilde{H} = \tilde{T} + \tilde{V}_{\text{NN}} + \tilde{V}_{\text{NNN}}$
- observables: energies  $E_n$ , moments  $\langle \widehat{\Psi}_n | \tilde{A} | \widehat{\Psi}_n \rangle$ , transitions  $|\langle \widehat{\Psi}_k | \tilde{A} | \widehat{\Psi}_n \rangle|^2$   
to be confronted with data

**HOWEVER**

# Modern Nuclear Structure – Ab Initio

## HOWEVER, there are conceptual problems

- realistic  $\tilde{V}_{NN}$  not unique !  
different phase-shift equivalent  $\tilde{V}_{NN}, \tilde{V}'_{NN}, \tilde{V}''_{NN}$  describe equally well the 2-body system
  - $\tilde{V}_{NN} + \tilde{V}_{NNN} \iff \tilde{V}'_{NN} + \tilde{V}'_{NNN}$   
each NN-interaction needs its NNN-part to describe equally well the 3-body system
- ➔ in nuclear structure theory there is **not the one** genuine NN or NNN force

# Modern Nuclear Structure – Ab Initio

and there are technical problems

- $\tilde{H} |\widehat{\Psi}_n\rangle = E_n |\widehat{\Psi}_n\rangle$  cannot be solved numerically for larger mass numbers

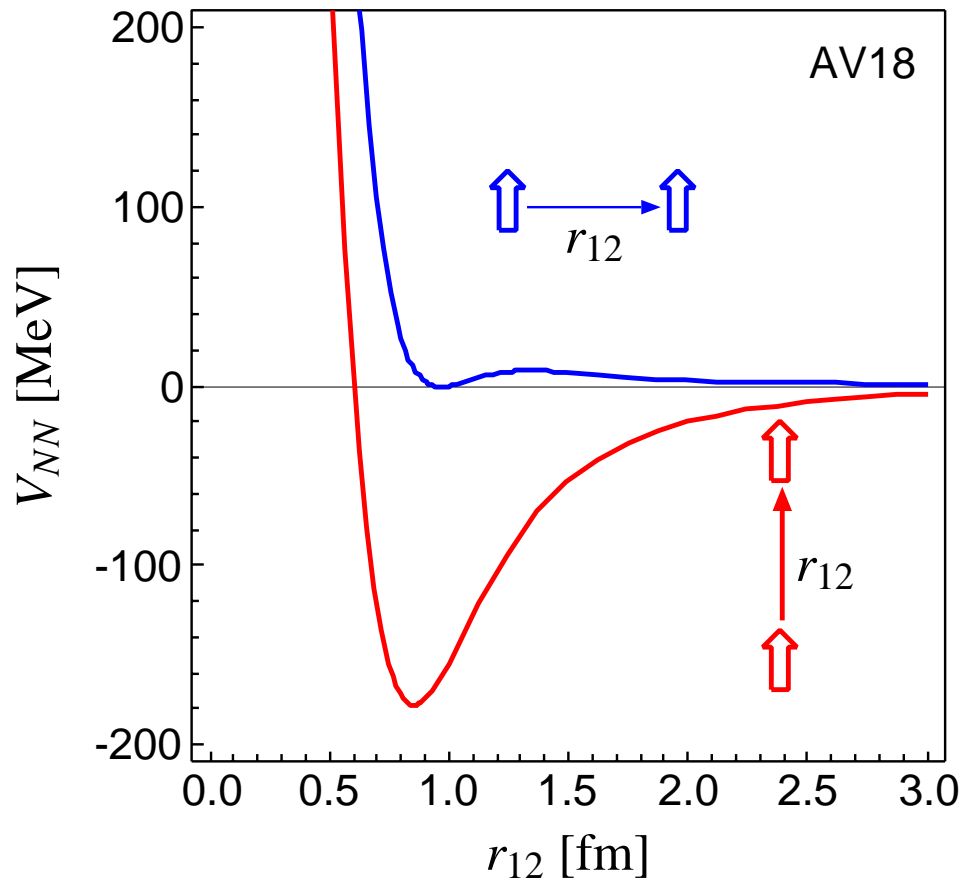
**Why ?**



# 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  $\approx 0.5$  fm

➔ **central correlations**

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

➔ **tensor correlations**

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

# Modern Nuclear Structure – Ab Initio

and there are technical problems

- $\tilde{H} |\widehat{\Psi}_n\rangle = E_n |\widehat{\Psi}_n\rangle$  cannot be solved numerically for larger mass numbers

**Solution:** treat short-range correlations by effective interactions

- Approximation: Hilbert space  $\mathcal{H} = \mathcal{H}_{\text{low-}k} \oplus \mathcal{H}_{\text{high-}k}$

$$\tilde{H}^{\text{eff}} |\Psi_n\rangle = E_n |\Psi_n\rangle \quad \text{with } |\Psi_n\rangle \in \mathcal{H}_{\text{low-}k}$$

- Unitary transformation  $|\widehat{\Psi}_n\rangle = \tilde{U} |\Psi_n\rangle$  such that

$$\tilde{H}^{\text{eff}} = \tilde{U}^\dagger \tilde{H} \tilde{U} \quad \text{does not connect } \mathcal{H}_{\text{low-}k} \text{ with } \mathcal{H}_{\text{high-}k}$$

sounds great, but many-body forces appear

$$\tilde{H}^{\text{eff}} = \tilde{T} + \tilde{V}_{\text{NN}}^{\text{eff}} + \tilde{V}_{\text{NNN}}^{\text{eff}} + \tilde{V}_{\text{NNNN}}^{\text{eff}} + \tilde{V}_{\text{NNNNN}}^{\text{eff}} + \dots$$

- Other observables  $\tilde{A}^{\text{eff}} = \tilde{U}^\dagger \tilde{A} \tilde{U}$

$\mathcal{H}_{\text{low-}k}$  Hilbert space:  
Harmonic Oscillator Basis

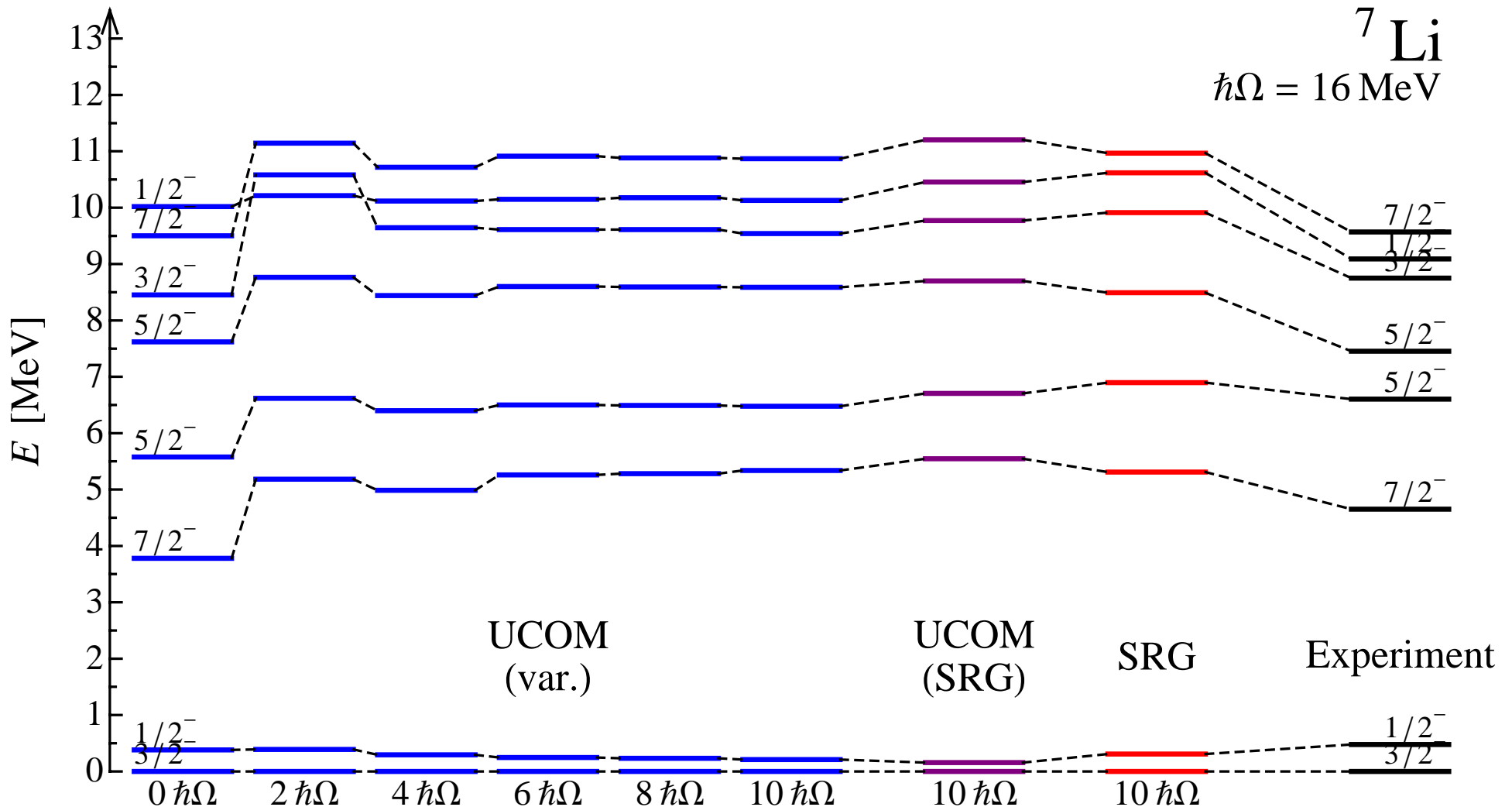


**No-Core Shell Model**

**Hartree Fock**

# NCSM for ${}^7\text{Li}$

$$H_{\text{eff}} = T + V_{\text{NN}}^{\text{eff}}$$

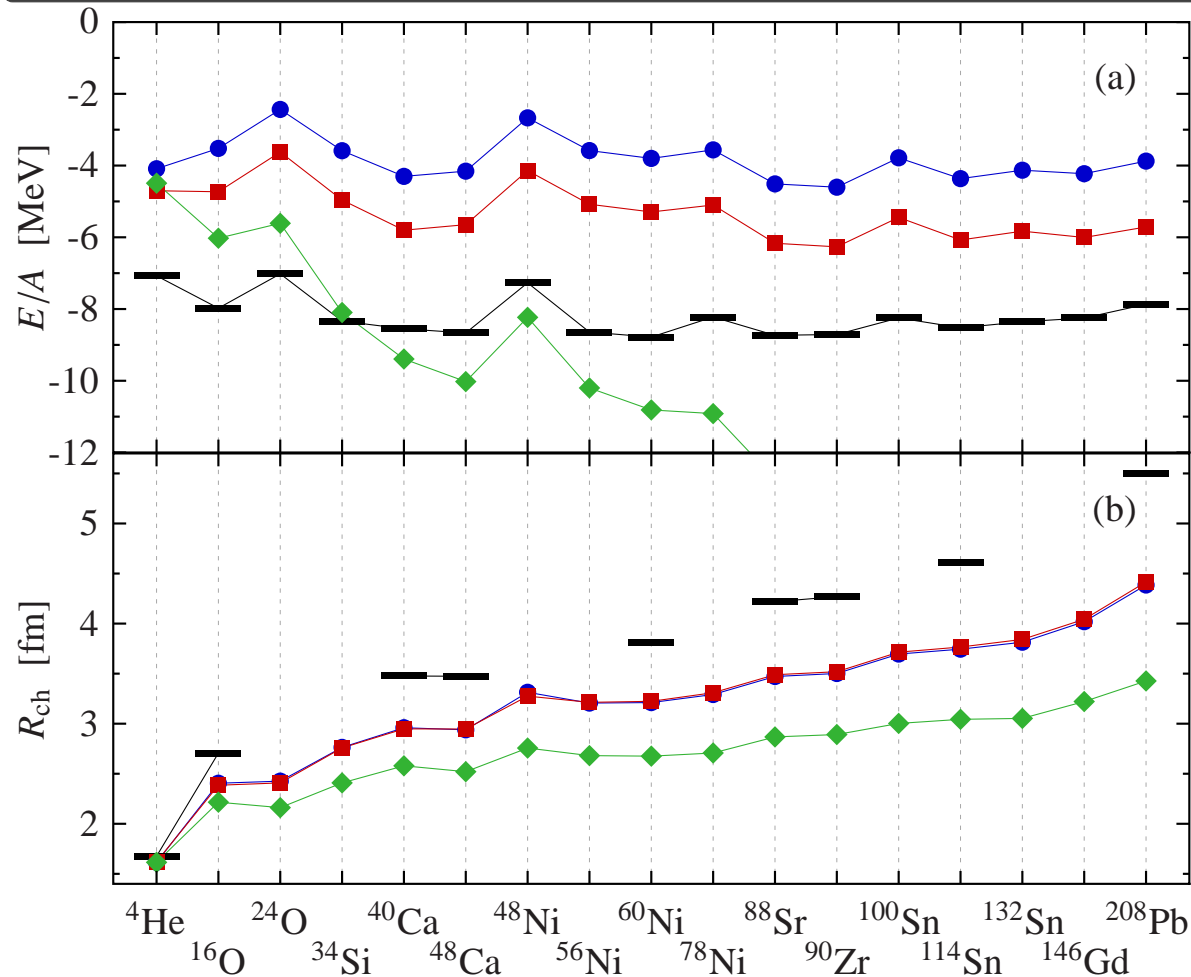


- fast convergence of spectra, no scattering to high- $k$

# Hartree-Fock

$$H_{\text{eff}} = T + V_{\text{NN}}^{\text{eff}}$$

➔ Ab-Initio HF for A = 4 to 208



long-range correlations are missing

UCOM(var.)  
UCOM(SRG)  
SRG

Only two-body part  $V_{\text{NN}}^{\text{eff}}$   
but three- and higher-body eff. interactions cannot be completely neglected especially for SRG (repulsive)

$\mathcal{H}_{\text{low-}k}$  Hilbert space:

**F**ermionic **M**olecular **D**ynamics



**FMD** many-body wave functions

**Restore** symmetries by projections

**V**ariation **A**fter **P**rojection (**VAP**)

**Configuration** mixing

# FMD Many-Body Hilbert Space

## Fermionic

Slater determinant

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

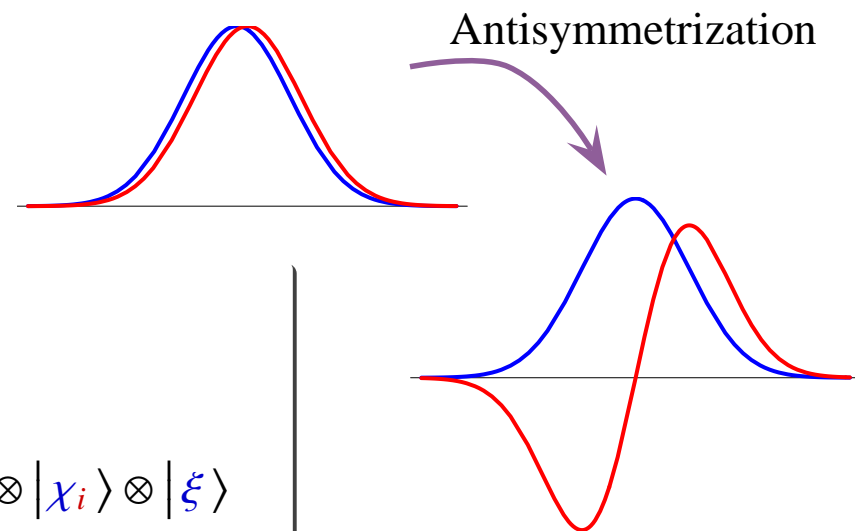
➔ antisymmetrized A-body state

## Molecular

single-particle states

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

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



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

## Dynamics in Hilbert space

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

$$|\Psi; J^\pi M\rangle = \sum_{a, K'} \psi_{aK'} P_{MK'}^{J^\pi} P^{P=0} |Q^{(a)}\rangle$$

variational principle →  $Q^{(a)} = \{q_v^{(a)}, v=1 \cdots A\}, \psi_{aK'}$

# Multi-Configuration Mixing

➤ most general projected state for multi-configuration calculations

$$|\Psi; J^\pi M\rangle = \sum_{aK} \psi_{aK} \tilde{P}^\pi \tilde{P}_{MK}^J \tilde{P}^{P=0} |Q^{(a)}\rangle$$

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

## Multi-configuration calculations

$$\tilde{H} |J^\pi M, n\rangle = E_n^{J^\pi} |J^\pi M, n\rangle$$

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

$$\sum_{bK'} \langle Q^{(a)} | \tilde{H} \tilde{P}_{KK'}^{J^\pi} \tilde{P}^{P=0} | Q^{(b)} \rangle \cdot c_{bK'}^{(n)} = E_n^{J^\pi} \sum_{bK'} \langle Q^{(a)} | \tilde{P}_{KK'}^{J^\pi} \tilde{P}^{P=0} | Q^{(b)} \rangle \cdot c_{bK'}^{(n)}$$

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

$$|J^\pi M, n\rangle = \sum_{bK'} c_{bK'}^{(n)} \tilde{P}^\pi \tilde{P}_{MK'}^J \tilde{P}^{P=0} |Q^{(b)}\rangle$$



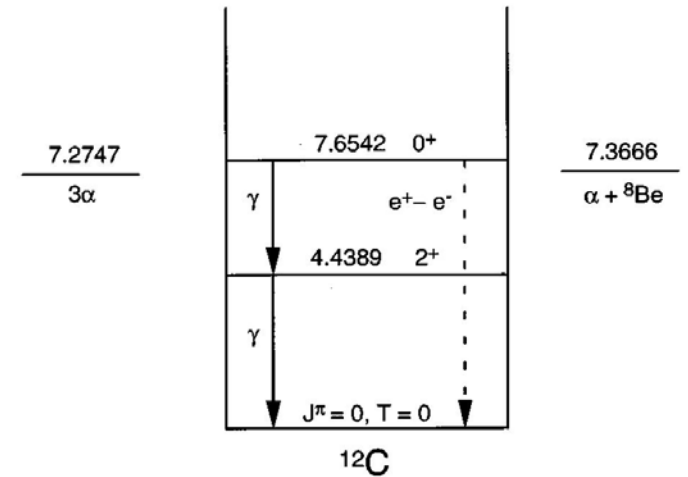
# Cluster States in $^{12}\text{C}$



## Astrophysical Motivation

## Structure

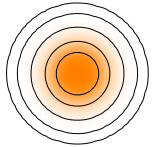
- Is the Hoyle state a  $\alpha$ -cluster state ?
- Other excited  $0^+$  and  $2^+$  states
- ➔ Analyze wave functions in harmonic oscillator basis



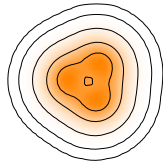
# FMD - Variation, PAV $\pi$ , Multiconfig.

PAV

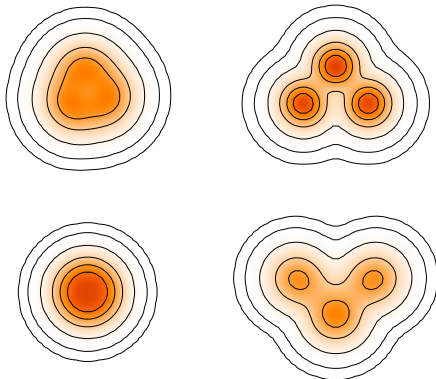
$^{12}\text{C}$



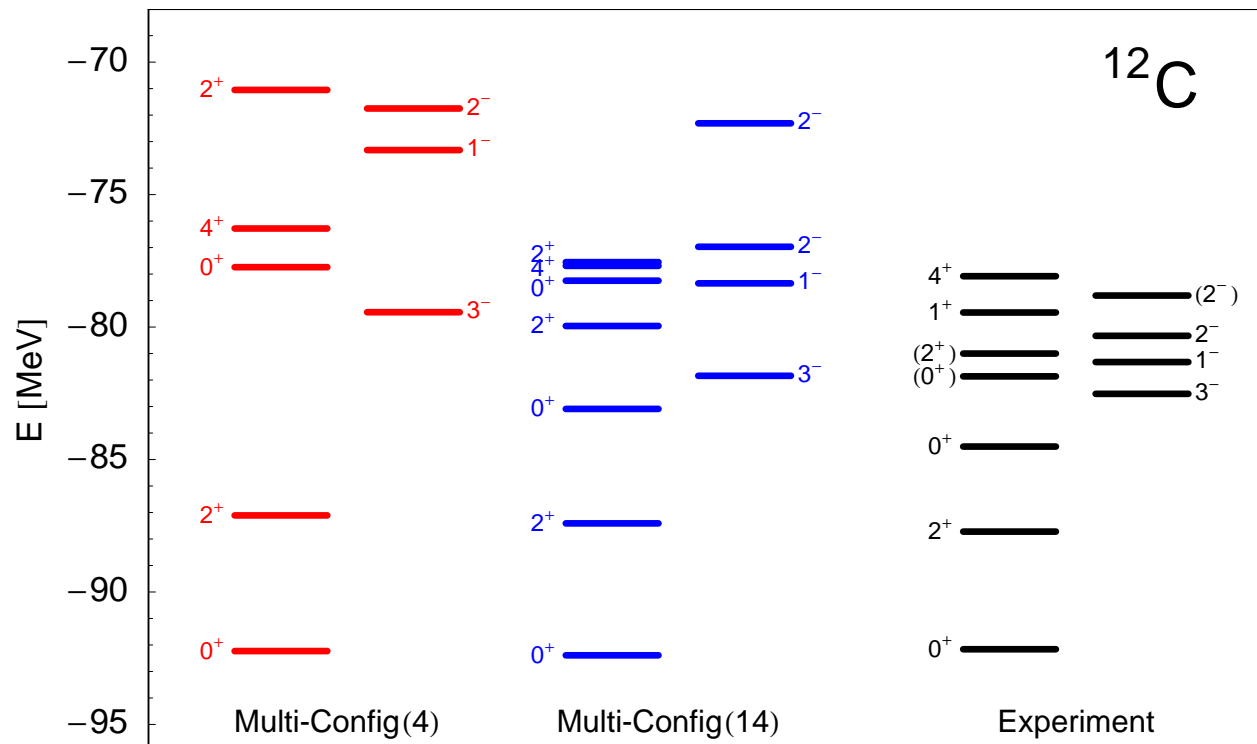
PAV $\pi$



Multiconfig(4)

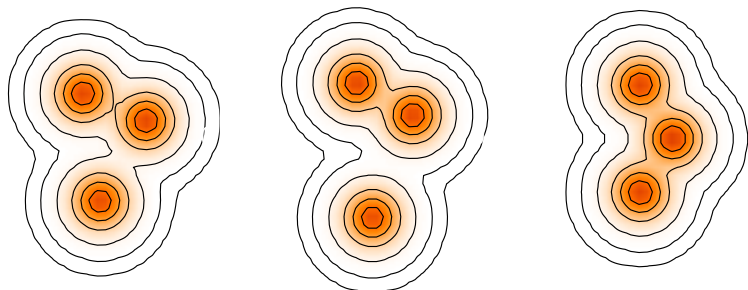


	$E$ [MeV]	$r_{charge}$ [fm]	$B(E2)$ [ $e^2\text{fm}^4$ ]
PAV	-81.4	2.36	-
PAV $\pi$	-88.5	2.51	36.3
Multiconfig(4)	-92.2	2.52	42.8
Multiconfig(14)	-92.4	2.52	42.9
Exp	-92.2	2.47	$39.7 \pm 3.3$



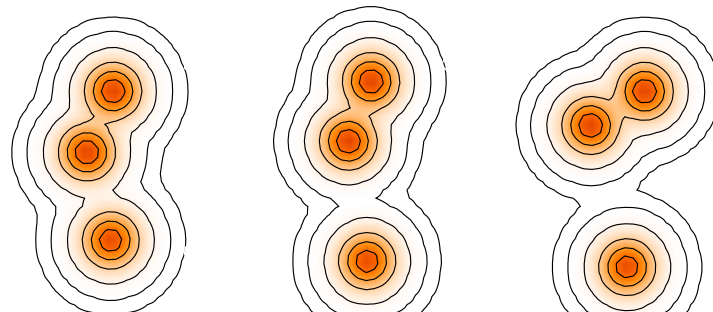
# $^{12}\text{C}$ $0^+$ states

## $0_2^+$ Hoyle state



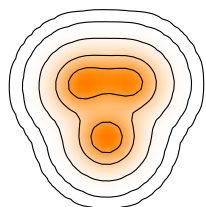
$$|\langle \cdot | 0_2^+ \rangle| = 0.76 \quad |\langle \cdot | 0_2^+ \rangle| = 0.71 \quad |\langle \cdot | 0_2^+ \rangle| = 0.50$$

## $0_3^+$ state

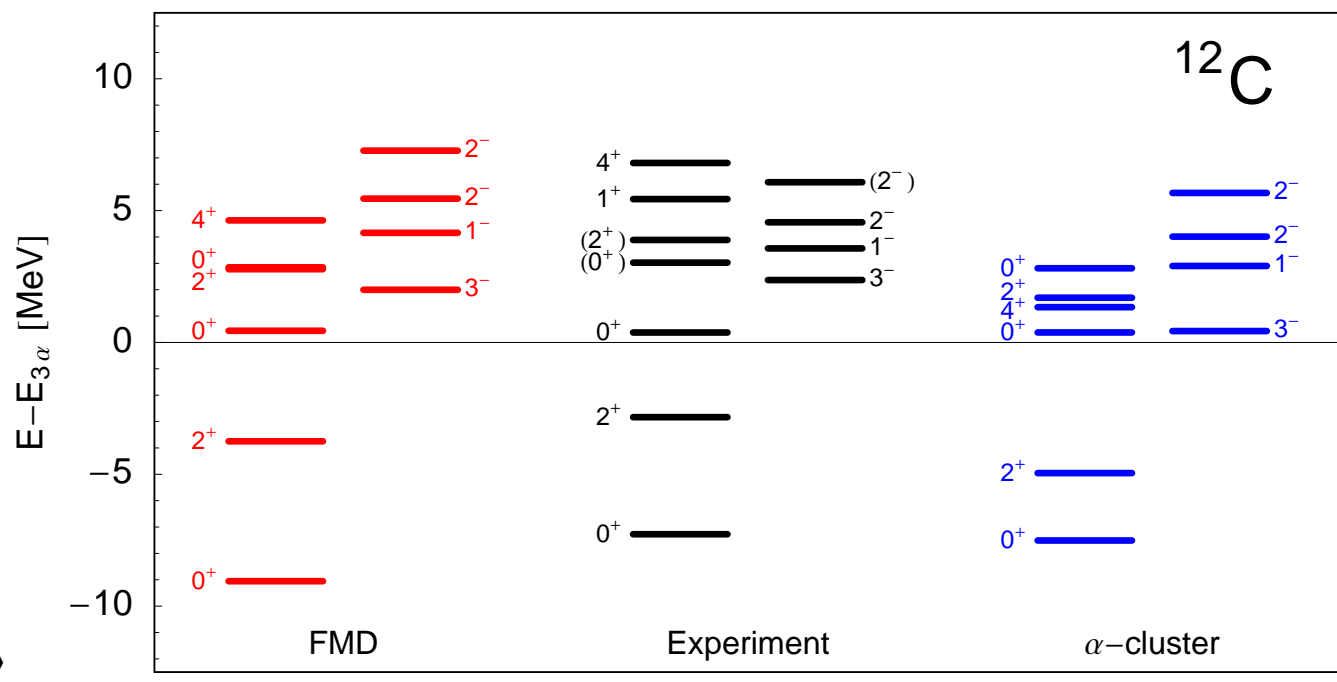


$$|\langle \cdot | 0_3^+ \rangle| = 0.69 \quad |\langle \cdot | 0_3^+ \rangle| = 0.65 \quad |\langle \cdot | 0_3^+ \rangle| = 0.44$$

## $0_1^+$ ground state

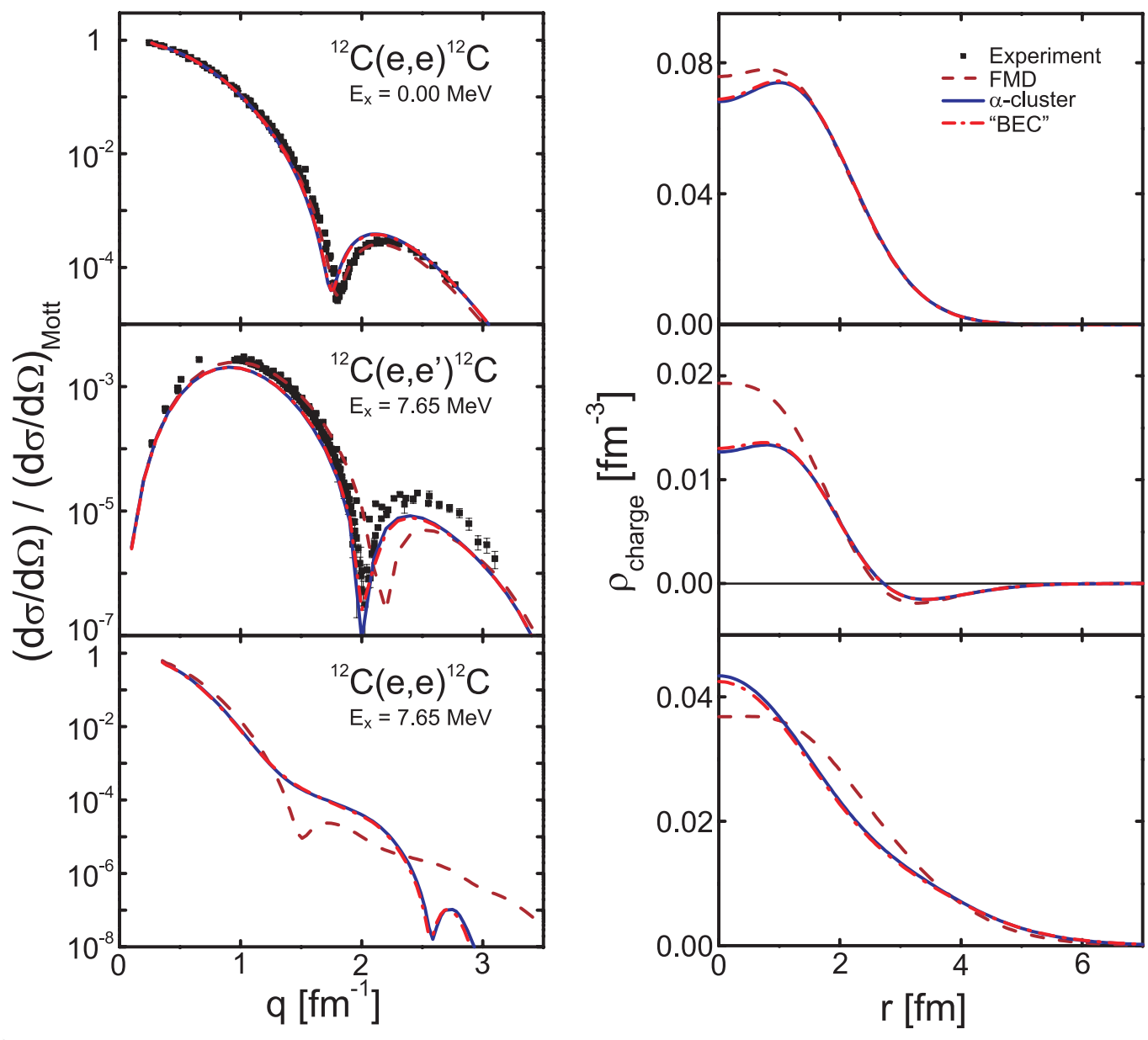


$$|\langle \cdot | 0_1^+ \rangle| = 0.94$$



$$|J^\pi M, n\rangle = \sum_{a, K'} c_{aK'}^{(n)} P_{MK'}^{J^\pi} P^{\mathbf{P}=0} |Q^{(a)}\rangle$$

# $^{12}\text{C}$ Hoyle State in Electron Scattering



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

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

- compare to experiment in Distorted Wave Born Approximation
- $\alpha$ -cluster and "BEC" calculated with mod. Volkov interaction

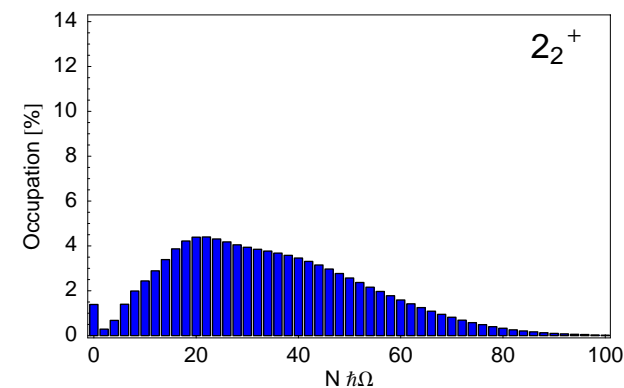
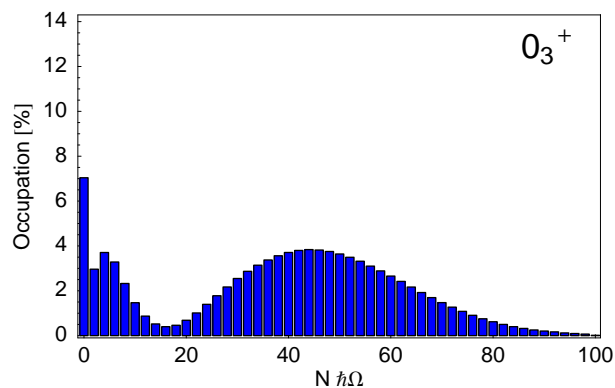
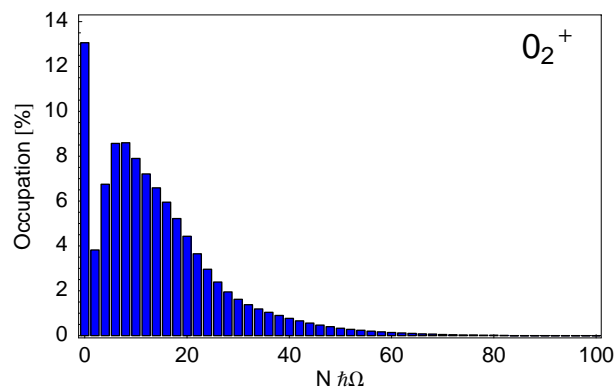
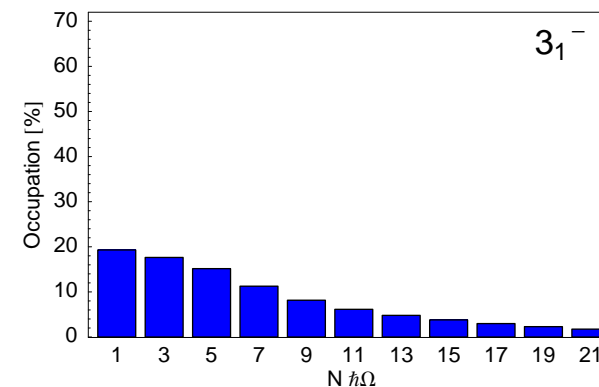
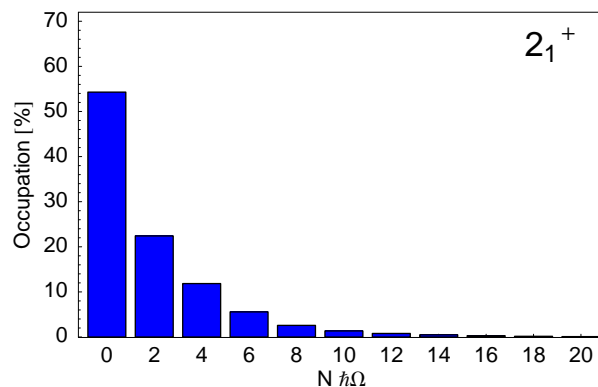
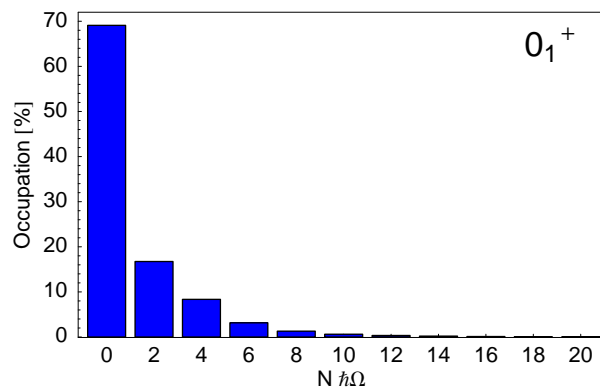
M. Chernykh, H. Feldmeier,  
P. von Neumann-Cosel, T. Neff,  
A. Richter, PRL **98**, 032501  
(2007)

# Harmonic Oscillator $N \hbar\Omega$ Excitations

Occupation probabilities of spaces with  $N$  harmonic oscillator quanta

$$\text{Occ}(N) = \langle \Psi | \delta \left( \sum_{i=1}^A \left( \frac{H^{HO}(i)}{\hbar\Omega} - 3/2 \right) - N \right) | \Psi \rangle$$

FMD



# $\mathcal{H}_{\text{low-}k}$ Hilbert space: Fermionic Molecular Dynamics



## Beryllium Isotopes

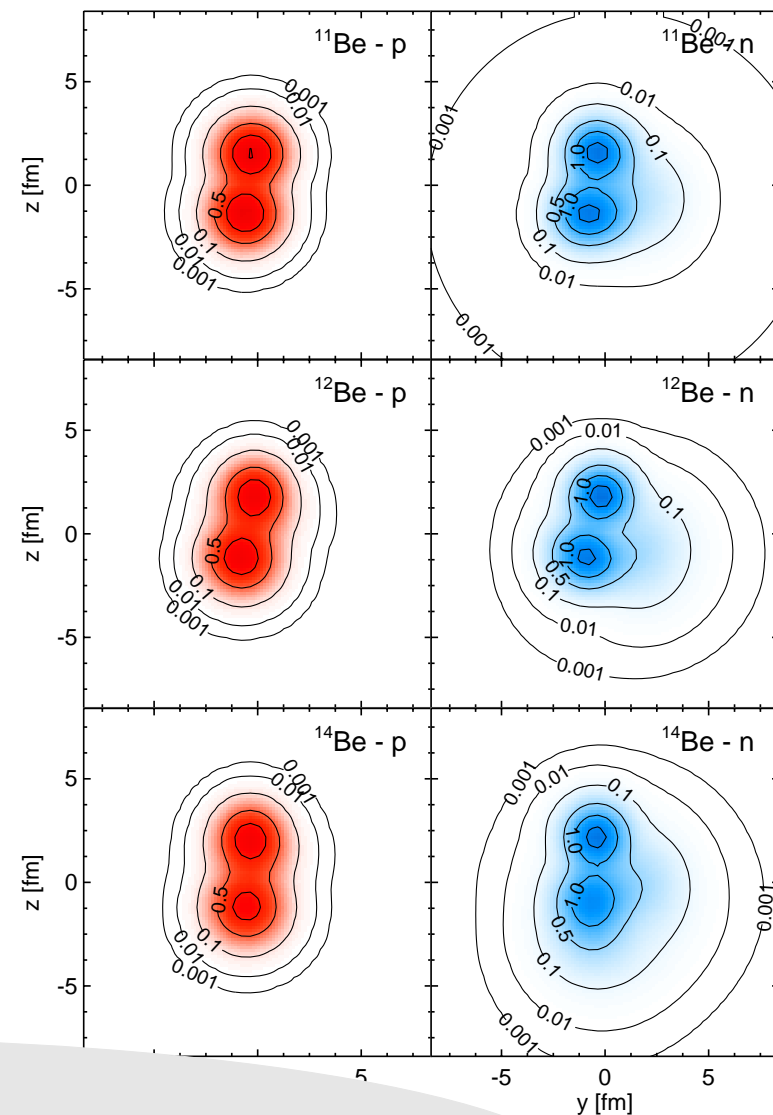
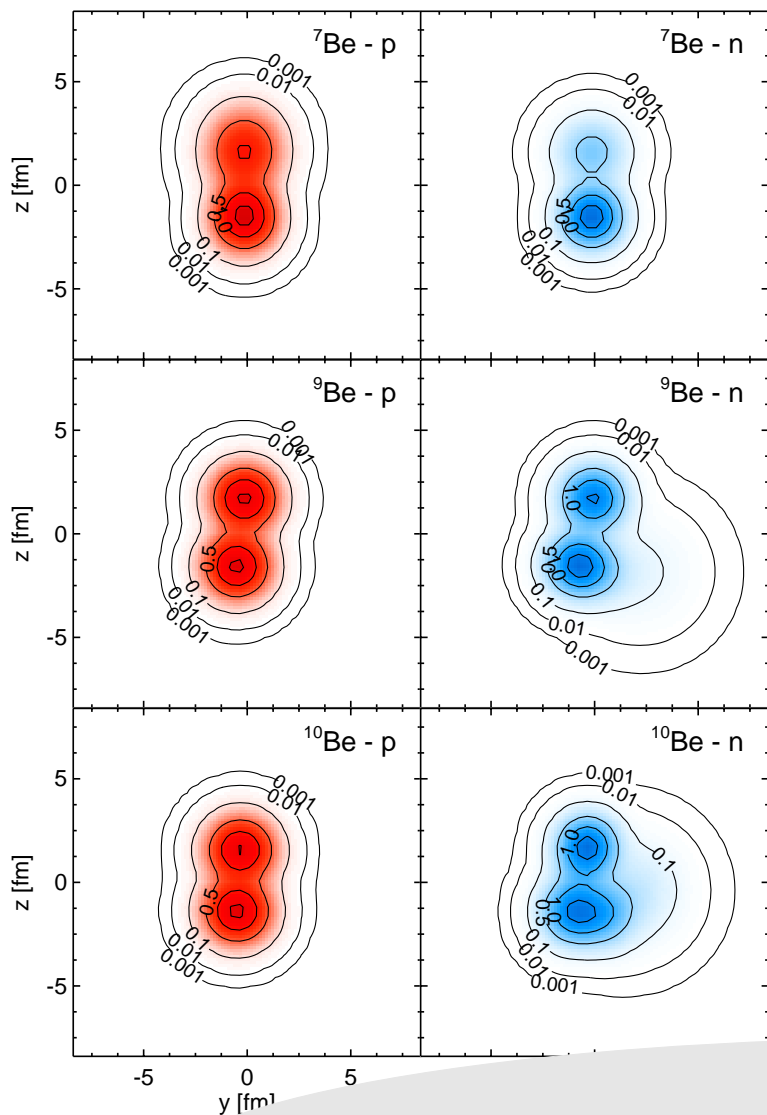
- $\alpha$ -clustering, halos in  $^{11}\text{Be}$  and  $^{14}\text{Be}$ ,  $N = 8$  shell closure ?

## Observables

- energies
- charge and matter radii, electromagnetic transitions

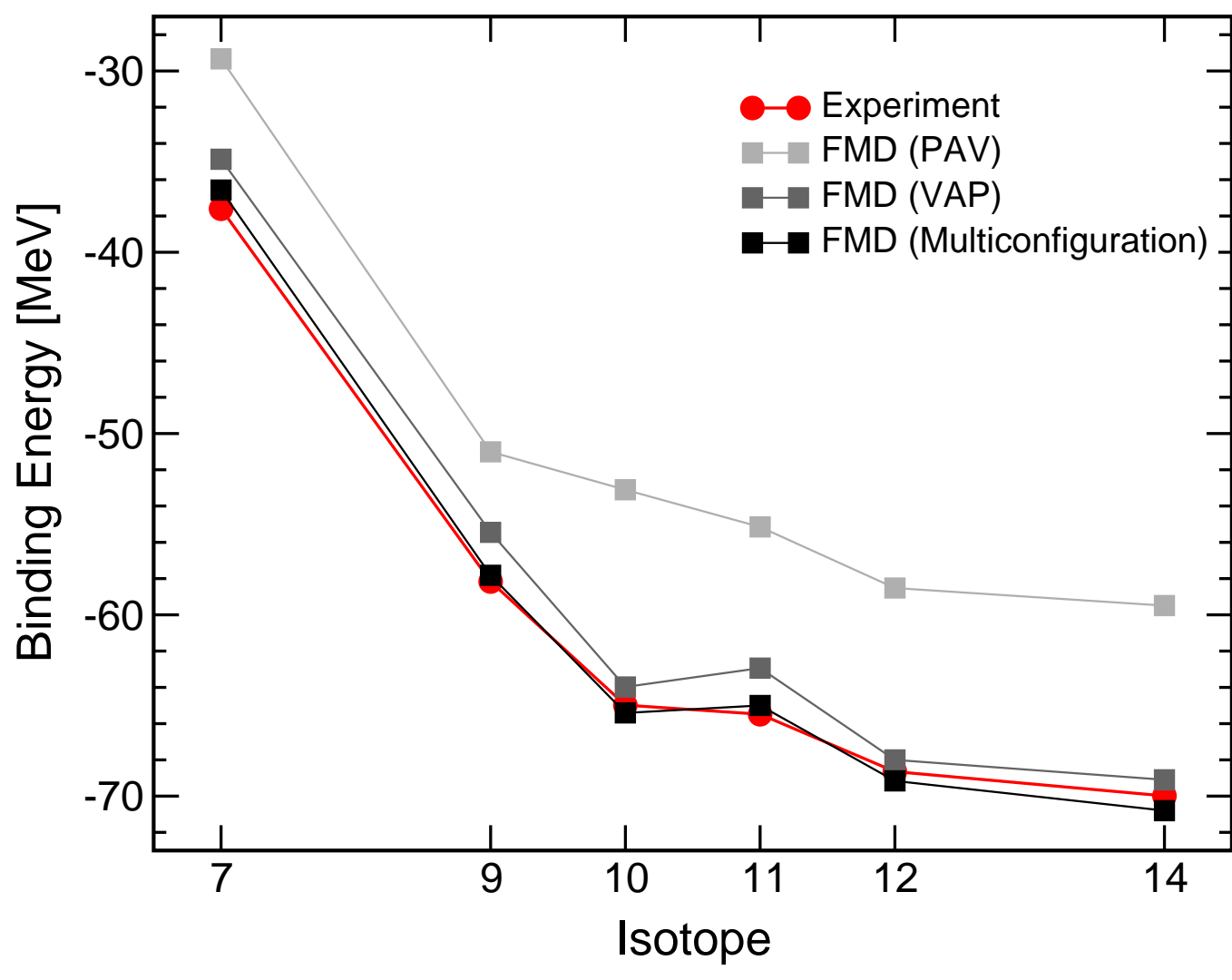
Thomas Neff  
Results still preliminary !

# Variation after Projection



- cluster structure shows up in VAP calculations
- *s*-wave configuration dominant in  $^{11}\text{Be}$

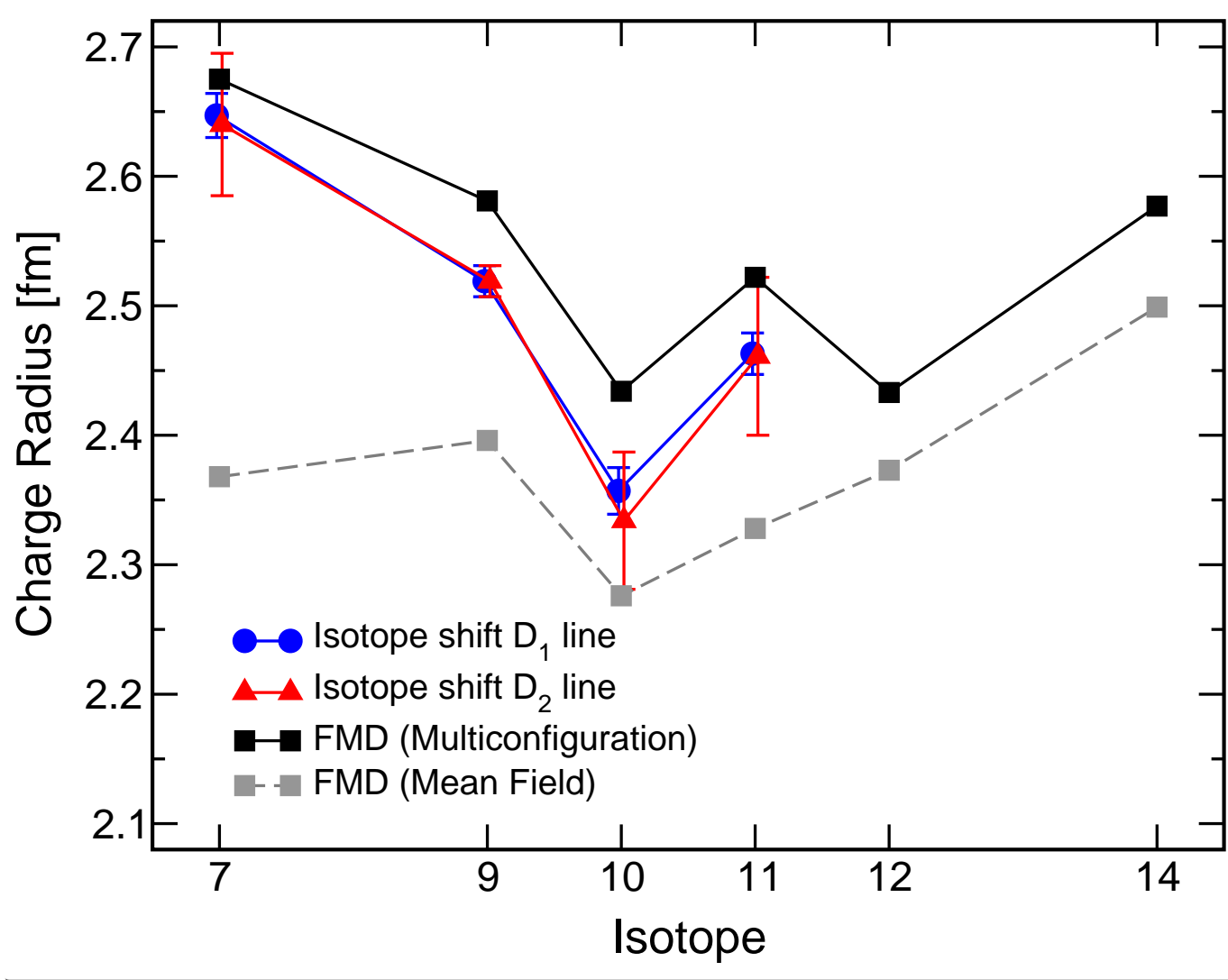
# Binding energies



- large correlation energies due to cluster structure
- loosely bound systems gain most by configuration mixing

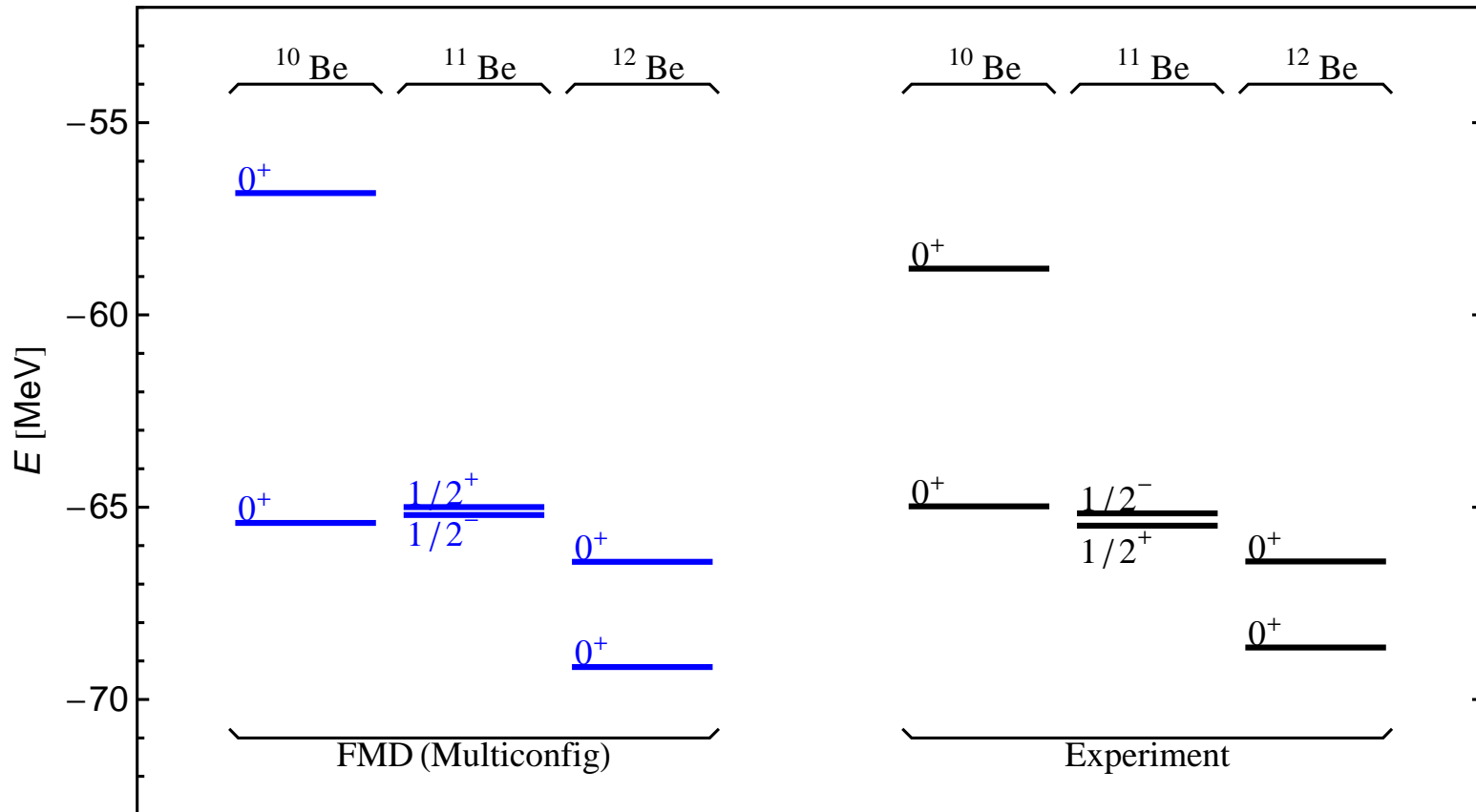


# Beryllium Isotopes Charge Radii



Nörtershäuser *et al.*, Phys. Rev. Lett. **102**, 243002 (2009)

Zakova, Neff, *et al.*, J. Phys. G, accepted for publication



- "almost correct" level ordering in  $^{11}\text{Be}$
- $^{12}\text{Be}$  ground state dominated by  $p^2$  configuration, sizeable admixture of  $s^2$  and  $d^2$  configurations which strongly mix

# Electromagnetic transitions

$^{10}\text{Be}$

	FMD(Multiconfig)	Experiment
$B(E2; 2_1^+ \rightarrow 0_1^+)$	$11.27 e^2\text{fm}^4$	$10.2 \pm 1.0 e^2\text{fm}^4$
$B(E2; 0_2^+ \rightarrow 2_1^+)$	$4.99 e^2\text{fm}^4$	$3.2 \pm 1.9 e^2\text{fm}^4$
$B(E1; 0_2^+ \rightarrow 1_1^-)$	$0.013 e^2\text{fm}^2$	$0.013 \pm 0.004 e^2\text{fm}^2$

$^{11}\text{Be}$

	FMD(Multiconfig)	Experiment
$B(E1; 1/2_1^+ \rightarrow 1/2_1^-)$	$0.020 e^2\text{fm}^2$	$0.099 \pm 0.010 e^2\text{fm}^2$

$^{12}\text{Be}$

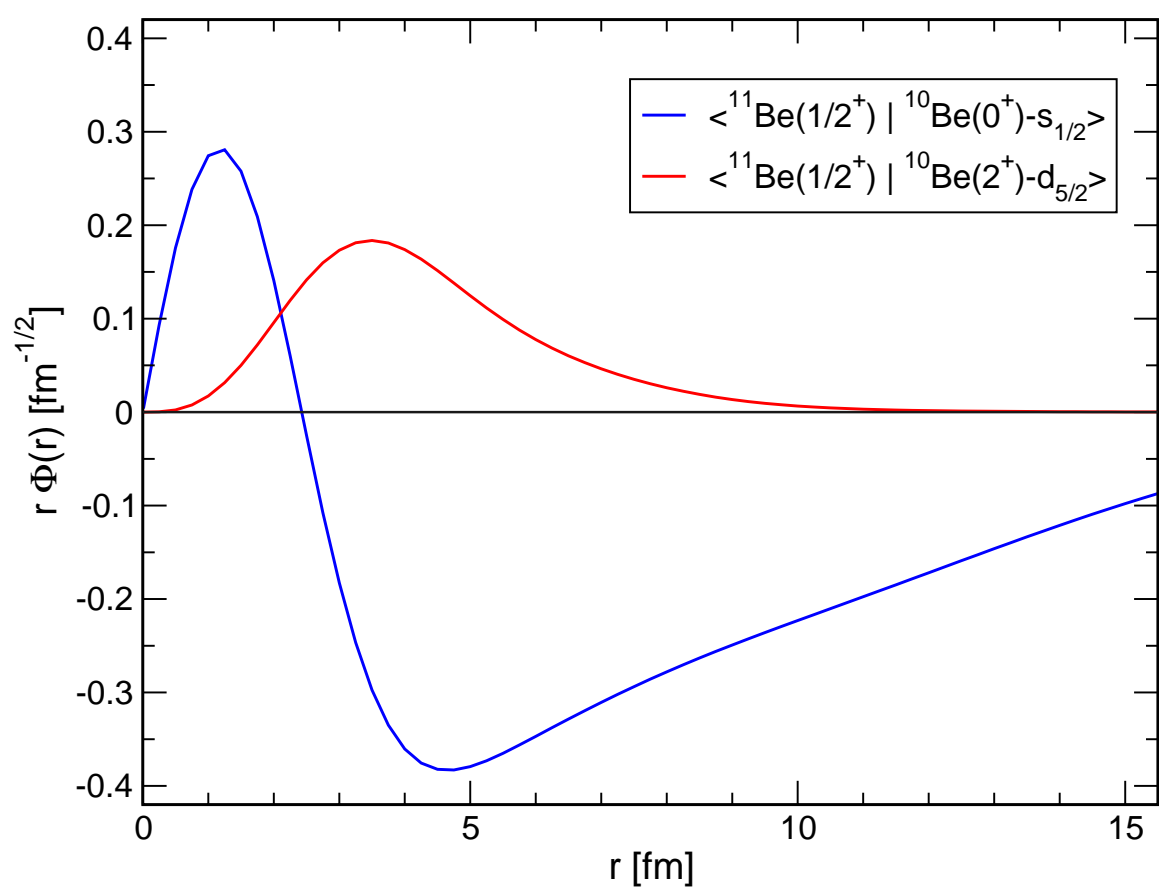
	FMD(Multiconfig)	Experiment
$B(E2; 2_1^+ \rightarrow 0_1^+)$	$8.27 e^2\text{fm}^4$	$8.0 \pm 3.0 e^2\text{fm}^4$
$B(E2; 0_2^+ \rightarrow 2_1^+)$	$6.50 e^2\text{fm}^4$	$7.0 \pm 0.6 e^2\text{fm}^4$
$M(E0; 0_1^+ \rightarrow 0_2^+)$	$1.05 e\text{fm}^2$	$0.87 \pm 0.03 e\text{fm}^2$
$B(E1; 0_1^+ \rightarrow 1_1^-)$	$0.08 e^2\text{fm}^2$	$0.051 \pm 0.003 e^2\text{fm}^2$

Nakamura *et al.*, Phys. Lett. **B394**, 11 (1997).

Shimoura *et al.*, Phys. Lett. **B654**, 87 (2007).

Iwasaki *et al.*, Phys. Lett. **B491**, 8 (2000).

# $^{11}\text{Be}$ - $^{10}\text{Be}$ Overlaps



- extended  $s$ -wave halo
- $s_{1/2}$  spectroscopic factor overestimated compared to results obtained from knockout and transfer reactions

## Spectroscopic Factors

$^{11}\text{Be}$	$^{10}\text{Be}$	$l_j$	S
$1/2^+$	$0^+$	$s_{1/2}$	0.937
	$2^+$	$d_{5/2}$	0.094
	$2^+$	$d_{3/2}$	0.007
$5/2^+$	$0^+$	$d_{5/2}$	0.543
	$2^+$	$s_{1/2}$	0.329
	$2^+$	$d_{5/2}$	0.243
$1/2^-$	$0^+$	$p_{1/2}$	0.805
	$2^+$	$p_{3/2}$	0.779

# Reactions



## Program

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

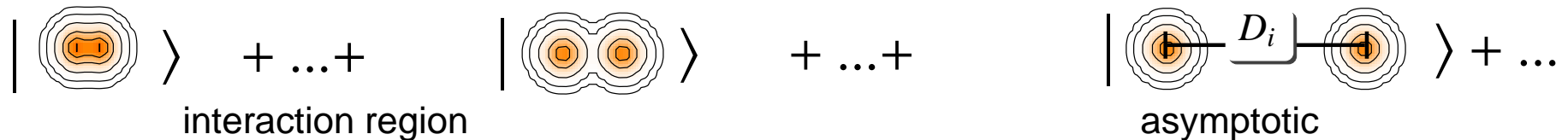
${}^3\text{He}(\alpha, \gamma){}^7\text{Be}$  reaction

# Many-Body Hilbert Space for Scattering

## Localized FMD states can represent many-body scattering states

- ➔ asymptotic states product of “frozen” FMD states  $(\mathcal{A} |^3\text{He}, -D_i/2\rangle \otimes |^4\text{He}, +D_i/2\rangle)$
- ➔ FMD states for compound system in the interaction region  $(|^7\text{Be}\rangle, |^7\text{Be}^*\rangle \dots)$

scattering state:



## Boundary conditions

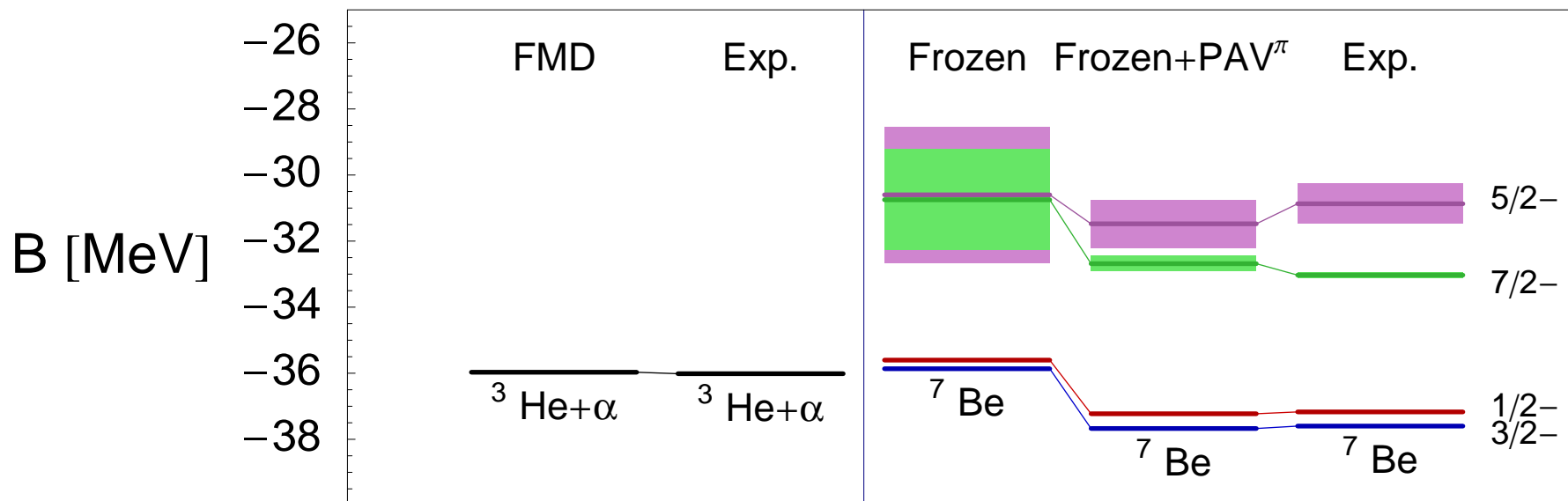
- matching to the Coulomb solution of two point-like nuclei
- ➔ phase shifts for scattering or widths of resonances

# $^7\text{Be}$ Levels Bound and in Continuum

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

$$\langle r | \Psi, [\ell \frac{1}{2}] J^\pi \rangle \xrightarrow{r \rightarrow \infty} iF_\ell(kr) + G_\ell(kr), \quad k = +\sqrt{2\mu Z}$$

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



interaction slightly adjusted  
to give correct threshold

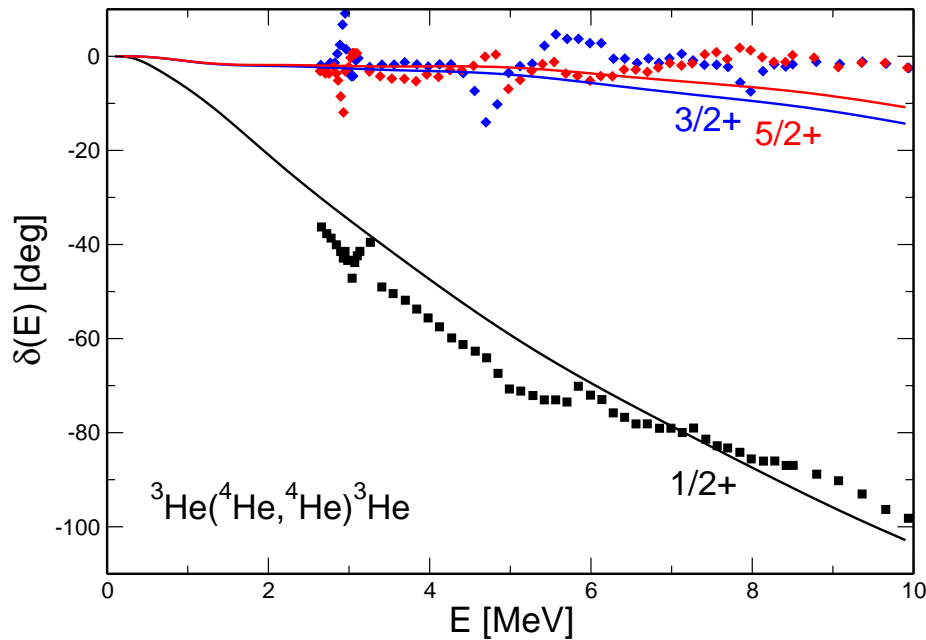
# $^3\text{He} - ^4\text{He}$ phase shifts

- boundary condition Coulomb scattering solutions

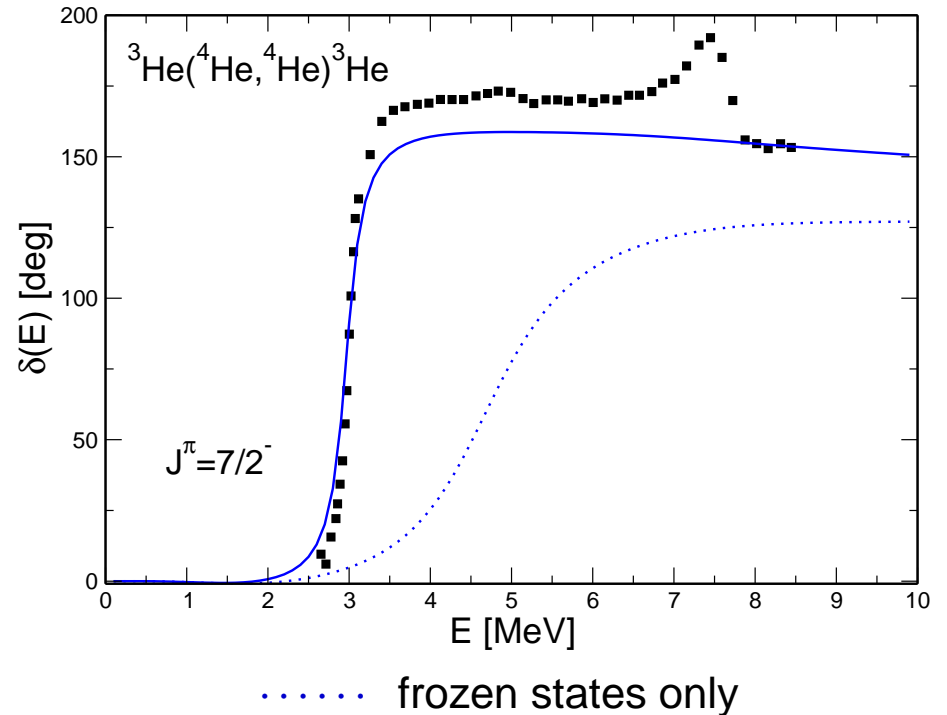
$$\langle r | \Psi, [\ell \frac{1}{2}] J^\pi \rangle \xrightarrow{r \rightarrow \infty} F_\ell(kr) + \tan(\delta_\ell(k)) G_\ell(kr), \quad k = +\sqrt{2\mu E}$$

➔ phase shift  $\delta(E)$

non-resonant



resonant

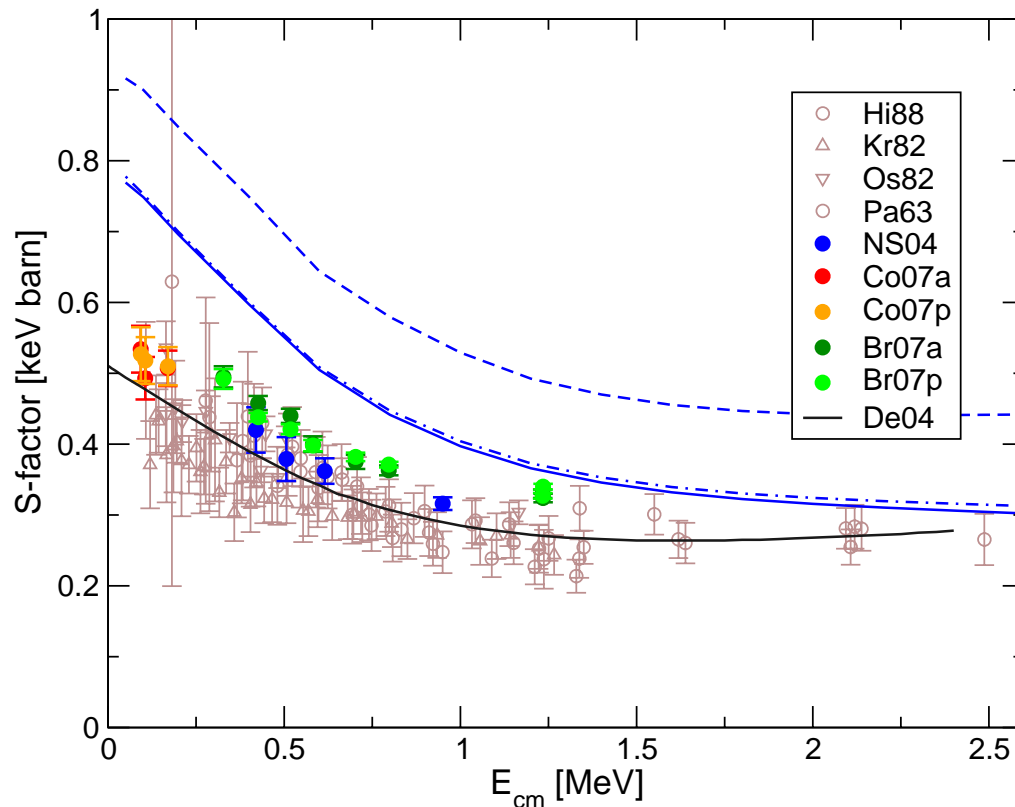




# S-Factor of Radiative Capture

*preliminary*

- Capture from  $1/2^+$ ,  $3/2^+$  and  $5/2^+$  scattering states into  $3/2^-$  and  $1/2^-$  bound states
- ${}^7\text{Be}$  described by single  $\text{PAV}\pi$  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 (—)  
Descouvemont et al. (2004)

# Concluding Remarks

## How to build a nuclear theory

- 1) Choose proper relevant degrees of freedom  
e.g. c.m. positions & spins of nucleons,  
one-body & pairing densities for larger nuclei
- 2) Find corresponding Hamiltonian (energy expressed in terms of deg. of freedom)
- 3) Calculate observables: energies, transitions, moments, cross sections, ...  
compare with data, make predictions

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- 2) Find corresponding Hamiltonian (energy expressed in terms of deg. of freedom)
- 3) Calculate observables: energies, transitions, moments, cross sections, ...  
compare with data, make predictions

## Nucleons are complex many-body systems, not point like

- ➔ NN-interaction is not a priori given, not fundamental  
is an effective interaction, depends on many-body Hilbert space
- ➔ NNN-interactions are needed  
 $(\tilde{V}_{NN} + \tilde{V}_{NNN})$  has to be treated consistently
- ➔ 2- and 3-body systems do not uniquely fix  $(\tilde{V}_{NN} + \tilde{V}_{NNN})$

# Concluding Remarks

## Novel concepts & methods progressed nuclear structure substantially in the last decade

- Chiral-PT, NN + NNN consistent
- Phase-shift equivalent low-momentum effective interactions  
UCOM, SRG,  $V_{\text{low-}k}$ , tame short-range correlations
- Exact few-body methods, Faddeev Yakubowski, hyperspherical harmonics, ...
- No-core shell model, Coupled Cluster, Importance sampling, ...  
medium and long-range correlations by configuration mixing
- Exotic states, clusters, halos, require non-standard Hilbert spaces, FMD, ...
- First ab initio microscopic nucleus-nucleon scattering, nucleus-nucleus scattering
- Ab initio energy density functionals ?
- ...

**FAIR will be a key promoter  
driving nuclear structure theory to new frontiers**

# Thanks to my Collaborators

- A. Cribeiro, K. Langanke, T. Neff, D. Weber  
GSI Darmstadt
- H. Hergert, R. Roth  
Institut für Kernphysik, TU Darmstadt

# Helium Isotopes ${}^4\text{He}$ – ${}^8\text{He}$

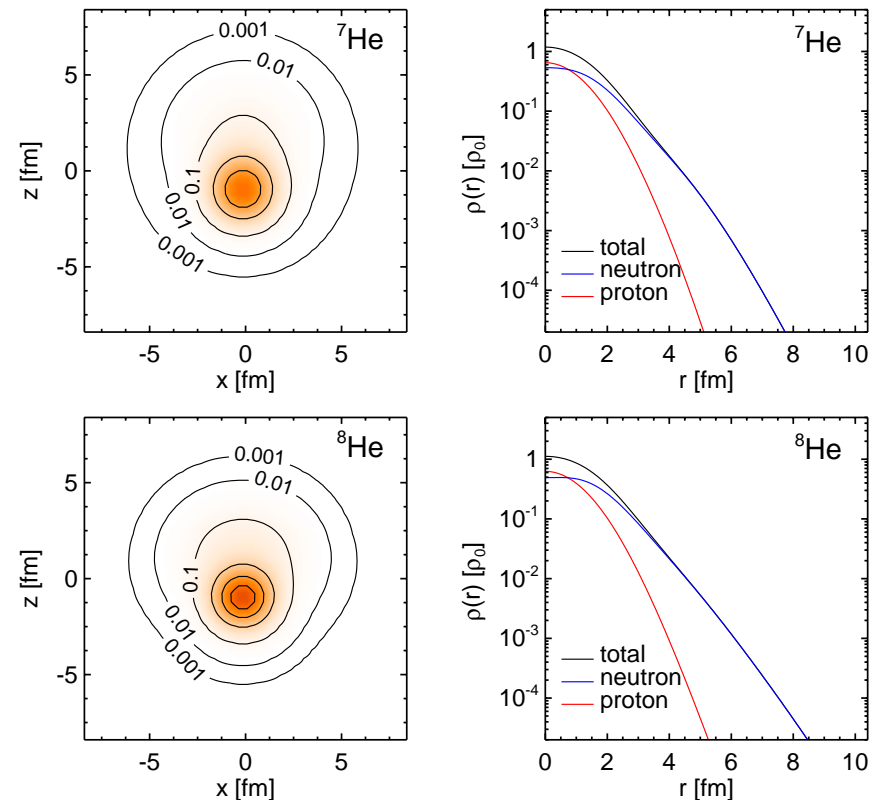
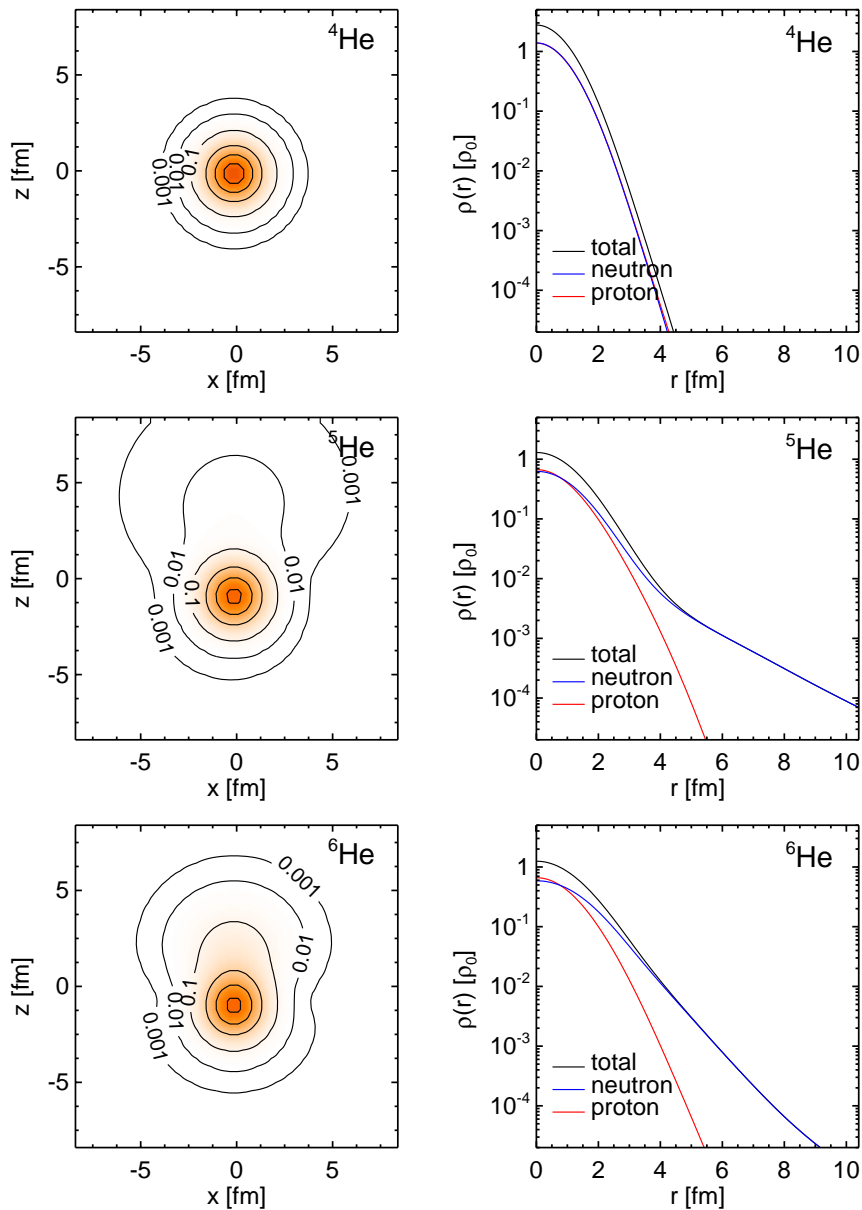


## Structure

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

## Observables

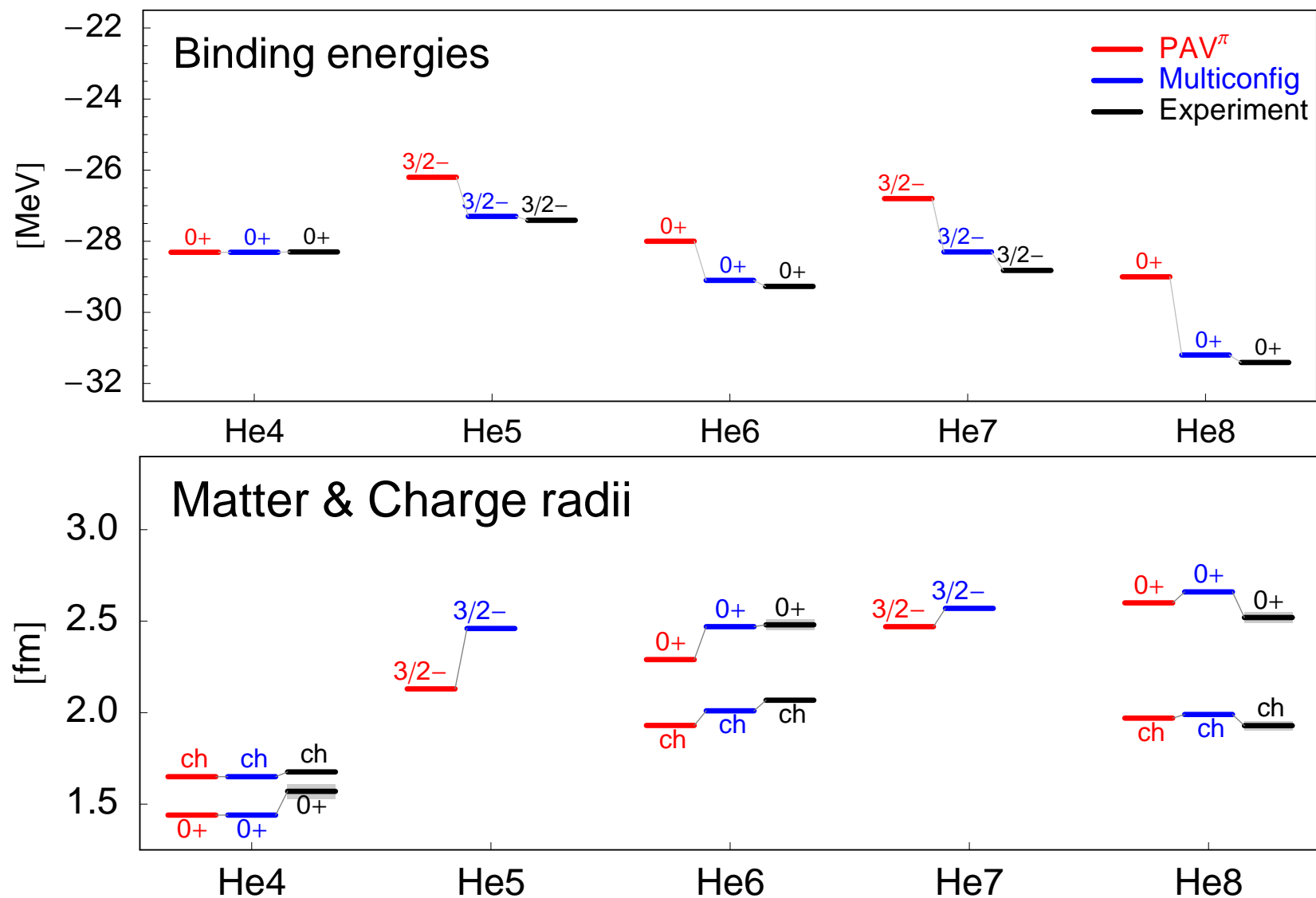
- Charge radii
- Matter radii
- Proton, neutron densities



- intrinsic densities of VAP $^{\pi}$  states  

$$|Q^{\pm}\rangle = \frac{1}{2} (1 \pm \Pi) |Q\rangle$$
- radial densities from multiconfiguration calculations

# Helium Isotopes

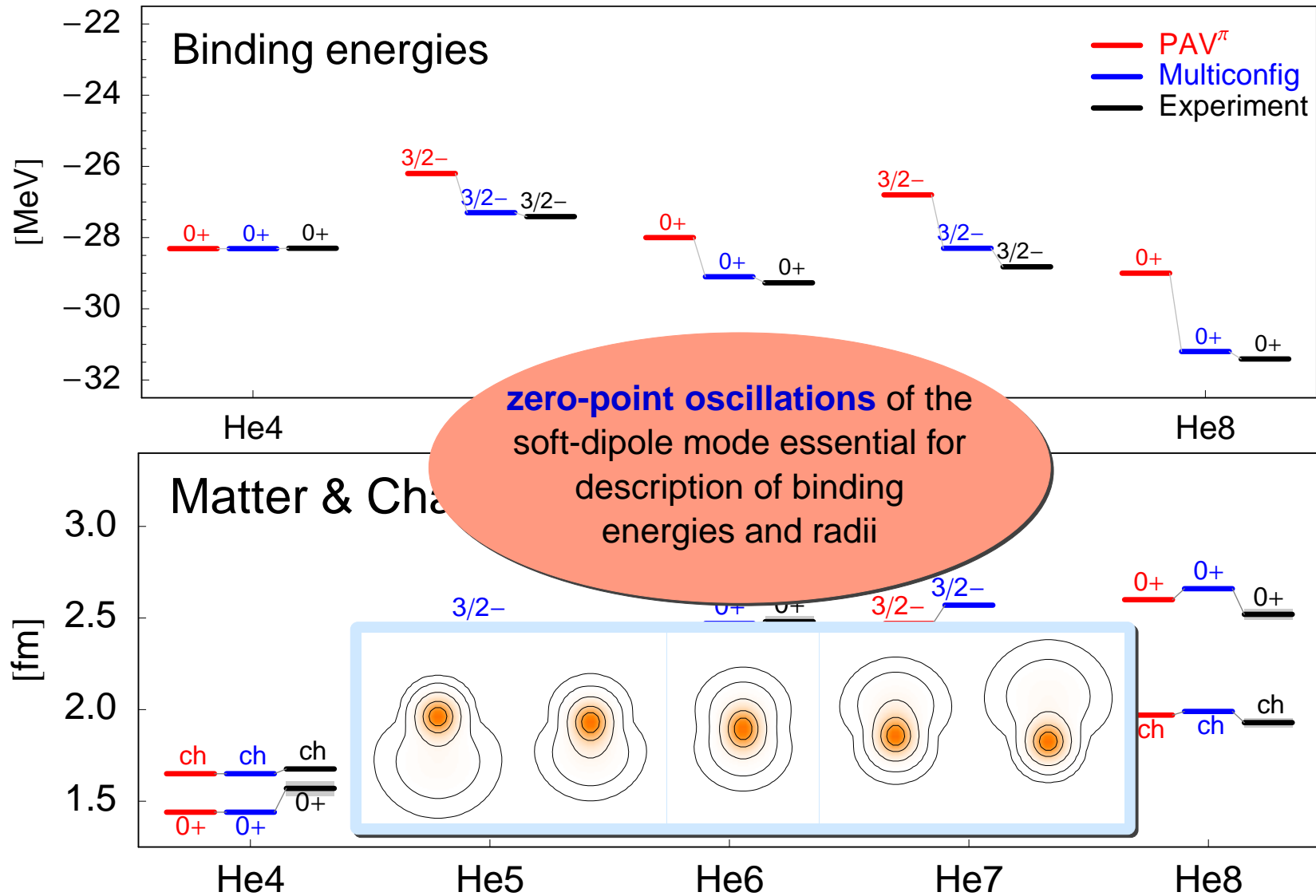


Exp: Ozawa,Suzuki,Tanihata, NPA**693**(2001)32; Raman,Nestor,Tikkanen, Atomic Data and Nucl. Data Tables **78**(2001)1

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



# Helium Isotopes



Exp: Ozawa,Suzuki,Tanihata, NPA**693**(2001)32; Raman,Nestor,Tikkanen, Atomic Data and Nucl. Data Tables **78**(2001)1

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

# Neon Isotopes $^{17}\text{Ne}$ – $^{22}\text{Ne}$



## Structure

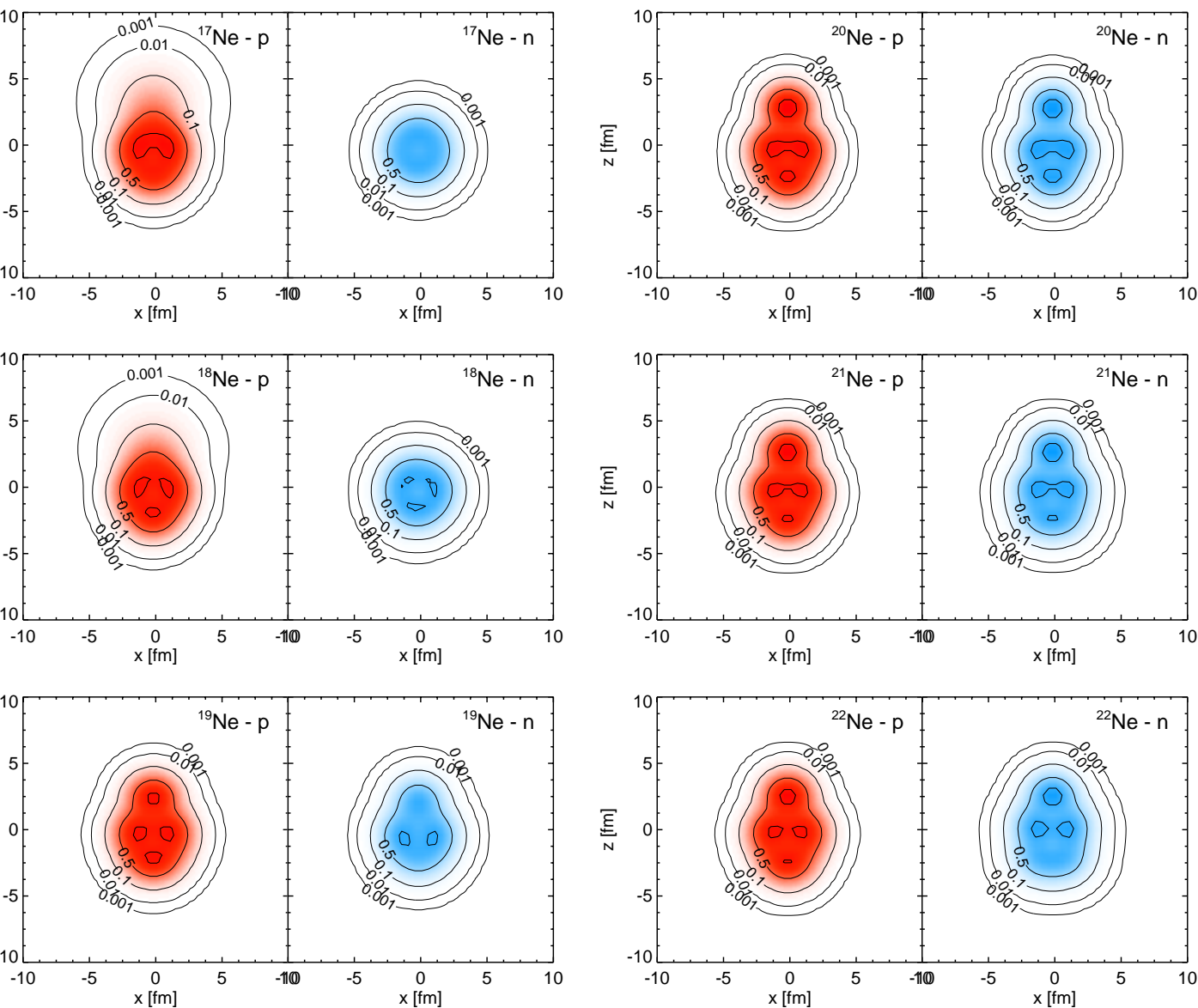
- $s^2/d^2$  occupation in  $^{17}\text{Ne}$  and  $^{18}\text{Ne}$
- $^3\text{He}$  and  $^4\text{He}$  cluster admixtures

## Observables

- Charge Radii
- Matter Radii
- Is  $^{17}\text{Ne}$  a Halo nucleus ?

# Neon Isotopes

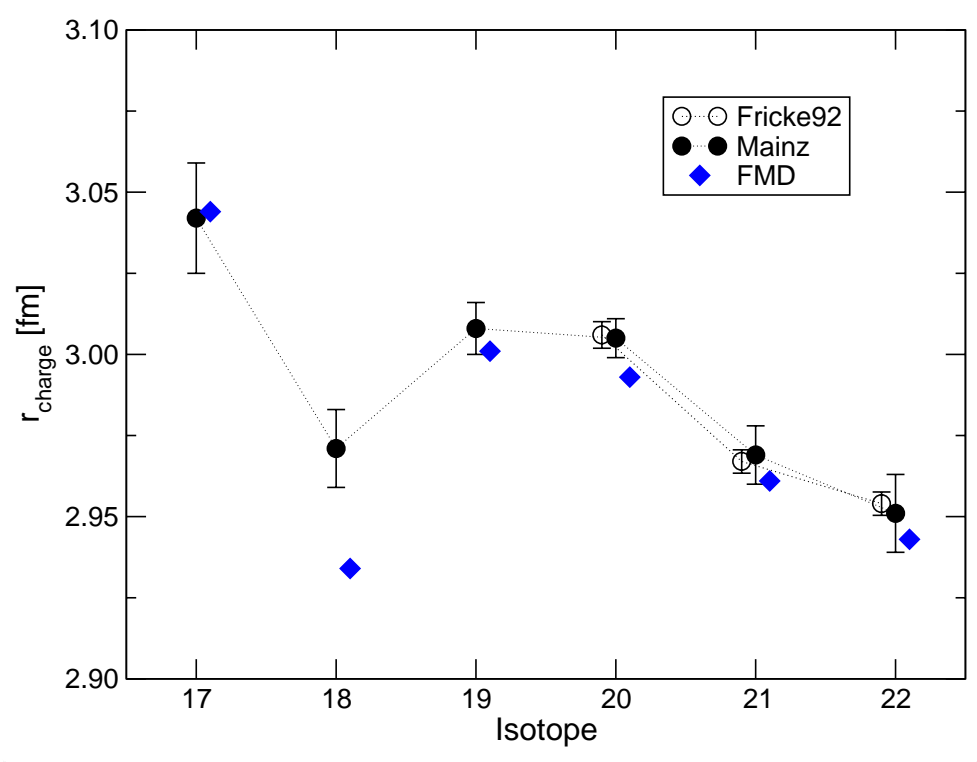
# Variation after Parity Projection VAP $\pi$



- 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  $^{17,18}\text{Ne}$
- explicit cluster configurations:
  - $^{17}\text{Ne}$ :  $^{14}\text{O}-^3\text{He}$
  - $^{18}\text{Ne}$ :  $^{14}\text{O}-^4\text{He}$
  - $^{19}\text{Ne}$ :  $^{16}\text{O}-^3\text{He}$ ,  $^{15}\text{O}-^4\text{He}$
  - $^{20}\text{Ne}$ :  $^{16}\text{O}-^4\text{He}$
  - $^{21}\text{Ne}$ : “ $^{17}\text{O}$ ”- $^4\text{He}$
  - $^{22}\text{Ne}$ : “ $^{18}\text{O}$ ”- $^4\text{He}$

$|Q^\pm\rangle$  minima

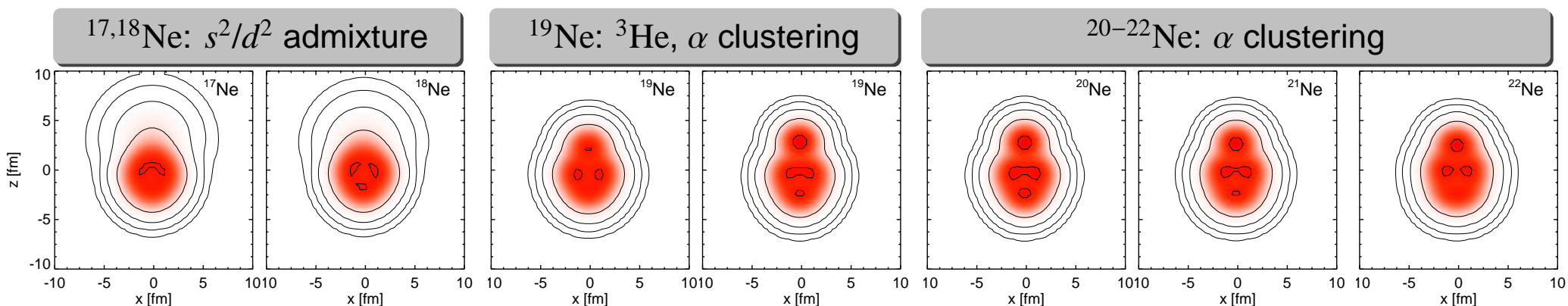
Intrinsic proton/neutron densities of dominant FMD state



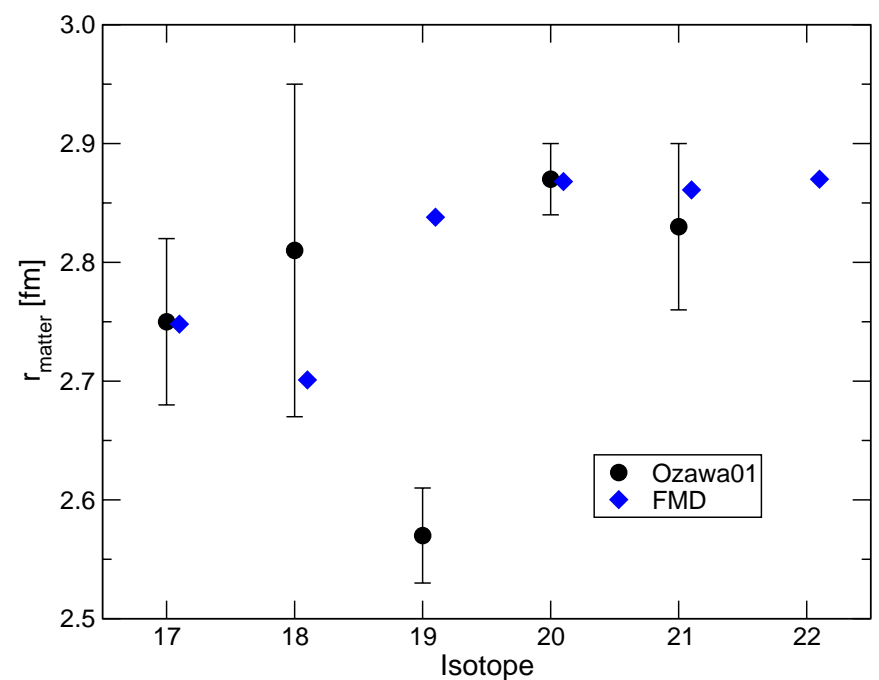
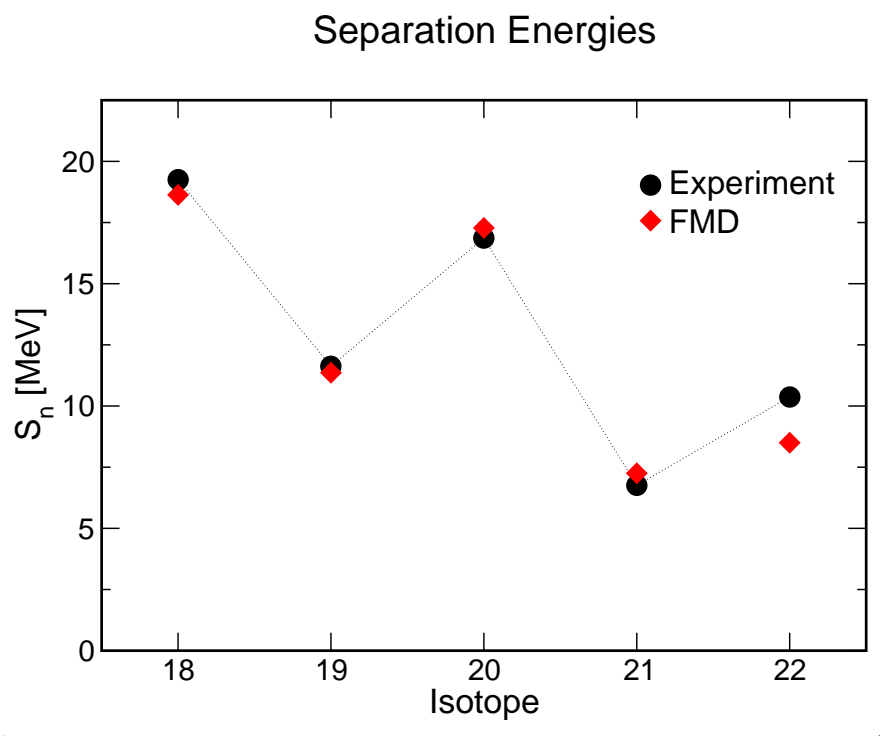
- charge radii of  $^{17,18}\text{Ne}$  depend strongly on  $s^2/d^2$  occupations
- cluster admixtures responsible for large charge radii in  $^{19-22}\text{Ne}$

- measurements of charge radii by COLLAPS@ISOLDE

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



# ● Separation Energies and Matter Radii



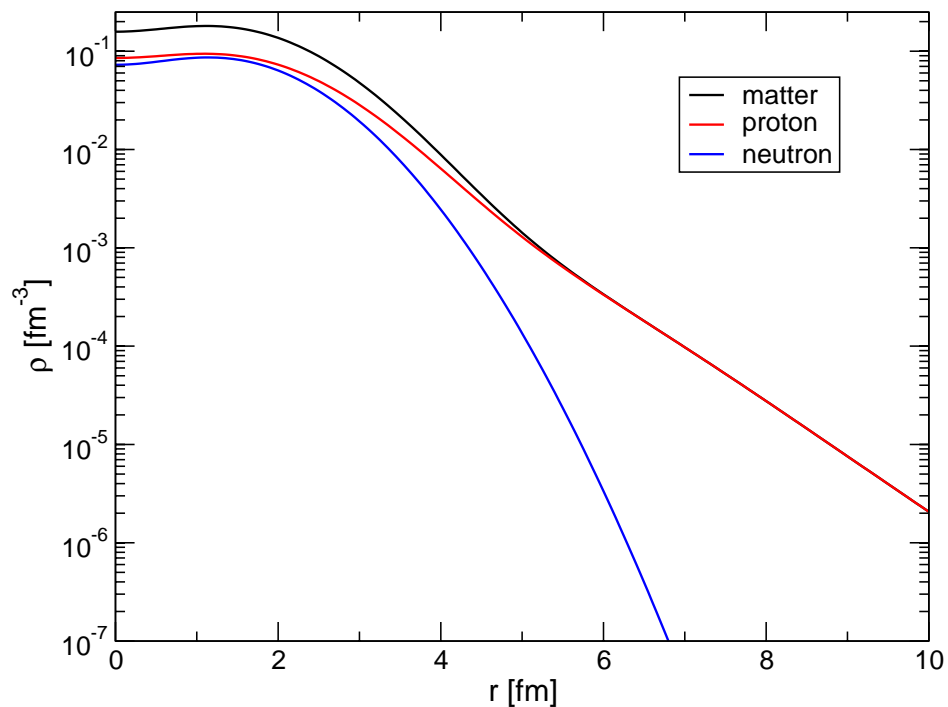
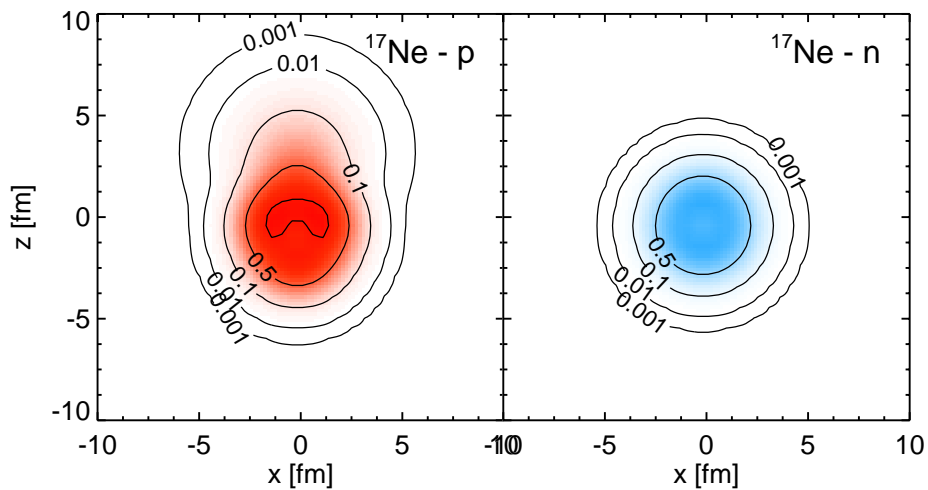
- matter radii from interaction cross sections

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

- good agreement with exception of  $^{19}\text{Ne}$

# Neon Isotopes

## $^{17}\text{Ne}$ Halo ?



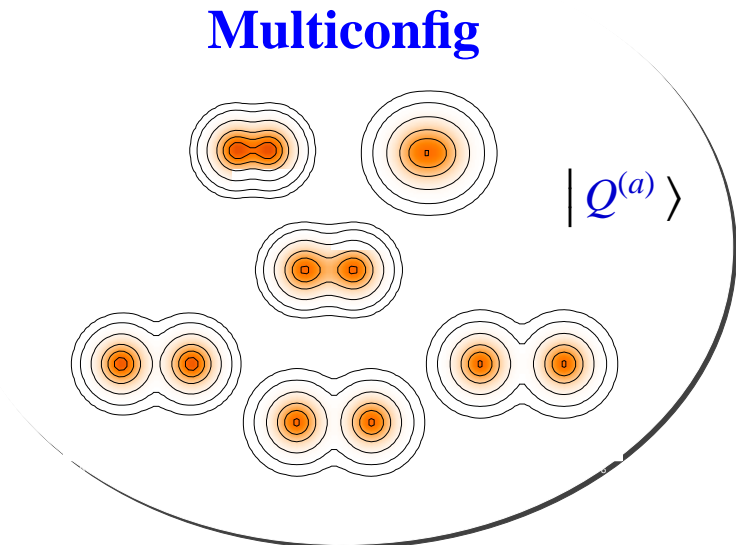
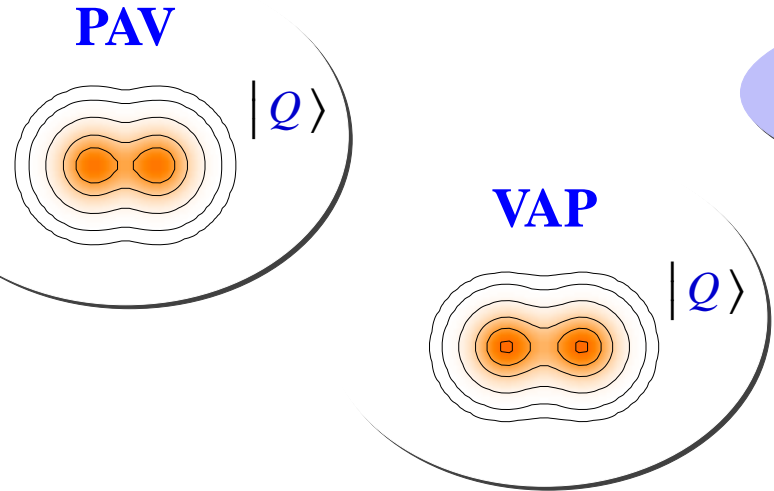
	FMD	Experiment
$r_{\text{ch}}[\text{fm}]$	3.03	3.042(17)
$r_{\text{mat}}[\text{fm}]$	2.75	2.75(7)
$B(E2; \frac{1}{2}^- \rightarrow \frac{3}{2}^-)[e^2\text{fm}^4]$	76.7	$66^{+18}_{-25}$
$B(E2; \frac{1}{2}^- \rightarrow \frac{5}{2}^-)[e^2\text{fm}^4]$	119.8	124(18)
occupancy $s^2$	40%	
occupancy $d^2$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

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

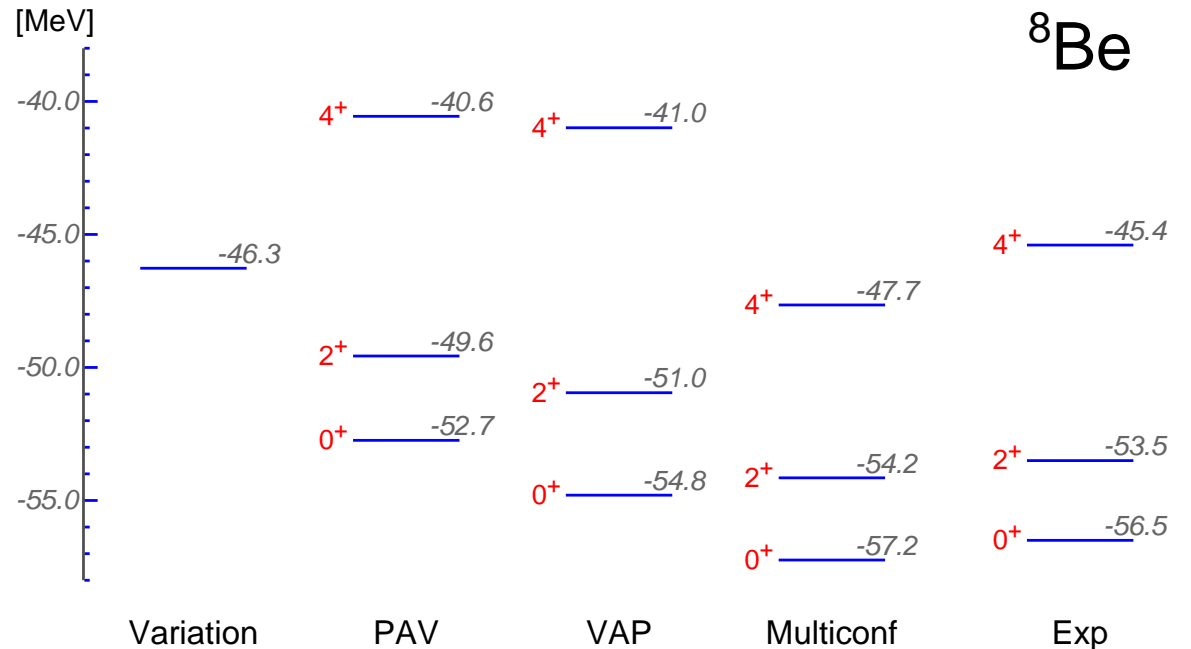
# FMD - Projection, Variation after Proj., Multiconfiguration

## Radius and Quadrupole Moment as Generator Coordinates

	$r_{charge}$ [fm]	$Q$ [ $\text{fm}^2$ ]	$B(E2)$ [ $e^2\text{fm}^4$ ]
PAV	2.39	-6.25	9.31
VAP	2.49	-8.02	15.36
Multiconfig	2.74	-11.88	30.39



$$|J^\pi M, n\rangle = \sum_{a, K'} c_{aK'}^{(n)} P_{MK'}^{J^\pi} P^{\mathbf{P}=0} |Q^{(a)}\rangle$$



# Collective Coordinate Representation

## Size Measure

➔ Operator  $\tilde{B}$  measures extension of the system

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

## Asymptotic Interpretation $r \gg R_{C1} + R_{C2}$

➔ Eigenvalues relate to relative distance  $r$  (for each  $J^\pi M$ )

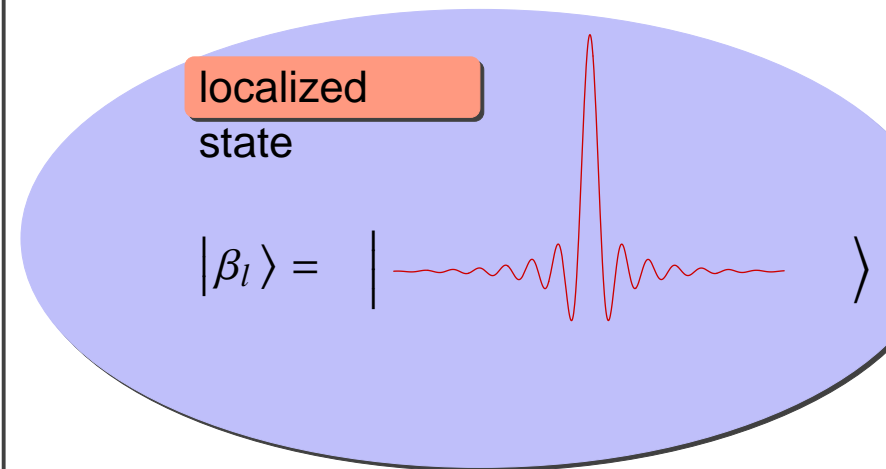
$$\tilde{B} |\beta_l\rangle = \beta_l |\beta_l\rangle$$

$$\Rightarrow \beta(r) = \frac{1}{A} \left( \frac{A_1 A_2}{A} r^2 + A_1 R_{C1}^2 + A_2 R_{C2}^2 \right) \Rightarrow r_l \leftrightarrow \beta_l$$

➔ Eigenvectors are localized in  $\beta$  and  $r$

$$\langle \beta_l | \tilde{B}^2 | \beta_l \rangle - \langle \beta_l | \tilde{B} | \beta_l \rangle^2 = 0$$

$$\Rightarrow \Psi(r_l) := \langle \beta_l | J^\pi M; \Psi \rangle \text{ relative wave function}$$

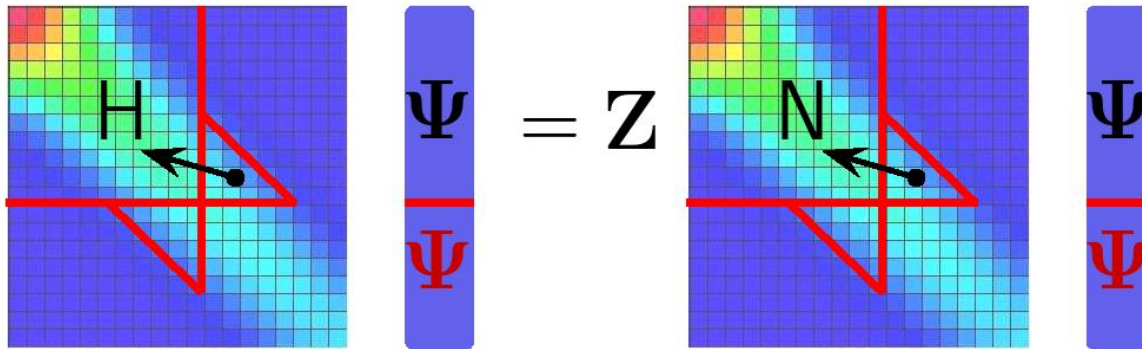




# Boundary Conditions 1

## Implement boundary conditions using the Collective Coordinate Representation

- Eigenvalue problem for scattering state  $|J^\pi M; \Psi\rangle$



$$|J^\pi M; \Psi\rangle = \sum_{aK}^N \psi_{aK} P_{MK}^{J^\pi} P^{P=0} |Q^{(a)}\rangle + \sum_{aK=N+1}^{N+n} \psi_{aK} P_{MK}^{J^\pi} P^{P=0} |Q^{(a)}\rangle$$

- Express unknown  $\psi_{aK}$  by known asymptotic solution  $\langle r | w \rangle = w(r)$  like

$$\frac{\langle \beta_N | [H, B]^s | J^\pi M; \Psi \rangle}{\langle \beta_N | J^\pi M; \Psi \rangle} \stackrel{!}{=} \frac{\langle r_N | \left[ \frac{1}{2\mu} \left( -\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} \right) + \frac{Z_1 Z_2 e^2}{r}, \beta(r) \right]^s | w \rangle}{\langle r_N | w \rangle} \quad s = 1, \dots, n$$

FMD many-body world = asymptotic point charge world

- ➔ Hamiltonian and Overlap matrix get modified  
both depend on complex eigenvalue  $Z$

# Boundary Conditions 2

## Different boundary conditions — Different physical situations

- **Whittaker** function

$$\langle r | w \rangle = W_\ell(kr) , \quad k = +\sqrt{-2\mu E}$$

- ➔ **bound state** with tail tunneling into Coulomb barrier,  $E < 0$

- **outgoing** Coulomb scattering solution

$$\langle r | w \rangle = iF_\ell(kr) + G_\ell(kr) , \quad k = +\sqrt{2\mu Z}$$

- ➔ **Gamov state** with resonance energy and width  $Z = E - i\Gamma/2$

- Coulomb **scattering** solution with phase shift

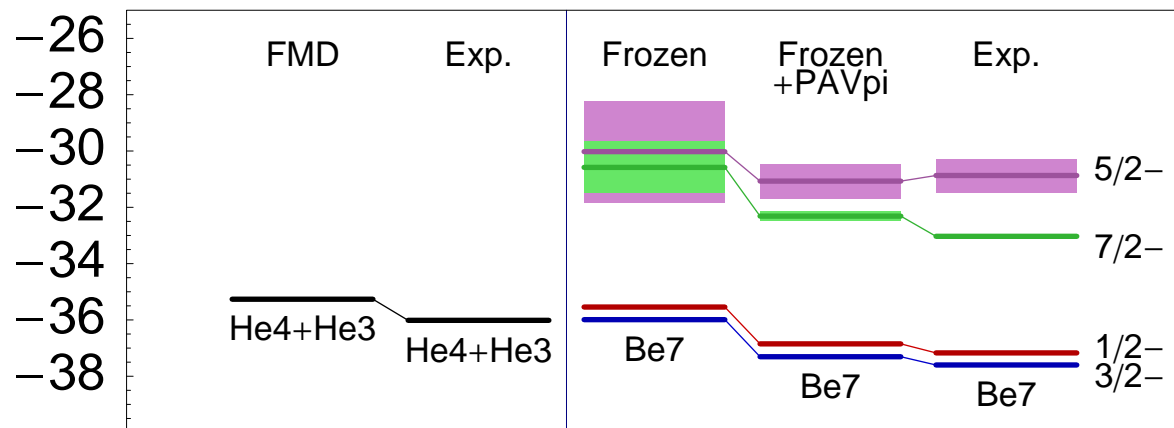
$$\langle r | w \rangle = F_\ell(kr) + \tan(\delta_\ell(E)) G_\ell(kr) , \quad k = +\sqrt{2\mu E}$$

- ➔ **continuum solution** with phase shift  $\delta_\ell(E)$ ,  $E > 0$

# $^7\text{Be}$ Levels Bound and in Continuum

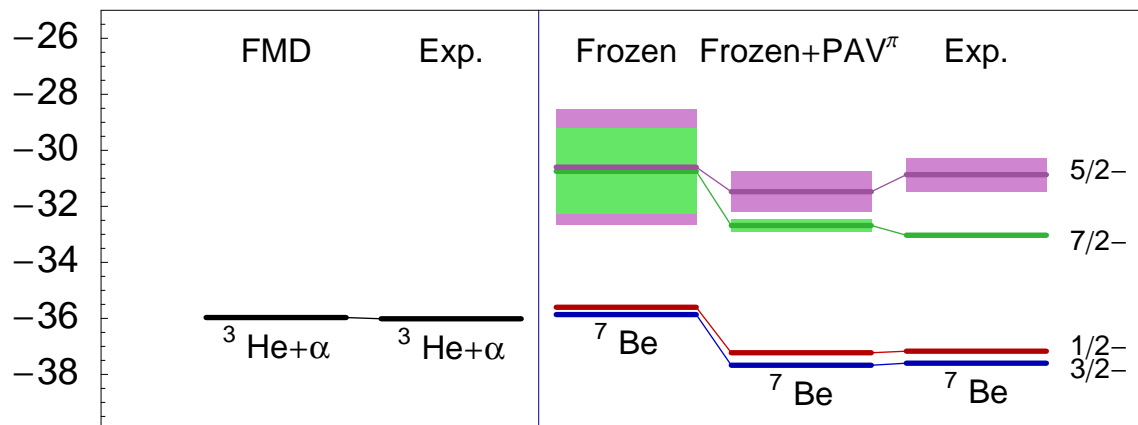
- implement boundary conditions using the **Gamov** state, outgoing only
- ➔ Hamiltonian and Overlap matrix get modified, complex eigenvalue

Binding energies

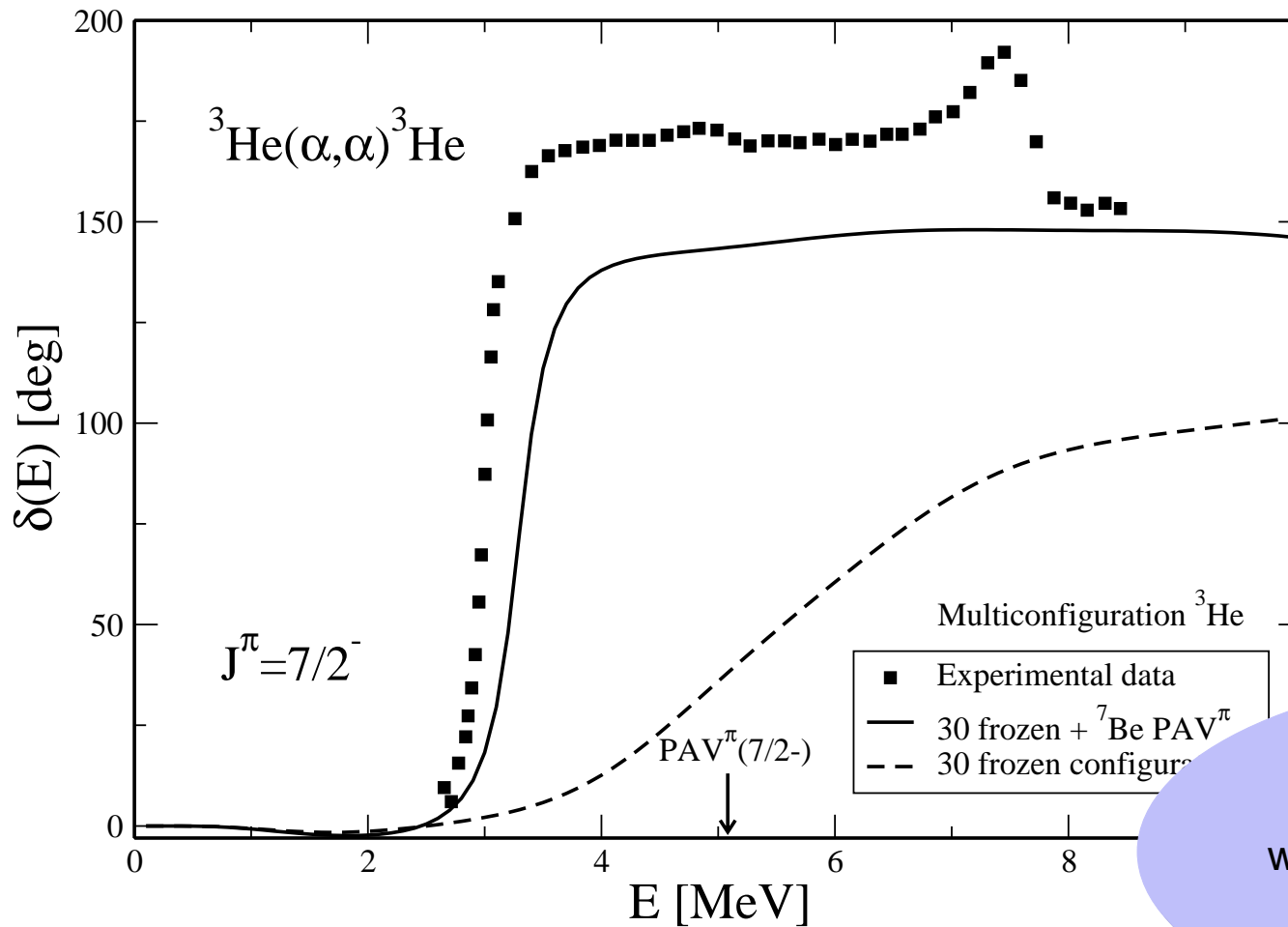


- single Slater determinant gives poor description for  $^3\text{He}$
- ➔ use multiconfiguration state for  $^3\text{He}$

[MeV]

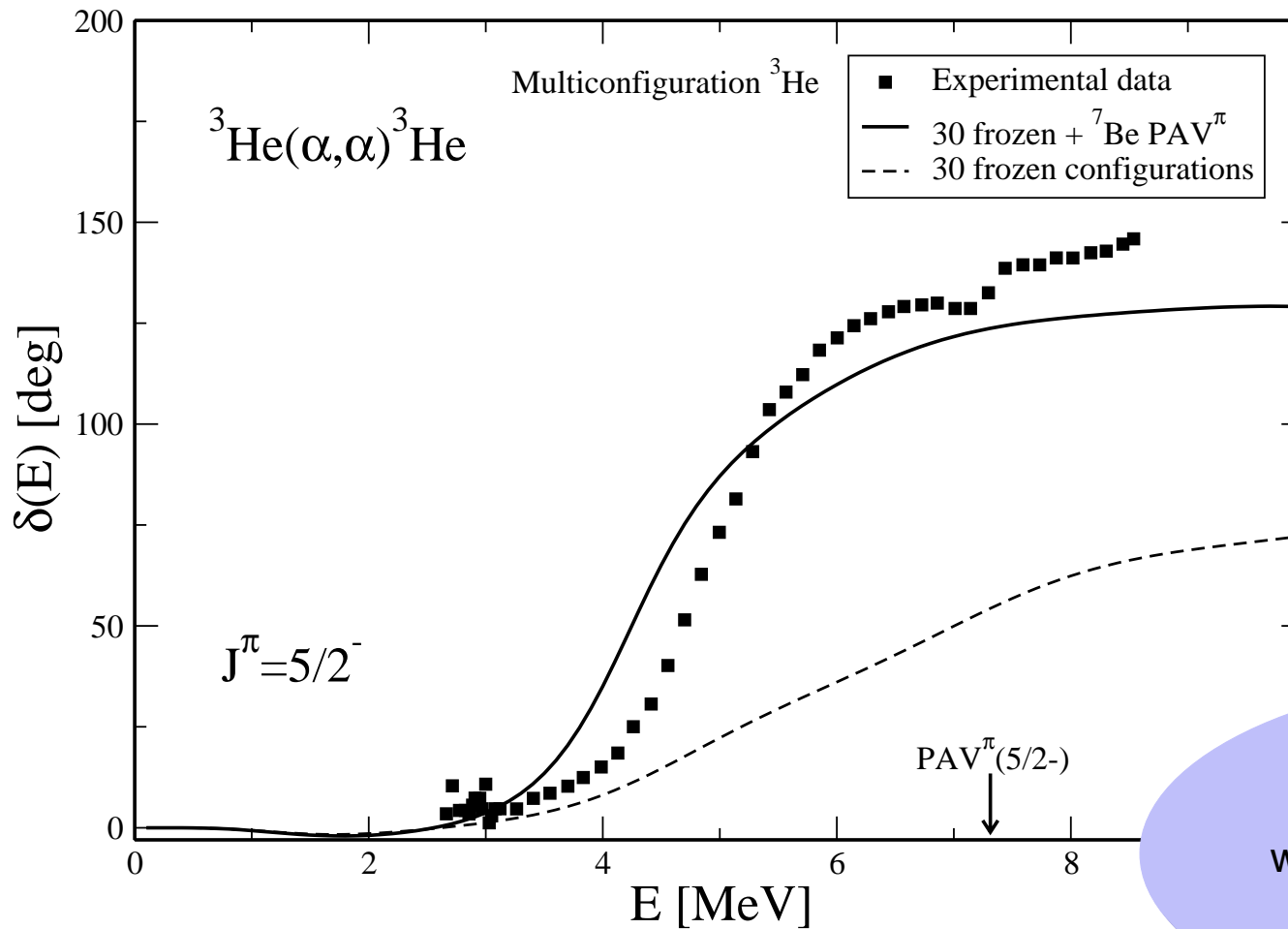


# ${}^7\text{Be}$ Phase Shift $7/2^-$ Resonance



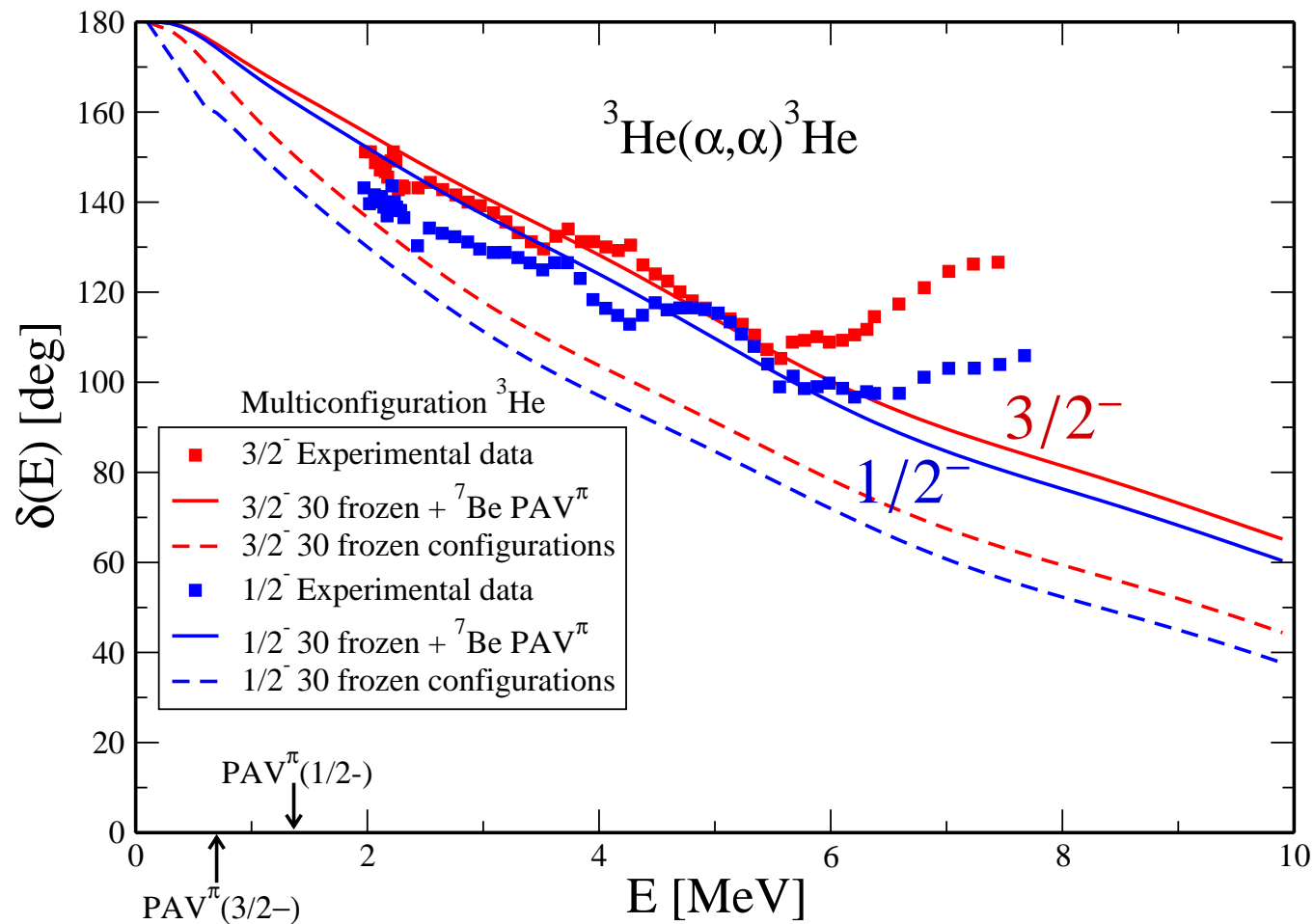
★ Resonance ★  
 wave function large in interior  
 $\text{PAV}^\pi$  state essential

# ${}^7\text{Be}$ Phase Shift $5/2^-$ Resonance

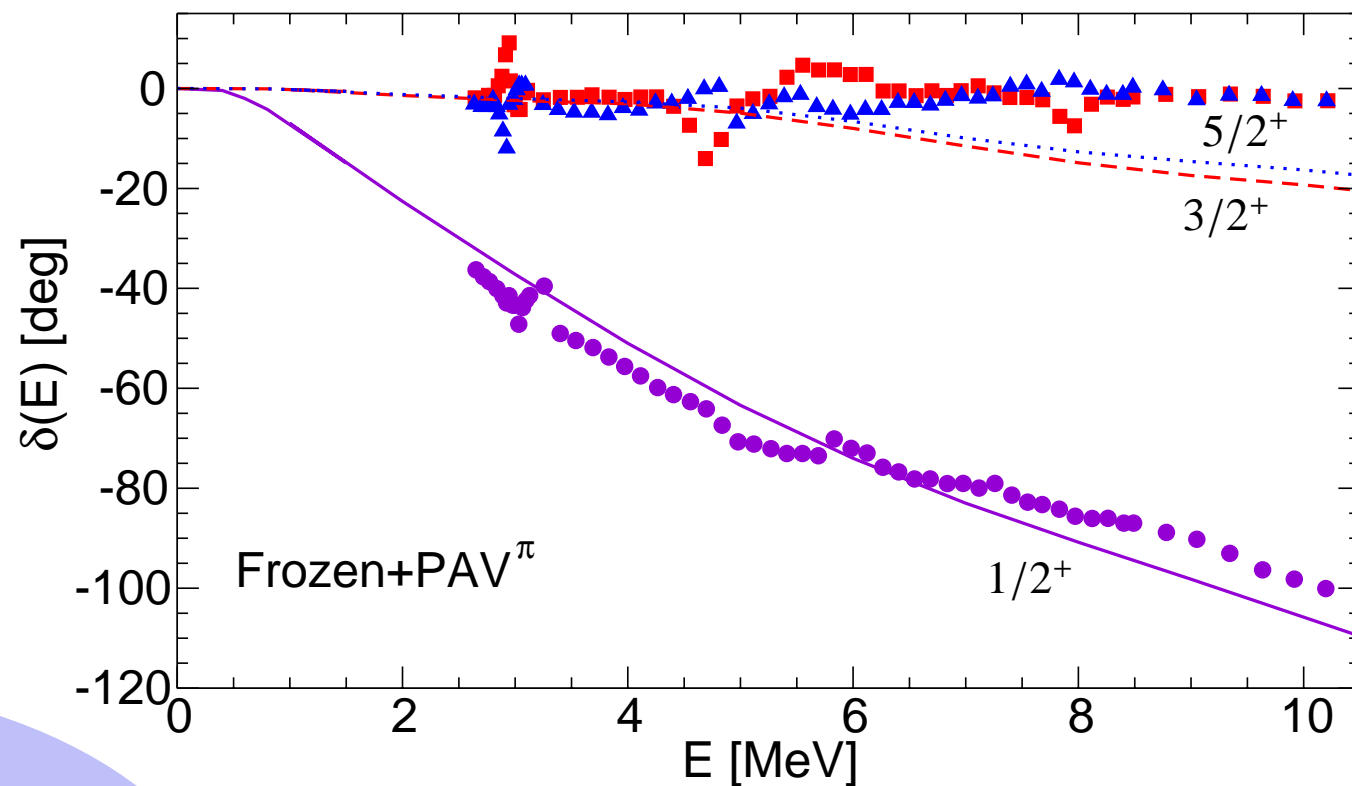


★ **Resonance** ★  
 wave function large in interior  
 PAV $^\pi$  state essential

# $^7\text{Be}$ Phase Shifts, nonresonant



# ${}^7\text{Be}$ Phase Shifts, nonresonant

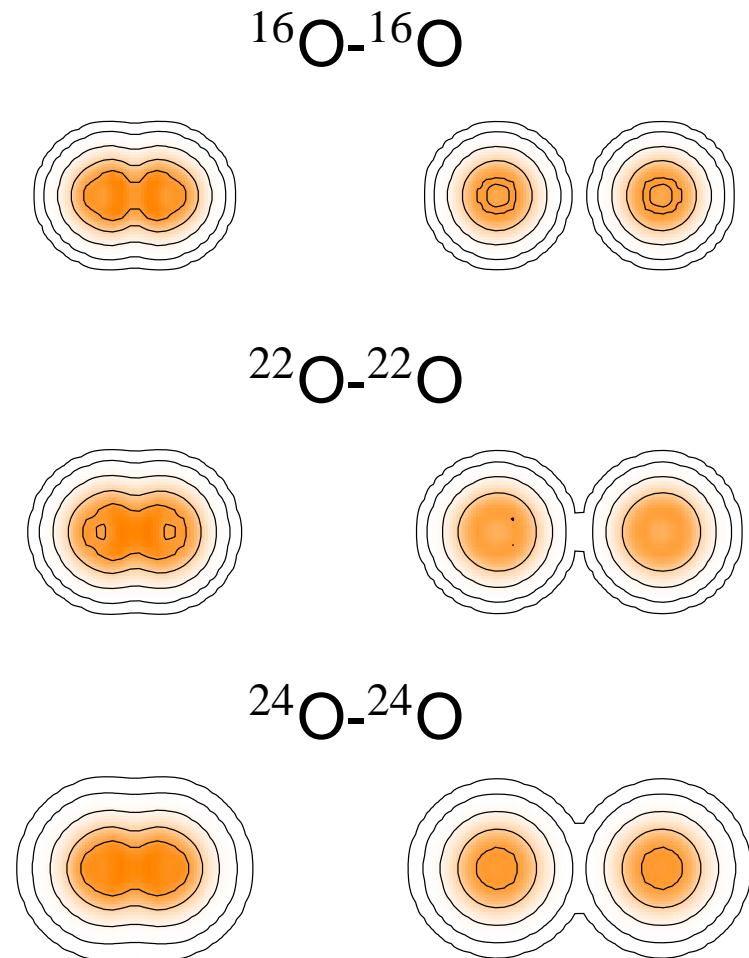
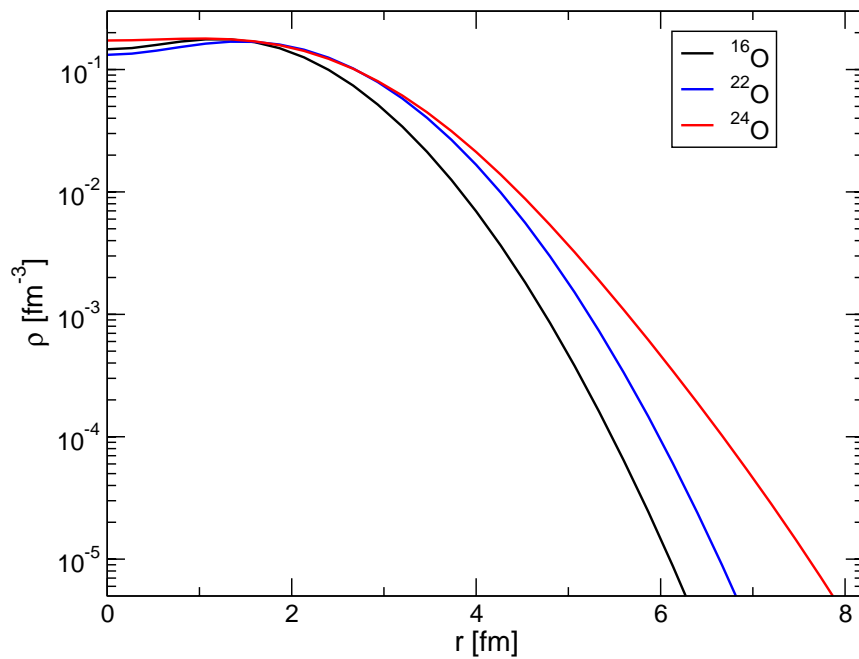


➤ remaining task:

calculate **dipole transitions** from the scattering states to the bound states to obtain the cross-sections and the **S-factor**

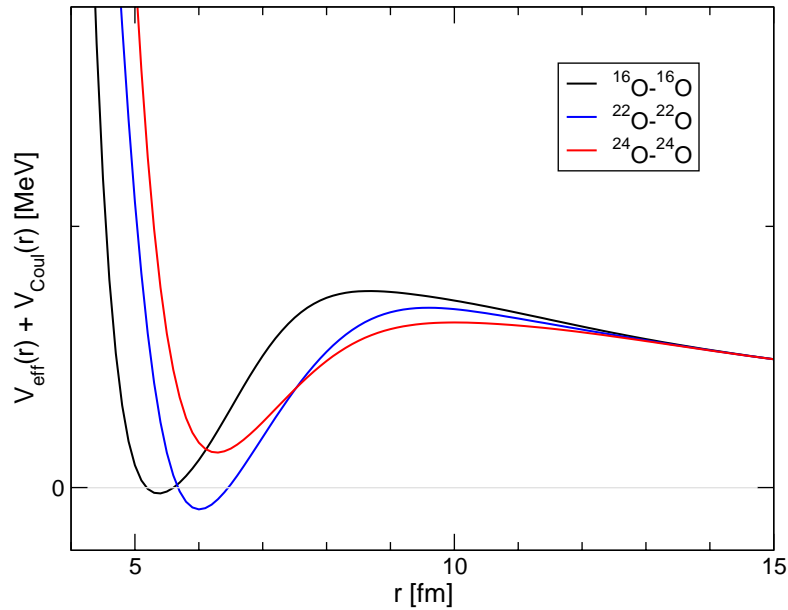
# Microscopic Nucleus-Nucleus Interactions

- Fermionic Molecular Dynamics (FMD) many-body states
- Effective nucleon-nucleon interaction derived from realistic Argonne V18 interaction





# S-Factors



Microscopically derived  
Nucleus-Nucleus potentials

Astrophysical S-factor

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

