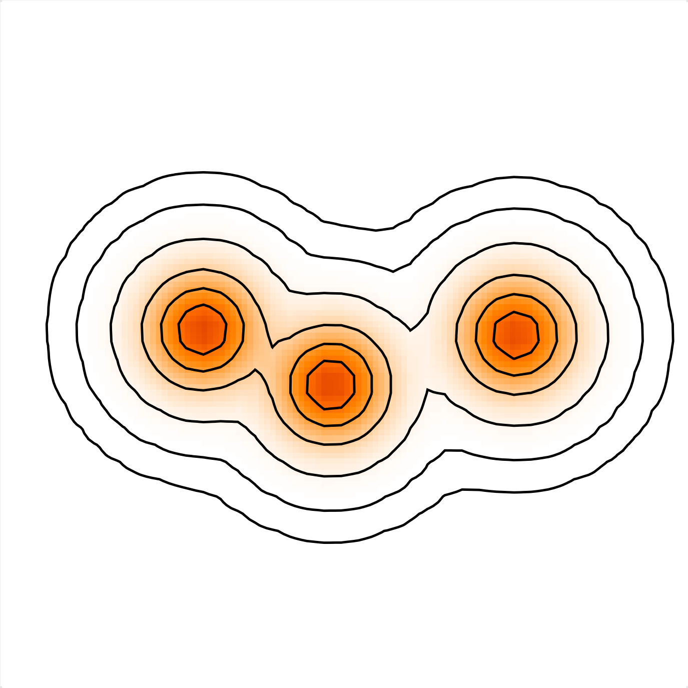
# Halo and Cluster Structures
# in
# Fermionic Molecular Dynamics


Hans Feldmeier, GSI, Darmstadt


Halo 06

ECT*, Trento

Oct. 30 – Nov. 03, 2006



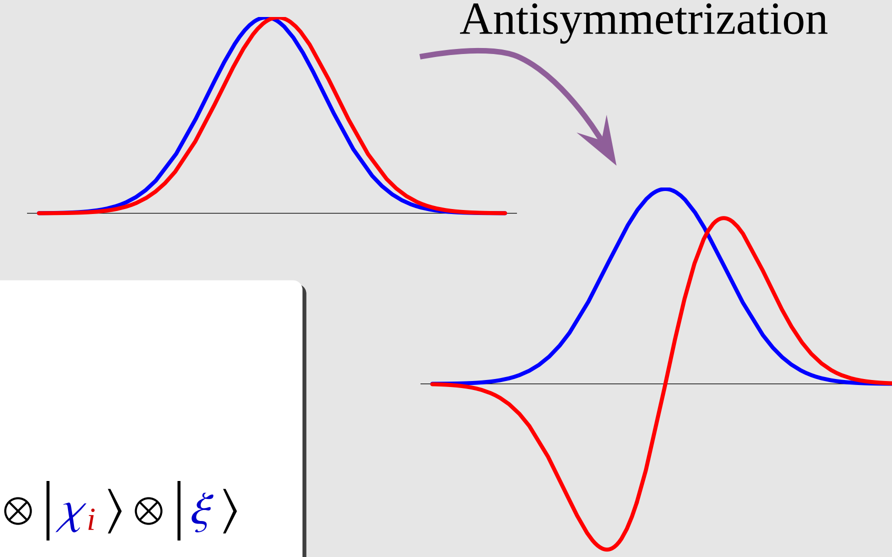
# FMD - Hilbert Space

## Fermionic

Slater determinant

$$\big|\, Q \,\big\rangle = \underset{\sim}{\mathcal{A}}\Big(\big|\, q_1 \,\big\rangle \otimes \cdots \otimes \big|\, q_A \,\big\rangle\Big)$$

➨ antisymmetrized $A$-body state




## Molecular

single-particle states

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

➨ 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 $\big|\, Q^{(a)} \,\big\rangle$

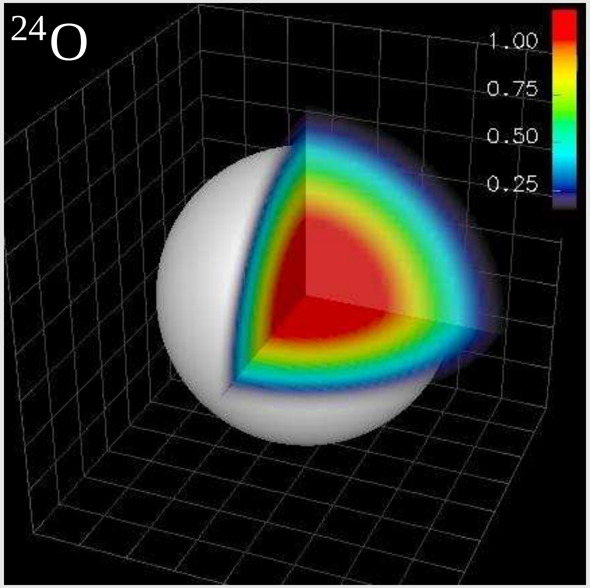
$$\big|\, \Psi; J^\pi M \,\big\rangle = \sum_{a,K'} \psi_{a,K'} \, \underset{\sim}{P}^{J^\pi}_{MK'} \underset{\sim}{P}^{\mathbf{P}=0} \big|\, Q^{(a)} \,\big\rangle$$

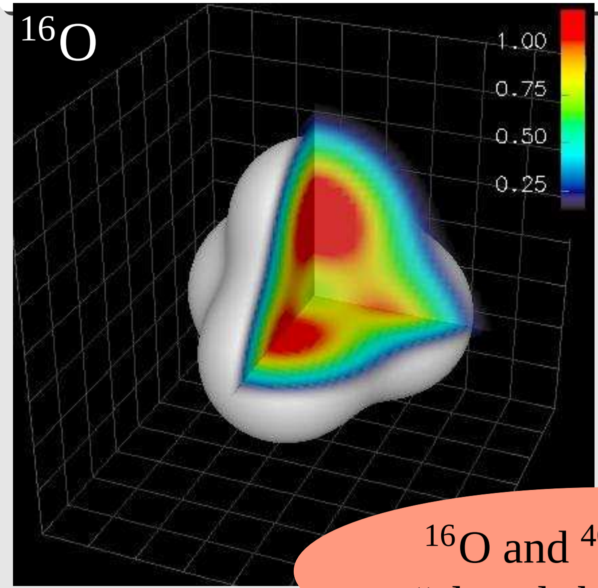
variational principle $\rightarrow$ $Q^{(a)} = \{\, q^{(a)}_\nu, \nu = 1 \cdots A \,\},\ \psi_{a,K'}$

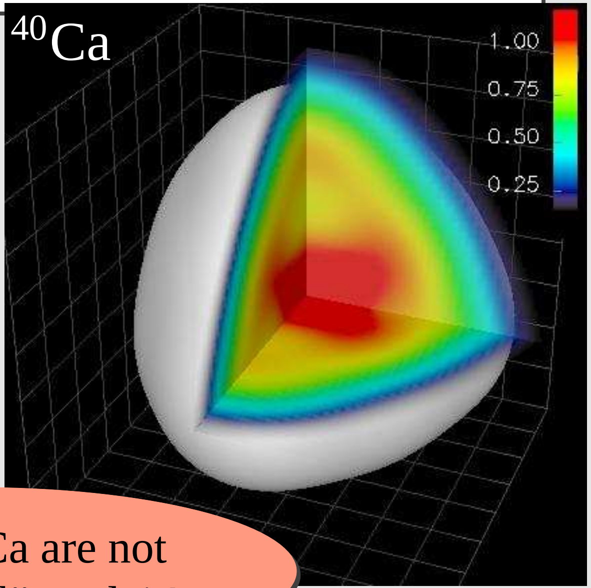
# Nucleon-Nucleon Potential

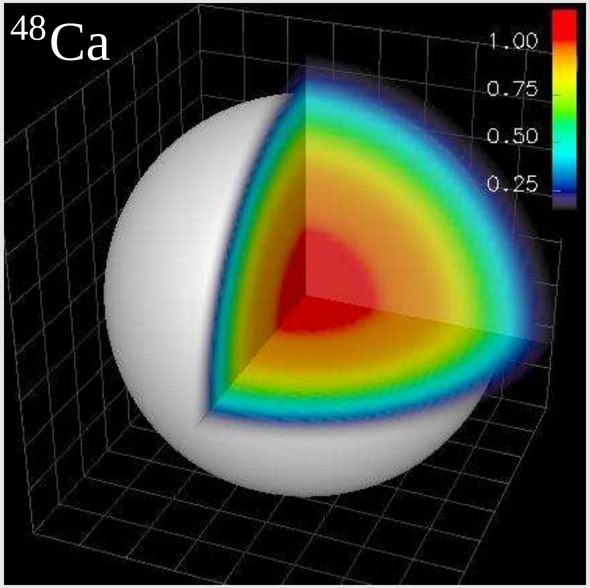
## Effective two-body interaction

- correlated 2-body interaction $\widehat{\underset{\sim}{H}} = \underset{\sim}{C}^{\dagger} \underset{\sim}{H}\, \underset{\sim}{C} = \underset{\sim}{T} + \underset{\sim}{V}_{UCOM}$ treats short range repulsive and tensor correlations
- additional small 2-body correction (momentum-dependent and spin-orbit) to make up for 3-body forces and long range tensor correlations
- fit correction term to binding energies and radii of "closed-shell" nuclei
- altogether a **15%** correction to the *ab-initio* $\underset{\sim}{V}_{UCOM}$




$^{16}$O and $^{40}$Ca are not "closed shell" 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
  - linear momentum
  - angular-momentum
- projected state

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

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

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

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

## Variation After Projection (VAP)

- effect of projection can be large
- perform 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)
- perform true VAP

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

# Multi-Configuration Mixing

- most general projected state for multi-configuration calculations

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

- 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

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

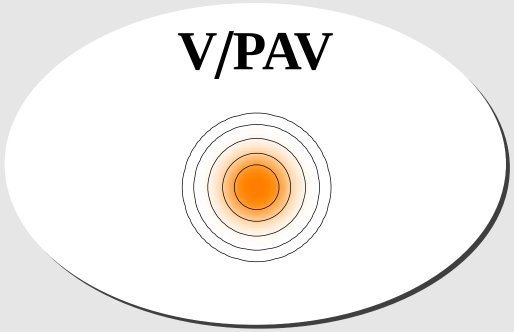
- **diagonalize** Hamiltonian in this set of nonorthogonal projected intrinsic states

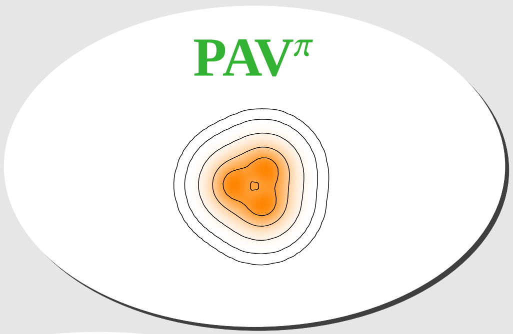
$$\sum_{K'b} \left\langle Q^{(a)} \right| \underset{\sim}{H} \underset{\sim}{P}^{J^\pi}_{KK'} \underset{\sim}{P}^{\mathbf{P}=0} \left| Q^{(b)} \right\rangle \cdot c^{(n)}_{K'b} = E_n^{J^\pi} \sum_{K'b} \left\langle Q^{(a)} \right| \underset{\sim}{P}^{J^\pi}_{KK'} \underset{\sim}{P}^{\mathbf{P}=0} \left|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

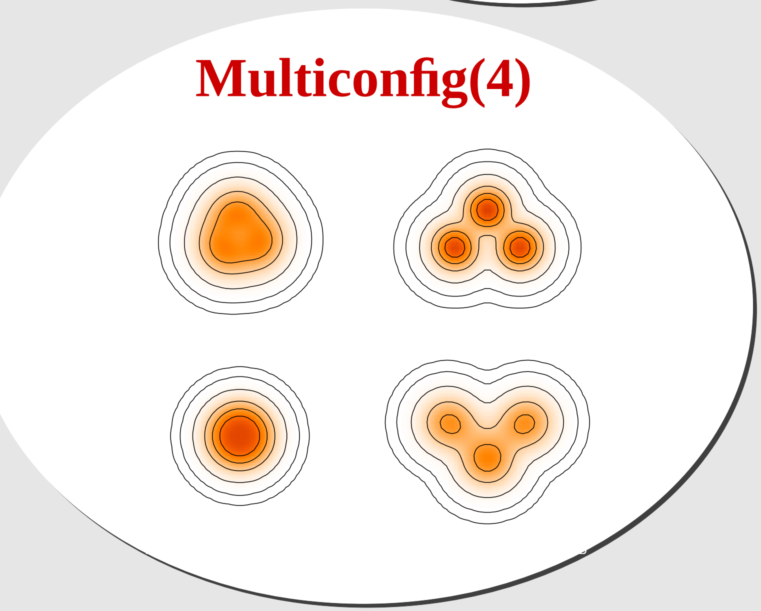
- energy levels $E_n^{J^\pi}$ and eigenstates $\left| J^\pi M, n \right\rangle$ describing nuclear many-body system

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

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

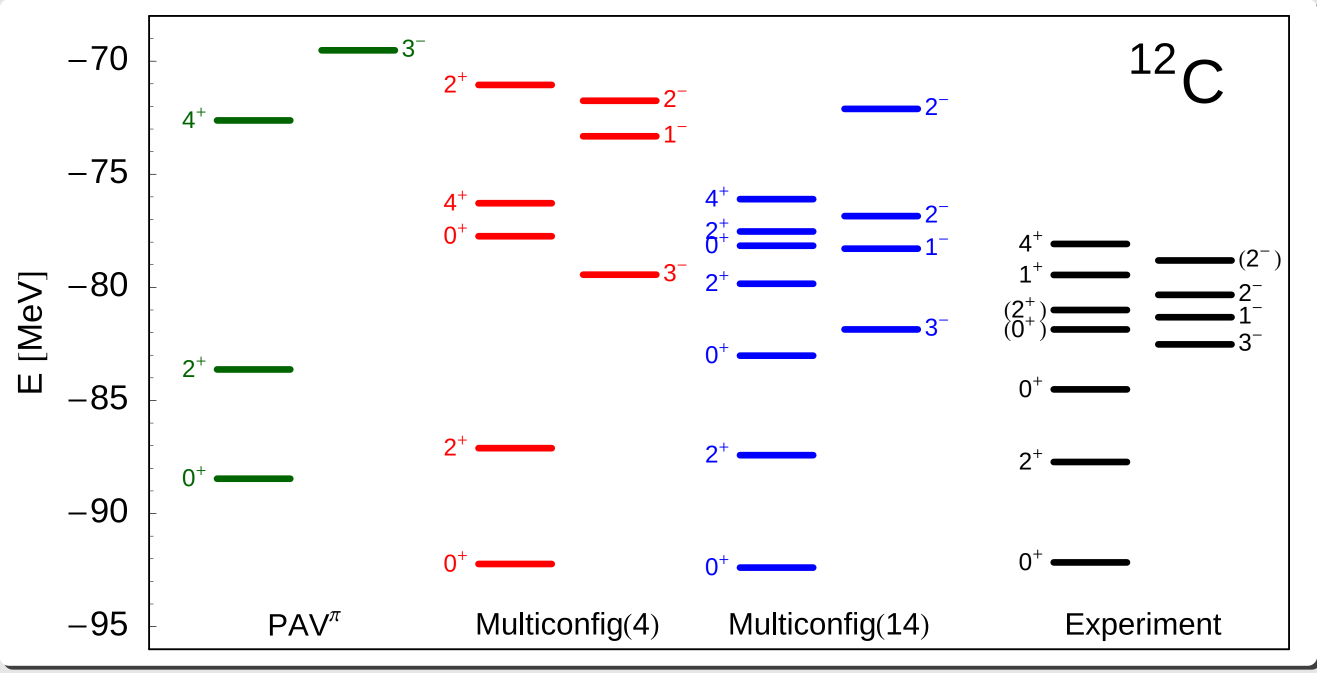


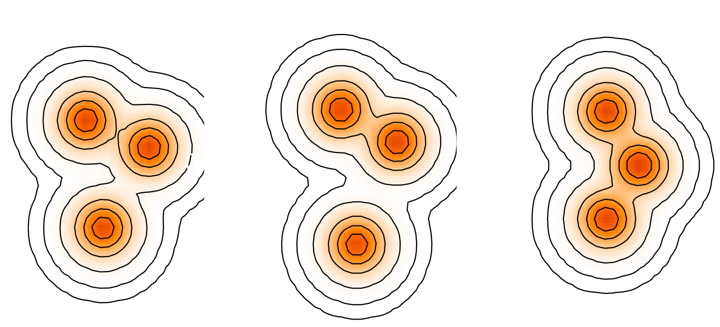

$^{12}$C

| | $E$ [MeV] | $r_{charge}$ [fm] | $B(E2)$ [$e^2$fm$^4$] |
|---|---|---|---|
| V/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 |



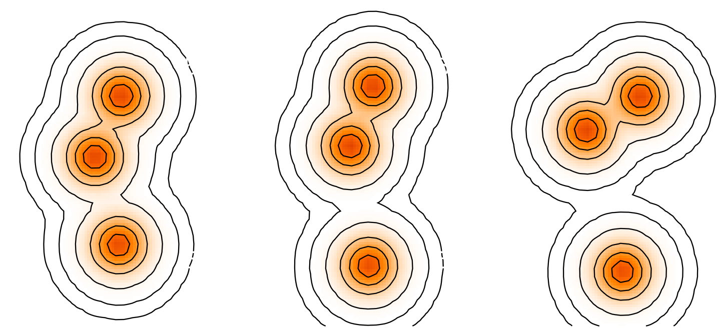
# $^{12}$C excited $0^+$ and $2^+$ states

## $0_2^+$ state



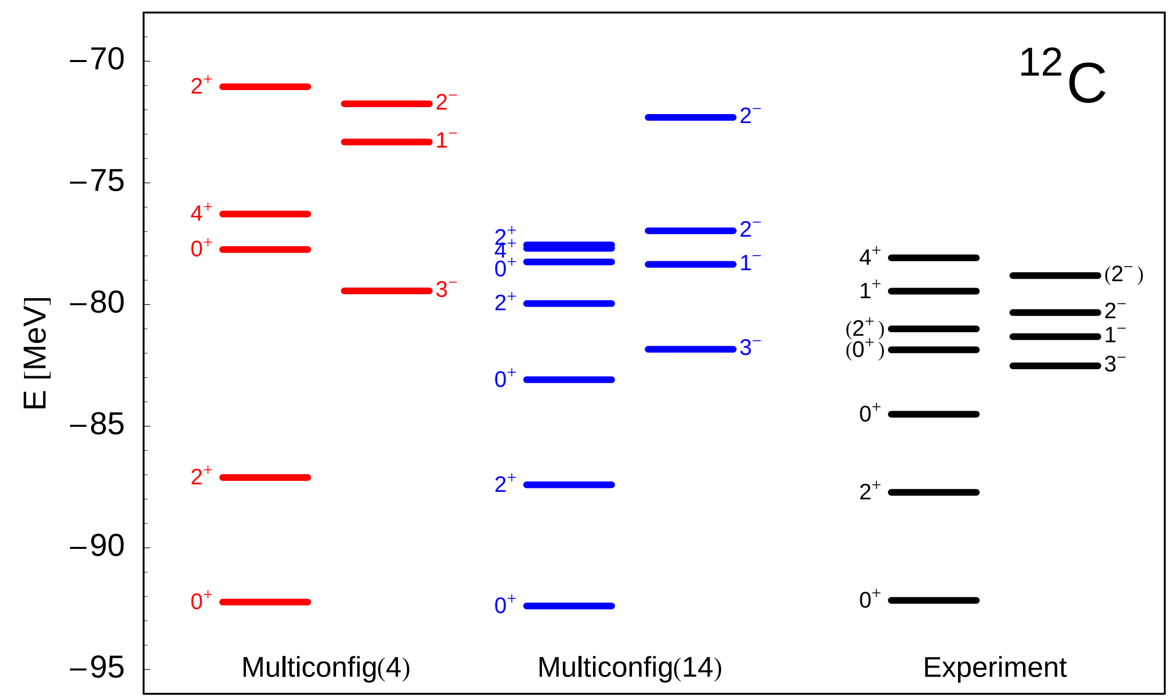
$|\langle \cdot | 0_2^+ \rangle| = 0.76$ $|\langle \cdot | 0_2^+ \rangle| = 0.71$ $|\langle \cdot | 0_2^+ \rangle| = 0.50$

## $0_3^+$ state

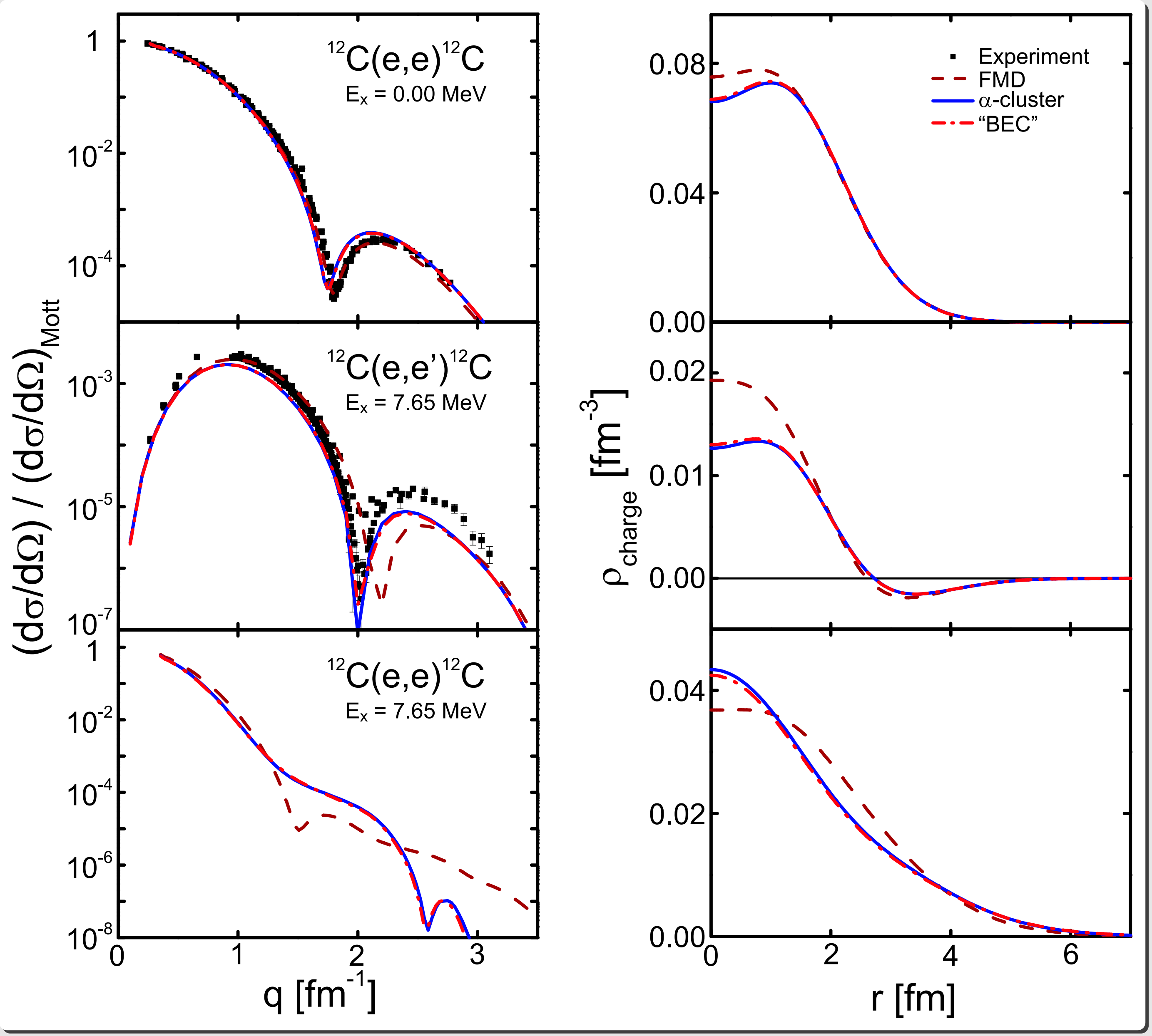


$|\langle \cdot | 0_3^+ \rangle| = 0.69$ $|\langle \cdot | 0_3^+ \rangle| = 0.65$ $|\langle \cdot | 0_3^+ \rangle| = 0.44$

| | Multiconfig | Experiment |
|---|---|---|
| $E_b$ [MeV] | 92.4 | 92.2 |
| $r_{charge}$[fm] | 2.52 | 2.47 |
| $B(E2)(0_1^+ \rightarrow 2_1^+)$ [$e^2$fm$^4$] | 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

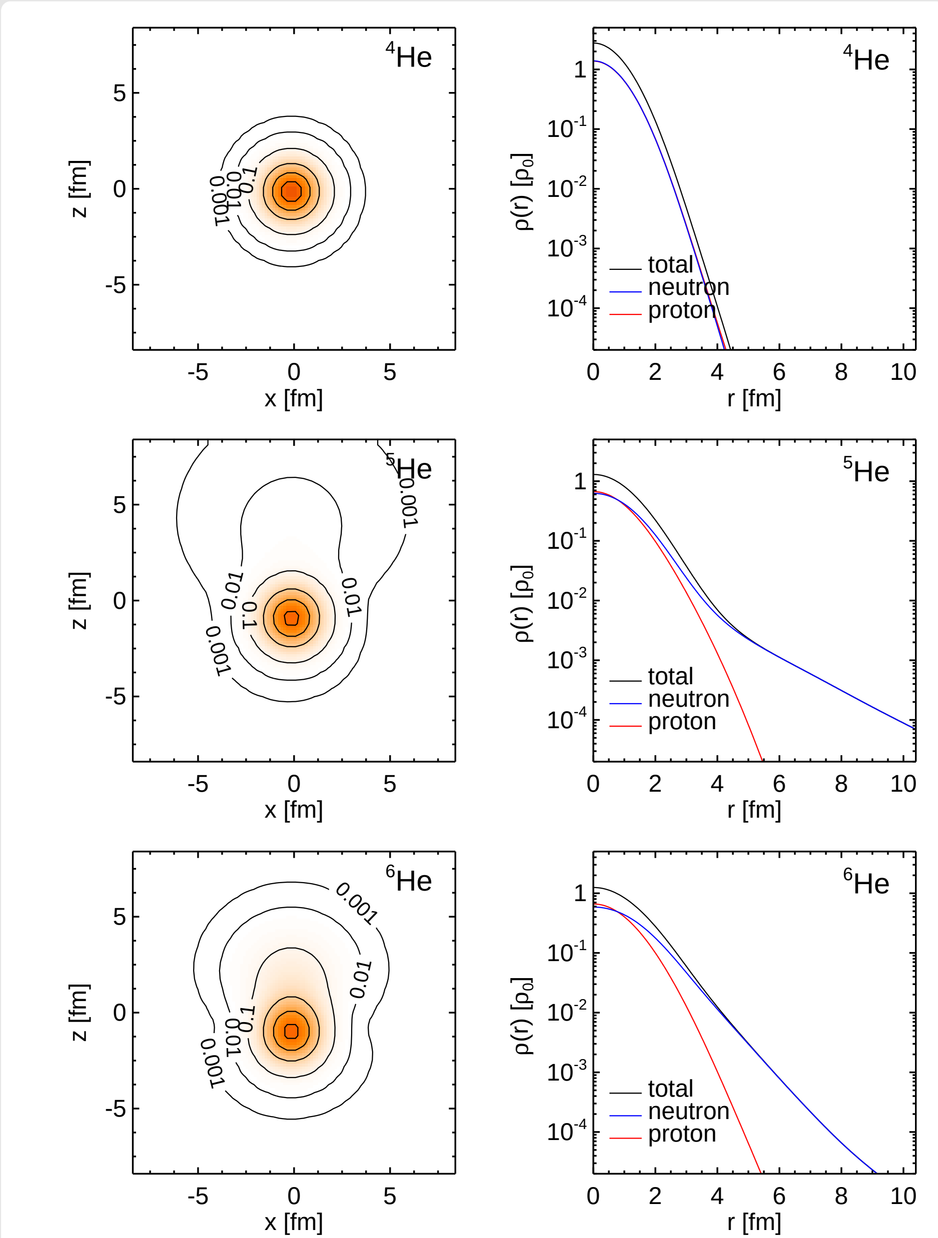
- $\alpha$-cluster and "BEC" calculated with mod. Volkov interation

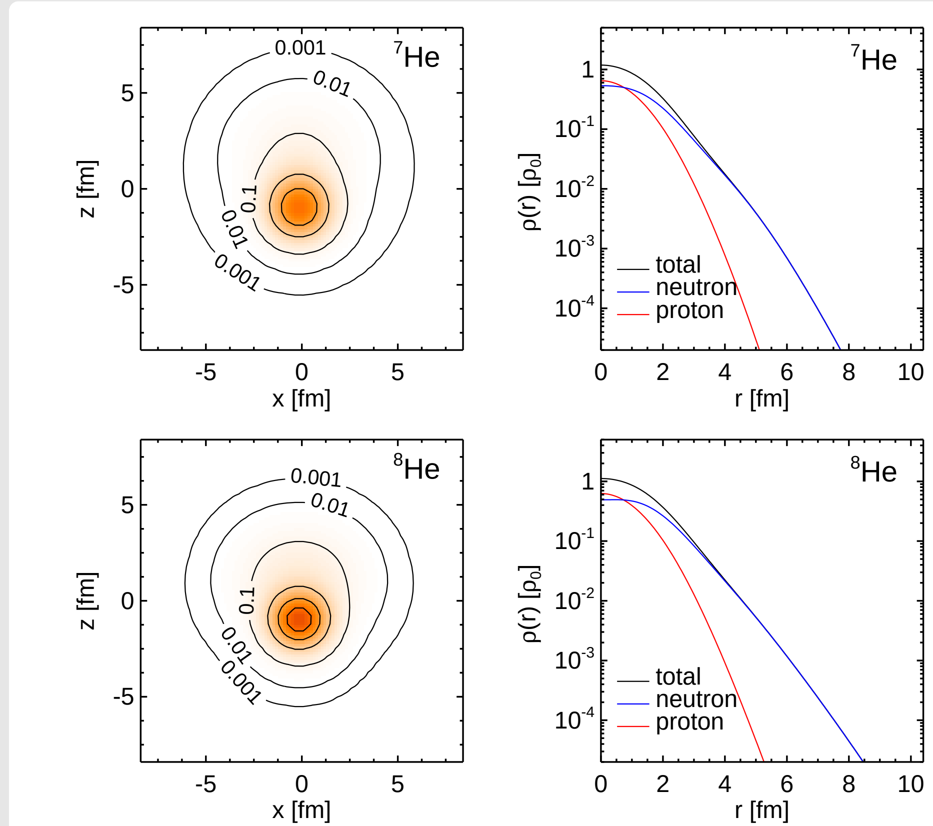
M. Chernykh, P. von Neumann-Cosel, A. Richter et al. submitted to PRL

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

# Helium Isotopes

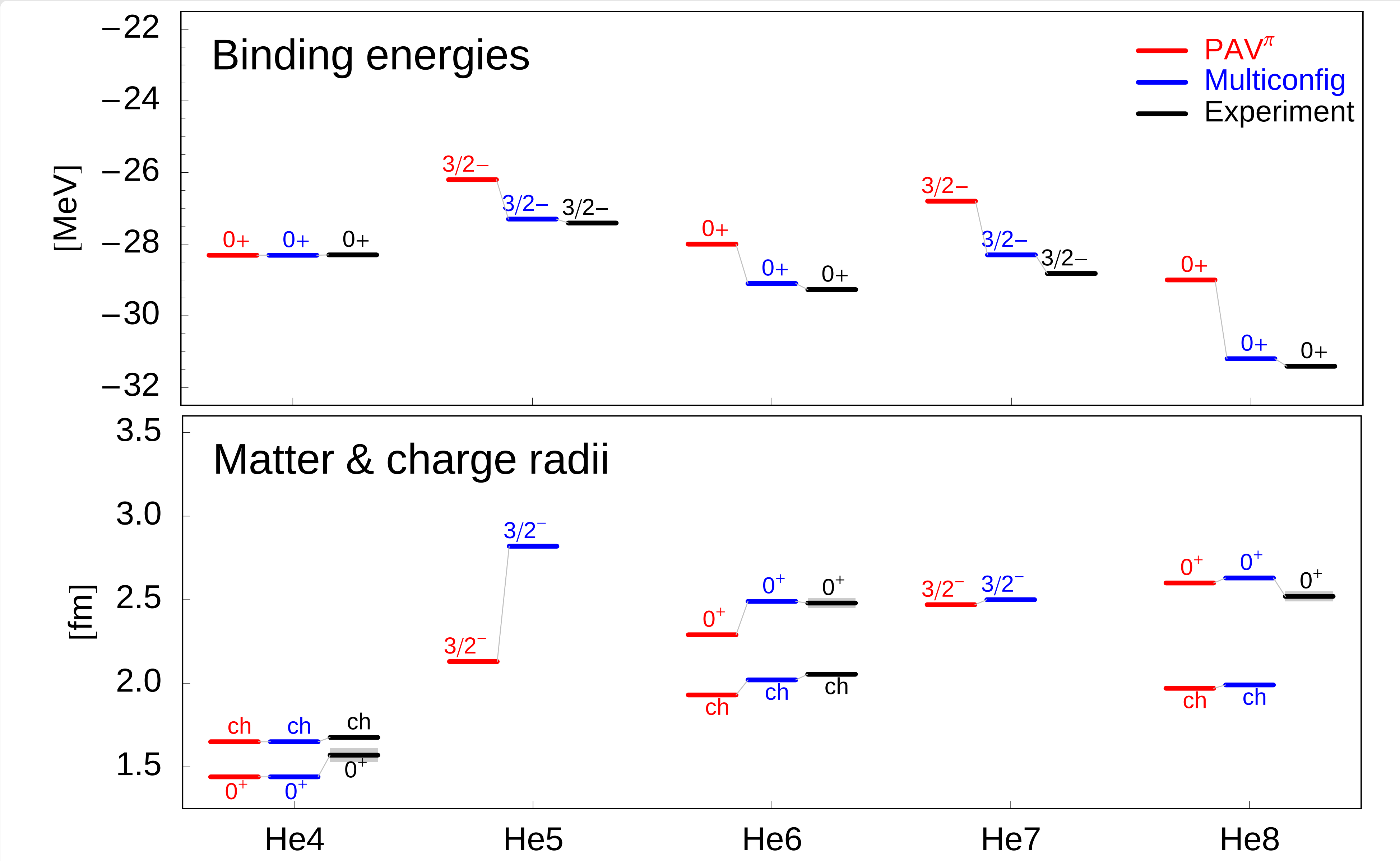
**dipole and quadrupole constraints**



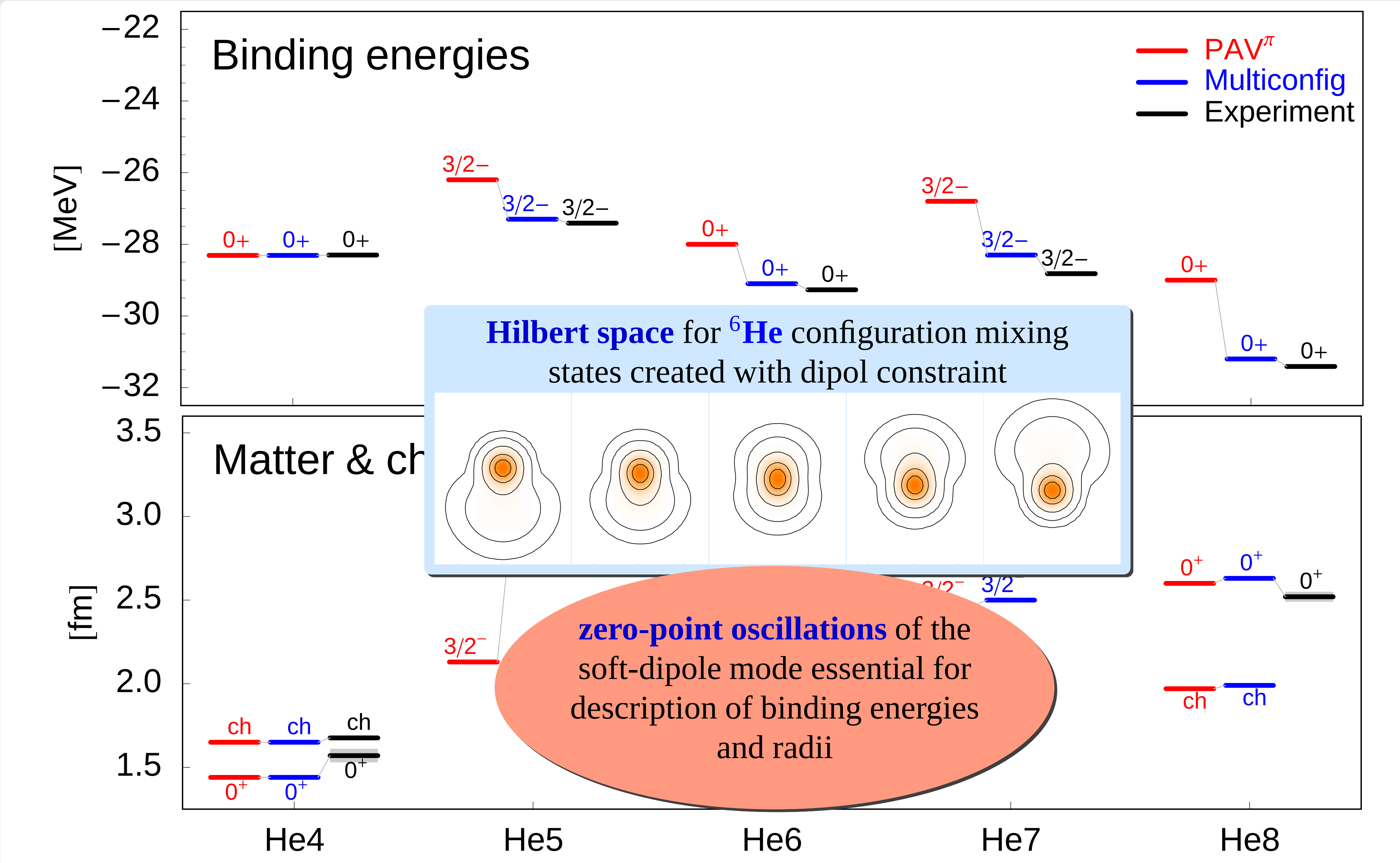

- intrinsic densities of VAP$^{\pi}$ states
  $\left| Q^{\pm} \right\rangle = \frac{1}{2}\left(1 \pm \underset{\sim}{\Pi}\right)\left| Q \right\rangle$
- radial densities from multiconfiguration calculations

# Helium Isotopes




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

# Helium Isotopes - Multi-Configuration Mixing

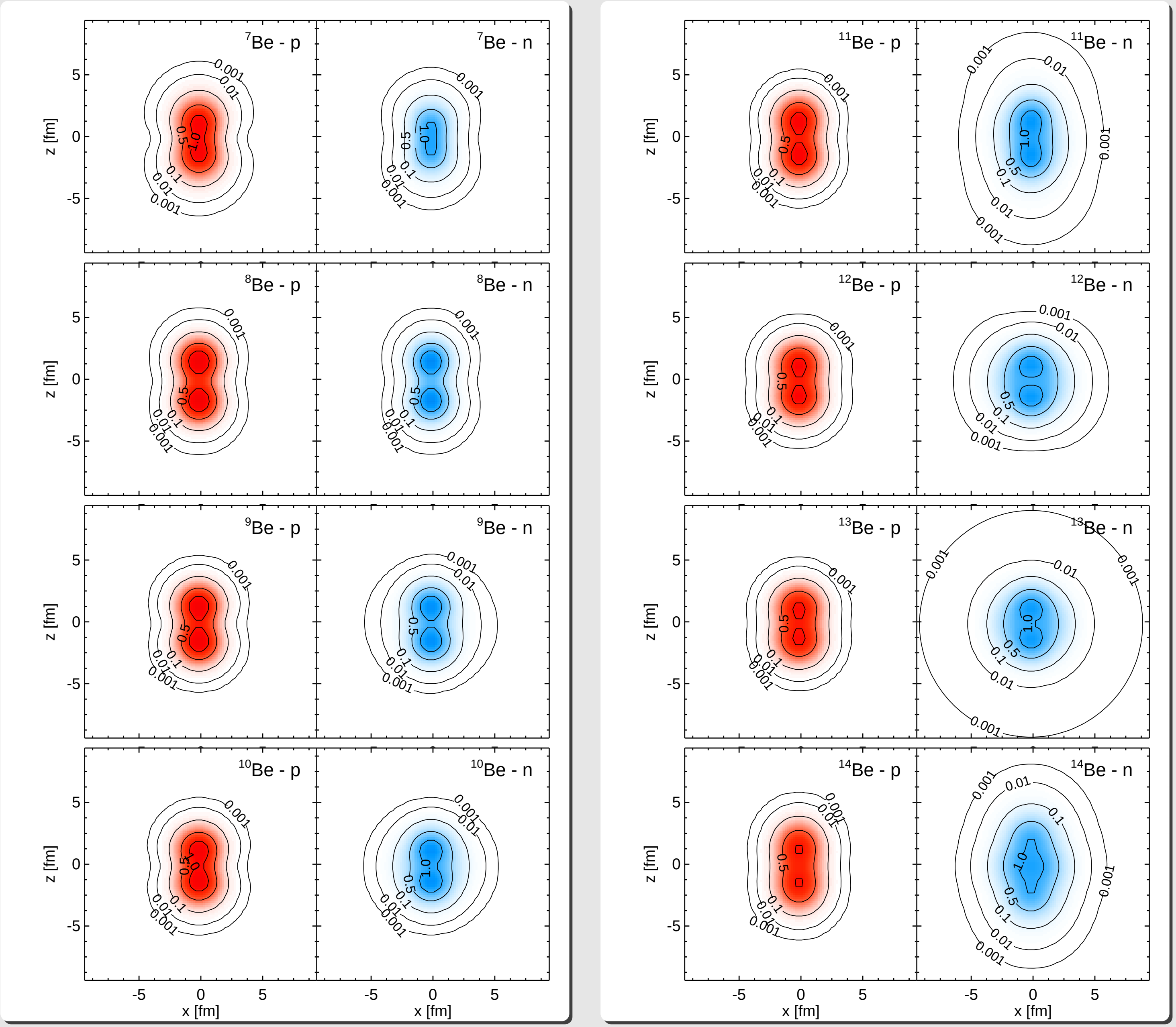



**Hilbert space** for $^6$**He** configuration mixing
states created with dipol constraint

**zero-point oscillations** of the soft-dipole mode essential for description of binding energies and radii

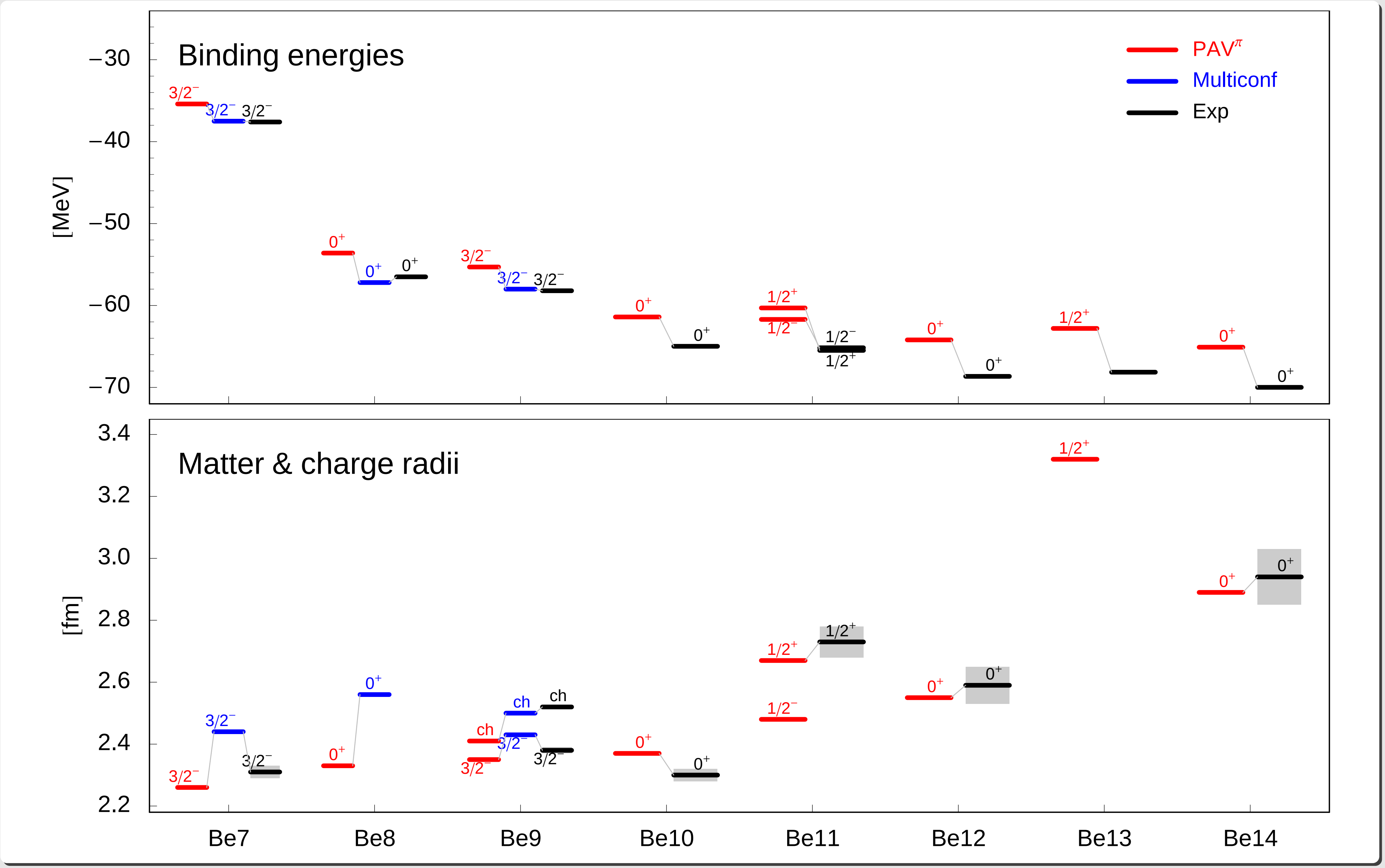
Exp: Ozawa,Suzuki,Tanihata, NP**A693**(2001)32; Raman,Nestor,Tikkanen, Atomic Data and Nucl. Data Tables **78**(2001)1

# Beryllium Isotopes



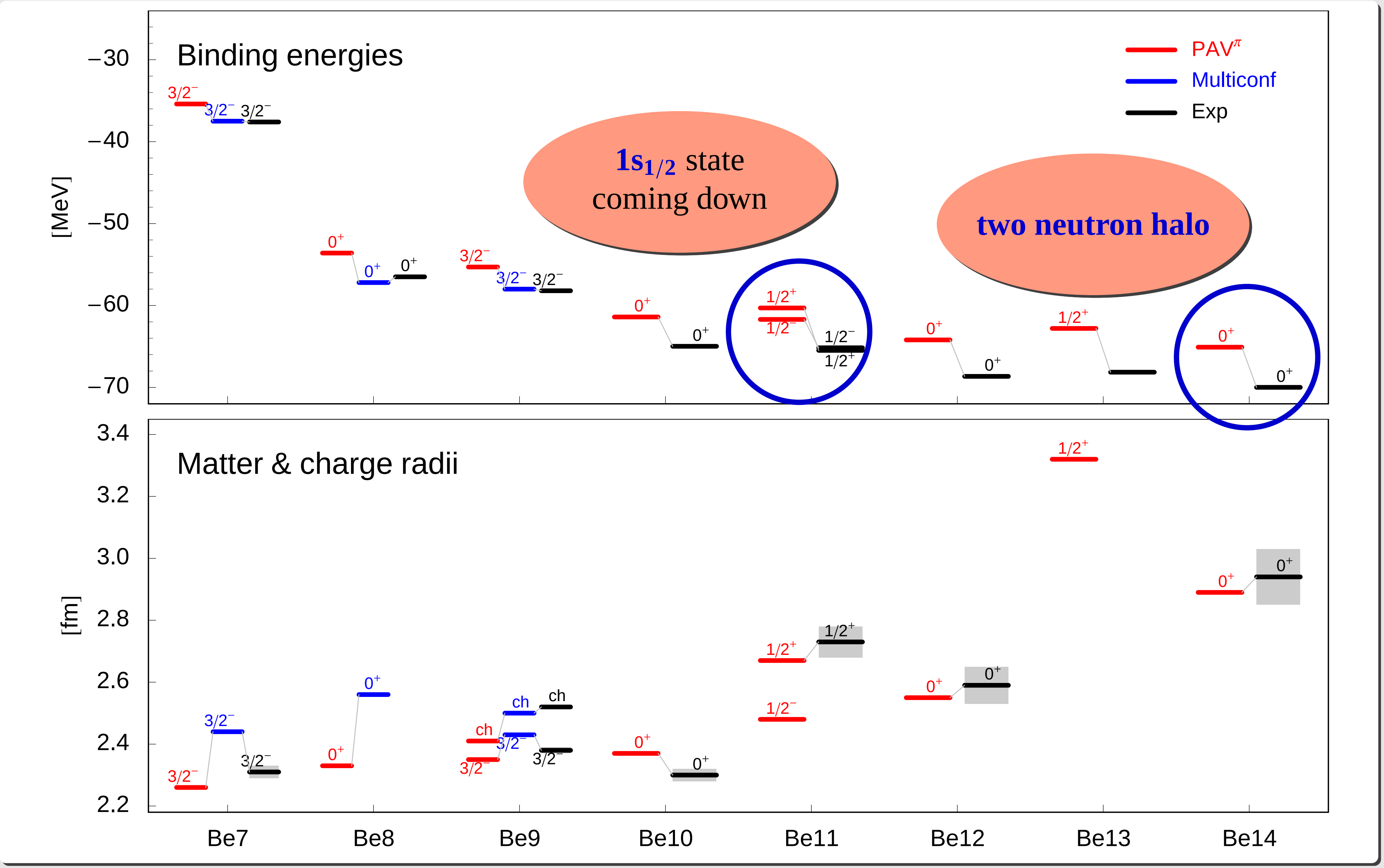

cluster structure changes with addition of neutrons

# Beryllium Isotopes




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

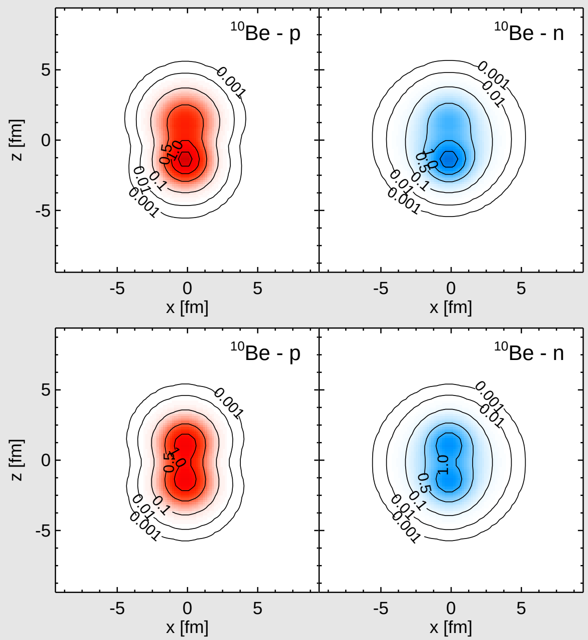
# Beryllium Isotopes



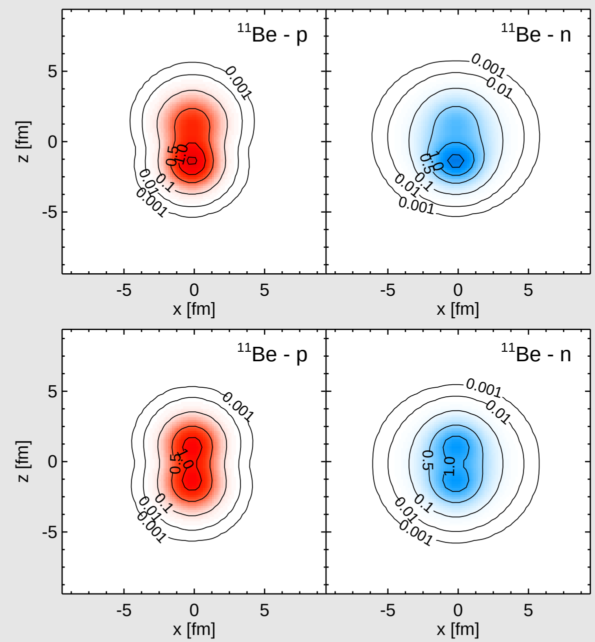

Exp: Ozawa,Suzuki,Tanihata, NP**A693**(2001)32; Raman,Nestor,Tikkanen, Atomic Data and Nucl. Data Tables **78**(2001)1

# $^{11}$Be positive parity intruder

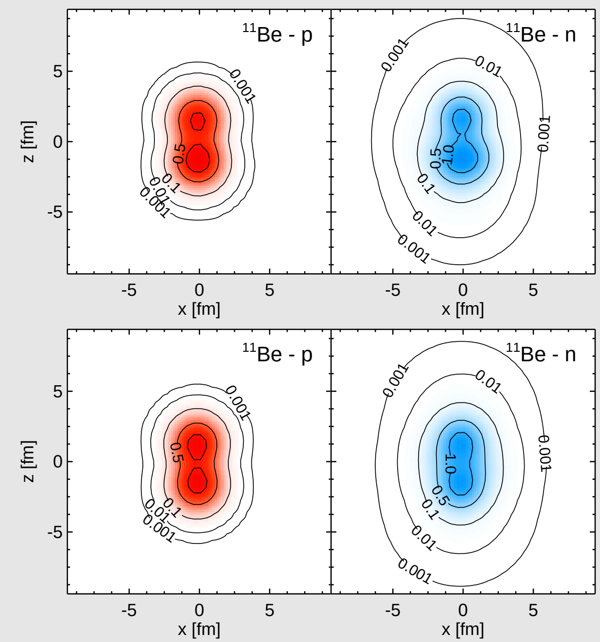
## $^{10}$Be

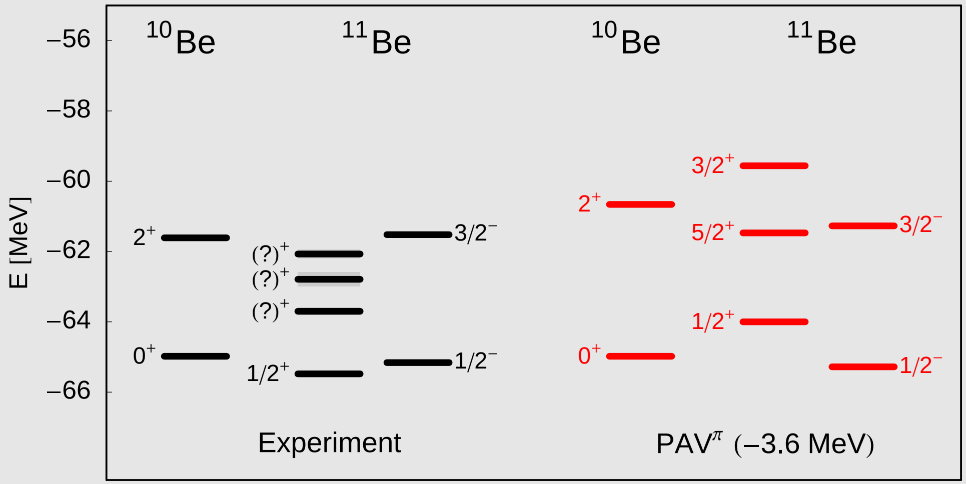


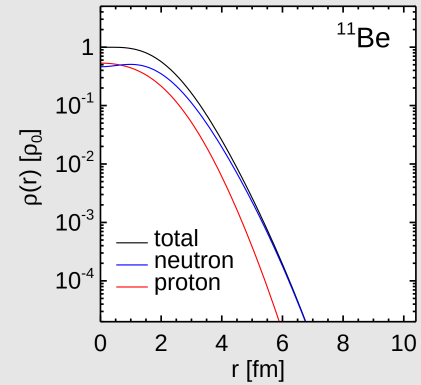

## $^{11}$Be **negative parity**

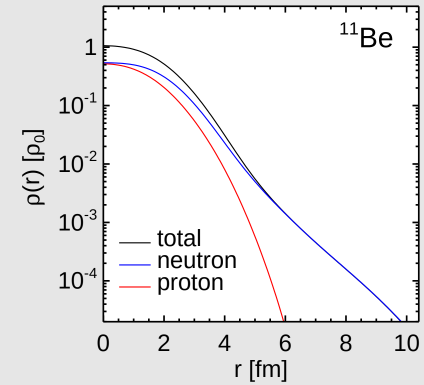



## $^{11}$Be **positive parity**



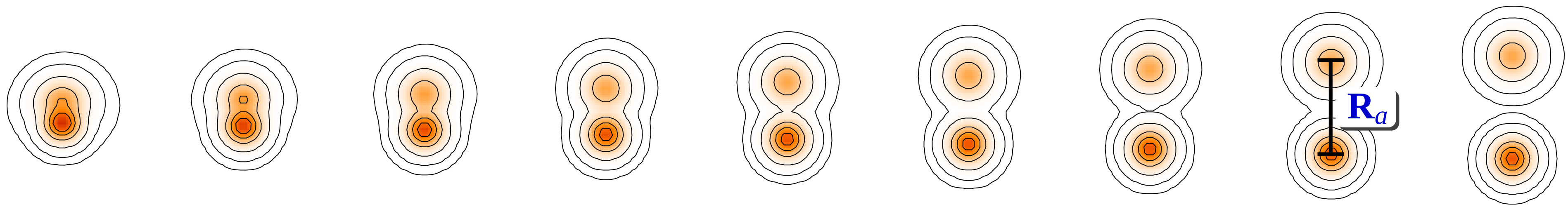




➡ $1/2^+$ state has a neutron halo

# Many-Body Hilbert Space for Scattering

➨ localized FMD wave packets can represent

**A:** two nuclei at a distance **R** $\big| Q^{(a)} \big\rangle = \underset{\sim}{\mathcal{A}} \big| Q_{C1}, -\mathbf{R}_a/2 \big\rangle \otimes \big| Q_{C2}; \mathbf{R}_a/2 \big\rangle$ ("frozen states")

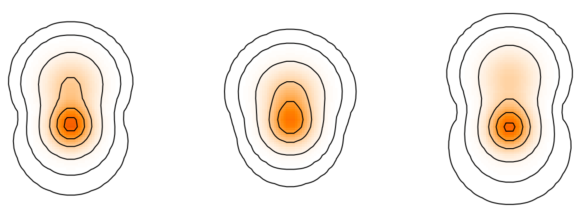



interaction region

asymptotic channel

boundary condition

**B:** compact configurations, lowest PAV$^\pi$ state, GCM states $\big| Q^{(a)} \big\rangle = \Big\{ \big| Q^{\pm} \big\rangle, \big| Q^{(a)}_{GCM} \big\rangle \; \dots \Big\}$



improved representation of interaction region

# Collective Coordinate Representation

## Size Measure

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

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

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

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

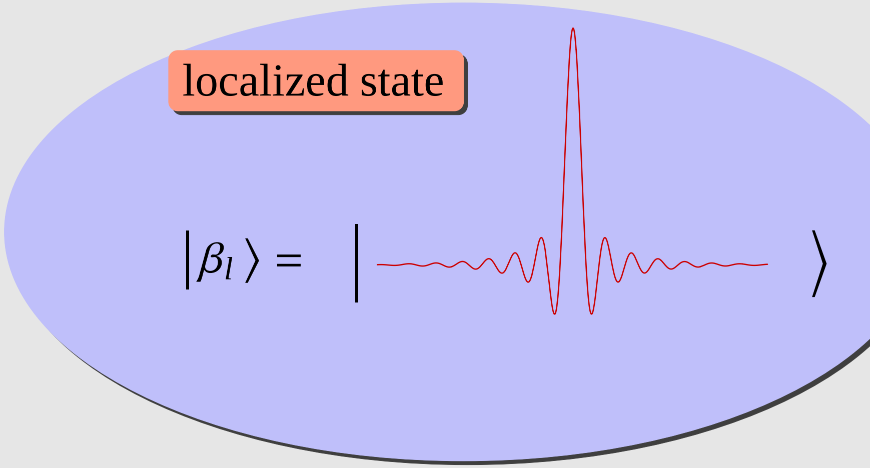
$$\underset{\sim}{B} \left|\beta_l\right\rangle = \beta_l \left|\beta_l\right\rangle$$

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

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

$$\left\langle \beta_l \middle| \underset{\sim}{B}^2 \middle| \beta_l \right\rangle - \left\langle \beta_l \middle| \underset{\sim}{B} \middle| \beta_l \right\rangle^2 = 0$$

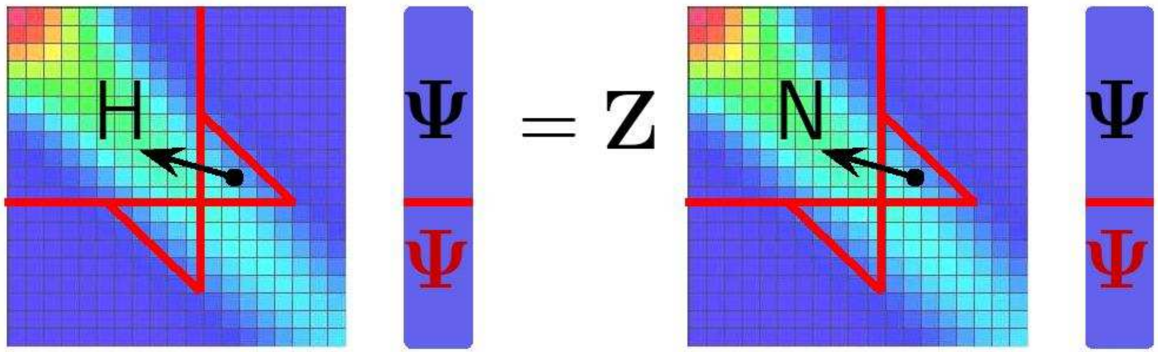
$$\Rightarrow \Psi(r_l) := \left\langle \beta_l \middle| J^\pi M; \Psi \right\rangle$$ **relative wave function**



# Boundary Conditions 1

## Implement boundary conditions using the Collective Coordinate Representation

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




$$\big| J^\pi M; \Psi \big\rangle = \sum_{aK}^{N} \psi_{aK} \, \underset{\sim}{P}^{J^\pi}_{MK} \underset{\sim}{P}^{\mathbf{P}=0} \big| Q^{(a)} \big\rangle + \sum_{aK=N+1}^{N+n} \psi_{aK} \, \underset{\sim}{P}^{J^\pi}_{MK} \underset{\sim}{P}^{\mathbf{P}=0} \big| Q^{(a)} \big\rangle$$

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

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

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

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

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

- **outgoing** Coulomb scattering solution

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

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

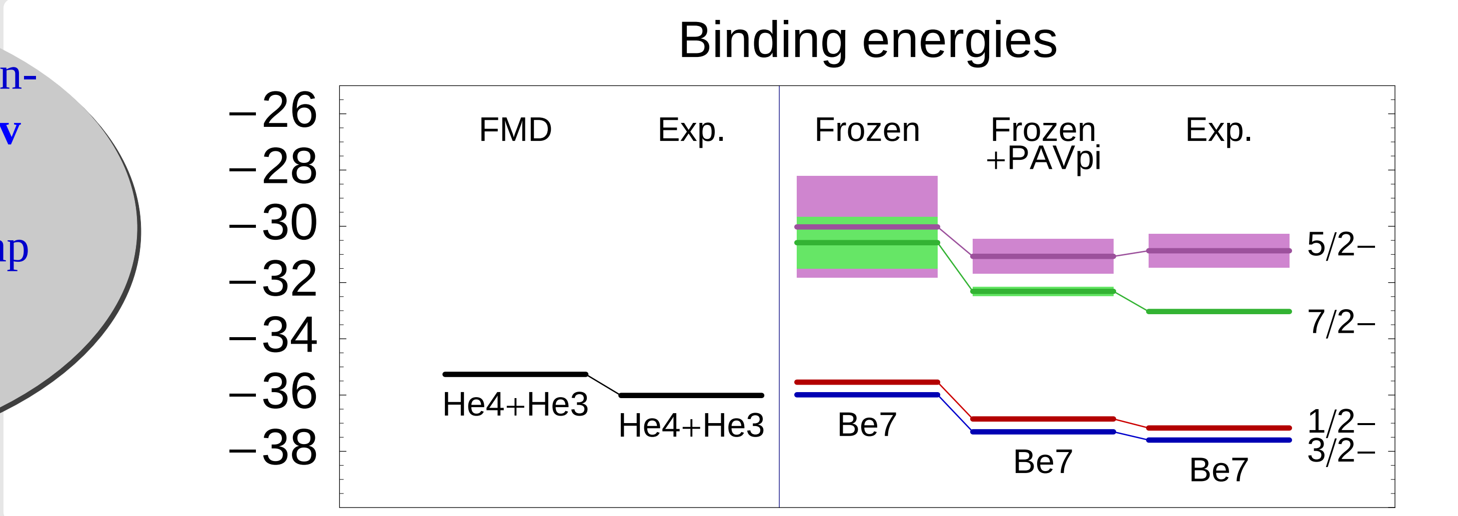
- Coulomb **scattering** solution with phase shift

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

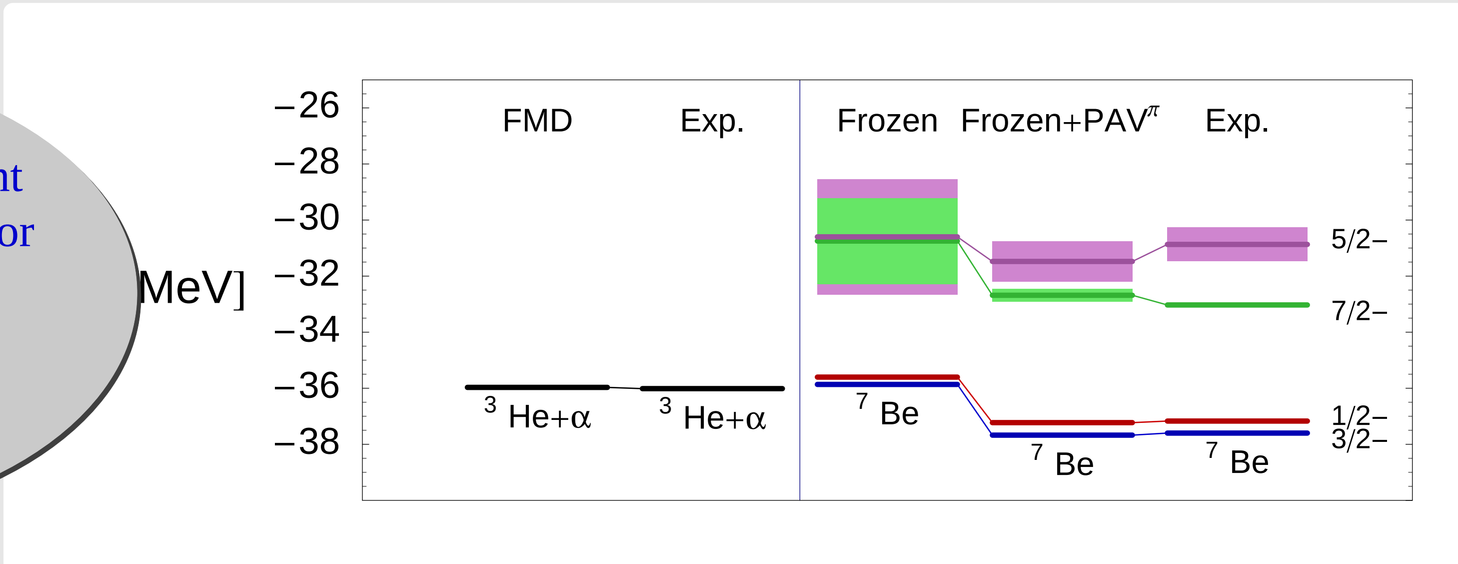
➨ **continuum solution** with phase shift $\delta_\ell(E)$, $E > 0$

# $^7$Be Levels Bound and in Continuum

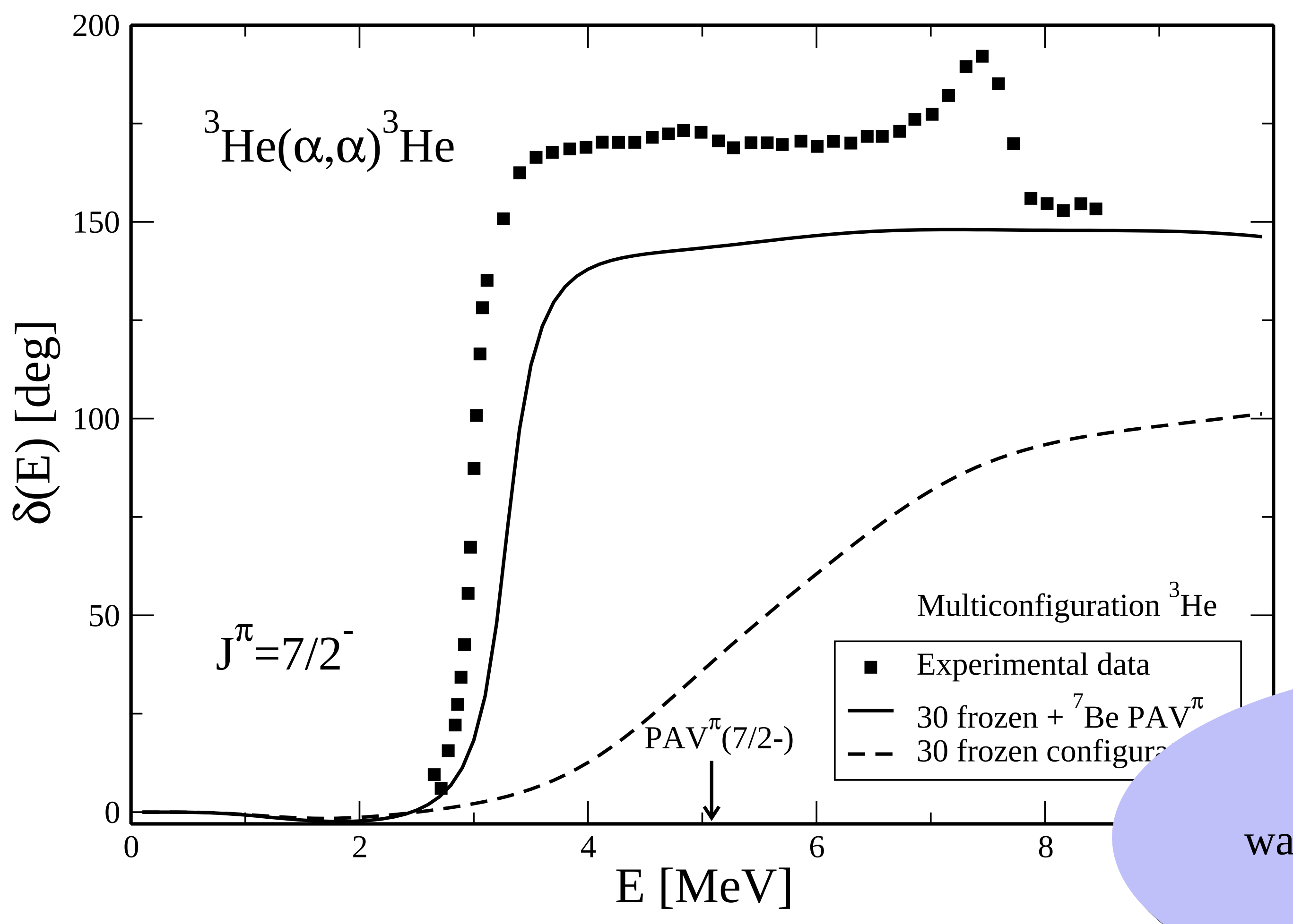
- implement boundary conditions using the **Gamov** state, outgoing only
- ➨ Hamiltonian and Overlap matrix get modified, complex eigenvalue




- single Slater determinant gives poor description for $^3$He
- ➨ use multiconfiguration state for $^3$He



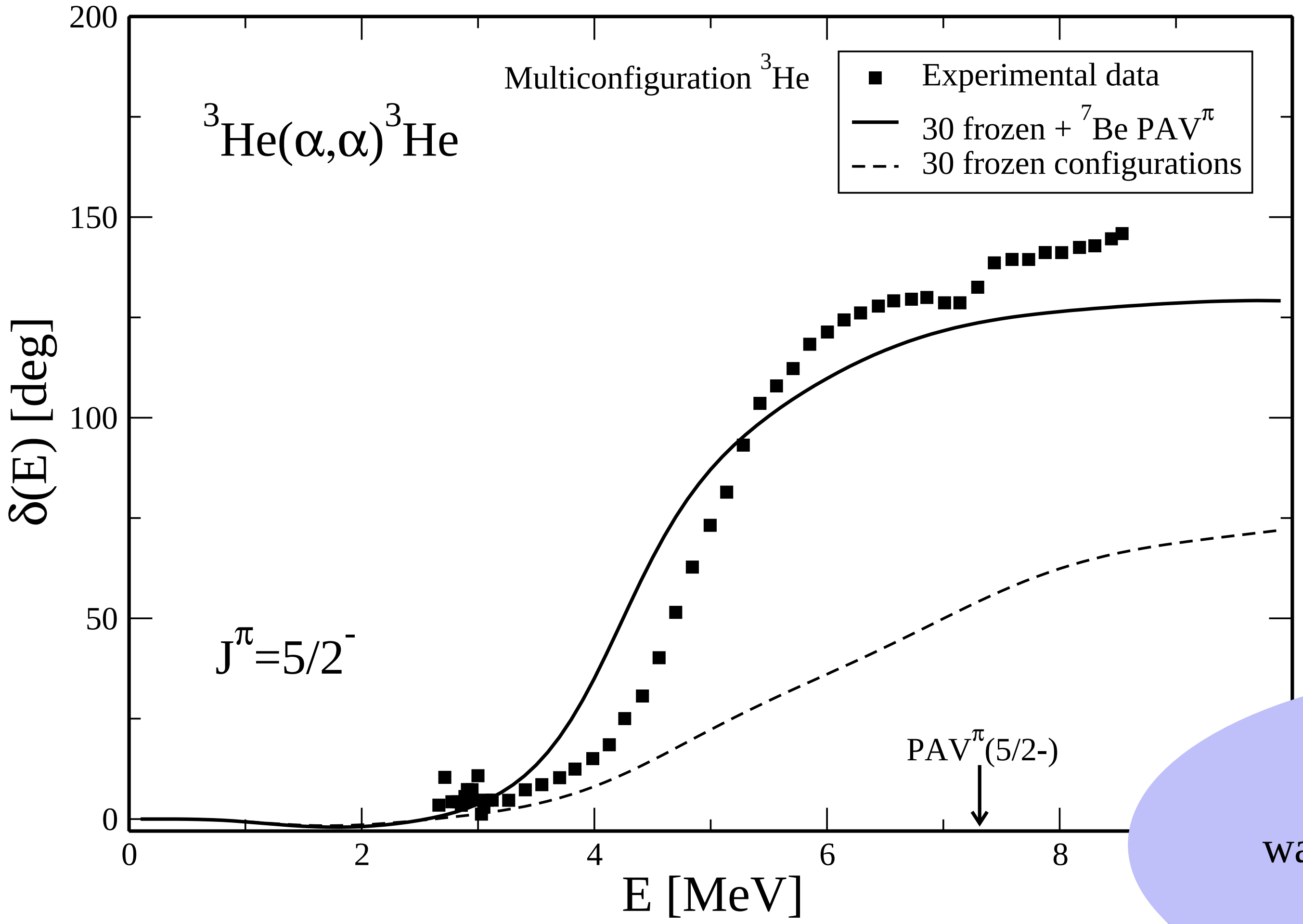
# $^7$Be Phase Shift $7/2^-$ Resonance




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

Data: R. J. Spiger, T. A. Tombrello, Phys. Rev. 163(1967)162

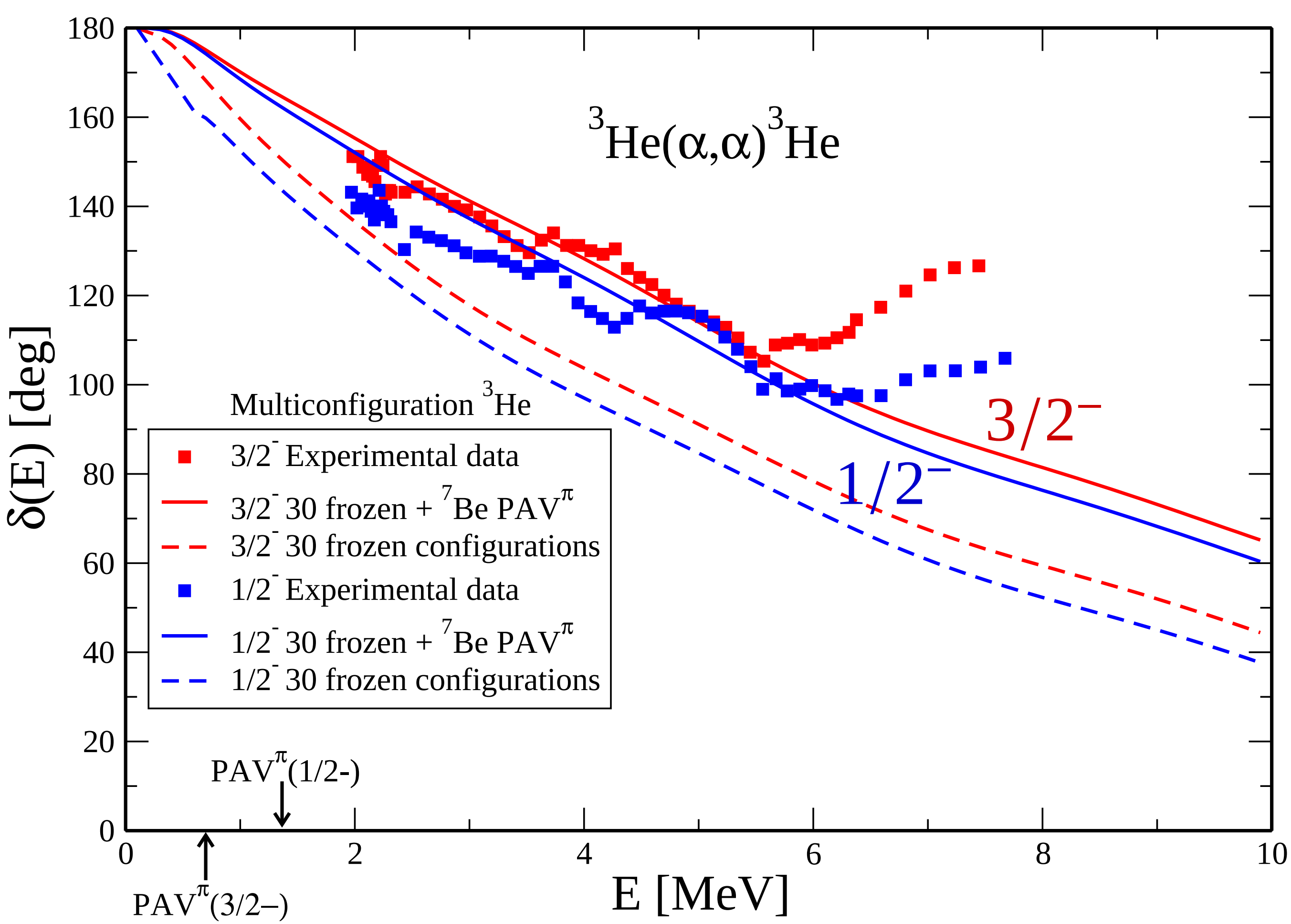
# $^7$Be Phase Shift $5/2^-$ Resonance




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

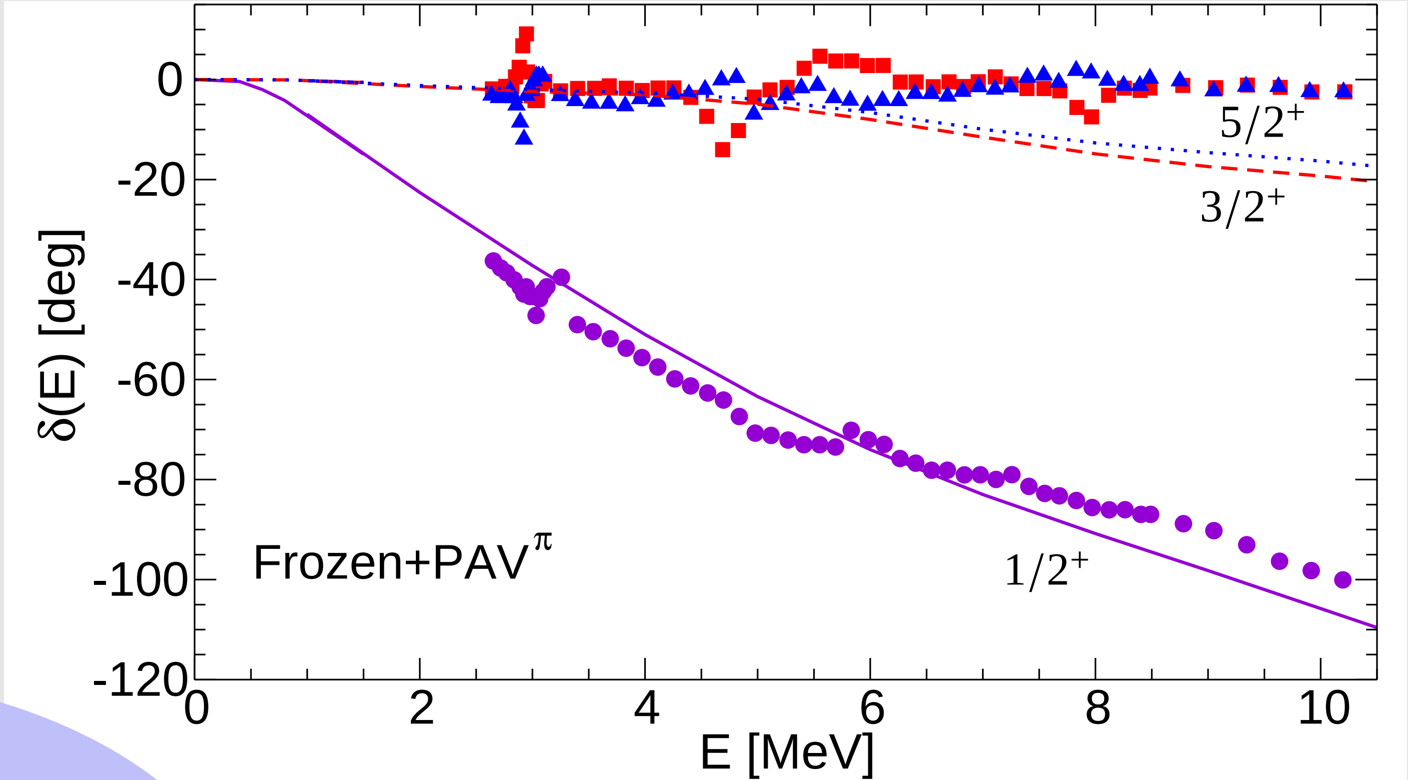
Data: R. J. Spiger, T. A. Tombrello, Phys. Rev. 163(1967)162

# $^7$Be Phase Shifts, nonresonant




Data: R. J. Spiger, T. A. Tombrello, Phys. Rev. 163(1967)162

# $^7$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**

Data: R. J. Spiger, T. A. Tombrello, Phys. Rev. 163(1967)162

# Summary

## Unitary Correlation Operator Method

- explicit description of short-range central and tensor correlations
- phase-shift equivalent correlated interaction $V_{\mathrm{UCOM}}$
- $V_{\mathrm{UCOM}}$ used in Hartree-Fock + many-body pertubation theory, no-core shell model, RPA ... (see talk of Robert Roth)

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

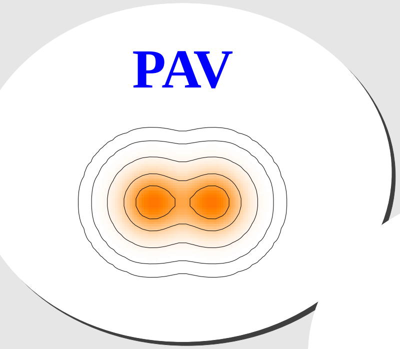
- Structure of light nuclei
- Halos and clustering
- Resonances, scattering states, reactions

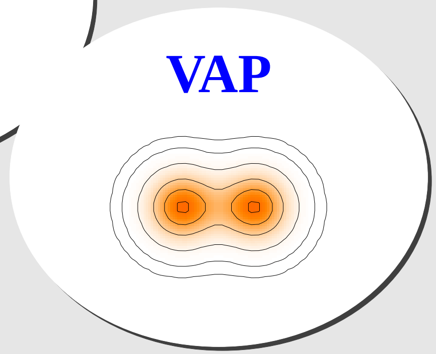
**Microscopic unified approach for nuclear structure and reactions**

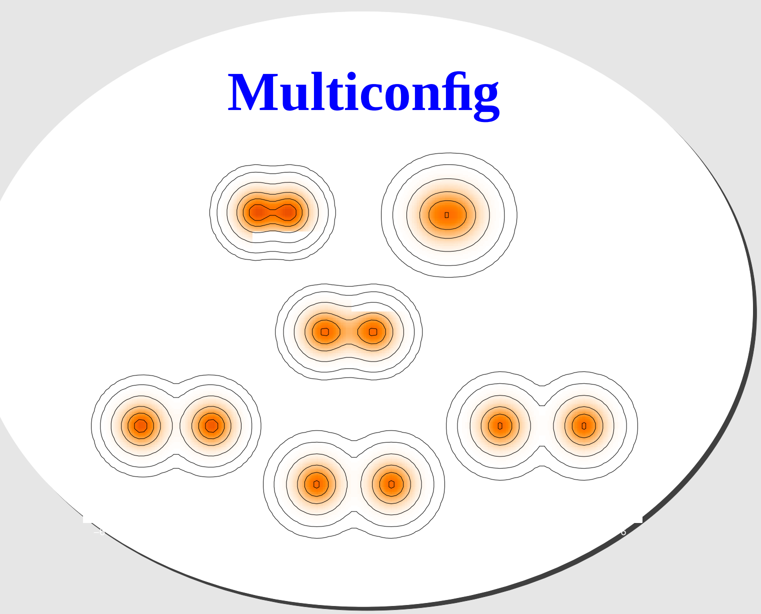
# Collaborators

- S. Bacca, C. Barbieri, A. Cribeiro, R. Cussons,
  K. Langanke, G. Martinez Pinedo, C. Özen, T. Milosic, R. Torabi
  GSI Darmstadt
- T. Böhlen, P. Hedfeld, H. Hergert, N. Paar, P. Papakonstantinou,
  R. Roth, A. Zapp
  Institut für Kernphysik, TU Darmstadt
- T. Neff
  NSCL, Michigan State University

# FMD - Projection, Variation after Proj., Multiconfiguration




## Radius and Quadrupole Moment as Generator Coordinates

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