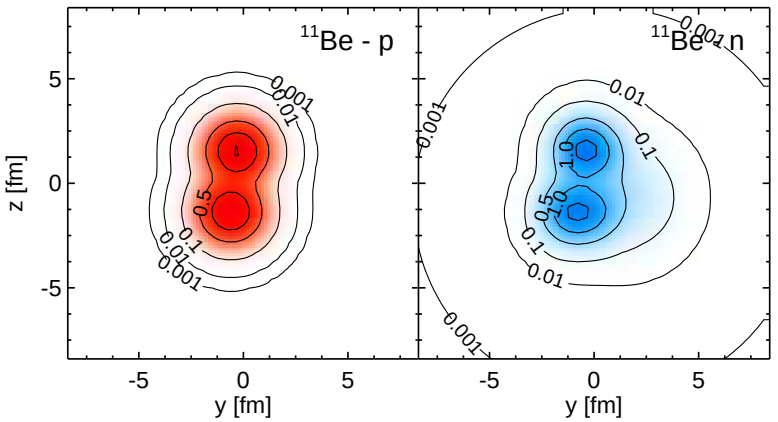
Beryllium Isotopes studied in Fermionic Molecular Dynamics



Thomas Neff

2nd EMMI-EFES Workshop on Neutron-Rich Exotic Nuclei EENEN10

RIKEN, Tokyo
June 16, 2010

HELMHOLTZ ASSOCIATION

GSI

Overview

Effective Nucleon-Nucleon interaction:

Unitary Correlation Operator Method

Roth, Neff, Feldmeier, Prog. Part. Nucl. Phys. 65 (2010) 50

- **Short-range Central and Tensor Correlations**
- ***ab initio* Few-Body Calculations**

Many-Body Method:

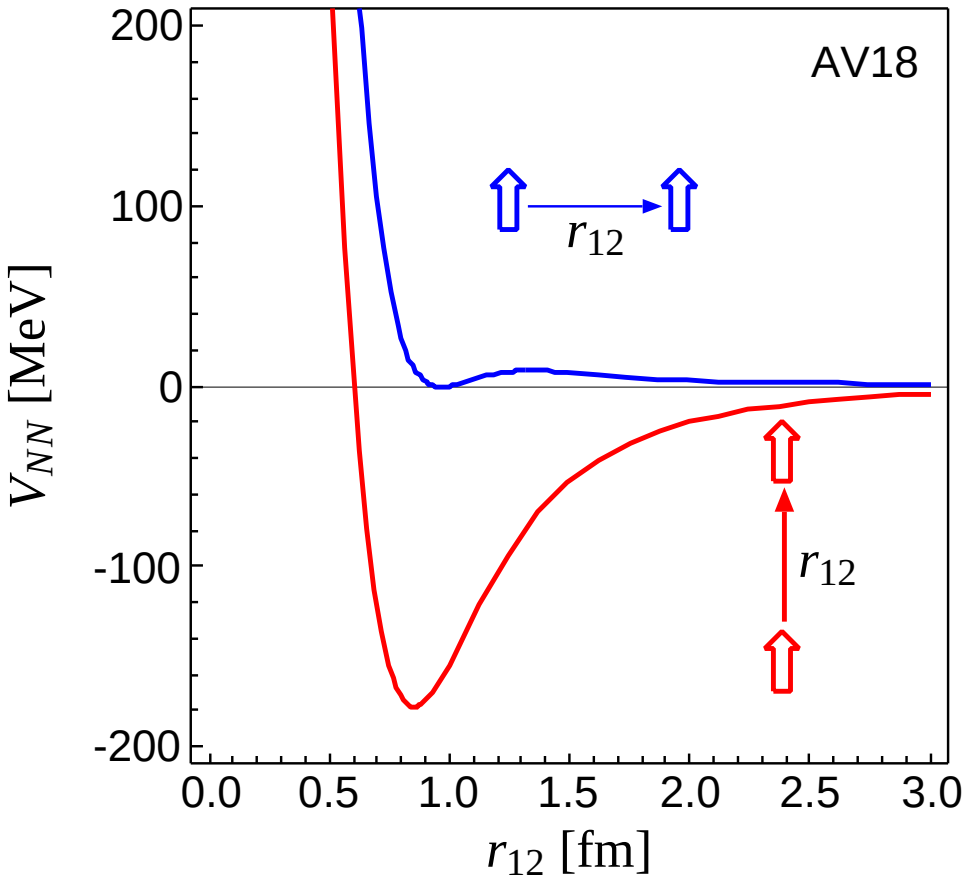
Fermionic Molecular Dynamics

- **Model**
- **Beryllium Isotopes**

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**

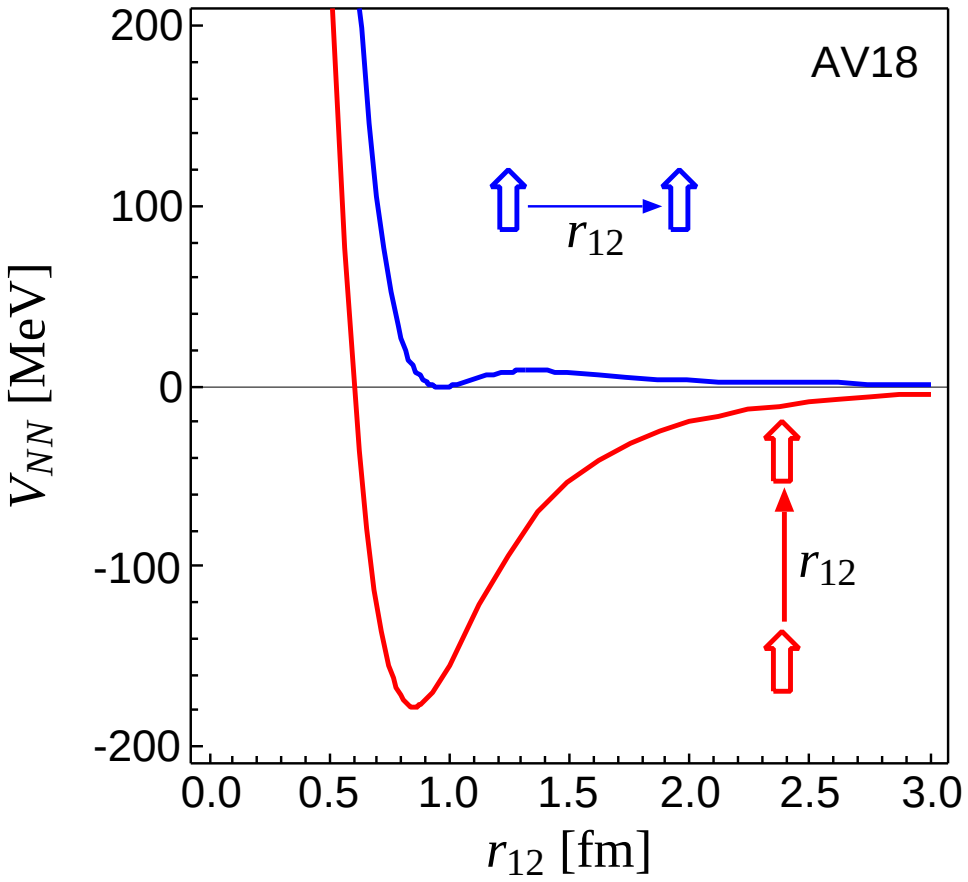
- strong dependence on the orientation of the spins due to the tensor force

➨ **tensor correlations**

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**

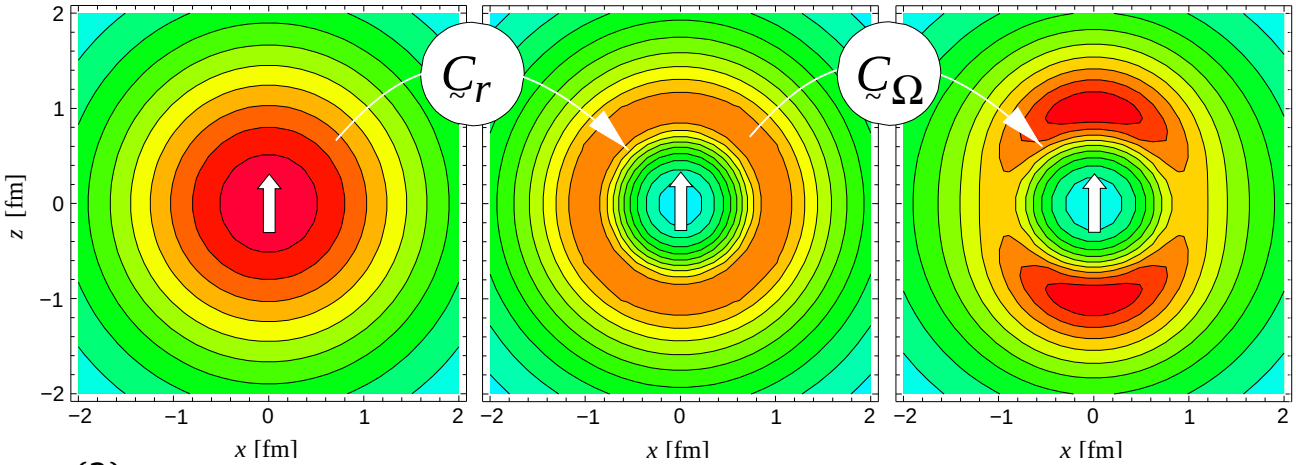
- strong dependence on the orientation of the spins due to the tensor force

➨ **tensor correlations**

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

Realistic Effective Interaction

two-body densities



$\rho^{(2)}_{S,T}(\mathbf{r}_1 - \mathbf{r}_2) \quad S = 1, M_S = 1, T = 0$

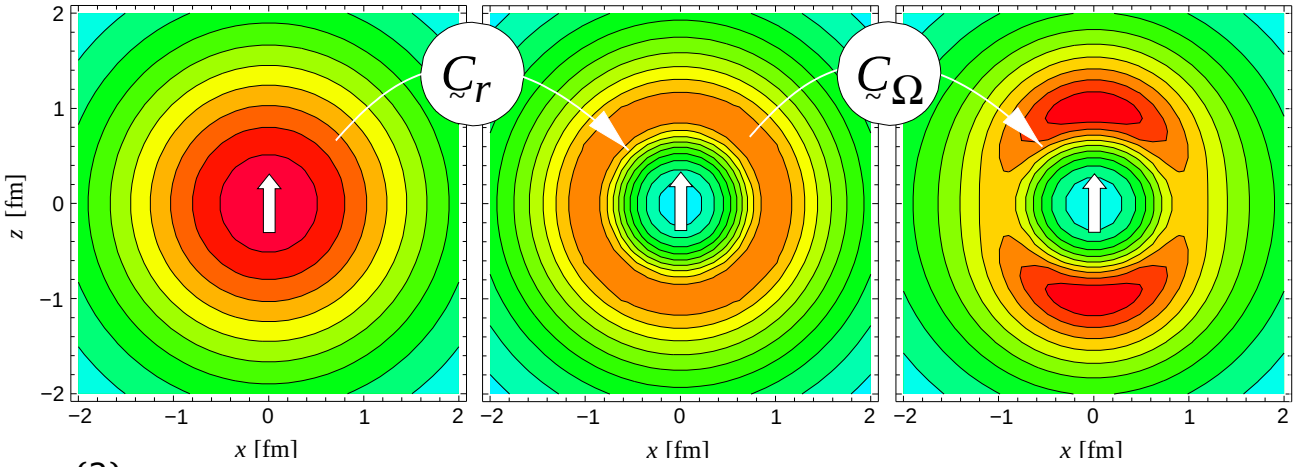
central correlator C_r shifts density out of the repulsive core

tensor correlator C_Ω aligns density with spin orientation

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

Realistic Effective Interaction

two-body densities



$\rho^{(2)}_{S,T}(\mathbf{r}_1 - \mathbf{r}_2) \quad S = 1, M_S = 1, T = 0$

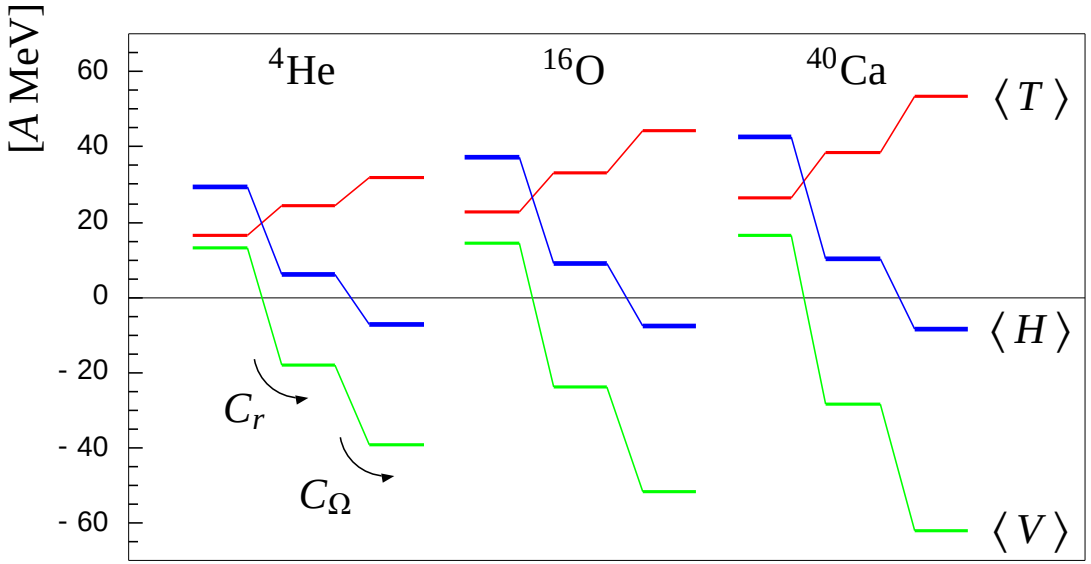
central correlator C_r shifts density out of the repulsive core

tensor correlator C_Ω aligns density with spin orientation

both central and tensor correlations are essential for binding

energies

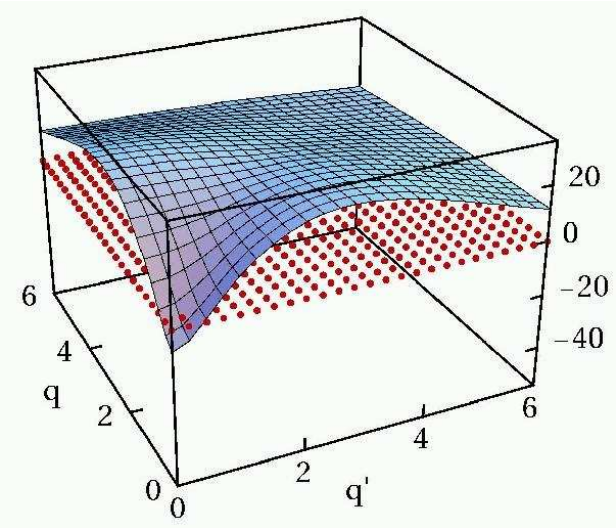
$0\hbar\omega$ Harmonic Oscillator



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

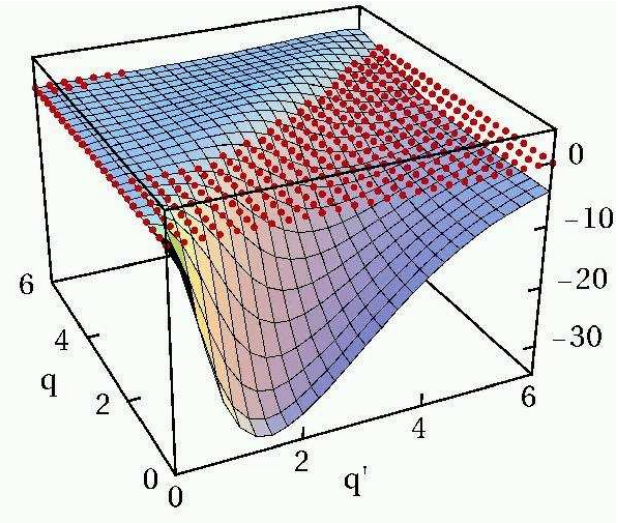
Correlated Interaction in Momentum Space

$^3S_1$ bare



bare interaction has **strong off-diagonal** matrix elements connecting to high momenta

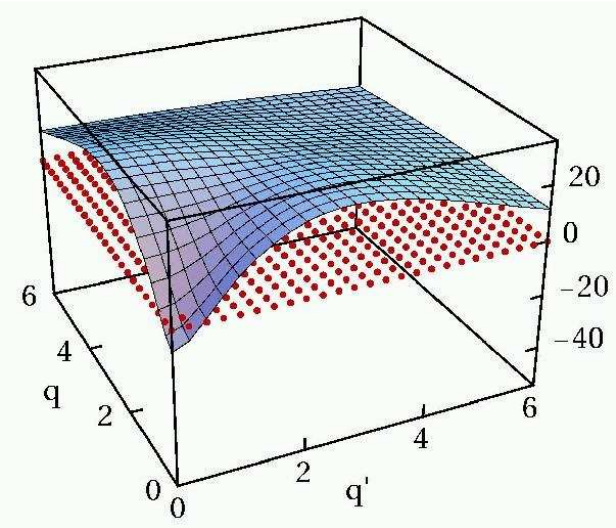
$^3S_1$ - $^3D_1$ bare



Roth, Hergert, Papakonstaninou, Neff, Feldmeier, Phys. Rev. C **72**, 034002 (2005)

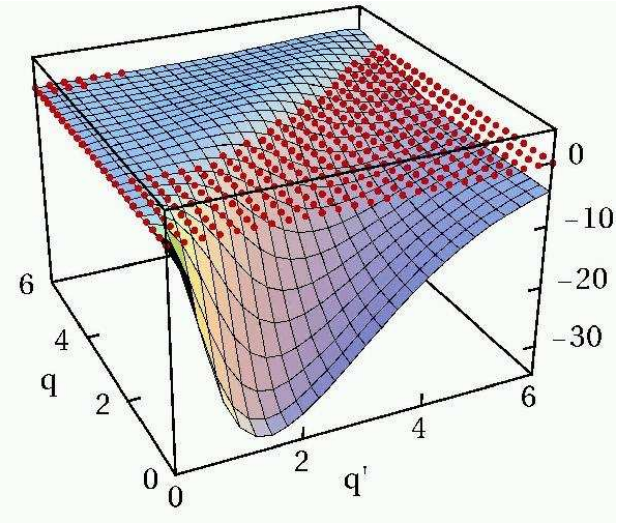
Correlated Interaction in Momentum Space

$^3S_1$ bare

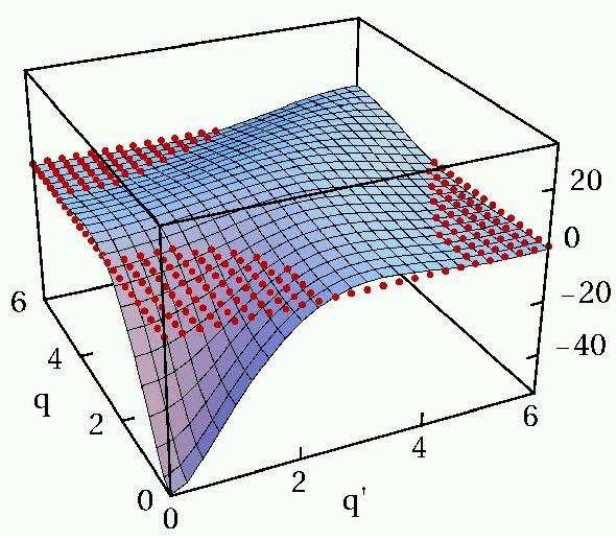


bare interaction has **strong off-diagonal** matrix elements connecting to high momenta

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



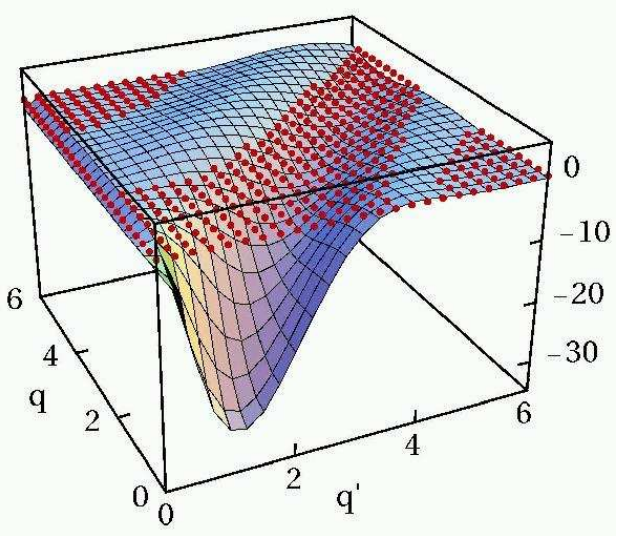
$^3S_1$ correlated



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

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

$^3S_1$ - $^3D_1$ correlated

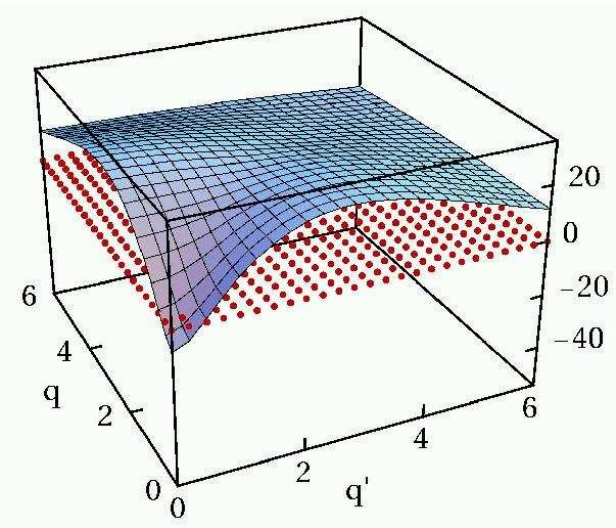


Roth, Hergert, Papakonstaninou, Neff, Feldmeier, Phys. Rev. C **72**, 034002 (2005)

Unitary Correlation Operator Method

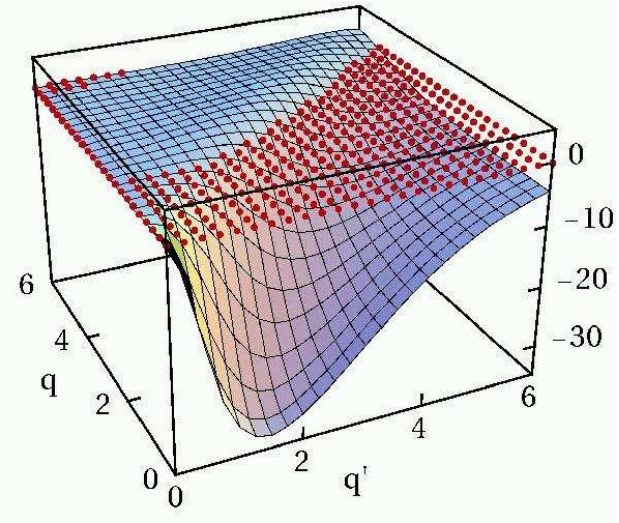
Correlated Interaction in Momentum Space

$^3S_1$ bare

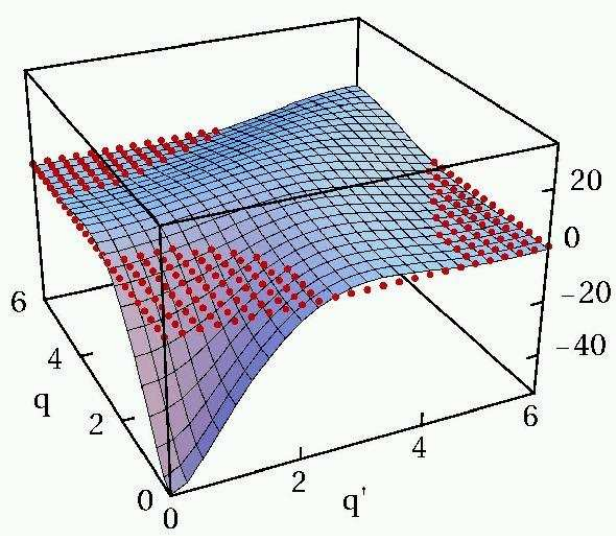


bare interaction has **strong off-diagonal** matrix elements connecting to high momenta

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

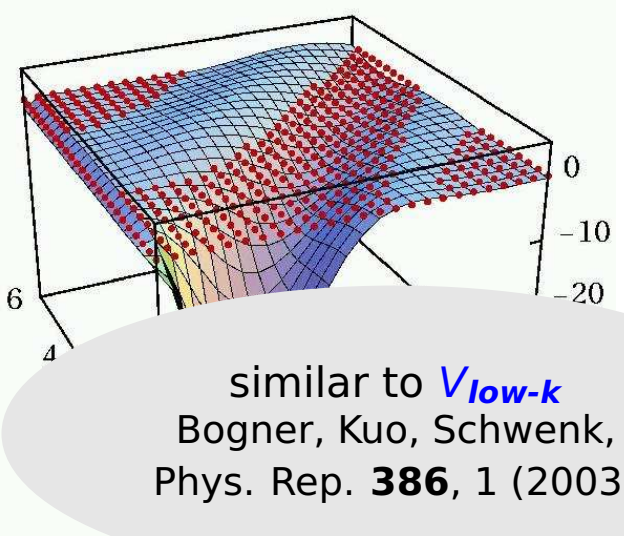


$^3S_1$ correlated



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

$^3S_1$ - $^3D_1$ correlated



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

similar to $V_{low\text{-}k}$
Bogner, Kuo, Schwenk, Phys. Rep. **386**, 1 (2003)

Roth, Hergert, Papakonstaninou, Neff, Feldmeier, Phys. Rev. C **72**, 034002 (2005)

Fermionic Molecular Dynamics

Motivation

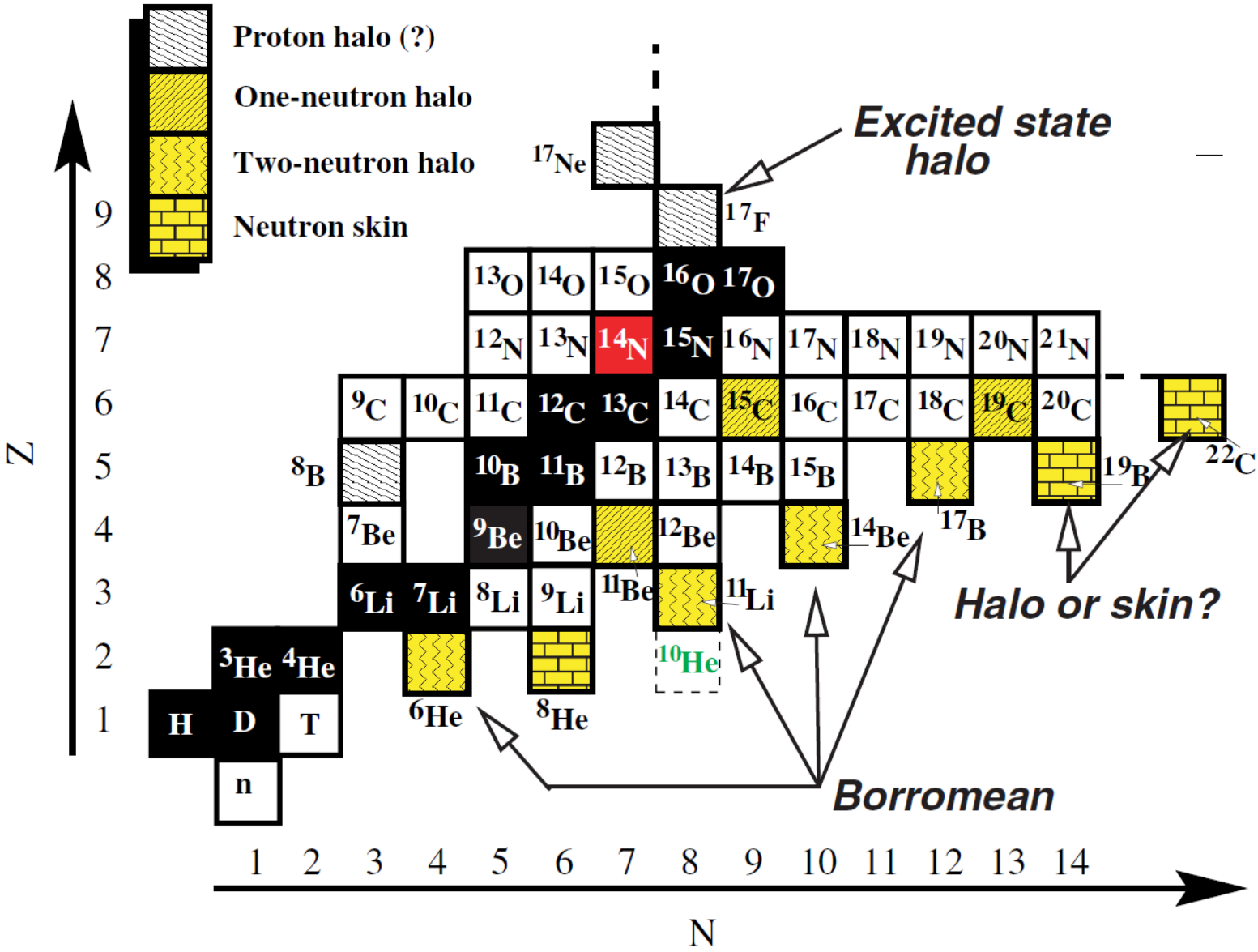
FMD Wave Functions

Nucleon-Nucleon Interaction

Mean-Field Calculations

**Projection After Variation,
Variation After Projection
and Multiconfiguration**

Exotica: Special Challenges



Al-Khalili, Nunes, J. Phys. G **29**, R89 (2003)

Fermionic Molecular Dynamics

Fermionic

Slater determinant

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

- antisymmetrized A-body state

Feldmeier, Schnack, Rev. Mod. Phys. **72** (2000) 655

Neff, Feldmeier, Nucl. Phys. **A738** (2004) 357

Fermionic Molecular Dynamics

Fermionic

Slater determinant

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

- antisymmetrized A-body state

Molecular

single-particle states

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

- 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
- use one or two wave packets for each single particle state

Feldmeier, Schnack, Rev. Mod. Phys. **72** (2000) 655

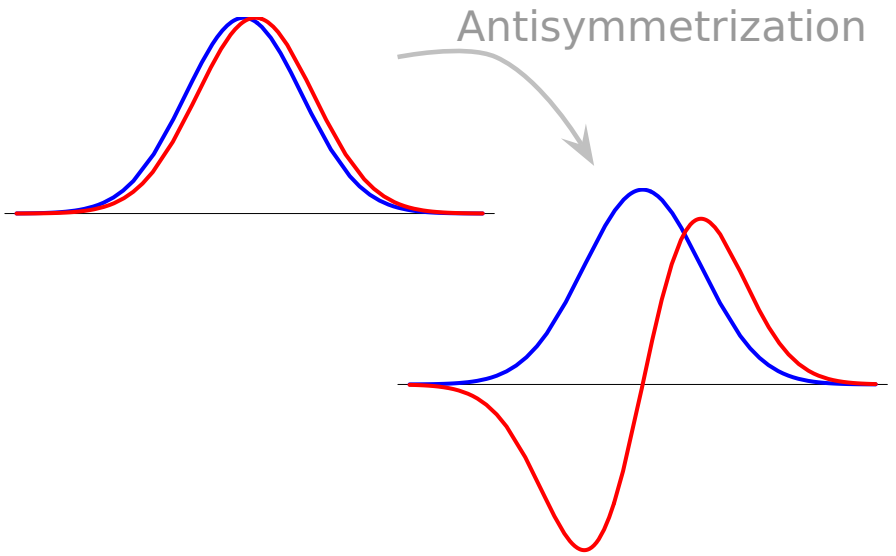
Neff, Feldmeier, Nucl. Phys. **A738** (2004) 357

Fermionic Molecular Dynamics

Fermionic

Slater determinant

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



- antisymmetrized A-body state

Molecular

single-particle states

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

- 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
- use one or two wave packets for each single particle state

Feldmeier, Schnack, Rev. Mod. Phys. **72** (2000) 655

Neff, Feldmeier, Nucl. Phys. **A738** (2004) 357

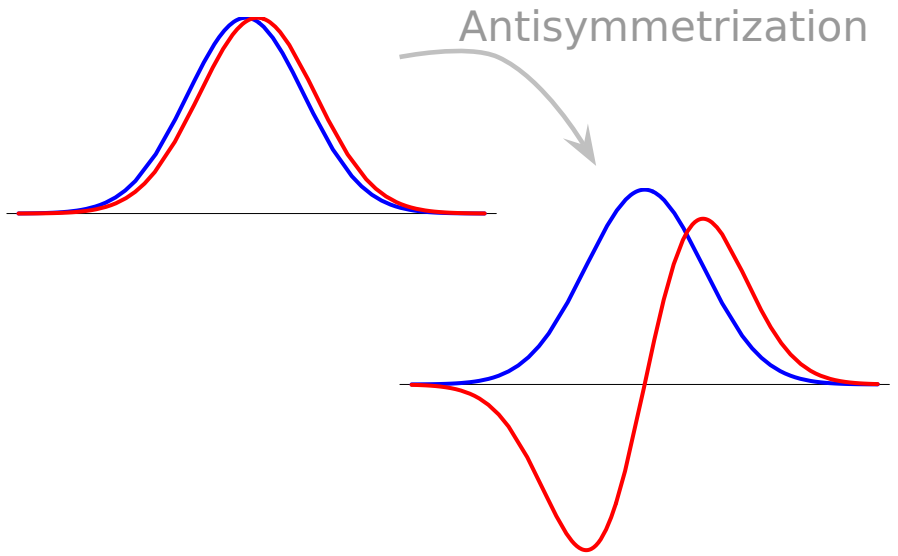
FMD

Fermionic Molecular Dynamics

Fermionic

Slater determinant

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



- antisymmetrized A-body state

Molecular

single-particle states

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

- 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
- use one or two wave packets for each single particle st

see also
Antisymmetrized Molecular Dynamics
H. Horiuchi, Y. Kanada-En'yo

Feldmeier, Schnack, Rev. Mod. Phys. **72** (2000) 655

Neff, Feldmeier, Nucl. Phys. **A738** (2004) 357

Effective interaction based on V_{UCOM}

Effective two-body interaction

- FMD model space can't describe correlations induced by residual medium-long ranged tensor forces

➨ use **long ranged tensor correlator – "low cutoff"** to partly account for that

- no three-body forces: missing spin-orbit strength, saturation properties

➨ 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)

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

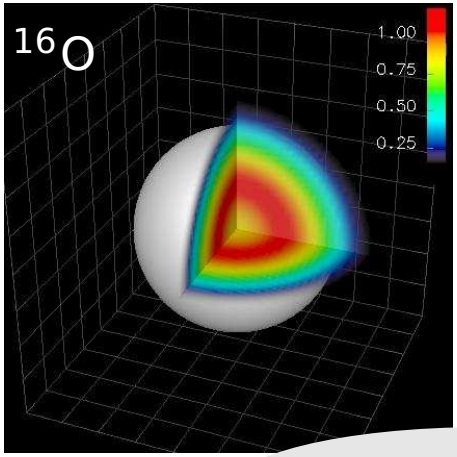
Mean-Field Calculations

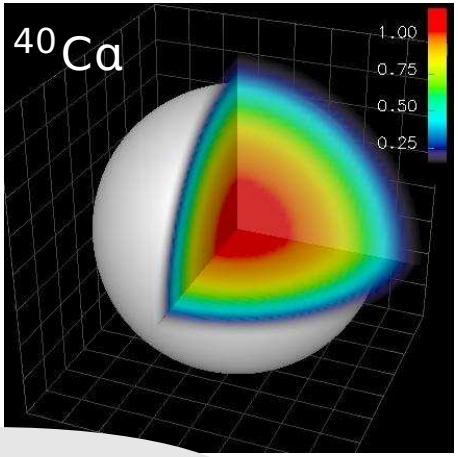
Minimization

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

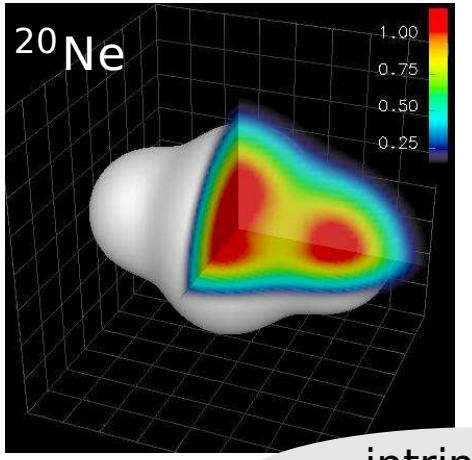
$$\min_{\{q_k\}} \frac{\langle Q \left| \underset{\sim}{H} - \underset{\sim}{T}_{cm} \right| Q \rangle}{\langle Q \left| Q \right\rangle}$$

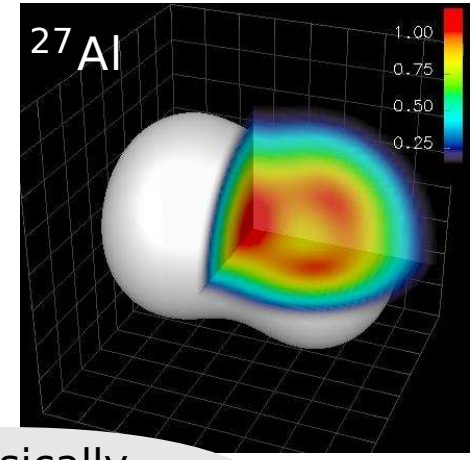
- this is a Hartree-Fock calculation in our particular single-particle basis
- the mean-field may break the symmetries of the Hamiltonian





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

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

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

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

PAV, VAP and Multiconfiguration

Projection After Variation (PAV)

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

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

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

Variation After Projection (VAP)

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

- effect of projection can be large
- full Variation after Angular Momentum and Parity Projection (VAP) for light nuclei

- 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 for heavier 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

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

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

Variation After Projection (VAP)

- effect of projection can be large
- full Variation after Angular Momentum and Parity Projection (VAP) for light nuclei

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

- 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 for heavier nuclei

Multiconfiguration Calculations

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

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

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

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

Beryllium Isotopes

Questions

- **α-clustering, halos in ^{11}Be and ^{14}Be, $N = 8$ shell closure ?**

Calculation

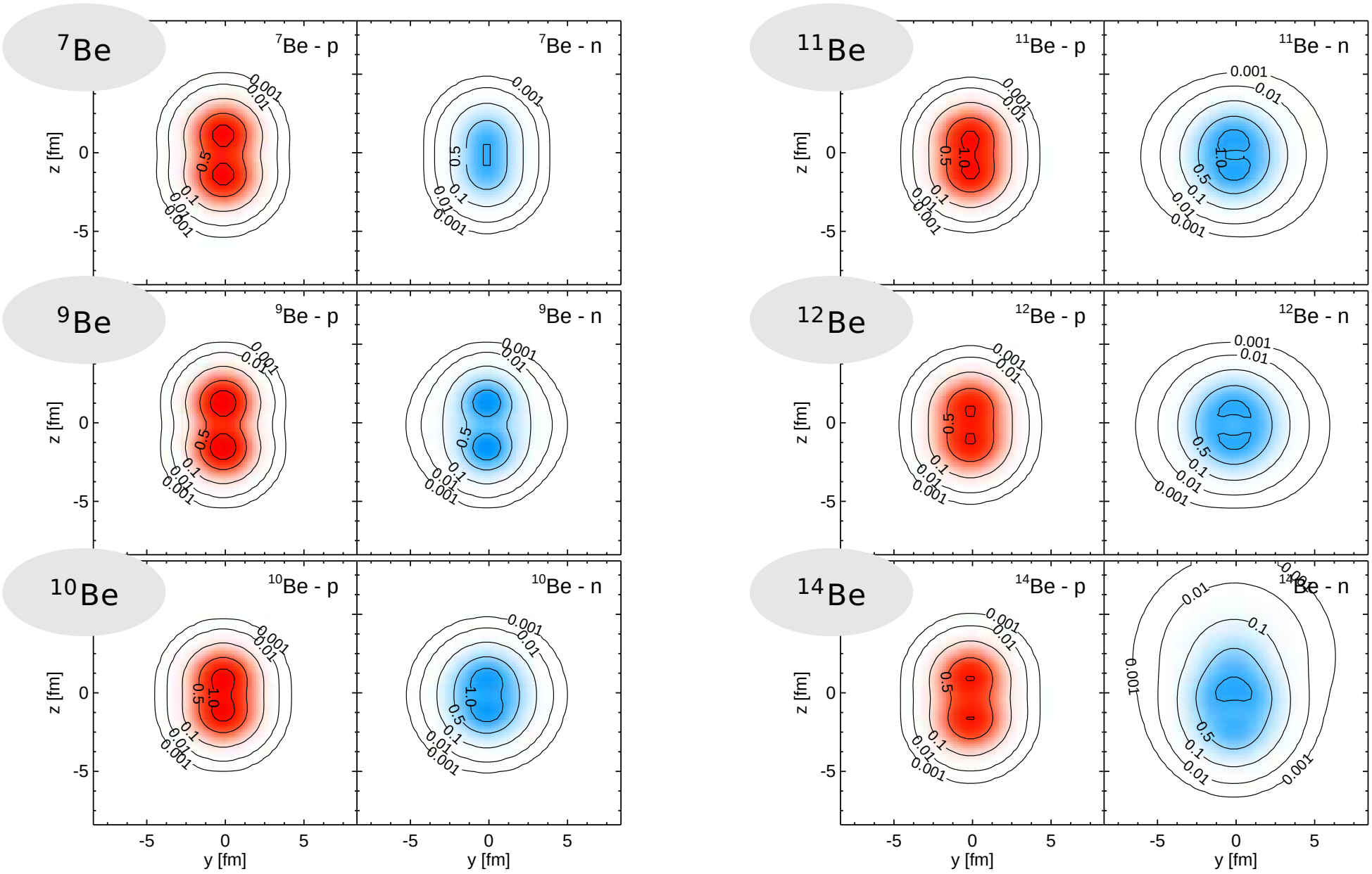
- **FMD wave functions with two Gaussians per sp-state**
- **mean field, variation after projection, variation after multiconfiguration mixing**
- **VAP and multiconfiguration-VAP configurations with mean proton distance as generator coordinate**

Observables

- **energies**
- **charge and matter radii, electromagnetic transitions**

Beryllium Isotopes

Mean field

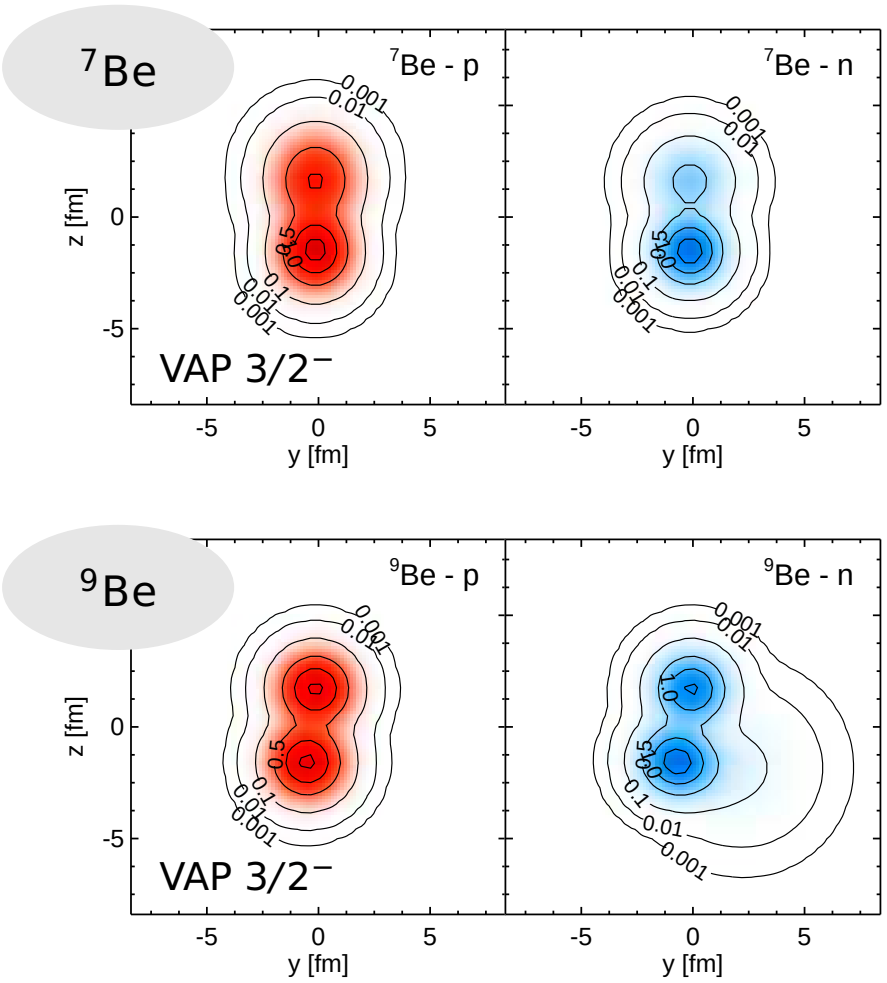


Variation after Projection

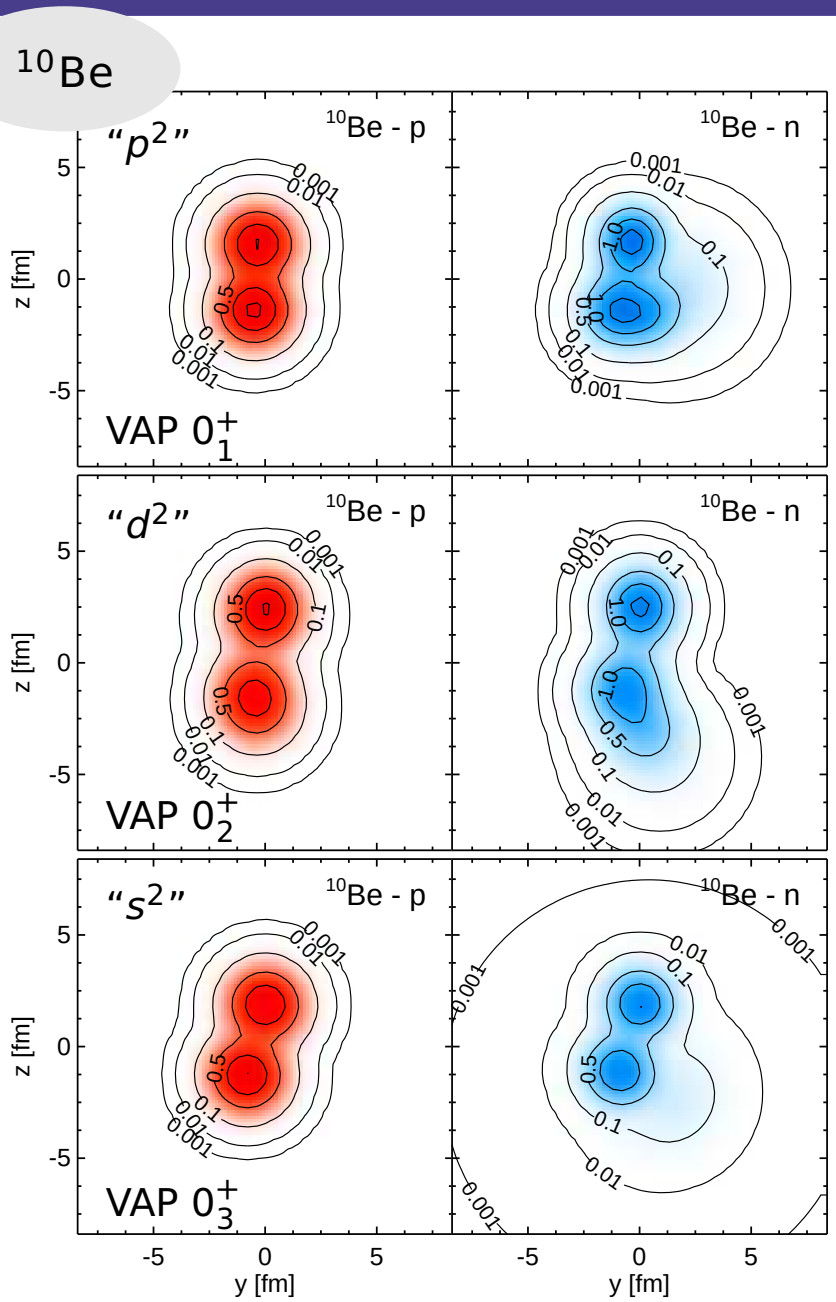
- create configurations by variation after parity and angular momentum projection

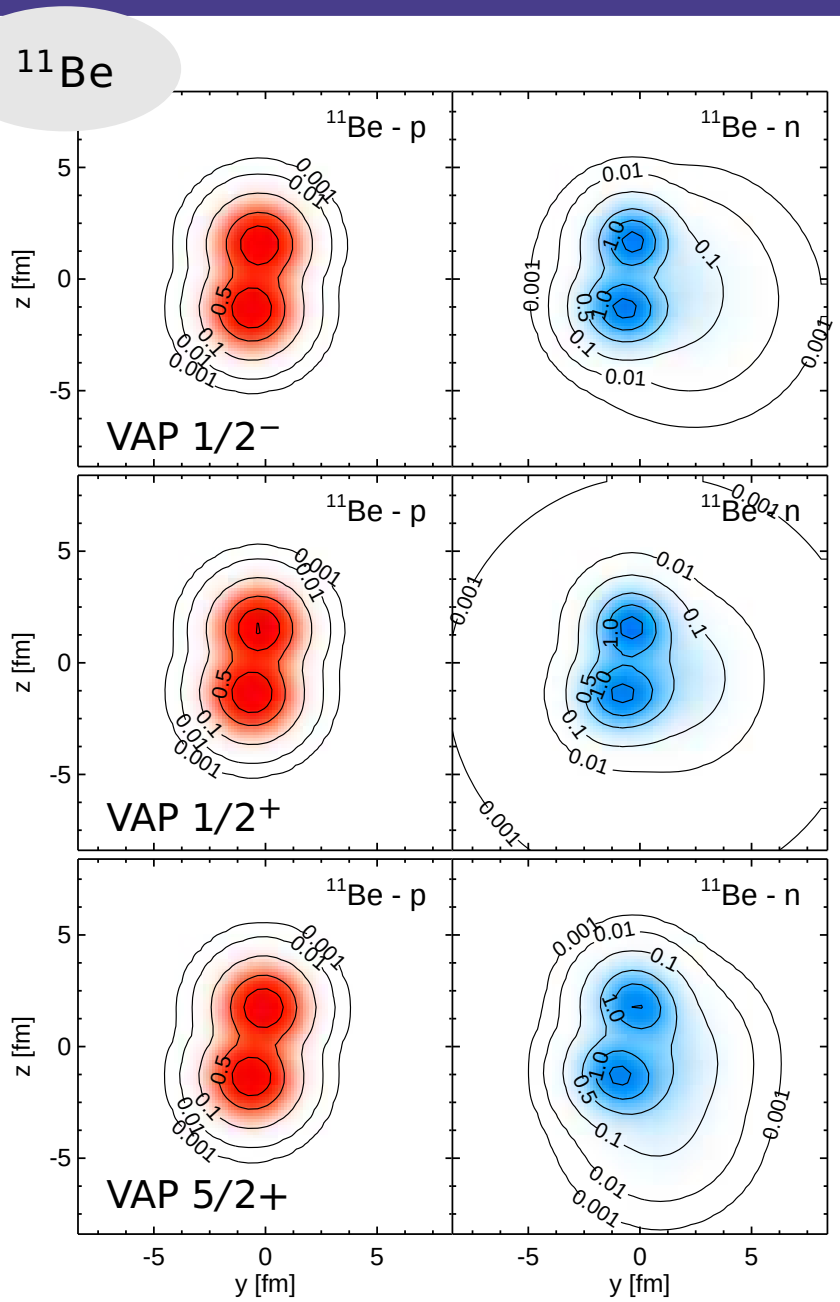
➨ large gain in binding energy compared to mean-field result

➨ intrinsic states show pronounced cluster structure. Parameters of ^{4}He and ^{3}He clusters are close to those of the free clusters

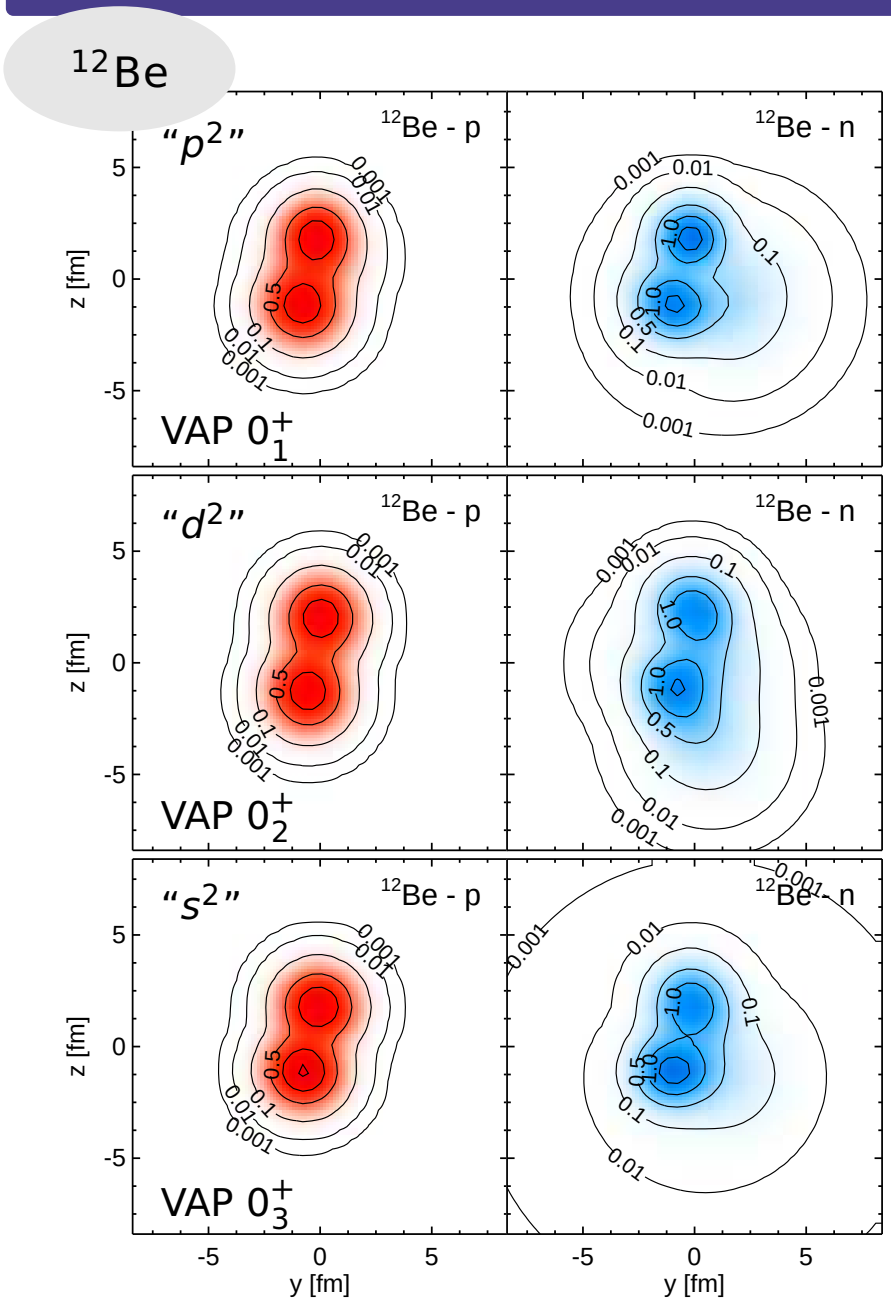


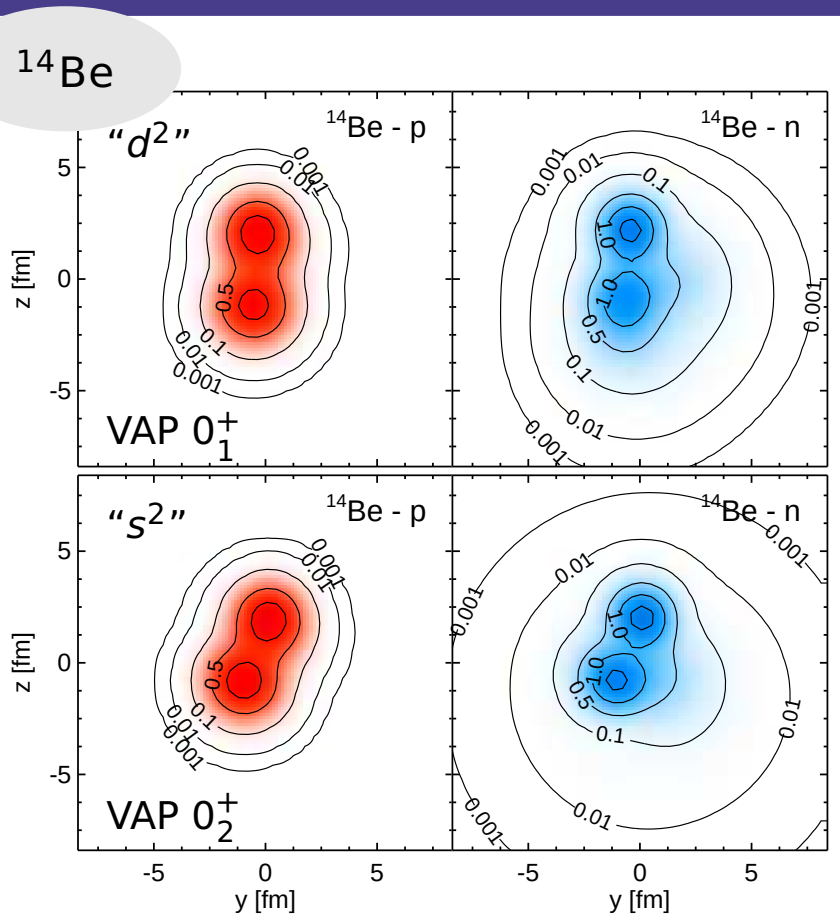
Variation after Projection



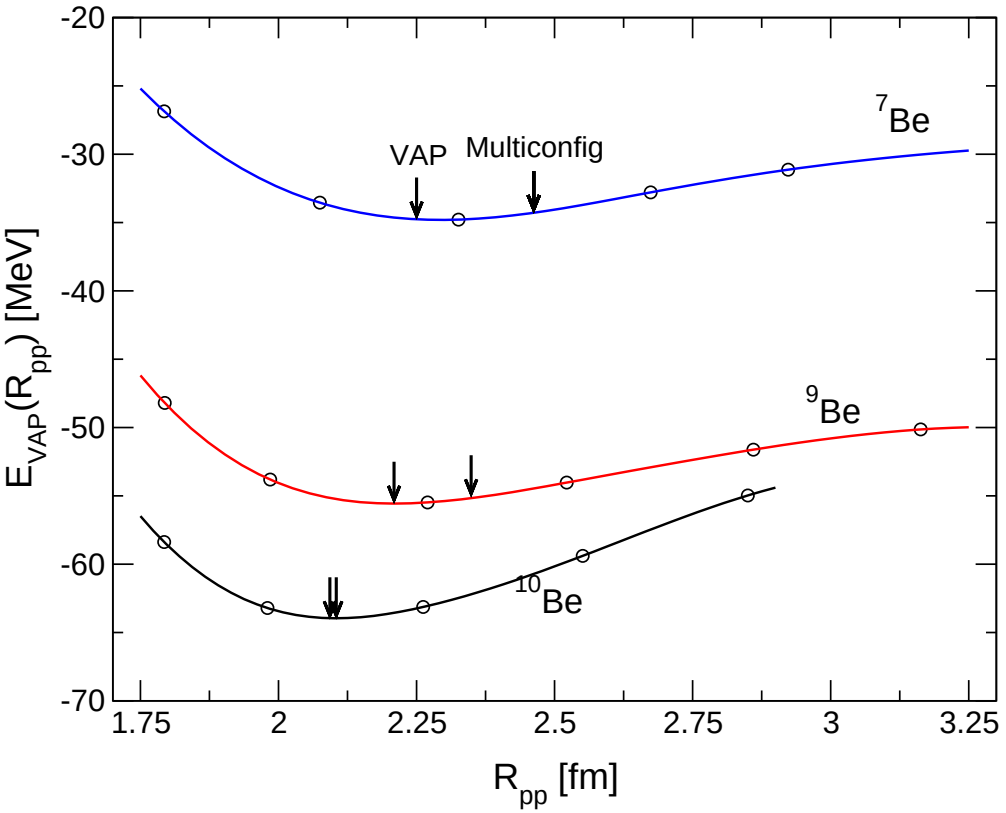


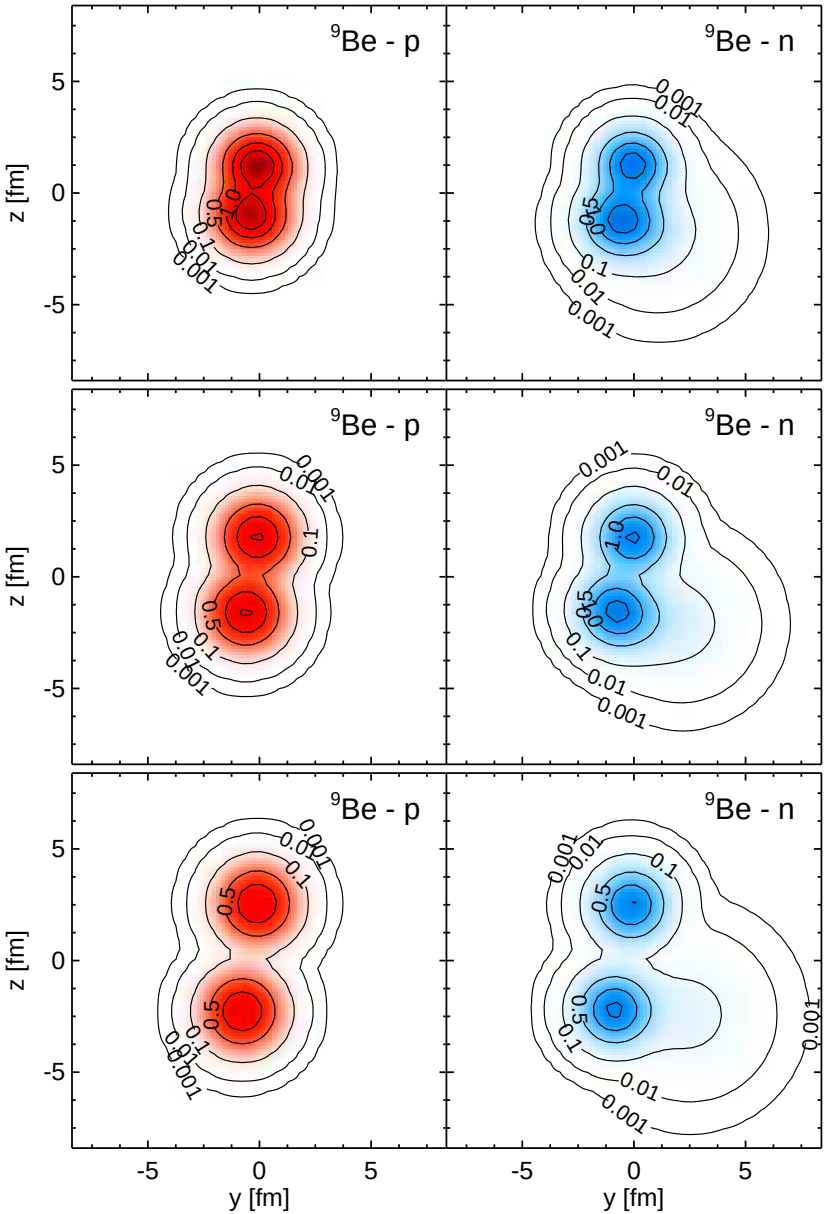
Variation after Projection





Mean proton distance as generator coordinate



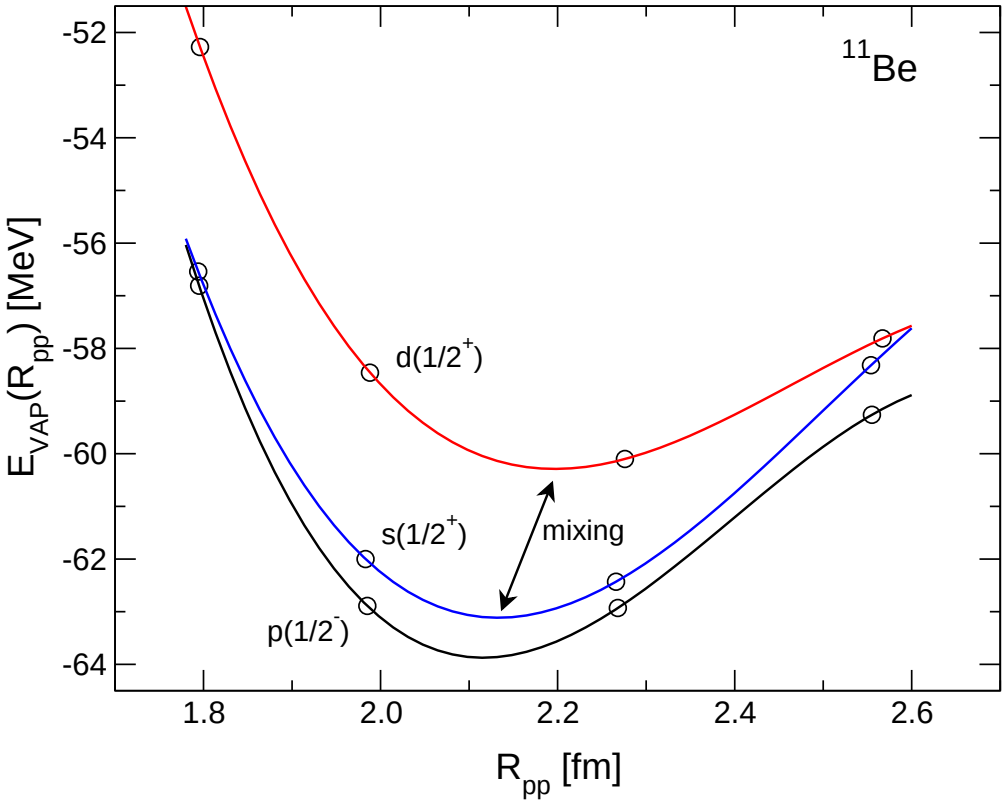


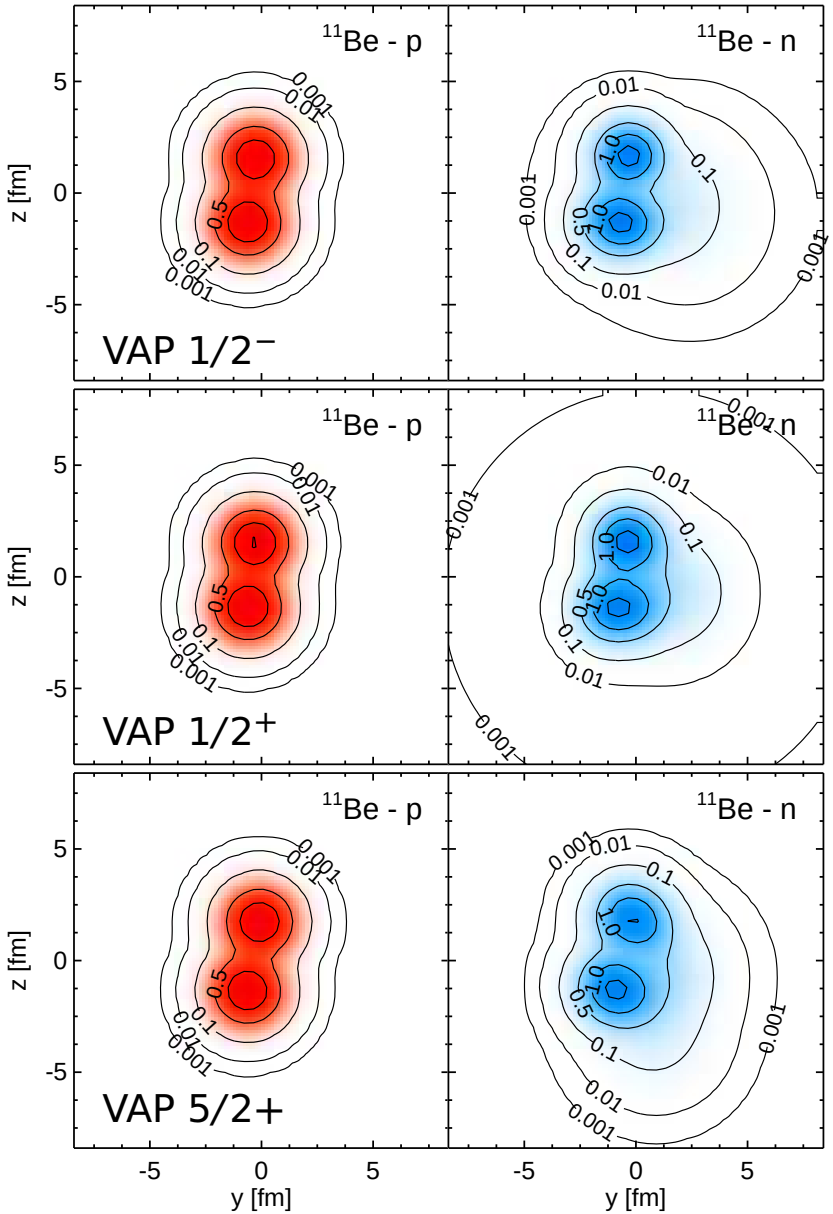
Mean proton distance

$$R_{pp}^2 = \frac{1}{Z^2}\langle \sum_{i<j}^{\text{protons}} (\mathbf{r}_i - \mathbf{r}_j)^2 \rangle$$

R_{pp} as a measure of
α-cluster distance

Mean proton distance as generator coordinate

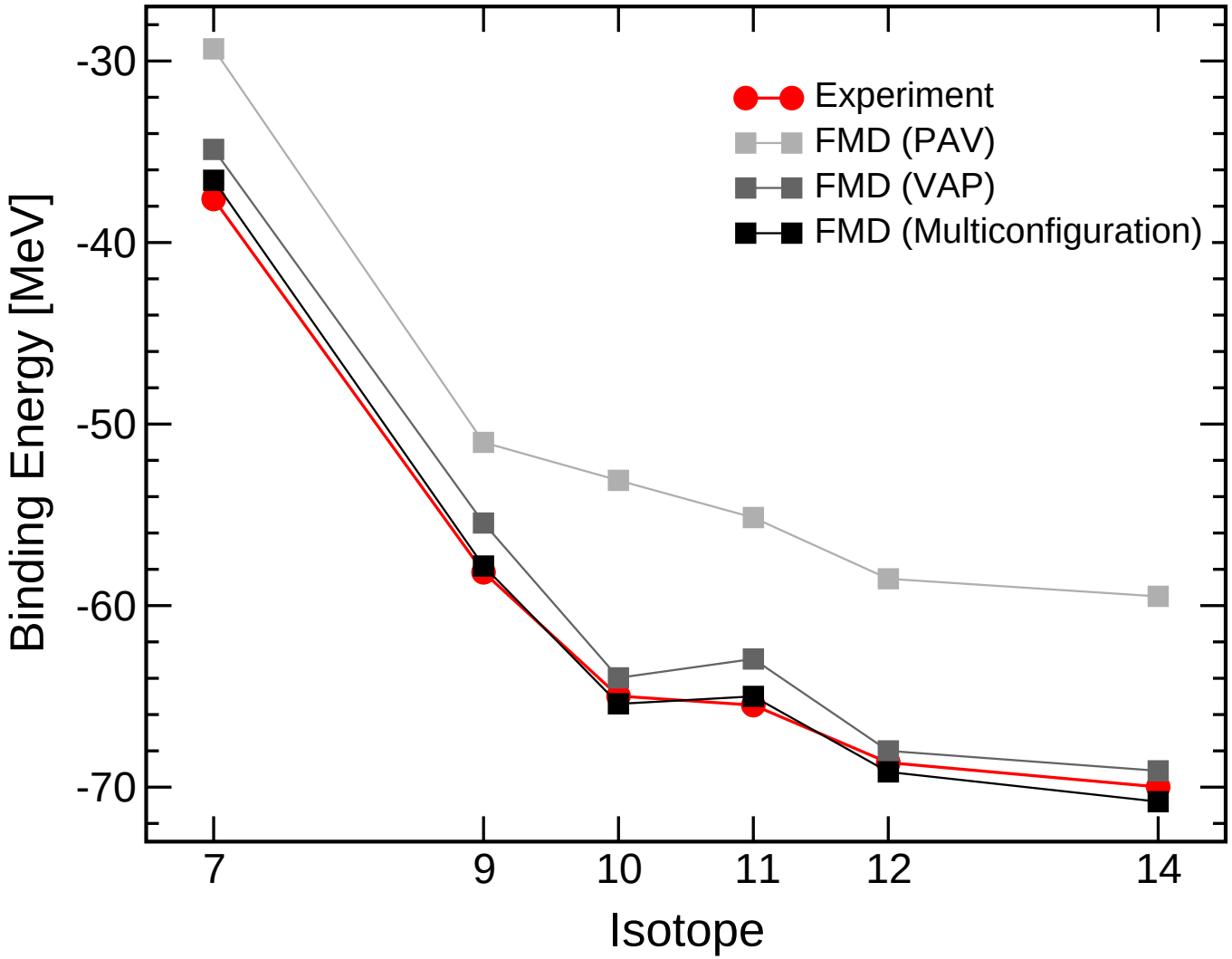




^{11}Be – "*p*", "*s*" and "*d*"-configurations

- "*s*"- and "*d*"-configurations will mix in 1/2$^+$ state
- energy surfaces for "*p*" and "*s*" similar to those in ^{10}Be
- "*d*" surface has minimum at larger cluster distance → *d*-configuration has a polarized ^{10}Be core

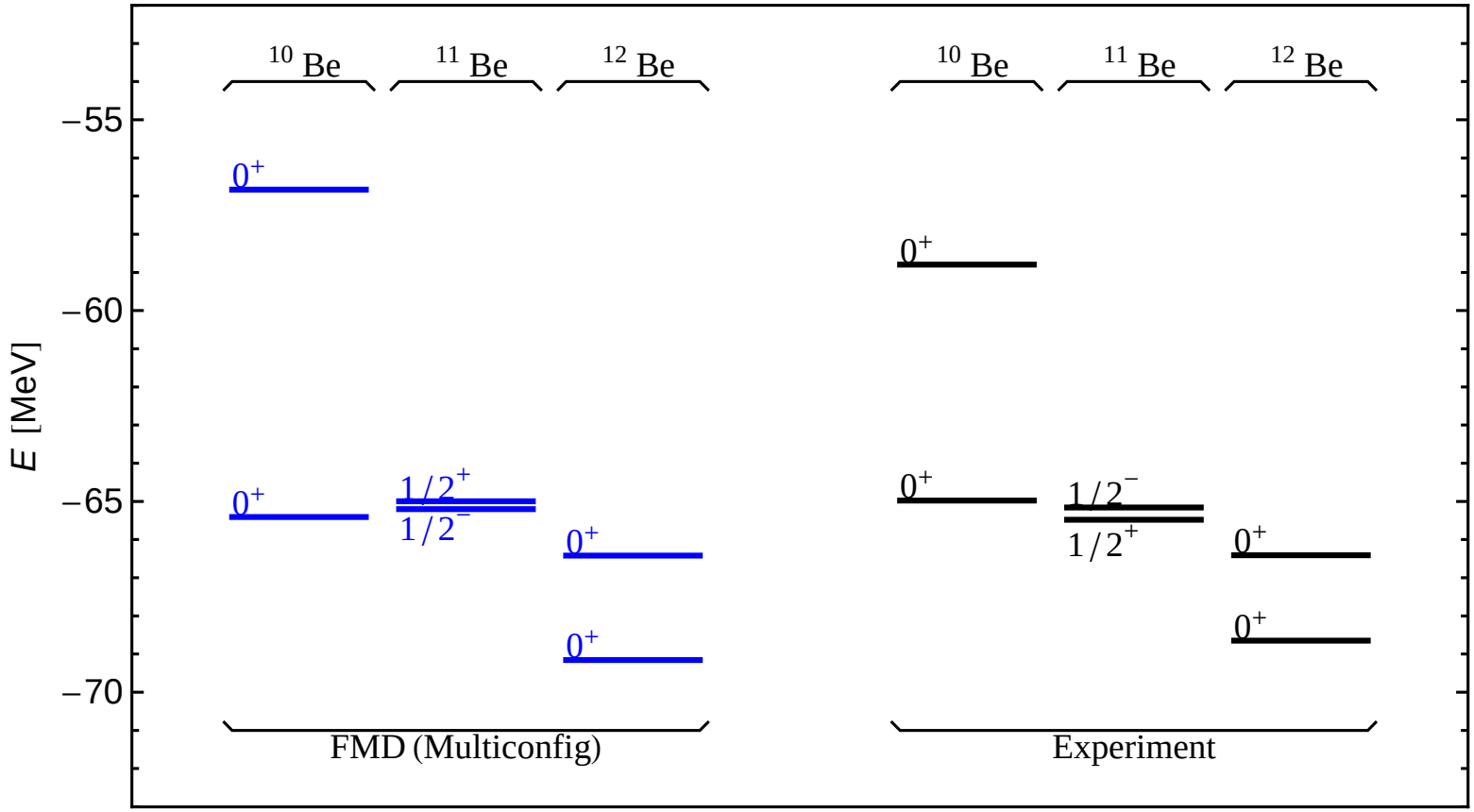
Binding energies



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

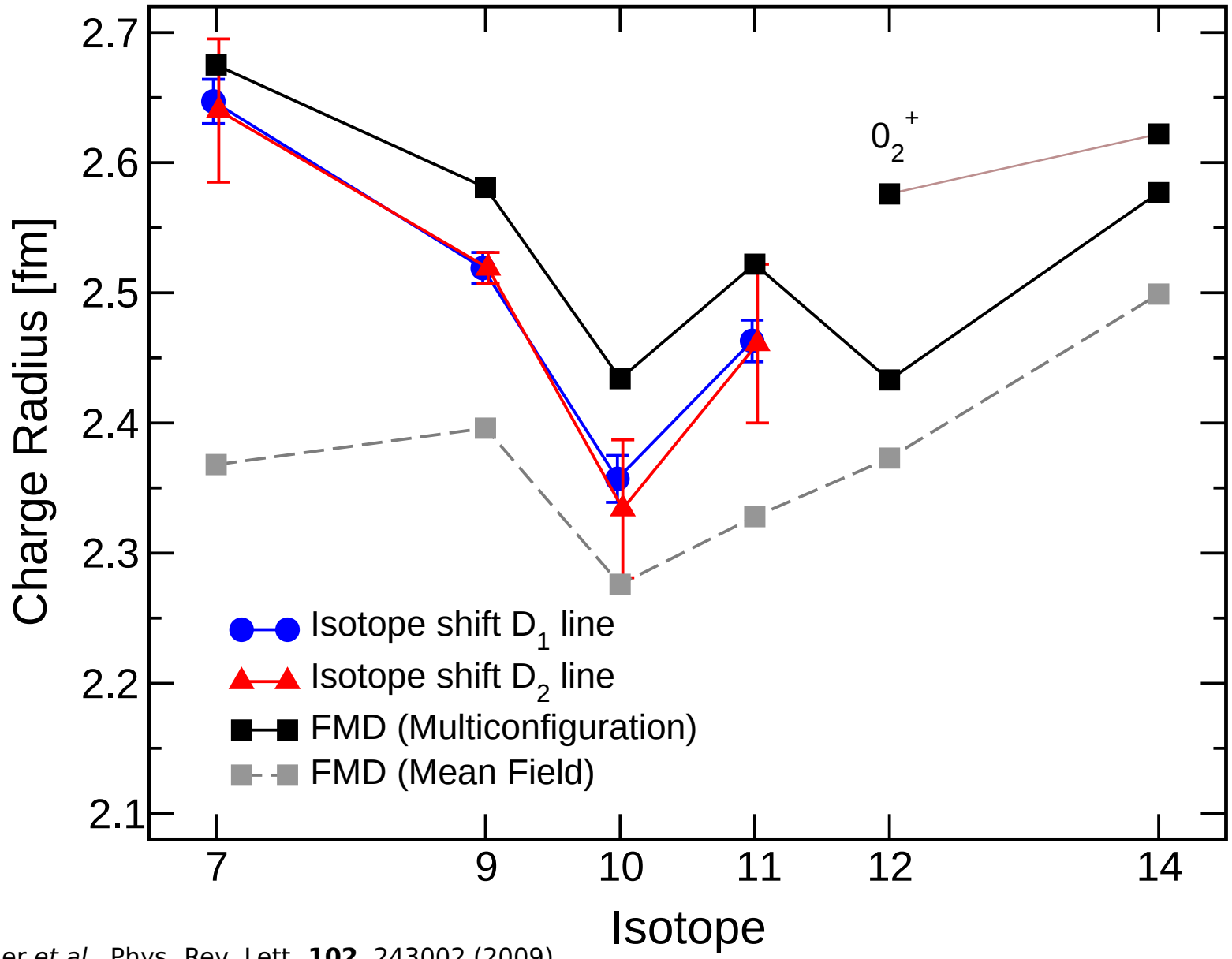
Beryllium Isotopes

$N = 8$ Shell Closure ?



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

Beryllium Isotopes
Charge Radii

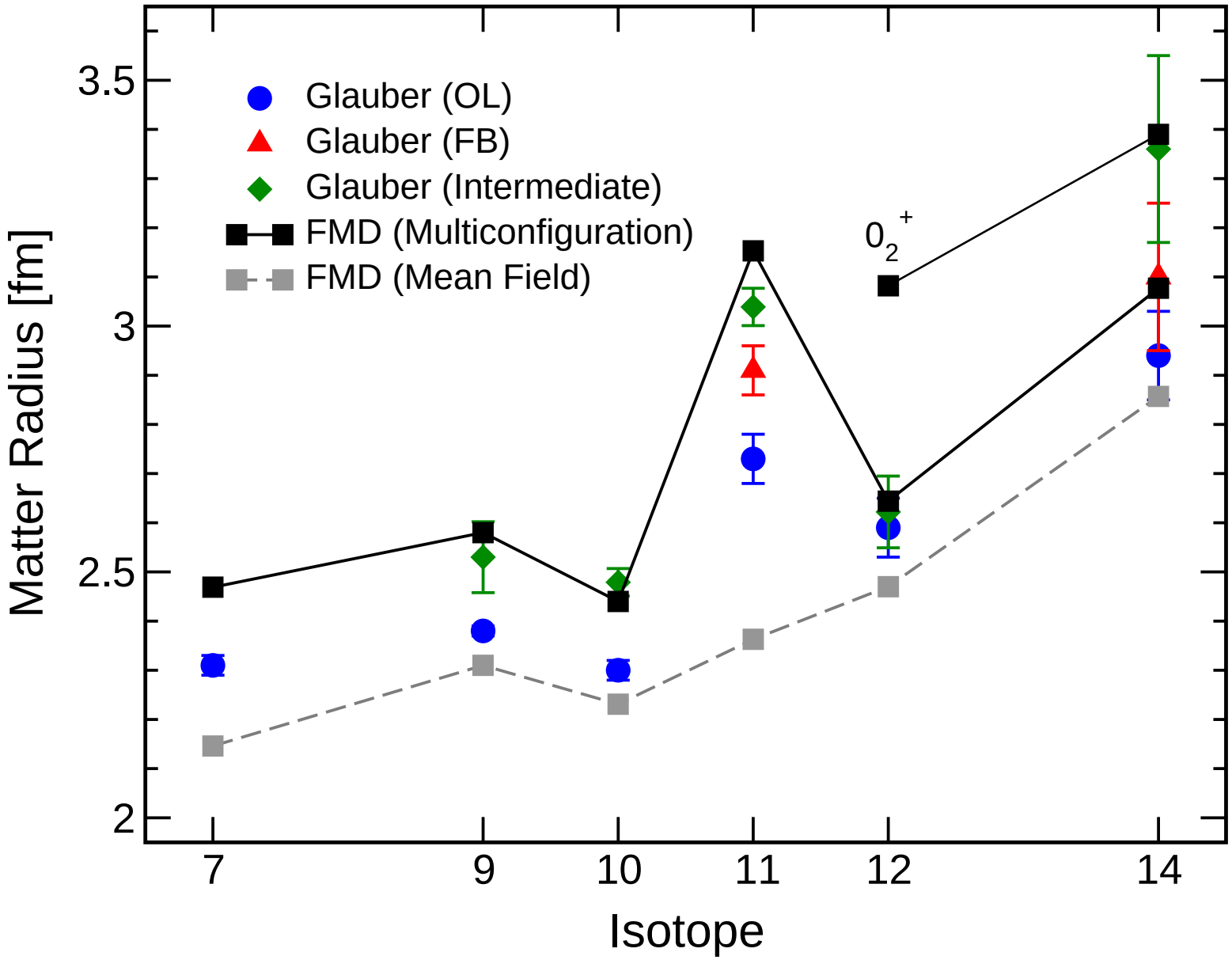


Nörtershäuser *et al.*, Phys. Rev. Lett. **102**, 243002 (2009)

Zakova, Neff, *et al.*, J. Phys. G **37**, 055107 (2010)

Beryllium Isotopes

Matter Radii



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

Electromagnetic transitions

^{10}Be

	FMD(Multiconfig)	Experiment
$B(E2; 2_1^+ \to 0_1^+)$	11.27 e^2fm^4	9.2 ± 0.3 e^2fm^4
$B(E2; 2_2^+ \to 0_1^+)$	1.00 e^2fm^4	0.11 ± 0.02 e^2fm^4
$B(E2; 0_2^+ \to 2_1^+)$	4.99 e^2fm^4	3.2 ± 1.9 e^2fm^4
$B(E1; 0_2^+ \to 1_1^-)$	0.013 e^2fm^2	0.013 ± 0.004 e^2fm^2

^{11}Be

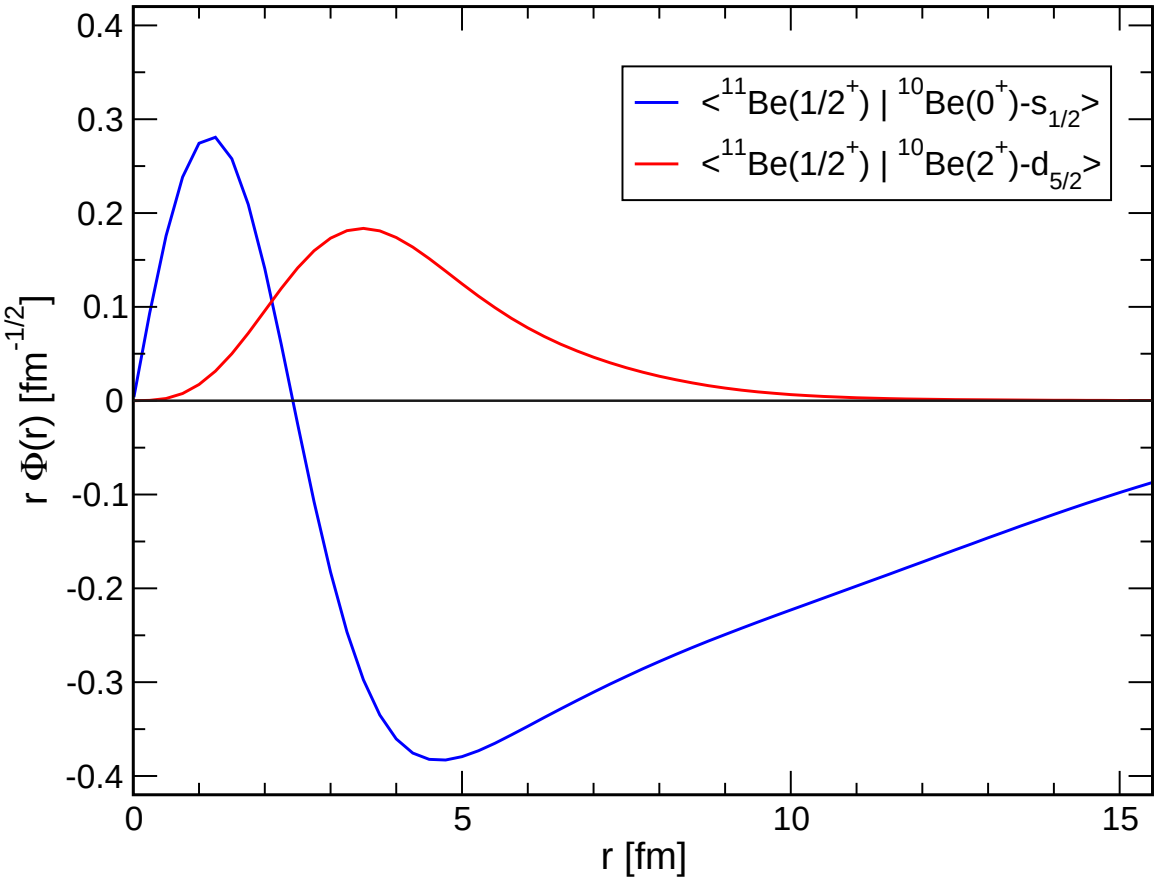
	FMD(Multiconfig)	Experiment
$B(E1; 1/2_1^+ \to 1/2_1^-)$	0.020 e^2fm^2	0.099 ± 0.010 e^2fm^2

^{12}Be

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

McCutchan *et al.*. Phys. Rev. Lett. **103**, 192501 (2009).
Nakamura *et al.*, Phys. Lett. **B394**, 11 (1997).
Shimoura *et al.*, Phys. Lett. **B654**, 87 (2007).
Iwasaki *et al.*, Phys. Lett. **B491**, 8 (2000).
Imai *et al.*, Phys. Lett. **B673**, 179 (2009).

^{11}Be-^{10}Be **Overlaps**



Spectroscopic Factors

^{11}Be	^{10}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

- extended *s*-wave halo
- $s_{1/2}$ spectroscopic factor larger than results obtained from knockout and transfer reactions

Summary

Unitary Correlation Operator Method

- Explicit description of short-range central and tensor correlations
- Decouples low- and high-momentum modes

Fermionic Molecular Dynamics

- Microscopic many-body approach using Gaussian wave-packets
- Projection and multiconfiguration mixing
- Consistent description of well bound states with shell structure and loosely bound states of cluster or halo nature

Beryllium Isotopes

- α-clustering, dissappearance of $N = 8$ shell closure
- s-wave halo in ^{11}Be, spectroscopic amplitudes
- ^{12}Be ground state dominantly p^2 – consistent with matter radius, waiting for charge radius measurement
- charge and matter radii, electromagnetic transitions

Thanks

to my Collaborators

S. Bacca, A. Cribeiro, R. Cussons, H. Feldmeier, P. J. Ginsel, B. Hellwig, K. Langanke, R. Torabi, D. Weber

GSI Darmstadt

H. Hergert, R. Roth

Institut für Kernphysik, TU Darmstadt