Cluster States in ^{12}C and neighboring nuclei

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Our Aim:

Solve the
nuclear many-body problem for
bound-states, resonances and scattering states
with realistic NN interactions

Many-Body Method

Fermonic Molecular Dynamics
(FMD)

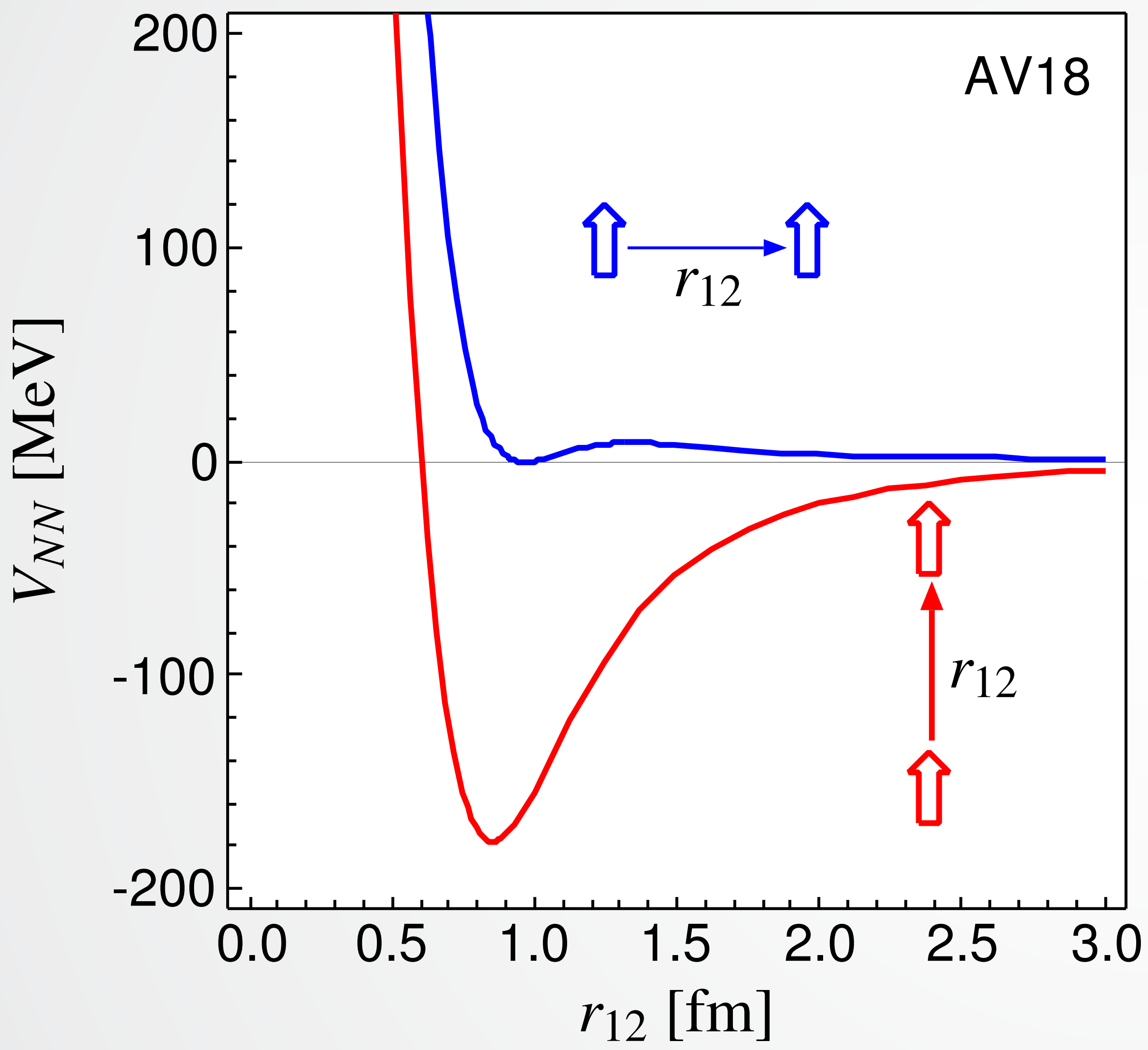
↔

Effective Interaction

Unitary Correlation Operator Method
(UCOM)

Unitary Correlation Operator Method

S=1, T=0



- **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** (mainly from π-exchange) → **tensor correlations**
- the nuclear force will induce strong short-range correlations in the nuclear wave function

$$\hat{S}_{12} = 3(\boldsymbol{\sigma}_1 \cdot \hat{\mathbf{r}}_{12})(\boldsymbol{\sigma}_2 \cdot \hat{\mathbf{r}}_{12}) - (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2)$$

Unitary Correlation Operator Method

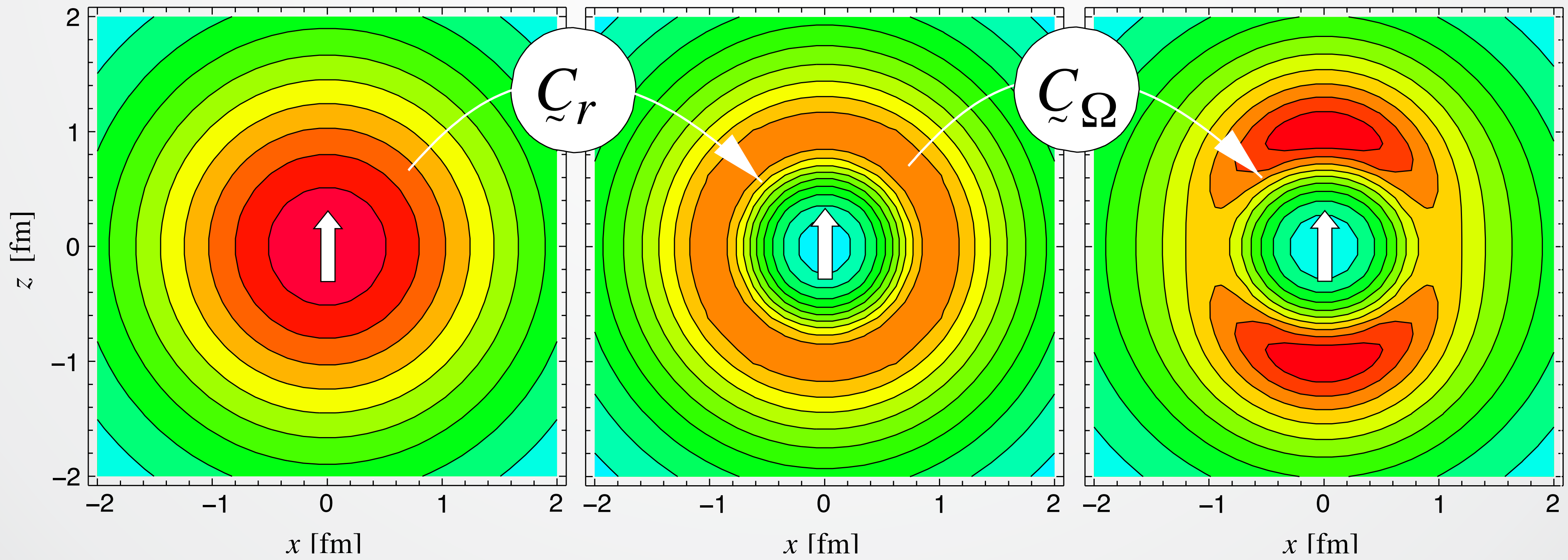
Correlation Operator

$$\hat{C} = \hat{C}_\Omega \hat{C}_r$$

Correlated Hamiltonian

$$\hat{C}^\dagger(\hat{T} + \hat{V})\hat{C} = \hat{T} + \hat{V}_{\mathrm{UCOM}} + \ldots$$

Central correlator shifts nucleons apart,
Tensor correlator aligns nucleons with spin



Clustering in Light Nuclei

- Many-body methods based on harmonic oscillator basis have difficulties describing clustering
- (Microscopic) Cluster models are successful to describe many properties of cluster states for example in ^{12}C but rely on phenomenological interactions
- Gaussian wave-packet basis (AMD and FMD) allows consistent microscopic description with both single-particle and cluster degrees of freedom

^{12}C and the Hoyle state

- ^{12}C and especially the Hoyle state is the prototype for clustering
- Compare cluster model picture with FMD calculations
- Use ^{8}Be+alpha channels to describe continuum

Is the Hoyle state special? What about cluster states in ^{11}C?

- alpha-cluster models obviously do not work, we will combine FMD with explicit cluster configurations
- In ^{11}C the $^{7}Be+^{4}He$ is the first open channel, $^{8}Be+^{3}He$ is not far away
- Can we understand the low-lying positive parity states?

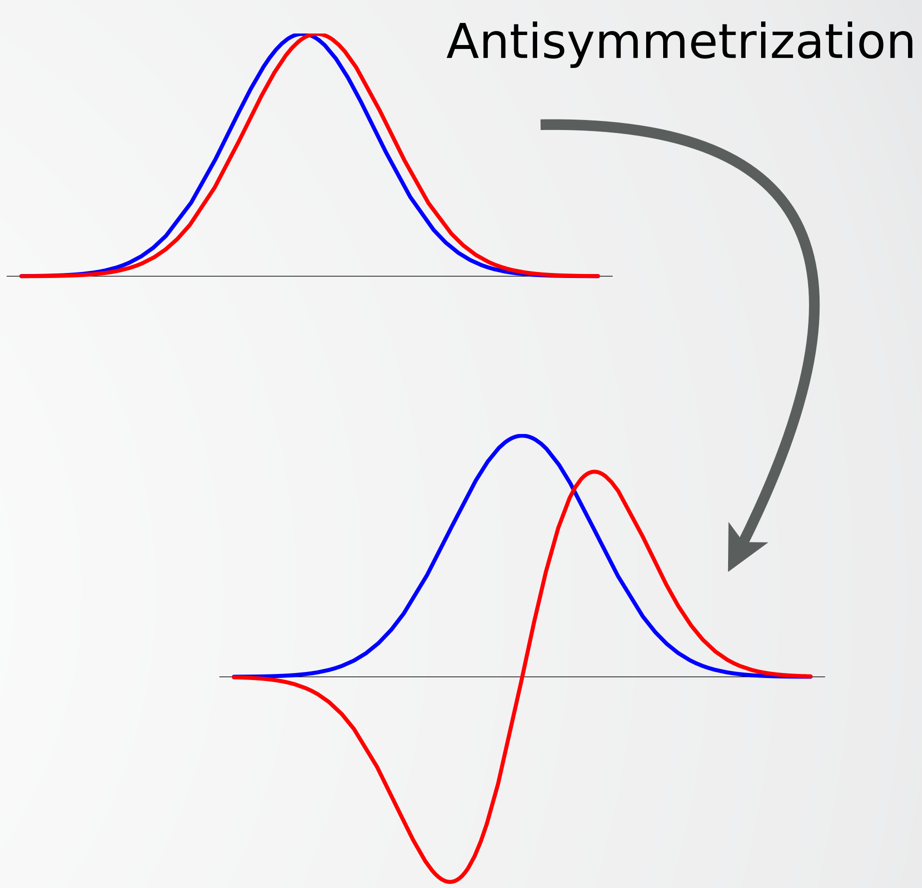
Fermionic Molecular Dynamics

Fermionic

Intrinsic many-body states

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

are antisymmetrized *A*-body states



Molecular

Single-particle states

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

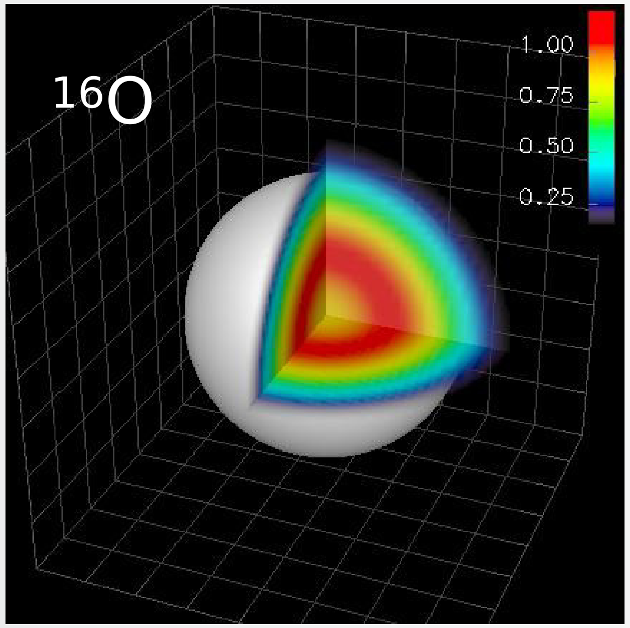
- Gaussian wave-packets in phase-space (complex parameter $\mathbf{b}_i$ encodes mean position and mean momentum), spin is free, isospin is fixed
- width a_i is an independent variational parameter for each wave packet
- use one or two wave packets for each single particle state

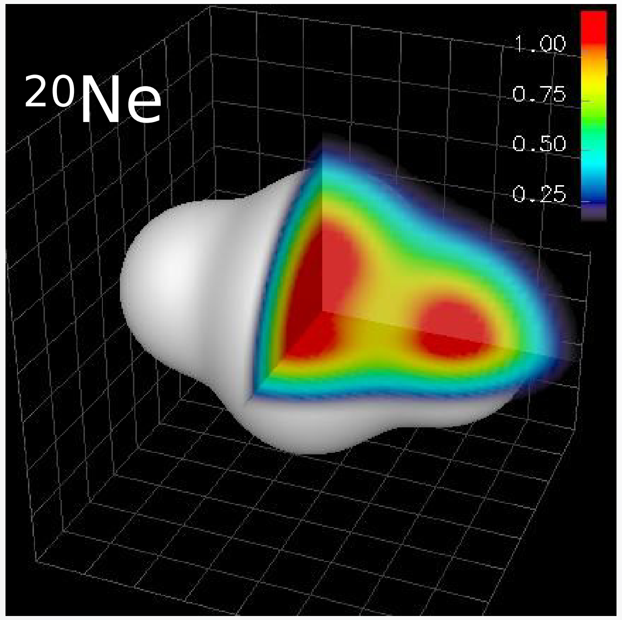
FMD basis contains **harmonic oscillator shell model** and **Brink-type cluster** configurations as limiting cases

Projection after Variation

Variation and Projection

- minimize the energy of the intrinsic state
- intrinsic state may break symmetries of Hamiltonian
- restore inversion, translational and rotational symmetry by **projection on parity**, **angular (and linear) momentum**





Variation

$$\min_{\{q_\nu\}} \frac{\langle Q | \hat{H} - \hat{T}_{\mathrm{cm}} | Q \rangle}{\langle Q | Q \rangle}$$

Projection

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

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

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

Generator coordinates

- use generator coordinates (radii, quadrupole or octupole deformation, strength of spin-orbit force) to create additional basis states

Variation after Projection

Variation after Projection

- Correlation energies can be quite large for well deformed and/or clustered states
- For light nuclei it is possible to perform real variation after projection
- Can be combined with generator coordinate method

Multiconfiguration Mixing

- Set of N intrinsic states optimized for different spins and parities and for different values of generator coordinates are used as basis states
- Diagonalize in set of projected basis states

Variation

$$\min_{\{q_\nu\}} \frac{\langle Q | \hat{H} - \hat{T}_{\mathrm{cm}} | Q \rangle}{\langle Q | Q \rangle}$$

Variation after Projection

$$\min_{\{q_\nu, {c^\alpha}_K\}} \frac{\sum_{KK'} {c^\alpha}_K^\star \langle Q | (\hat{H} - \hat{T}_{\mathrm{cm}}) \hat{P}^\pi {\hat{P}^J}_{KK'} | Q \rangle {c^\alpha}_{K'}}{\sum_{KK'} {c^\alpha}_K^\star \langle Q | \hat{P}^\pi {\hat{P}^J}_{KK'} | Q \rangle {c^\alpha}_{K'}}$$

(Intrinsic) Basis States

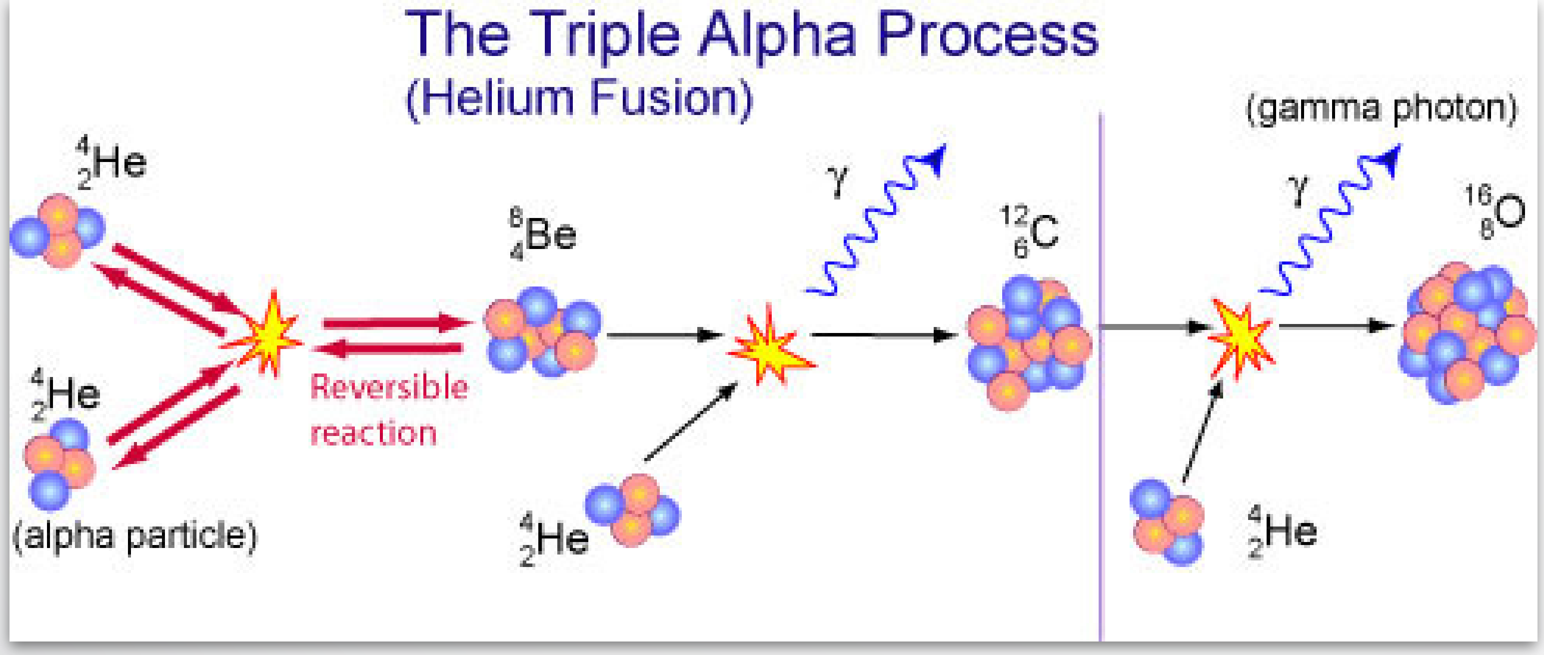
$$\left\{ \left| Q^{(a)} \right\rangle, a = 1, \ldots, N \right\}$$

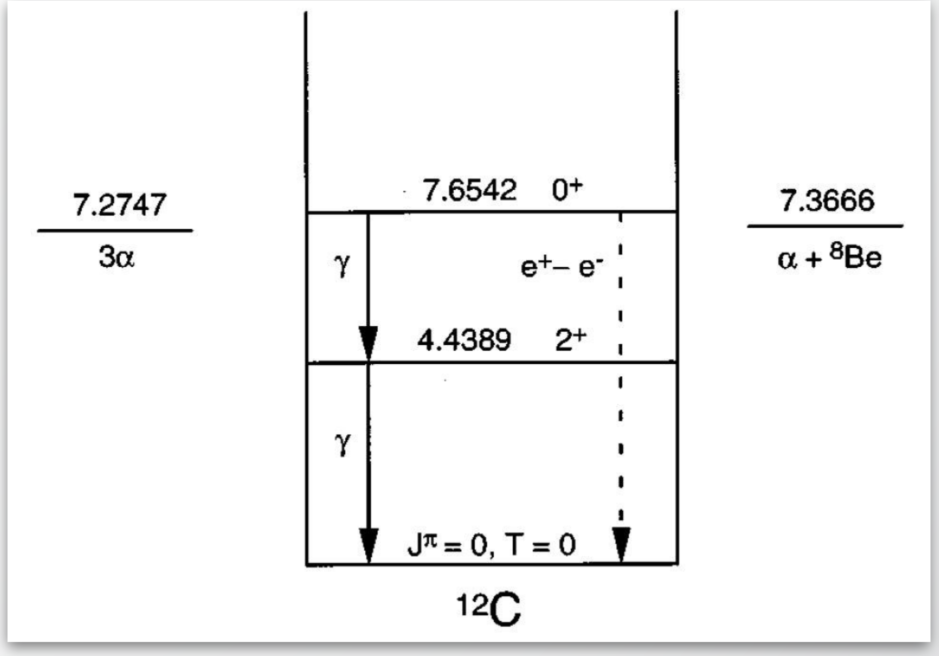
Generalized Eigenvalue Problem

$$\sum_{K'b} \underbrace{\left\langle Q^{(a)} \middle| \hat{H} \hat{P}^\pi {\hat{P}^J}_{KK'} \hat{P}^{\mathbf{P}=0} \middle| Q^{(b)} \right\rangle}_{\text{Hamiltonian kernel}} {c^\alpha}_{K'b} = E^{J^\pi \alpha} \sum_{K'b} \underbrace{\left\langle Q^{(a)} \middle| \hat{P}^\pi {\hat{P}^J}_{KK'} \hat{P}^{\mathbf{P}=0} \middle| Q^{(b)} \right\rangle}_{\text{norm kernel}} {c^\alpha}_{K'b}$$

Cluster States in ^{12}C

FMD versus traditional Cluster Model Calculations



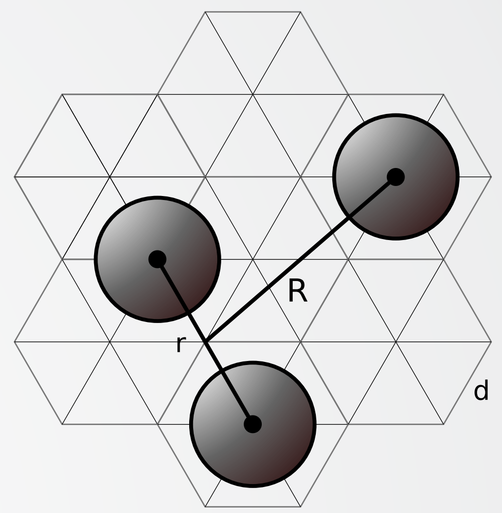


^{12}C: Microscopic α-Cluster Model

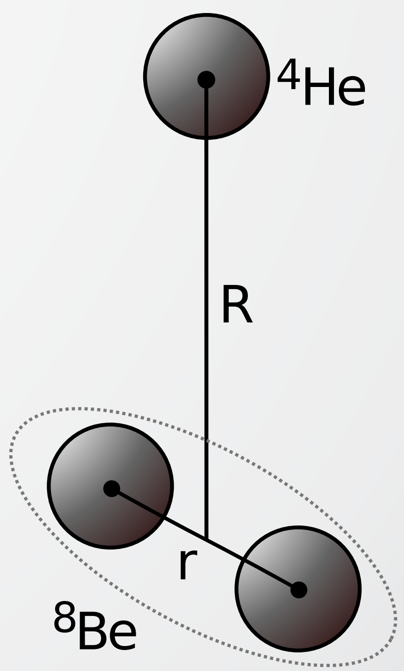
- ^{12}C is described as a system of three α-particles
- α-particles are given by HO $(0s)^4$ wave functions
- wave function is fully antisymmetrized
- effective Volkov nucleon-nucleon interaction adjusted to reproduce α-α and ^{12}C ground state properties

- Internal region: **α's on triangular grid**
- External region: **^{8}Be(0^+,2^+,4^+)-α configurations**

Internal Region



External Region



$$\left|\Psi^{3\alpha}_{JMK\pi}(\mathbf{R}_1,\mathbf{R}_2,\mathbf{R}_3)\right\rangle = \hat{P}^{\pi}\hat{P}^{J}_{MK}\hat{\mathcal{A}}\left\{\left|\Psi_\alpha(\mathbf{R}_1)\right\rangle \otimes \left|\Psi_\alpha(\mathbf{R}_2)\right\rangle \otimes \left|\Psi_\alpha(\mathbf{R}_3)\right\rangle\right\}$$

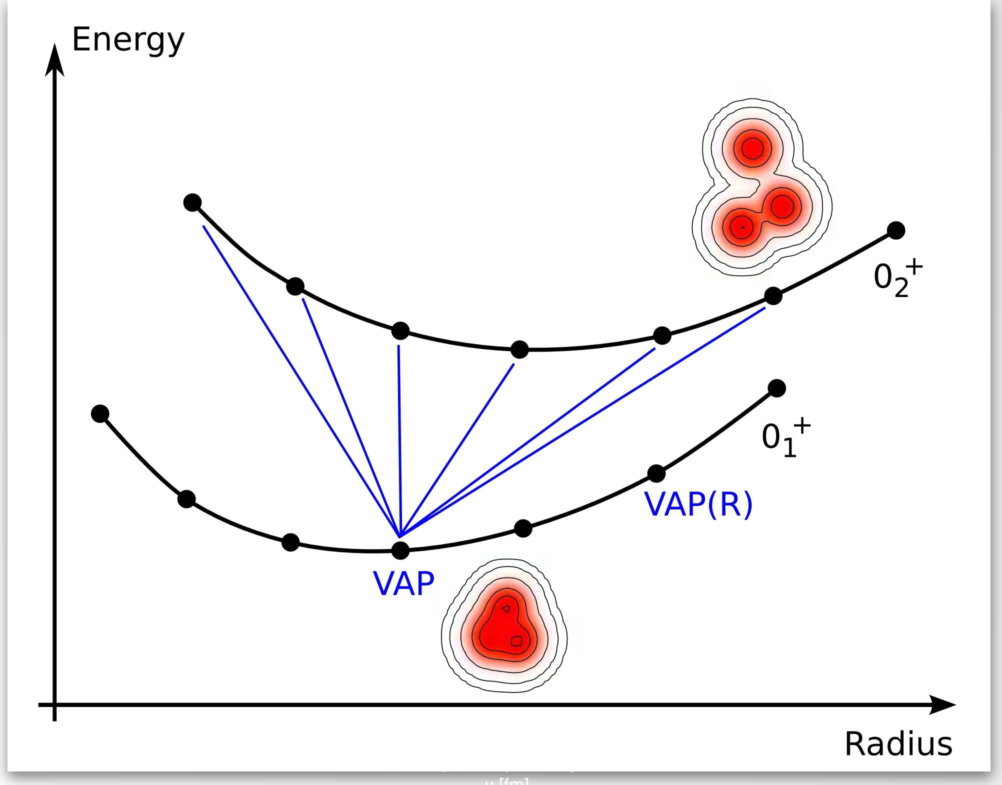
Double Projection

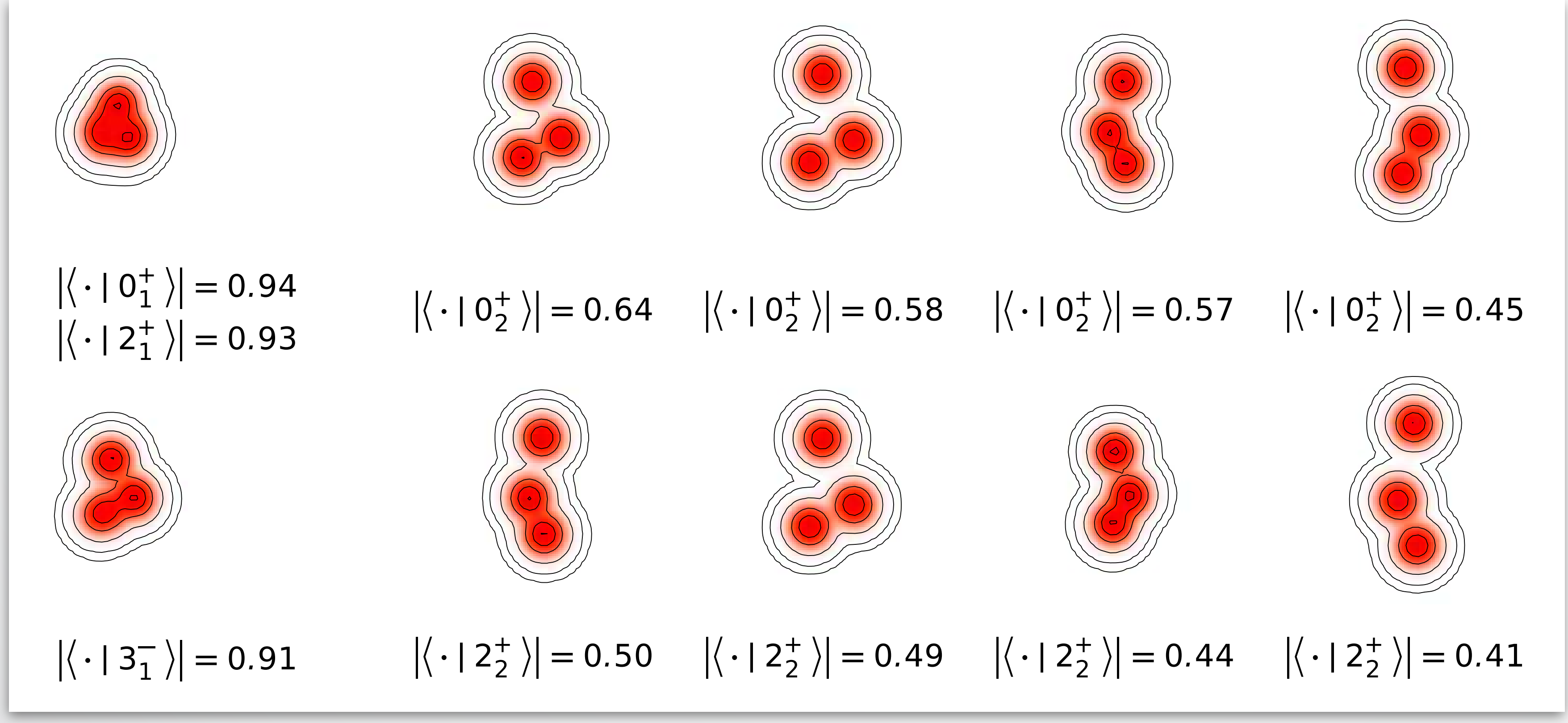
$$\left|\Psi^{^8\mathrm{Be}}_{IK}\right\rangle = \sum_i \hat{P}^{I}_{K0}\hat{\mathcal{A}}\left\{\left|\Psi_\alpha(-\tfrac{r_i}{2}\mathbf{e}_z)\right\rangle \otimes \left|\Psi_\alpha(+\tfrac{r_i}{2}\mathbf{e}_z)\right\rangle\right\} c^I_i$$

$$\left|\Psi^{^8\mathrm{Be},\alpha}_{IK;JM\pi}(R_j)\right\rangle = \hat{P}^{\pi}\hat{P}^{J}_{MK}\hat{\mathcal{A}}\left\{\left|\Psi^{^8\mathrm{Be}}_{IK}(-\tfrac{R_j}{3}\mathbf{e}_z)\right\rangle \otimes \left|\Psi_\alpha(+\tfrac{2R_j}{3}\mathbf{e}_z)\right\rangle\right\}$$

^{12}C: FMD + ^{8}Be-^{4}He Cluster Configurations

- **AV18 UCOM(SRG)** (α=0.20 fm^4) interaction — Increase strength of spin-orbit force by a factor of two to partially account for omitted three-body forces
- Internal region: FMD basis states obtained by **VAP** with radius as generator coordinate for **first 0^+, 1^+, 2^+, …**, perform VAP for **second 0^+, 1^+, 2^+, …** with radius as generator coordinate
- External region: **$^{8}Be(0^+,2^+,4^+)$-α configurations**, polarization effects in ^{8}Be are important





Basis states are not orthogonal !

0^+_2 and 2^+_2 states have no rigid intrinsic structure

^{12}C: Matching to Coulomb Asymptotics

- asymptotically only Coulomb interaction between ^{8}Be and α
- calculate spectroscopic amplitudes with RGM wavefunction
- use microscopic ***R*-matrix** method to match logarithmic derivative of spectroscopic amplitudes to Coulomb solutions

Bound states (Whittaker)

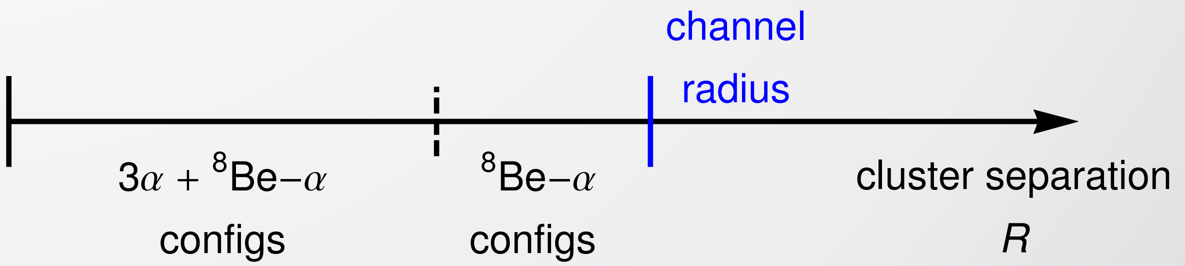
$$\psi_c(r) = A_c \frac{1}{r} W_{-\eta_c, L_c+1/2}(2\kappa_c r), \qquad \kappa_c = \sqrt{-2\mu(E-E_c)}$$

Resonances (purely outgoing Coulomb - complex energy)

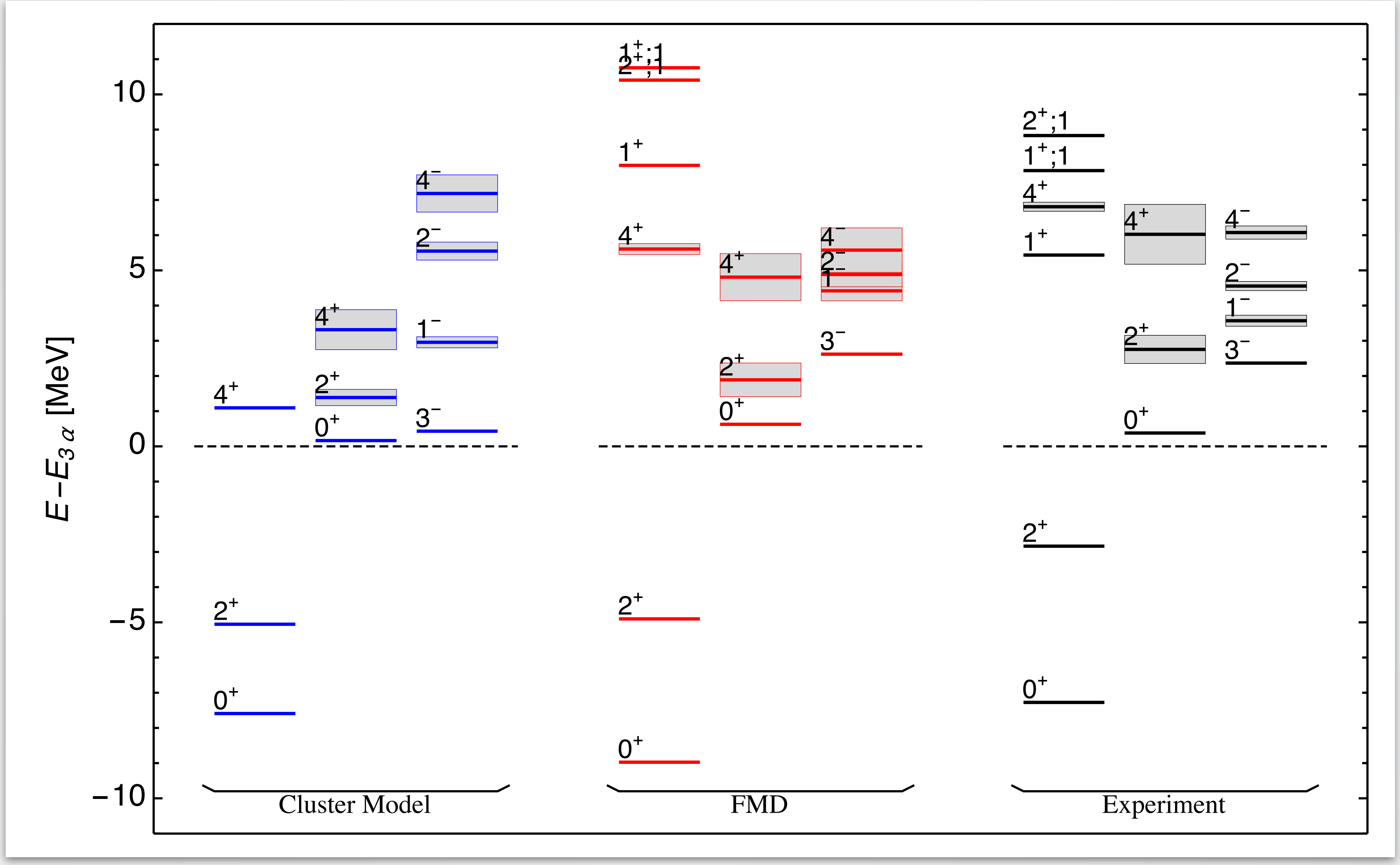
$$\psi_c(r) = A_c \frac{1}{r} O_{L_c}(\eta_c, k_c r), \qquad k_c = \sqrt{2\mu(E-E_c)}$$

Scattering States (incoming + outgoing Coulomb)

$$\psi_c(r) = \frac{1}{r}\left\{\delta_{L_c,L_0} I_{L_c}(\eta_c, k_c r) - S_{c,c_0} O_{L_c}(\eta_c, k_c r)\right\}, \qquad k_c = \sqrt{2\mu(E-E_c)}$$



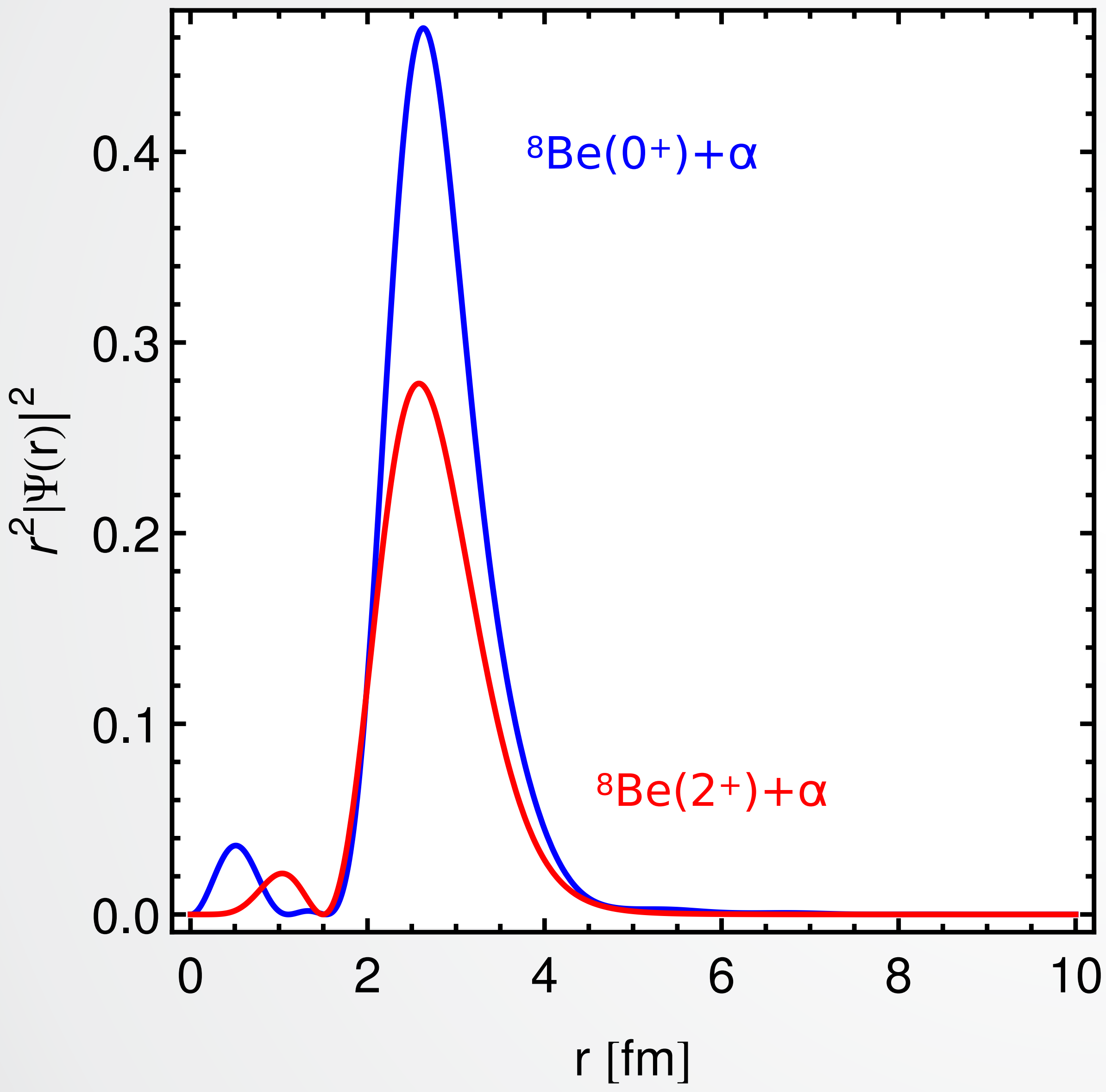
^{12}C: Spectrum including Continuum



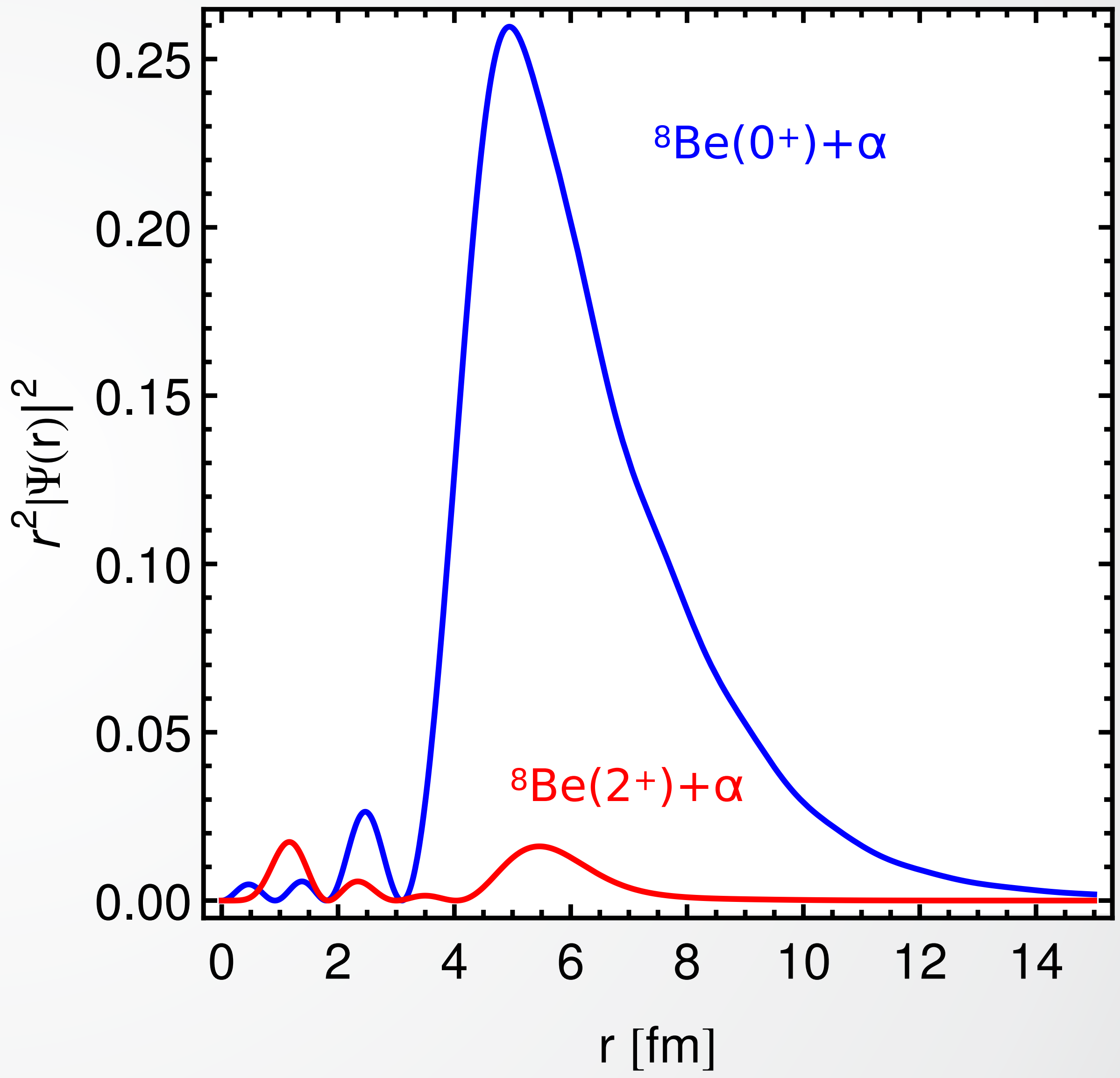
- FMD provides a consistent description of *p*-shell states, negative parity states and cluster states

^{12}C: ^{8}Be-α Spectroscopic Amplitudes

Ground State



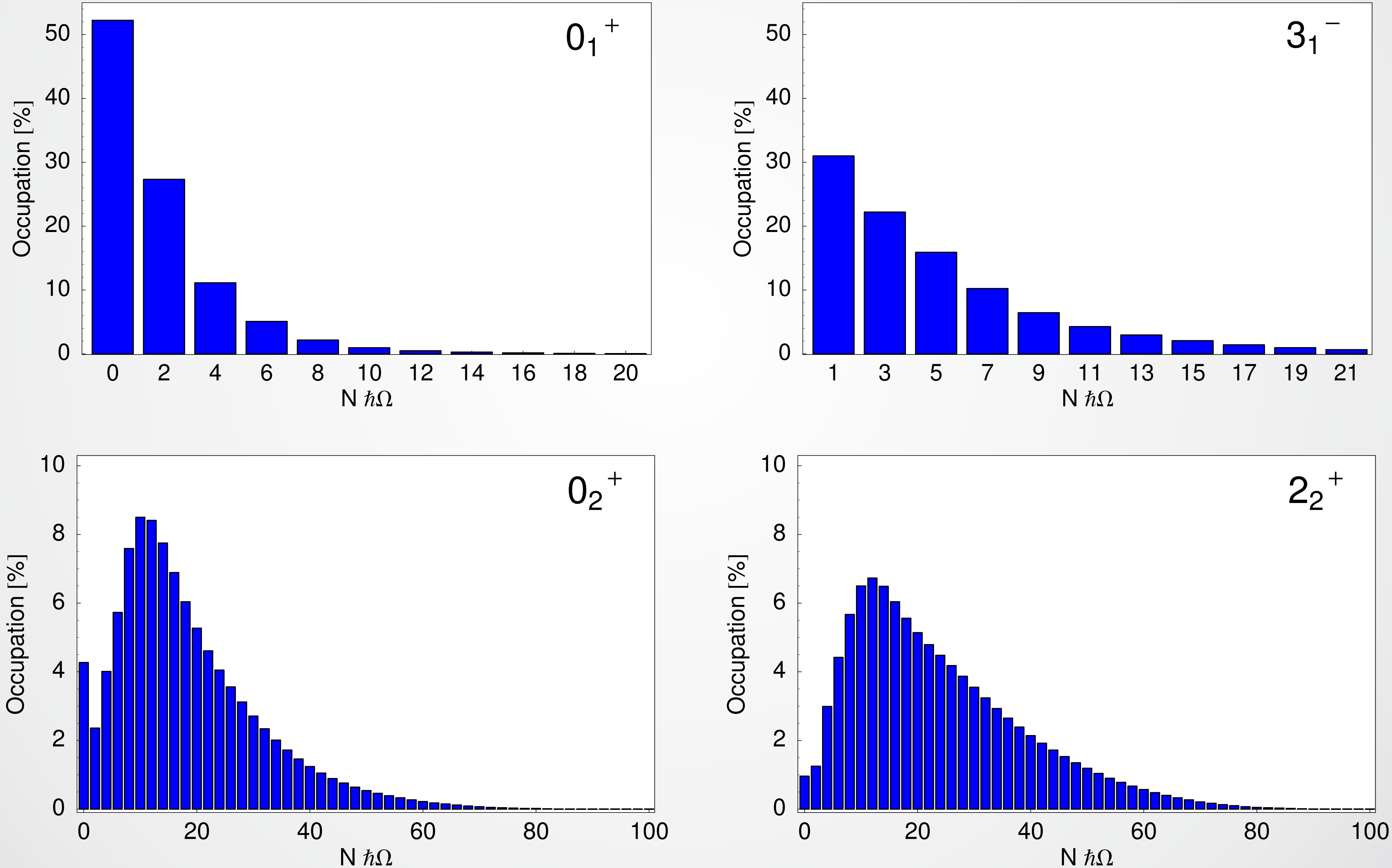
Hoyle State



- Ground state overlap with $^{8}Be(0^+)+\alpha$ and $^{8}Be(2^+)+\alpha$ configurations of similar magnitude
- Hoyle state overlap dominated by $^{8}Be(0^+)+\alpha$ configurations, large spatial extension

^{12}C: $N\hbar\Omega$ Decomposition

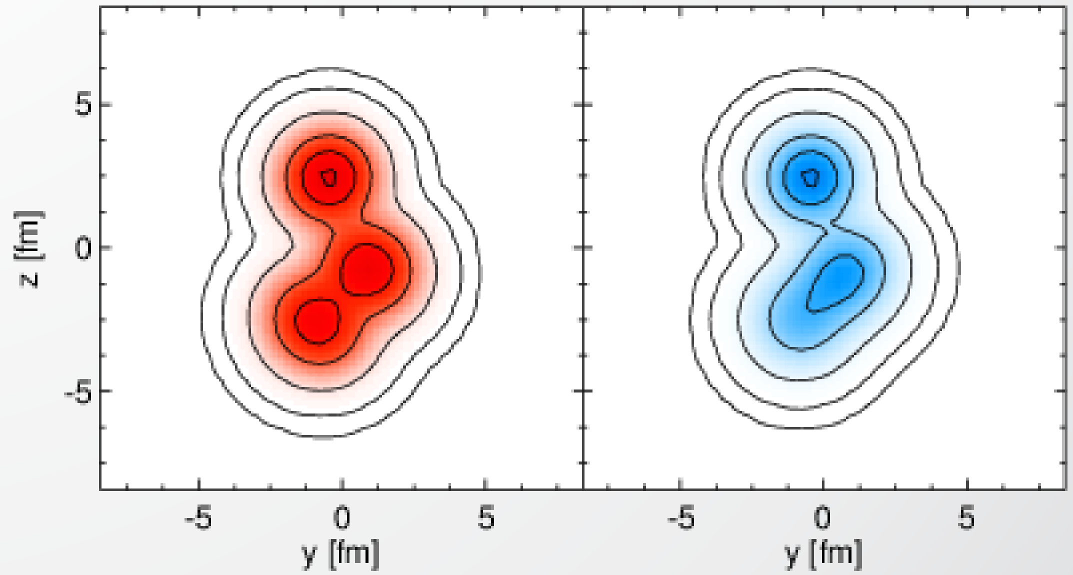
$$\mathrm{Occ}(N) = \left\langle \Psi \middle| \delta\Big(\sum_i (\hat{H}_i^{HO}/\hbar\Omega - 3/2) - N\Big) \middle| \Psi \right\rangle$$



Cluster States in ^{11}C

FMD + explicit cluster configurations

- Is the Hoyle state in ^{12}C special? Are there analogue states in ^{11}C?
- $^{7}Be+^{4}He$ is the first open channel, $^{8}Be+^{3}He$ is not far away
- Unnatural parity states and clustering



^{11}C: Outline of Calculation

I) FMD Calculation using VAP basis states

- Perform VAP calculations for the first couple of eigenstates for each spin and parity
- Can we observe the appearance of cluster structures?
- This provides only a relatively small set of basis states especially for loosely bound and spatially extended states

II) FMD cluster model calculations with ^{7}Be-^{4}He and ^{8}Be-^{3}He configs

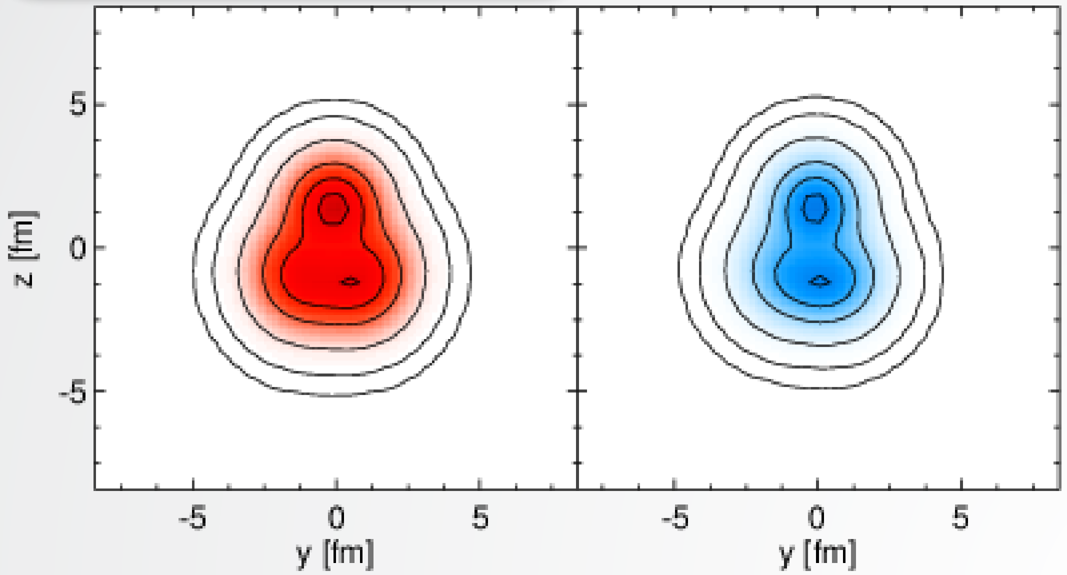
- $^{7}Be(3/2-,1/2-)$ clusters described using a superposition of $^{7}Be(3/2^{-})$ VAP state and an extended ^{4}He-^{3}He config
- $^{8}Be(0+,2+)$ clusters described using a superposition of $^{8}Be(0^{+})$ VAP state and an extended ^{4}He-^{4}He config
- Double-projection of ^{7}Be-^{4}He and ^{8}Be-^{3}He configs at distances of D=1.5, …, 9.0 fm

III) Full calculation with combined VAP and Cluster basis states

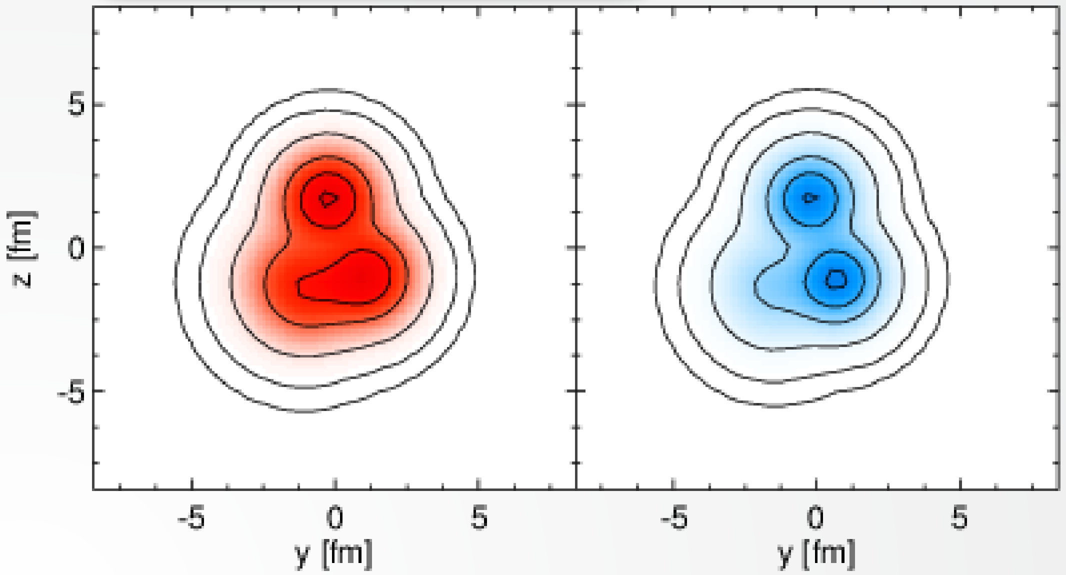
- Basis is overcomplete
- Cluster configs become orthogonal at large distances where the overlap between the clusters vanishes

^{11}C: FMD Variation after Projection

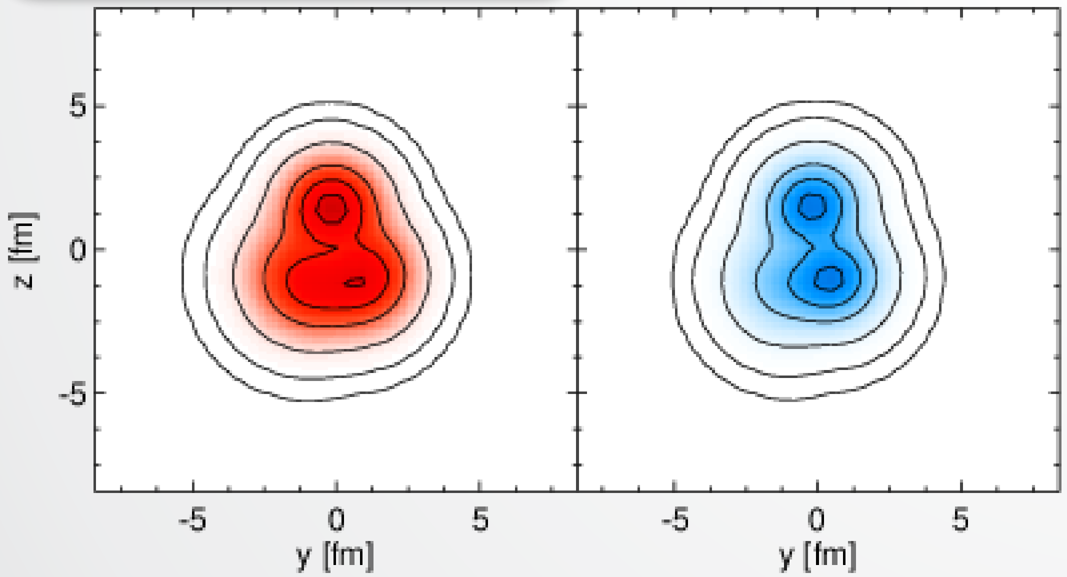
first $3/2^-$



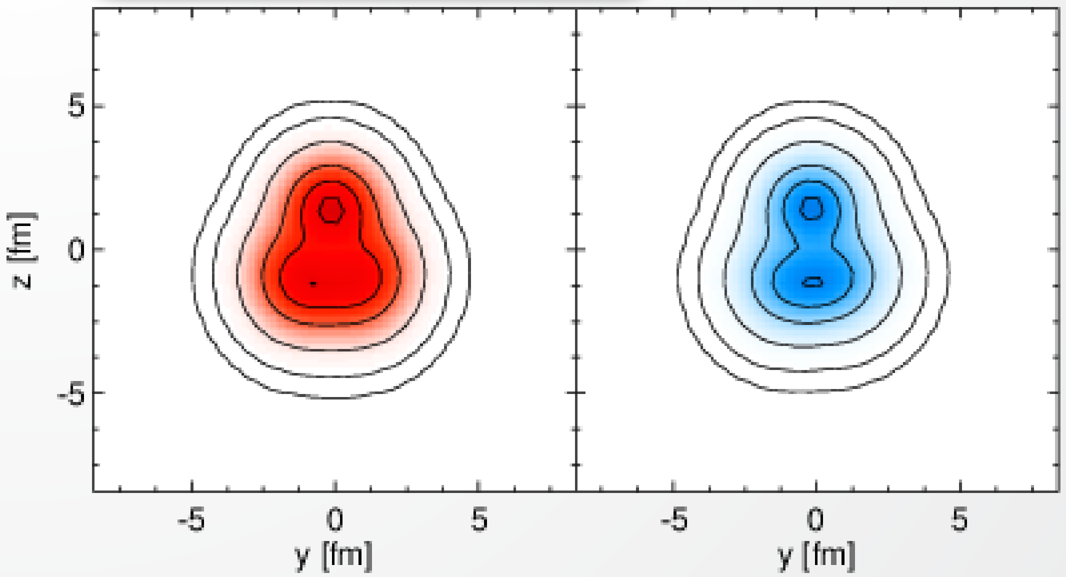
second $3/2^-$



first $1/2^-$



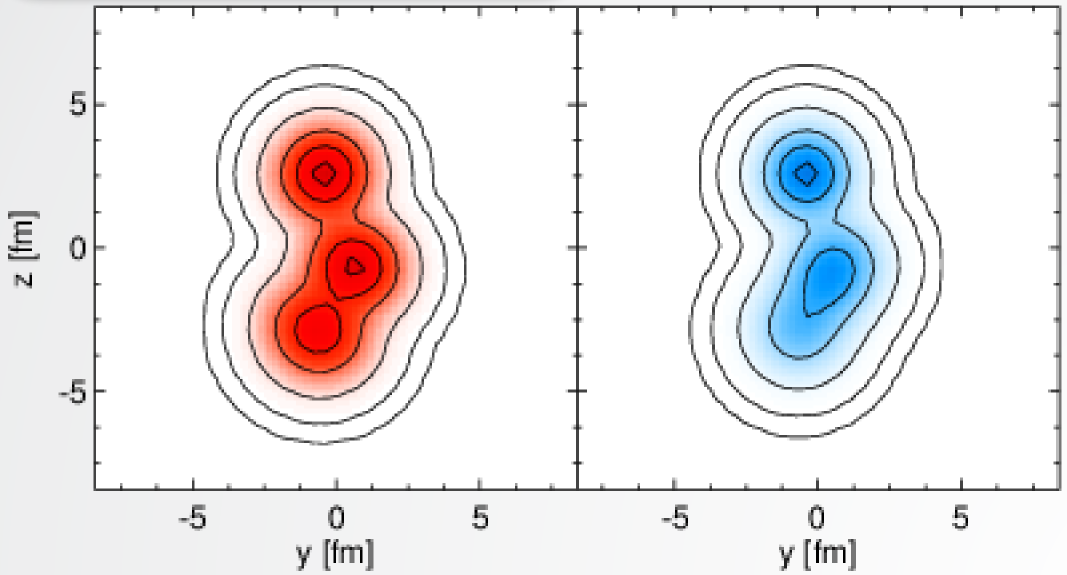
first $5/2^-$



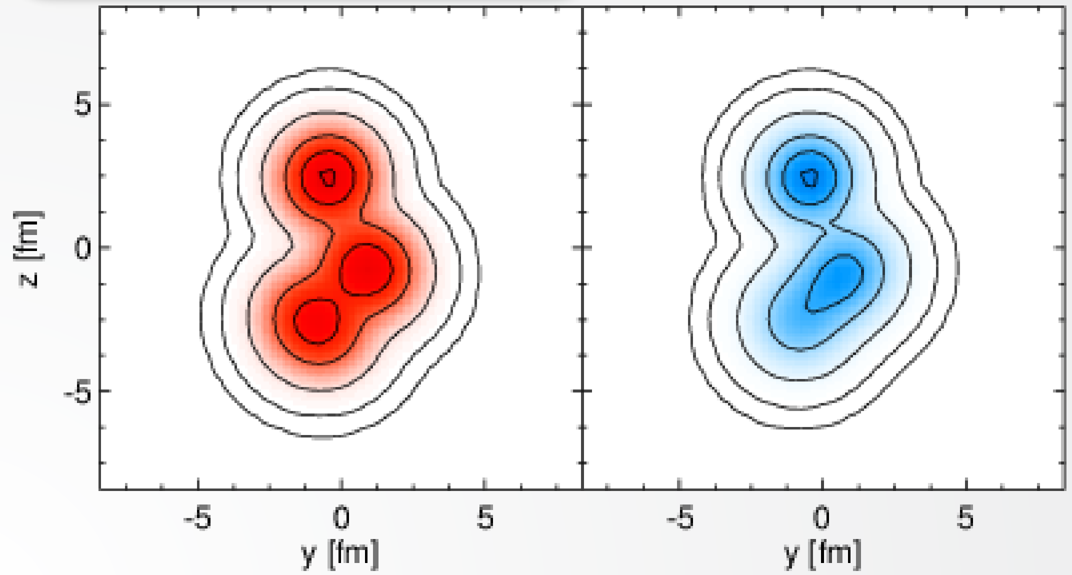
p-shell states with some hint of clustering

^{11}C: FMD Variation after Projection

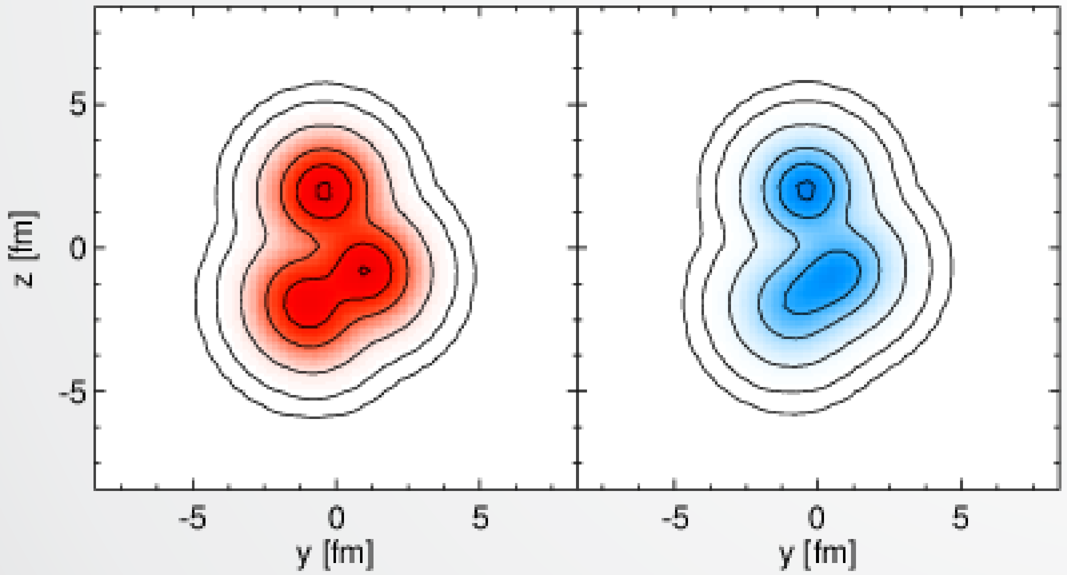
first 1/2+



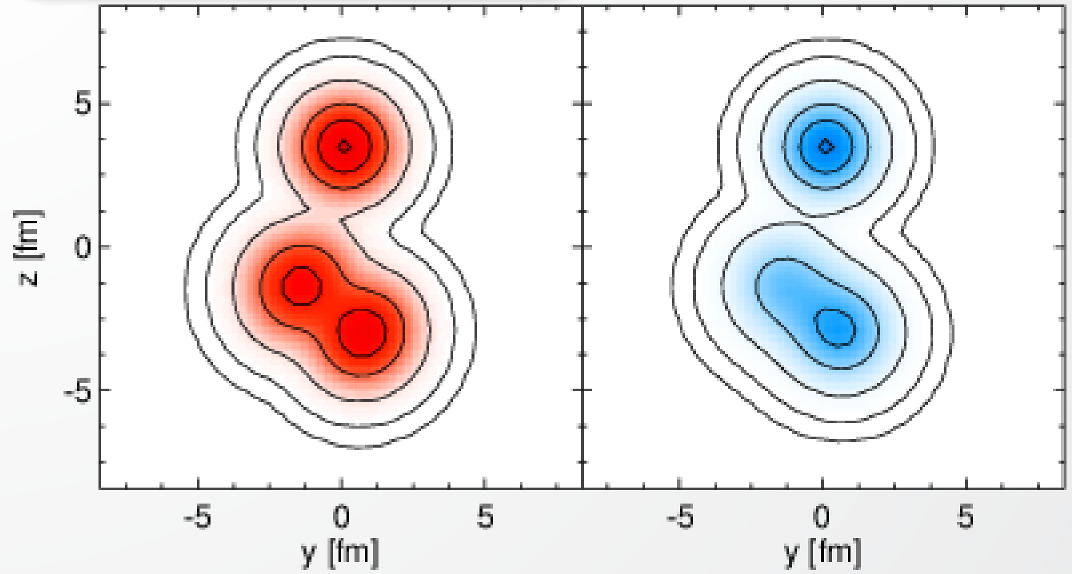
third 3/2-



first 5/2+

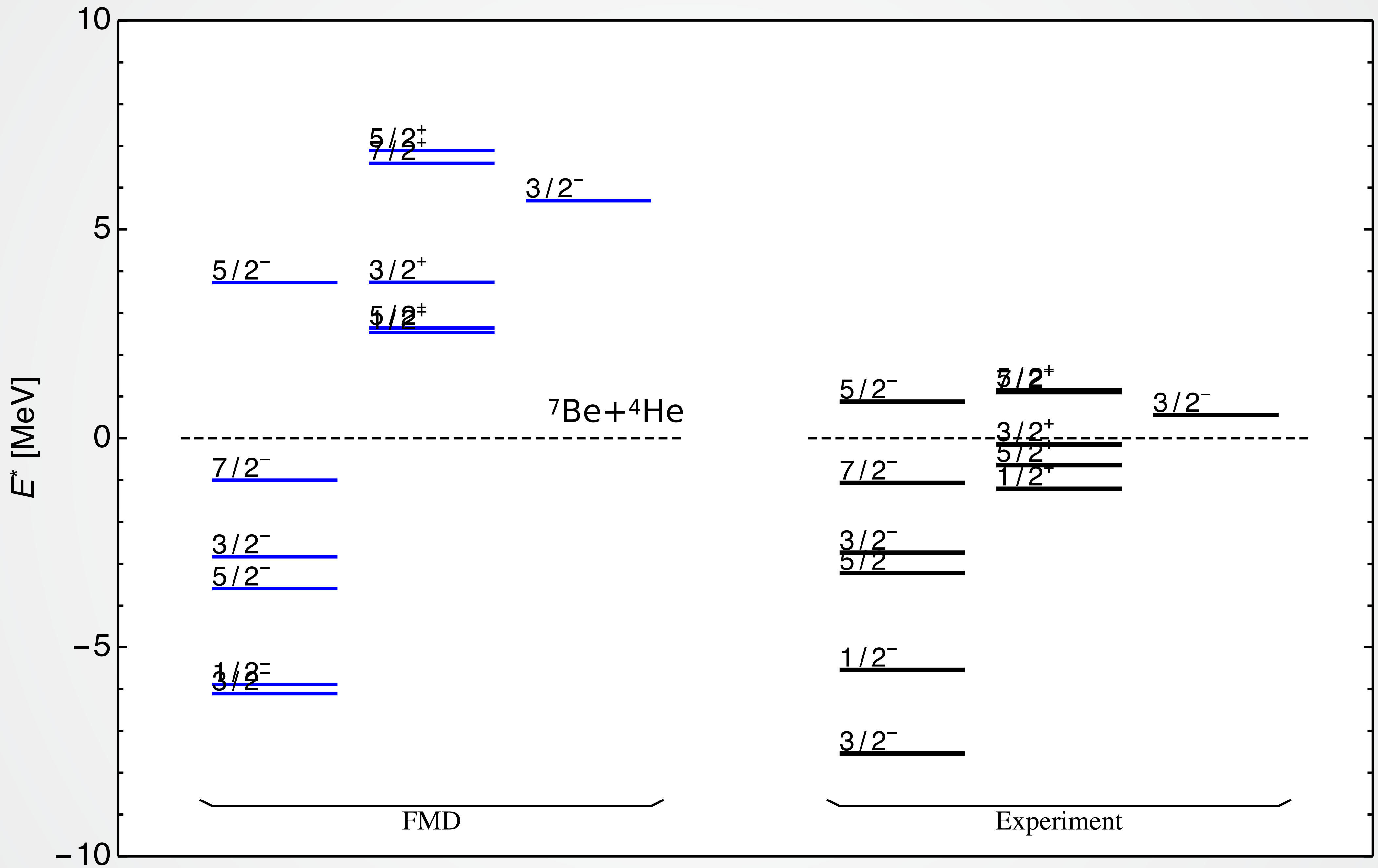


fourth 3/2-



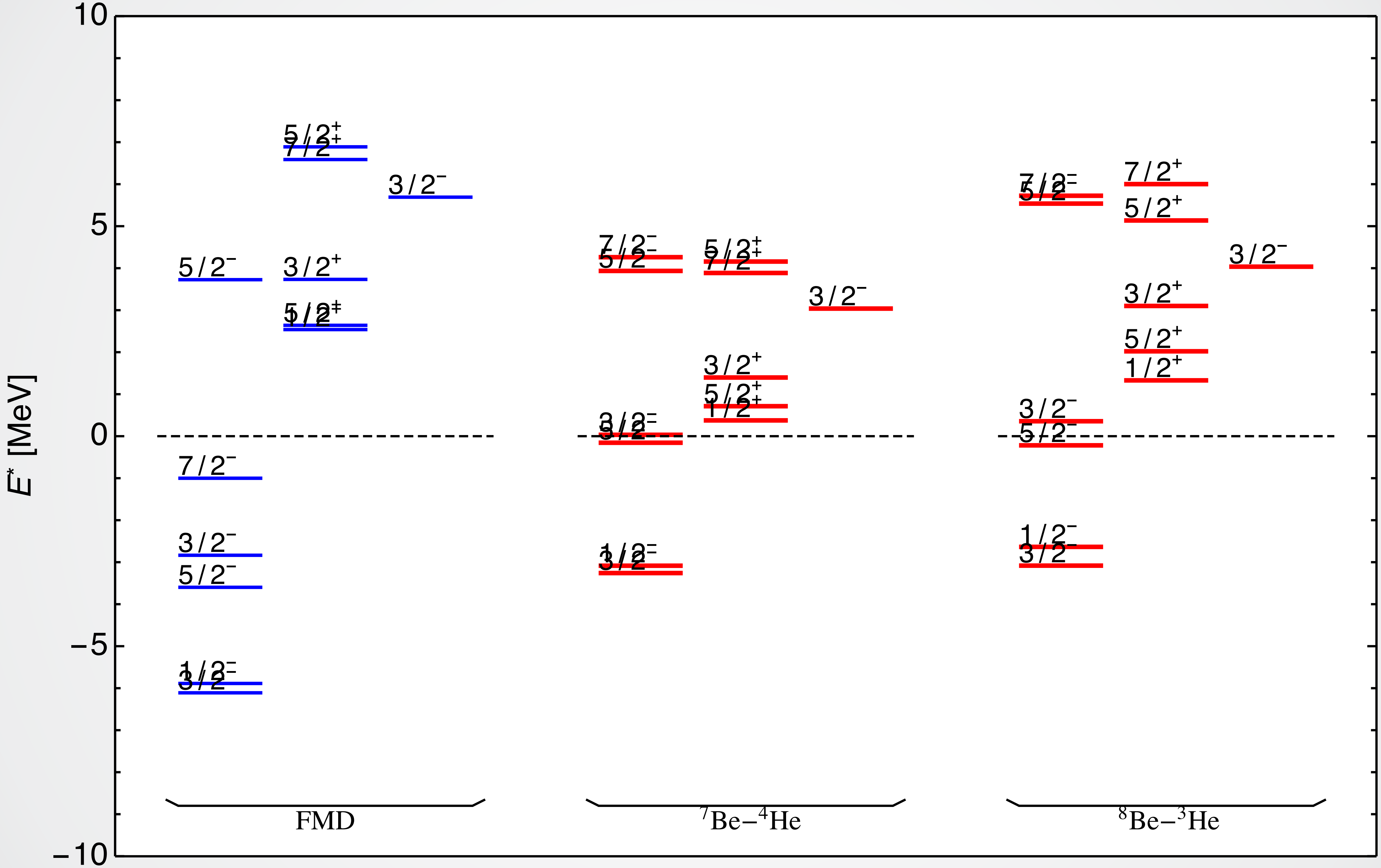
states with well defined cluster structure

^{11}C: Diagonalization with FMD VAP States



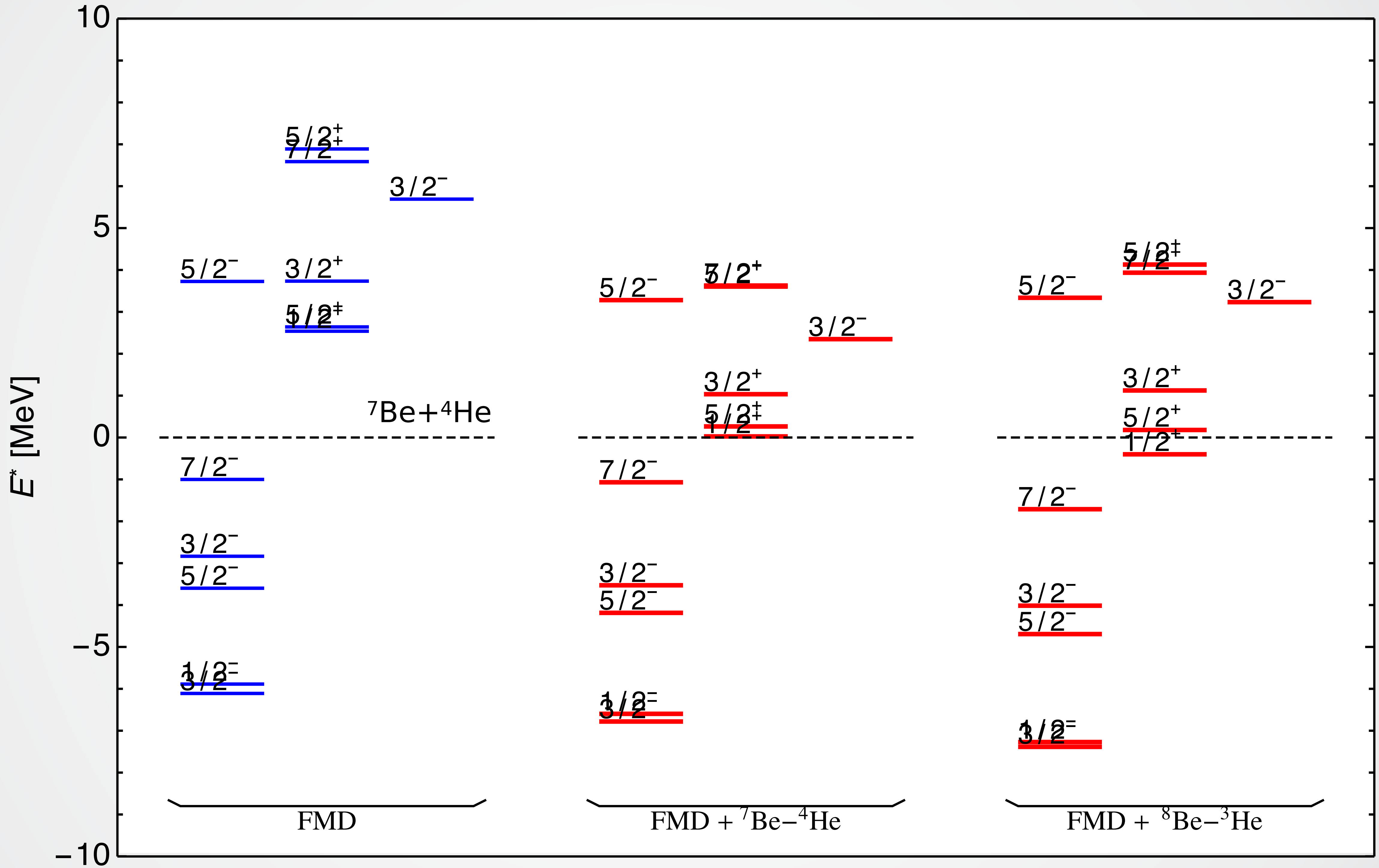
clustered states too high in energy

^{11}C: FMD vs Cluster Configurations



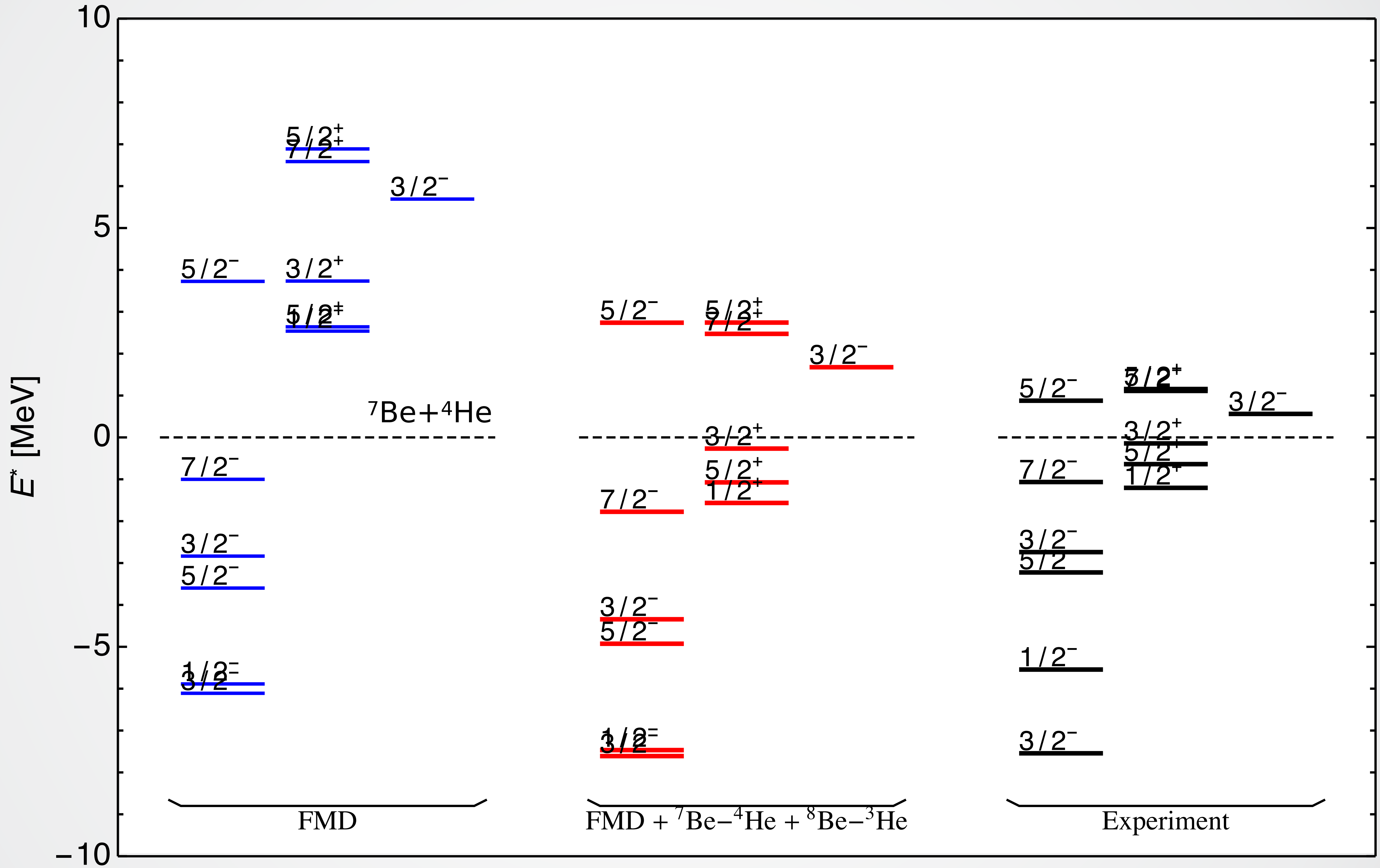
worse for p-shell states, better for clustered states

^{11}C: FMD plus Cluster Configurations



improves both p-shell and clustered states

^{11}C: Full Calculation



consistent picture of p-shell and clustered states

^{11}C: Cluster Ovlaps

	$^{7}Be(3/2^{-})$-^{4}He	$^{7}Be(3/2^{-},1/2^{-})$-^{4}He	$^{8}Be(0^{+})$-^{3}He	$^{8}Be(0^{+},2^{+})$-^{3}He
$3/2^{-}$	0.83	0.85	0.62	0.82
$1/2^{-}$	0.86	0.88	0.62	0.79
$5/2^{-}$	0.81	0.82	0.01	0.78
second $3/2^{-}$	0.76	0.86	0.14	0.82
third $3/2^{-}$	0.76	0.80	0.11	0.37
$1/2^{+}$	0.72	0.86	0.56	0.77
$5/2^{+}$	0.88	0.90	0.54	0.77

- Be careful with interpretation — because of antisymmetrization a large overlap with cluster configurations does not necessarily mean that the state is well clustered
- More interesting than these spectroscopic factors would be spectroscopic amplitudes / ANCs / alpha-widths — work in progress
- Calculate alpha-capture rate $^{7}Be(\alpha,\gamma)^{11}C$

Summary

Summary

- FMD with Gaussian wave-packets allows microscopic description of clustering
- Variation after angular momentum and parity projection is essential to get good basis states
- Explicit cluster configurations are needed to describe the asymptotic behavior of wave functions
- Cluster configurations like ^{8}Be-^{4}He, ^{7}Be-^{4}He or ^{8}Be-^{3}He require double-projection
- Match to Coulomb asymptotics for scattering and resonance properties
- Extension to reactions straightforward

- Hoyle state in ^{12}C has no well defined intrinsic state — superposition of many triangular three-alpha configurations — large overlap with ^{8}Be(0^{+})+^{4}He cluster configurations
- The third 3/2^{-} state in ^{11}C above the alpha-threshold has a ^{7}Be(3/2^{-})+^{4}He structure similar to the Hoyle state with its ^{8}Be+^{4}He structure
- The positive parity states in ^{11}C also show pronounced clustering