The role of clustering in structure and reactions of light nuclei

Thomas Neff
GSI Helmholtzzentrum für Schwerionenforschung, Darmstadt

Workshop on
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Nuclear structure and decay, heavy-ion collisions, and astrophysics ”
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GSI theory

HELMHOLTZ GEMEINSCHAFT

Our Aim:

Solve the
nuclear many-body problem for exotic nuclei
with (realistic) NN interaction

Many-Body Method

Fermonic Molecular Dynamics
(FMD)

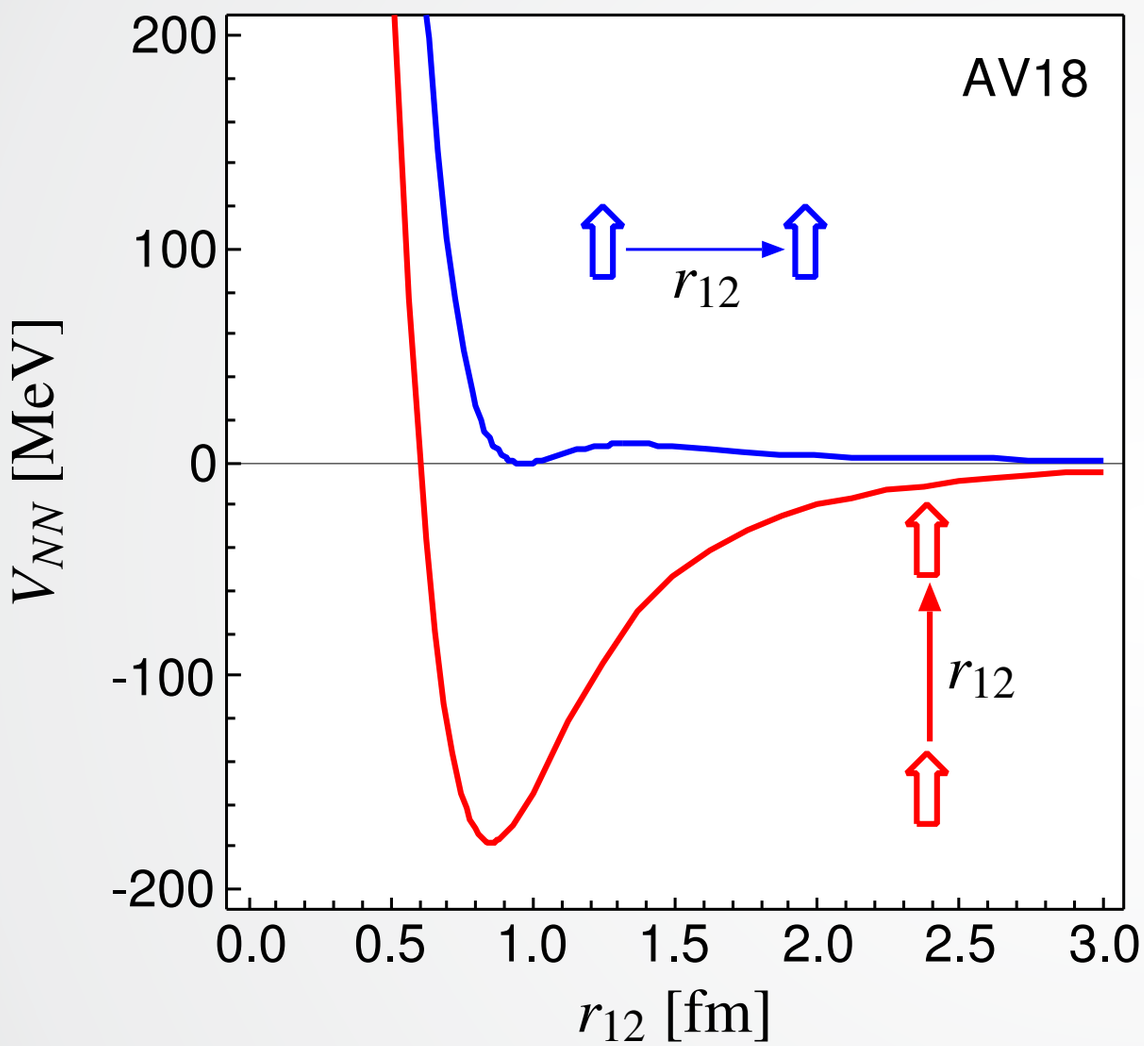
↔

Realistic Effective Interaction

Unitary Correlation Operator Method
(UCOM)

Nucleon-Nucleon Interaction

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

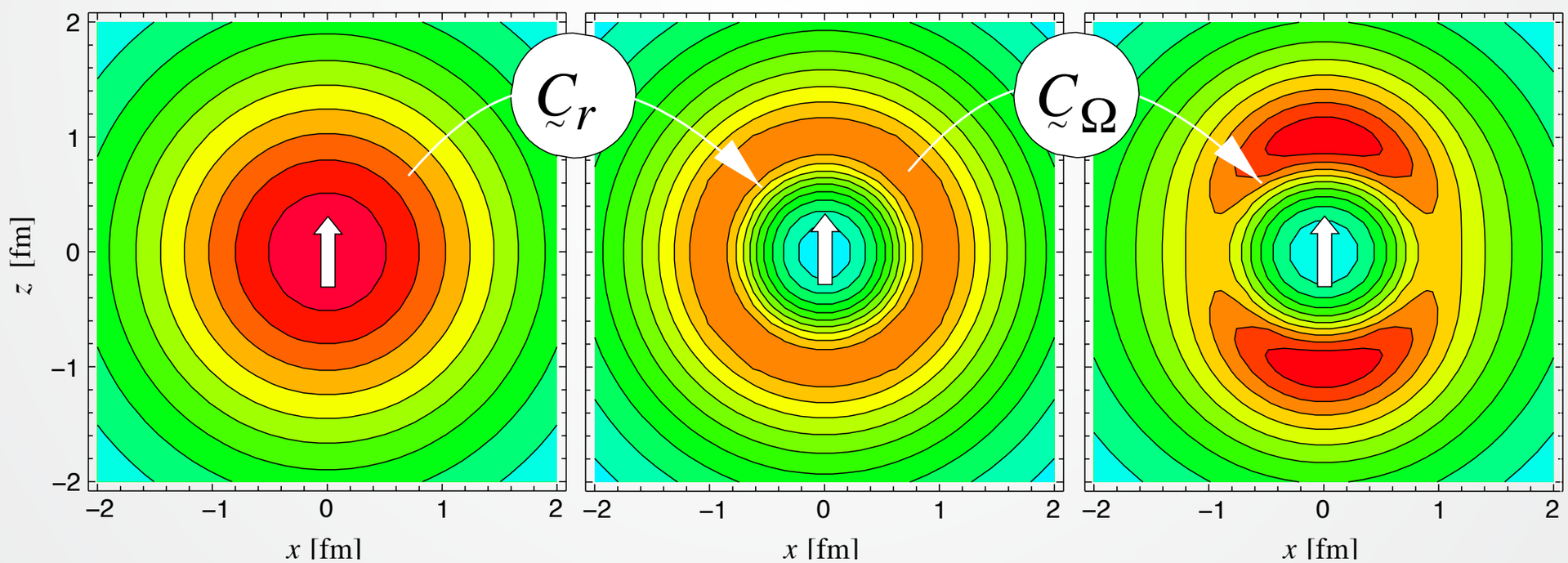
Correlation Operator

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

Correlated Hamiltonian

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

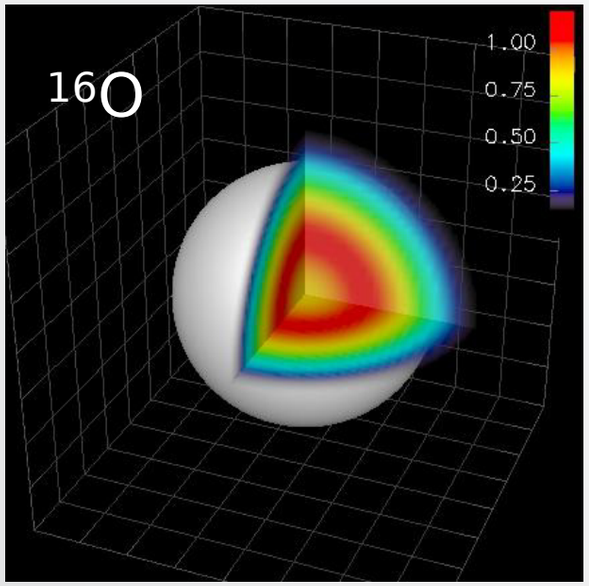
Central correlator shifts nucleons apart,
Tensor correlator aligns nucleons with spin

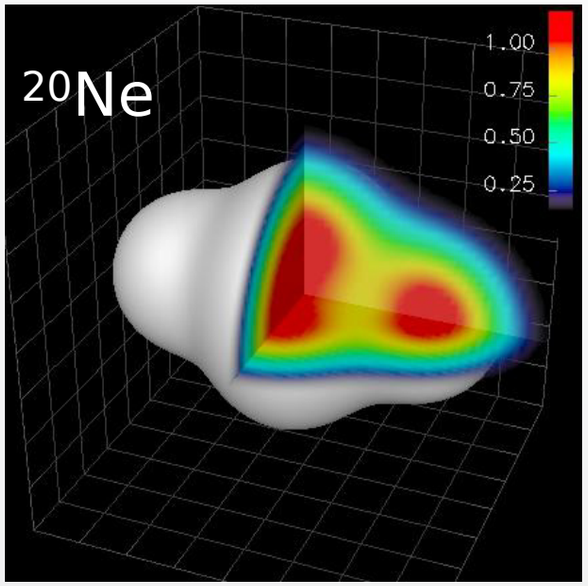


- realistic two-body spin-orbit force is too weak, use phenomenogical correction for heavier nuclei in the *p*-shell

Fermionic Molecular Dynamics

Nuclear structure calculations with a Gaussian wave-packet basis





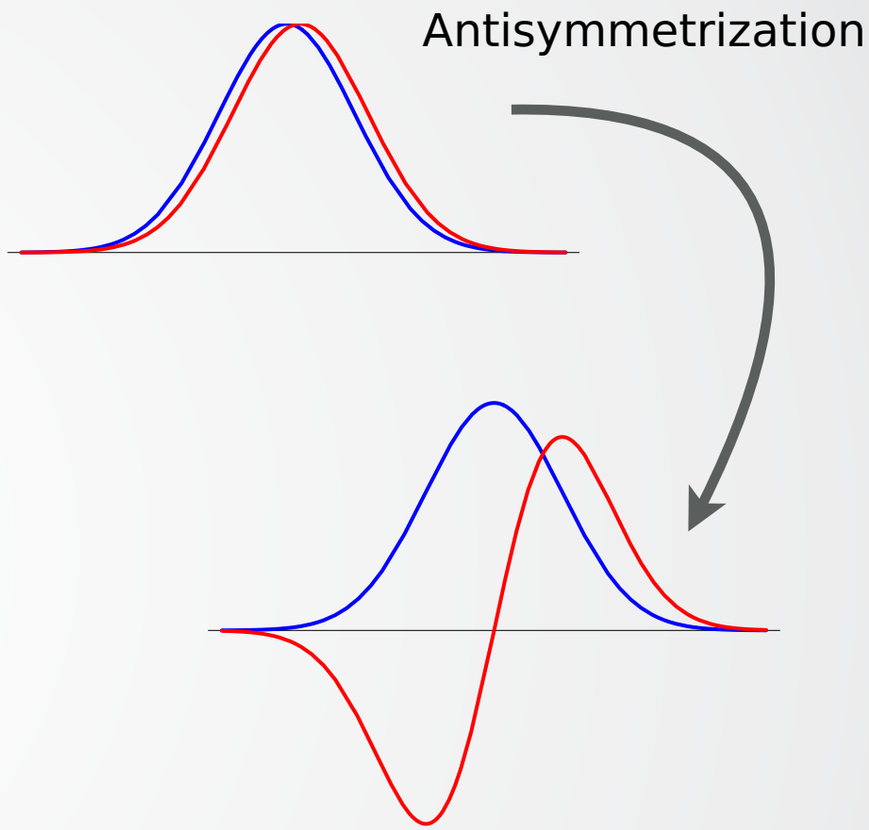
Fermionic Molecular Dynamics

Fermionic

Intrinsic many-body states

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

are antisymmetrized A-body states



Molecular

Single-particle states

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

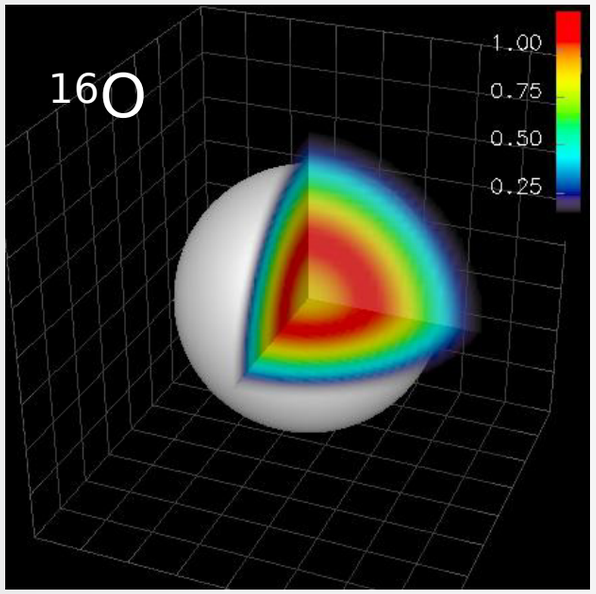
- Gaussian wave-packets in phase-space (complex parameter $\mathbf{b}_i$ encodes mean position and mean momentum), spin is free, isospin is fixed
- width a_i is an independent variational parameter for each wave packet
- use one or two wave packets for each single particle state

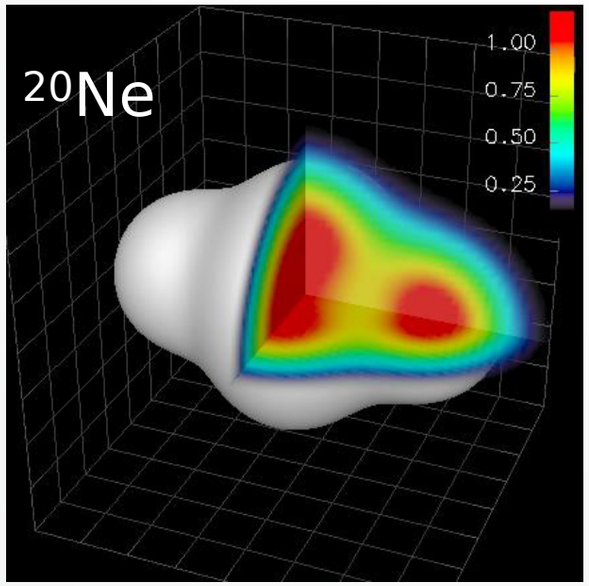
FMD basis contains **harmonic oscillator shell model** and **Brink-type cluster** configurations as limiting cases

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**





Generator coordinates

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

Variation

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

Projection

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

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

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

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

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

^{8}Be: GCM/RGM and Antisymmetrization

- Describe ^{8}Be by superposition of ^{4}He clusters at distances R_i

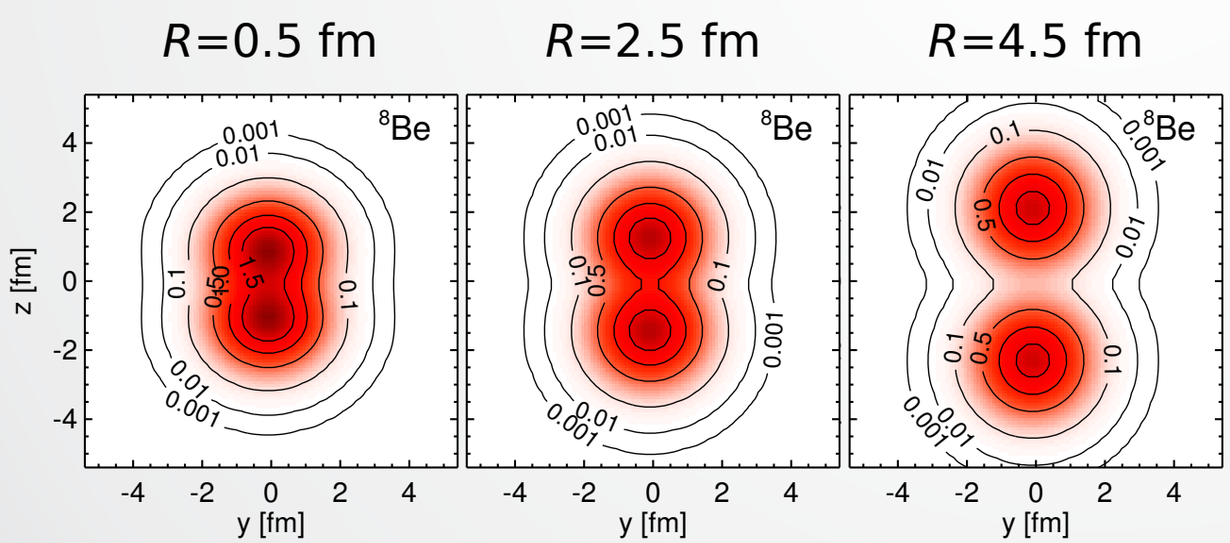
$$\left|\Psi_{\mathrm{GCM}}\right\rangle = \sum_i c_i \hat{\mathcal{A}}\left\{\left|\Psi_\alpha(-\mathbf{R}_i/2)\right\rangle \otimes \left|\Psi_\alpha(+\mathbf{R}_i/2)\right\rangle\right\}$$

- This can be rewritten using intrinsic ^{4}He wavefunctions and the relative motion given by a RGM wavefunction

$$\left\langle \boldsymbol{\rho}, \xi_a, \xi_b, \mathbf{X}\middle|\Psi_{\mathrm{GCM}}\right\rangle = \int d^3r\, \Phi_{\mathrm{GCM}}(\mathbf{r})\, \hat{\mathcal{A}}\left\{\delta(\boldsymbol{\rho}-\mathbf{r})\Phi_\alpha(\xi_a)\Phi_\alpha(\xi_b)\right\} \Psi_{\mathrm{cm}}(\mathbf{X})$$

with

$$\Phi_{\mathrm{GCM}}(\mathbf{r}) = \sum_i c_i \left(\frac{\mu_A}{\pi a}\right)^{3/4} \exp\left\{-\mu_A \frac{(\mathbf{r}-\mathbf{R}_i)^2}{2a}\right\}$$



compare with **THSR** wavefunction

$$\Phi_{\mathrm{THSR}}(\mathbf{r}) = \exp\left\{-\frac{r_x^2+r_y^2}{b^2+\beta_x{}^2} - \frac{r_z^2}{b^2+\beta_z{}^2}\right\}$$

^{8}Be: From RGM to α-α Wavefunction

- RGM basis states

$$\left\langle \boldsymbol{\rho}, \xi_a, \xi_b \middle| \Phi_{\alpha\alpha}(\mathbf{r}) \right\rangle = \hat{\mathcal{A}} \left\{ \delta(\boldsymbol{\rho} - \mathbf{r}) \Phi_\alpha(\xi_a) \Phi_\alpha(\xi_b) \right\}$$

- RGM norm kernel

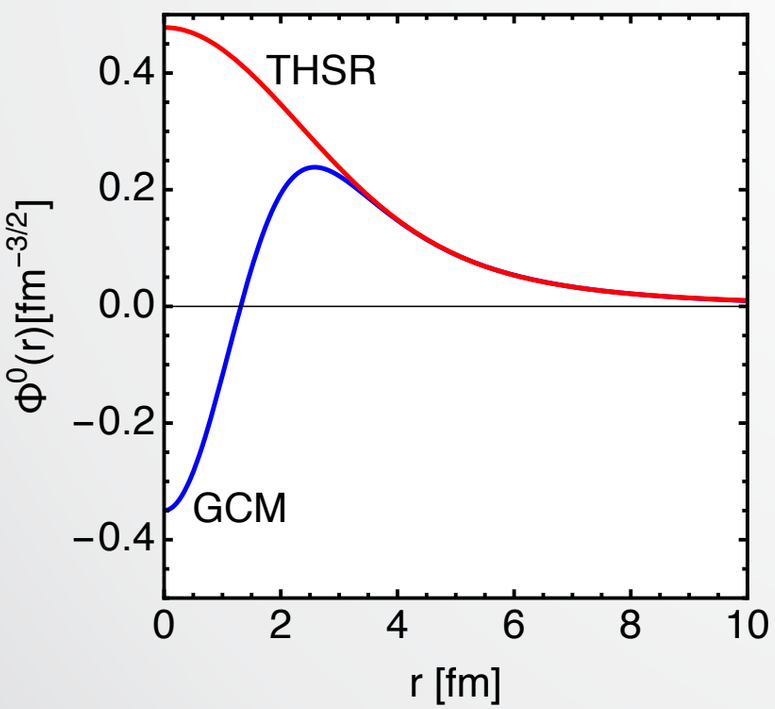
$$N(\mathbf{r}, \mathbf{r}') = \left\langle \Phi_{\alpha\alpha}(\mathbf{r}) \middle| \Phi_{\alpha\alpha}(\mathbf{r}') \right\rangle$$

- Wavefunction for relative motion of two point-like α's

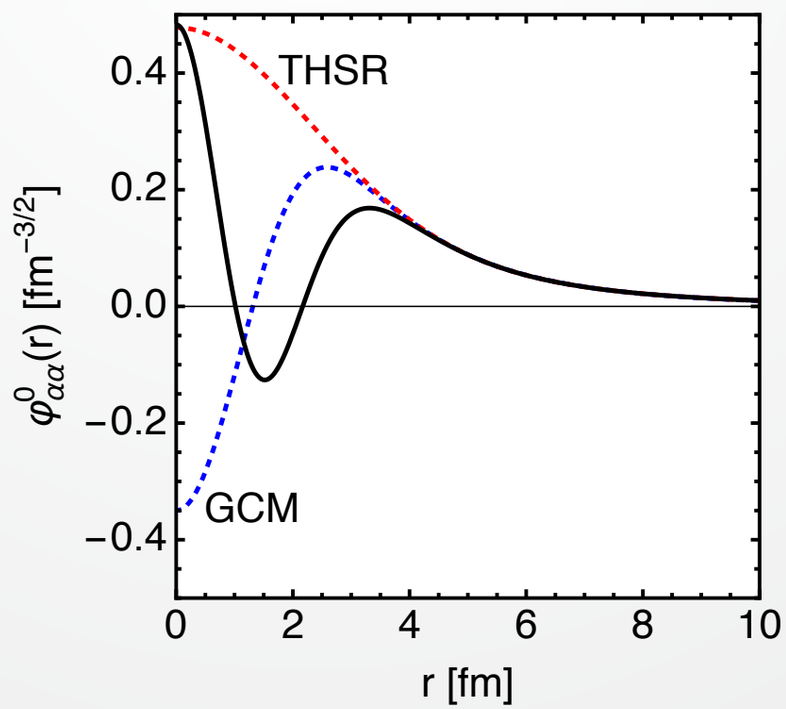
$$\phi_{\alpha\alpha}(\mathbf{r}) = \int d^3r' \, N^{-1/2}(\mathbf{r}, \mathbf{r}') \, \Phi_{GCM/THSR}(\mathbf{r}')$$

α-α wavefunction
up to 4 fm governed by
antisymmetrization

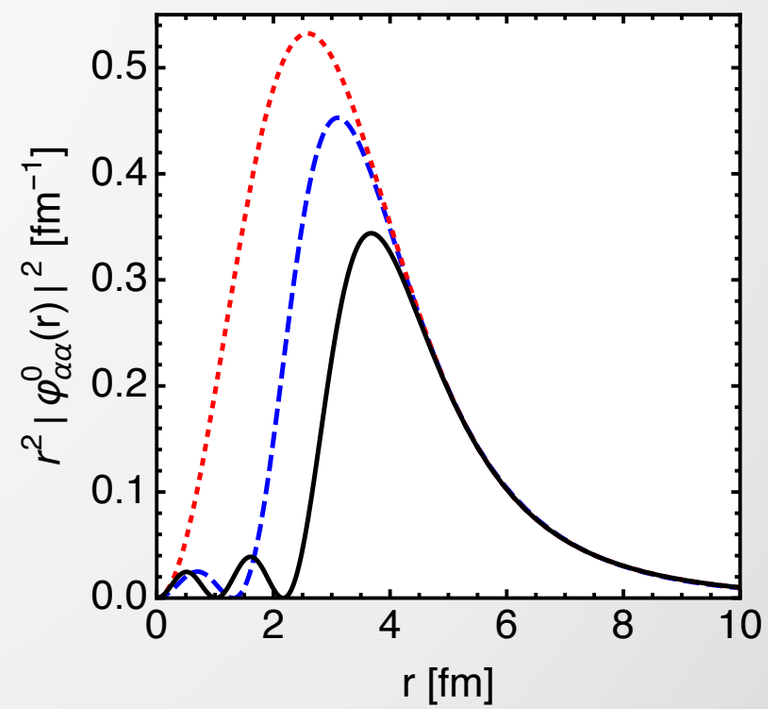
RGM wavefunction



α-α wavefunction



α-α density



$^3He(\alpha,\gamma)^7Be$ and $^3H(\alpha,\gamma)^7Li$

Radiative Capture

PRL **106,** 042502 (2011) PHYSICAL REVIEW LETTERS week ending 28 JANUARY 2011

Microscopic Calculation of the $^3He(\alpha, \gamma)^7Be$ and $^3H(\alpha, \gamma)^7Li$ Capture Cross Sections Using Realistic Interactions

Thomas Neff*

GSI Helmholtzzentrum für Schwerionenforschung GmbH, Planckstraße 1, 64291 Darmstadt, Germany

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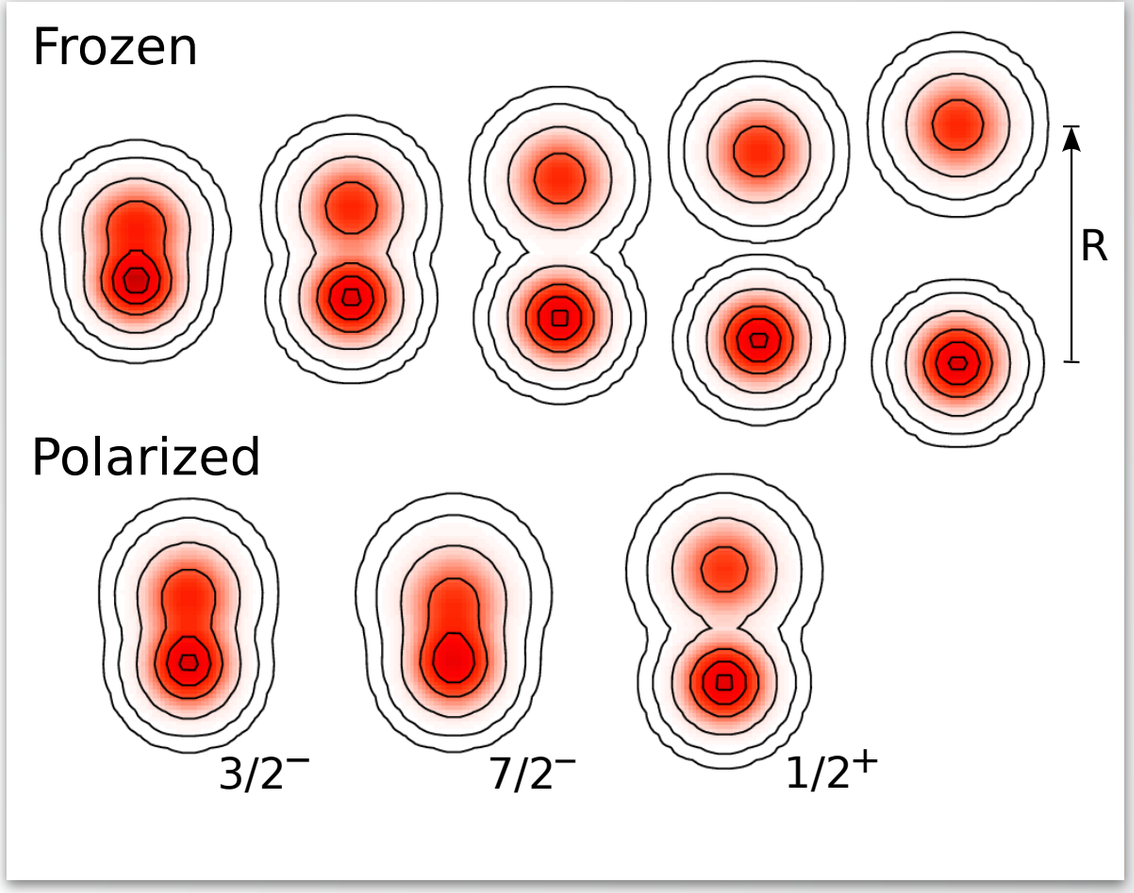
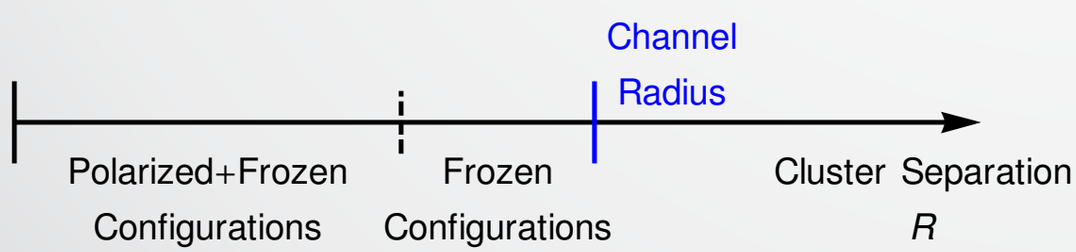
FMD Basis States

- FMD wave functions use **Gaussian wave packets** as single-particle basis states
- Many-body basis states are Slater determinants projected on parity, angular momentum and total linear momentum
- FMD basis contains both harmonic oscillator and Brink-type cluster wave functions as special cases

- a realistic low-momentum interaction is obtained from the Argonne v_{18} interaction by the Unitary Correlation Operator Method in two-body approximation



- **Polarized** configurations are obtained by **variation after projection** for all spins and parities
- **Frozen** configurations are generated from ^{4}He and ^{3}He ground states
- at the channel radius many-body wave functions are matched to Whittaker and Coulomb solutions for point-like clusters with the ***R*-matrix** method



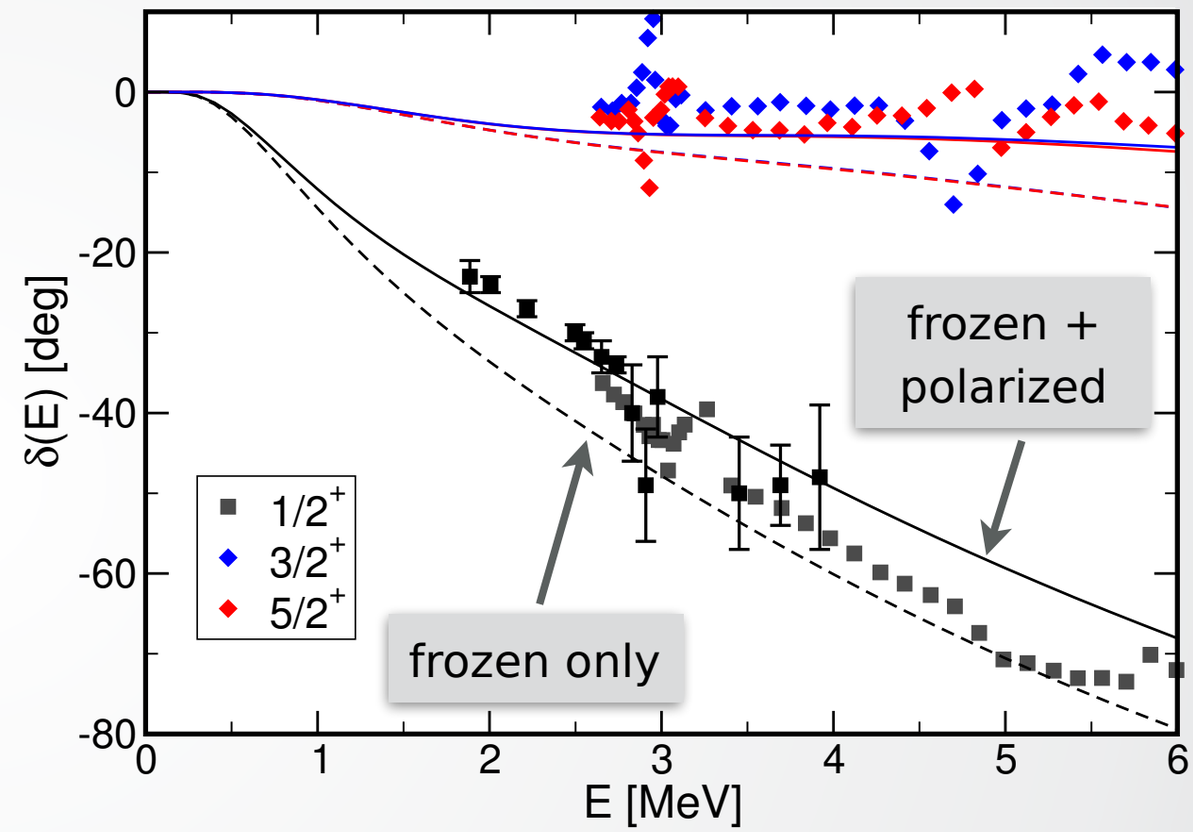
Bound and Scattering States

Bound States

		FMD	Experiment
^{7}Be	$E_{3/2^-}$ [MeV]	-1.49	-1.59
	$E_{1/2^-}$ [MeV]	-1.31	-1.15
	r_{ch} [fm]	2.67	2.647(17)
	Q [e fm^2]	-6.83	-
^{7}Li	$E_{3/2^-}$ [MeV]	-2.39	-2.467
	$E_{1/2^-}$ [MeV]	-2.17	-1.989
	r_{ch} [fm]	2.46	2.444(43)
	Q [e fm^2]	-3.91	-4.00(3)

- centroid energy of bound states well reproduced, splitting between $3/2^-$ and $1/2^-$ states too small
- charge radii and quadrupole moment test the tails of bound state wave functions

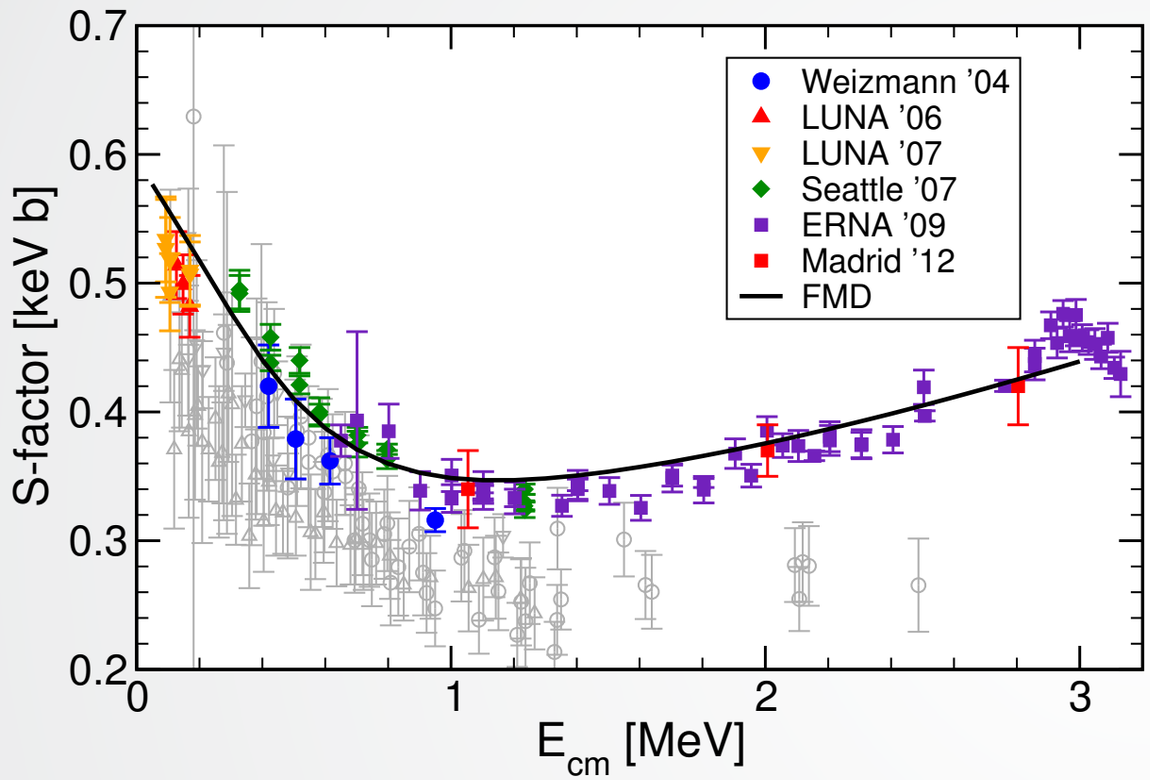
Scattering States



- *s*- and *d*-wave capture dominate at small energies
- polarized configurations are important for describing the phase shifts

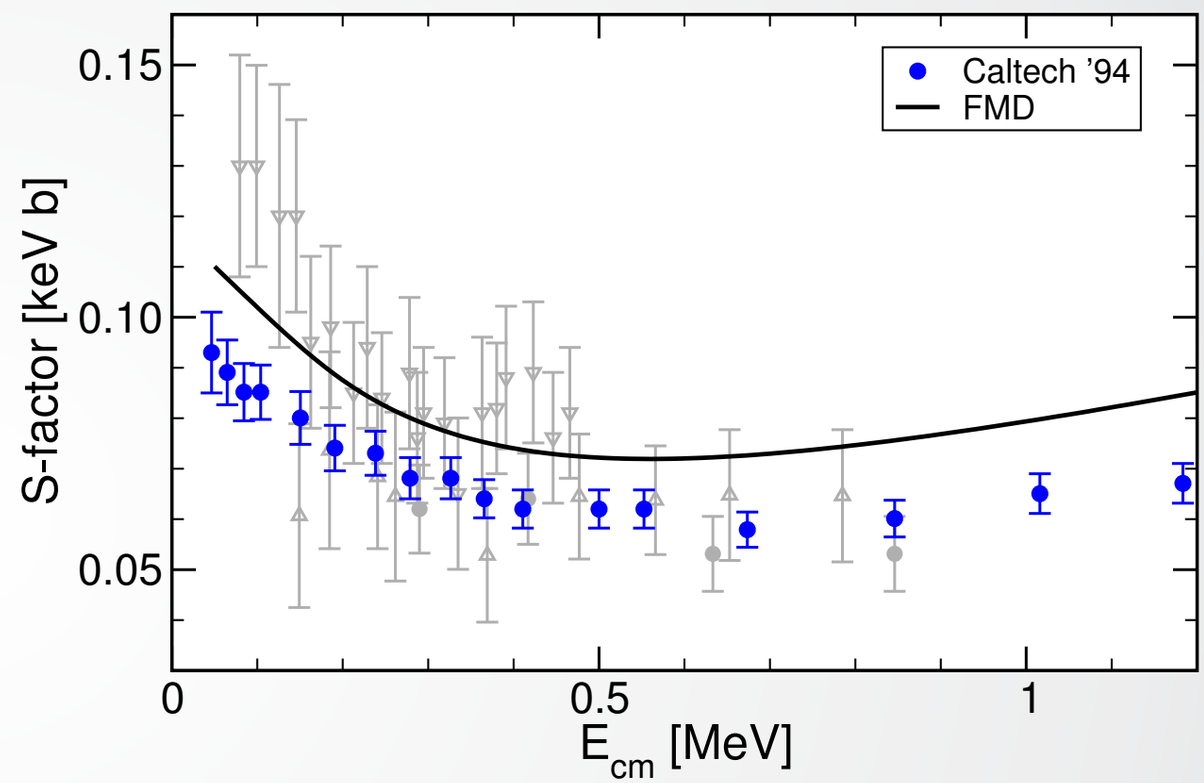
Capture Cross Section

$^3He(\alpha,\gamma)^7Be$



- good agreement with new high quality $^3He(\alpha,\gamma)^7Be$ data regarding both energy dependence and normalization

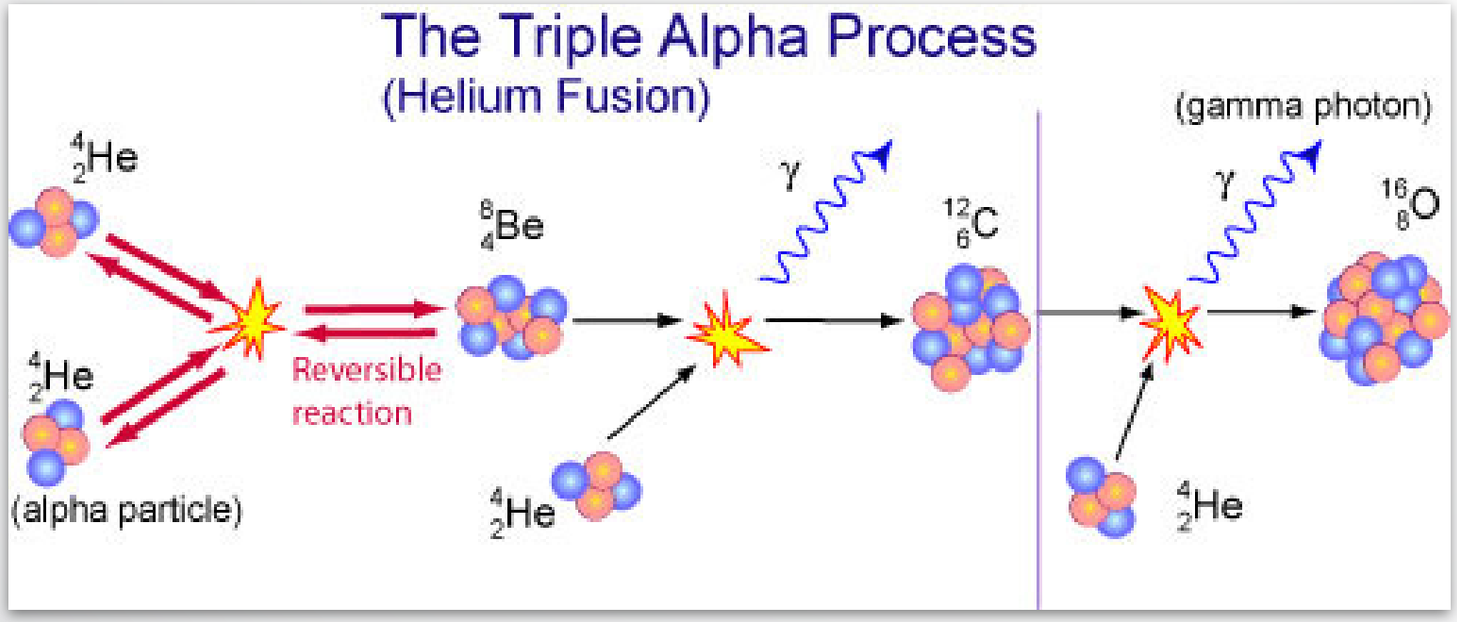
$^3H(\alpha,\gamma)^7Li$

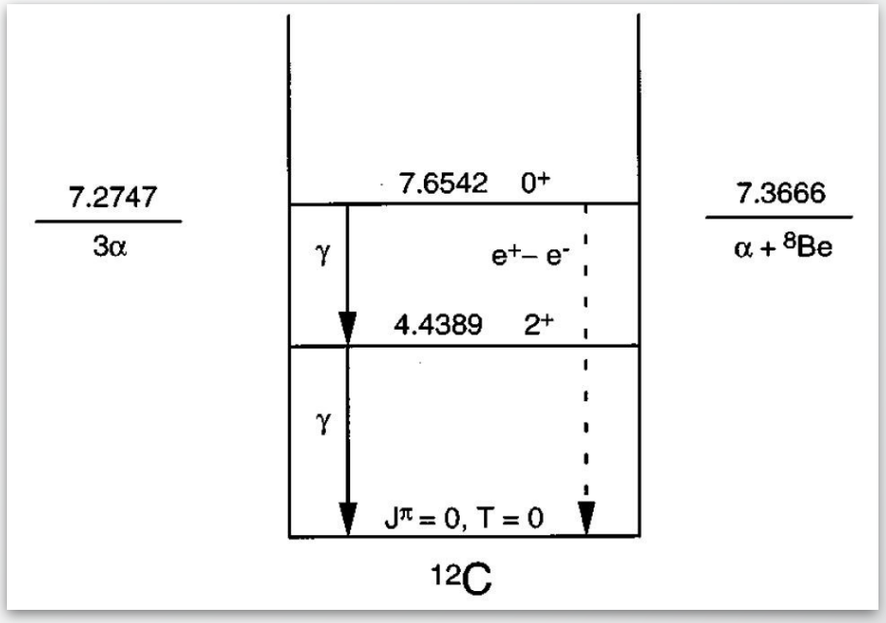


- calculations reproduce energy dependence but not normalization of $^3H(\alpha,\gamma)^7Li$ data by Brune *et al.*

Cluster States in ^{12}C

FMD and Cluster Model Calculations



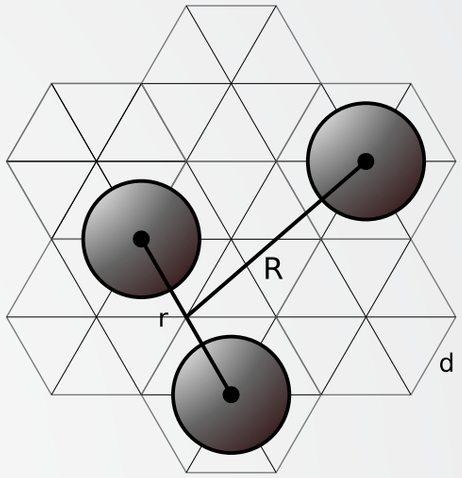


^{12}C: Microscopic α-Cluster Model

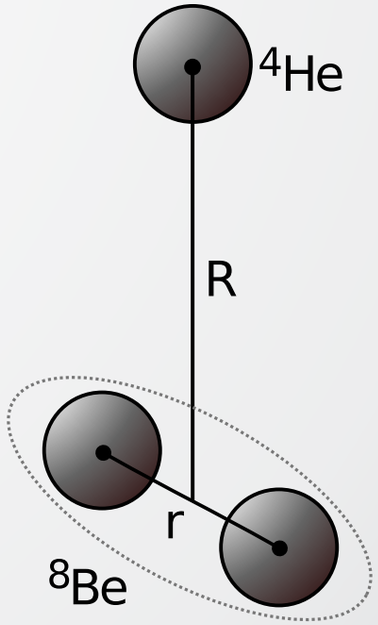
- ^{12}C is described as a system of three α-particles
- α-particles are given by HO $(0s)^4$ wave functions
- wave function is fully antisymmetrized
- effective Volkov nucleon-nucleon interaction adjusted to reproduce α-α and ^{12}C ground state properties

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

Internal Region



External Region



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

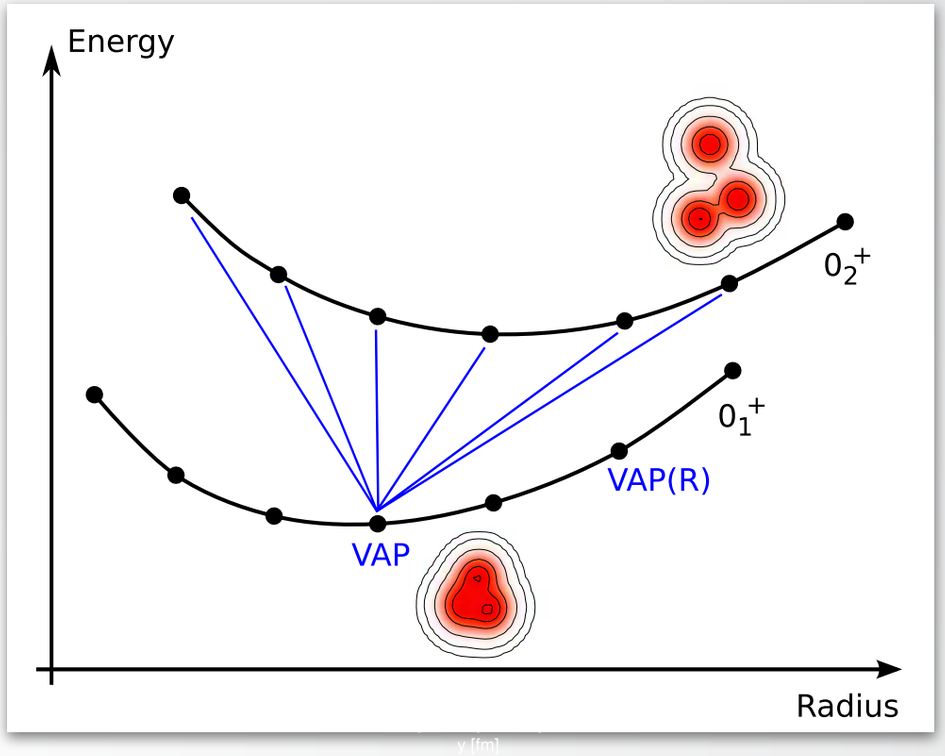
Double Projection

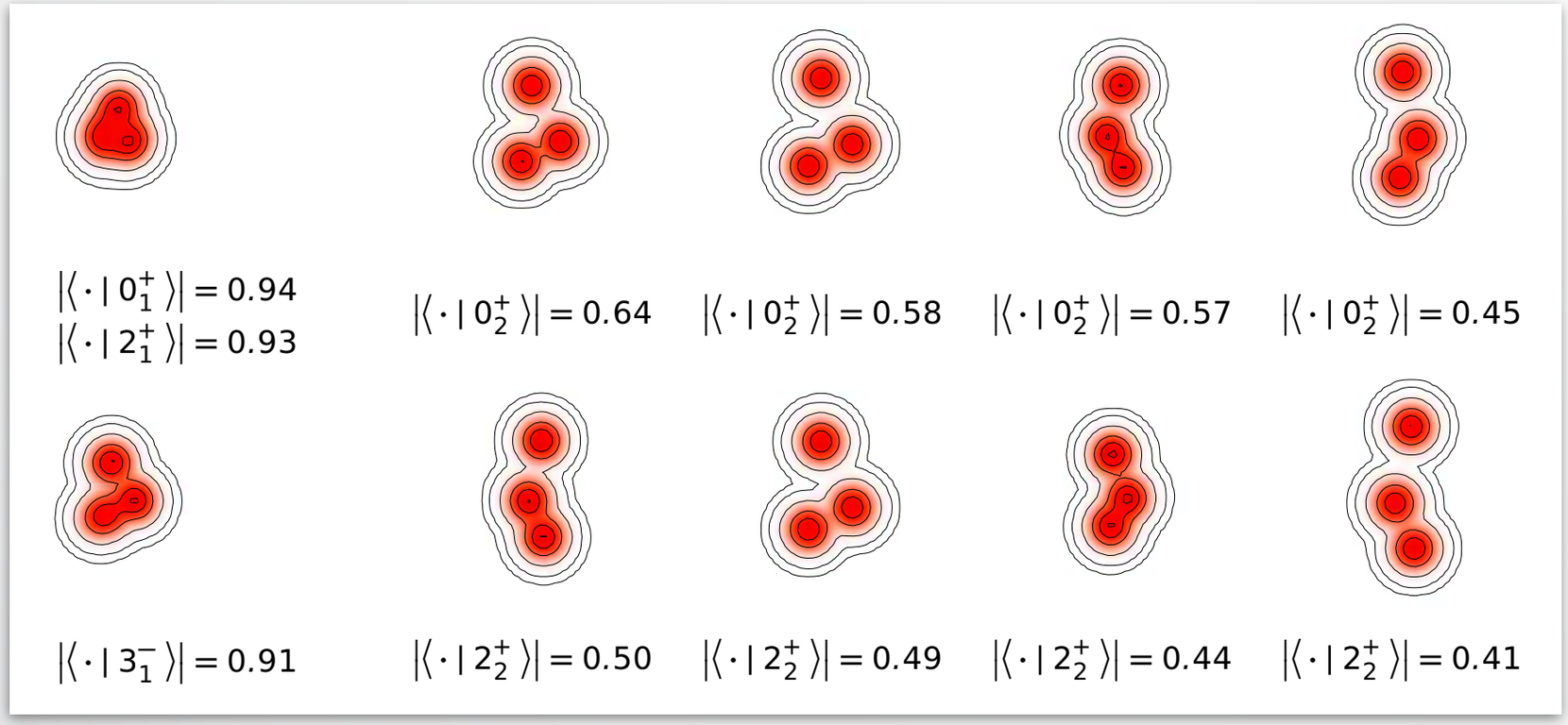
$$\left|\Psi^{^8\mathrm{Be}}_{IK}\right\rangle = \sum_i \hat{P}^{I}_{K0}\hat{\mathcal{A}}\left\{\left|\Psi_\alpha(-\tfrac{r_i}{2}\mathbf{e}_z\right\rangle \otimes \left|\Psi_\alpha(+\tfrac{r_i}{2}\mathbf{e}_z\right\rangle\right\} c^I_i$$

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

^{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)

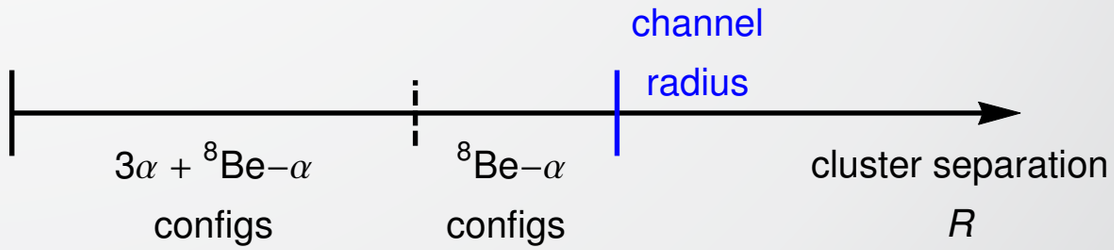
$$\psi_c(r) = A_c \frac{1}{r} W_{-\eta_c, L_c+1/2}(2\kappa_c r), \qquad \kappa_c = \sqrt{-2\mu(E-E_c)}$$

Resonances (purely outgoing Coulomb - complex energy)

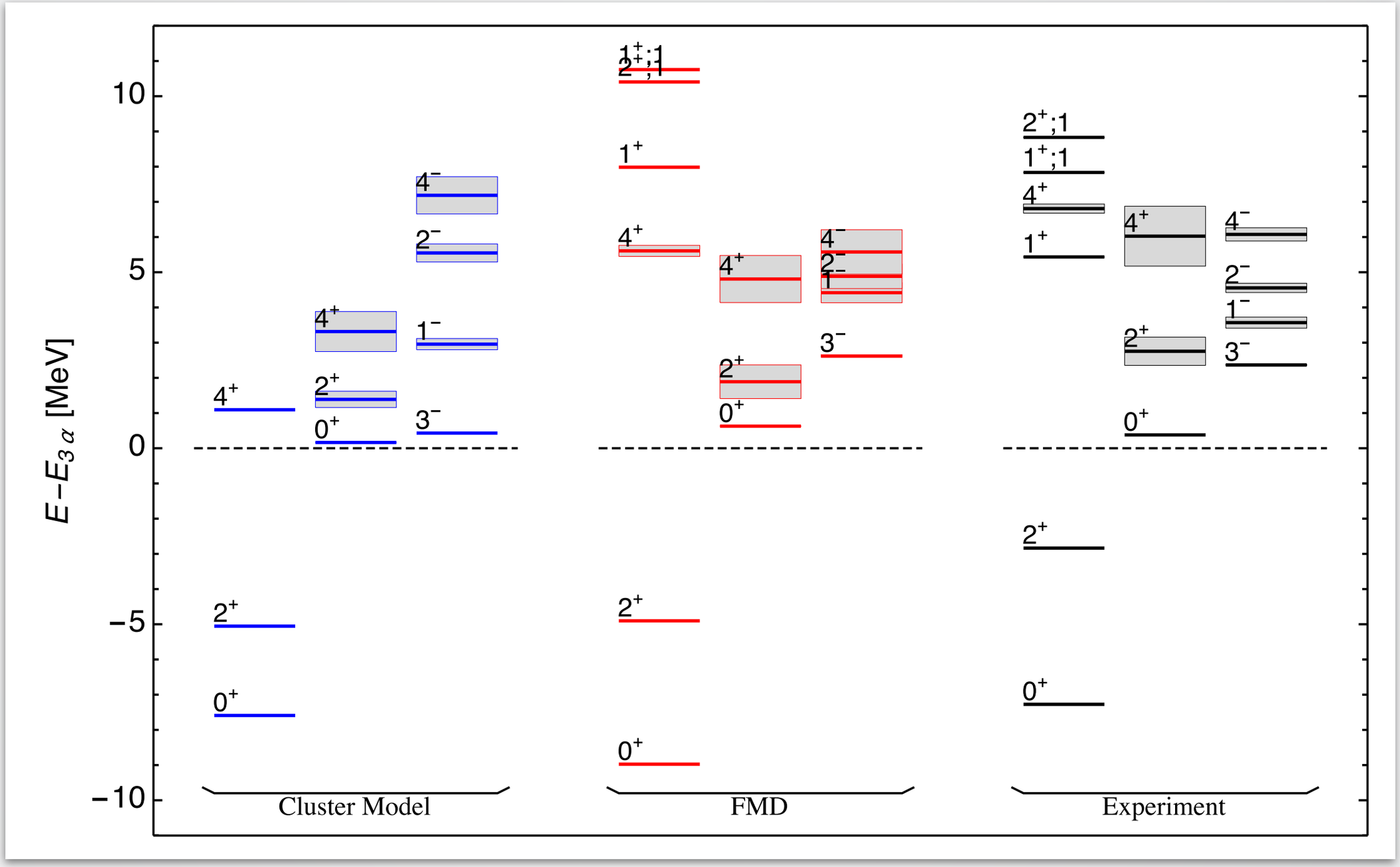
$$\psi_c(r) = A_c \frac{1}{r} O_{L_c}(\eta_c, k_c r), \qquad k_c = \sqrt{2\mu(E-E_c)}$$

Scattering States (incoming + outgoing Coulomb)

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



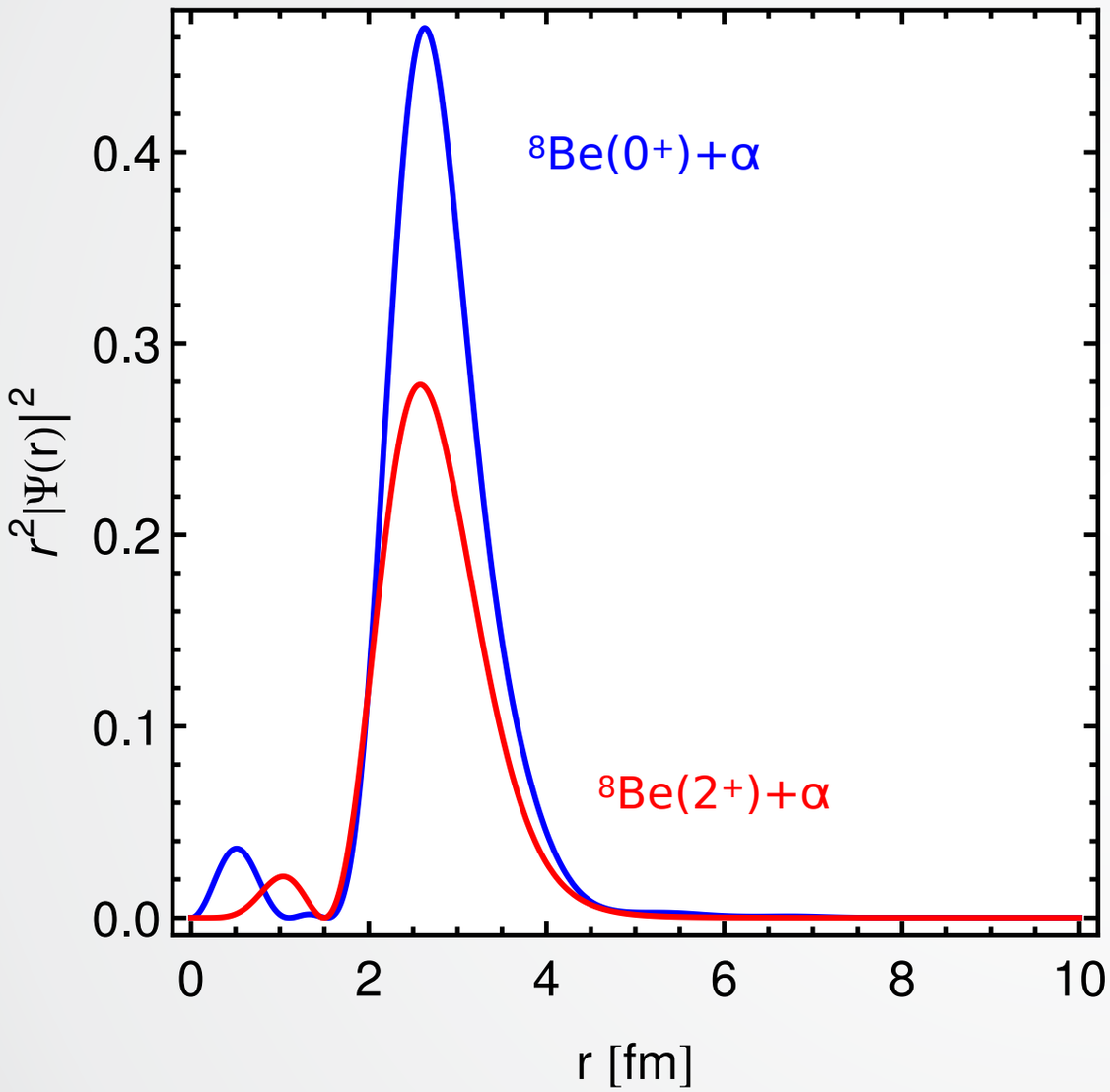
^{12}C: Spectrum including Continuum



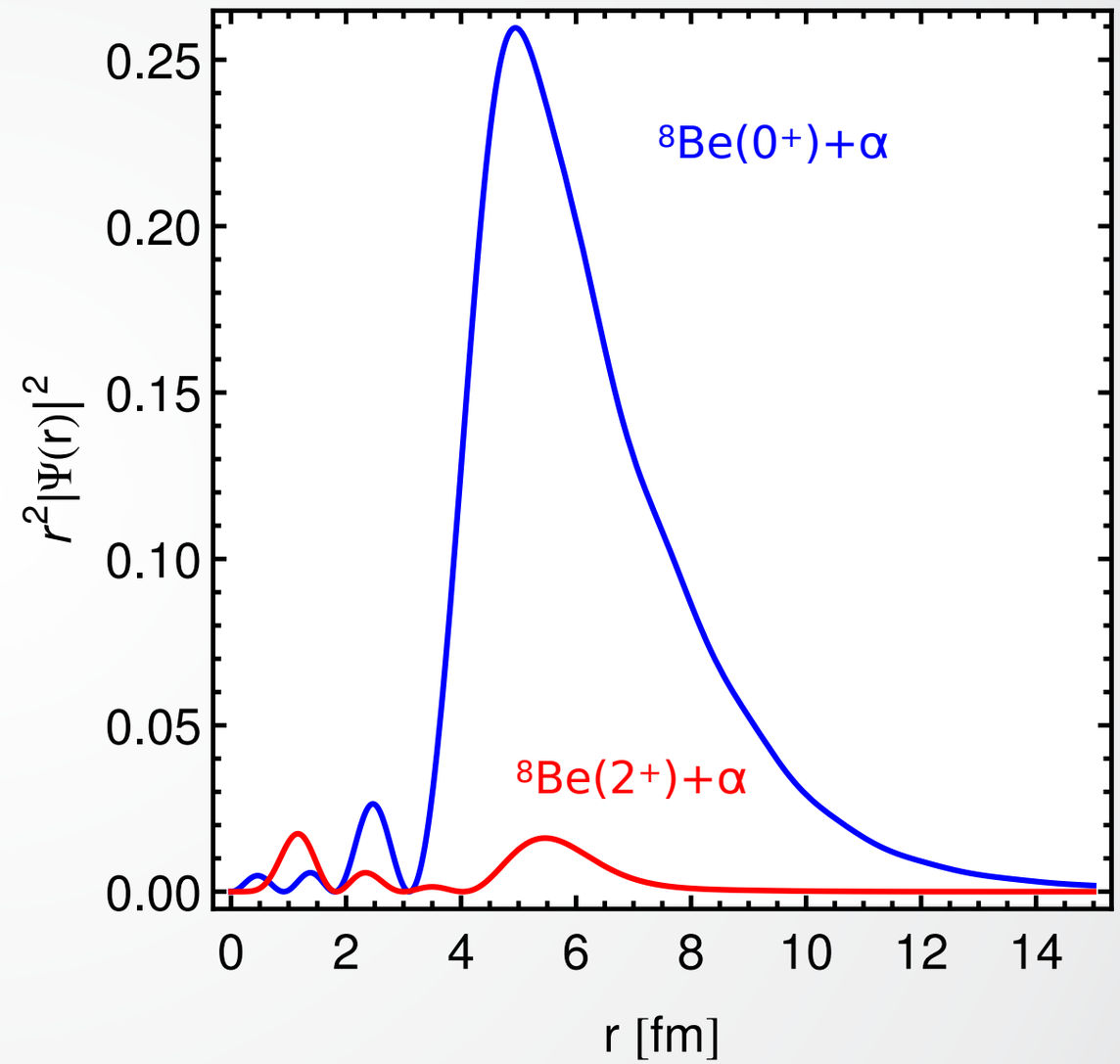
- FMD provides a consistent description of *p*-shell states, negative parity states and cluster states

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

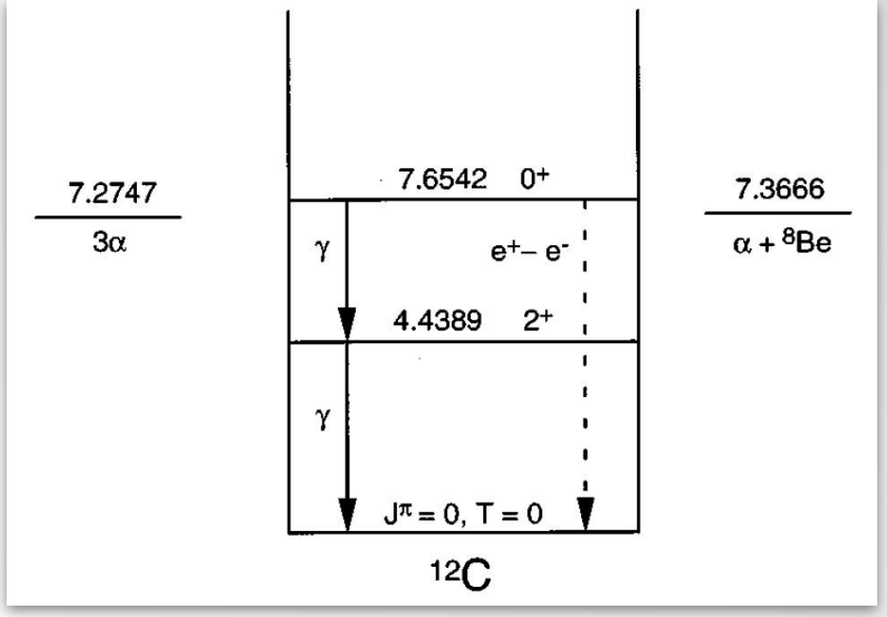
Ground State



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



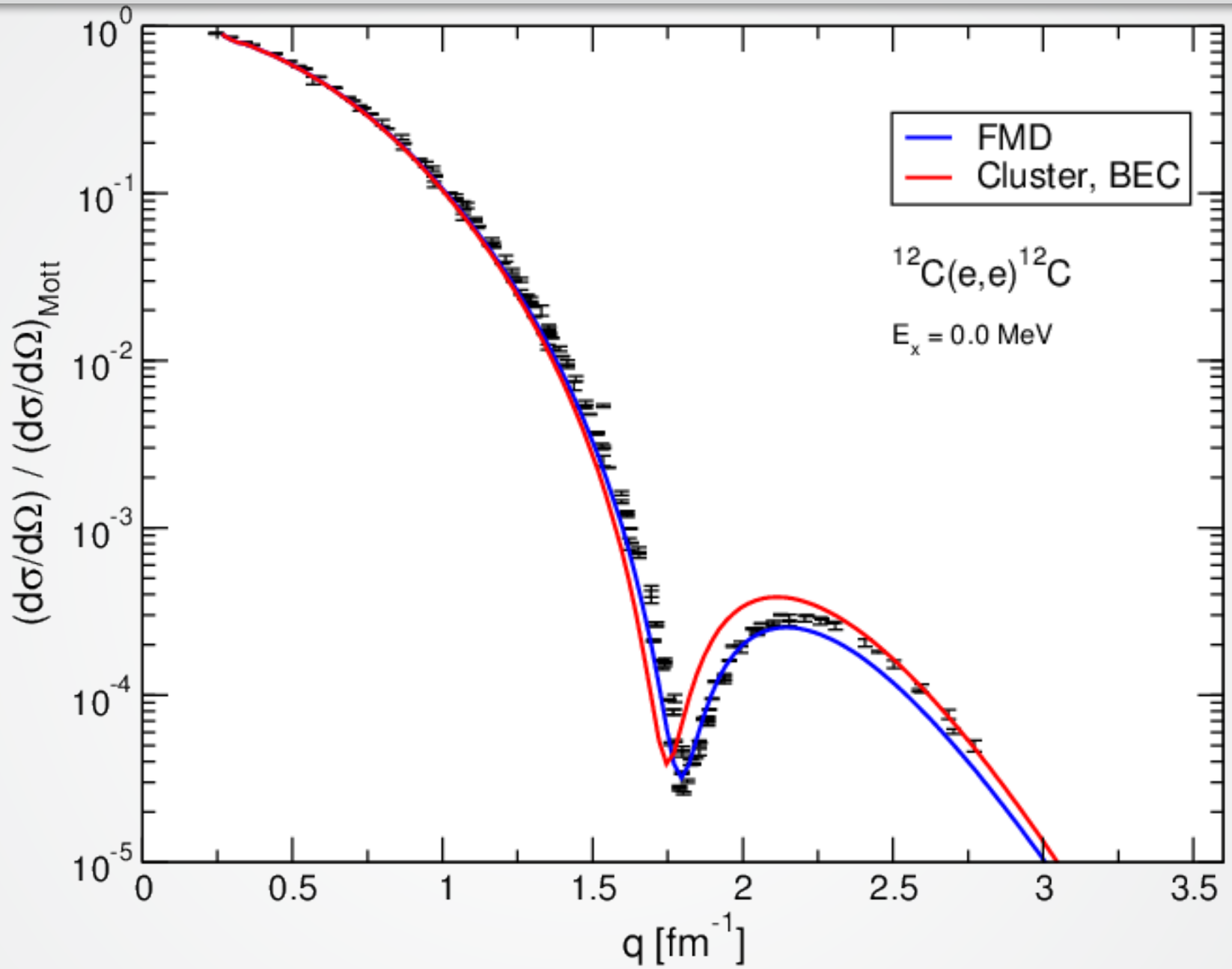
Electron scattering on ^{12}C

FMD and Cluster Model Calculations

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

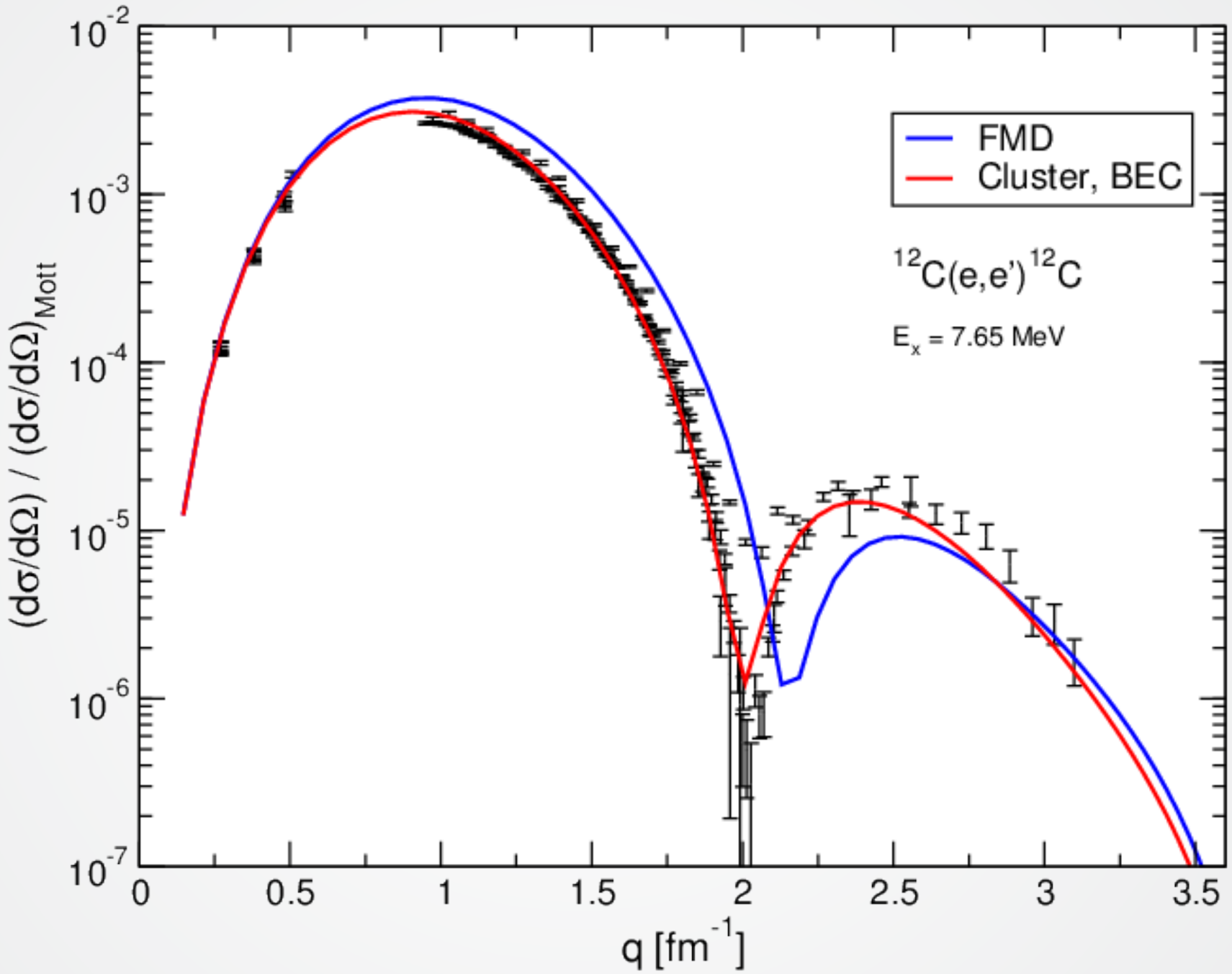
M. Chernykh, H. Feldmeier, T. Neff, P. von Neumann-Cosel, A. Richter, Phys. Rev. Lett. **105** (2010) 022501

^{12}C: Elastic Cross Section



- Using DWBA to calculate the theoretical cross sections
- FMD doing a little bit better in reproducing the cross section

^{12}C: Inelastic Cross Section



- Inelastic cross section rather well described, confirming the dilute nature of the Hoyle state

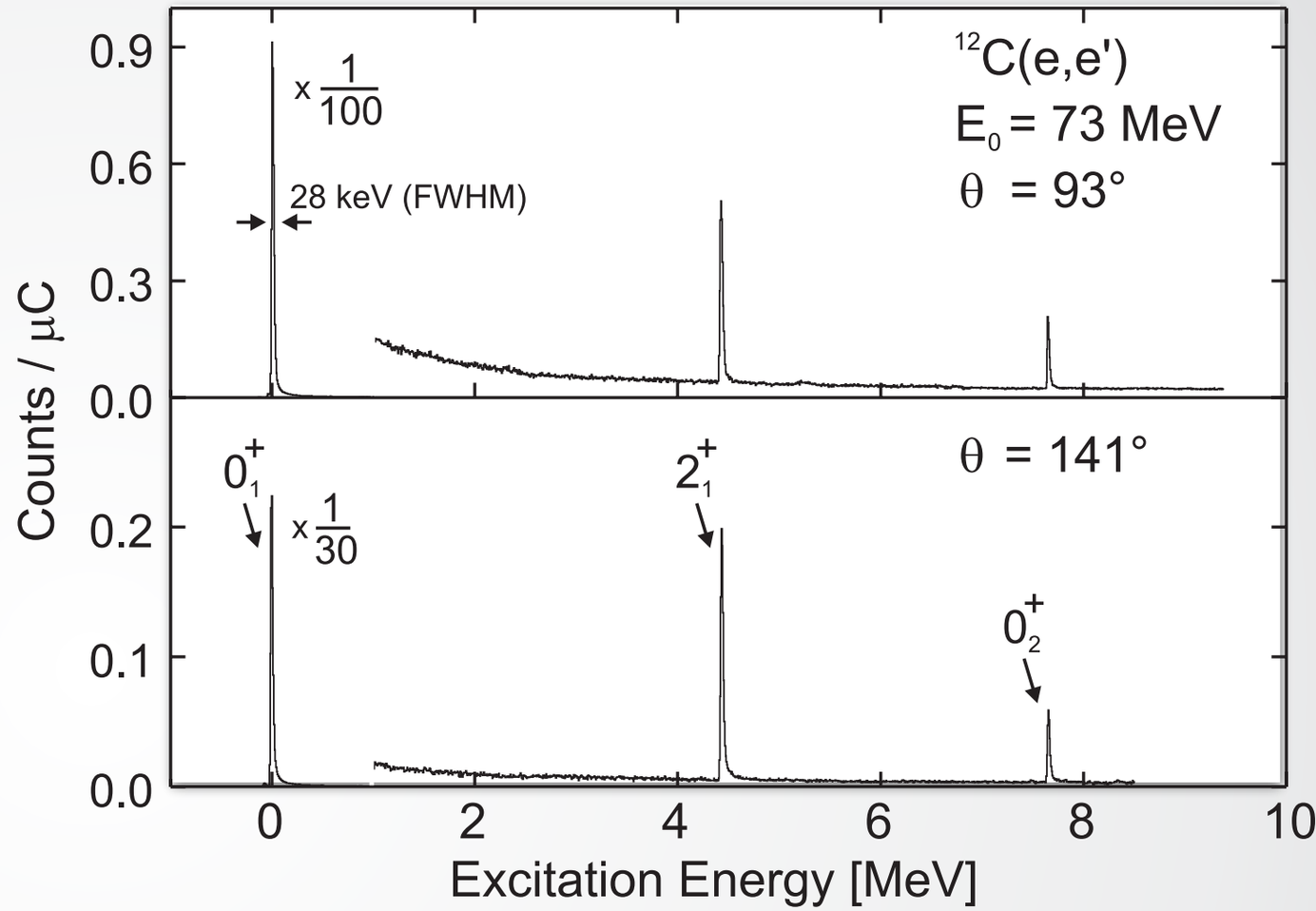
^{12}C: Inelastic Formfactor revisited

Motivation

- Astrophysics requires a precision value for the monopole matrix element
- Literature values differed by up to 10%

Our Approach

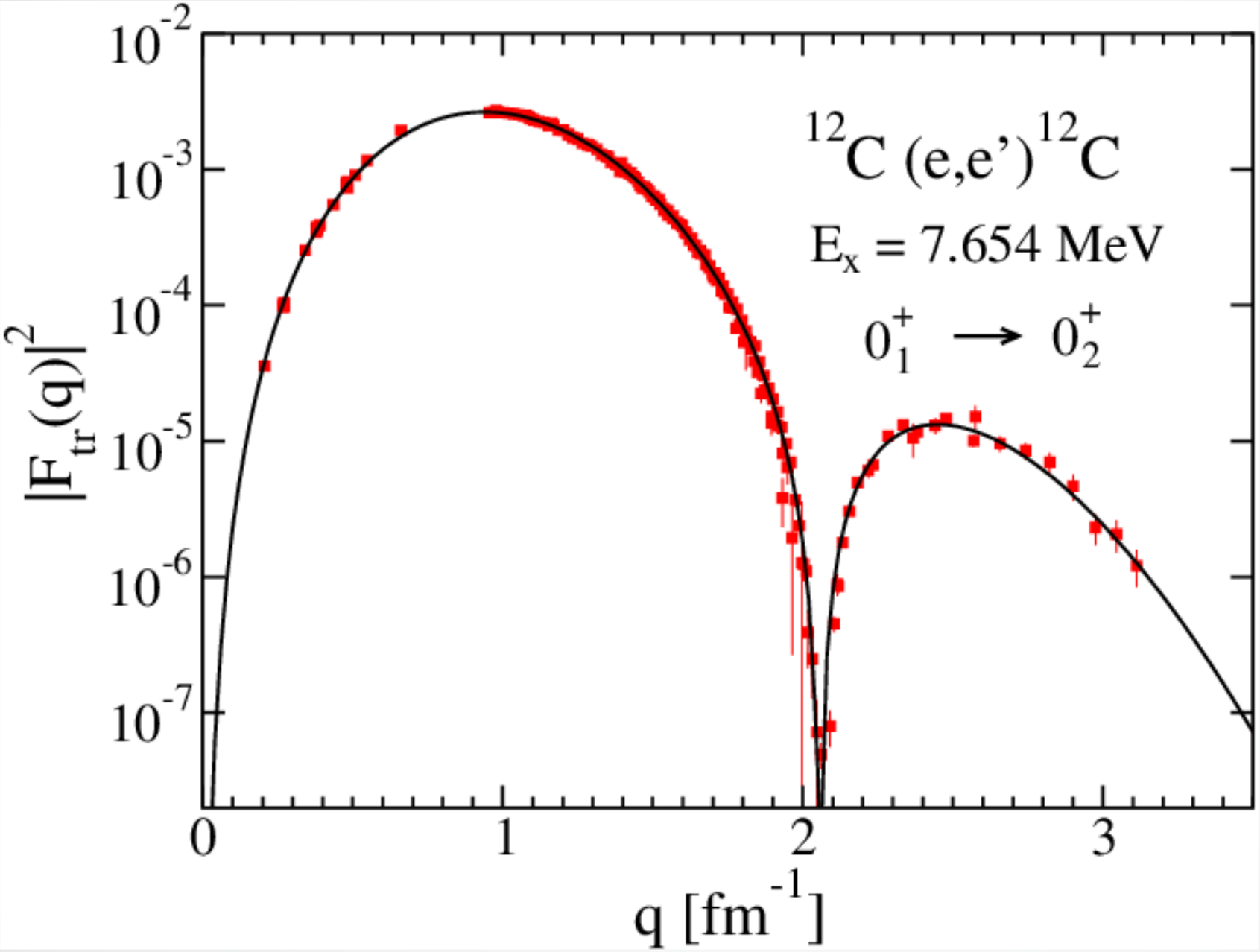
- Add new electron scattering data from Darmstadt at low momentum transfer
- Use a model independent approach to extract form factor/transition density
- Self-consistent calculation in DWBA
- Compare extraction from low-momentum data only with global form factor fit



$$F_{\mathrm{tr}}(q) = \frac{4\pi}{Z} \int_0^\infty \rho_{\mathrm{tr}}(r)\, j_0(qr)\, r^2\, dr$$

$$\left|F_{\mathrm{tr}}^{\mathrm{exp}}(q_i)\right|^2 = \frac{4\pi}{Z^2} B(C0, q_i, E_{0i})\, \frac{B^{\mathrm{PWBA}}(q_i)}{B^{\mathrm{DWBA}}(q_i, E_{0i})}$$

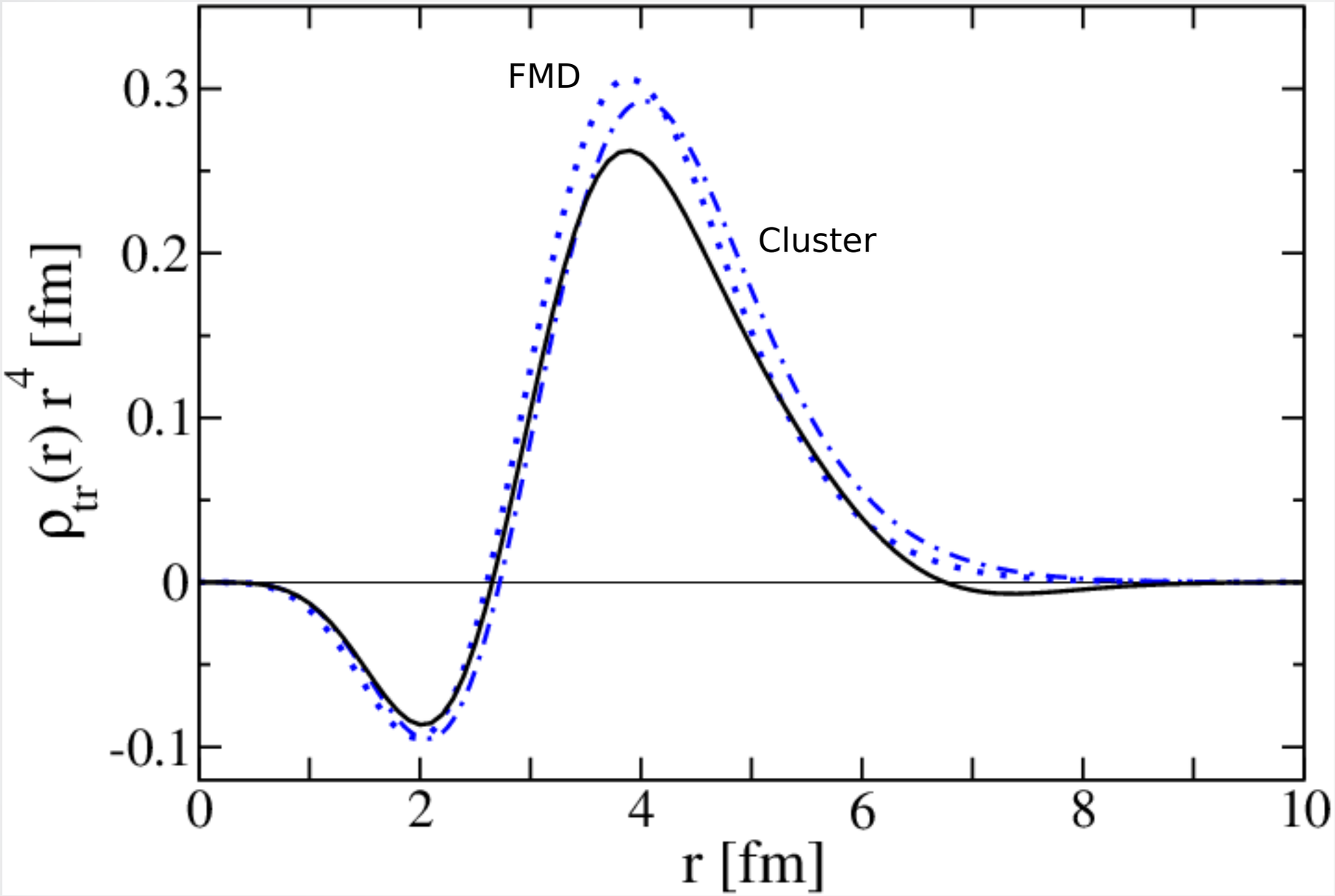
^{12}C: Reanalyzed Monopole Form Factor



- Model independent ansatz:
  best fit with 6 parameters (b, c_1 … c_5)

$$F_{tr}(q) = \frac{1}{Z}\, e^{-\frac{1}{2}(b\,q)^2} \sum_{n=1}^{n_{max}} c_n\, (b\,q)^{2n}$$

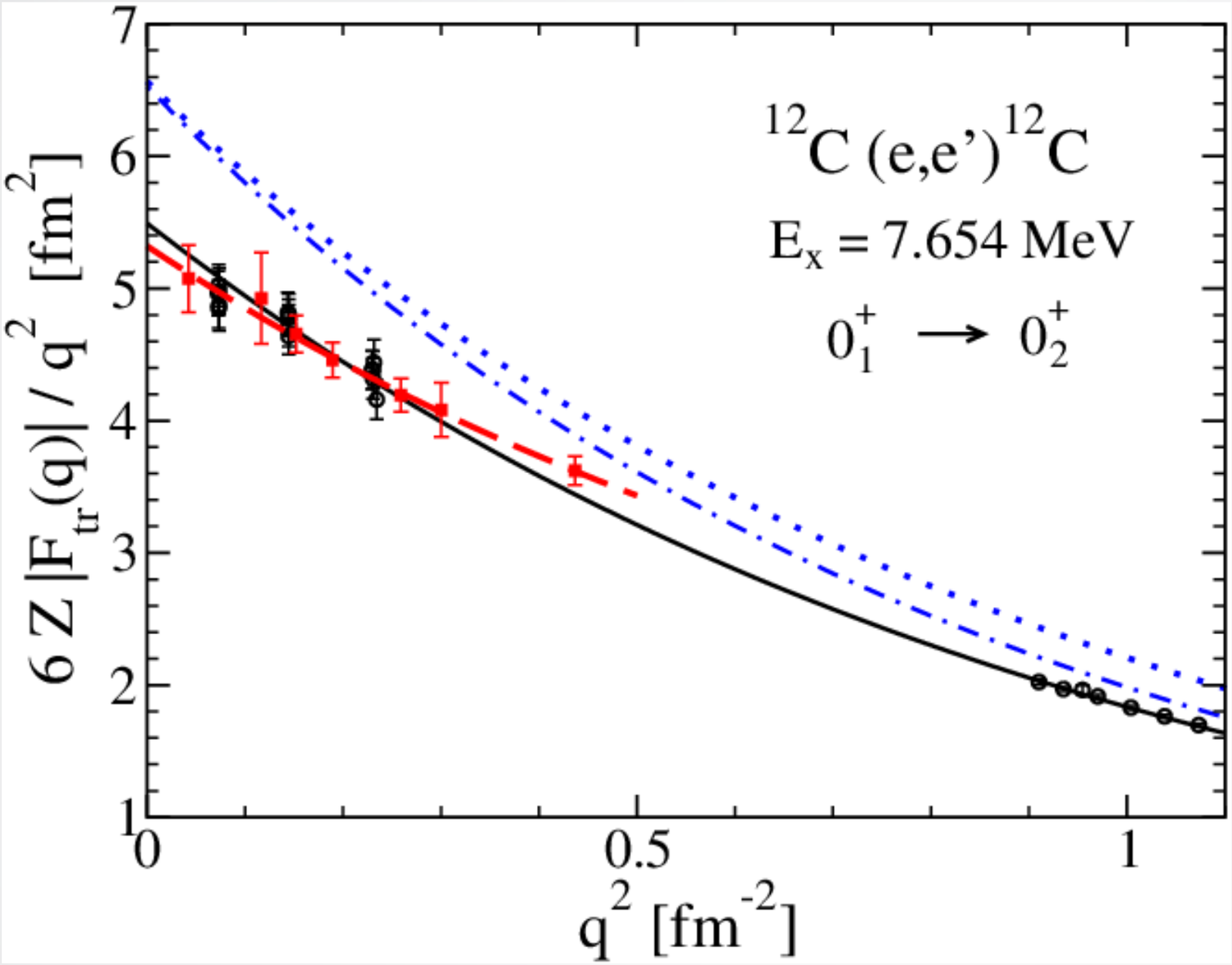
^{12}C: Transition Densities



- Models agree reasonably well with extracted transition density, deviations at large distances

$$\rho_{\mathrm{tr}}(r) = \frac{1}{b^3}\, \mathrm{e}^{-\frac{1}{2}(\frac{r}{b})^2} \sum_{n=0}^{n_{\max}} d_n \left(\frac{r}{b}\right)^{2n}$$

Monopole Matrix Element



Extract monopole matrix element from low-momentum data

$$-6Z\frac{F_{\mathrm{tr}}(q)}{q^2} = \langle r^2 \rangle_{\mathrm{tr}} - \frac{q^2}{20}\langle r^4 \rangle_{\mathrm{tr}} + \ldots$$

$$M(E0) = (5.29 \pm 0.14)\,\mathrm{fm}^2$$

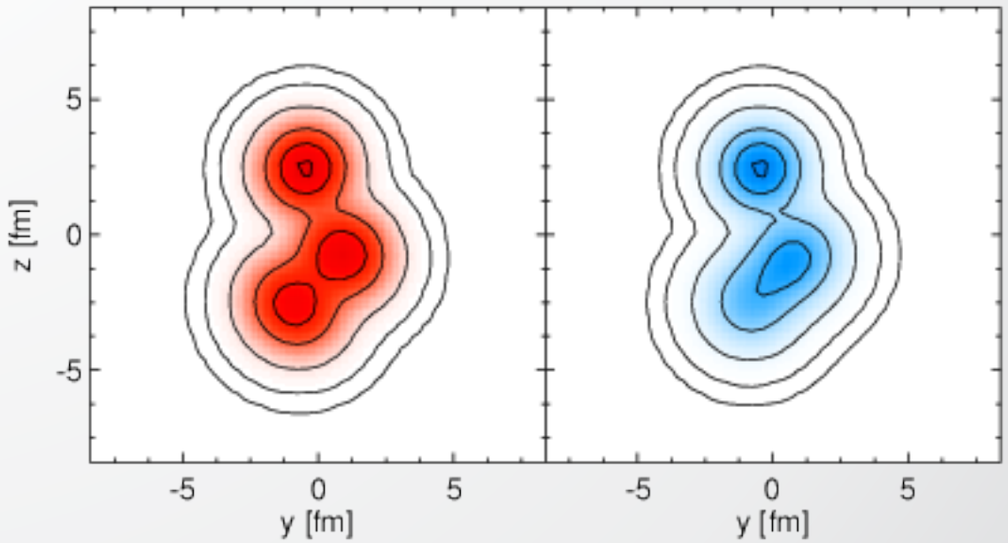
Extract monopole matrix element from global fit

$$M(E0) = (5.47 \pm 0.09)\,\mathrm{fm}^2$$

- Due to experimental error bars the fit to low-momentum data is less precise than the extraction from the global fit

Cluster States in ^{11}C

FMD + Cluster Configurations



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

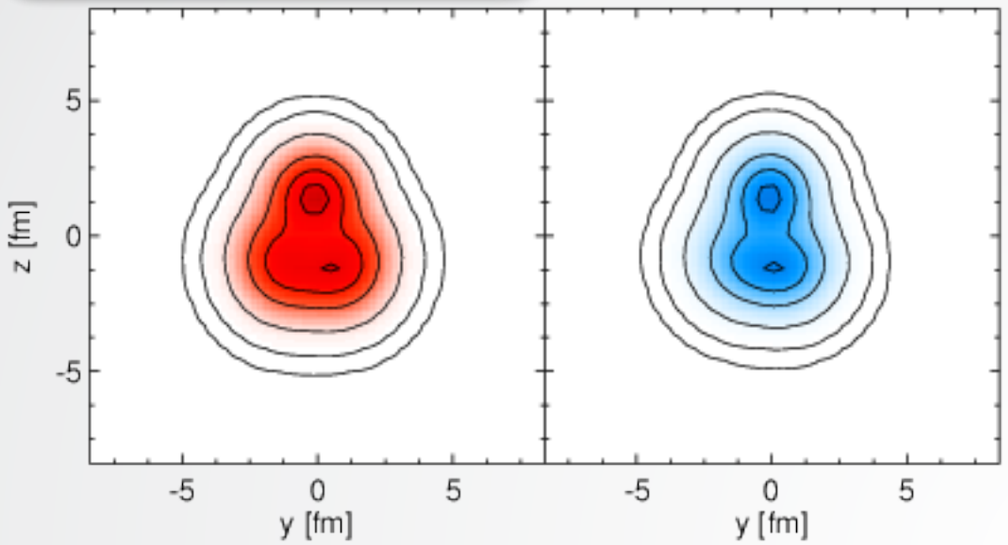
- ^{7}Be(3/2-,1/2-) clusters described using a superposition of ^{7}Be(3/2^{-}) VAP state and an extended ^{4}He-^{3}He config
- ^{8}Be(0+,2+) clusters described using a superposition of ^{8}Be(0^{+}) VAP state and an extended ^{4}He-^{4}He config
- Double-projection of ^{7}Be-^{4}He and ^{8}Be-^{3}He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

III) Full calculation with combined FMD and Cluster basis states

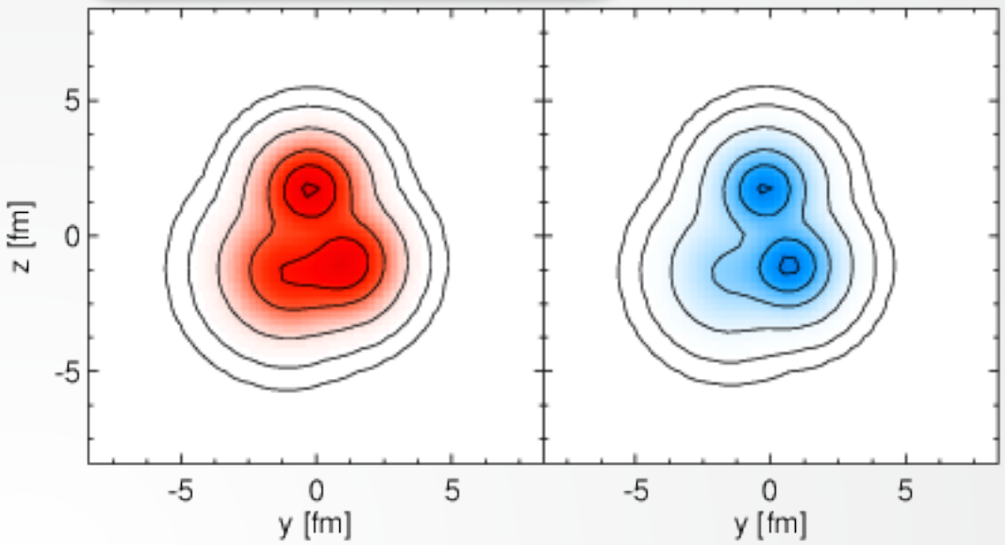
- Basis is overcomplete
- Cluster configs become orthogonal at large distances where the overlap between the clusters vanishes

^{11}C: FMD Variation after Projection

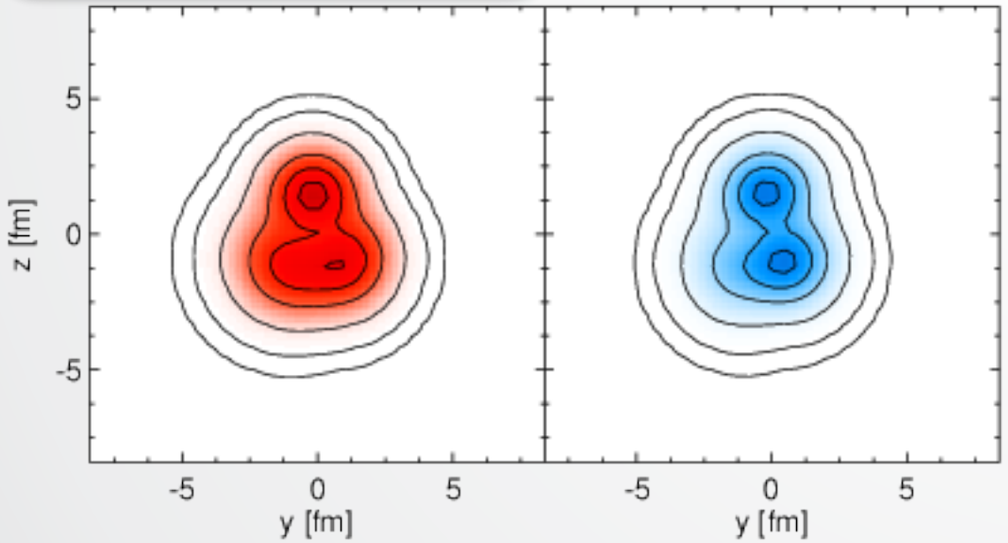
first $3/2^-$



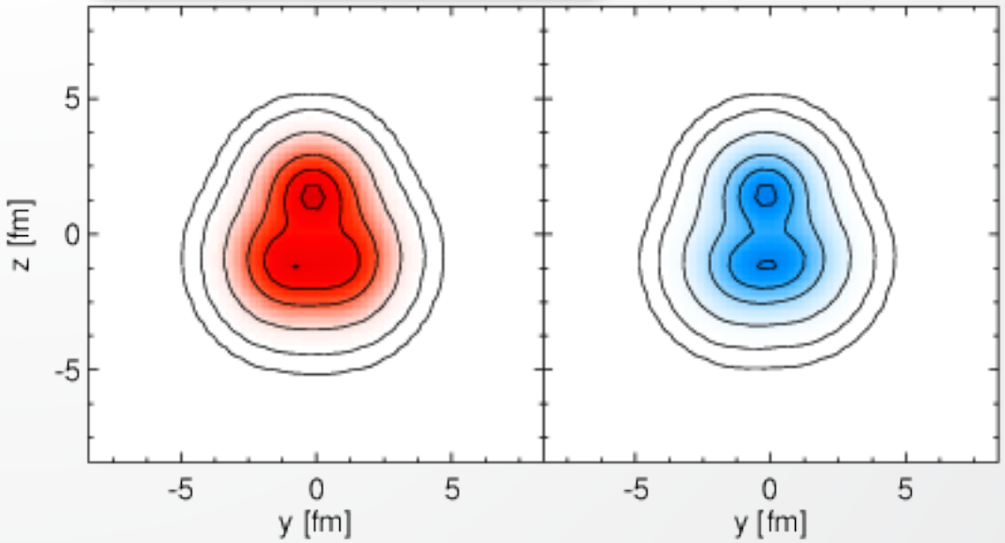
second $3/2^-$



first $1/2^-$



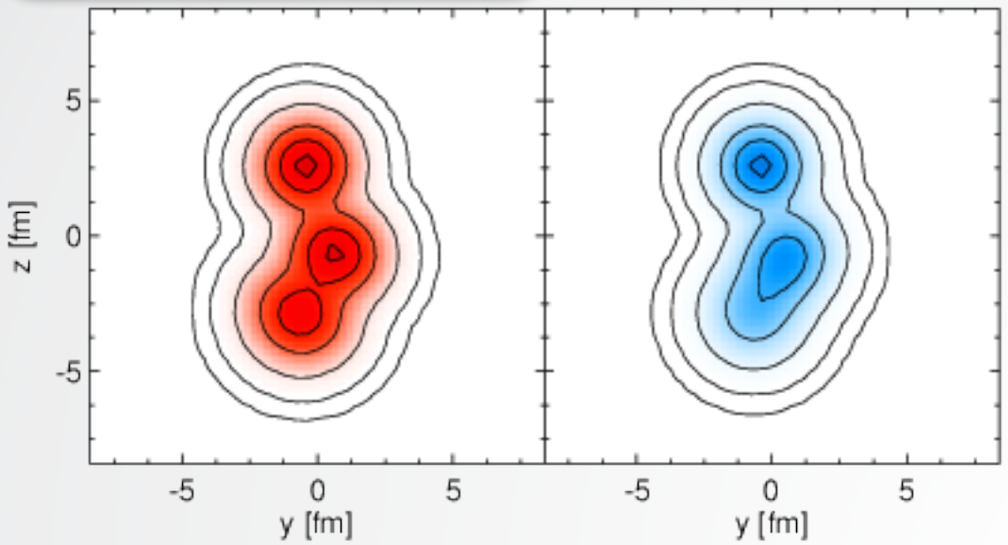
first $5/2^-$



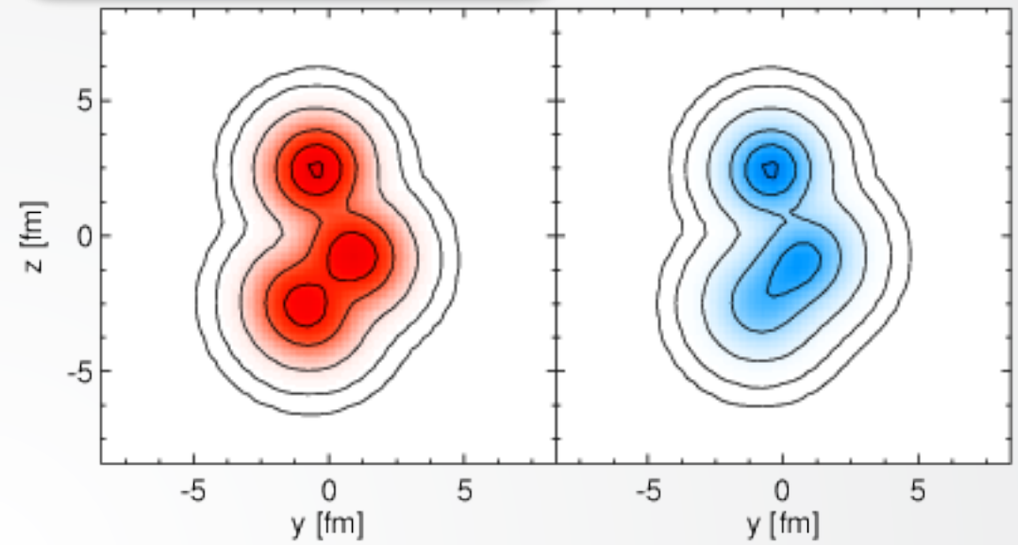
p-shell states with some hint of clustering

^{11}C: FMD Variation after Projection

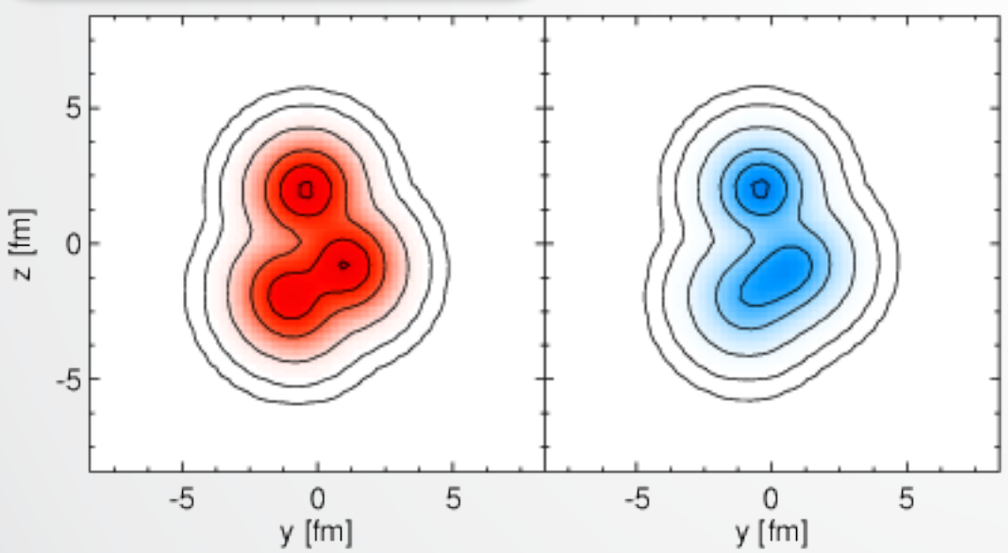
first $1/2^+$



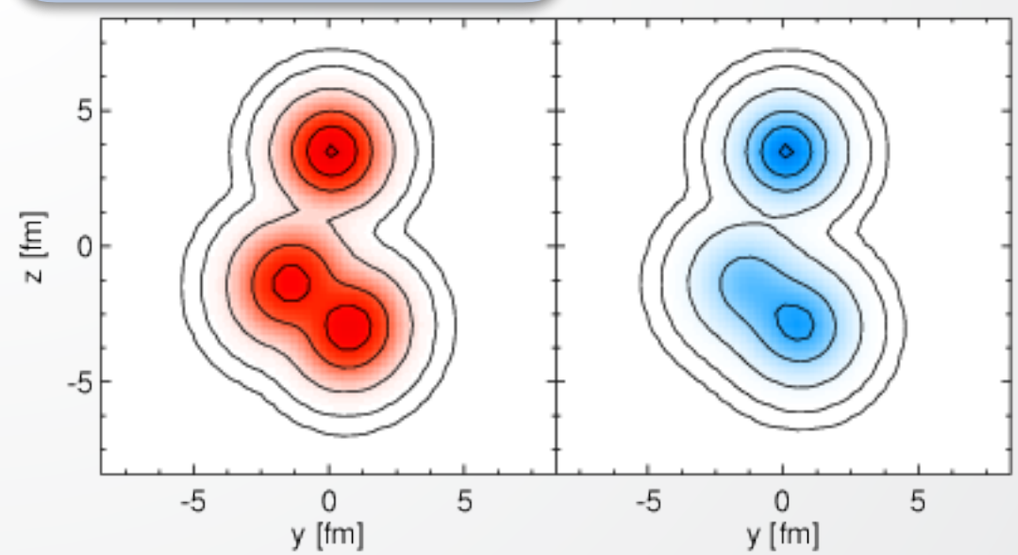
third $3/2^-$



first $5/2^+$

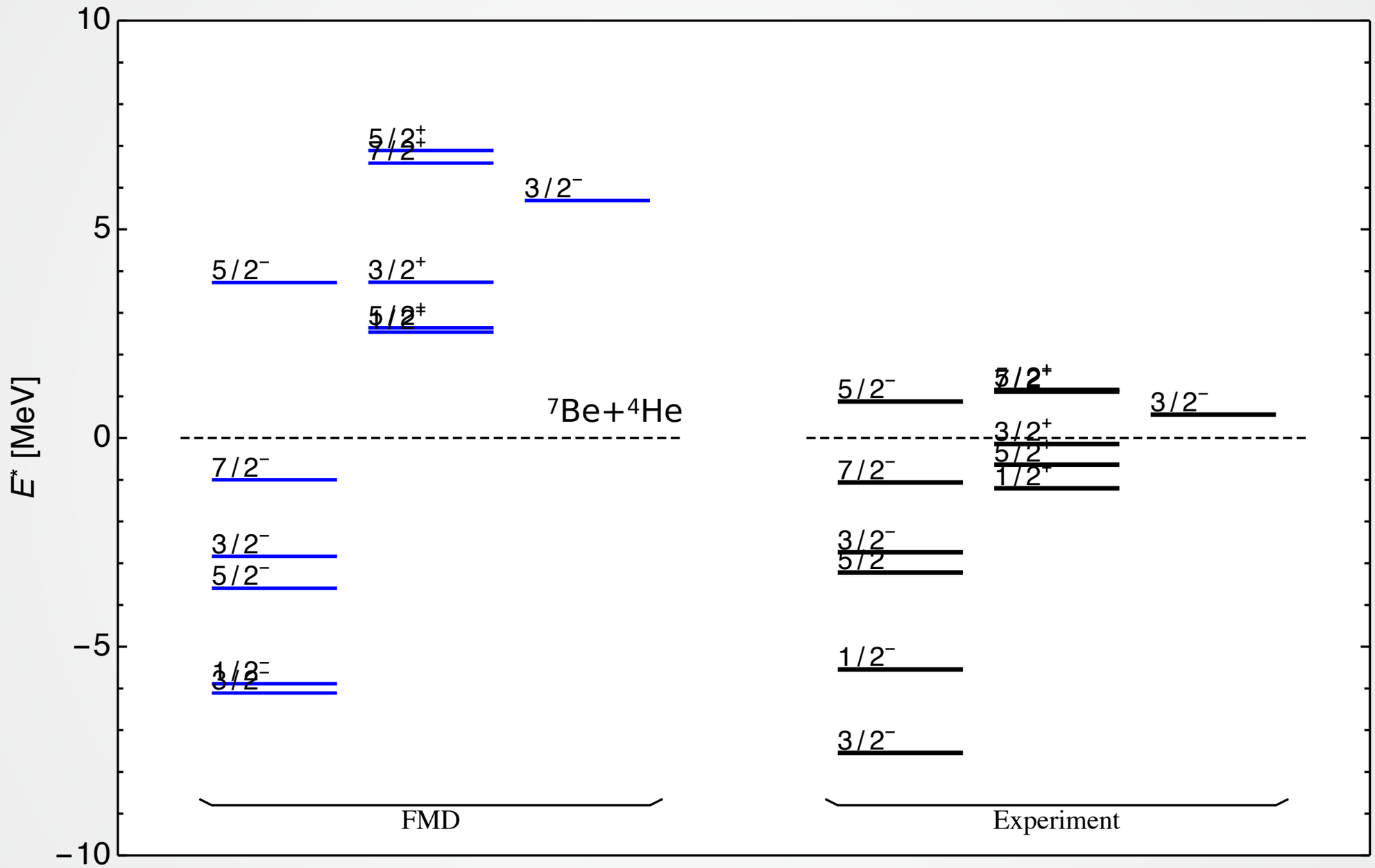


fourth $3/2^-$



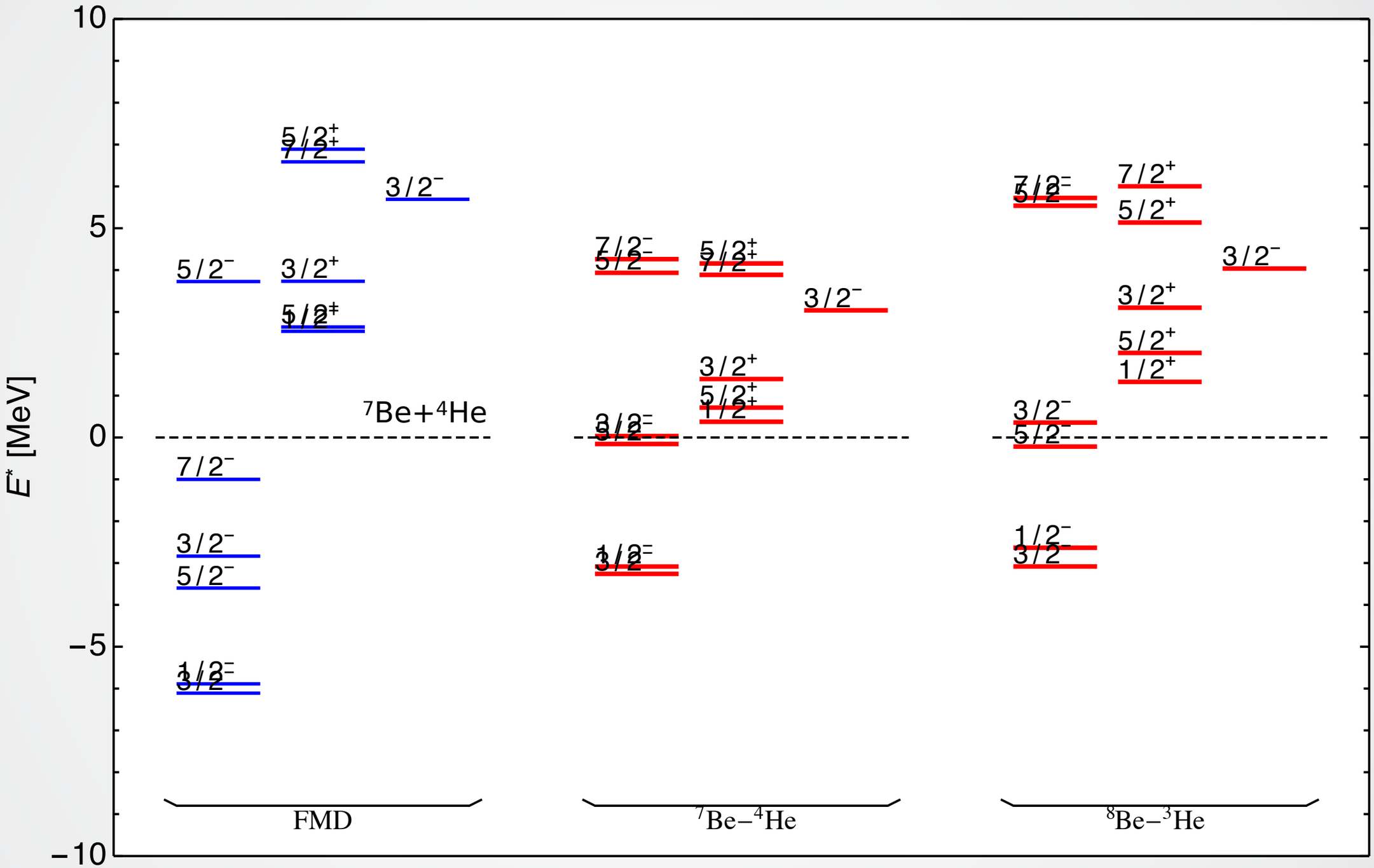
states with apparent cluster structure

^{11}C: Diagonalization with FMD VAP States



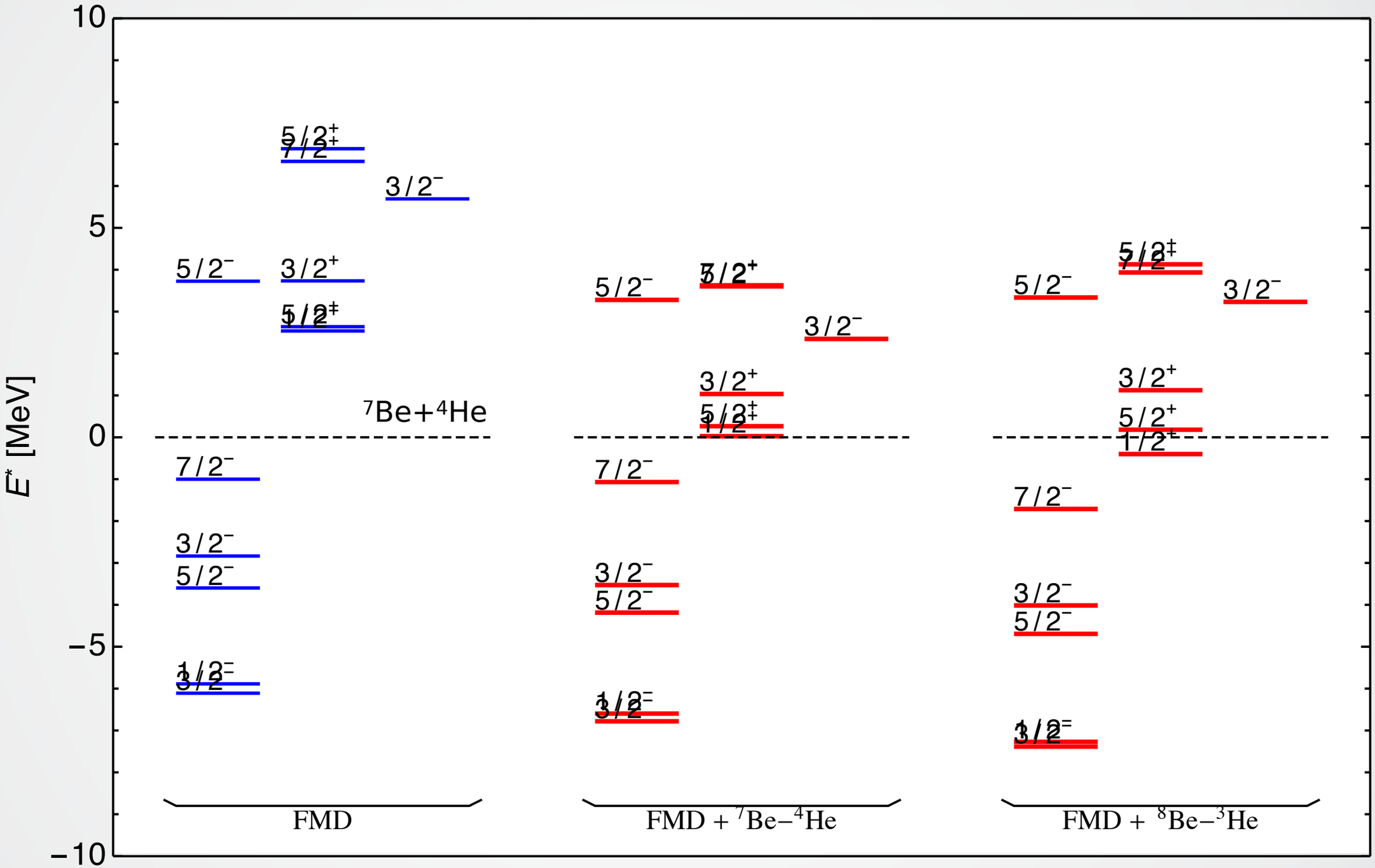
clustered states are well above threshold

^{11}C: FMD vs (FMD)-Cluster Model



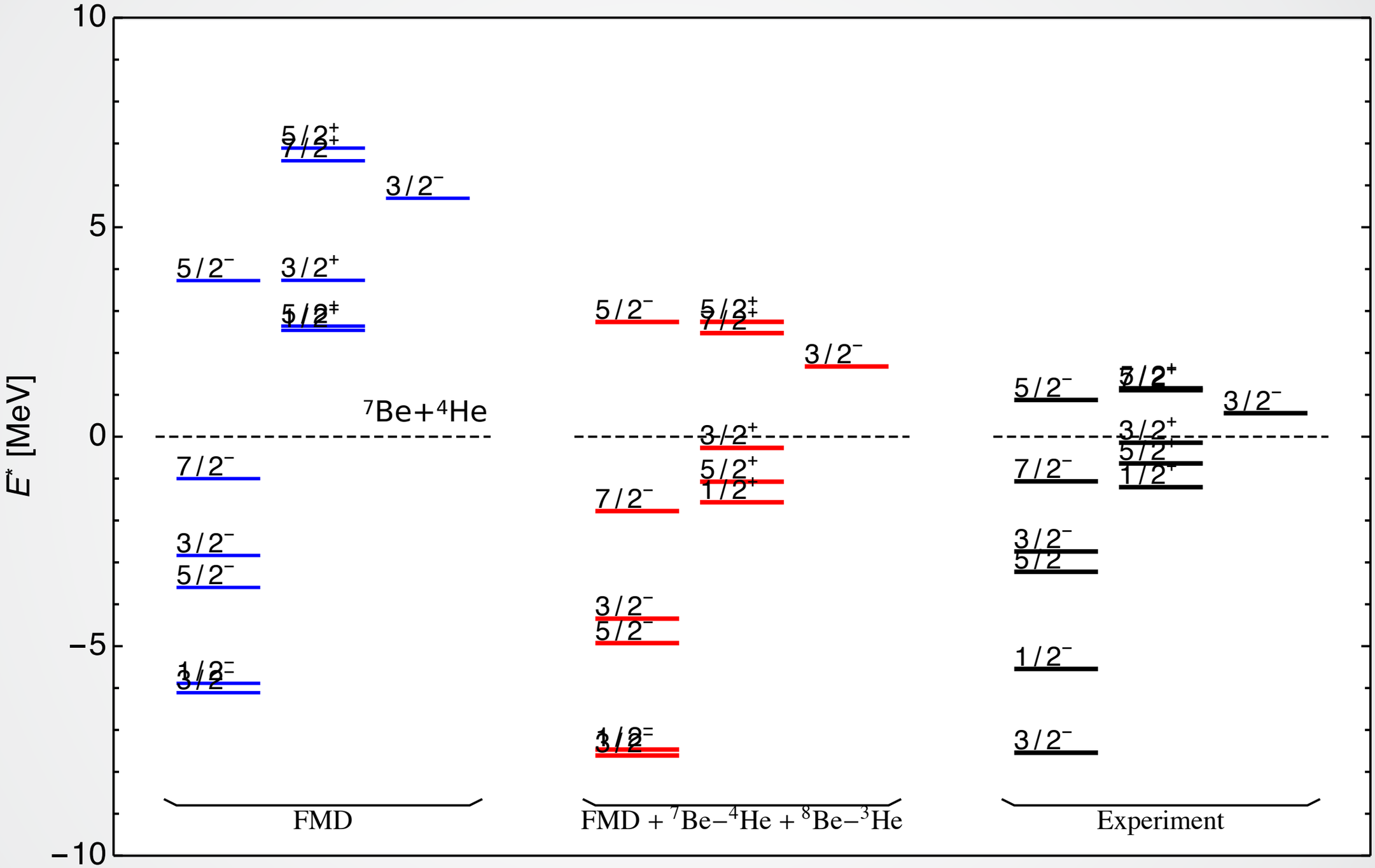
worse for p-shell states, better for clustered states

^{11}C: FMD plus (FMD)-Cluster Model



improves both p-shell and clustered states

^{11}C: FMD vs Full Calculation



consistent picture of p-shell and clustered states

Summary and Conclusions

Unitary Correlation Operator Method

- Explicit description of short-range central and tensor correlations

Fermionic Molecular Dynamics

- Gaussian wave-packet basis contains HO shell model and Brink-type cluster states
- R-matrix method for description of continuum states

^{3}He(α,γ)^{7}Be Capture Reaction

- Consistent description of bound-state properties, phase shifts and capture cross section
- Good agreement with ^{3}He(α,γ)^{7}Be data, but normalization off for ^{3}H(α,γ)^{7}Li

Cluster states in ^{12}C and ^{11}C

- Compare α-cluster model and FMD
- Consistent picture for ground state band, negative parity states and cluster states in the continuum
- The importance of ^{8}Be+^{4}He cluster structures in ^{12}C and ^{7}Be+^{4}He and ^{8}Be+^{3}He cluster structures in ^{11}C
- Careful evaluation of electron scattering data to extract the monopole matrix element