Microscopic calculations for structure and reactions of light nuclei

Thomas Neff

GSI Helmholtzzentrum für Schwerionenforschung, Darmstadt

Workshop on

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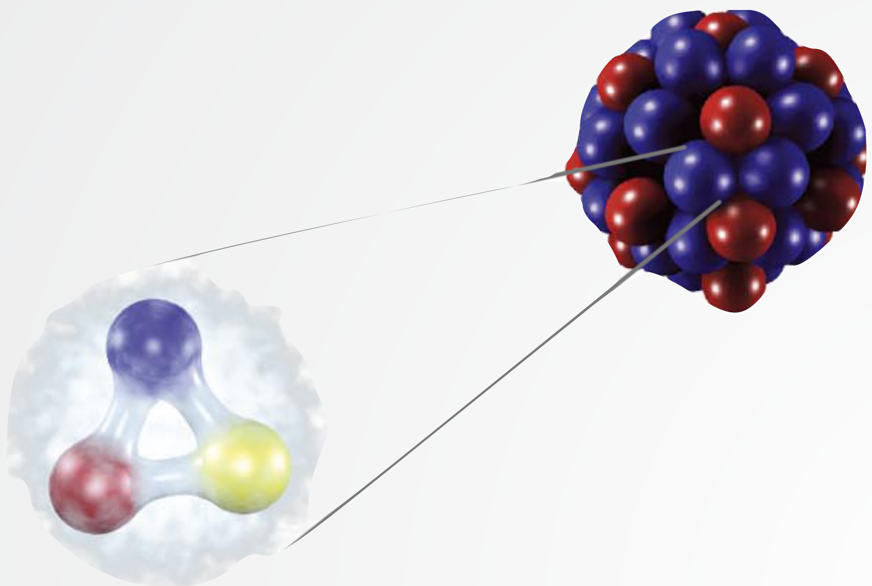
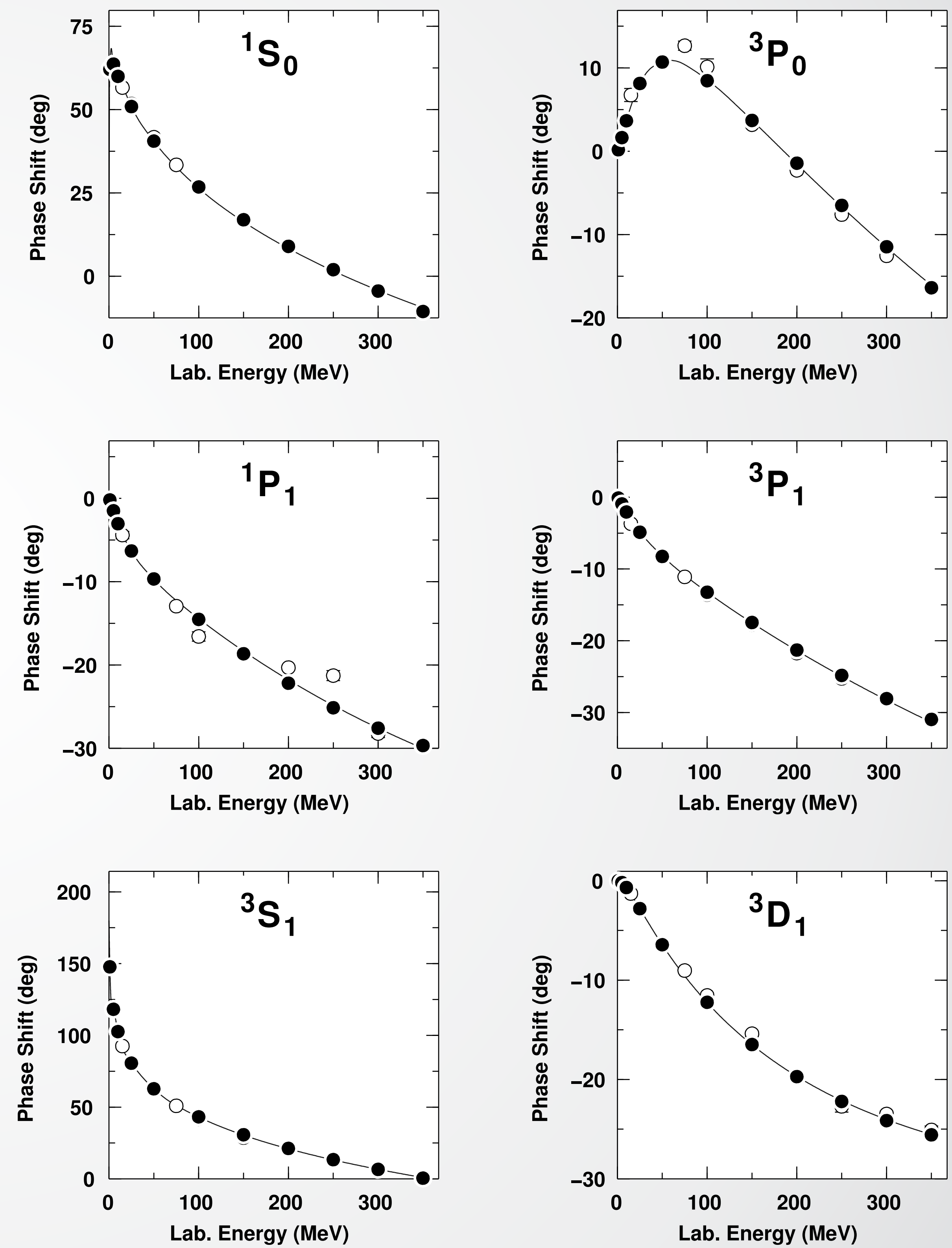
Our Aim:

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

Many-Body Method $\longleftrightarrow$ Effective Interaction

Nucleon-Nucleon Interaction

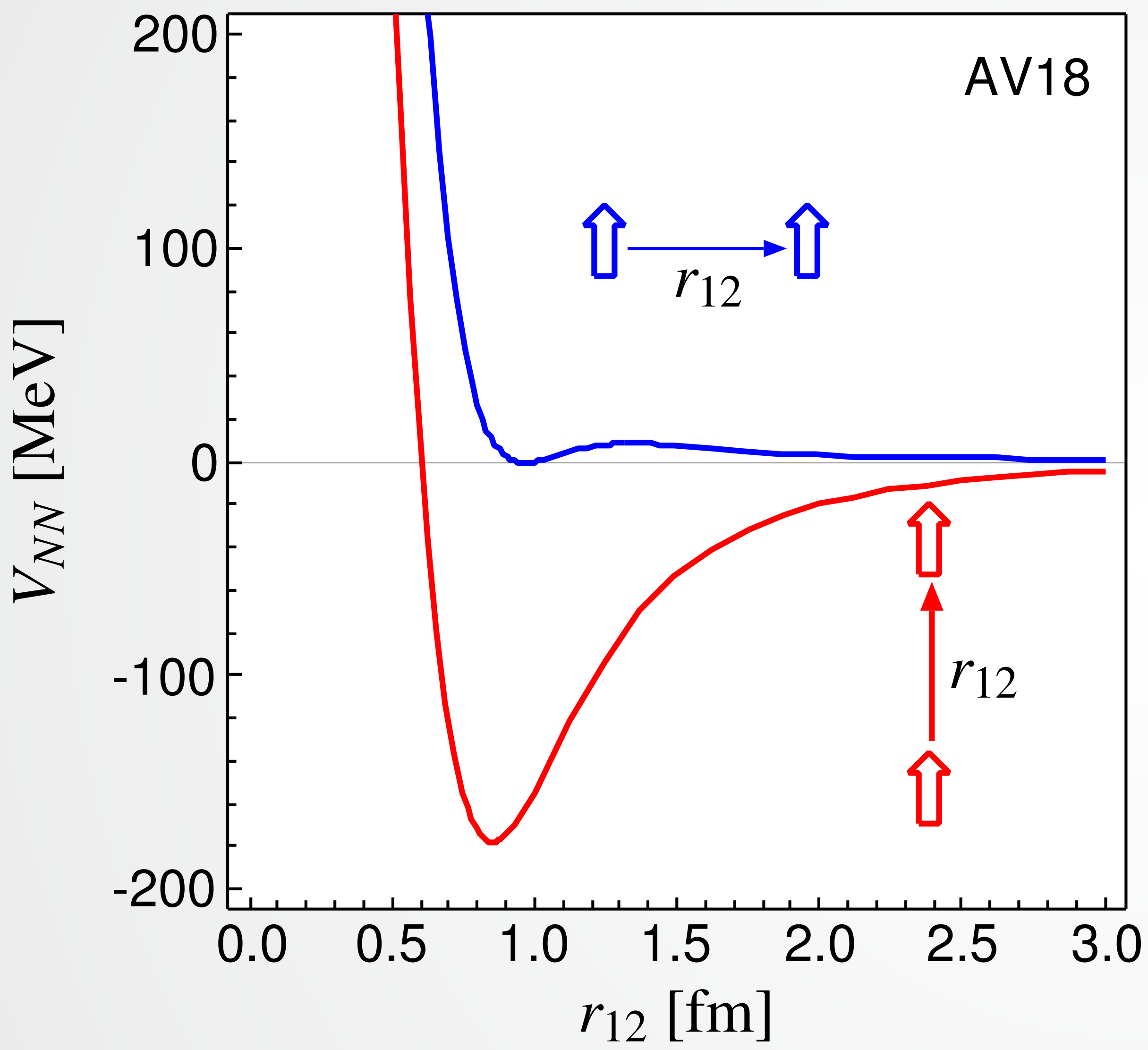




- Nucleons are not point-like, complicated quark and gluon sub-structure
- Nucleon-nucleon (NN) interaction: residual interaction
- Calculation within QCD not possible yet → construct **realistic NN potentials** …
- describe two-nucleon properties (scattering, deuteron) with high accuracy
- high-momentum and off-shell behavior not constrained by scattering data

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

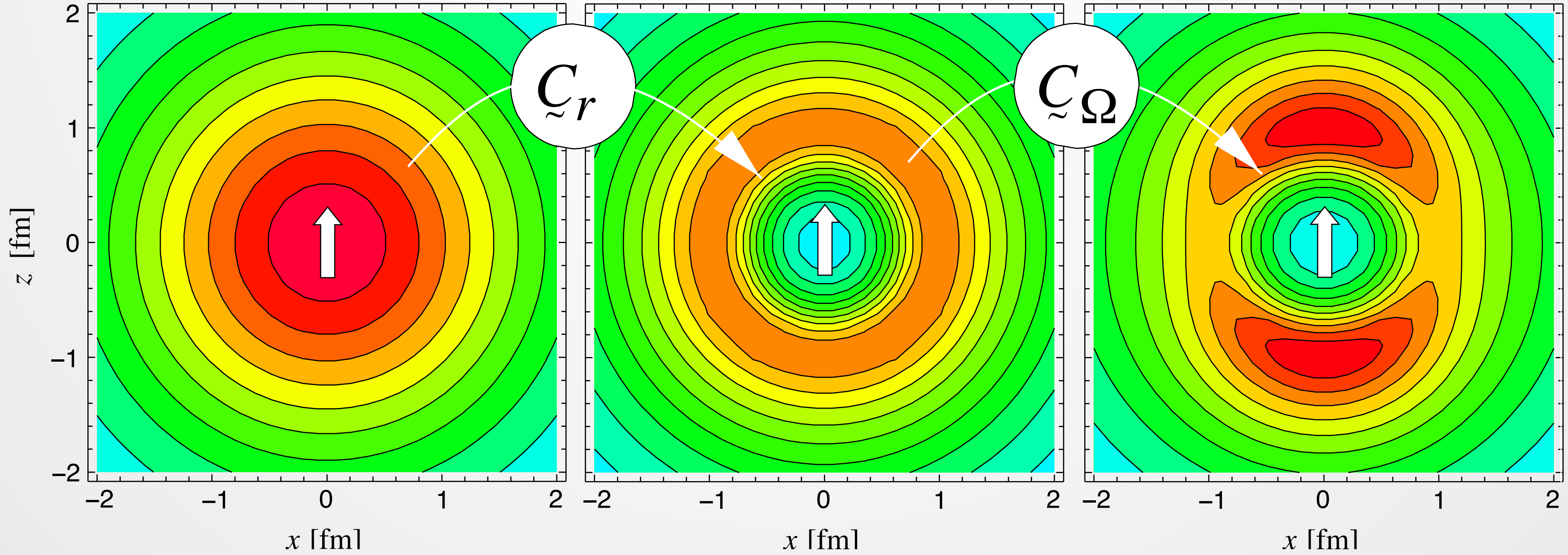
Correlation Operator

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

Correlated Hamiltonian

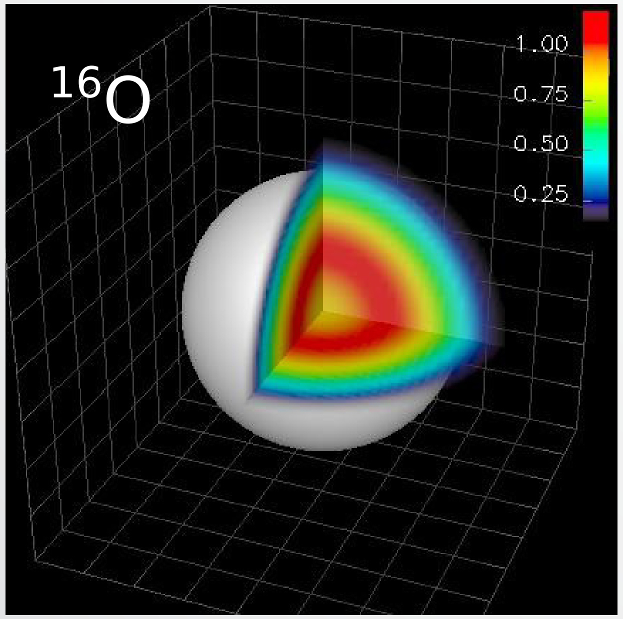
$$\hat{C}^\dagger(\hat{T} + \hat{V})\hat{C} = \hat{T} + \hat{V}_{\mathrm{UCOM}} + \ldots$$

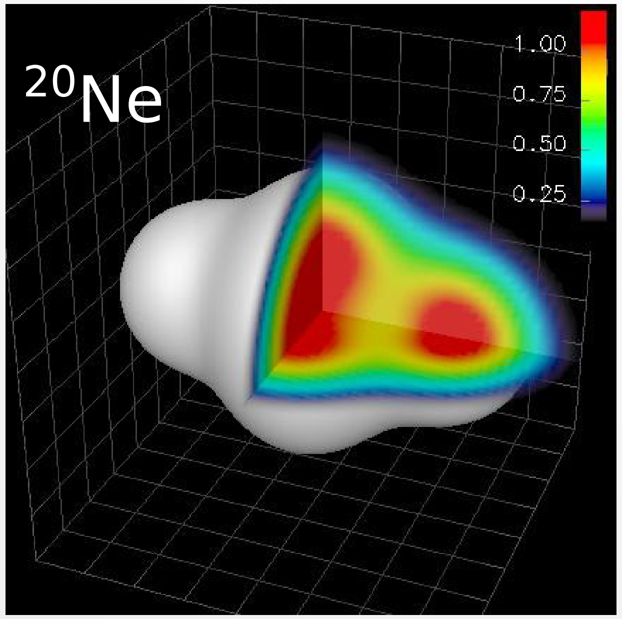
Central correlator shifts nucleons apart,
Tensor correlator aligns nucleons with spin



Fermionic Molecular Dynamics

Many-body Method using Gaussian wave-packet basis





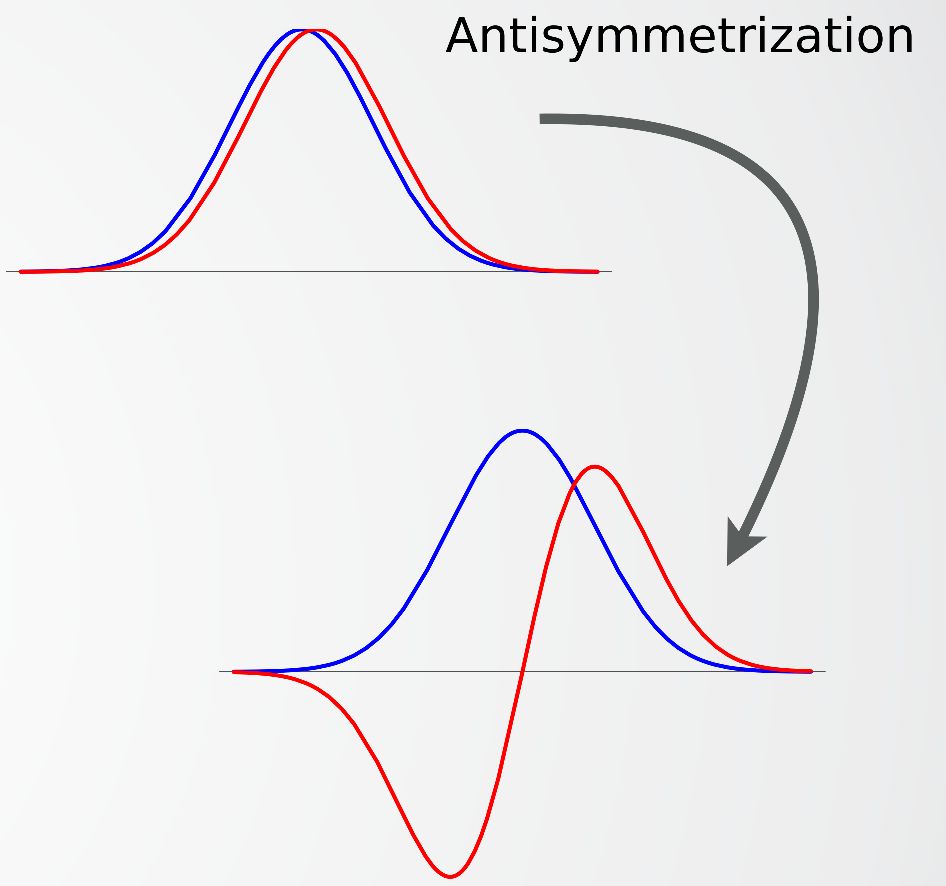
Fermionic Molecular Dynamics

Fermionic

Intrinsic many-body states

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

are antisymmetrized A-body states



Molecular

Single-particle states

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

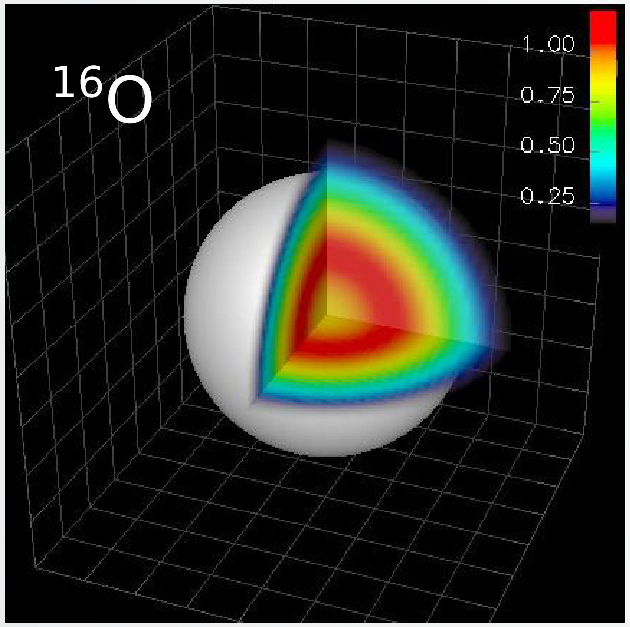
- Gaussian wave-packets in phase-space (complex parameter $\mathbf{b}_i$ encodes mean position and mean momentum), spin is free, isospin is fixed
- width a_i is an independent variational parameter for each wave packet
- use one or two wave packets for each single particle state

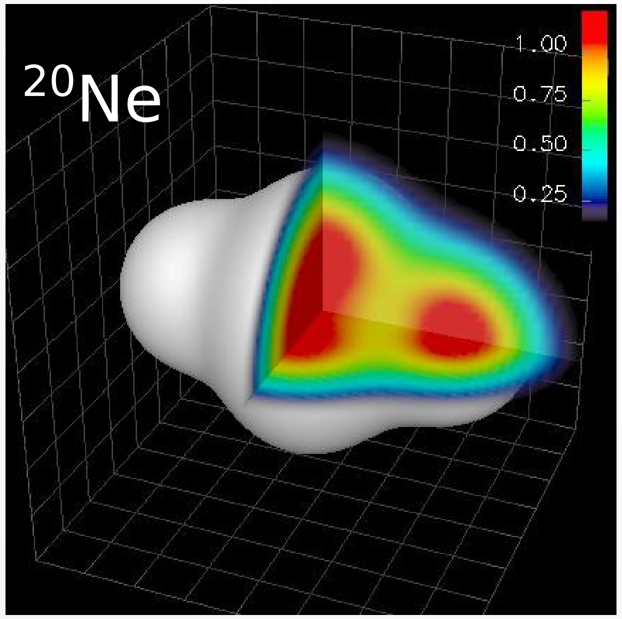
FMD basis contains **harmonic oscillator shell model** and **Brink-type cluster** configurations as limiting cases

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

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

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

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

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

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

Variation after Projection

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

(Intrinsic) Basis States

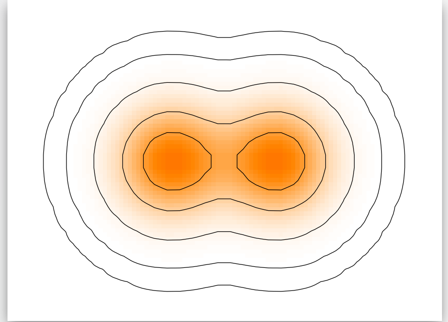
$$\left\{ \left| Q^{(a)} \right\rangle, a = 1, \ldots, N \right\}$$

Generalized Eigenvalue Problem

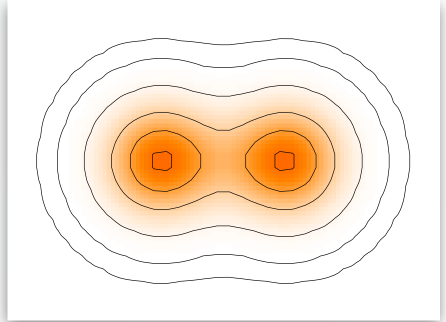
$$\sum_{K'b} \underbrace{\left\langle Q^{(a)} \middle| \hat{H} \hat{P}^\pi {\hat{P}^J}_{KK'} \hat{P}^{\mathbf{P}=0} \middle| Q^{(b)} \right\rangle}_{\text{Hamiltonian kernel}} {c^\alpha}_{K'b} = E^{J^\pi \alpha} \sum_{K'b} \underbrace{\left\langle Q^{(a)} \middle| \hat{P}^\pi {\hat{P}^J}_{KK'} \hat{P}^{\mathbf{P}=0}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

^{8}Be: PAV/VAP/Multiconfiguration Mixing

V/PAV

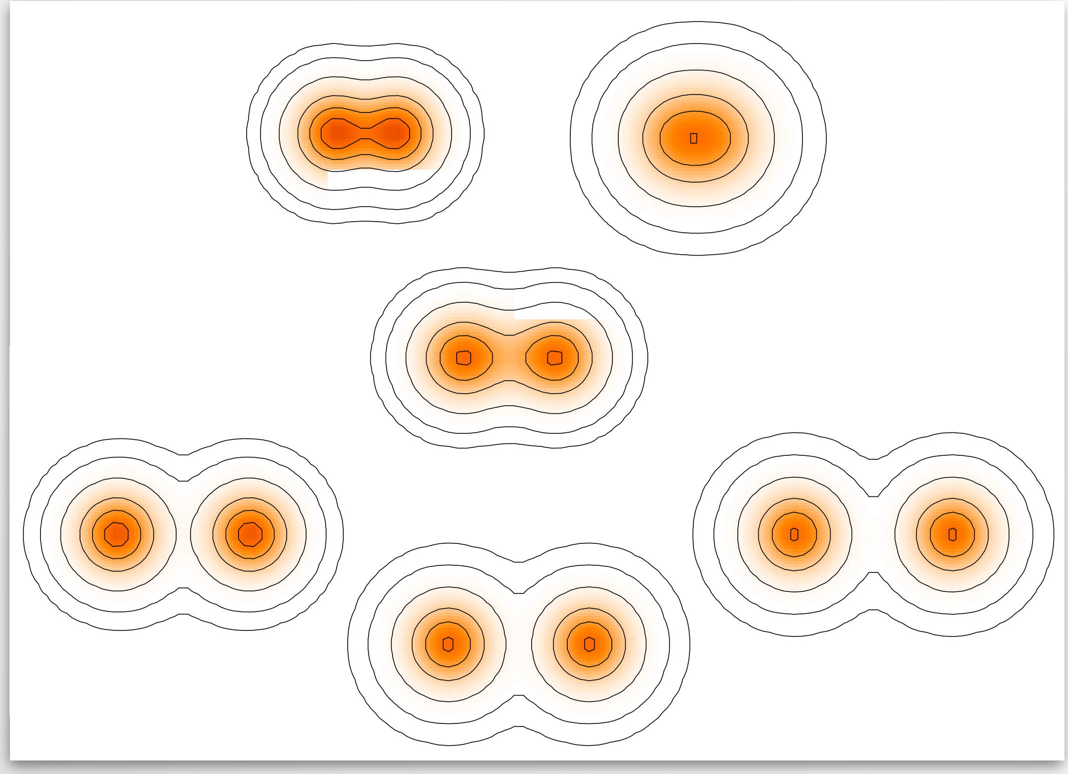


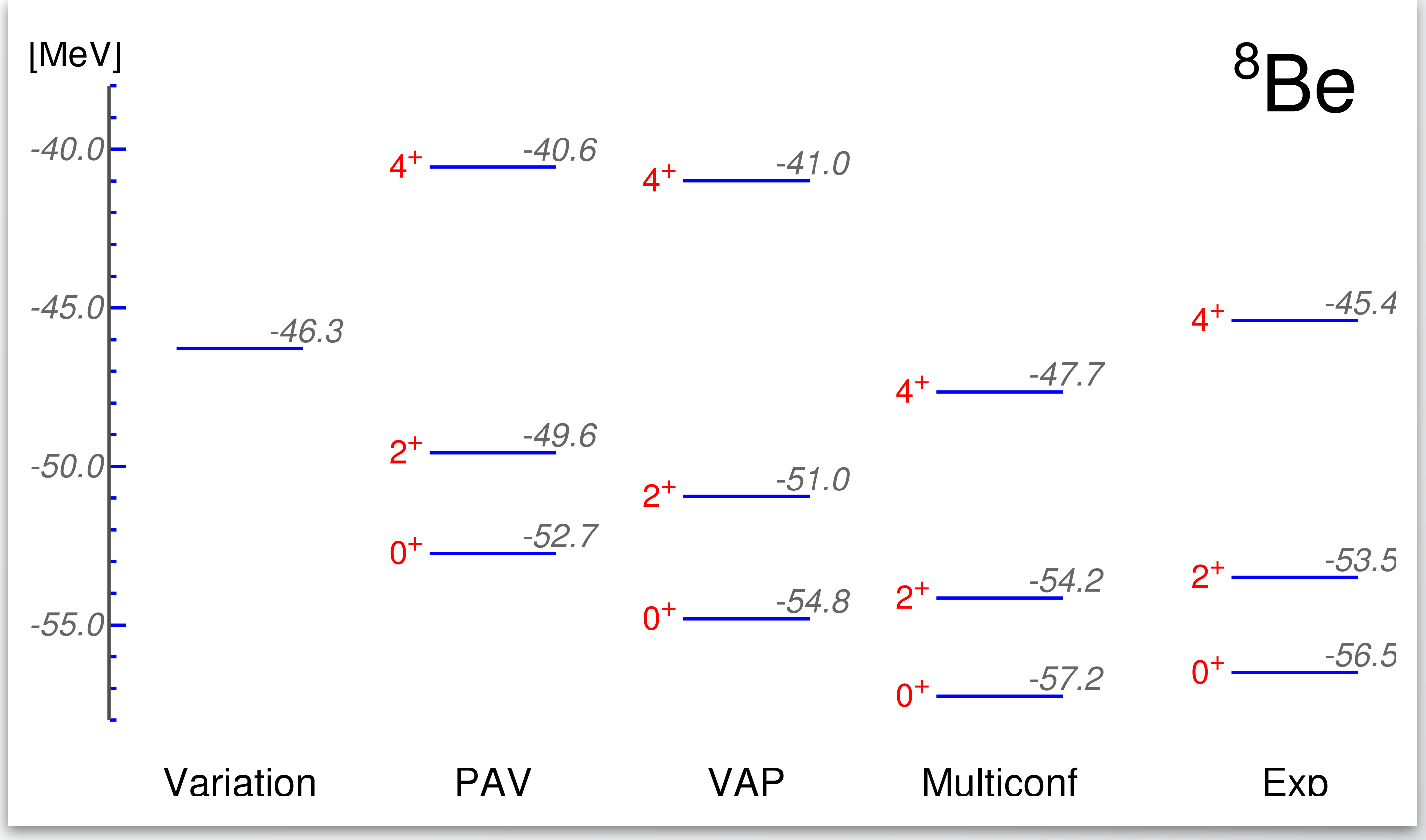
VAP



	E_b [MeV]	r_{ch} [fm]	$B(E2)$ [e^2 fm^4]
PAV	52.7	2.39	9.3
VAP	54.8	2.49	15.4
Multiconfig	57.2	2.74	30.4
Exp.	56.5		

Multiconfiguration Mixing





^{3}He(α,γ)^{7}Be and ^{3}H(α,γ)^{7}Li Radiative Capture

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

Microscopic Calculation of the ^{3}He(α, γ)^{7}Be and ^{3}H(α, γ)^{7}Li Capture Cross Sections Using Realistic Interactions

Thomas Neff*

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

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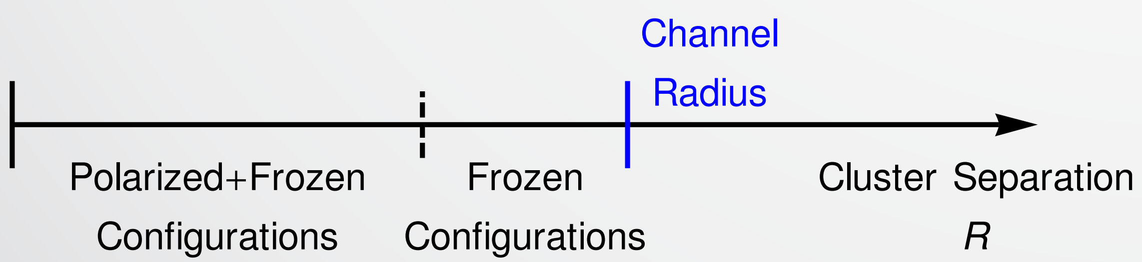
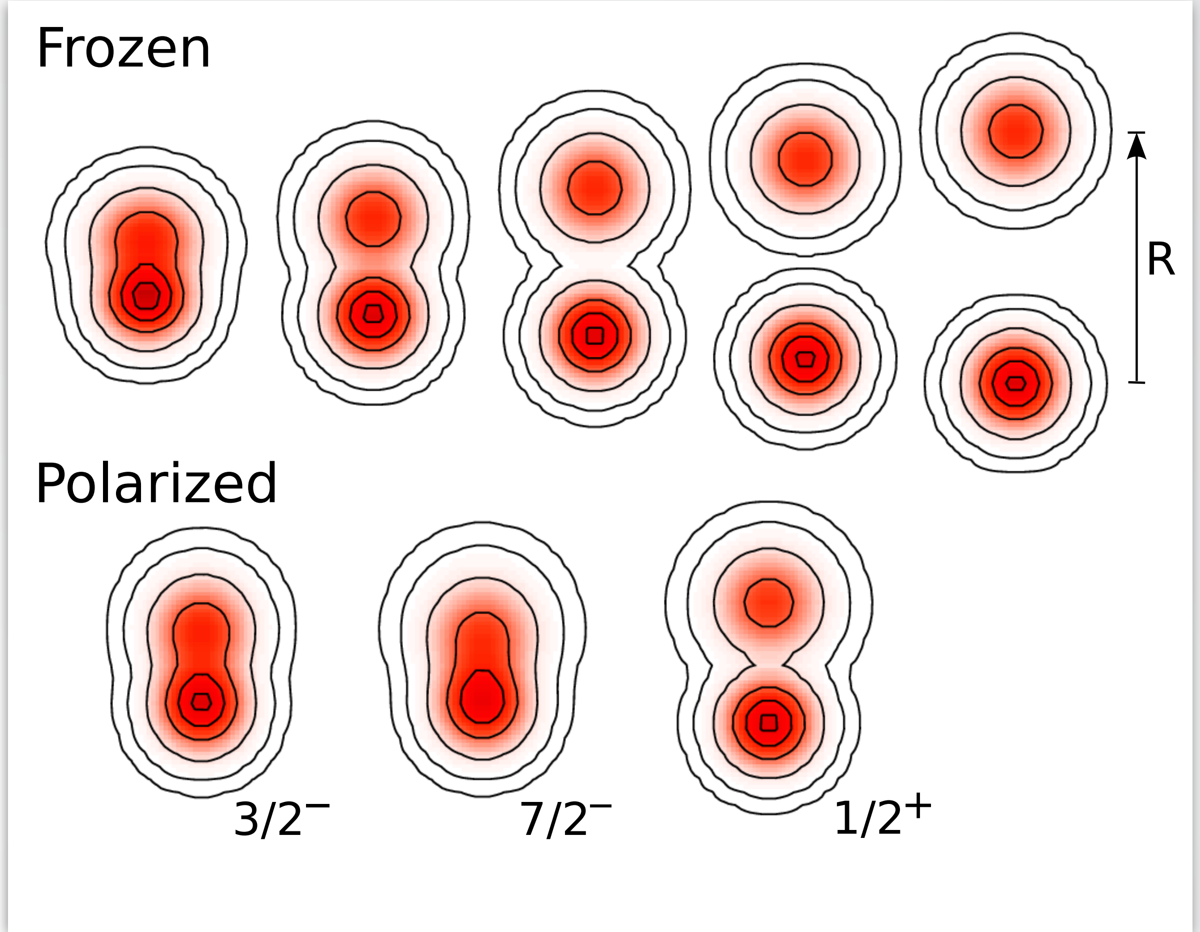
FMD Basis States

- 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

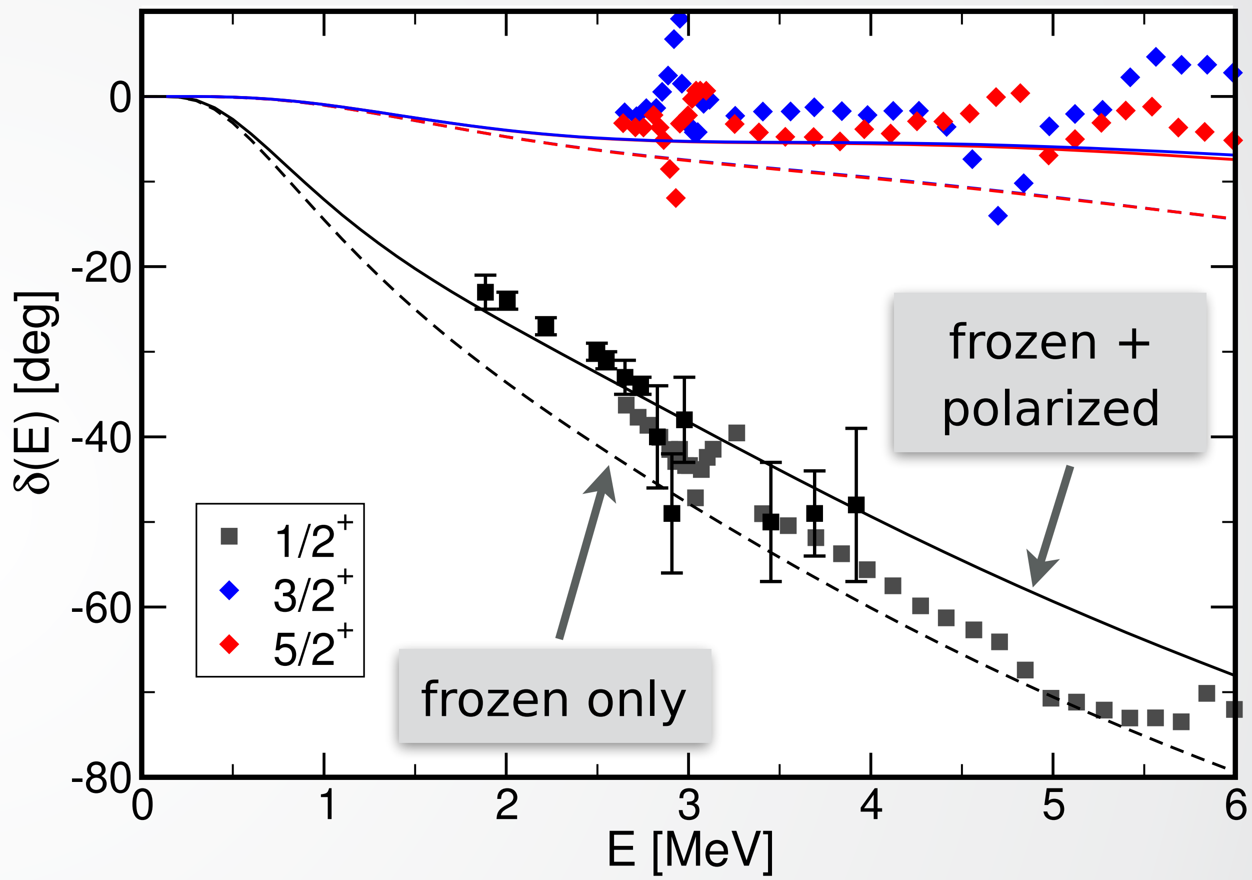
Bound and Scattering States

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

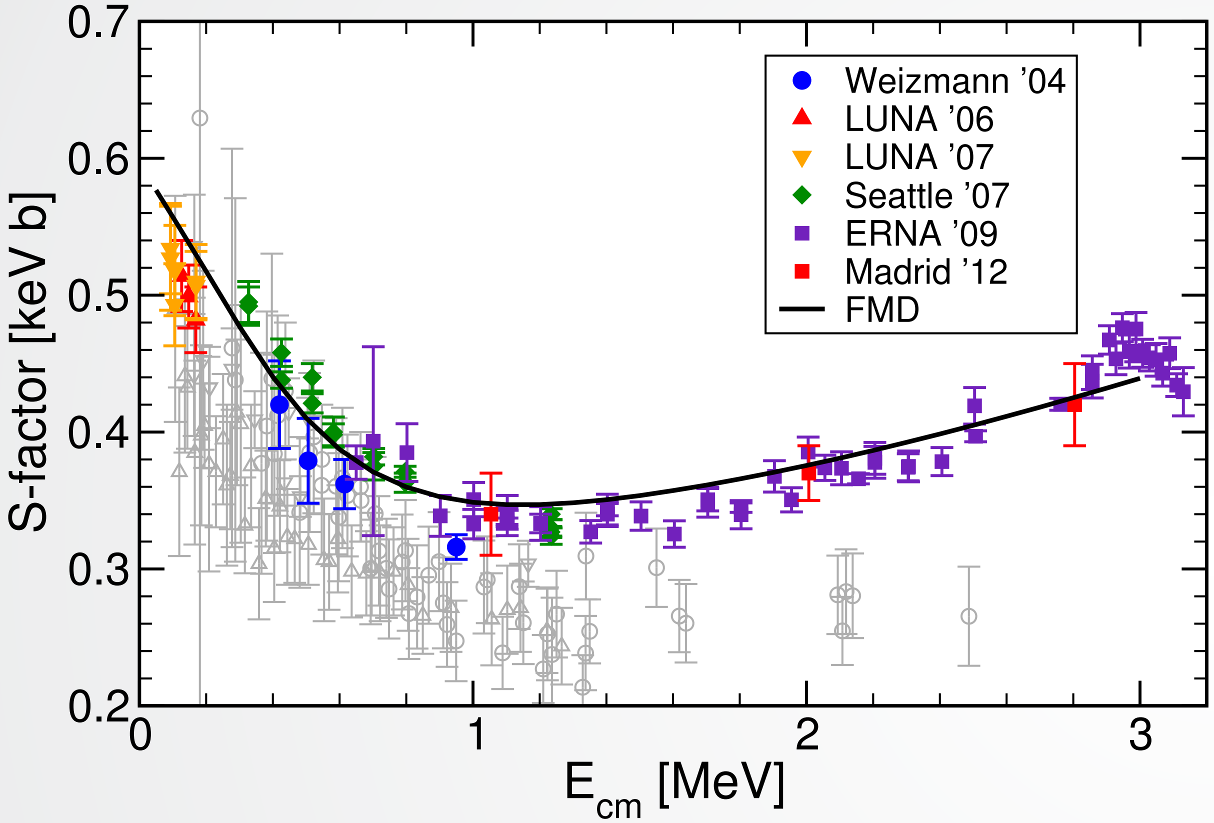
Scattering States



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

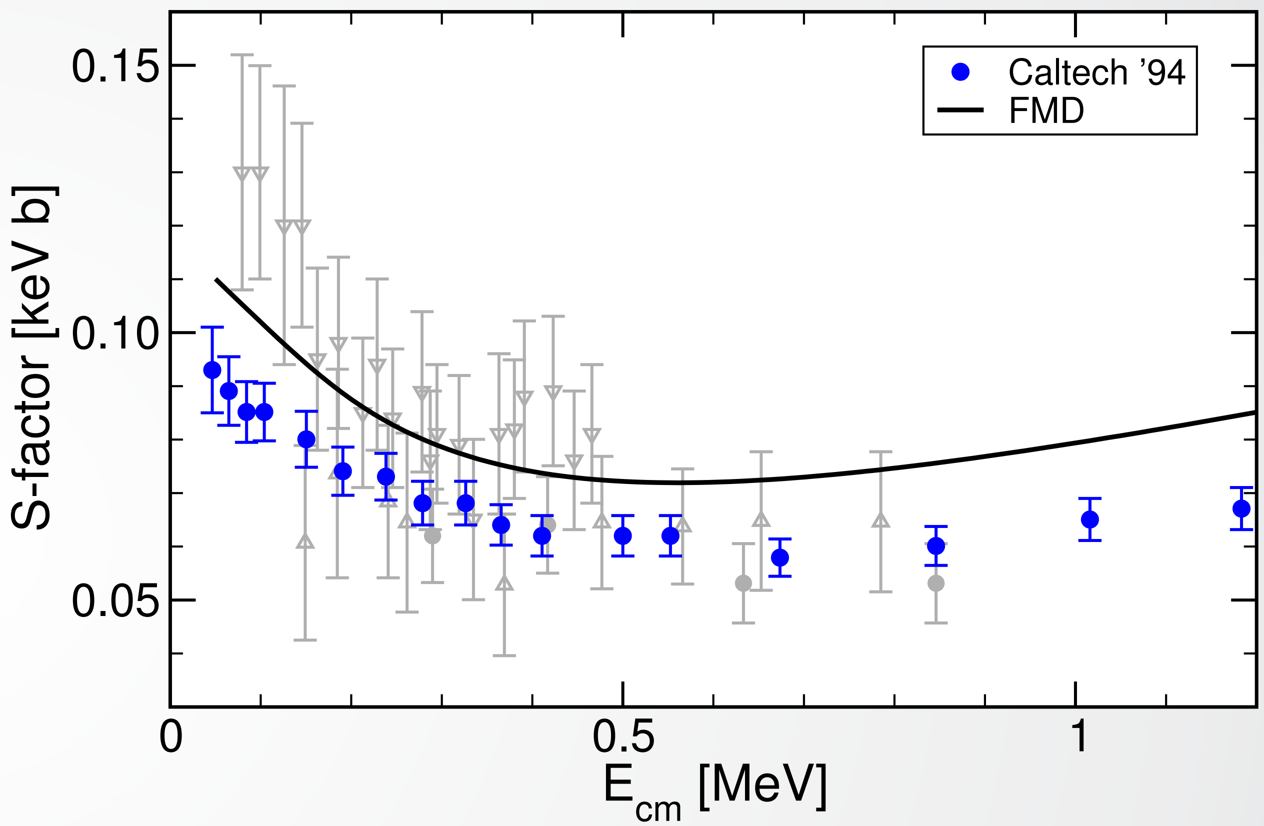
Capture Cross Section

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



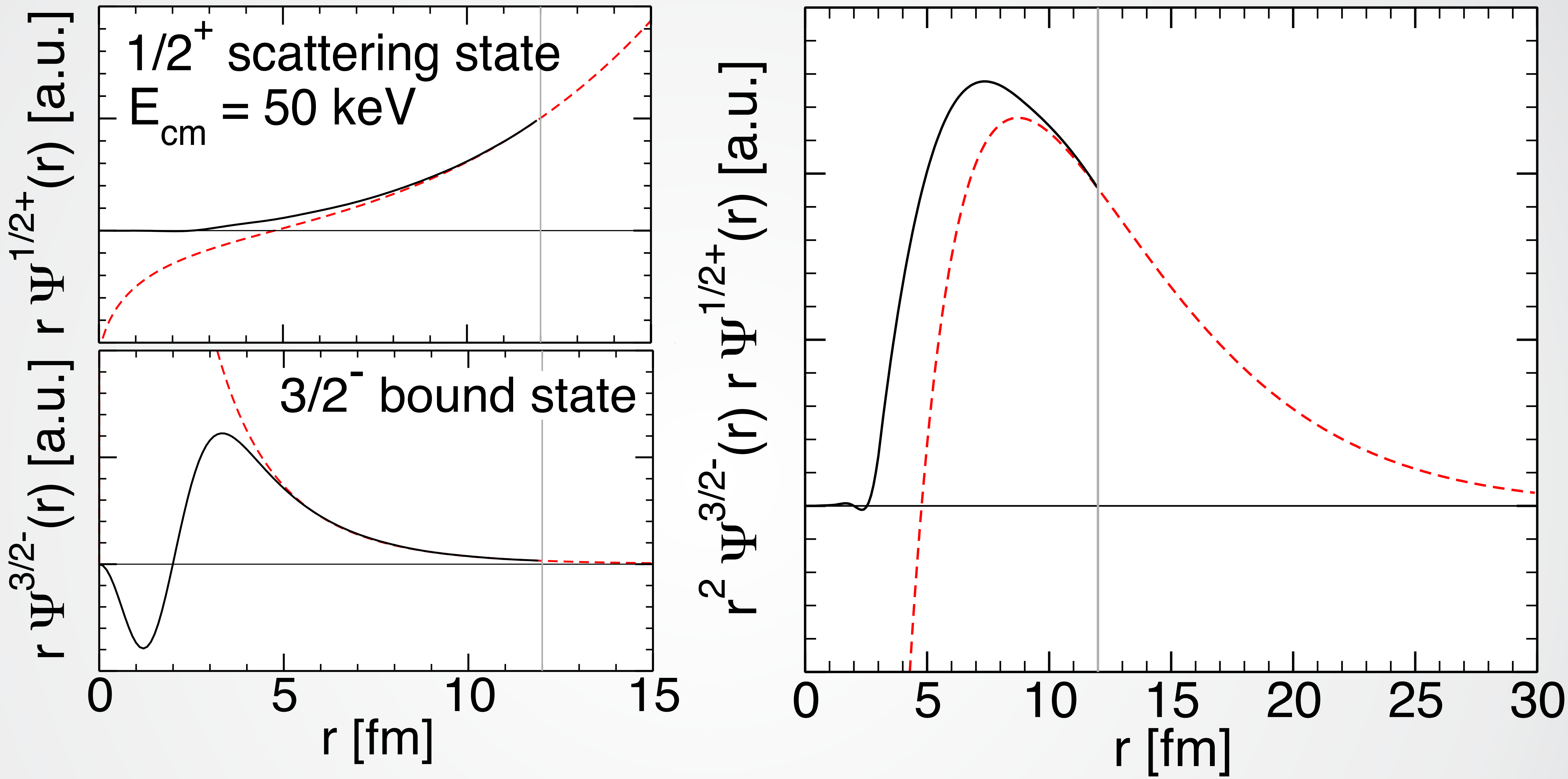
- good agreement with new high quality $^3He(\alpha,\gamma)^7Be$ data regarding both energy dependence and normalization

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



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

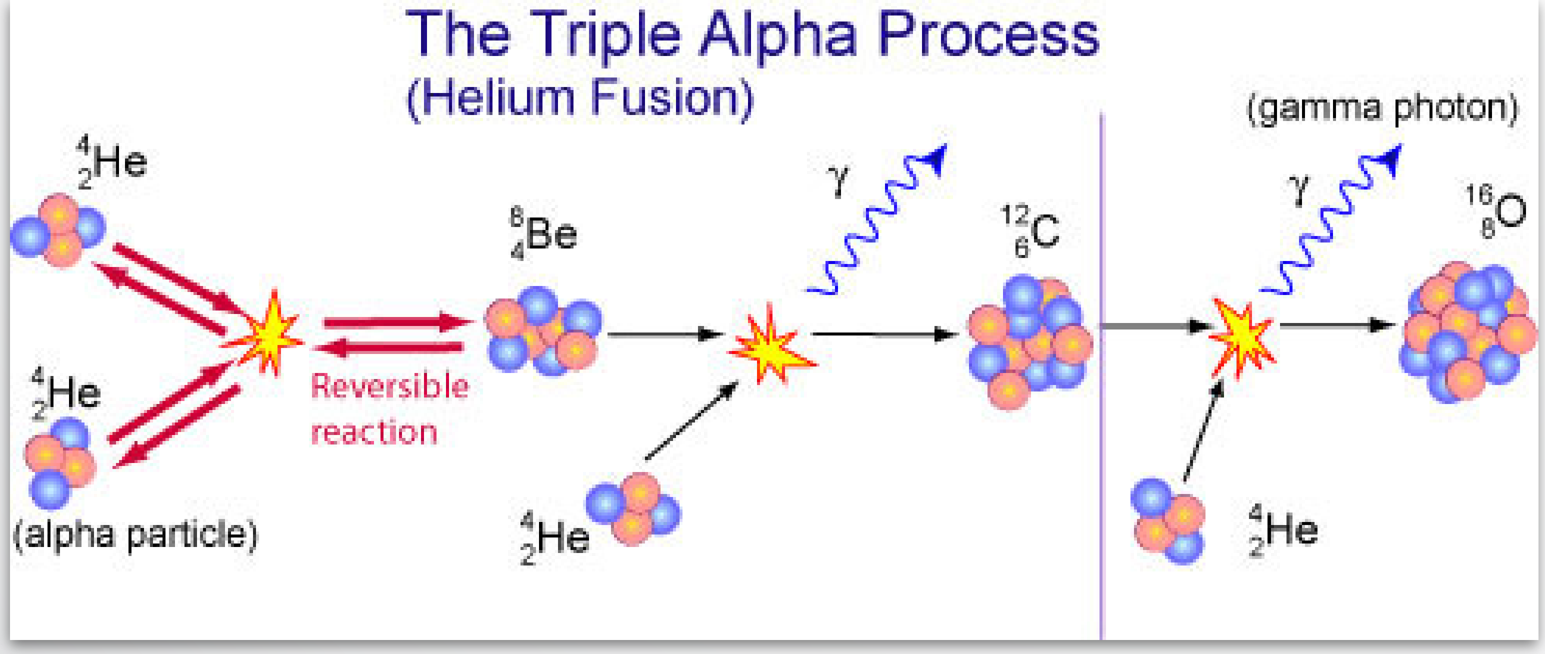
Overlap functions and Matrixelements

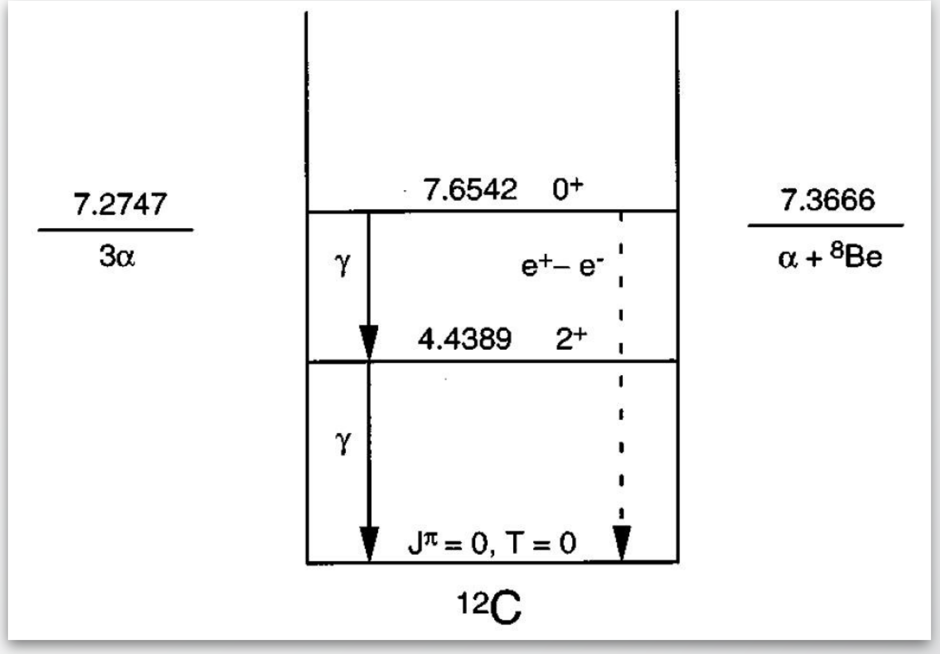


- Overlap functions from projection on RGM-cluster states
- Dipole matrix elements calculated from overlap functions reproduce full calculation within 2%
- cross section depends significantly on internal part of wave function, description as an "external" capture is too simplified

Cluster States in ^{12}C

FMD and Cluster Model Calculations



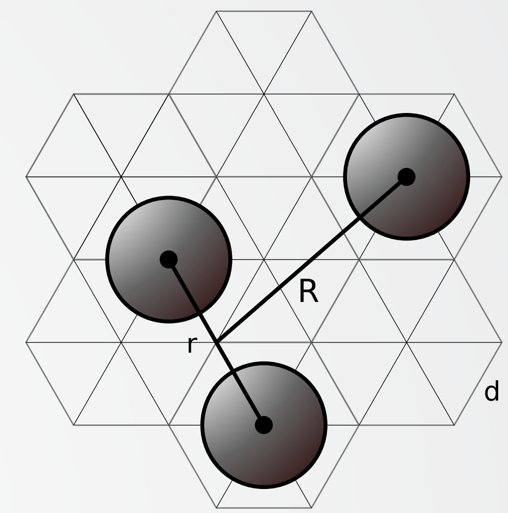


^{12}C: Microscopic α-Cluster Model

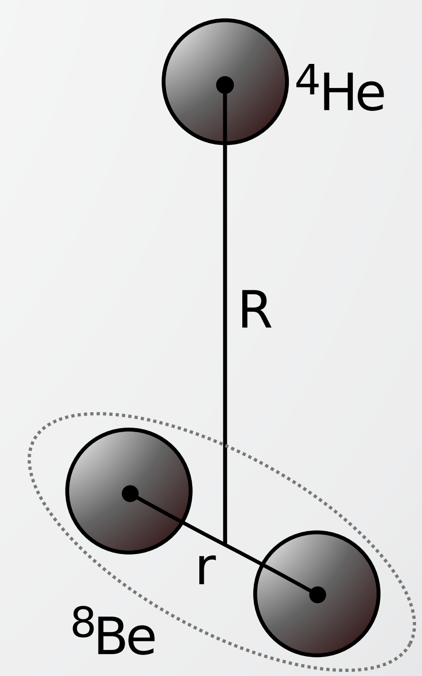
- ^{12}C is described as a system of three α-particles
- α-particles are given by HO $(0s)^4$ wave functions
- wave function is fully antisymmetrized
- effective Volkov nucleon-nucleon interaction adjusted to reproduce α-α and ^{12}C ground state properties

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

Internal Region



External Region



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

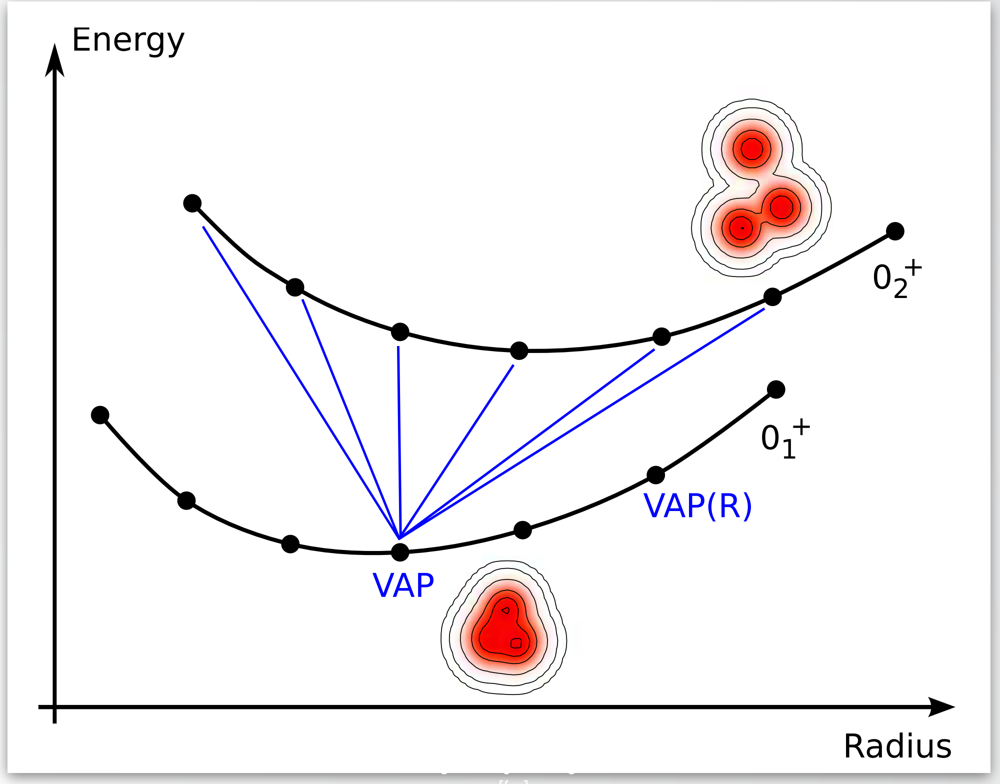
Double Projection

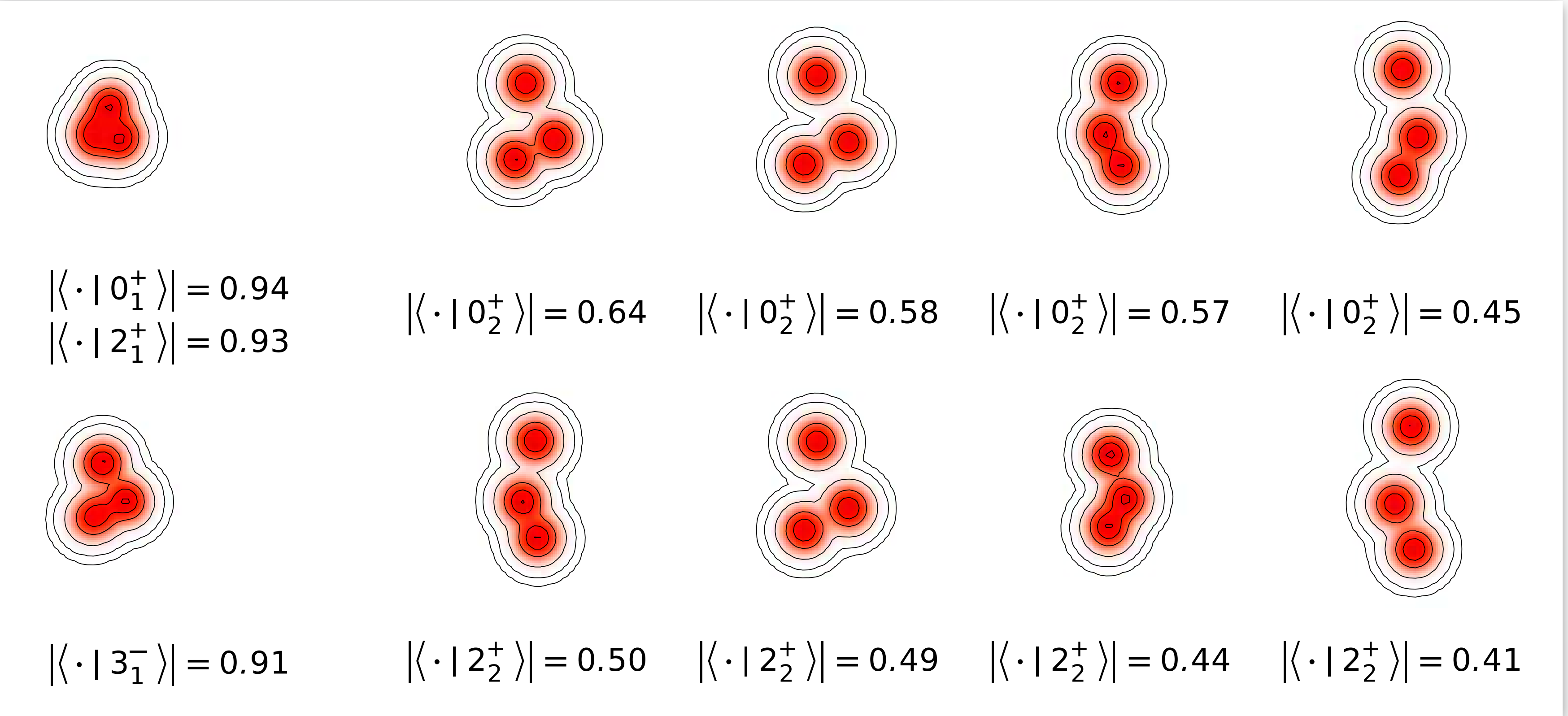
$$\left|\Psi^{^8\mathrm{Be}}_{IK}\right\rangle = \sum_i \hat{P}^{I}_{K0}\hat{\mathcal{A}}\left\{\left|\Psi_\alpha(-\tfrac{r_i}{2}\mathbf{e}_z\right\rangle \otimes \left|\Psi_\alpha(+\tfrac{r_i}{2}\mathbf{e}_z\right\rangle\right\} c^I_i$$

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

^{12}C: FMD

- **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)

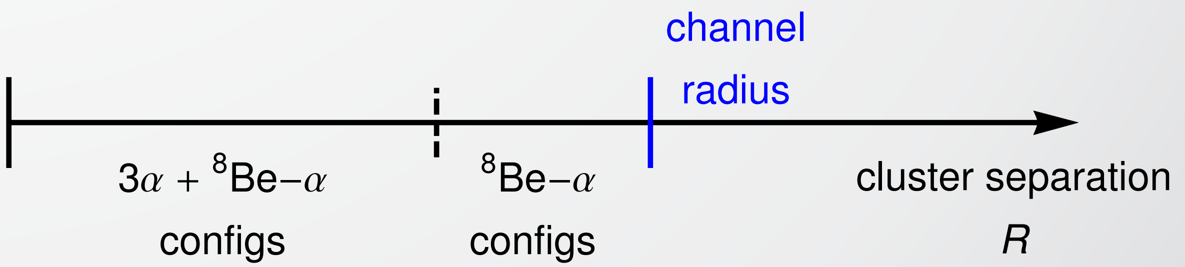
$$\psi_c(r) = A_c \frac{1}{r} W_{-\eta_c, L_c+1/2}(2\kappa_c r), \qquad \kappa_c = \sqrt{-2\mu(E - E_c)}$$

Resonances (purely outgoing Coulomb - complex energy)

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

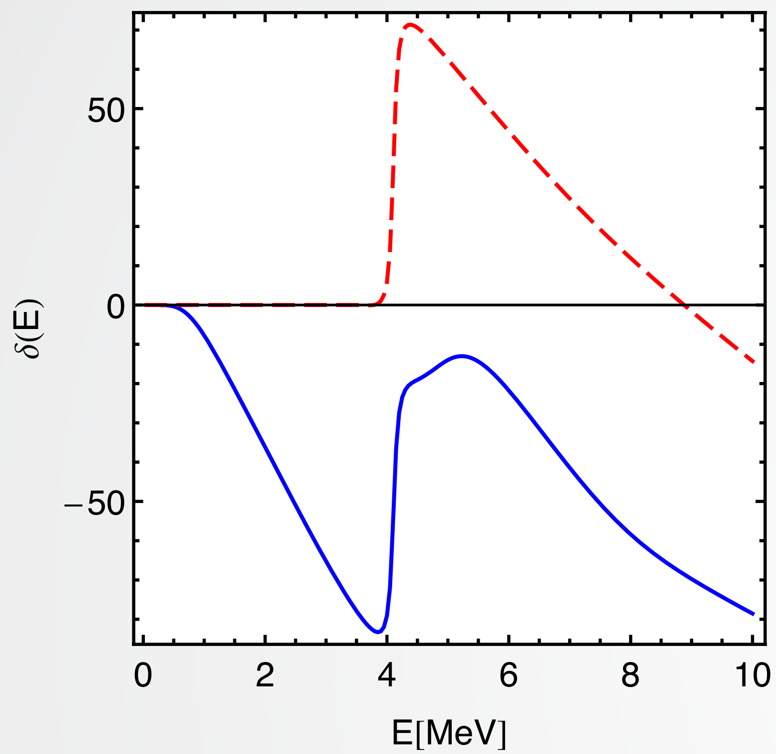
Scattering States (incoming + outgoing Coulomb)

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

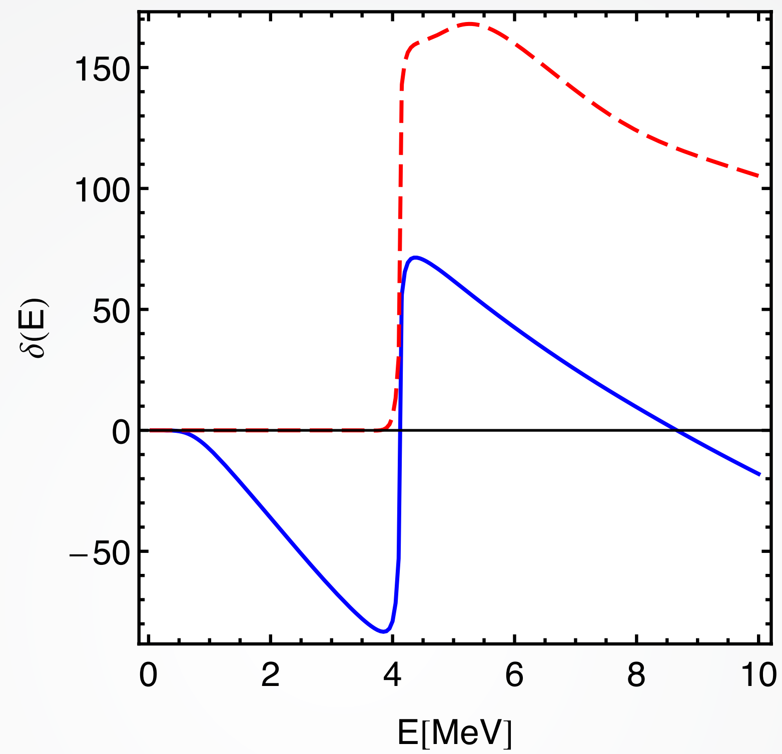


$^{8}Be(0_1^+,0_2^+)+\alpha$ Continuum: 0^+ Phaseshifts

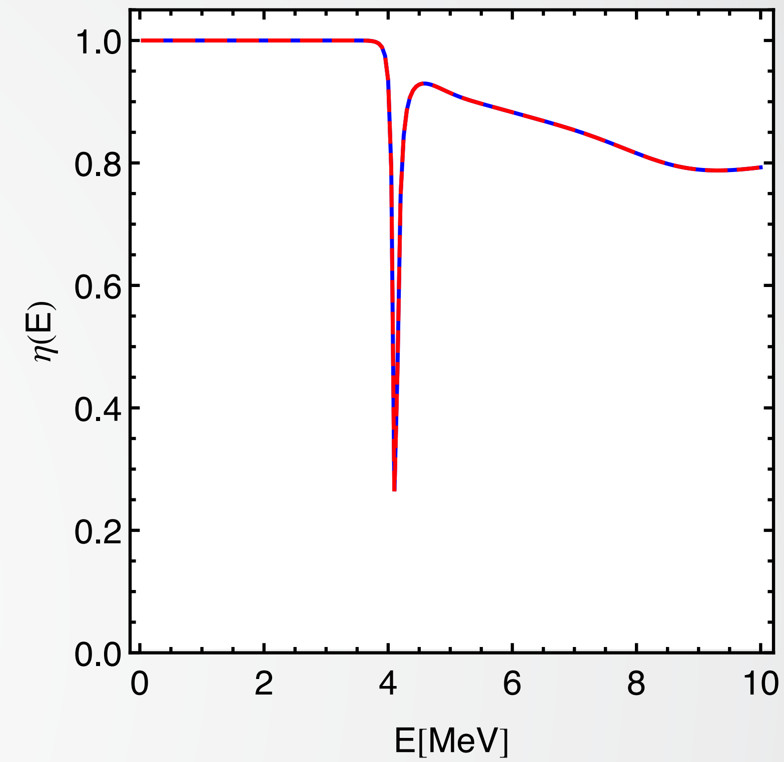
Eigenphaseshifts



Phaseshifts



Inelasticities



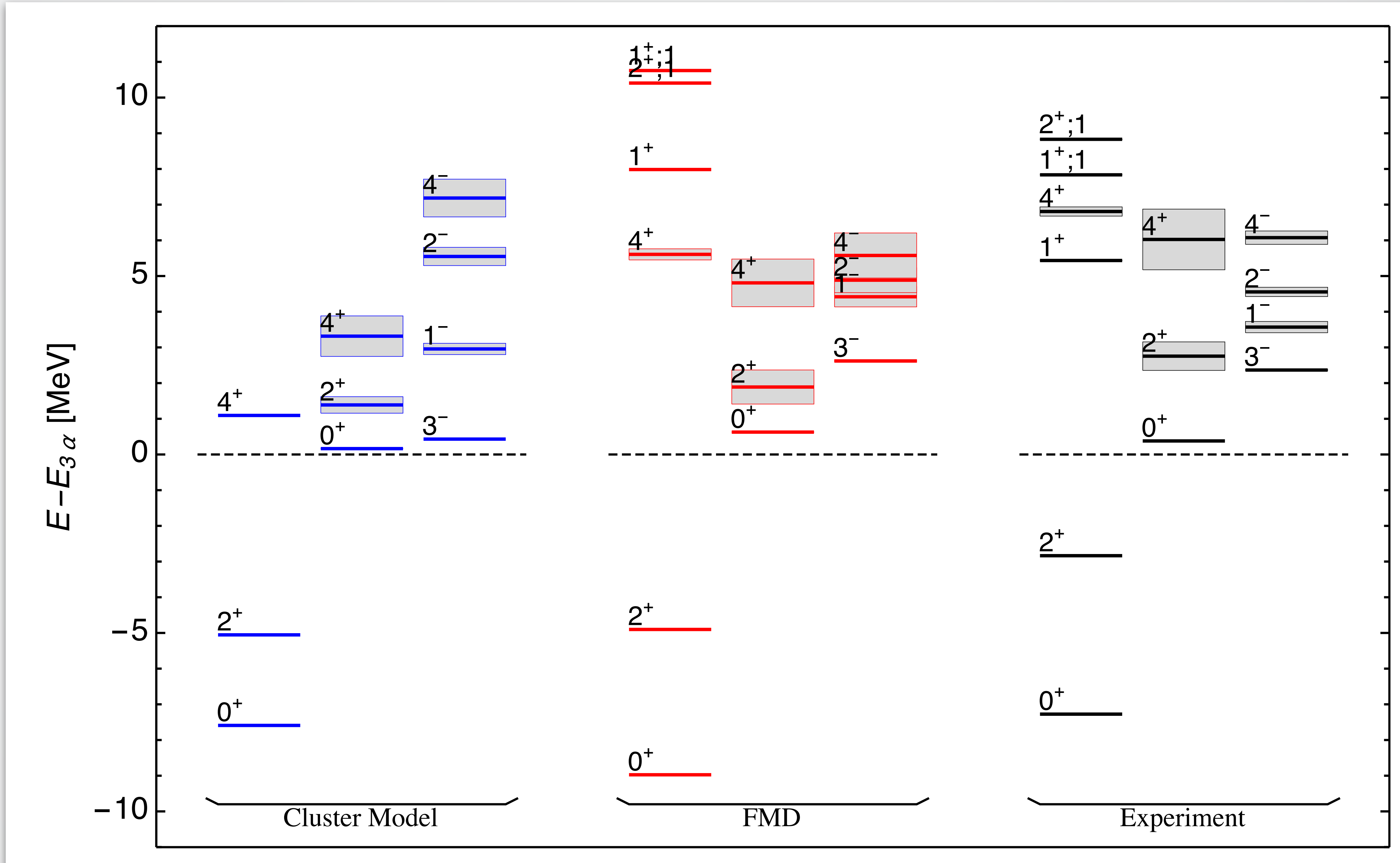
Gamow States

	E [MeV]	Γ_α [MeV]
0_2^+	0.29	$1.78\ 10^{-5}$
0_3^+	4.11	0.12
0_4^+	4.76	1.51

- Hoyle state missed when scanning the phase shifts
- non-resonant background
- strong coupling between $^{8}Be(0^+)$ and $^{8}Be(2^+)$ channel at 4.1 MeV

Cluster Model

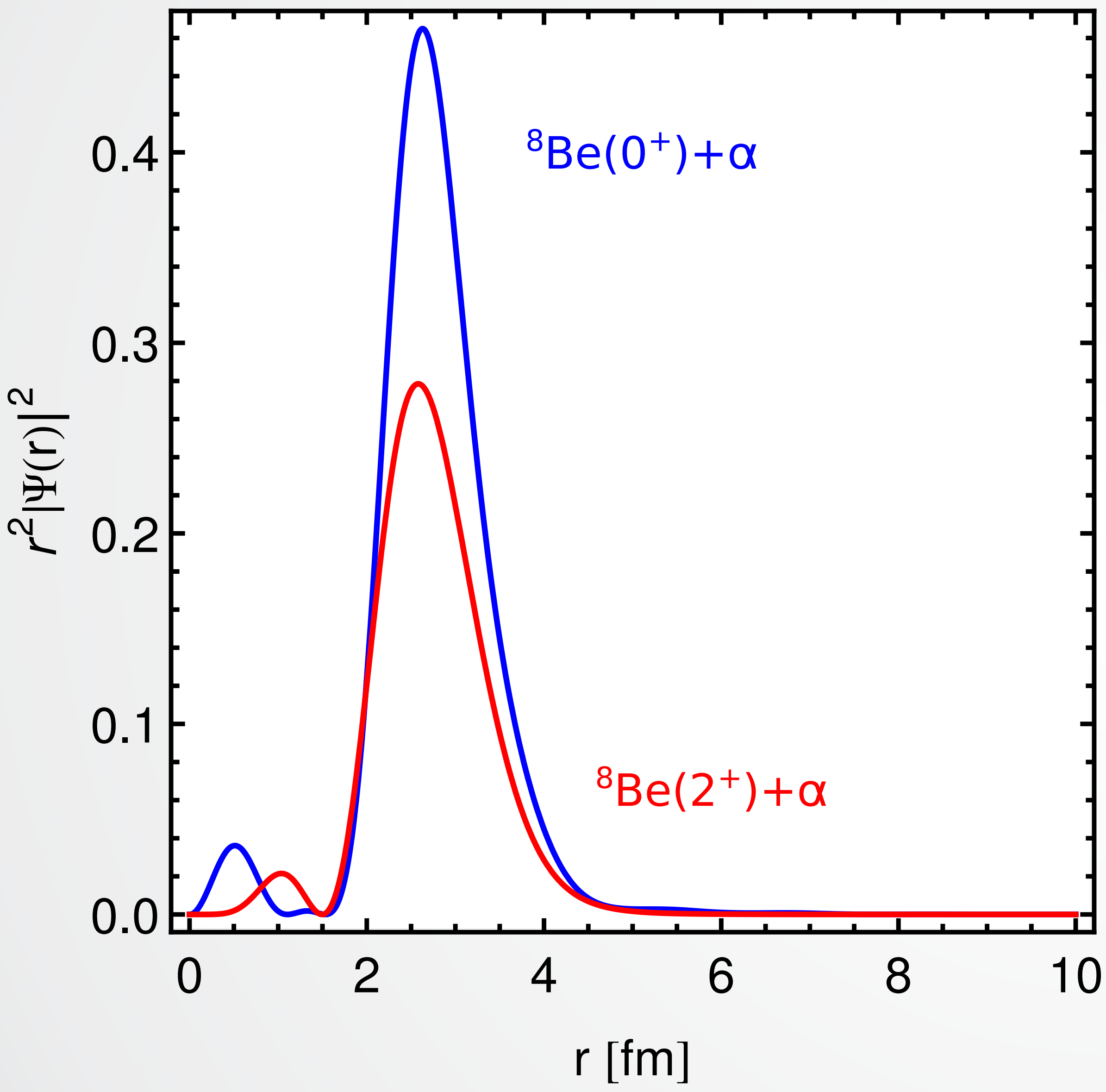
^{12}C: Spectrum



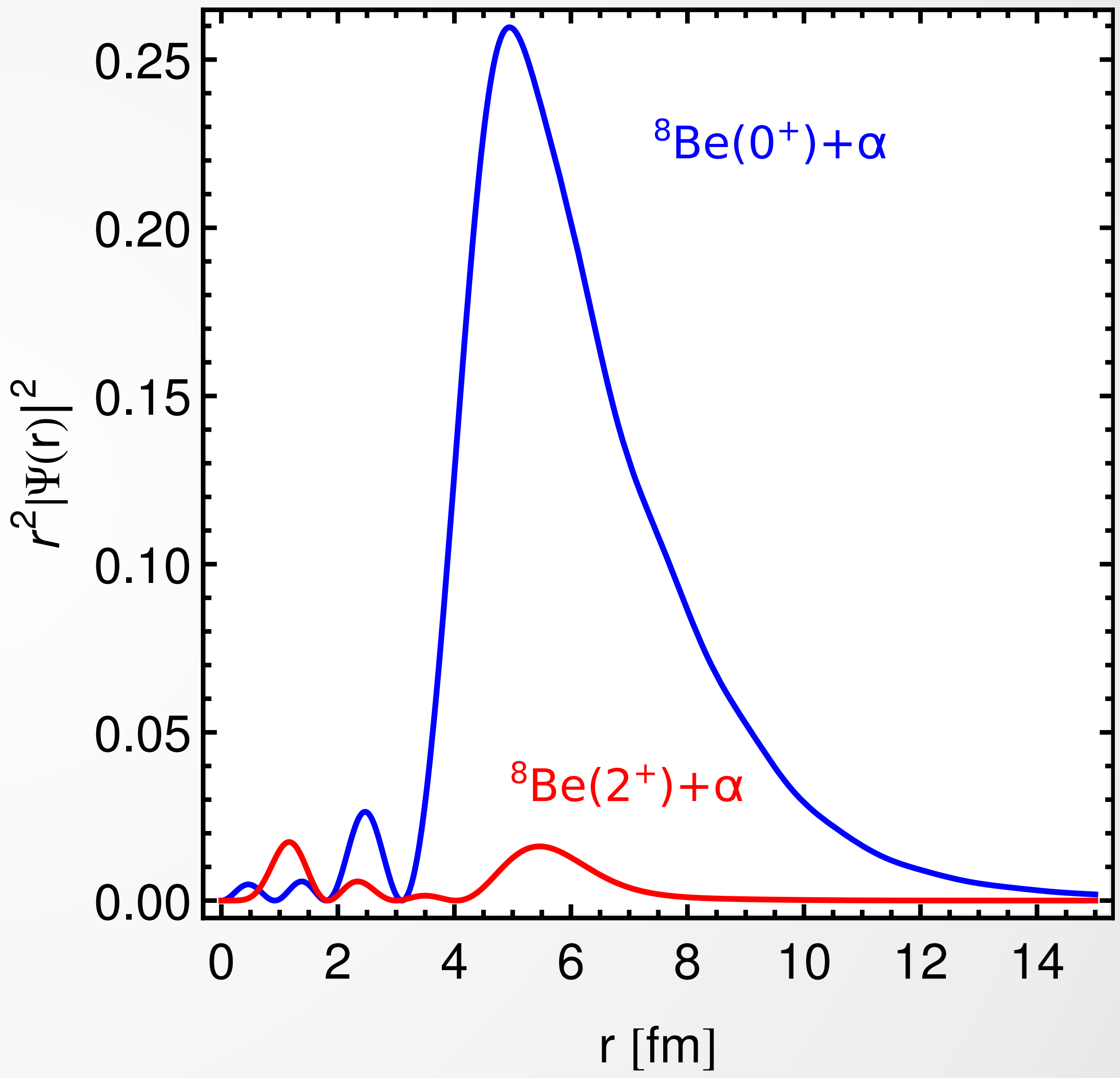
- FMD provides a consistent description of *p*-shell states, negative parity states and cluster states

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

Ground State

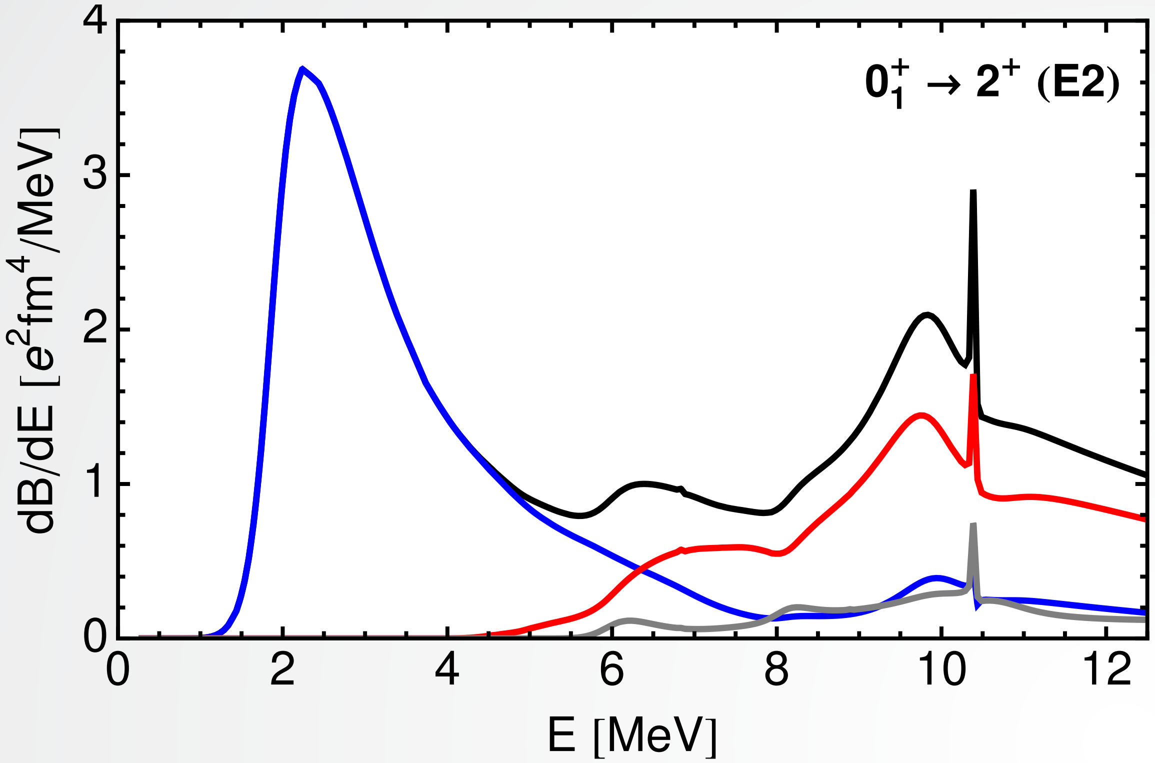


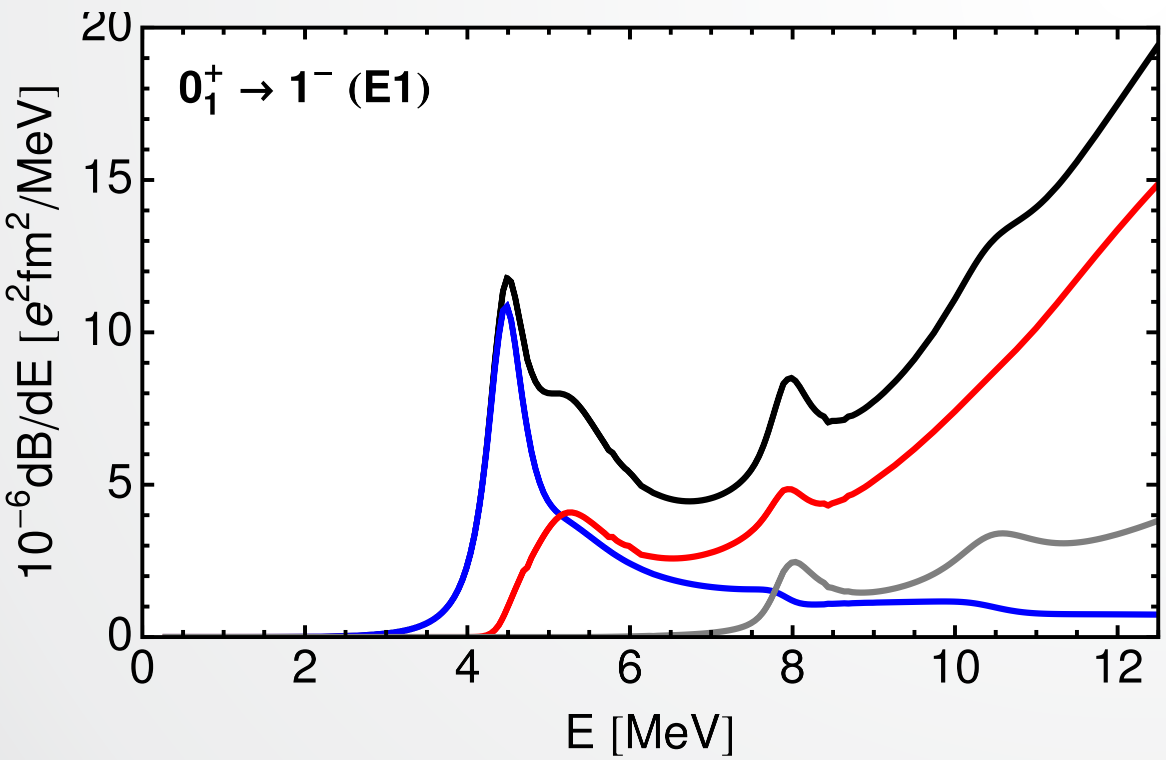
Hoyle State

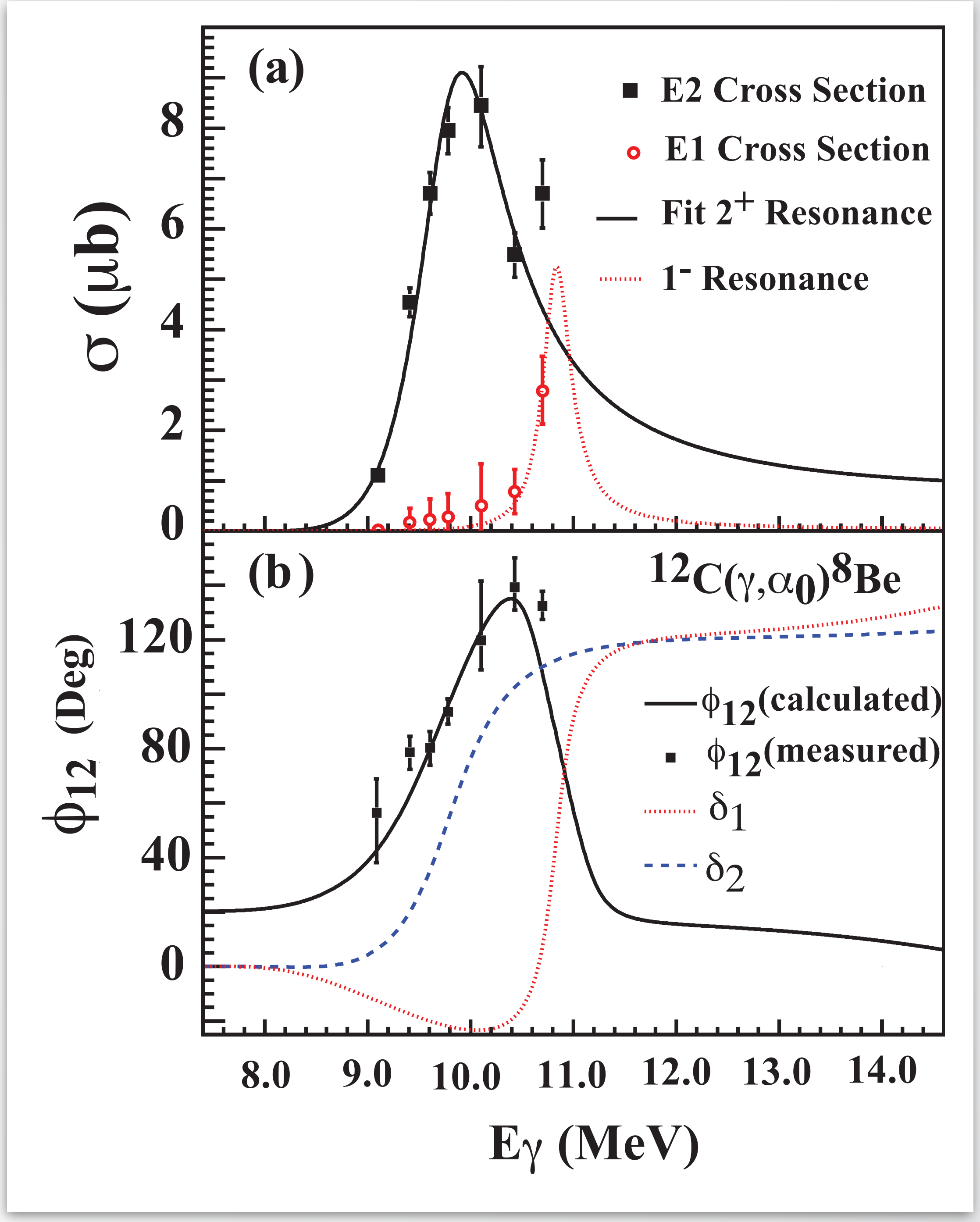


- Ground state overlap with ^{8}Be(0^{+})+α and ^{8}Be(2^{+})+α configurations of similar magnitude
- Hoyle state overlap dominated by ^{8}Be(0^{+})+α configurations, large spatial extension

^{12}C: Transitions into the Continuum



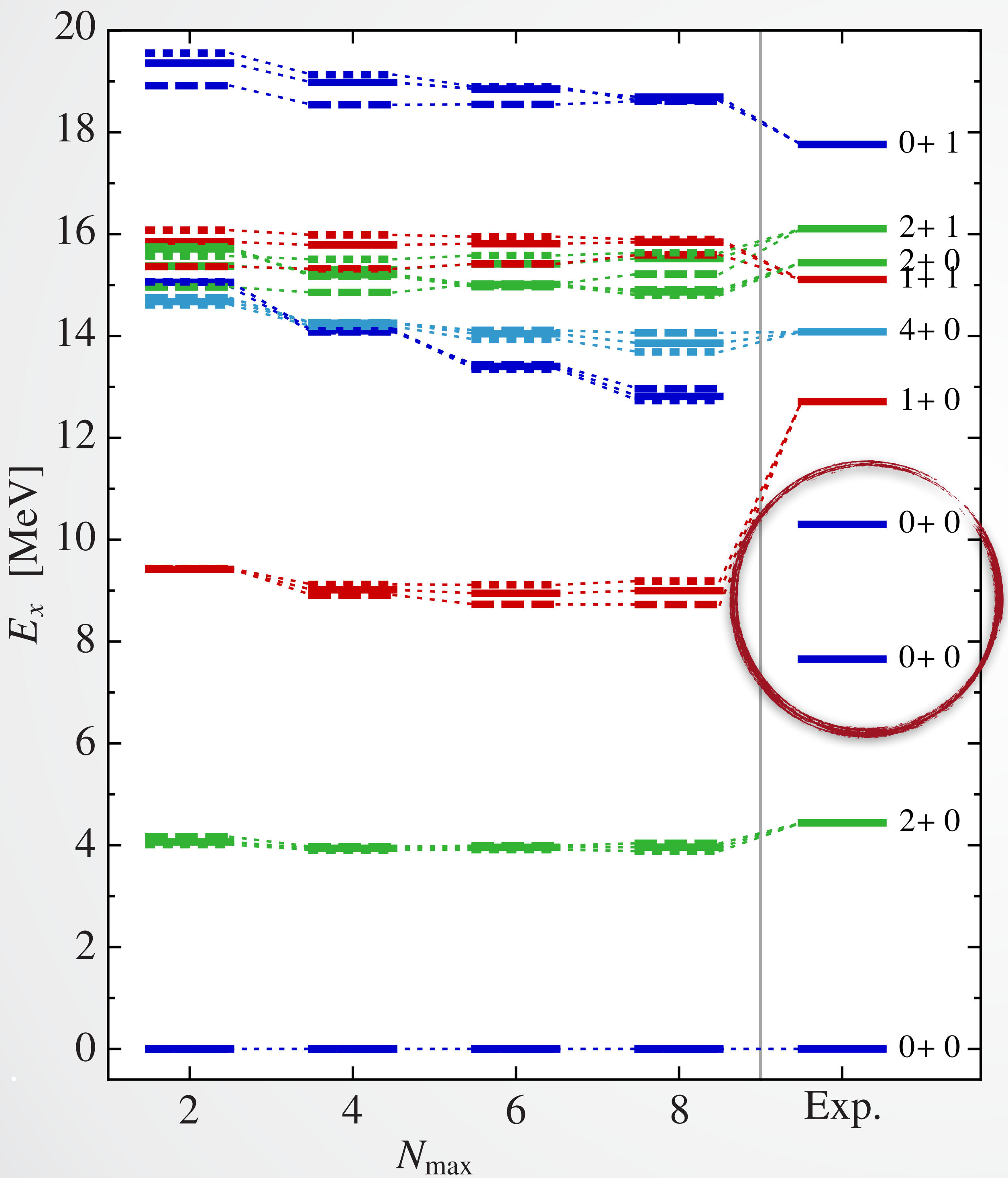




Zimmermann et al., Phys. Rev. Lett. **110**, 152502 (2013)

- E1 transition isospin-forbidden in cluster model

^{12}C: Cluster States in the Oscillator Basis ?



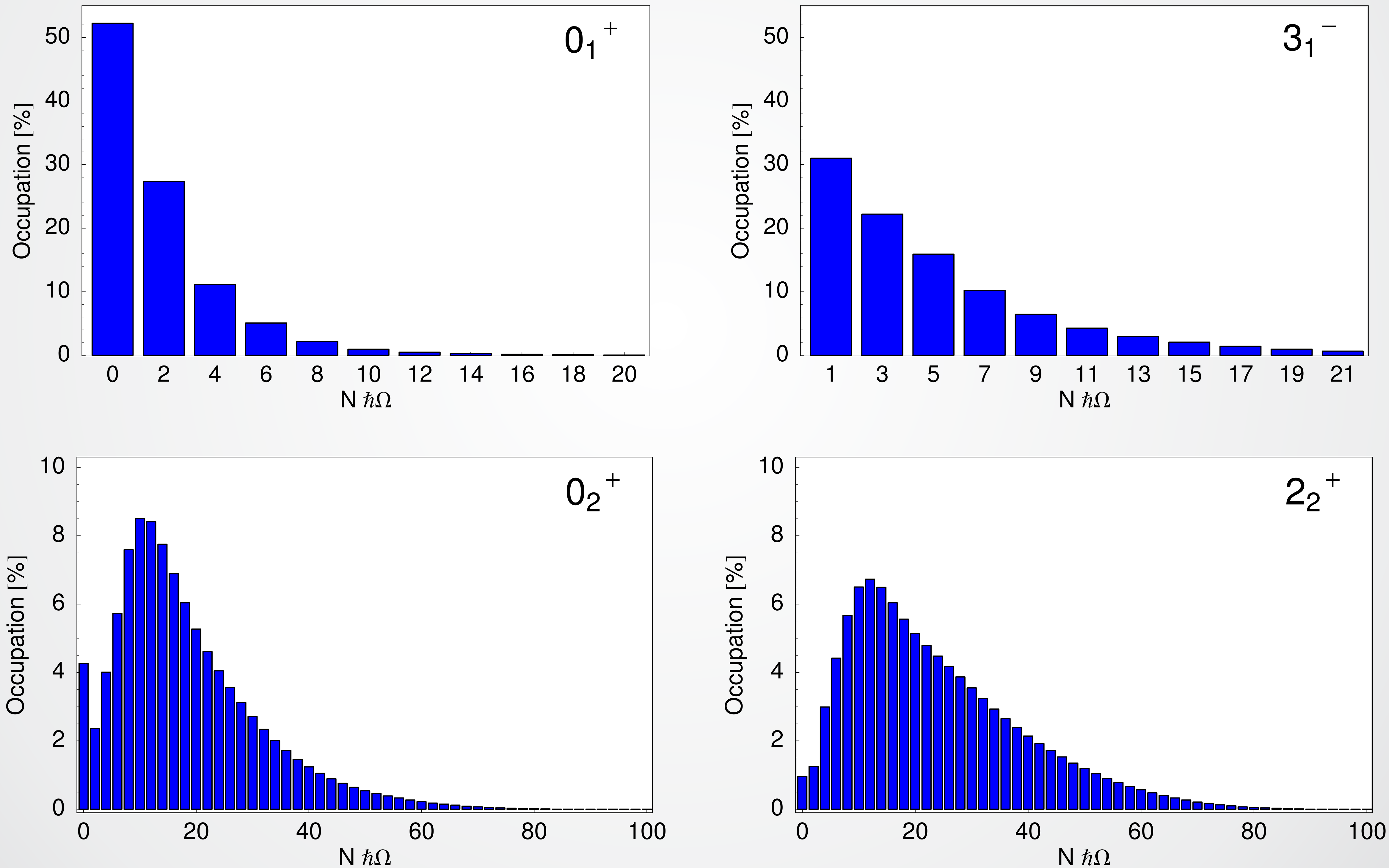
State of the art NCSM calculation with chiral NN+NNN forces

Hoyle state and other cluster states missing !

Maris, Vary, Calci, Langhammer, Binder, Roth, Phys. Rev. C **90**, 014314 (2014)

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

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



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

Continuum states in ^{12}C

- Compare α-cluster model and FMD
- Model space with ^{8}Be(0^{+},2^{+},...)+α configurations
- Consistent picture for ground state band, negative parity states and cluster states in the continuum
- Hoyle state band built on ^{8}Be(gs)+α