Microscopic description of nuclear structure and reactions with astrophysical applications

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Overview

Unitary Correlation Operator Method

Fermionic Molecular Dynamics

^{3}He(α,γ)^{7}Be Radiative Capture Reaction

- **bound and scattering states**
- **astrophysical S-factor**

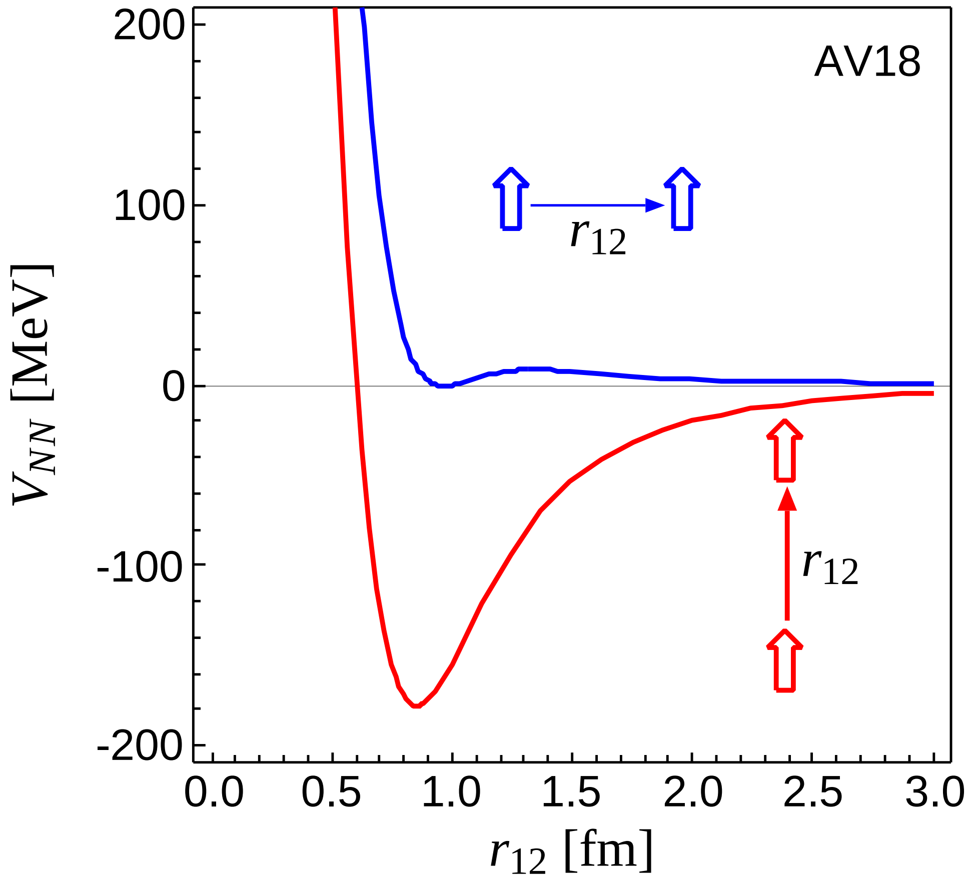
Cluster States in ^{12}C

- **FMD and microscopic cluster model**
- **electron scattering data – form factors**
- **include ^{8}Be+α continuum**

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**

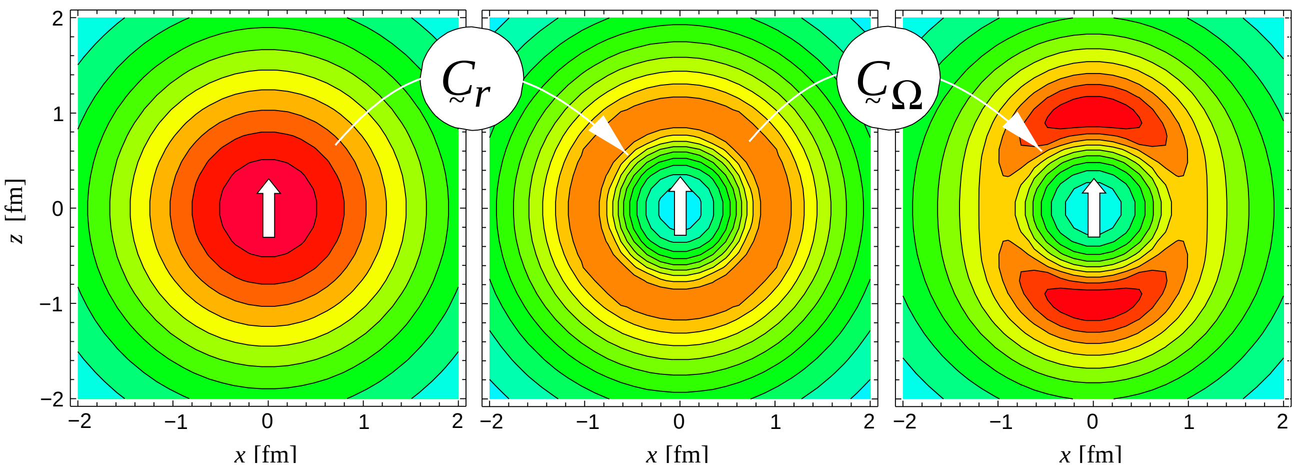
- strong dependence on the orientation of the spins due to the tensor force

➽ **tensor correlations**

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

Correlations and Energies

two-body densities



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

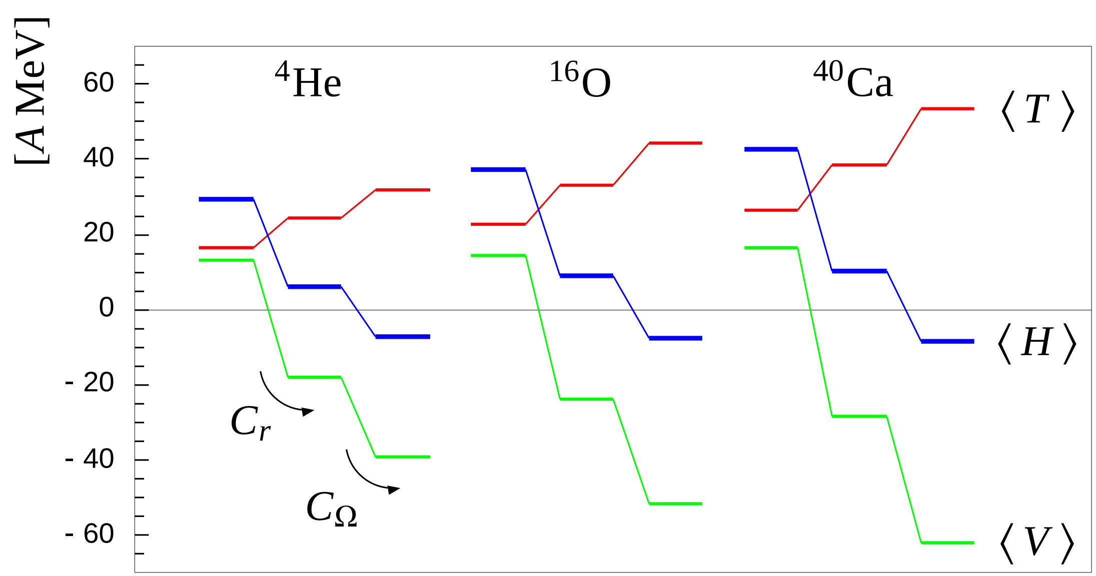
central correlator $\underset{\sim}{C}_{\mathbf{r}}$ shifts density out of the repulsive core

tensor correlator $\underset{\sim}{C}_{\boldsymbol{\Omega}}$ aligns density with spin orientation

both central and tensor correlations are essential for binding

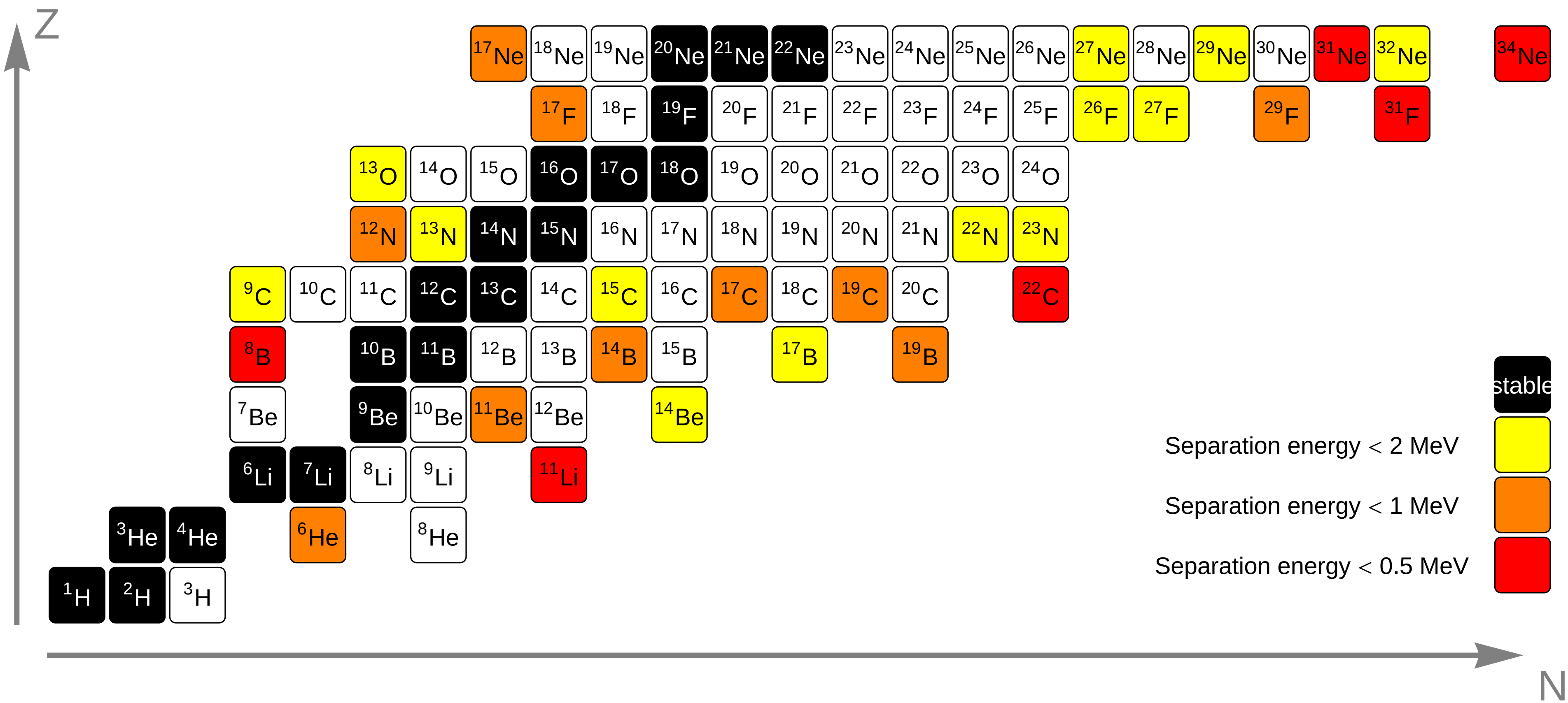
energies

$0\hbar\omega$ Harmonic Oscillator



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

Exotica: Special Challenges



- states close to one-nucleon, two-nucleon or cluster thresholds can have well developed **halo** or **cluster** structure
- these are hard to tackle in the harmonic oscillator basis

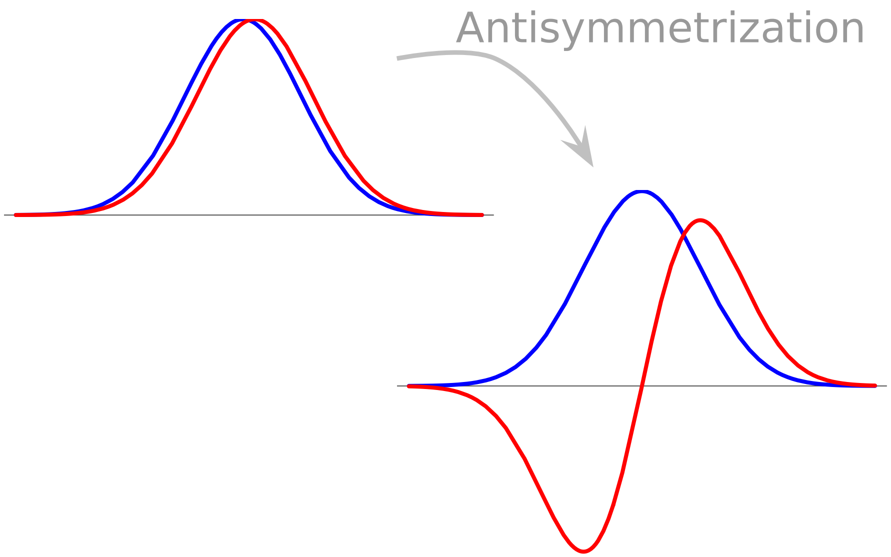
Fermionic Molecular Dynamics

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 s[tate]

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

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

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

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

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

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

Variation After Projection (VAP)

- effect of projection can be large
- **Variation after Angular Momentum and Parity Projection** (VAP) for light nuclei
- combine VAP with **constraints** on **radius**, **dipole** moment, **quadrupole** moment, . . . to generate additional configurations

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

Multiconfiguration Calculations

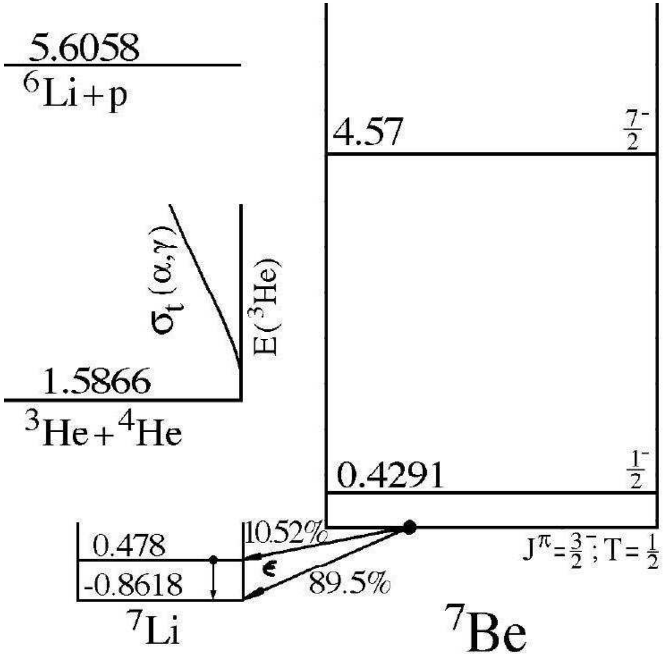
- **diagonalize** Hamiltonian in a set of projected intrinsic states

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

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

^{3}He(α,γ)^{7}Be radiative capture

one of the key reactions in the solar pp-chains



Effective Nucleon-Nucleon interaction:

UCOM(SRG) $\alpha = 0.20\ \mathrm{fm}^4$ – $\lambda \approx 1.5\ \mathrm{fm}^{-1}$

Many-Body Approach:

Fermionic Molecular Dynamics

- **Internal region: VAP configurations with radius constraint**
- **External region: Brink-type cluster configurations**
- **Matching to Coulomb solutions: Microscopic** R**-matrix method**

Results:

- ^{7}Be **bound and scattering states**
- **Astrophysical** S**-factor**

T. Neff, Phys. Rev. Lett. **106**, 042502 (2011)

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

FMD model space

Frozen configurations

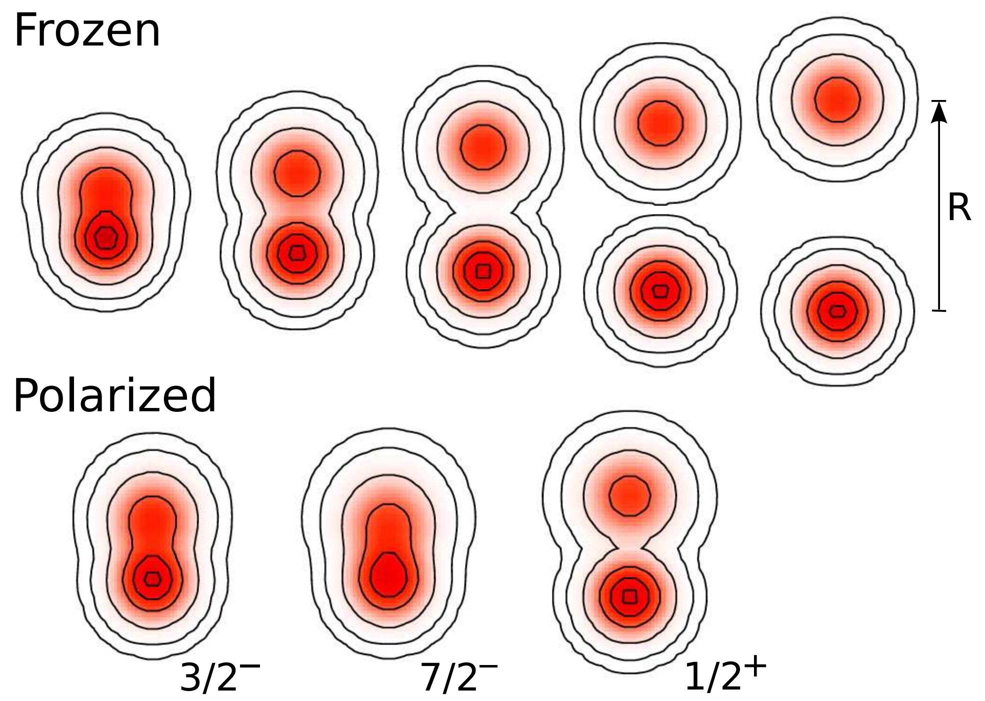
- 15 antisymmetrized wave function built with ^{4}He and ^{3}He FMD clusters up to channel radius a=12 fm

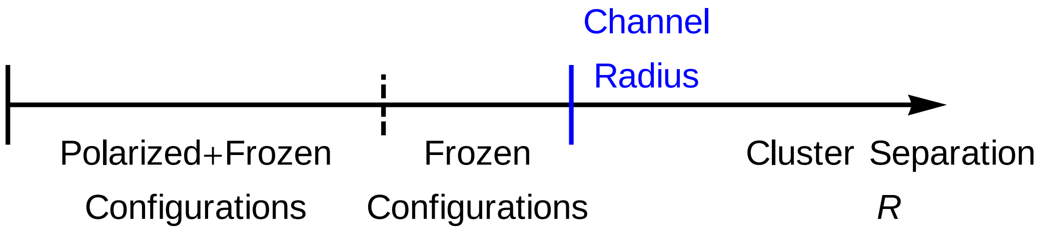
Polarized configurations

- 30 FMD wave functions obtained by VAP on $1/2^-$, $3/2^-$, $5/2^-$, $7/2^-$ and $1/2^+$, $3/2^+$ and $5/2^+$ combined with radius constraint in the interaction region

Boundary conditions

- Match relative motion of clusters at channel radius to Whittaker/Coulomb functions with the **microscopic *R*-matrix** method of the Brussels group
  D. Baye, P.-H. Heenen, P. Descouvemont





p-wave Bound and Scattering States

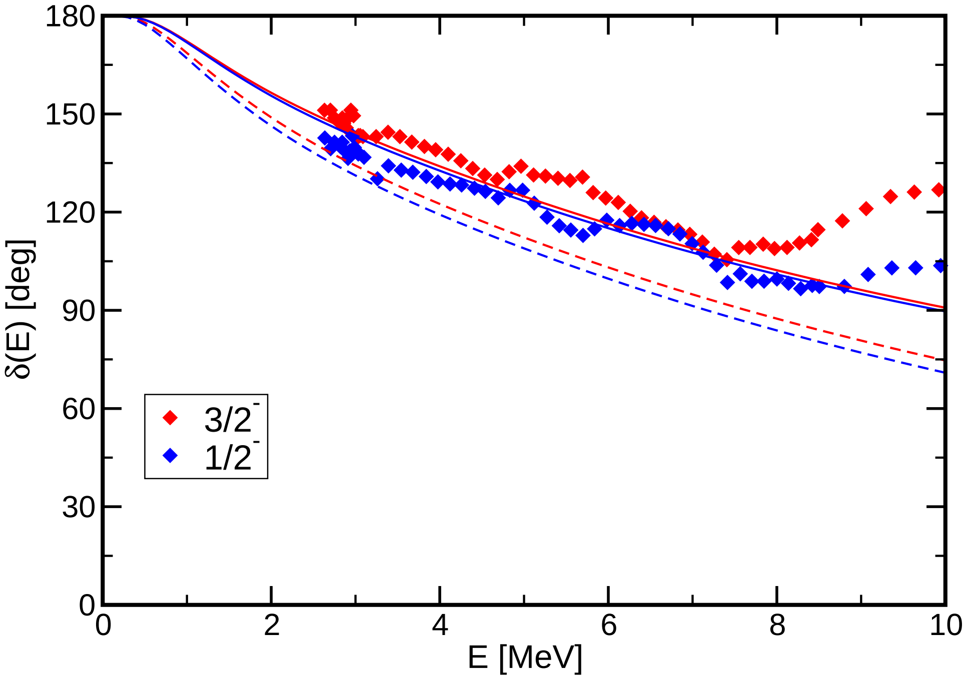
Bound states

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

- centroid of bound state energies well described if polarized configurations included
- tail of wave functions tested by charge radii and quadrupole moments

Phase shift analysis:

Spiger and Tombrello, PR **163**, 964 (1967)



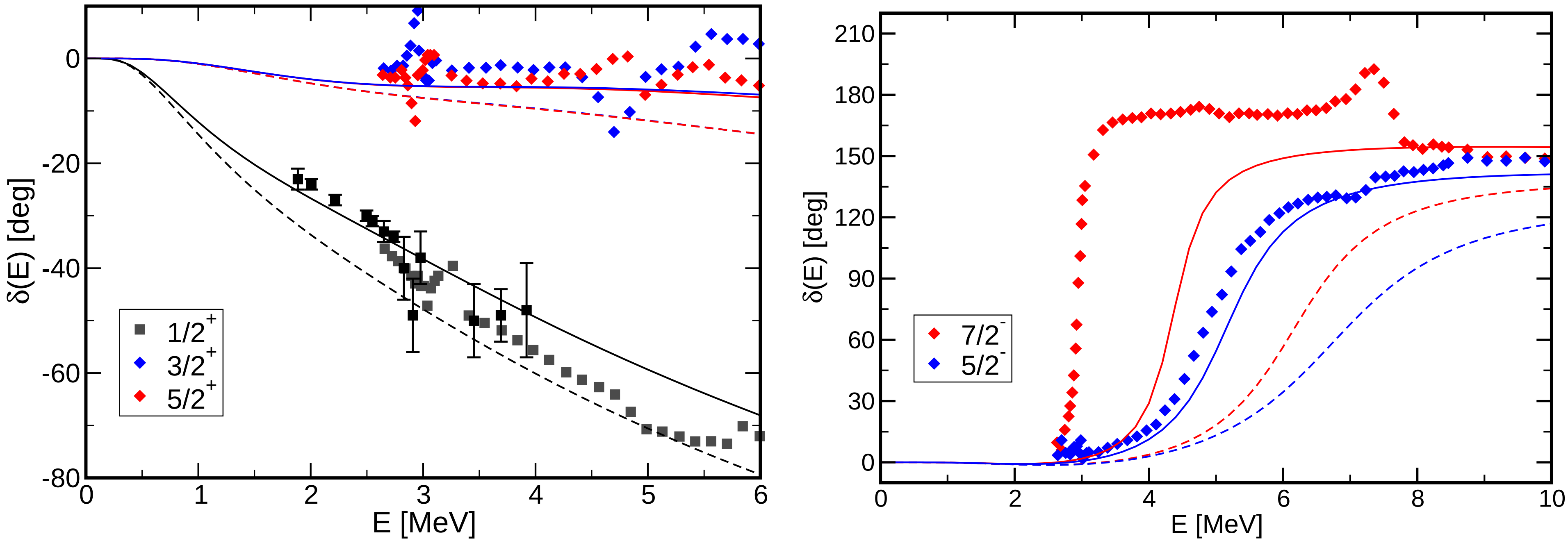
dashed lines – frozen configurations only

solid lines – polarized configurations in interaction region included

- Scattering phase shifts well described, polarization effects important

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

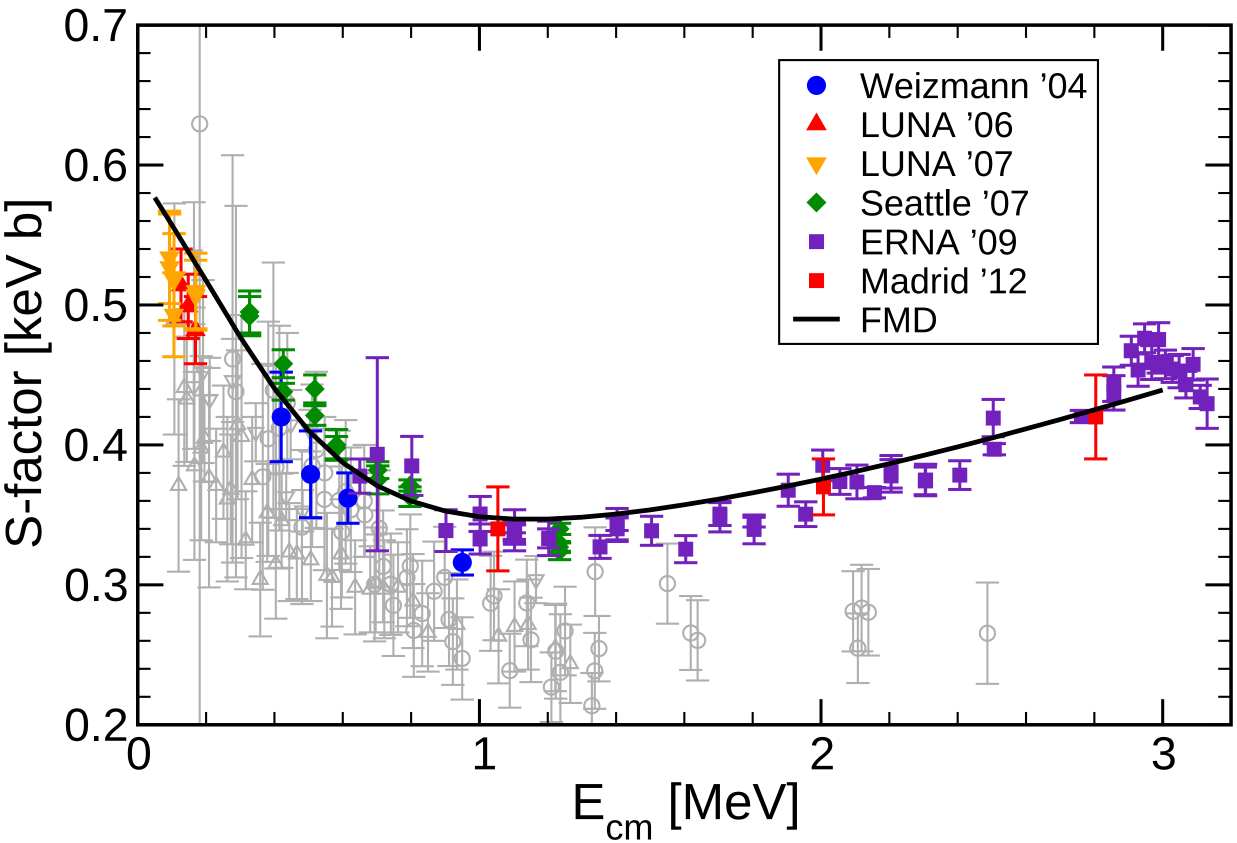
s-, *d*- and *f*-wave Scattering States



dashed lines – frozen configurations only – solid lines – FMD configurations in interaction region included

- polarization effects important
- *s*- and *d*-wave scattering phase shifts well described
- 7/2⁻ resonance too high, 5/2⁻ resonance roughly right, consistent with no-core shell model calculations

S-Factor



S-factor:

$$S(E) = \sigma(E) E \exp\{2\pi\eta\}$$

$$\eta = \frac{\mu Z_1 Z_2 e^2}{k}$$

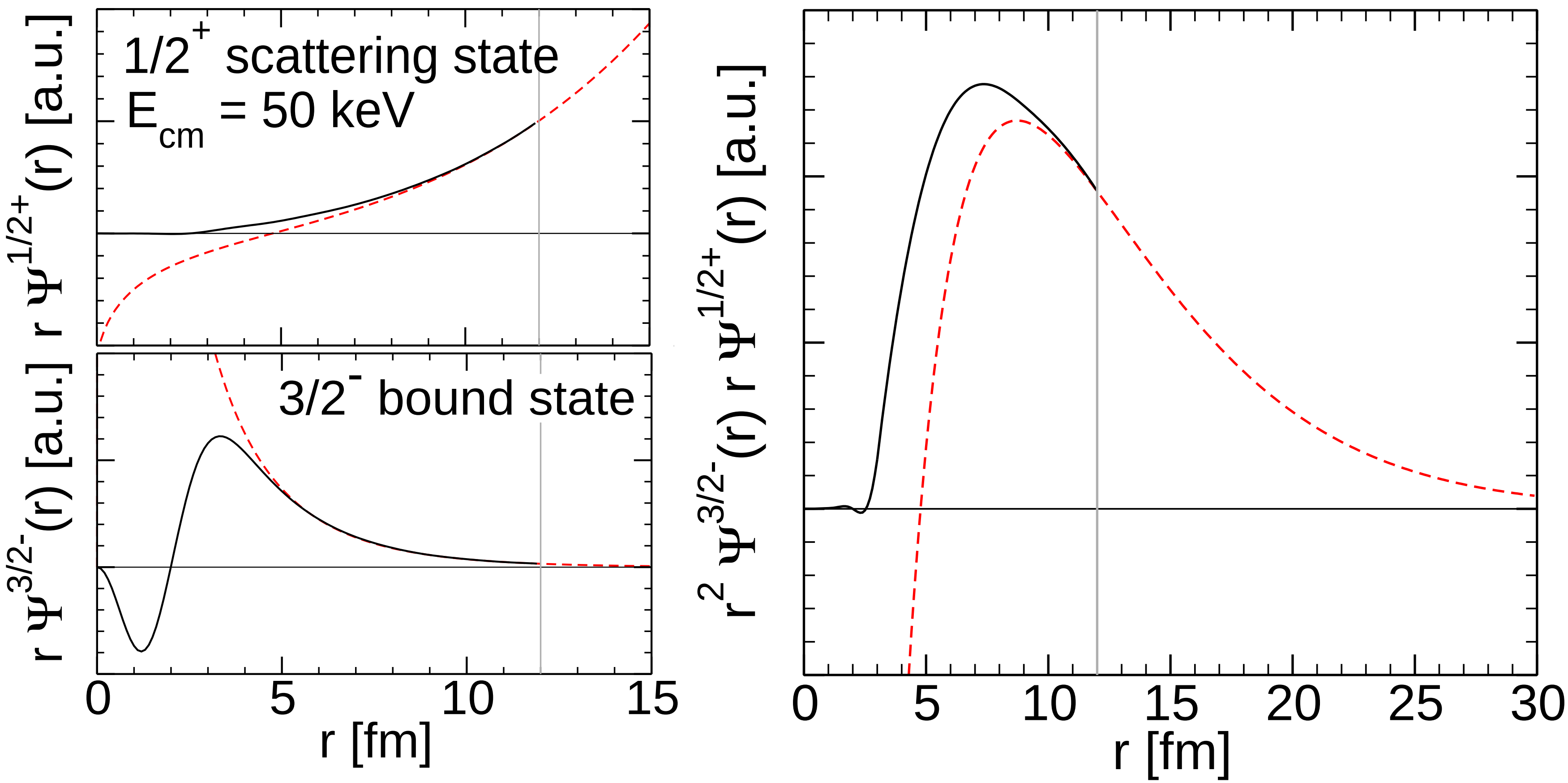
Nara Singh *et al.*, PRL **93**, 262503 (2004)
Bemmerer *et al.*, PRL **97**, 122502 (2006)
Confortola *et al.*, PRC **75**, 065803 (2007)
Brown *et al.*, PRC **76**, 055801 (2007)
Di Leva *et al.*, PRL **102**, 232502 (2009)
Carmona-Gallardo *et al.*, PRC **86**, 032801(R) (2012)

- dipole transitions from $1/2^+$, $3/2^+$, $5/2^+$ scattering states into $3/2^-$, $1/2^-$ bound states
- FMD is the only model that describes well the energy dependence and normalization of new high quality data
- fully microscopic calculation, bound and scattering states are described consistently

T. Neff, Phys. Rev. Lett. **106** (2011) 042502

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

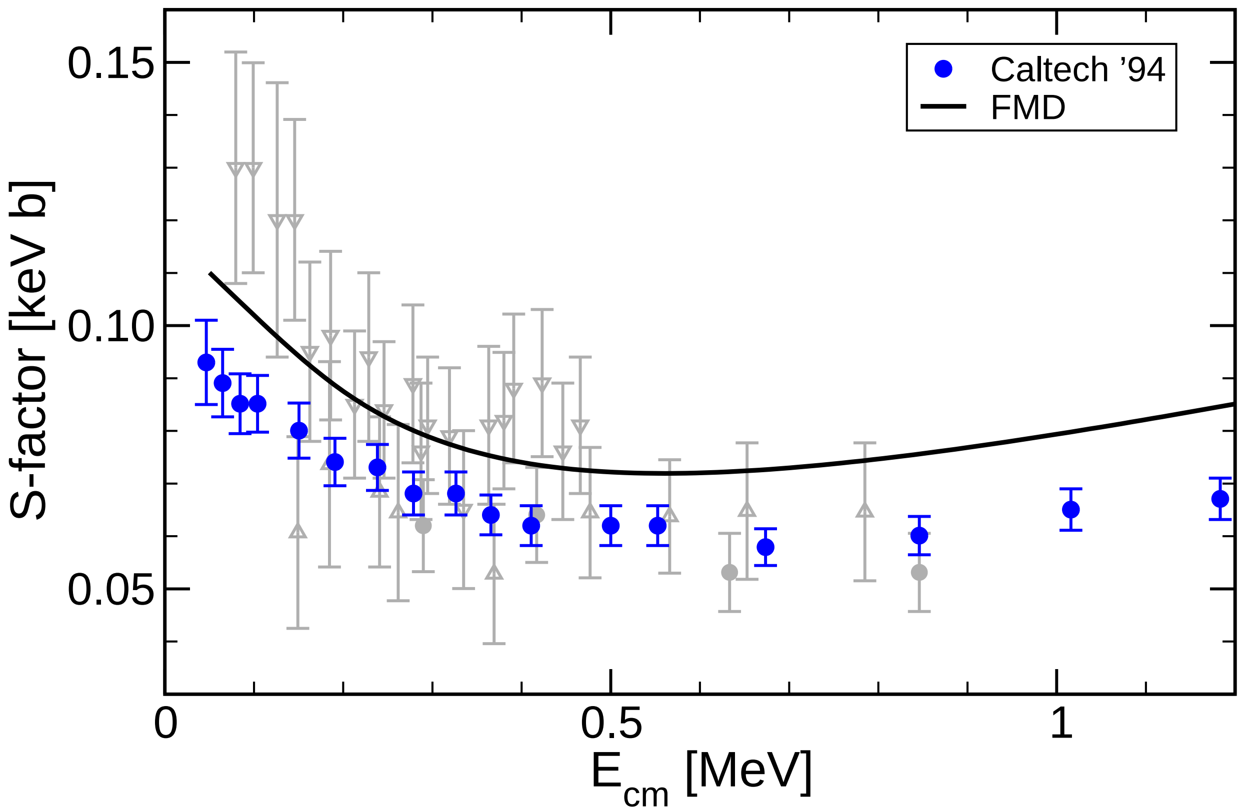
Overlap Functions and Dipole Matrixelements



- Overlap functions from projection on RGM-cluster states
- Coulomb and Whittaker functions matched at channel radius a=12 fm
- 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

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

S-Factor



S-factor:

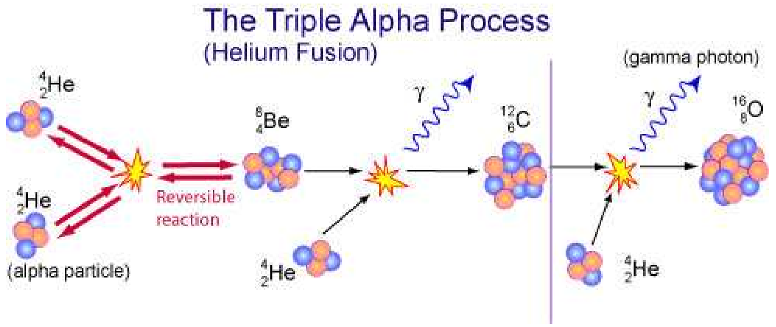
$$S(E) = \sigma(E) E \exp\{2\pi\eta\}$$

$$\eta = \frac{\mu Z_1 Z_2 e^2}{k}$$

Brune *et al.*, PRC **50**, 2205 (1994)

- isospin mirror reaction of $^{3}He(\alpha,\gamma)^{7}Be$
- ^{7}Li bound state properties and phase shifts well described

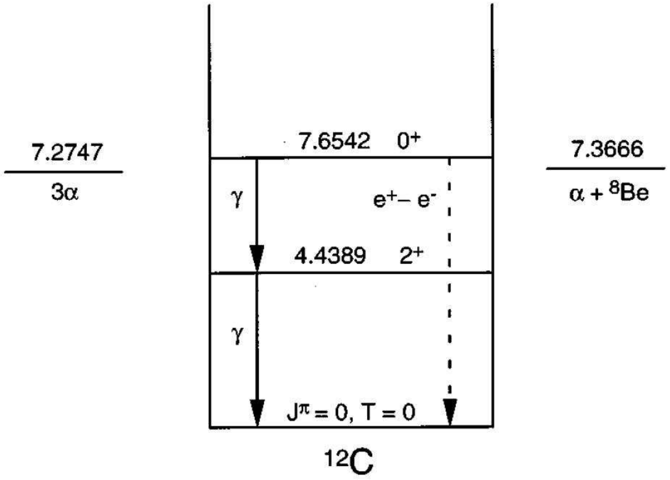
➽ FMD calculation describes energy dependence of Brune *et al.* data but cross section is larger by about 15%



Cluster States in ^{12}C

Astrophysical Motivation

- **Helium burning: triple alpha-reaction**



Structure

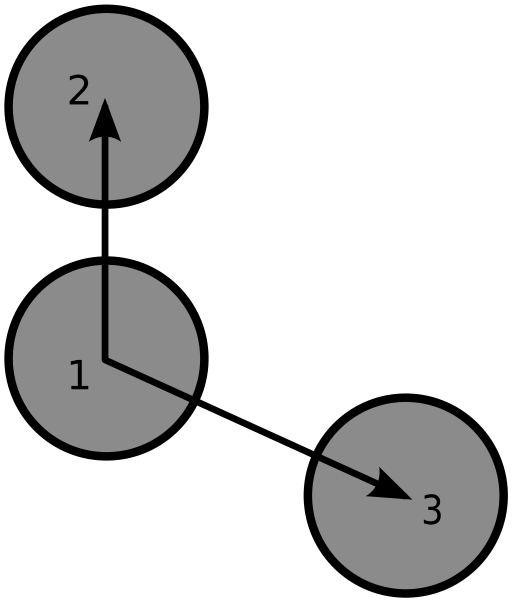
- **Is the Hoyle state a pure α-cluster state ?**
- **Other excited 0^+ and 2^+ states**

➽ **Compare FMD results to microscopic α-cluster model**

➽ **Intrinsic structure from two-body densities**

➽ **Analyze wave functions in harmonic oscillator basis**

Microscopic α-Cluster Model



$$R_{12} = (2, 4, \ldots, 10)\,\mathrm{fm}$$
$$R_{13} = (2, 4, \ldots, 10)\,\mathrm{fm}$$
$$\cos(\vartheta) = (1.0, 0.8, \ldots, -1.0)$$

alltogether 165 configurations

Kamimura, Nuc. Phys. **A351** (1981) 456

Funaki et al., Phys. Rev. C **67** (2003) 051306(R)

Basis States

- describe Hoyle State as a system of 3 ^{4}He nuclei

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

Volkov Interaction

- simple central interaction
- parameters adjusted to give reasonable α binding energy and radius, $\alpha - \alpha$ scattering data, adjusted to reproduce ^{12}C ground state energy

✘ only reasonable for ^{4}He, ^{8}Be and ^{12}C nuclei

‘BEC’ wave functions

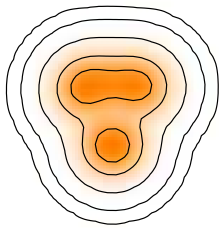
- interpretation of the Hoyle state as a Bose-Einstein Condensate of α-particles by Funaki, Tohsaki, Horiuchi, Schuck, Röpke
- same interaction and α-cluster parameters used

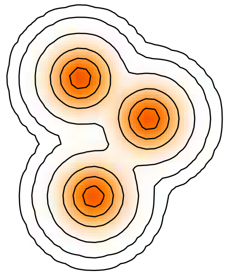
Cluster States in ^{12}C
FMD

Basis States

- 20 FMD states obtained in Variation after Projection on 0^+ and 2^+ with constraints on the radius
- 42 FMD states obtained in Variation after Projection on parity with constraints on radius and quadrupole deformation
- 165 α-cluster configurations

➻ projected on angular momentum and linear momentum

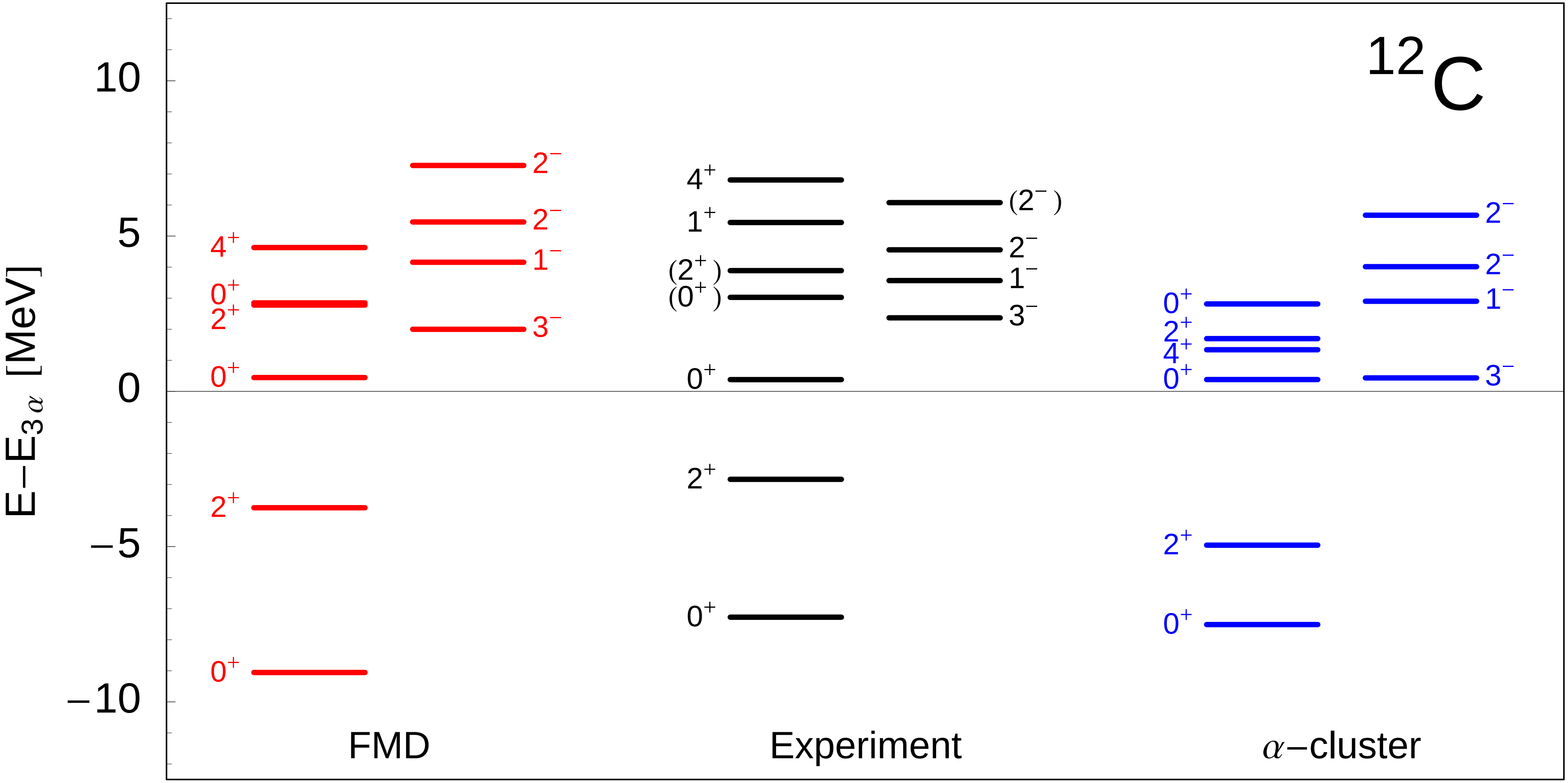




Interaction

- UCOM interaction (I_ϑ=0.30 fm^3 with phenomenological two-body correction term (momentum-dependent central and spin-orbit) fitted to doubly-magic nuclei
- not tuned for α-α scattering or ^{12}C properties

Comparison



^{12}C
10
5
0
−5
−10
E−E$_{3\alpha}$ [MeV]
FMD
Experiment
α−cluster
4$^+$
0$^+$
2$^+$
0$^+$
2$^+$
0$^+$
2$^-$
2$^-$
1$^-$
3$^-$
4$^+$
1$^+$
(2$^+$)
(0$^+$)
0$^+$
2$^+$
0$^+$
(2$^-$)
2$^-$
1$^-$
3$^-$
0$^+$
2$^+$
4$^+$
0$^+$
2$^+$
0$^+$
2$^-$
2$^-$
1$^-$
3$^-$

Comparison

	Exp[1]	Exp[2]	FMD	α-cluster	'BEC'[3]
$E(0_1^+)$	-92.16		-92.64	-89.56	-89.52
$E^*(2_1^+)$	4.44		5.31	2.56	2.81
$E(3\alpha)$	-84.89		-83.59	-82.05	-82.05
$E(0_2^+) - E(3\alpha)$	0.38		0.43	0.38	0.26
$E(0_3^+) - E(3\alpha)$	(3.0)	2.7(3)	2.84	2.81	
$E(2_2^+) - E(3\alpha)$	(3.89)	2.76(11)	2.77	1.70	
$r_{\mathrm{charge}}(0_1^+)$	2.47(2)		2.53	2.54	
$r(0_1^+)$			2.39	2.40	2.40
$r(0_2^+)$			3.38	3.71	3.83
$r(0_3^+)$			4.62	4.75	
$r(2_1^+)$			2.50	2.37	2.38
$r(2_2^+)$			4.43	4.02	
$M(E0, 0_1^+ \rightarrow 0_2^+)$	5.4(2)		6.53	6.52	6.45
$B(E2, 2_1^+ \rightarrow 0_1^+)$	7.6(4)		8.69	9.16	
$B(E2, 2_1^+ \rightarrow 0_2^+)$	2.6(4)		3.83	0.84	
$B(E2, 2_2^+ \rightarrow 0_1^+)$		0.73(13)	0.46	1.99	

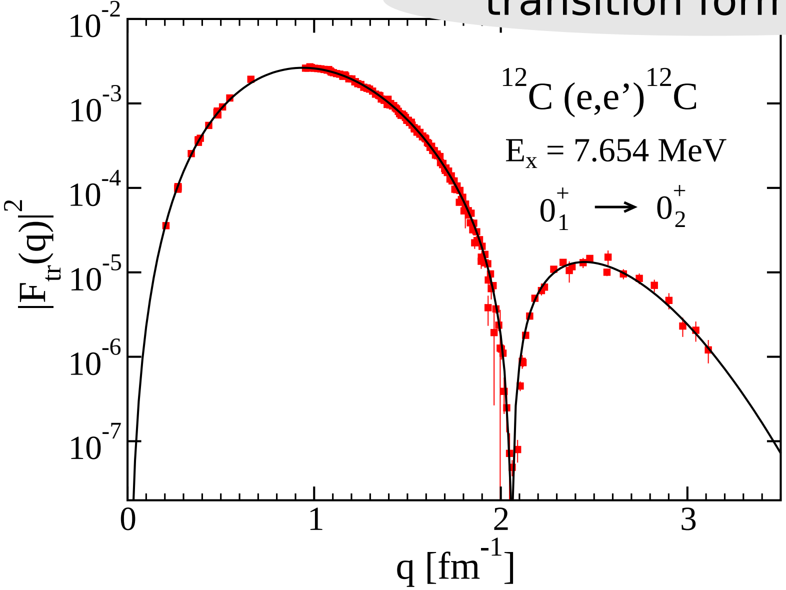
experimental situation for 0^+ and 2^+ states above threshold still not completely settled

calculated in bound state approximation

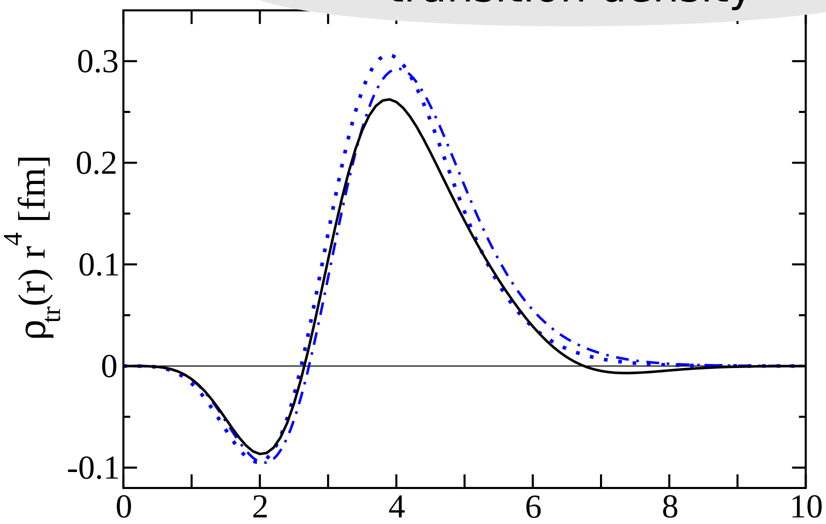
[1] Ajzenberg-Selove, Nuc. Phys. **A506**, 1 (1990)
[2] Itoh et al., Nuc. Phys. **A738**, 268 (2004), Zimmermann et al., Phys. Rev. Lett. **110**, 152502 (2013)
[3] Funaki et al., Phys. Rev. C **67**, 051306(R) (2003)

Monopole Matrix Element revisited

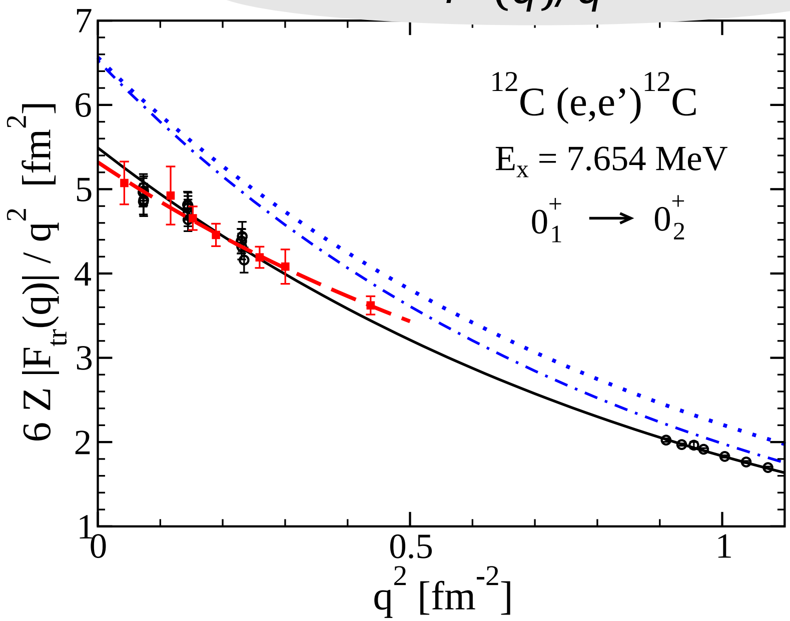
transition form factor



transition density



$F^2(q)/q^2$

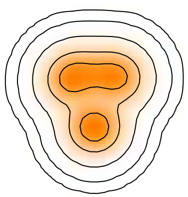


- $M(E0)$ determines the pair decay width
- model-independent self-consistent determination of transition form-factor/density in DWBA
- data at high momentum transfer necessary to constrain matrix element $M(E0) = 5.47 \pm 0.09\, e^2\mathrm{fm}^2$

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

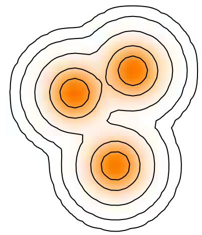
Important Configurations

- Calculate the overlap with FMD basis states to find the most important contributions to the Hoyle state

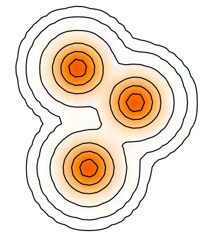


$\left|\langle \cdot \mid 0_1^+ \rangle\right| = 0.94$

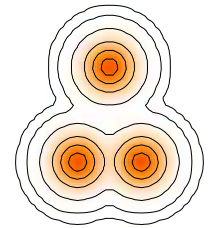
$\left|\langle \cdot \mid 2_1^+ \rangle\right| = 0.93$



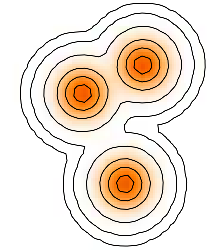
$\left|\langle \cdot \mid 0_2^+ \rangle\right| = 0.72$



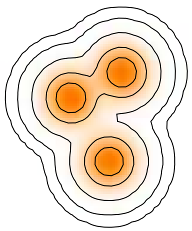
$\left|\langle \cdot \mid 0_2^+ \rangle\right| = 0.71$



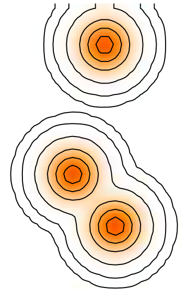
$\left|\langle \cdot \mid 0_2^+ \rangle\right| = 0.61$



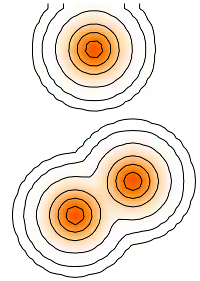
$\left|\langle \cdot \mid 0_2^+ \rangle\right| = 0.61$



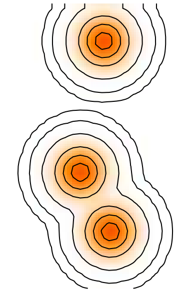
$\left|\langle \cdot \mid 3_1^- \rangle\right| = 0.83$



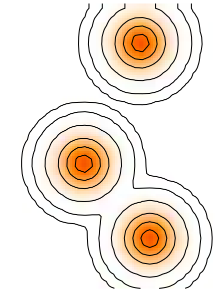
$\left|\langle \cdot \mid 0_3^+ \rangle\right| = 0.50$



$\left|\langle \cdot \mid 0_3^+ \rangle\right| = 0.49$



$\left|\langle \cdot \mid 0_3^+ \rangle\right| = 0.44$



$\left|\langle \cdot \mid 0_3^+ \rangle\right| = 0.41$

FMD basis states are not orthogonal!

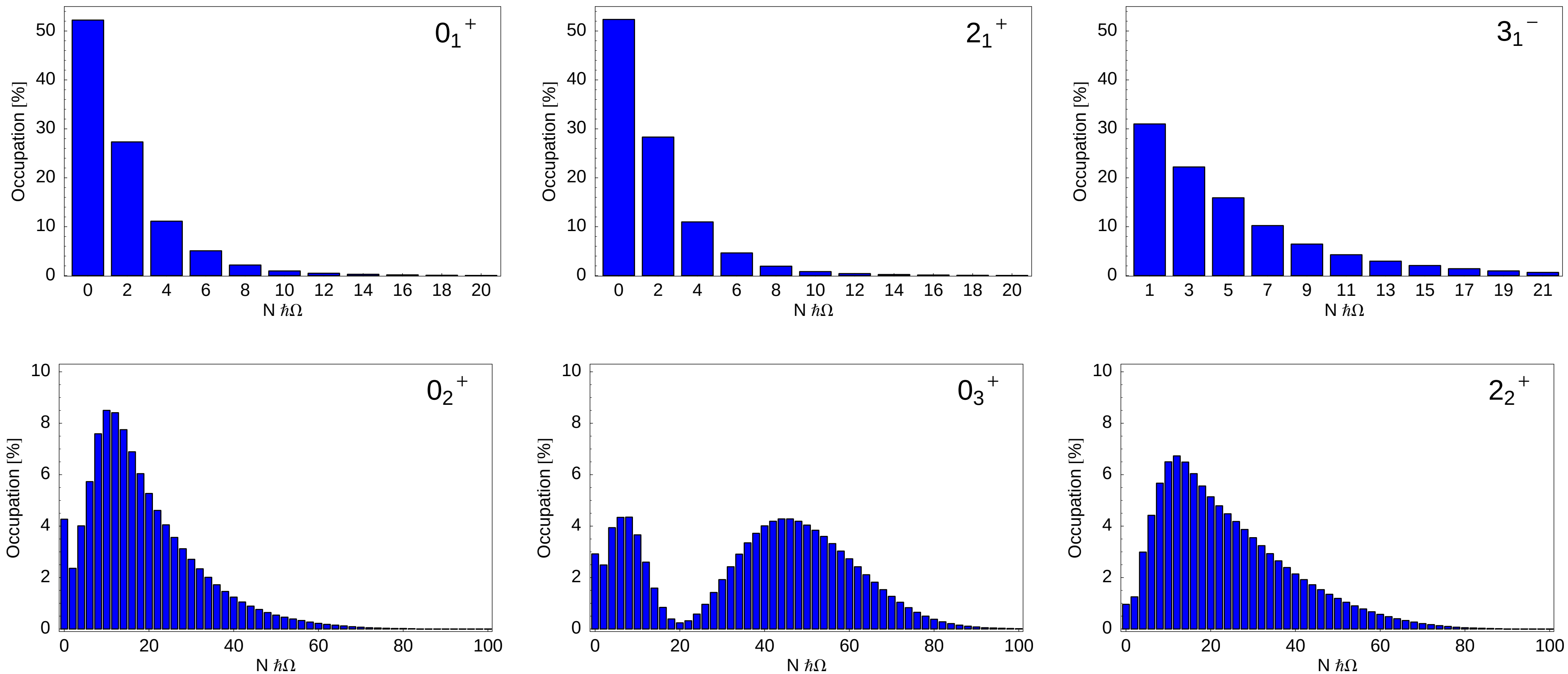
0_2^+ and 0_3^+ states have no rigid intrinsic structure

Harmonic Oscillator $N\hbar\Omega$ Excitations

Y. Suzuki *et al*, Phys. Rev. C **54**, 2073 (1996).

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

Cluster Model



Preliminary:
Include ^{8}Be-α continuum

How to treat the ^{12}C continuum above the 3-α threshold ?

- **In principle it should be described as a three-body continuum**
- **However ^{8}Be+α states are lower in energy than 3-α configurations up to pretty large hyperradii**
- **Approximation: consider ^{8}Be(0^{+}) and ^{8}Be(2^{+}) as bound states**
- **Could be considered as a microscopic CDCC approach**

^{8}Be-α wave functions

alpha-cluster model calculations with continuum:

Descouvemont, Baye, Phys. Rev. **C36**, 54 (1987)
Arai, Phys. Rev. **C74**, 064311 (2006)
Vasilevsky *et al.*, Phys. Rev. **C85**, 034318 (2012)

^{8}Be wave functions

- α-α configurations up to 9 fm distance, project on 0^+ and 2^+, $M = 0, 1, 2$

$$\left| {}^8\mathrm{Be}_{I,K} \right\rangle = P^I_{K0} \sum_i \left\{ \left| {}^4\mathrm{He}(-R_i/2\mathbf{e}_z) \right\rangle \otimes \left| {}^4\mathrm{He}(R_i/2\mathbf{e}_z \right\rangle \right\} c^J_i$$

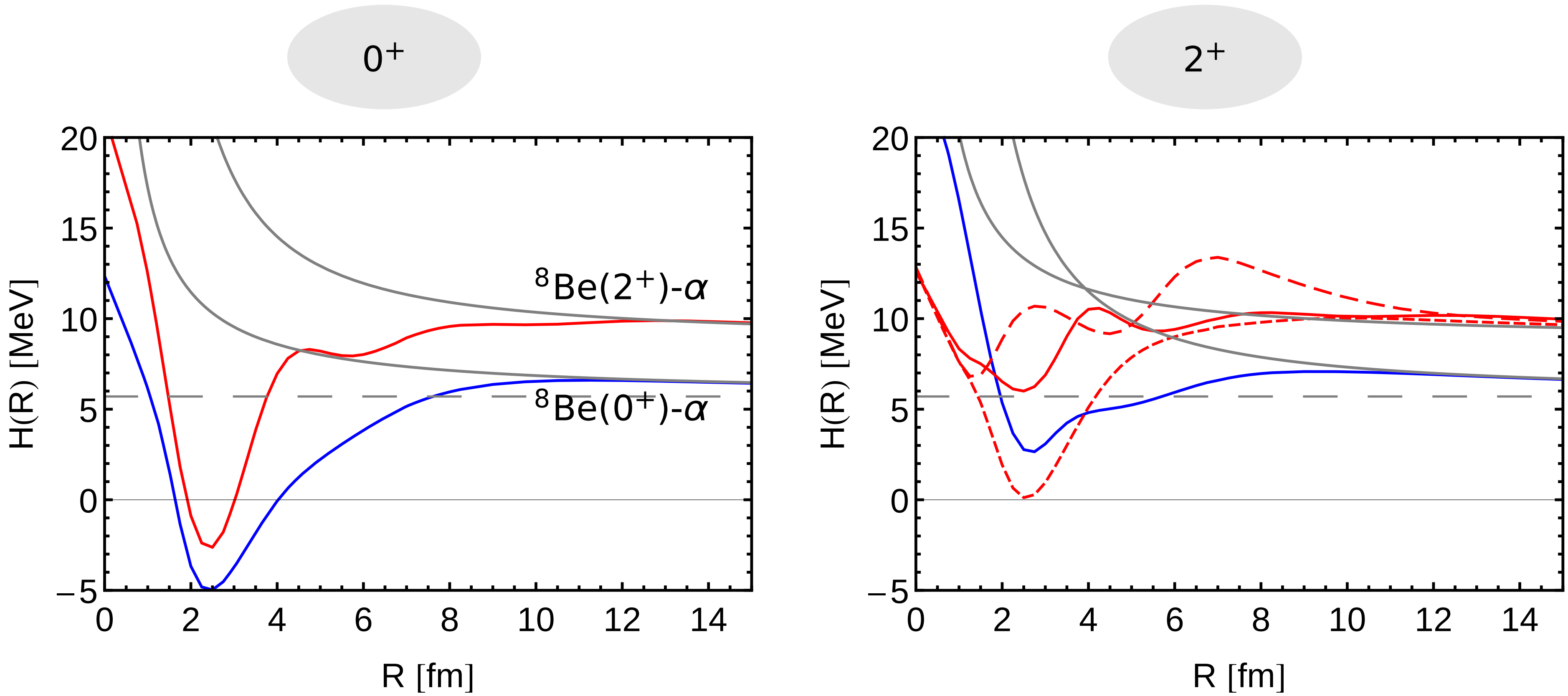
- reproduces ground state energy within 50 keV compared to full calculation

^{12}C configurations

- ^{8}Be(0^+,2^+) and α at distance R
- ^{8}Be(2^+) can have different orientations with respect to distance vector
- ^{8}Be(0^+,2^+)+α configurations have to be projected on total angular momentum

$$\left| {}^8\mathrm{Be}_{I,K}, {}^4\mathrm{He}; R; JM \right\rangle = P^J_{MK} \left\{ \left| {}^8\mathrm{Be}_{I,K}(-1/3R\mathbf{e}_z) \right\rangle \otimes \left| {}^4\mathrm{He}(2/3R\mathbf{e}_z) \right\rangle \right\}$$

GCM Energy Surfaces

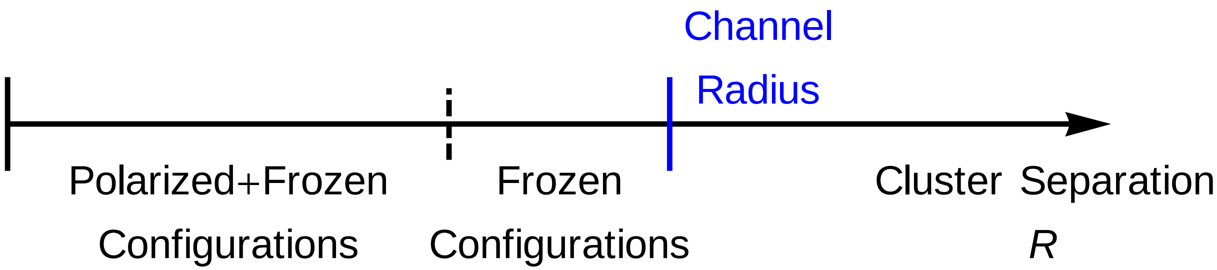


- energy surfaces contain localization energy for relative motion of ^{8}Be and α
- 2^+ energy surface depends strongly on orientation of ^{8}Be 2^+ state – $M = 2$ most attractive

Full calculation: Microscopic *R*-matrix Method

Model Space

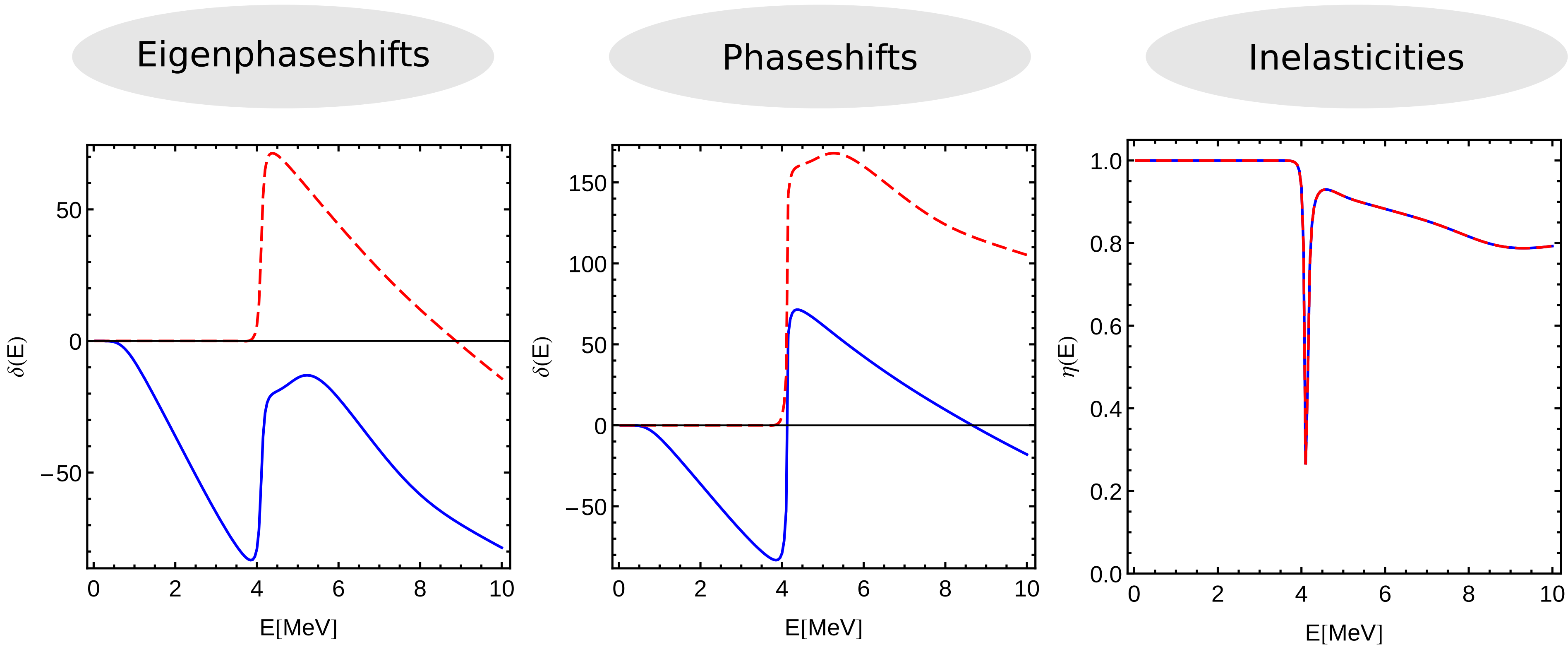
- Internal region in the cluster model: 3-α configurations on a grid
- External region: $^{8}\mathrm{Be}(0^{+}, 2^{+})$-$\alpha$ configurations
- Channel radius has to be large: only Coulomb interaction between ^{8}Be and α and Coulomb coupling between different ^{8}Be channels should be small
- Check that results are independent from channel radius: used $a = 16.5$ fm here



Scattering Solutions

- Obtain scattering matrix using multichannel microscopic *R*-matrix approach
  Descouvemont, Baye, Phys. Rept. 73, 036301 (2010)
- Diagonal phase shifts and inelastic parameters: $S_{ii} = \eta_i \exp\{2i\delta_i\}$
- Eigenphases: $S = V^{-1} D V, D_{\alpha\alpha} = \exp\{2i\delta_\alpha\}$

Cluster Model: ^{8}Be-α Continuum
0^+ Phase shifts



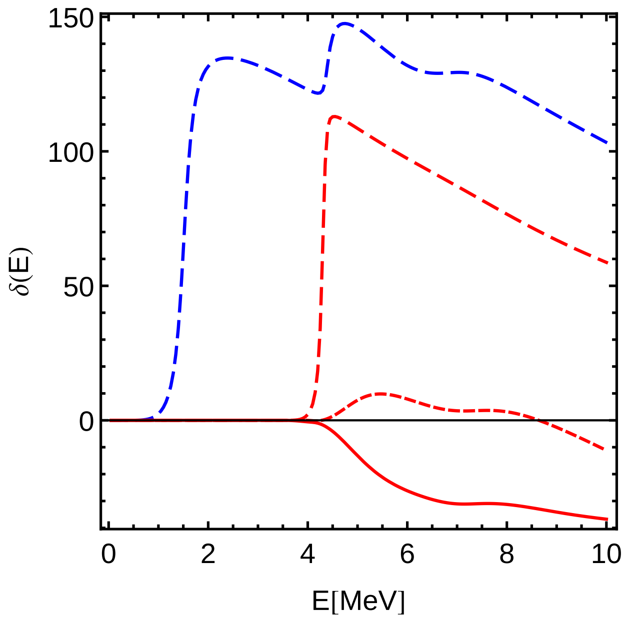
Gamow states

	E [MeV]	Γ [MeV]	
0^+_2	0.29	$1.78 \cdot 10^{-5}$	
0^+_3	4.11	0.12	
0^+_4	4.76	1.57	(?)

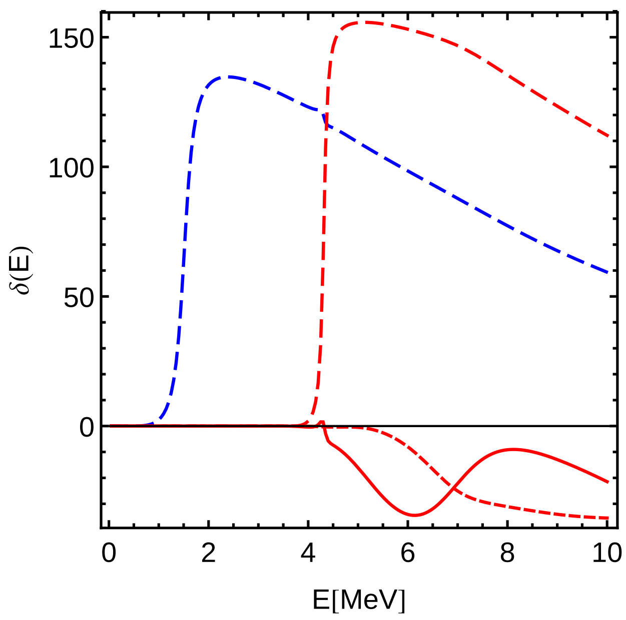
- non-resonant background
- strong coupling between ^{8}Be(0^+) and ^{8}Be(2^+) channel at 4.1 MeV
- Hoyle state not resolved in phase shifts
- stability of broad resonance with respect to channel radius ?

2^+ Phase shifts

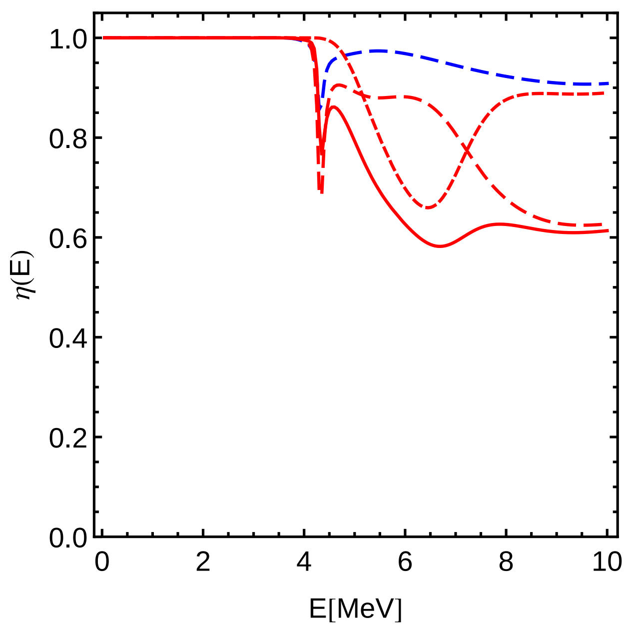
Eigenphaseshifts



Phaseshifts



Inelasticities



Gamow states

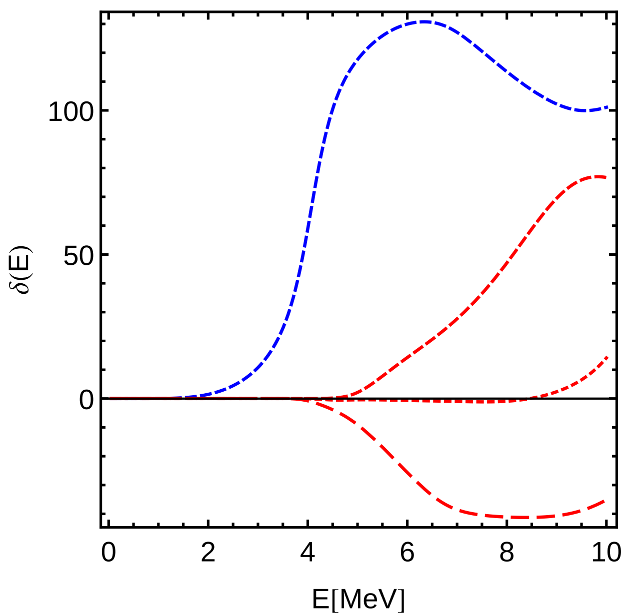
	E [MeV]	Γ [MeV]
2^+_2	1.51	0.32
2^+_3	4.31	0.14
...		

- non-resonant background
- strong $L = 2$ ^{8}Be(0^+) and ^{8}Be(2^+) resonances

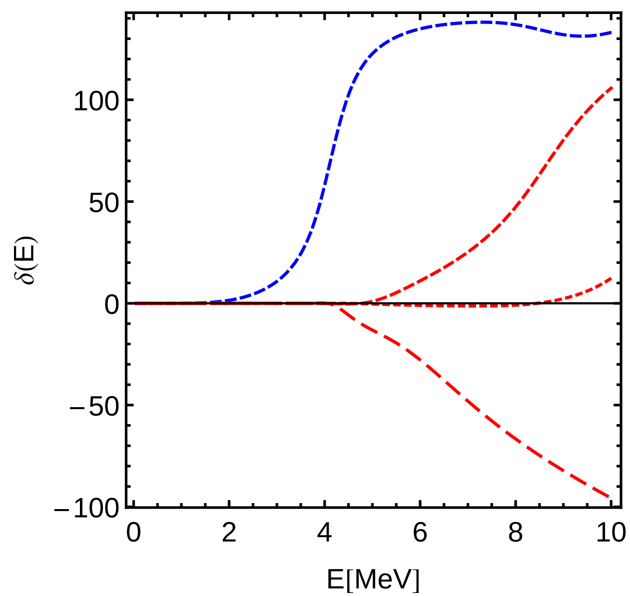
Cluster Model: ^{8}Be-α Continuum

4^+ Phase shifts

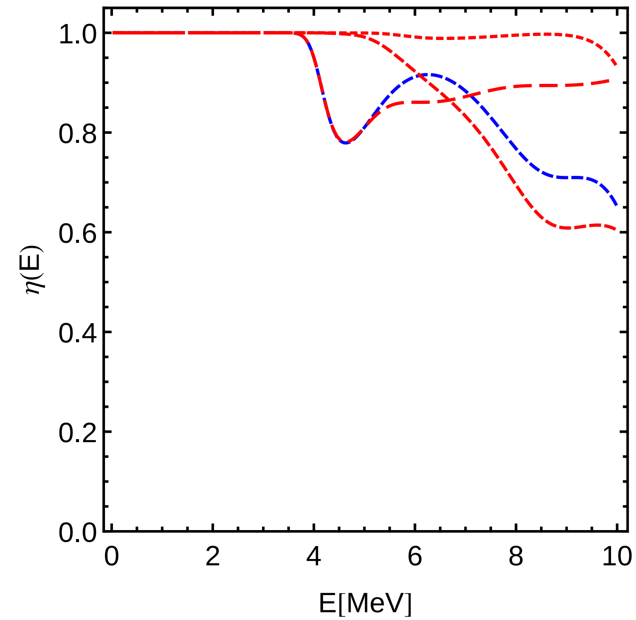
Eigenphaseshifts



Phaseshifts



Inelasticities



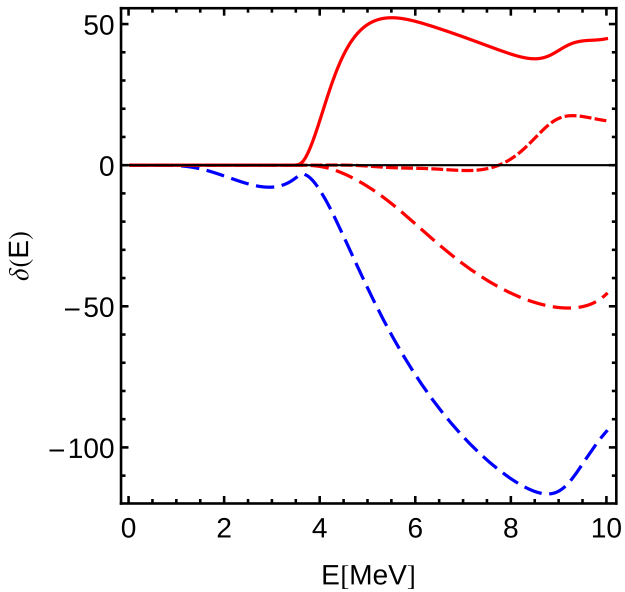
Gamow states

	E [MeV]	Γ [MeV]
4^+_1	1.17	$8.07\cdot 10^{-6}$
4^+_2	4.06	0.98
...		

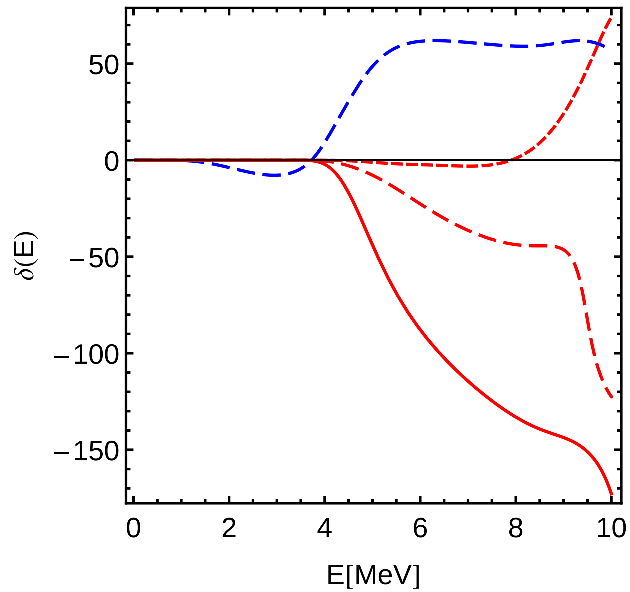
- 4_1 state very narrow, not resolved in phase shifts
- 4^+_2 state mostly ^{8}Be(0+)

Cluster Model: ^{8}Be-α Continuum
3^- Phase shifts

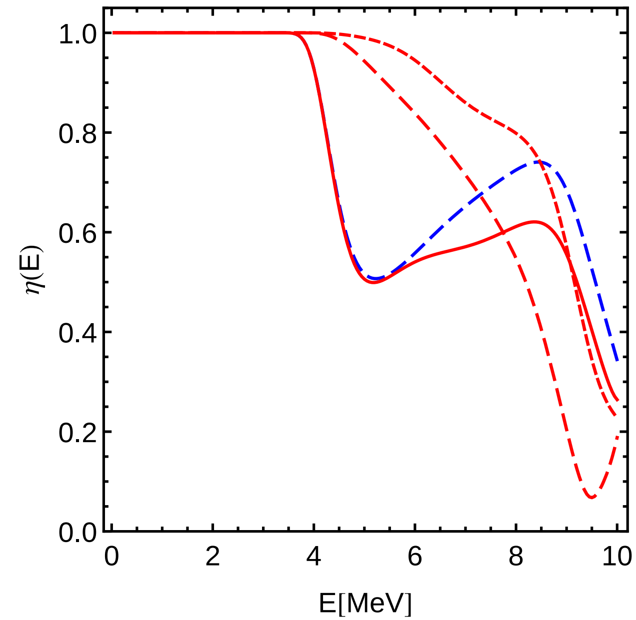
Eigenphaseshifts



Phaseshifts



Inelasticities



Gamow states

	E [MeV]	Γ [MeV]
3^+_1	0.54	$4.46 \cdot 10^{-6}$
...		

- 3_1 state very narrow, not resolved in phase shifts

Work in Progress:
FMD calculation with ^{8}Be-α Continuum

UCOM interaction

- **Correlation functions from SRG**
- **Modify strength of spin-orbit force to account for omitted three-body forces**

^{8}Be-α Continuum

- **To get a reasonable description of ^{8}Be it is essential to include polarized configurations**
- **Calculate strength distributions**
- **Investigate non-cluster states: non-natural parity states, $T = 1$ states, M1 transitions, ^{12}B and ^{12}N β-decay into ^{12}C, . . .**

Summary

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

^{3}He(α,γ)^{7}Be Radiative Capture

- Bound states, resonance and scattering wave functions
- S-Factor: energy dependence and normalization

Cluster States in ^{12}C

- Consistent description of ground state band and clustered states including the Hoyle state
- A proper treatment of the continuum above the 3-α threshold is necessary – first results with ^{8}Be(0^{+},2^{+})+α continuum in the cluster model

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