

Transitions to the Continuum in Fermionic Molecular Dynamics



Thomas Neff

FUSTIPEN Topical Meeting
“Future directions for nuclear structure and reaction theories”

GANIL, Caen, France

March 14-18, 2016



Overview



Realistic Effective Nucleon-Nucleon interaction:
Unitary Correlation Operator Method

Many-Body Approach:
Fermionic Molecular Dynamics

Applications:
 $^3\text{He}(\alpha, \gamma)^7\text{Be}$ Radiative Capture Reaction

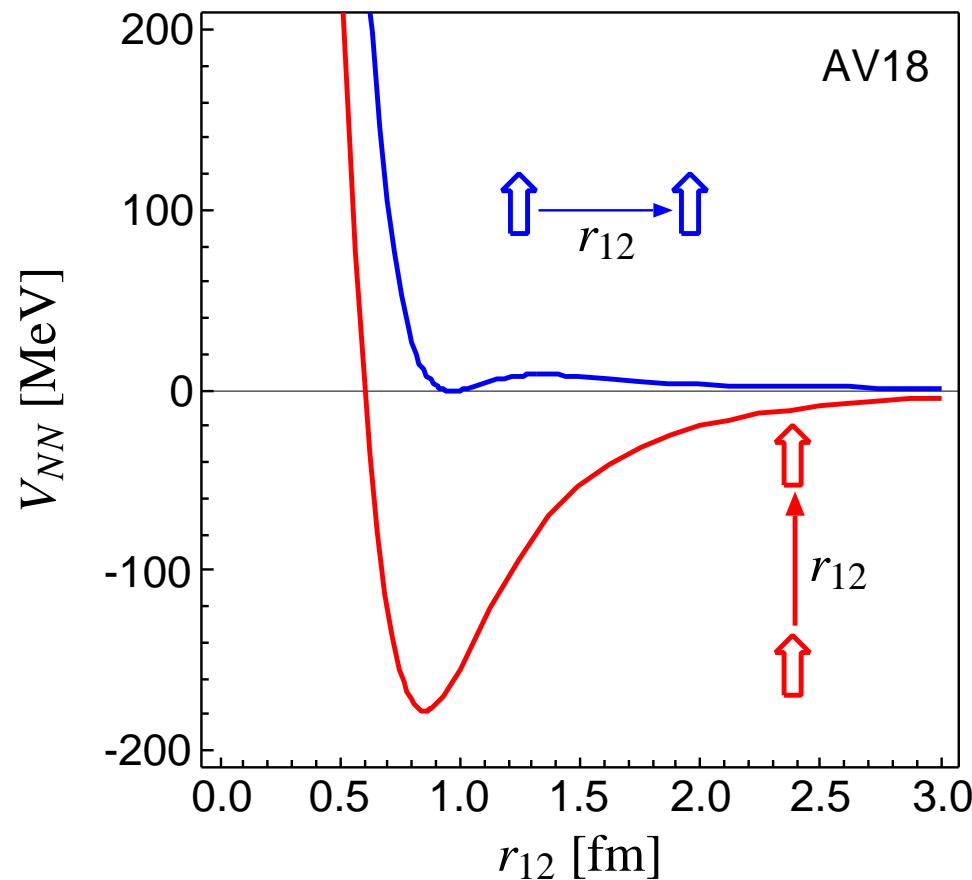
^{12}C in the Microscopic Cluster Model

^{12}C in Fermionic Molecular Dynamics

Nuclear Force

Argonne V18 ($T=0$)

spins aligned parallel or perpendicular to the relative distance vector



- strong repulsive core:
nucleons can not get closer
than ≈ 0.5 fm

► **central correlations**

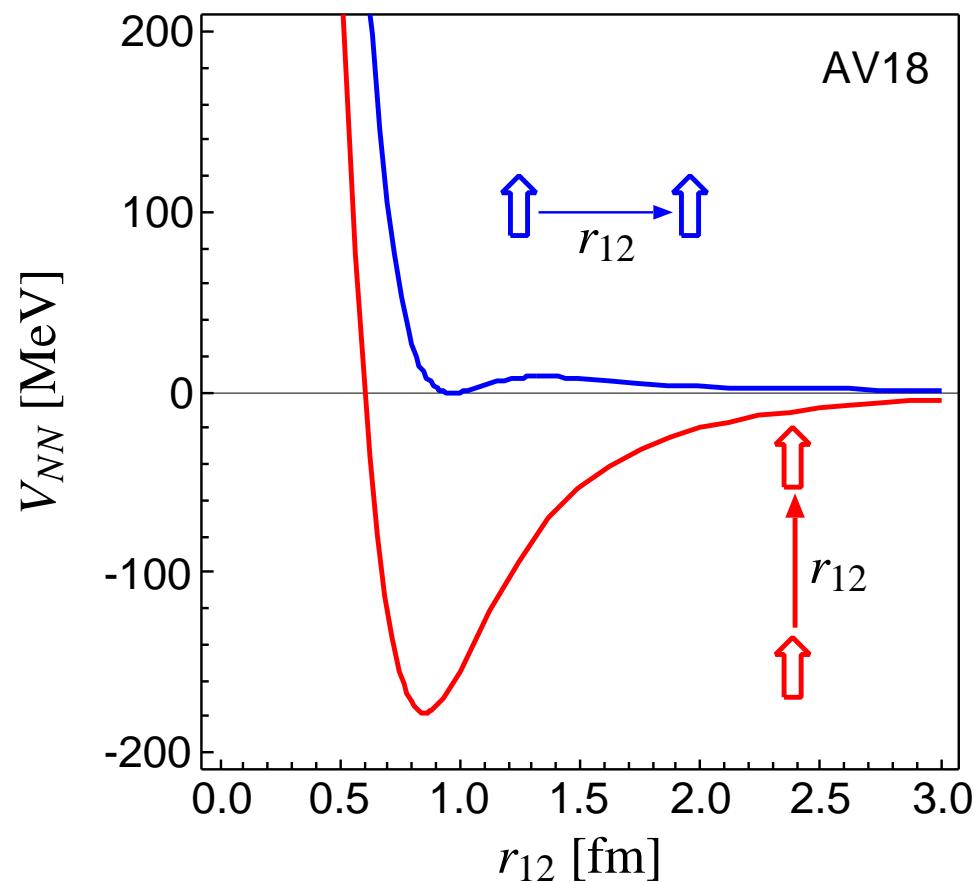
- strong dependence on the
orientation of the spins due
to the tensor force

► **tensor correlations**

Nuclear Force

Argonne V18 ($T=0$)

spins aligned parallel or perpendicular to the relative distance vector



- strong repulsive core:
nucleons can not get closer
than ≈ 0.5 fm

► **central correlations**

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

► **tensor correlations**

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

Unitary Correlation Operator Method

Correlation Operator

- induce short-range (two-body) central and tensor correlations into the many-body state

$$\tilde{C} = \tilde{\zeta}_\Omega \tilde{\zeta}_r = \exp[-i \sum_{i < j} \tilde{g}_{\Omega,ij}] \exp[-i \sum_{i < j} \tilde{g}_{r,ij}] \quad , \quad \tilde{C}^\dagger \tilde{C} = \mathbb{1}$$

- correlation operator should conserve the symmetries of the Hamiltonian and should be of finite-range

Correlated Operators

- correlated operators will have contributions in higher cluster orders

$$\tilde{C}^\dagger \tilde{Q} \tilde{C} = \hat{Q}^{[1]} + \hat{Q}^{[2]} + \hat{Q}^{[3]} + \dots$$

- two-body approximation: correlation range should be small compared to mean particle distance

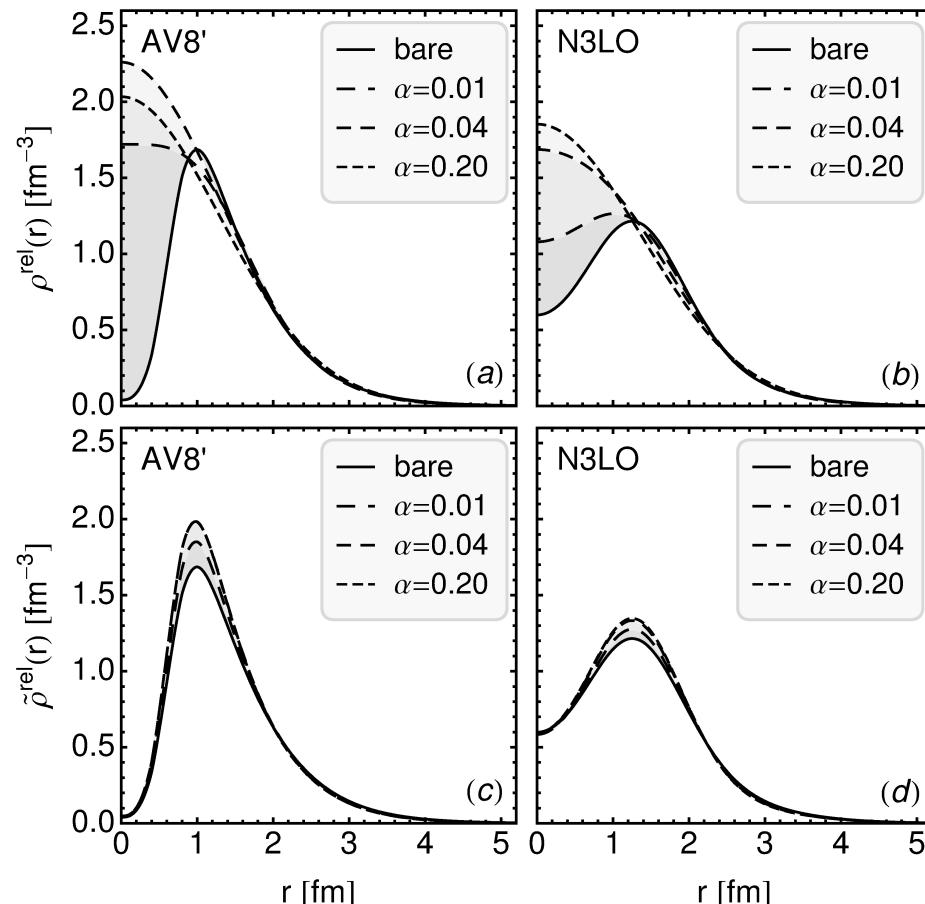
Correlated Interaction

$$\tilde{C}^\dagger (\tilde{T} + \tilde{V}) \tilde{C} = \tilde{T} + \tilde{V}_{\text{UCOM}} + \tilde{V}_{\text{UCOM}}^{[3]} + \dots$$

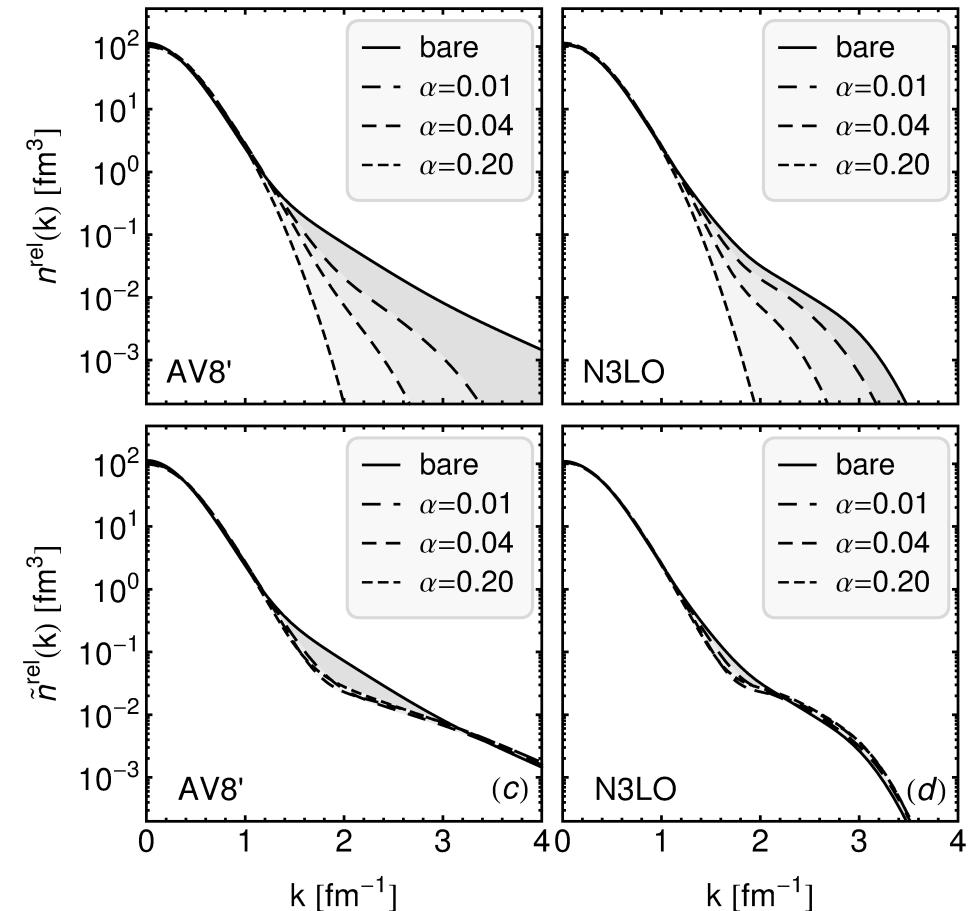
- correlated interaction **phase shift equivalent** to bare interaction by construction

SRG transformed Two-body densities in ${}^4\text{He}$

coordinate space



momentum space



- SRG transformation in two-body approximation
- High momentum components in wave function removed by SRG transformation
- High momentum information can be recovered with SRG transformed operators

•

Intrinsic Basis States

Fermionic

Slater determinant

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

- antisymmetrized A -body state

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

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

Intrinsic Basis States

Fermionic

Slater determinant

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

- antisymmetrized A -body state

Molecular

single-particle states

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

- 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

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

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

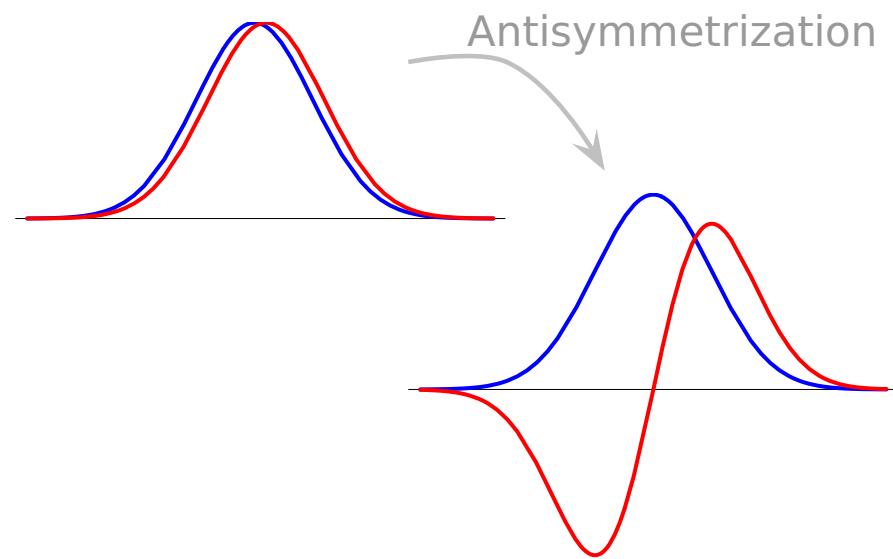
Intrinsic Basis States

Fermionic

Slater determinant

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

- antisymmetrized A -body state



Molecular

single-particle states

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

- 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

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

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

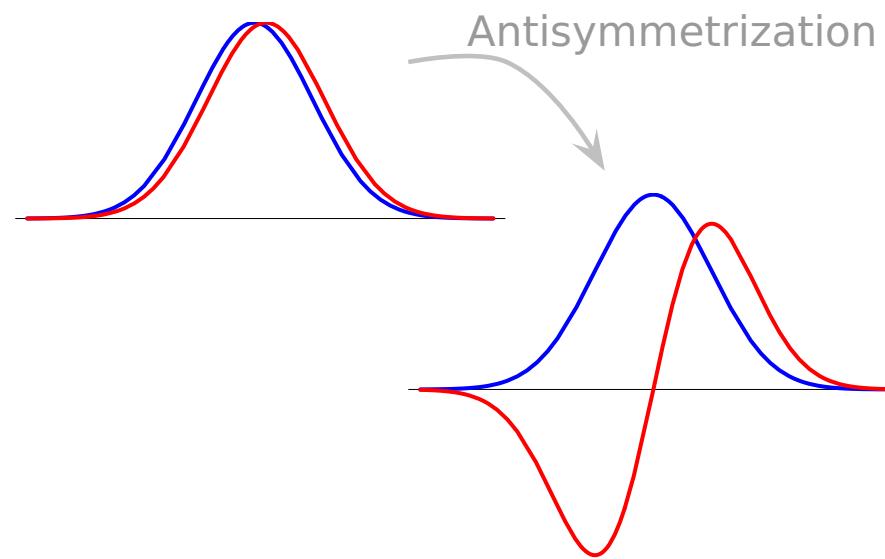
Intrinsic Basis States

Fermionic

Slater determinant

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

- antisymmetrized A -body state



Molecular

single-particle states

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

- 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 st

FMD basis contains
HO shell model and
microscopic cluster model
as limiting cases

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

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

Operator Representation of V_{UCOM}

$$\zeta^\dagger (\tilde{T} + \tilde{V}) \zeta = \tilde{T}$$

$$+ \sum_{ST} \hat{V}_c^{ST}(r) + \frac{1}{2} (\tilde{p}_r^2 \hat{V}_{p^2}^{ST}(r) + \hat{V}_{p^2}^{ST}(r) \tilde{p}_r^2) + \hat{V}_{l^2}^{ST}(r) \tilde{l}^2$$

one-body kinetic energy

$$+ \sum_T \hat{V}_{ls}^T(r) \tilde{l} \cdot \tilde{s} + \hat{V}_{l^2 ls}^T(r) \tilde{l}^2 \tilde{l} \cdot \tilde{s}$$

central potentials

$$+ \sum_T \hat{V}_t^T(r) \tilde{S}_{12}(\mathbf{r}, \mathbf{r}) + \hat{V}_{trp_\Omega}^T(r) \tilde{p}_r \tilde{S}_{12}(\mathbf{r}, \mathbf{p}_\Omega) + \hat{V}_{tll}^T(r) \tilde{S}_{12}(\mathbf{l}, \mathbf{l}) + \\ \hat{V}_{tp_\Omega p_\Omega}^T(r) \tilde{S}_{12}(\mathbf{p}_\Omega, \mathbf{p}_\Omega) + \hat{V}_{l^2 tp_\Omega p_\Omega}^T(r) \tilde{l}^2 \tilde{S}_{12}(\mathbf{p}_\Omega, \mathbf{p}_\Omega)$$

spin-orbit potentials

bulk of tensor force mapped onto central part
of correlated interaction

tensor correlations also change the spin-orbit
part of the interaction

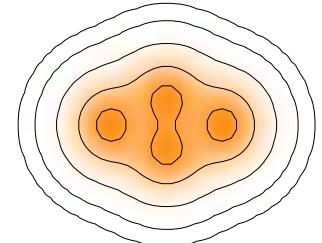
tensor potentials

- FMD

Symmetries and Projection

Breaking of symmetries

- Slater determinants $|Q\rangle$ may break symmetries of the Hamiltonian with respect to parity, rotations and translations



Projection

- Restore symmetries by projection

$$\tilde{P}^\pi = \frac{1}{2}(1 + \pi\tilde{\Pi}), \quad \tilde{P}_{MK}^J = \frac{2J+1}{8\pi^2} \int d^3\Omega D_{MK}^J(\Omega) \tilde{R}(\Omega), \quad \tilde{P}^{\mathbf{P}} = \frac{1}{(2\pi)^3} \int d^3X \exp\{-i(\tilde{\mathbf{P}} - \mathbf{P}) \cdot \mathbf{X}\}$$

Multiconfiguration Mixing

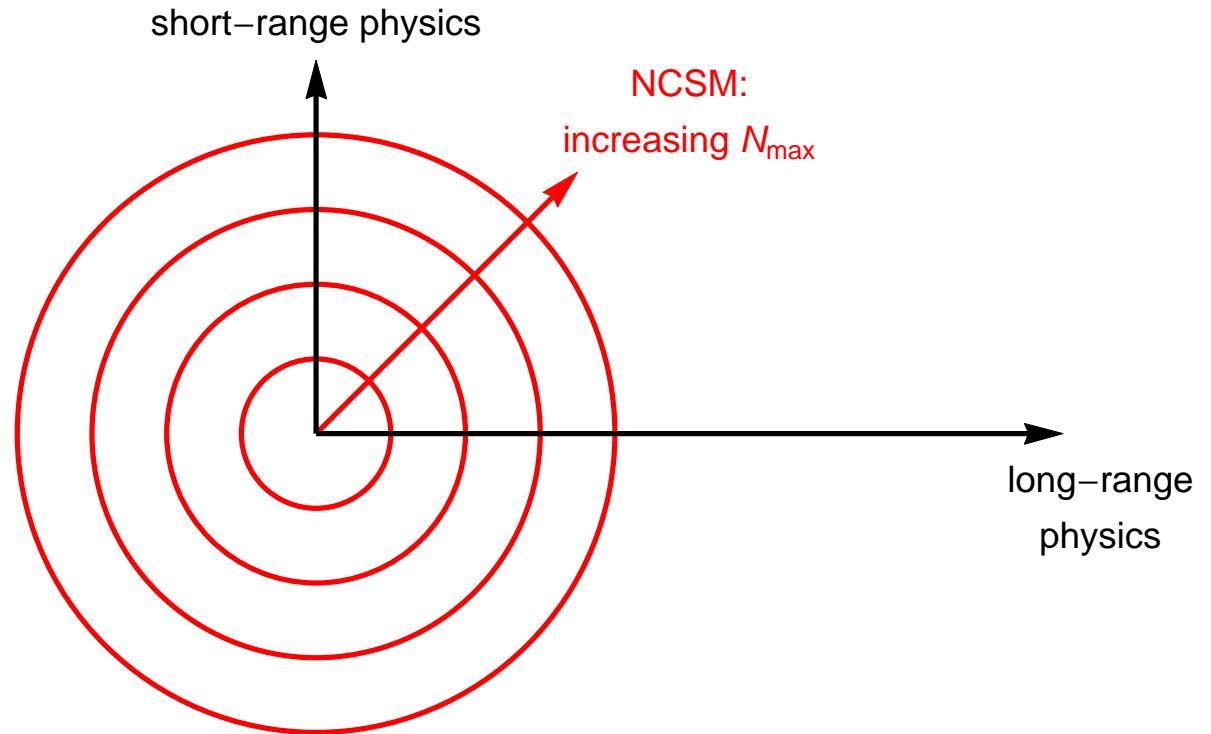
- **diagonalize** Hamiltonian in a set of projected intrinsic states $\{|Q^{(a)}\rangle, a = 1, \dots, N\}$

$$|\Psi; J^\pi Ma\rangle = \sum_{Ka} \tilde{P}^\pi \tilde{P}_{MK}^J \tilde{P}^{\mathbf{P}=0} |Q^{(a)}\rangle c_{Ka}^\alpha$$

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

FMD

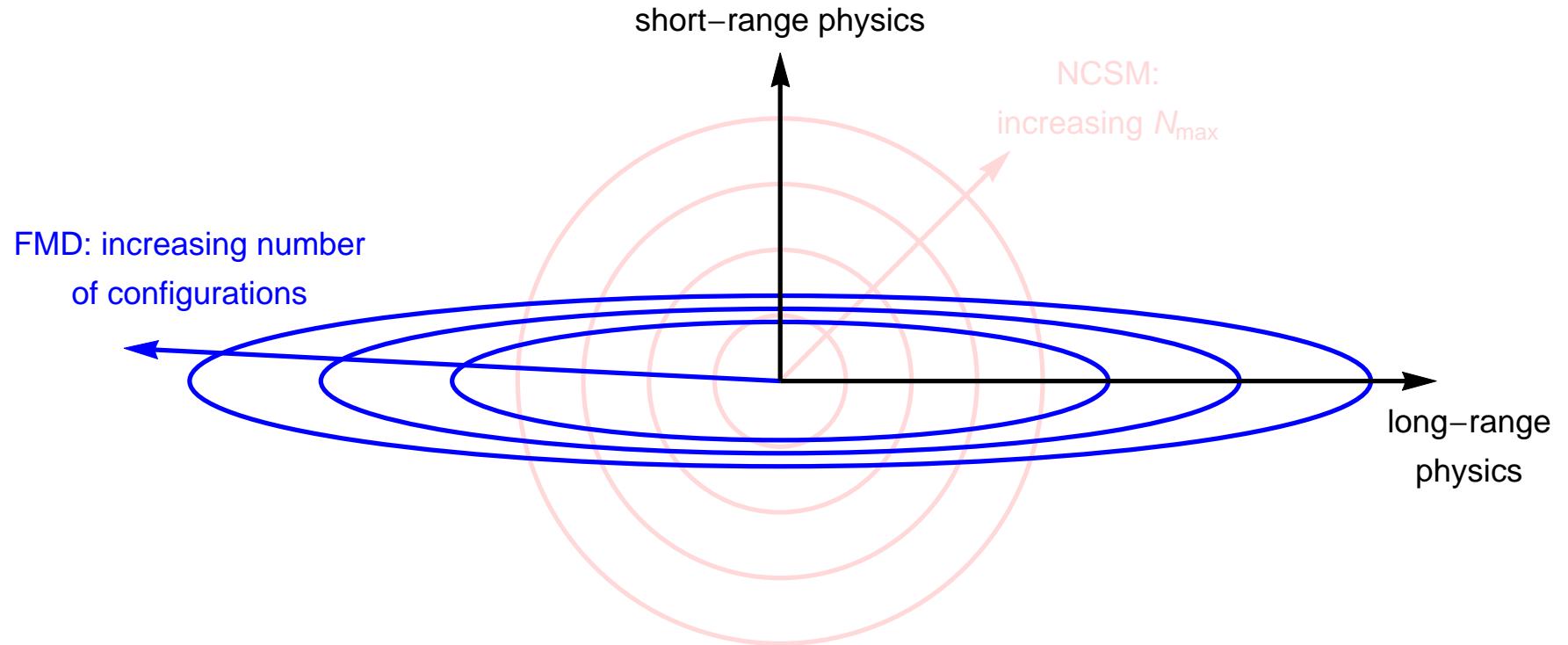
FMD vs NCSM model spaces



- NCSM allows good description of short-range physics, but long-range behavior suffers from harmonic oscillator asymptotics

• FMD

FMD vs NCSM model spaces



- NCSM allows good description of short-range physics, but long-range behavior suffers from harmonic oscillator asymptotics
- FMD allows to describe long-range physics by superposition of localized cluster configurations, but limited in description of short-range physics

$^3\text{He}(\alpha, \gamma)^7\text{Be}$ radiative capture

one of the key reactions in the solar pp-chains



Effective Nucleon-Nucleon interaction:

AV18-UCOM(SRG)

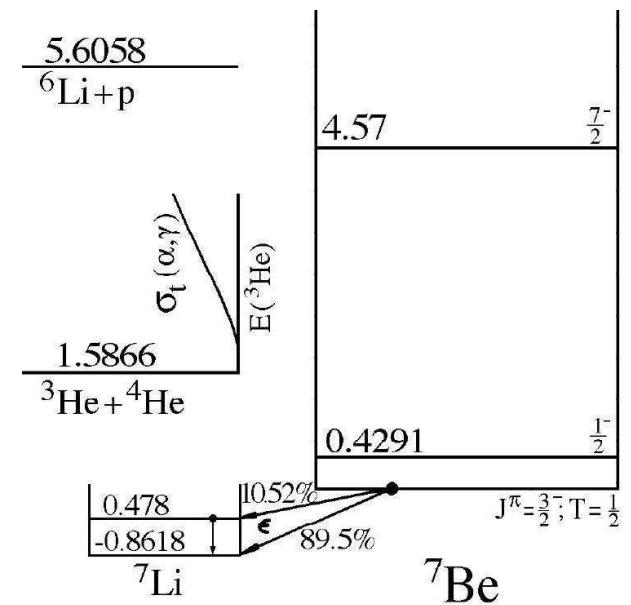
$$\alpha = 0.20 \text{ fm}^4 - \lambda \approx 1.5 \text{ fm}^{-1}$$

Many-Body Approach:

Fermionic Molecular Dynamics

- bound state wave functions
- scattering state wave functions
- electromagnetic transitions matrix elements between scattering and bound states

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



- ${}^3\text{He}(\alpha, \gamma){}^7\text{Be}$
- FMD model space

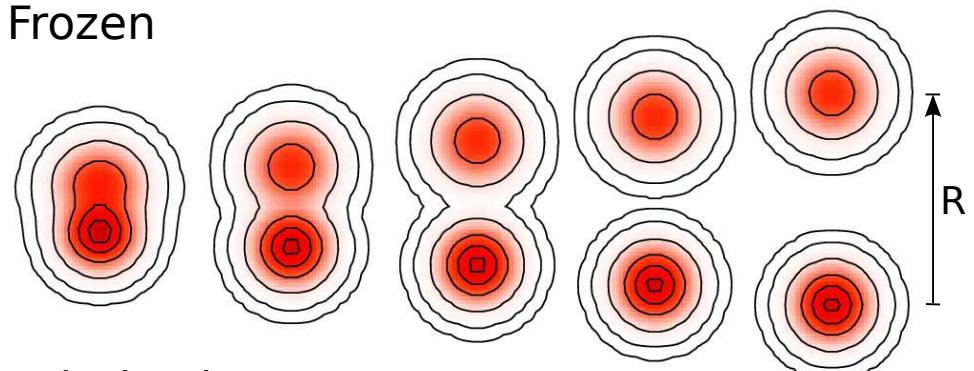
Frozen configurations

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

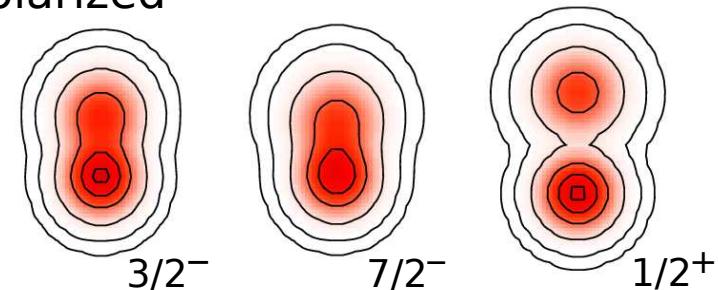
Polarized configurations

- FMD wave functions obtained by **Variation after Projection** 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

Frozen



Polarized



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

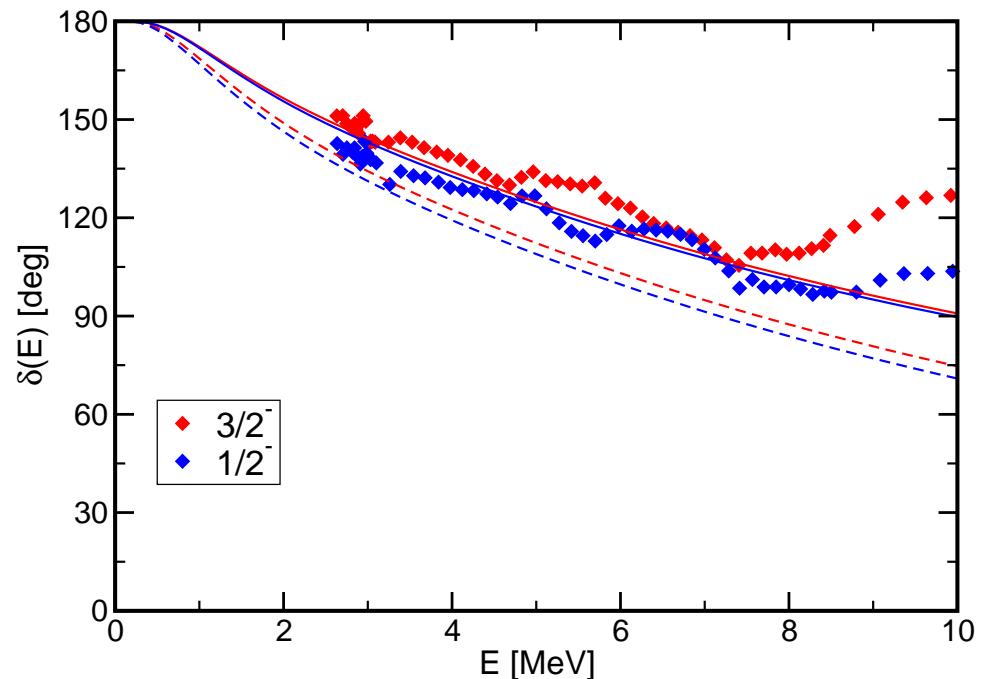
Bound states

		Experiment	FMD
^7Be	$E_{3/2^-}$	-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
^7Li	$E_{3/2^-}$	-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:

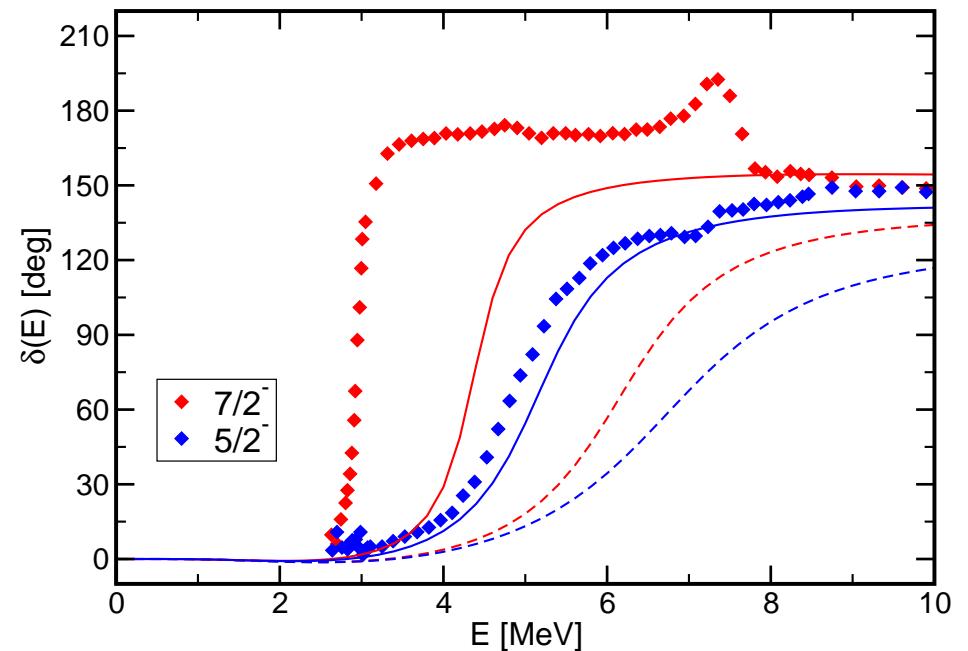
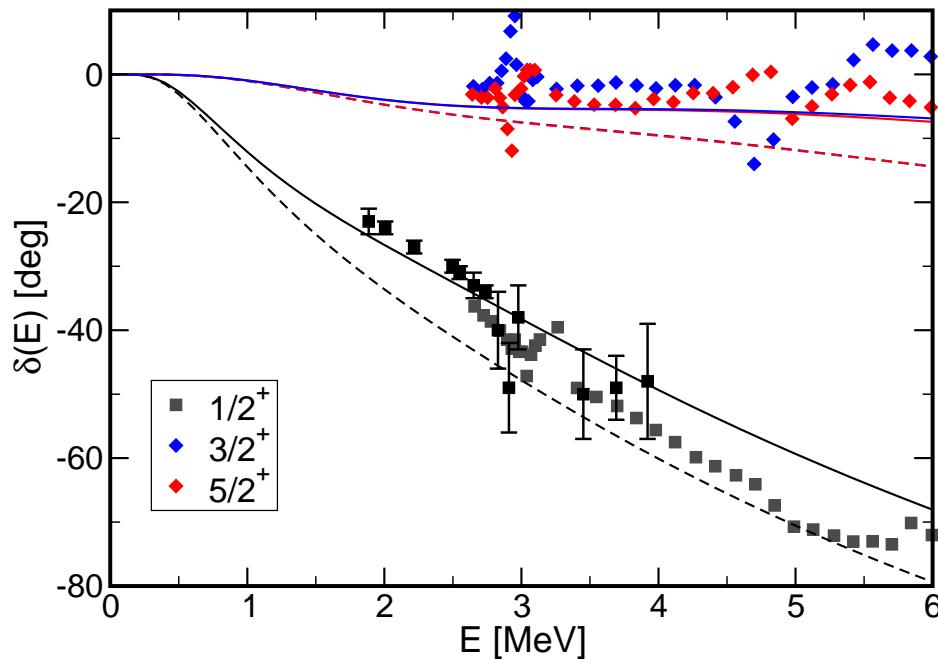
Spiger and Tombrello, PR **163**, 964 (1967)



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

- Scattering phase shifts well described, polarization effects important

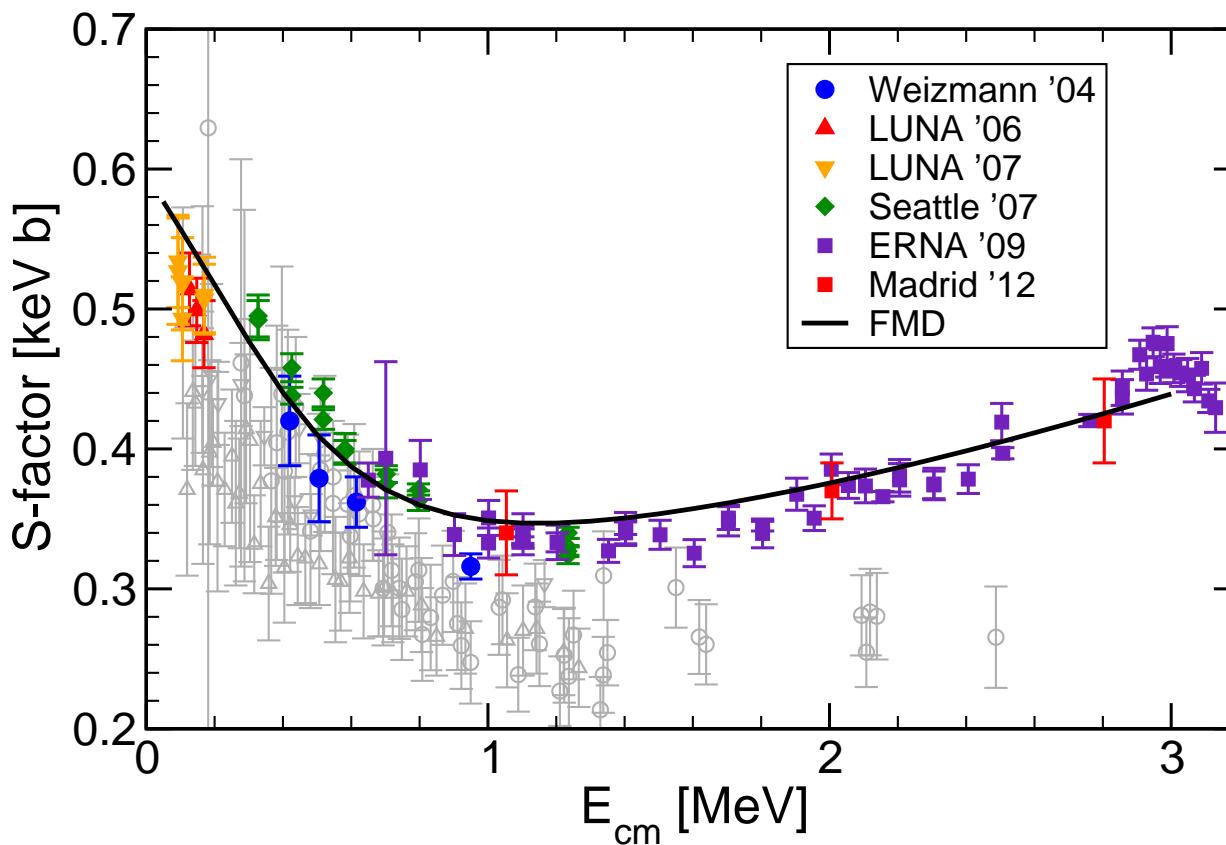
s-, *d*- and *f*-wave Scattering States



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
- *f*-wave splittings too small, additional spin-orbit strength from three-body forces expected

- $^3\text{He}(\alpha, \gamma)^7\text{Be}$
- S-Factor



S-factor:

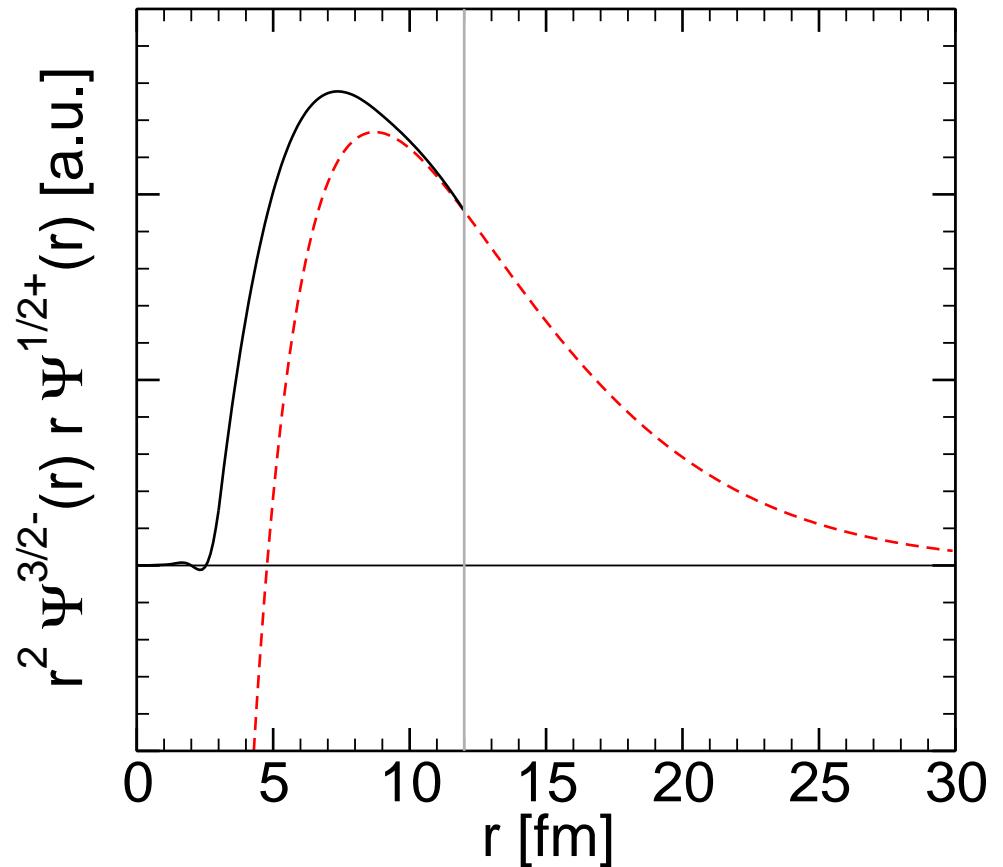
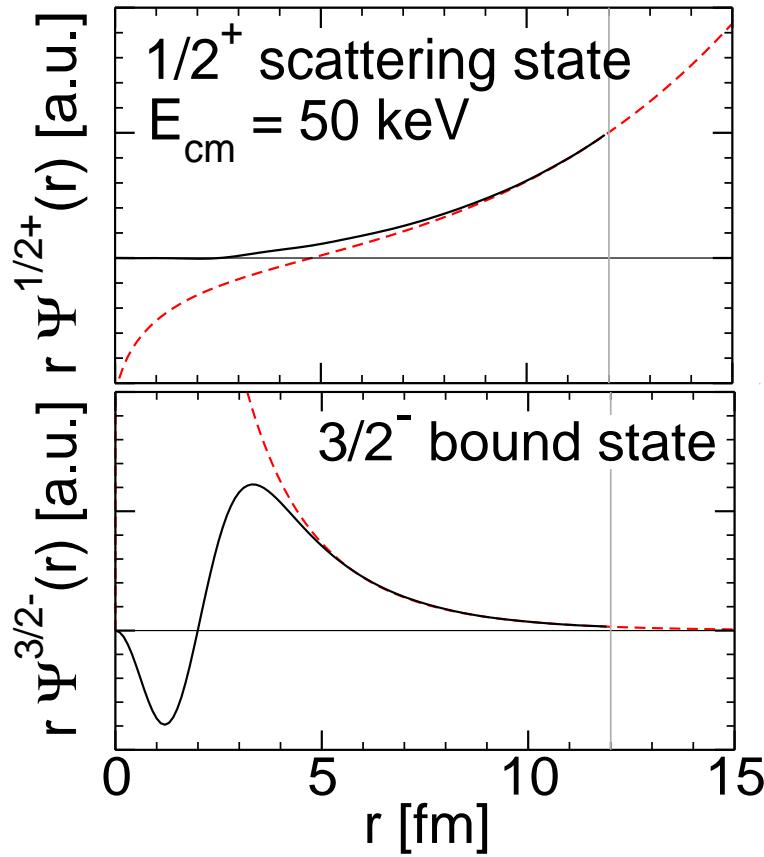
$$S(E) = \sigma(E)E \exp\{2\pi\eta\}$$

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

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)

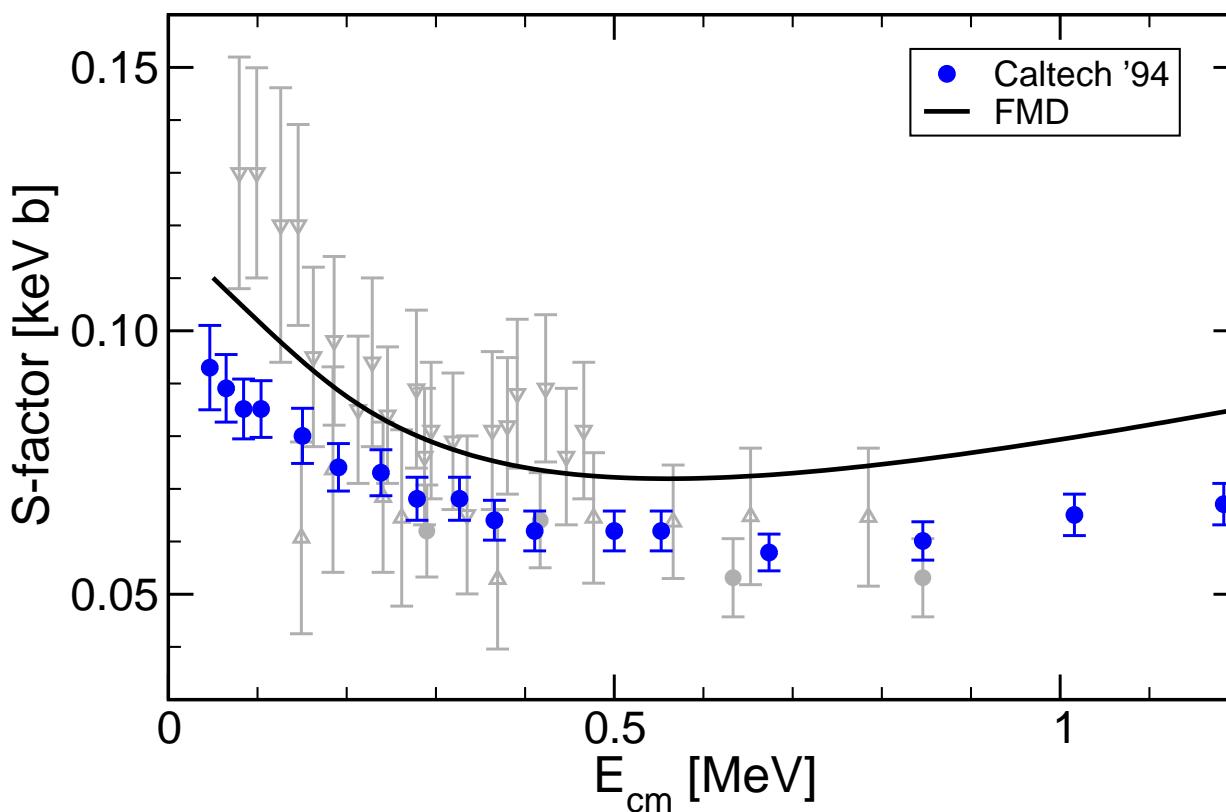
- dipole transitions from $1/2^+$, $3/2^+$, $5/2^+$ scattering states into $3/2^-$, $1/2^-$ bound states
- ➔ FMD is the only model that describes well the energy dependence and normalization of new high quality data
- ➔ fully microscopic calculation, bound and scattering states are described consistently

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

• $^3\text{H}(\alpha, \gamma)^7\text{Li}$
 • S-Factor



S-factor:

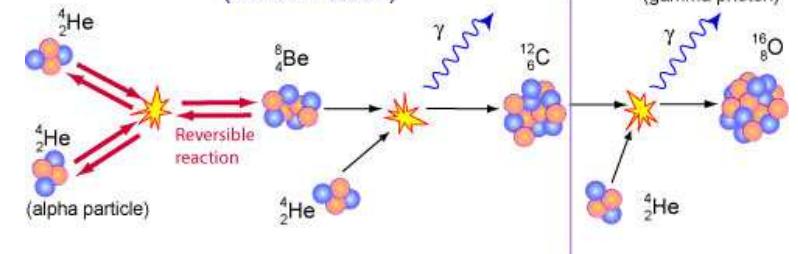
$$S(E) = \sigma(E)E \exp\{2\pi\eta\}$$

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

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

- isospin mirror reaction of $^3\text{He}(\alpha, \gamma)^7\text{Be}$
- ^7Li 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%

The Triple Alpha Process (Helium Fusion)

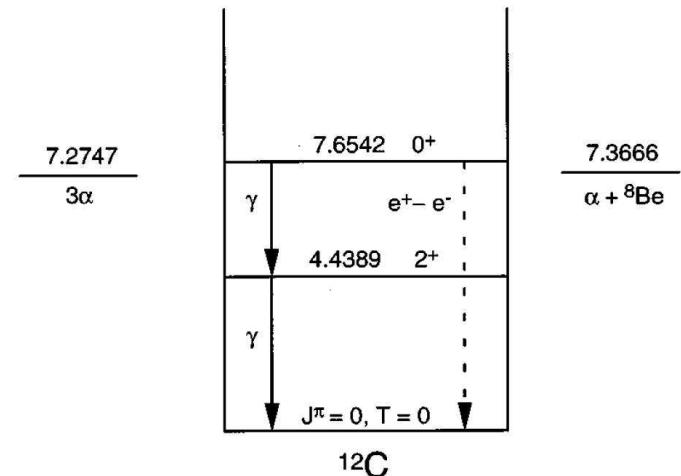


Cluster States in ^{12}C

• • • • • • • • • • • • • • • • • • • •

Structure

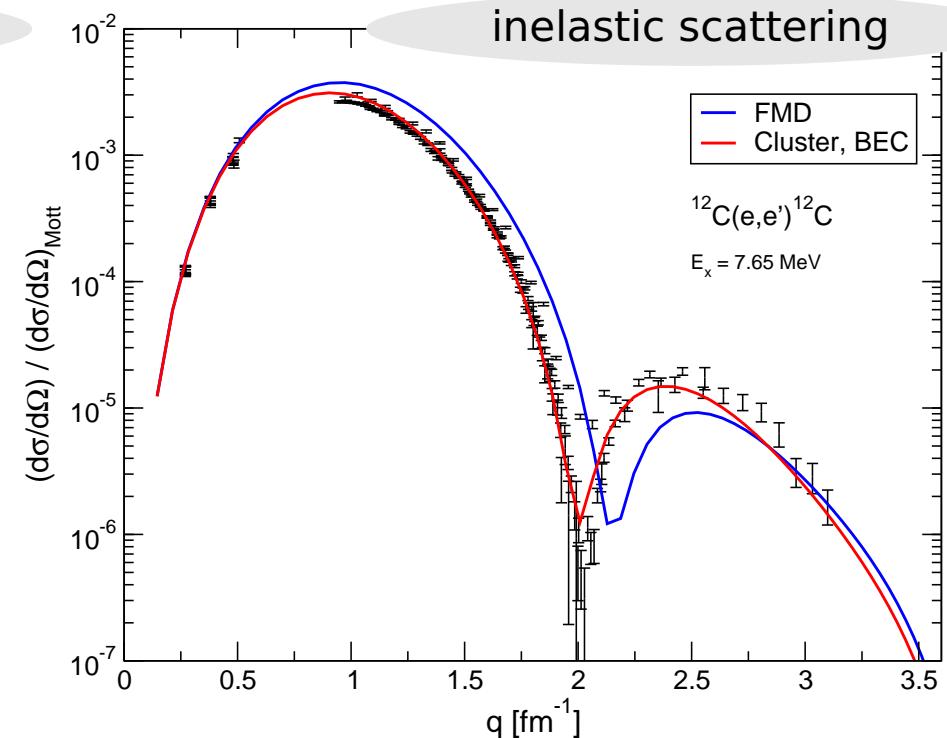
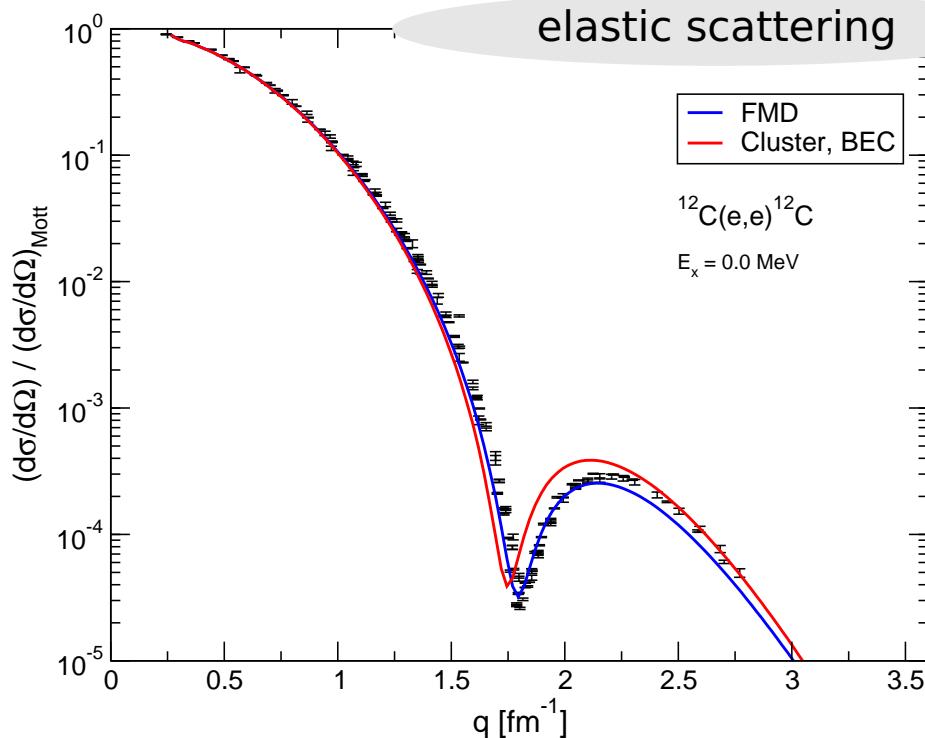
- Is the Hoyle state a pure α -cluster state ?
- Second 2^+ state
Zimmermann *et al.*, Phys. Rev. Lett. 110, 152502 (2013)
- Second 4^+ state
Freer *et al.*, Phys. Rev. C 83, 034314 (2011)
- Other states in the continuum
Fynbo *et al.*, ...



- Include continuum in the calculation!
- Compare microscopic α -cluster model and FMD

Chernykh, Feldmeier, Neff, von Neumann-Cosel, Richter,
Phys. Rev. Lett. (2007) 032501 (2007); Phys. Rev. Lett 105, 022501 (2010)
Neff, Feldmeier, arXiv:1409.3726

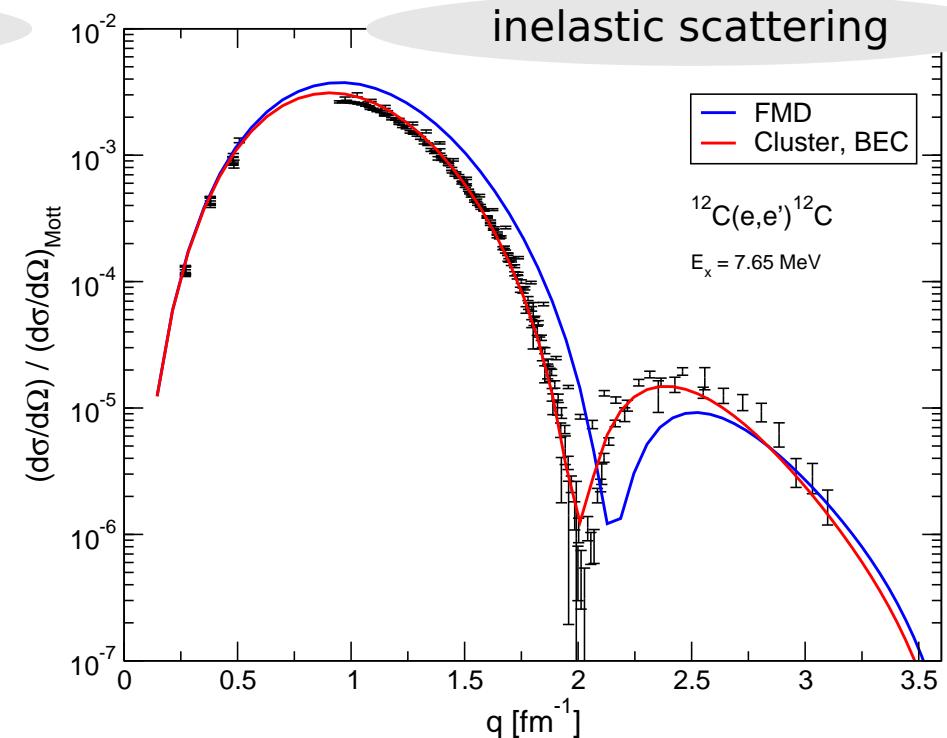
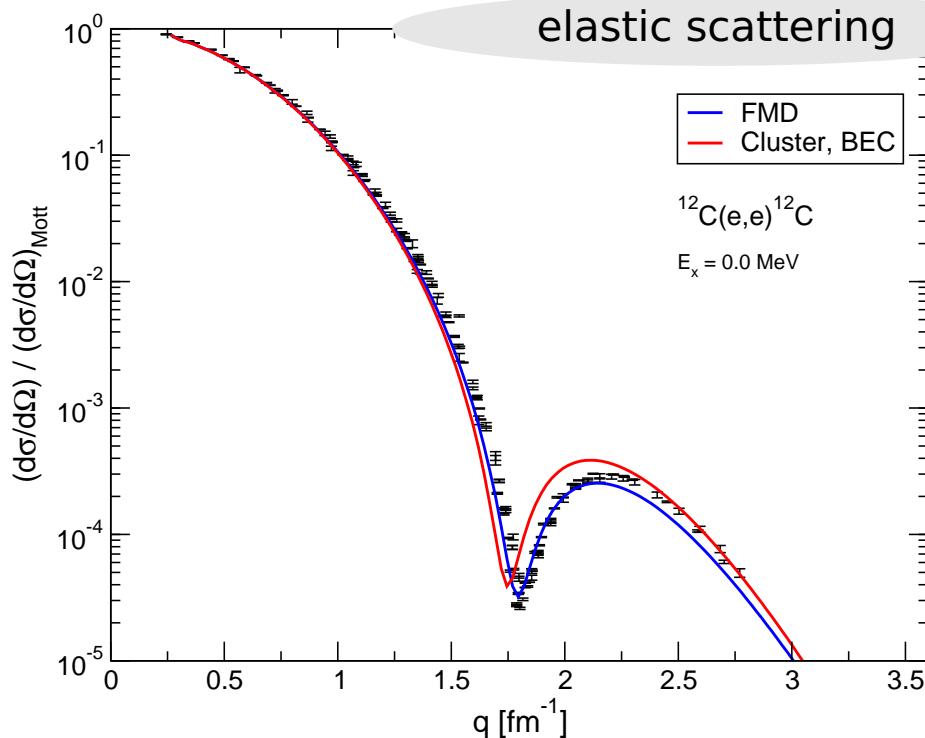
- Cluster States in ^{12}C
- Electron Scattering Data



- test wave functions with precise electron scattering data up to high momenta in Distorted Wave Born Approximation
- both FMD and cluster model give very large radii for the Hoyle state

- ➔ elastic cross section described very well by FMD
- ➔ agreement for the inelastic cross section data confirm the large size of the Hoyle state

- Cluster States in ^{12}C
- Electron Scattering Data



- test wave functions with precise electron scattering data up to high momenta in Distorted Wave Born Approximation
- both FMD and cluster model give very large radii for the Hoyle state

- ➔ elastic cross section described very well by FMD
- ➔ agreement for the inelastic cross section data confirm the large size of the Hoyle state

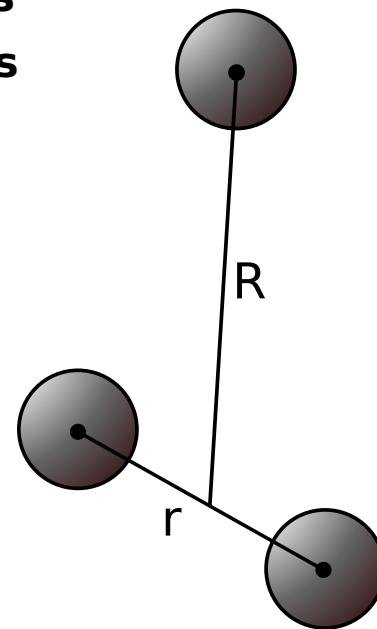
calculation was done in bound-state approximation

Microscopic α -cluster model



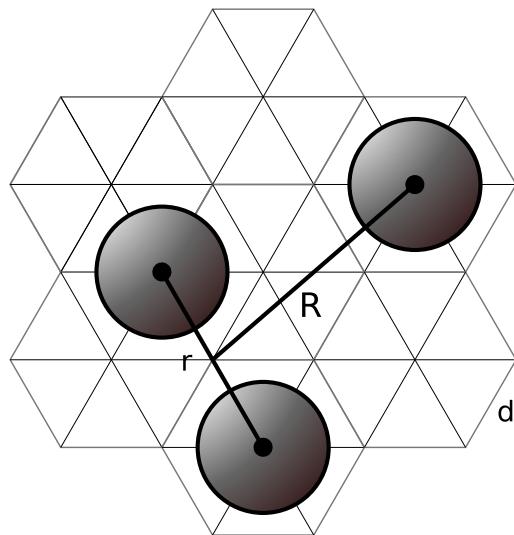
What are the degrees of freedom ?

- ^{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 nucleon-nucleon interaction adjusted to reproduce α - α and ^{12}C ground state properties
- include ^8Be - α channels for continuum



- Microscopic α -Cluster Model

Model space in internal region



$$\rho^2 = \frac{1}{2}\mathbf{r}^2 + \frac{2}{3}\mathbf{R}^2$$

Hyperradius

Model Space

- include all possible configurations on triangular grid ($d = 1.4$ fm) up to a certain hyperradius ρ
- no restriction on relative angular momenta

Basis States

- Intrinsic states are projected on parity and angular momentum

$$|\Psi_{JMK\pi}^{3\alpha}(\mathbf{R}_1, \mathbf{R}_2, \mathbf{R}_3)\rangle = P_{MK}^\pi \tilde{P}_{MK}^J \mathcal{A} \left\{ |\Psi^{^4\text{He}}(\mathbf{R}_1)\rangle \otimes |\Psi^{^4\text{He}}(\mathbf{R}_2)\rangle \otimes |\Psi^{^4\text{He}}(\mathbf{R}_3)\rangle \right\}$$

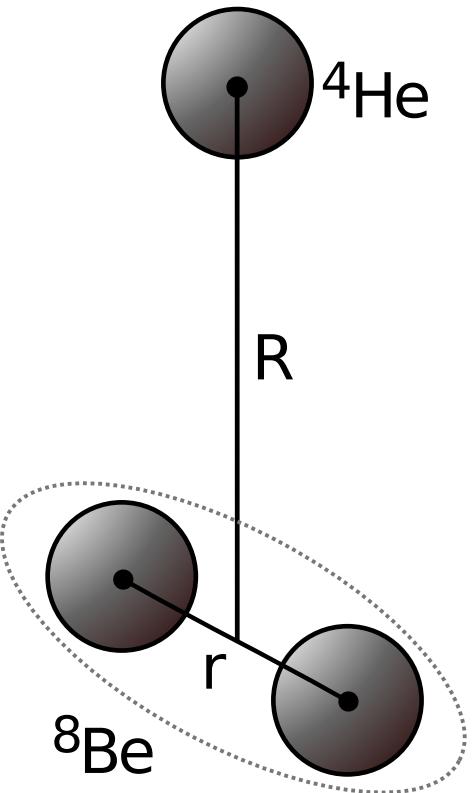
Volkov Interaction

- 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 ^4He , ^8Be and ^{12}C nuclei

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

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

- Microscopic α -Cluster Model
- Model space in external region



Model Space

- ${}^8\text{Be}-{}^4\text{He}$ cluster configurations with generator coordinate R
- ${}^8\text{Be}$ ground state (0_1^+) and pseudo states ($2_1^+, 0_2^+, 2_2^+, 4_1^+$) obtained by diagonalizing α - α configurations up to $r = 10 \text{ fm}$

Basis States

- ${}^{12}\text{C}$ basis states are obtained by **double projection**:
Project first ${}^8\text{Be}$

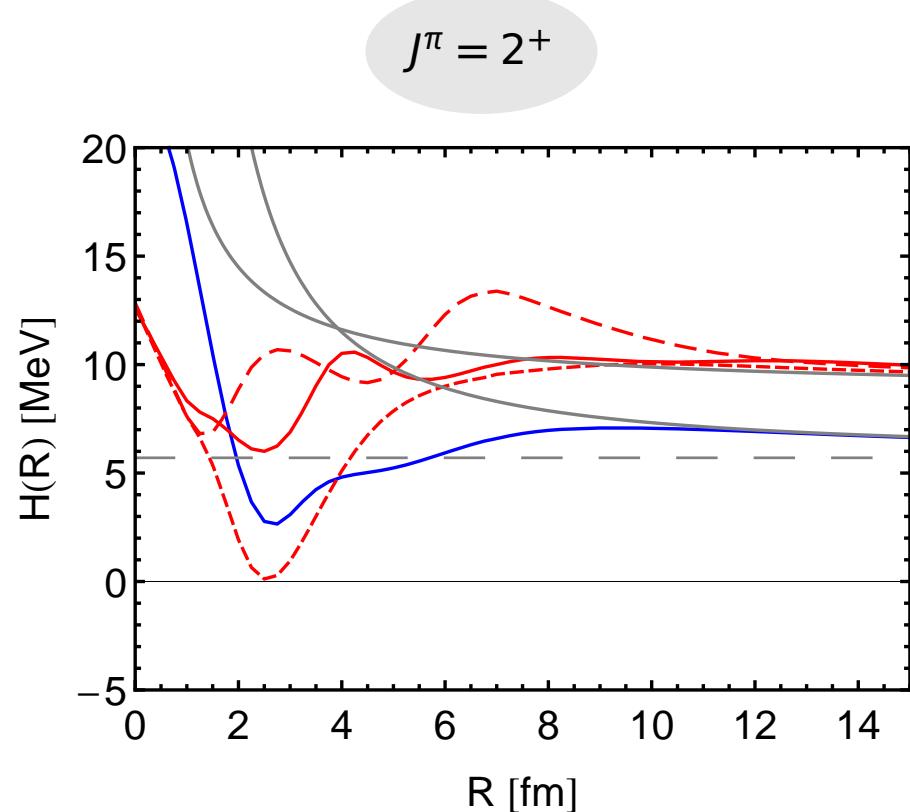
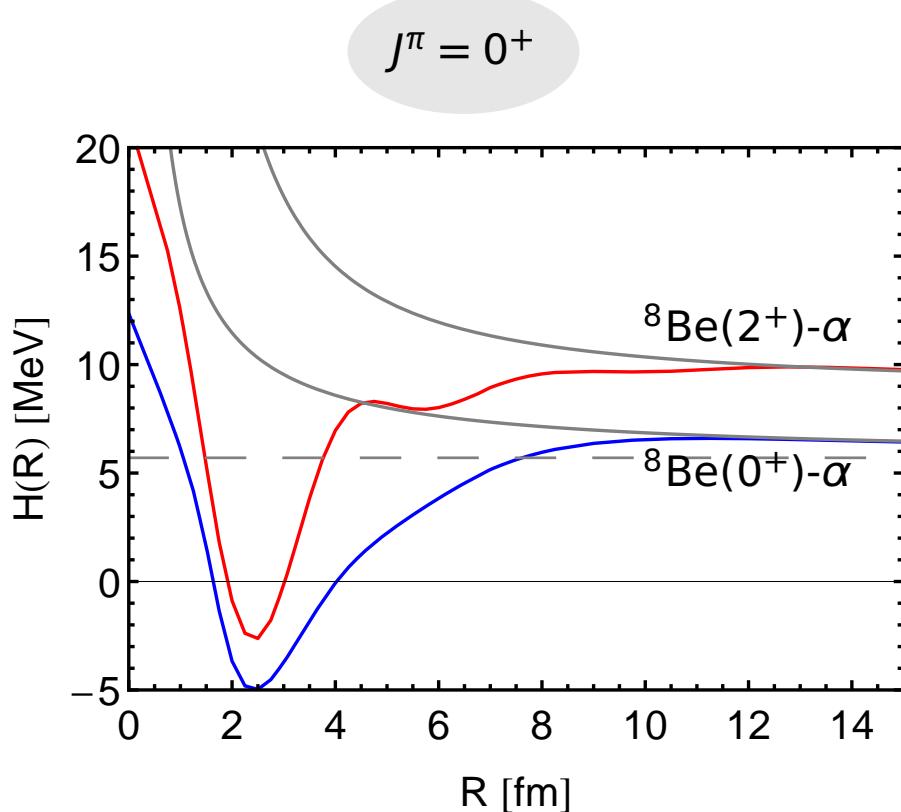
$$|\Psi_{IK}^{{}^8\text{Be}}\rangle = \sum_i P_{MK}^I \mathcal{A} \left\{ |\Psi^{{}^4\text{He}}(-\frac{r_i}{2}\mathbf{e}_z)\rangle \otimes |\Psi^{{}^4\text{He}}(+\frac{r_i}{2}\mathbf{e}_z)\rangle \right\} c_i^I$$

then the combined wave function

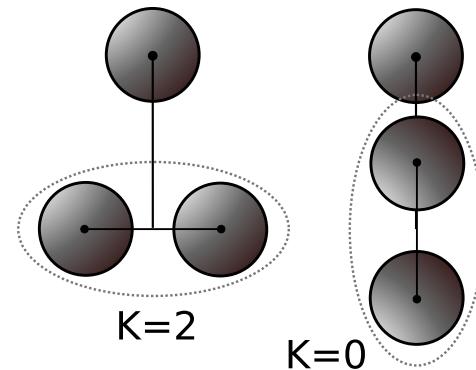
$$|\Psi_{IK;JM\pi}^{{}^8\text{Be}, {}^4\text{He}}(R_j)\rangle = P_{MK}^J \mathcal{A} \left\{ |\Psi_{IK}^{{}^8\text{Be}}(-\frac{R_j}{3}\mathbf{e}_z)\rangle \otimes |\Psi^{{}^4\text{He}}(+\frac{2R_j}{3}\mathbf{e}_z)\rangle \right\}$$

- will allow to match to Coulomb asymptotics

- Microscopic α -Cluster Model
- ${}^8\text{Be}-\alpha$ Energy Surfaces



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



- Microscopic α -Cluster Model

Bound state approximation – Convergence ?

	$\rho < 6 \text{ fm}$	$\rho < 6 \text{ fm}, R < 9 \text{ fm}$	$\rho < 6 \text{ fm}, R < 12 \text{ fm}$	$\rho < 6 \text{ fm}, R < 15 \text{ fm}$	Experiment
$E(0^+_1)$	-89.63	-89.64	-89.64	-89.64	-92.16
$E^*(2^+_1)$	2.53	2.54	2.54	2.54	4.44
$E^*(0^+_2), \Gamma_\alpha(0^+_2)$	8.53	7.82	7.78	7.76	$7.65, (8.5 \pm 1.0)10^{-6}$
$E^*(2^+_2), \Gamma_\alpha(2^+_2)$	10.11	9.18	9.08	8.93	10.03(11), 0.80(13) [3]
$r_{\text{charge}}(0^+_1)$	2.53	2.53	2.53	2.53	2.47(2)
$r(0^+_1)$	2.39	2.39	2.39	2.39	–
$r(0^+_2)$	3.21	3.68	3.78	3.89	–
$B(E2, 2^+_1 \rightarrow 0^+_1)$	9.03	9.12	9.08	9.08	7.6(4)
$M(E0, 0^+_1 \rightarrow 0^+_2)$	7.20	6.55	6.40	6.27	5.47(9) [2]
$B(E2, 2^+_2 \rightarrow 0^+_1)$	3.65	2.48	2.09	1.33	0.73(13) [3]

- properties of resonances (Hoyle state and second 2^+ state) can not be determined in bound state approximation in an unambiguous way

[1] Ajzenberg-Selove, Nuc. Phys. **A506**, 1 (1990)

[2] Chernykh et al., Phys. Rev. Lett. **105**, 022501 (2010)

[3] Zimmermann et al., Phys. Rev. Lett. **110**, 152502 (2013); these numbers are under discussion

- Microscopic α -cluster model
- Matching to Coulomb asymptotics

Model Space

- Internal region: 3- α configurations on a grid
- External region: ${}^8\text{Be}(0^+, 2^+, 4^+)$ - α configurations
- Asymptotically: only Coulomb interaction between ${}^8\text{Be}$ and ${}^4\text{He}$ clusters

GCM basis state expressed in RGM basis

- Microscopic GCM wave functions are functions of single-particle coordinates: internal wave functions of cluster, the relative motion of the clusters and the total center-of-mass motion are entangled
- Write GCM basis state in external region with RGM basis states

$$|\Psi_{IK;JM\pi}^{{}^8\text{Be}, {}^4\text{He}}(R_j)\rangle = \sum_L \begin{Bmatrix} I & L \\ K & 0 \end{Bmatrix} \int dr r^2 \Gamma_L(R_j; r) |\Phi_{(IL)JM\pi}^{{}^8\text{Be}, {}^4\text{He}}(r)\rangle \otimes |\Phi^{\text{cm}}\rangle$$

with ($\pi = (-1)^L$)

$$\langle \boldsymbol{\rho}, \xi_a, \xi_b | \Phi_{(IL)JM\pi}^{{}^8\text{Be}, {}^4\text{He}}(r) \rangle = \sum_{M_I, M_L} \begin{Bmatrix} I & L \\ M_I & M_L \end{Bmatrix} \tilde{A} \left\{ \frac{\delta(\rho - r)}{r^2} \Phi_{IM_I}^{{}^8\text{Be}}(\xi_a) \Phi^{{}^4\text{He}}(\xi_b) Y_{LM_L}(\hat{\rho}) \right\}$$

- asymptotically RGM states have good channel spin I and orbital angular momentum L

- Microscopic α -cluster model
- Matching to Coulomb asymptotics

RGM norm kernel and Overlap functions

- RGM norm kernel reflects effects of antisymmetrization, channel $c = (IL)J$

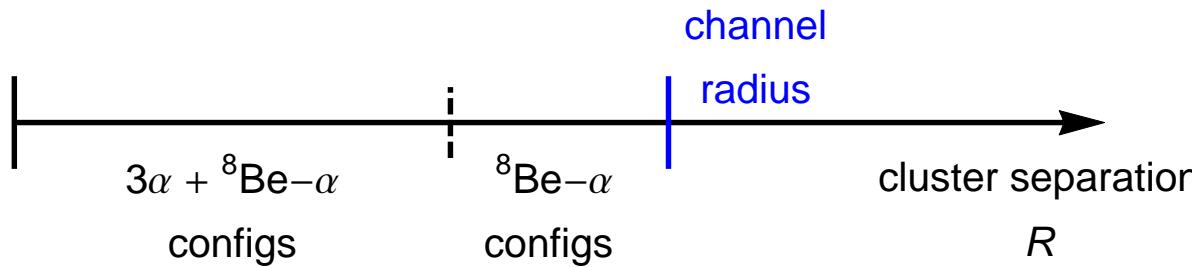
$$N_{c,c'}(r, r') = \langle \Phi_c(r) | \Phi_{c'}(r') \rangle \xrightarrow{r, r' \rightarrow \infty} \delta_{cc'} \frac{\delta(r - r')}{rr'}$$

- Overlap functions can be interpreted as wave functions for point-like clusters

$$\psi_c(r) = \int dr' r'^2 N_{c,c'}^{-1/2}(r, r') \langle \Phi_{c'}(r') | \Psi \rangle$$

Matching to the asymptotic solution

- Use multichannel microscopic R -matrix approach
Descouvemont, Baye, Phys. Rept. 73, 036301 (2010)
- Check that results are independent from channel radius: used $a = 16.5$ fm here



- Microscopic α -cluster model
- Matching to Coulomb asymptotics

Bound states

- Whittaker functions

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

Resonances

- purely outgoing Coulomb, k complex

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

Scattering states

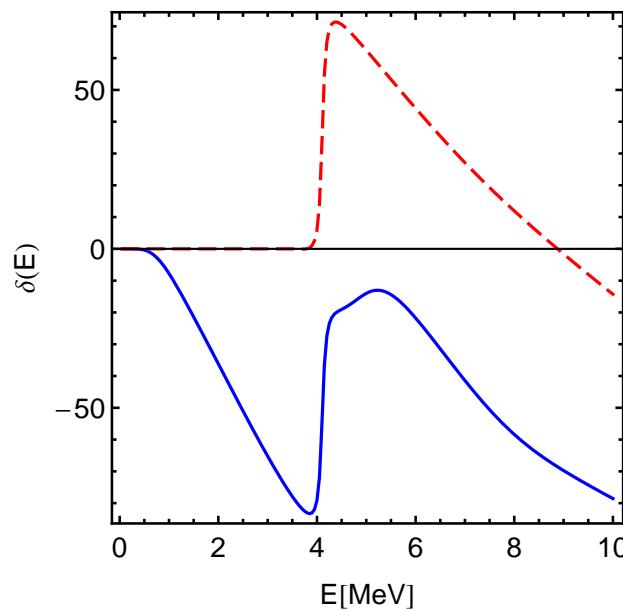
- in- and outgoing Coulomb (incoming channel c_0)

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

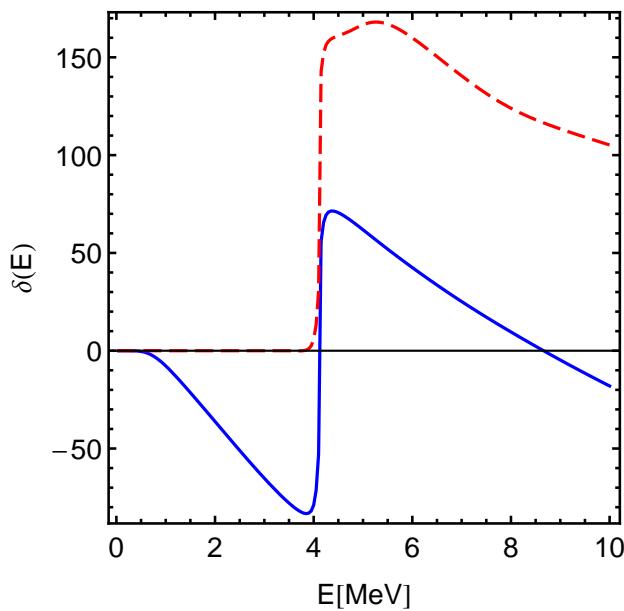
- Diagonal phase shifts and inelasticity parameters: $S_{cc} = \eta_c \exp\{2i\delta_c\}$
- Eigenphases: $S = U^{-1}DU, D_{\alpha\alpha} = \exp\{2i\delta_\alpha\}$

- Cluster Model: ${}^8\text{Be}(0_1^+, 2_1^+)$ - α Continuum
- 0^+ Phase shifts

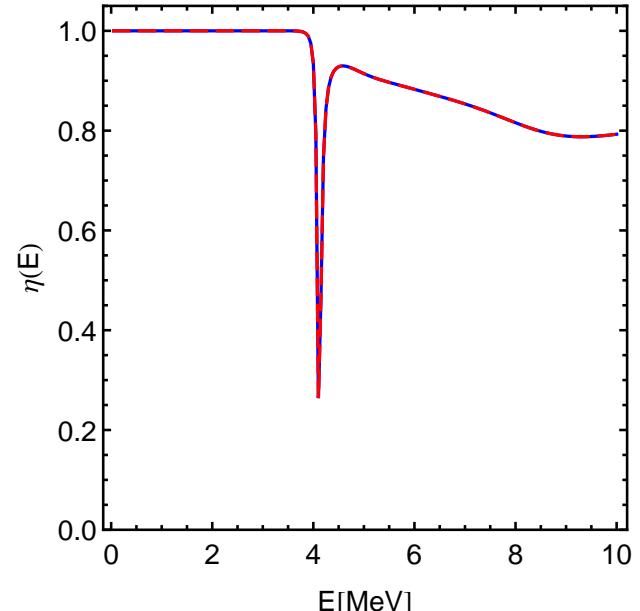
Eigenphaseshifts



Phaseshifts



Inelasticities



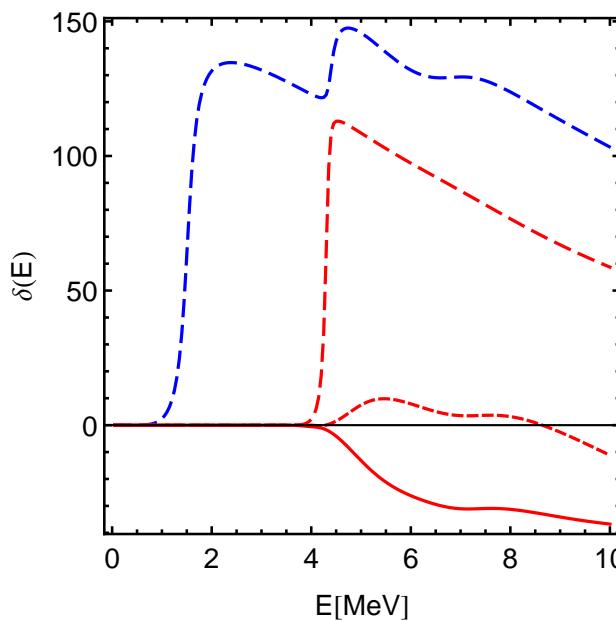
Gamow states

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

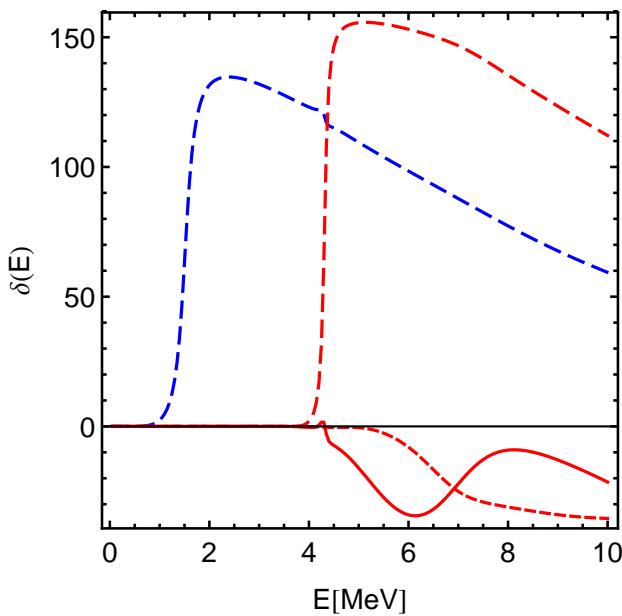
- Hoyle state missed when scanning the phase shifts
- non-resonant background
- strong coupling between ${}^8\text{Be}(0^+)$ and ${}^8\text{Be}(2^+)$ channel at 4.1 MeV

- Cluster Model: ${}^8\text{Be}(0_1^+, 2_1^+)$ - α Continuum
- 2^+ Phase shifts

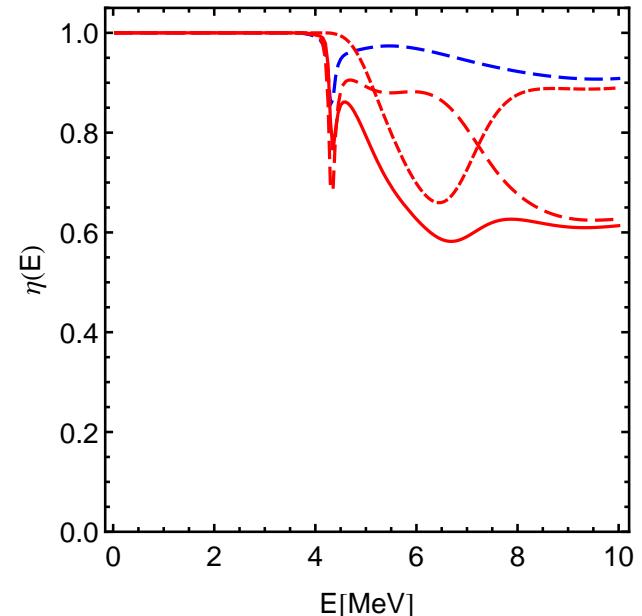
Eigenphaseshifts



Phaseshifts



Inelasticities



Gamow states

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

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

Work in Progress: FMD calculations with ^8Be - α continuum



UCOM interaction

- AV18 UCOM(SRG) ($\alpha=0.20 \text{ fm}^4$, $\lambda=1.5 \text{ fm}^{-1}$)
- Increase strength of spin-orbit force by a factor of two to partially account for omitted three-body forces

^8Be - α Continuum

- To get a good description of ^8Be 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 , ...

Model space in internal region

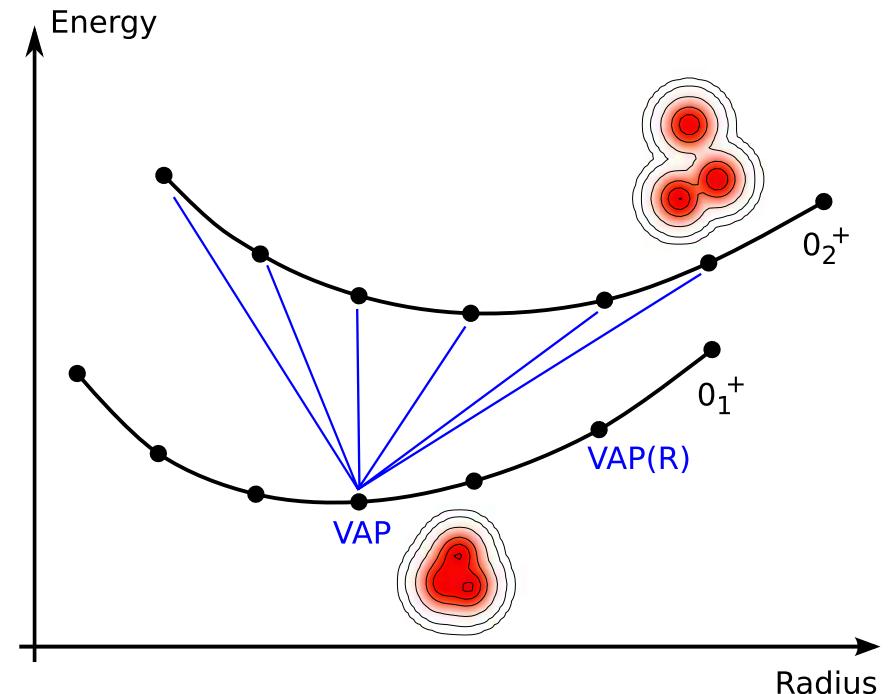
Model Space

- no assumption of α -clustering
- complete basis not feasible, find the “most important” basis states
- determine wave packet parameters by variation

VAP, VAP with constraints, Multiconfiguration-VAP

For each angular momentum ($0^+, 1^+, 2^+, \dots$)

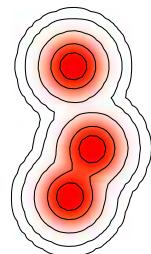
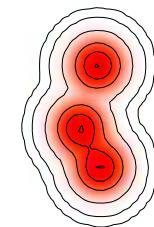
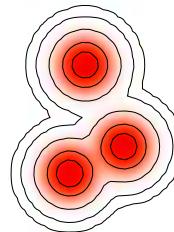
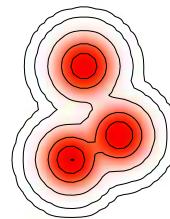
- **VAP**: vary energy of projected Slater determinant $\tilde{P}^\pi \tilde{P}_{MK}^\dagger |Q(q_i)\rangle$ with respect to all parameters q_i
- **VAP(R)**: create additional basis states by variation with a constraint on the radius of the intrinsic state
- **MC-VAP**: keep VAP state fix and vary the parameters of a second Slater determinant to minimize the energy of the second eigenstate in a multiconfiguration mixing calculation
- **MC-VAP(R)**: create additional basis states by adding a constraint on the radius of the second intrinsic state



- FMD

Important Configurations

- Calculate the overlap with FMD basis states to find the most important contributions to the eigenstates (in bound state approximation)



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

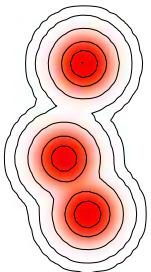
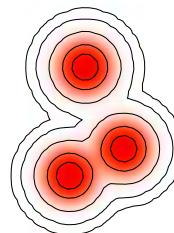
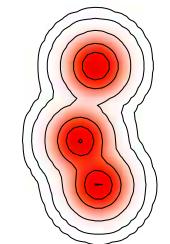
$$|\langle \cdot | 2_1^+ \rangle| = 0.93$$

$$|\langle \cdot | 0_2^+ \rangle| = 0.64$$

$$|\langle \cdot | 0_2^+ \rangle| = 0.58$$

$$|\langle \cdot | 0_2^+ \rangle| = 0.57$$

$$|\langle \cdot | 0_2^+ \rangle| = 0.45$$



$$|\langle \cdot | 3_1^- \rangle| = 0.91$$

$$|\langle \cdot | 2_2^+ \rangle| = 0.50$$

$$|\langle \cdot | 2_2^+ \rangle| = 0.49$$

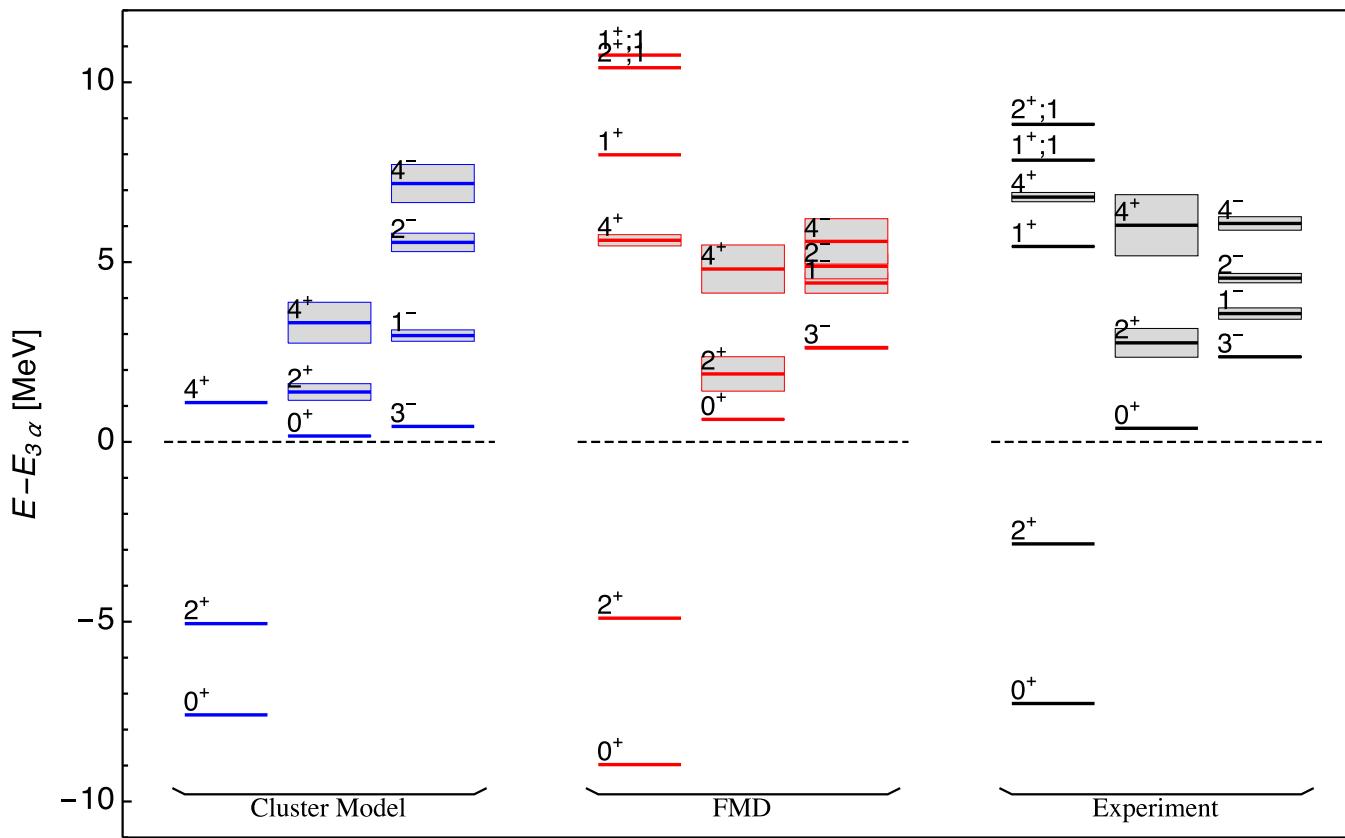
$$|\langle \cdot | 2_2^+ \rangle| = 0.44$$

$$|\langle \cdot | 2_2^+ \rangle| = 0.41$$

FMD basis states are not orthogonal!

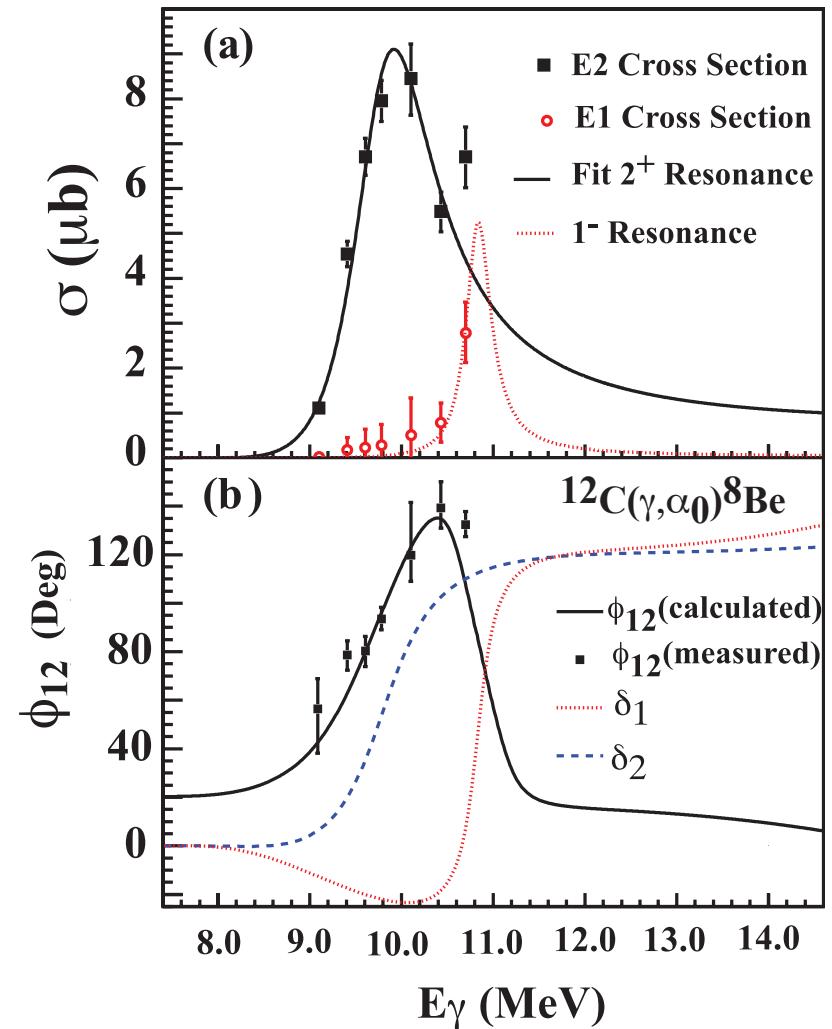
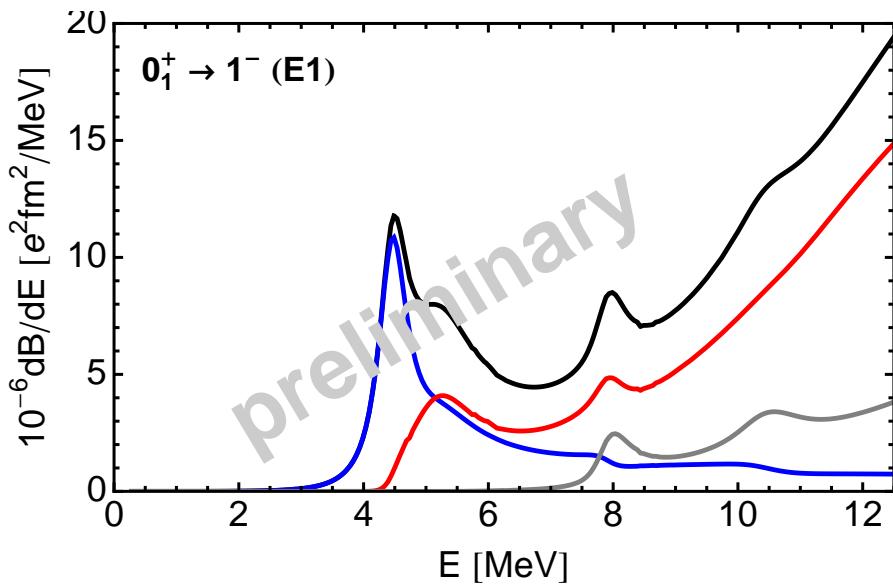
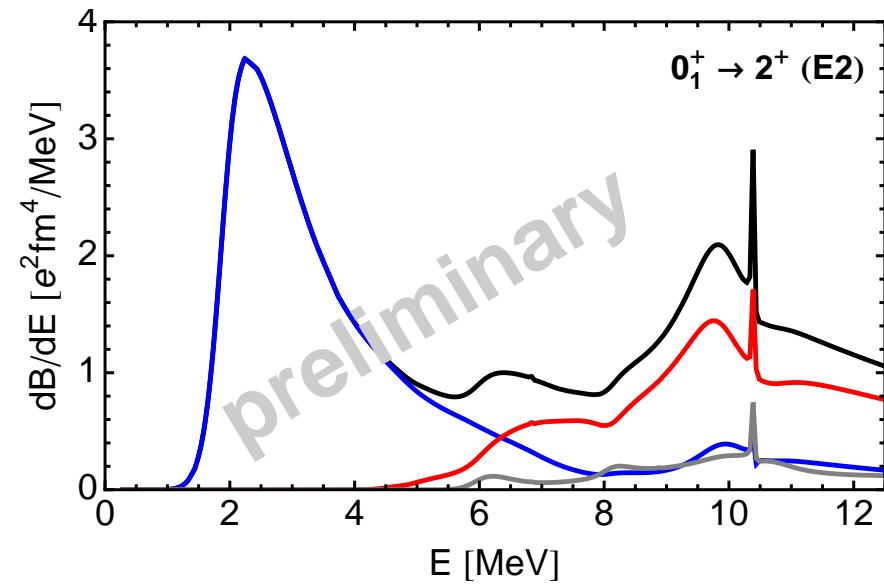
0_2^+ and 2_2^+ states have no rigid intrinsic structure

- FMD/Cluster Model: ${}^8\text{Be}-\alpha$ Continuum Spectrum



- FMD describes the ground state band, the cluster states related to the Hoyle state and the negative parity states reasonably well
- Spin-flip states ($1^+ T = 0, 1$ and $2^+ T = 1$) are somewhat too high in energy

- FMD: $^8\text{Be}-\alpha$ Continuum
- Strength distributions



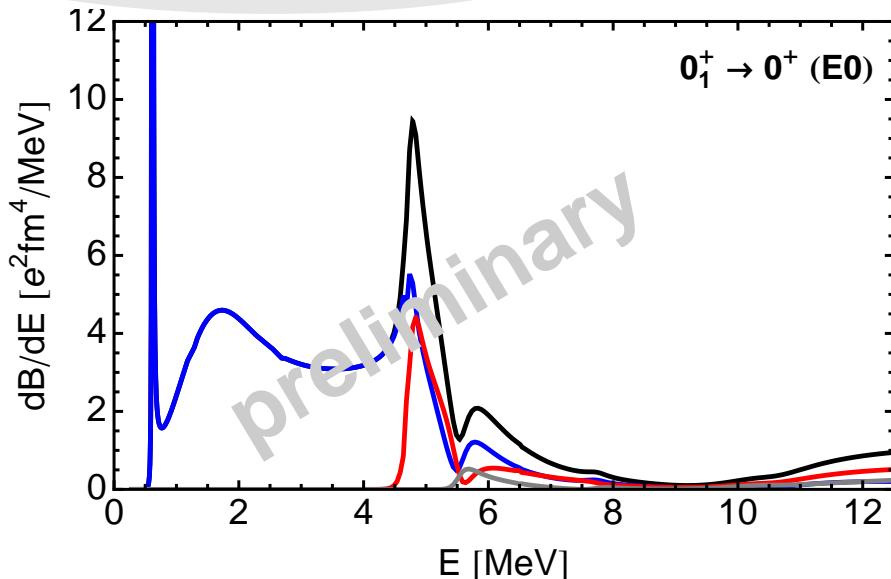
✗ E1 transition isospin-forbidden in cluster model !

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

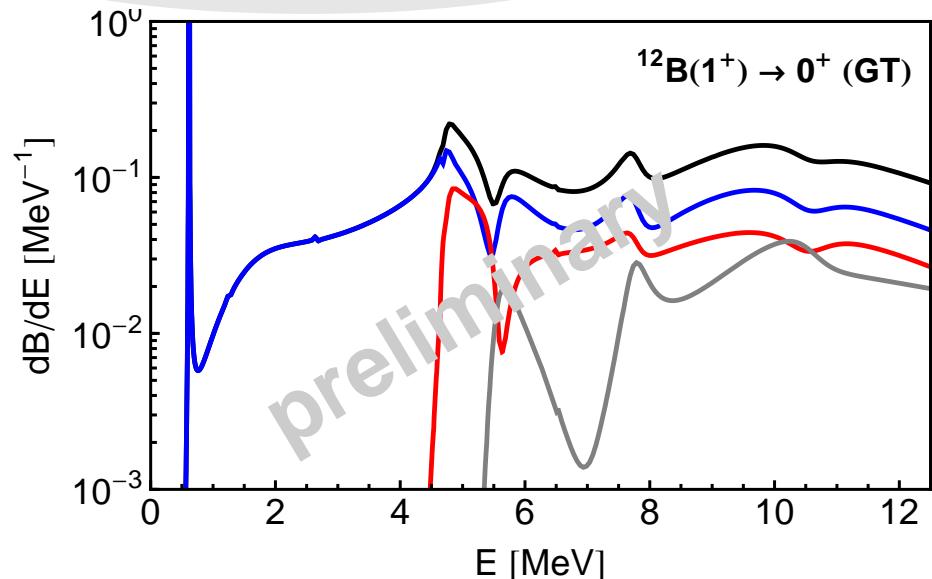
- FMD: ${}^8\text{Be}$ - α Continuum

Population of 0^+ continuum with different reactions

Monopole response



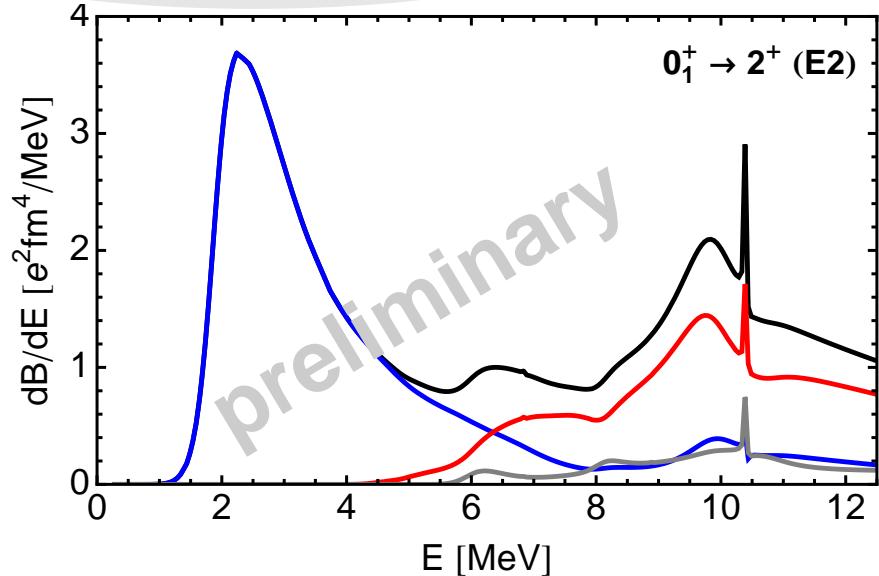
β -decay



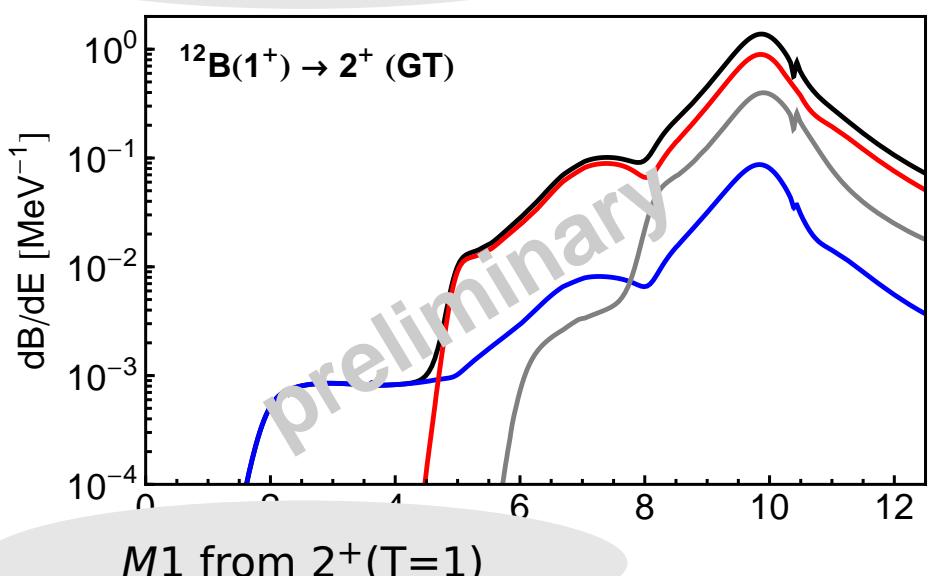
- GT transitions probe admixtures of “shell model” components
- Hoyle state populated in β -decay
- third 0^+ state decays through both ${}^8\text{Be}(0^+)$ - α and ${}^8\text{Be}(2^+)$ - α channels
– does this reflect a three-body resonance ?

- FMD: $^8\text{Be}-\alpha$ Continuum
- Population of 2^+ continuum with different reactions

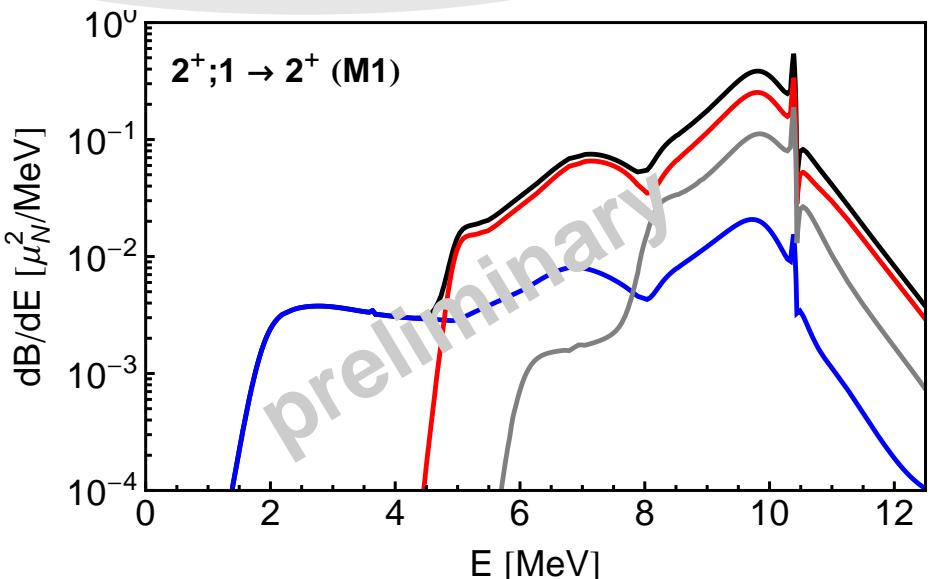
Quadrupole response



β -decay

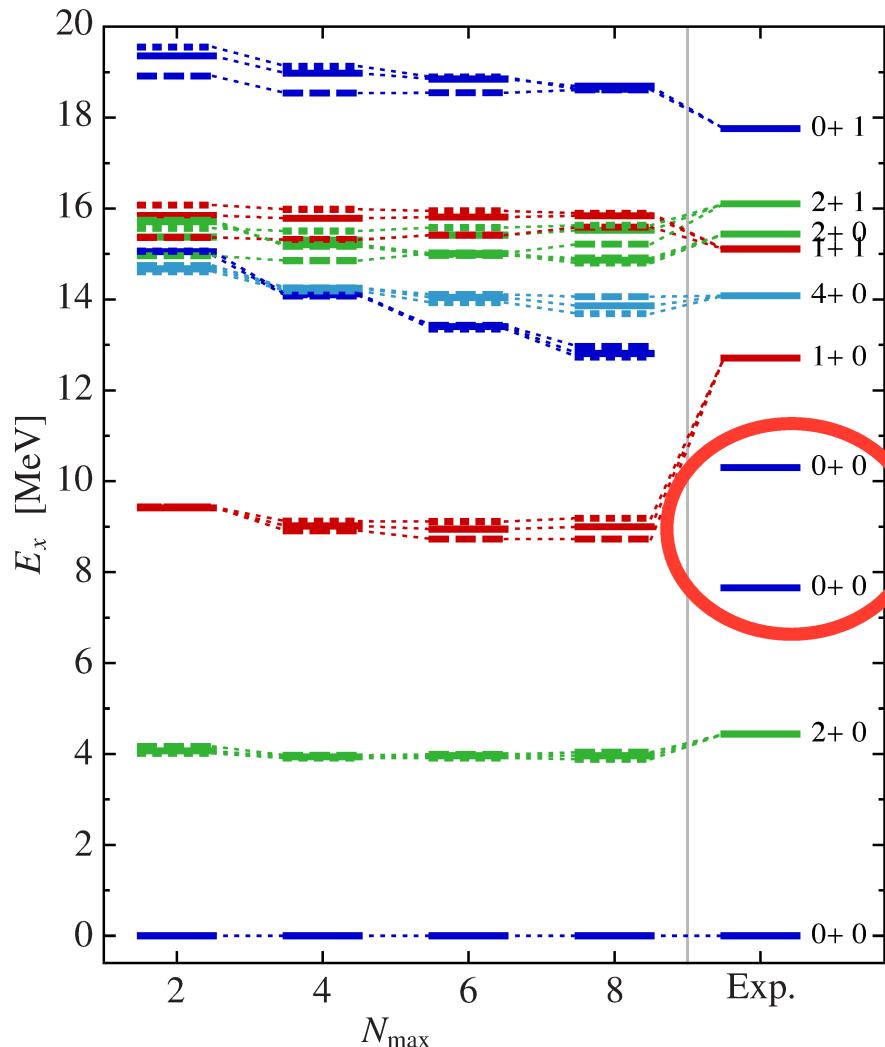


$M1$ from $2^+(T=1)$



- 2^+_2 state very weakly populated in β -decay and in $M1$ transitions
- β -decay and $M1$ transitions from $2^+(T=1)$ state strongly populate 2^+ states that decay mainly through $^8\text{Be}(2^+)-\alpha$

• ^{12}C Cluster States in *ab initio* approaches ?



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

Hoyle state and other
cluster states missing !

Lattice EFT

Green's Function
Monte Carlo

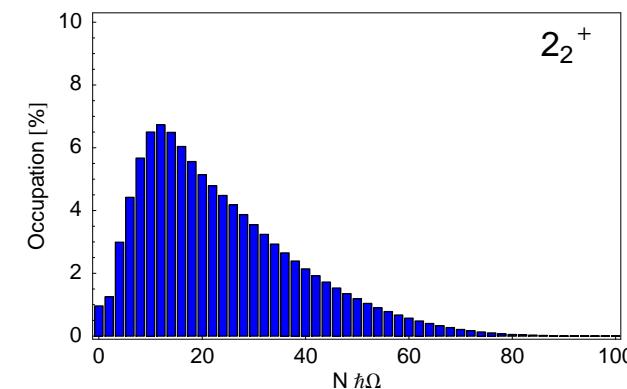
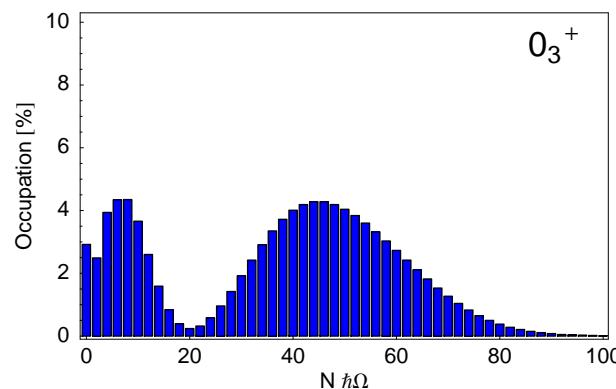
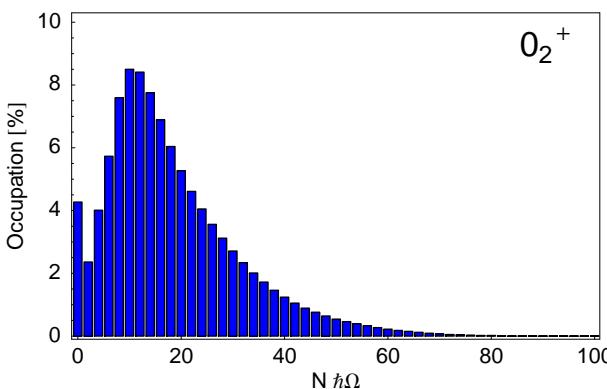
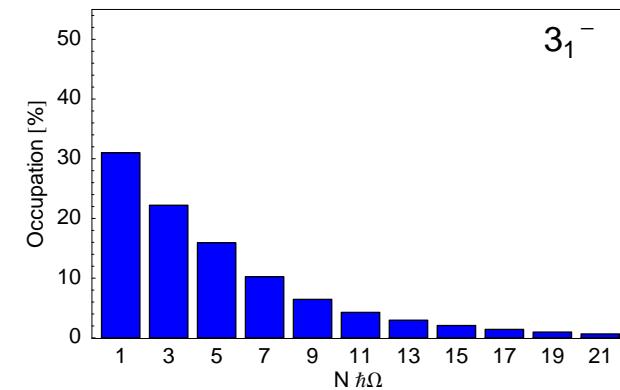
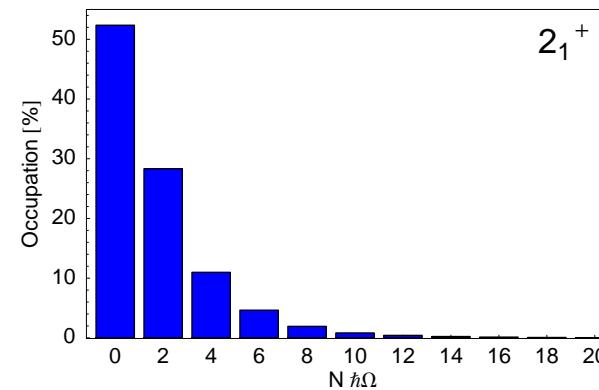
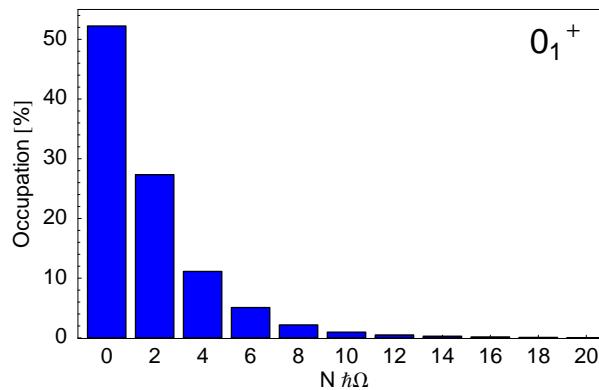
Maris, Vary, Calci, Langhammer, Binder, Roth, Phys. Rev. C **90**, 014314 (2014)

- Cluster States in ^{12}C
- Harmonic Oscillator $N\hbar\Omega$ Excitations

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

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

Cluster Model



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

$^3\text{He}(\alpha, \gamma)^7\text{Be}$ Radiative Capture

- Bound states, scattering states, capture cross sections

Microscopic cluster model for ^{12}C

- Model space with 3 α and $^8\text{Be}-\alpha$ configurations
- Matching with Coulomb continuum, resonances and scattering states
- Hoyle state band build on $^8\text{Be}(\text{gs})-\alpha$

FMD calculations for ^{12}C

- VAP and Multiconfig-VAP in internal region, $^8\text{Be}-\alpha$ in external region
 - Investigate EM and GT transitions to the continuum
- $^8\text{Be}-\alpha$ vs real three-body asymptotics ?