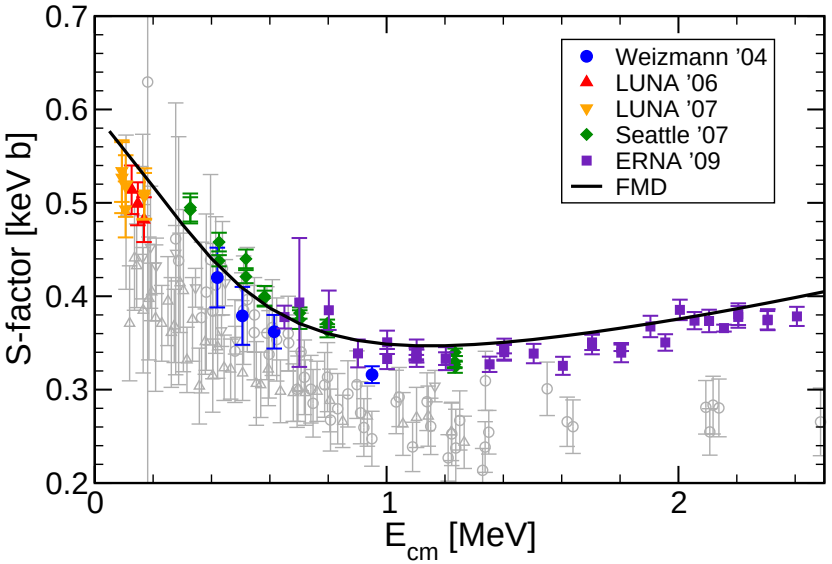
Microscopic calculation of the ^{3}He(α,γ)^{7}Be reaction rate



Thomas Neff

DREB 2012

Direct Reactions with Exotic Beams

Pisa, Italy

Mar 26-30, 2012

HELMHOLTZ ASSOCIATION

GSI

Overview

Introduction

Effective interaction and many-body approach

- **Unitary Correlation Operator Method**
- **Fermionic Molecular Dynamics**

Results

- **Bound and scattering states**
- **Astrophysical S-factor**

Discussion

- **Dipole matrix elements**
- **^{3}He(α,γ)^{7}Be vs. ^{3}H(α,γ)^{7}Li**

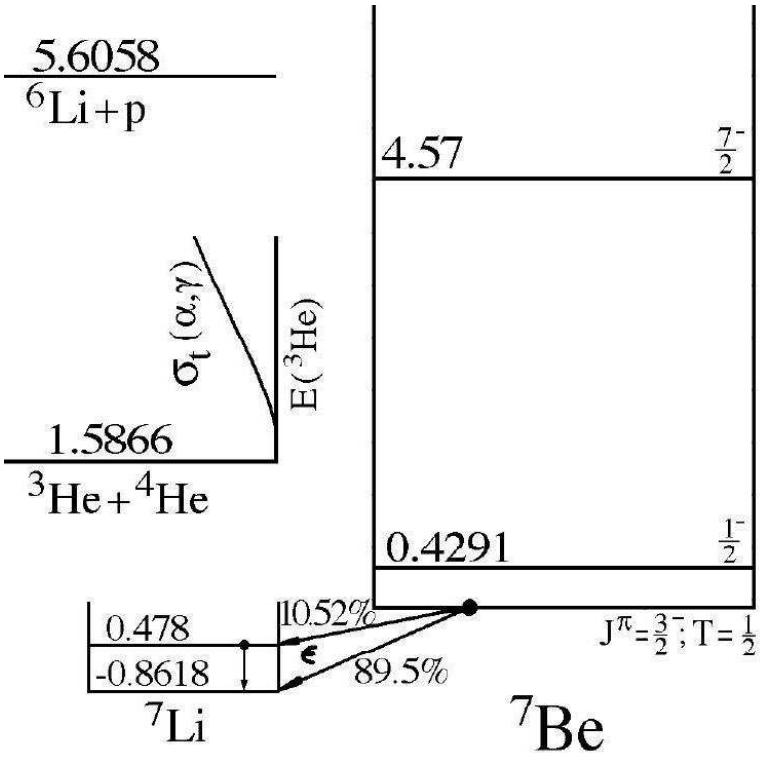
Introduction

Motivation

- ^{3}He(α,γ)^{7}Be one of the key reactions in the solar pp-chains
- in competetion with the ^{3}He(^{3}He,2p)^{4}He reaction it determines production of ^{7}Be and ^{8}B neutrinos

What is needed ?

- ^{7}Be bound state energies
- ^{7}Be bound state wave functions, ANC
- ^{3}He-^{4}He scattering states
- dipole matrix elements between bound and scattering states



Theoretical Approaches

Potential models (Kim *et al.* 1982, Mohr 2009, . . .)

- ^{4}He and ^{3}He are considered as point-like particles
- interacting via an effective nucleus-nucleus potential fitted to bound state properties and phase shifts
- ANCs calculated from *ab initio* wave functions (Nollett 2001, Navratil *et al.* 2007)

Microscopic Cluster Model (Tang *et al.* 1981, Langanke 1986, Kajino 1986 . . .)

- antisymmetrized wave function built with ^{4}He and ^{3}He clusters
- some attempts to include polarization effects by adding other channels like ^{6}Li plus proton
- interacting via an effective nucleon-nucleon potential, adjusted to describe bound state properties and phase shifts

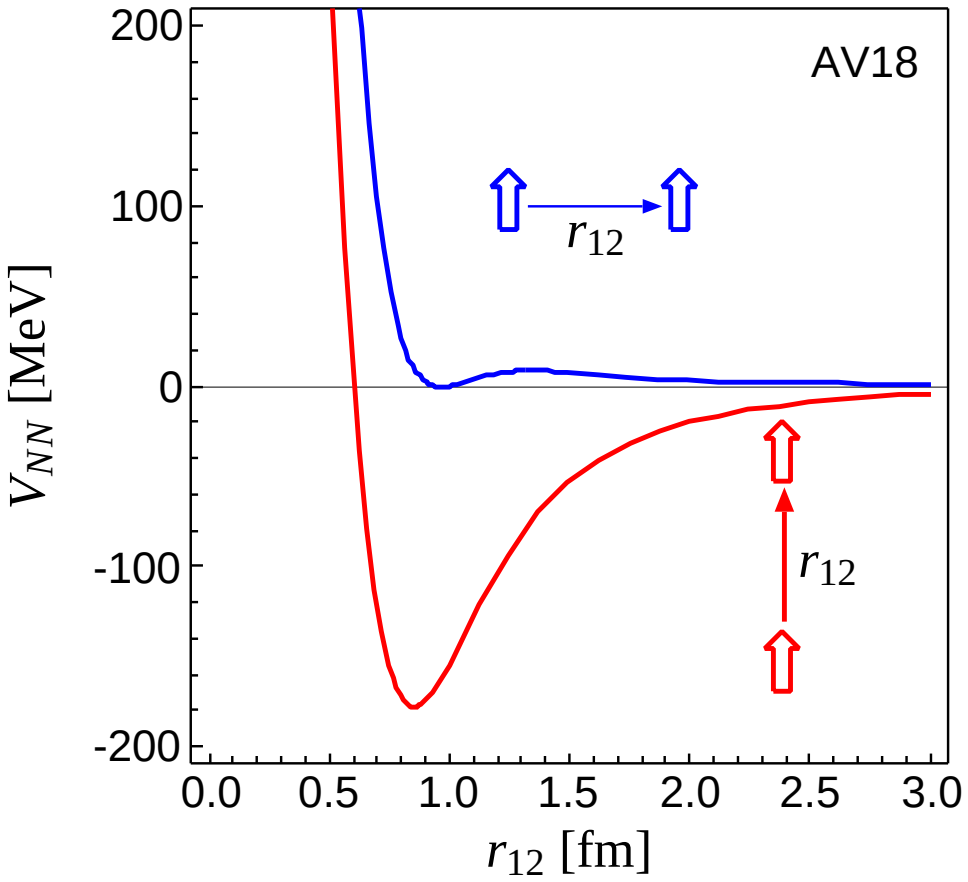
Our Aim

- fully microscopic wave functions with cluster configurations at large distances and additional polarized A-body configurations in the interaction region
- using a realistic effective interaction

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**

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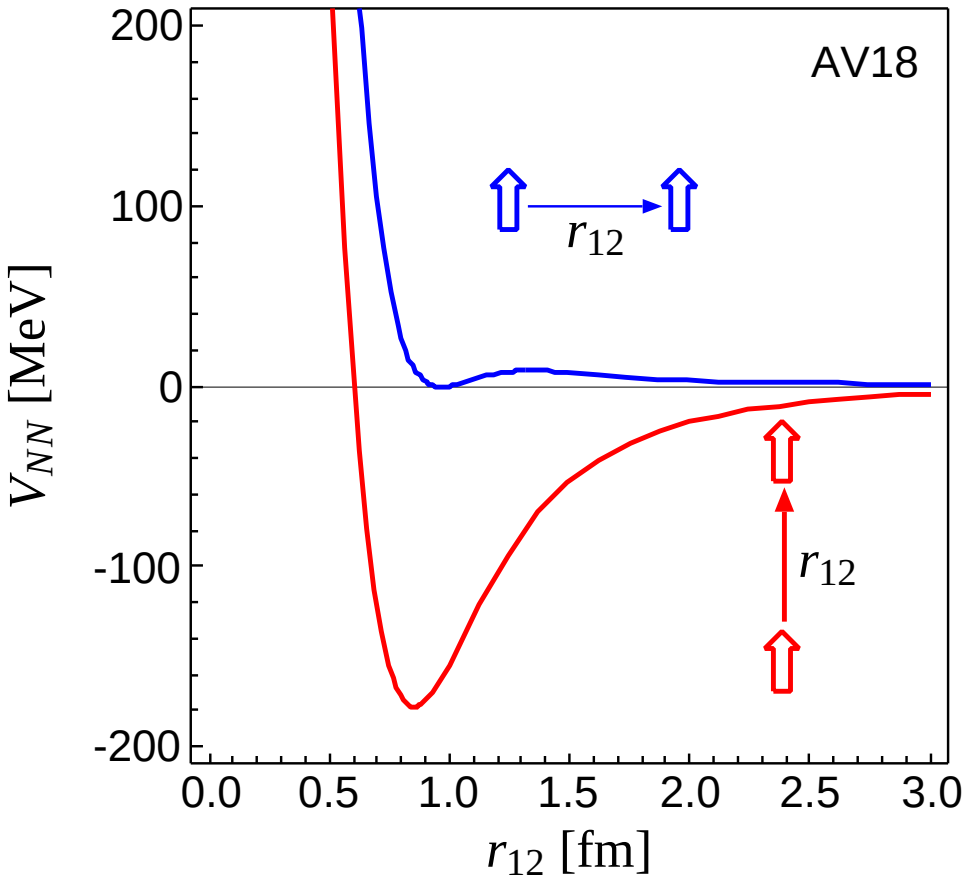

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➨ **central correlations**

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

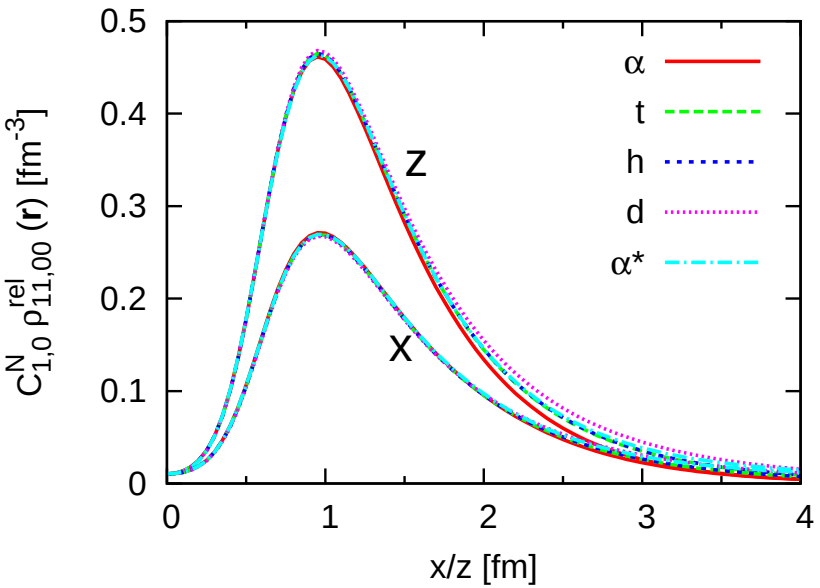
➨ **tensor correlations**

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

Universality of short-range correlations

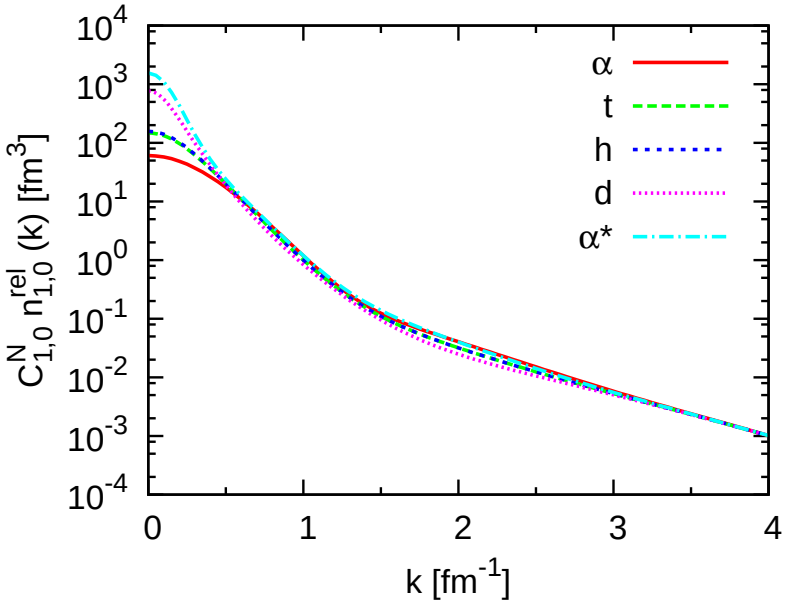
coordinate space

$S = 1, M_S = 1, T = 0$



momentum space

$S = 1, T = 0$



- normalize two-body density in coordinate space at r=1.0 fm
- normalized two-body densities in coordinate space are identical at short distances for all nuclei
- use the **same** normalization factor in momentum space – high momentum tails agree for all nuclei

Feldmeier, Horiuchi, Neff, Suzuki, Phys. Rev. C **84**, 054003 (2011)

Unitary Correlation Operator Method

Correlation Operator

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

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

- correlation operator should conserve the symmetries of the Hamiltonian and should be of finite-range, correlated interaction **phase shift equivalent** to bare interaction by construction

Correlated Operators

- correlated operators will have contributions in higher cluster orders

$$\underset{\sim}{C}^\dagger \underset{\sim}{O} \underset{\sim}{C} = \underset{\sim}{\hat{O}}^{[1]} + \underset{\sim}{\hat{O}}^{[2]} + \underset{\sim}{\hat{O}}^{[3]} + \ldots$$

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

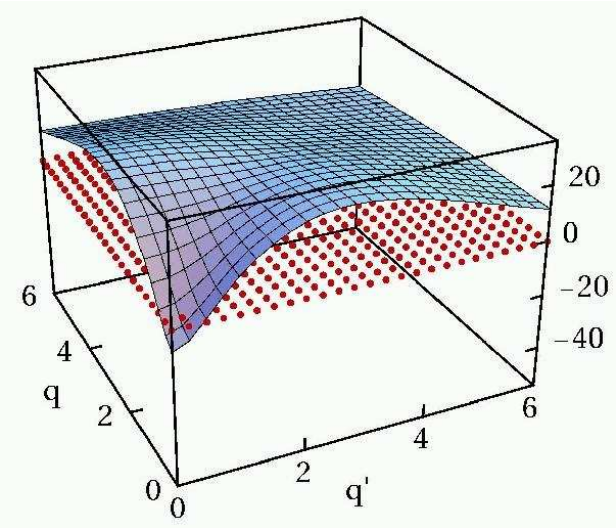
Correlated Interaction

$$\underset{\sim}{C}^\dagger \left(\underset{\sim}{T} + \underset{\sim}{V}\right) \underset{\sim}{C} = \underset{\sim}{T} + \underset{\sim}{V}_{\mathrm{UCOM}} + \underset{\sim}{V}^{[3]}_{\mathrm{UCOM}} + \ldots$$

Roth, Neff, Feldmeier, Prog. Part. Nucl. Phys. **65**, 50 (2010)

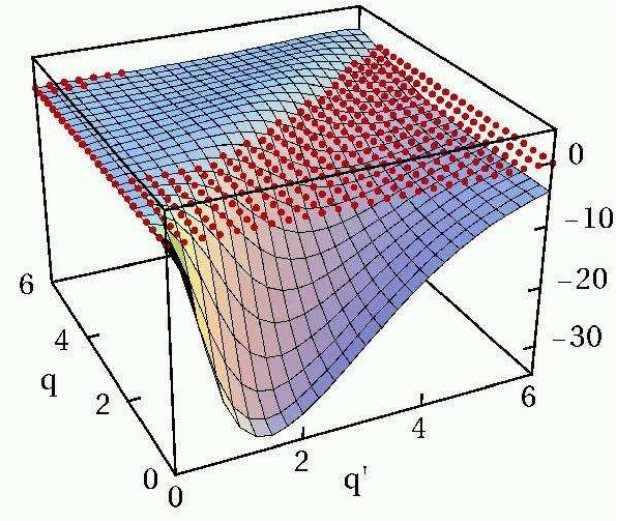
UCOM Interaction in Momentum Space $V(q, q')$

$^3S_1$ bare



bare interaction has **strong off-diagonal** matrix elements connecting to high momenta

$^3S_1$ - $^3D_1$ bare



Roth, Hergert, Papakonstaninou, Neff, Feldmeier, Phys. Rev. C **72**, 034002 (2005)

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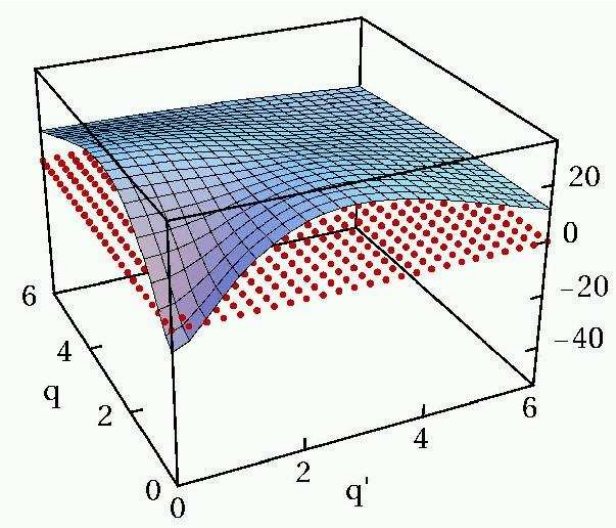

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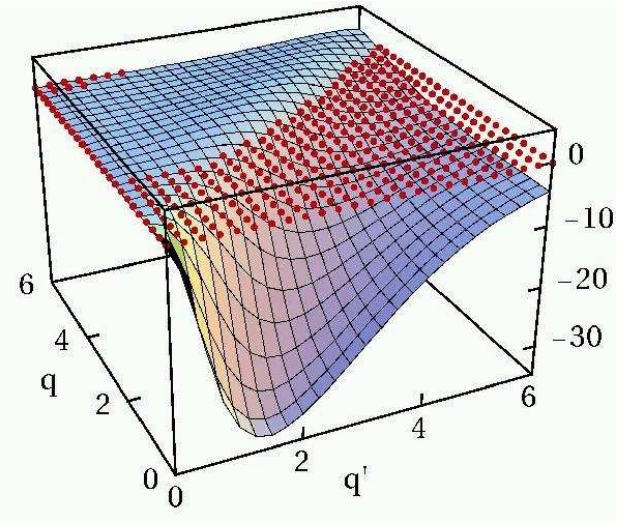
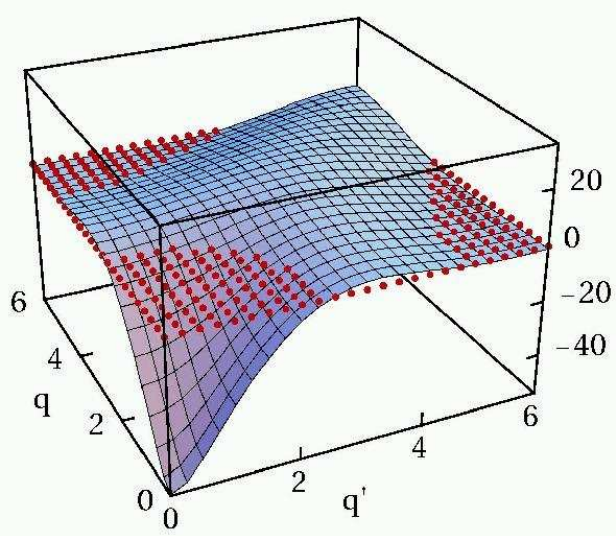
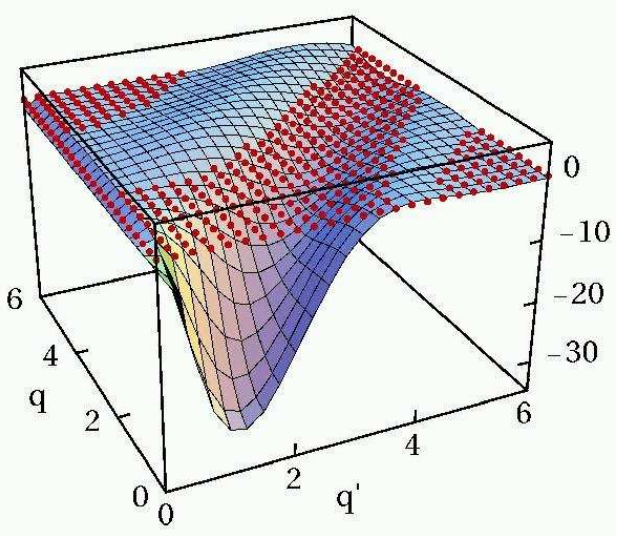


$^3S_1$ correlated



correlated interaction is **more attractive** at low momenta

$^3S_1$ - $^3D_1$ correlated



off-diagonal matrix elements connecting low- and high- momentum states are **strongly reduced**

Roth, Hergert, Papakonstaninou, Neff, Feldmeier, Phys. Rev. C **72**, 034002 (2005)

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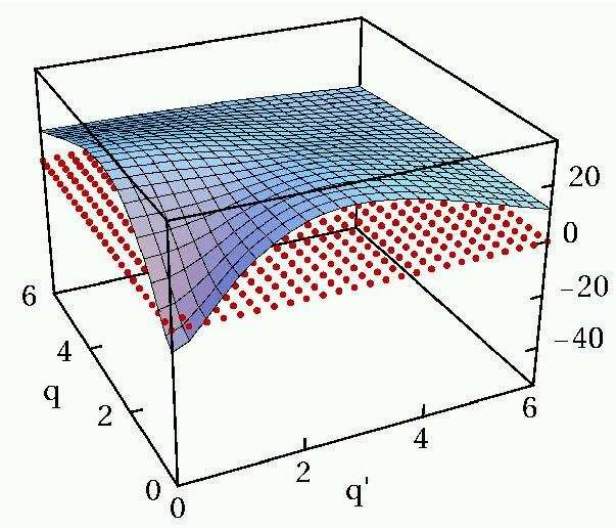

bare interaction has **strong off-diagonal** matrix elements connecting to high momenta

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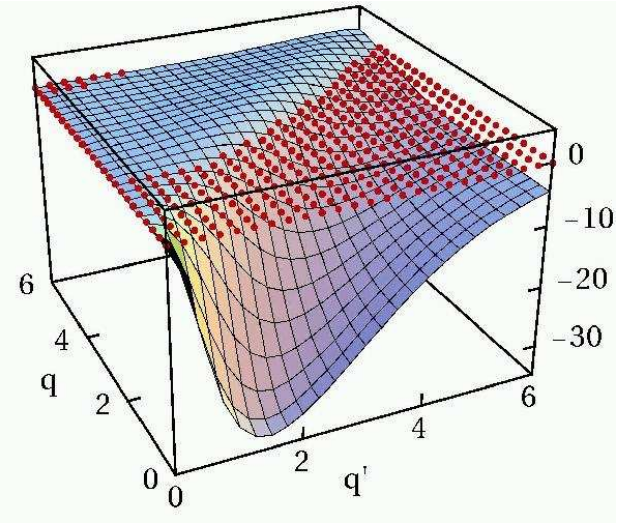

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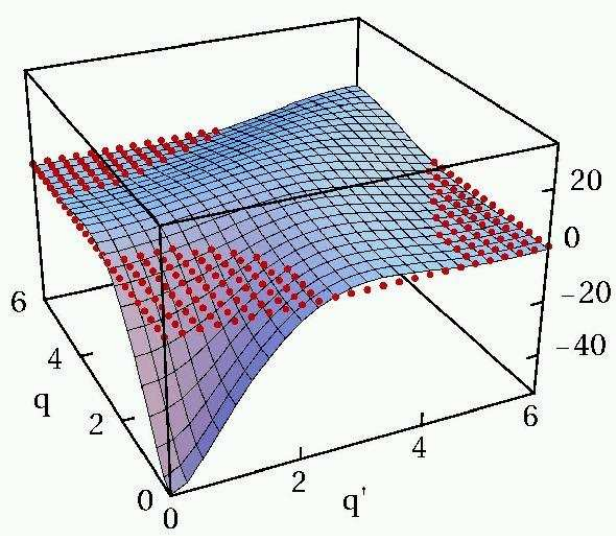

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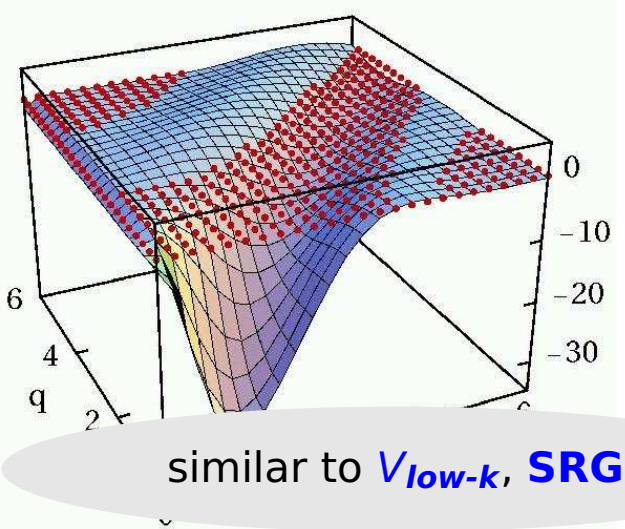
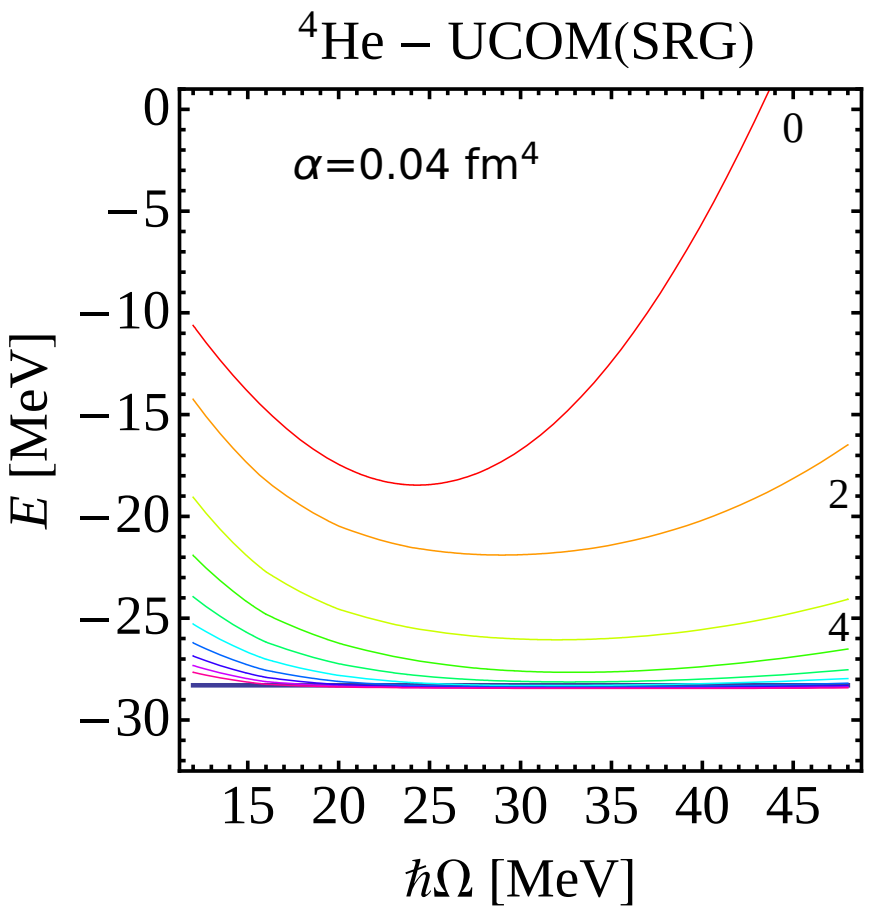


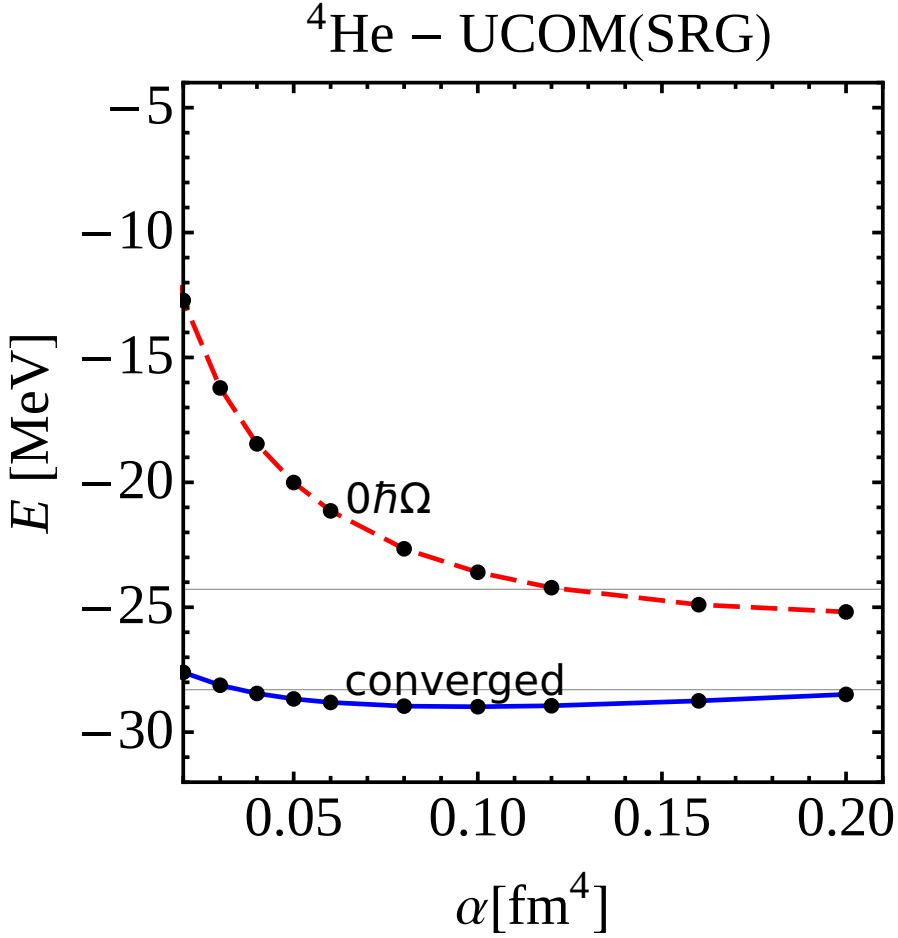
off-diagonal matrix elements connecting low- and high- momentum states are **strongly reduced**

similar to $V_{low\text{-}k}$, **SRG**

Roth, Hergert, Papakonstaninou, Neff, Feldmeier, Phys. Rev. C **72**, 034002 (2005)

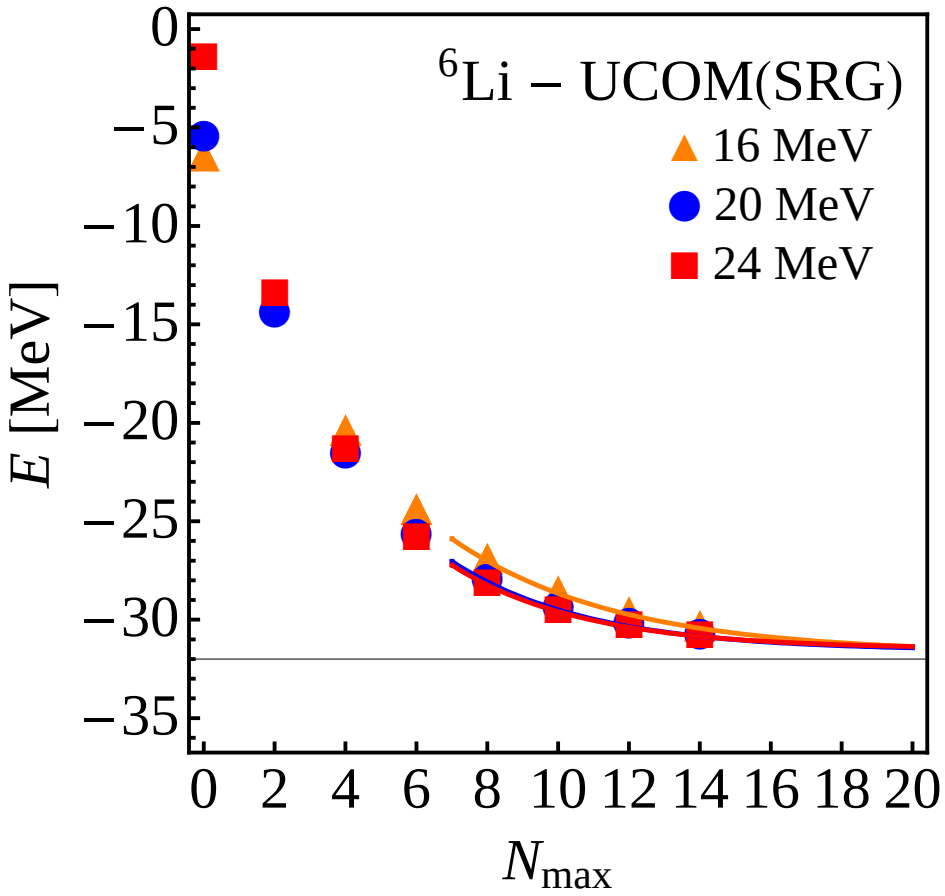
No-Core Shell Model Calculations

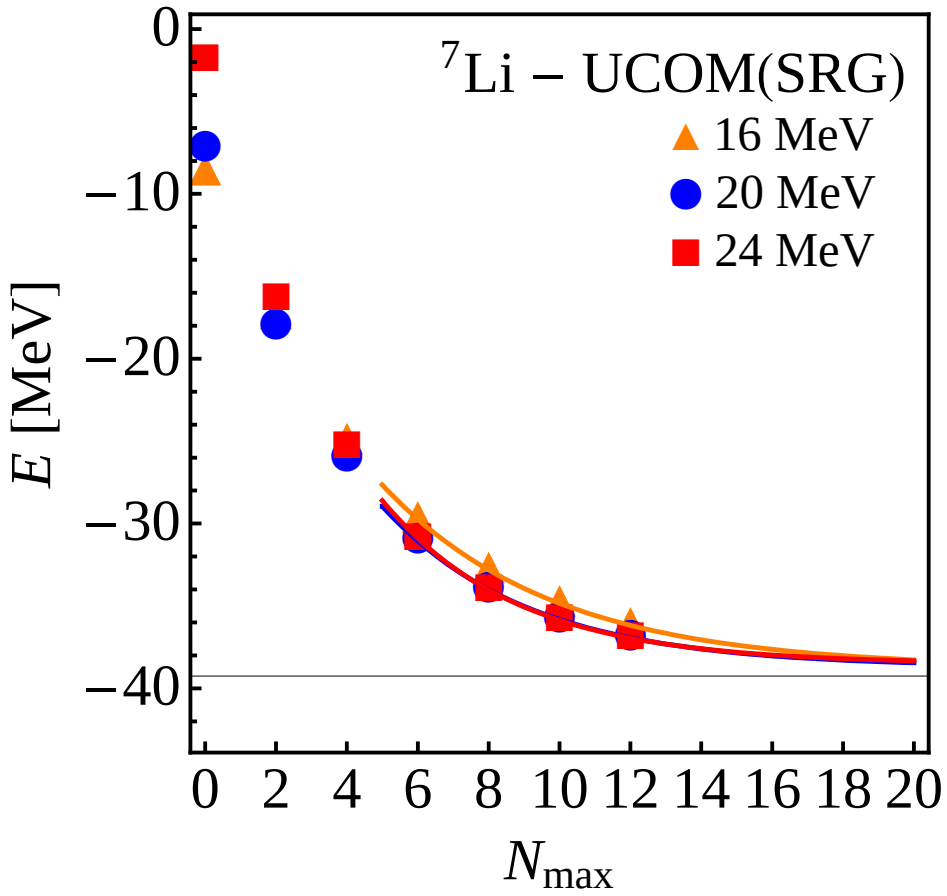




- convergence much improved compared to bare interaction
- effective interaction – in two-body approximation – converges to different energy then bare interaction
- transformed interaction can be tuned to obtain simultaneously (almost) exact ^{3}He and ^{4}He binding energies

NCSM ^{6}Li/^{7}Li ground state energy





- effective interaction also works reasonably well for heavier nuclei

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

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

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

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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 state

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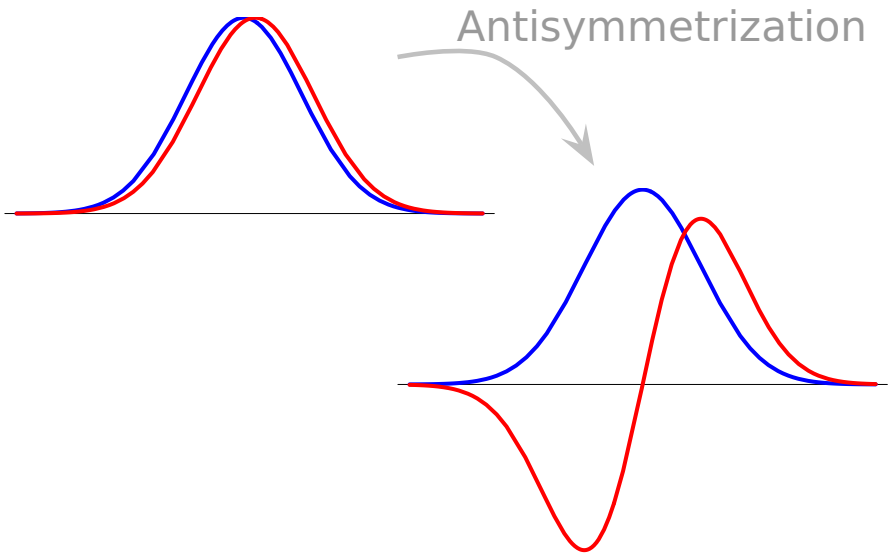

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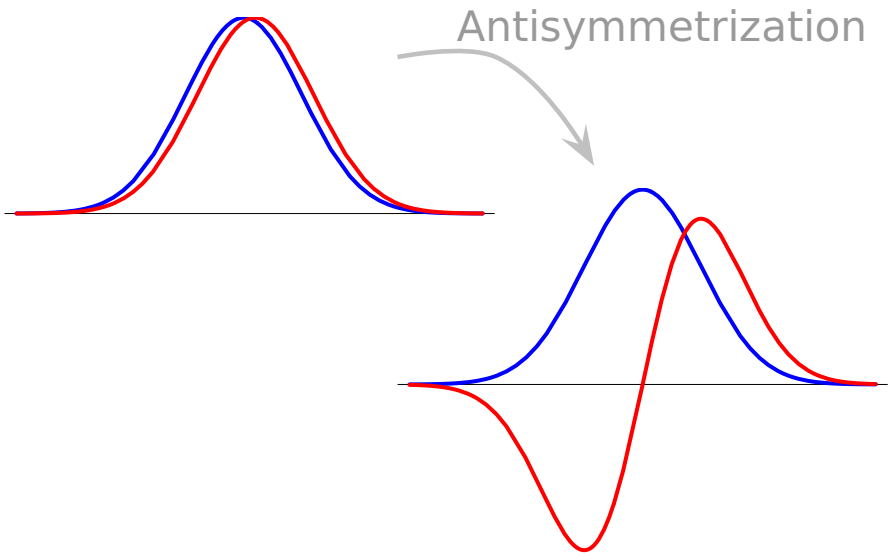

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see also
Antisymmetrized Molecular Dynamics
Horiuchi, Kanada-En'yo, Kimura, . . .

Feldmeier, Schnack, Rev. Mod. Phys. **72** (2000) 655
Neff, Feldmeier, Nucl. Phys. **A738** (2004) 357

Restoration of Symmetries

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

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

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

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

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Variation After Projection (VAP)

- effect of projection can be large
- full **Variation after Angular Momentum and Parity Projection** (VAP) for light nuclei

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- perform VAP in GCM sense by applying **constraints** on radius, dipole moment, quadrupole moment or octupole moment and minimizing the energy in the projected energy surface for heavier nuclei

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Multiconfiguration Calculations

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

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

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

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

FMD model space

Frozen configurations

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

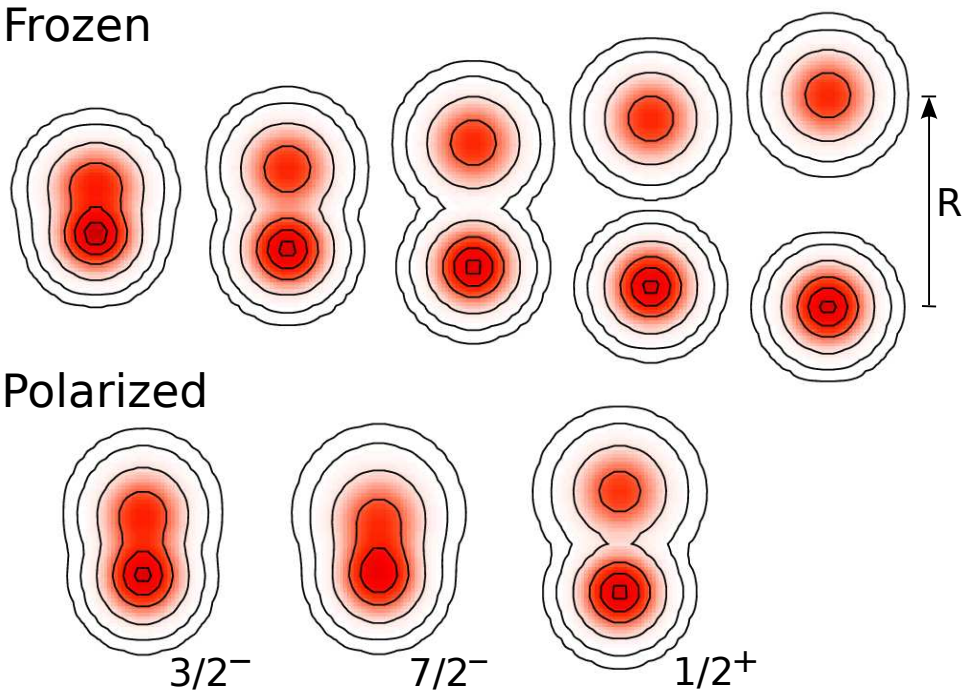
Polarized configurations

- 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

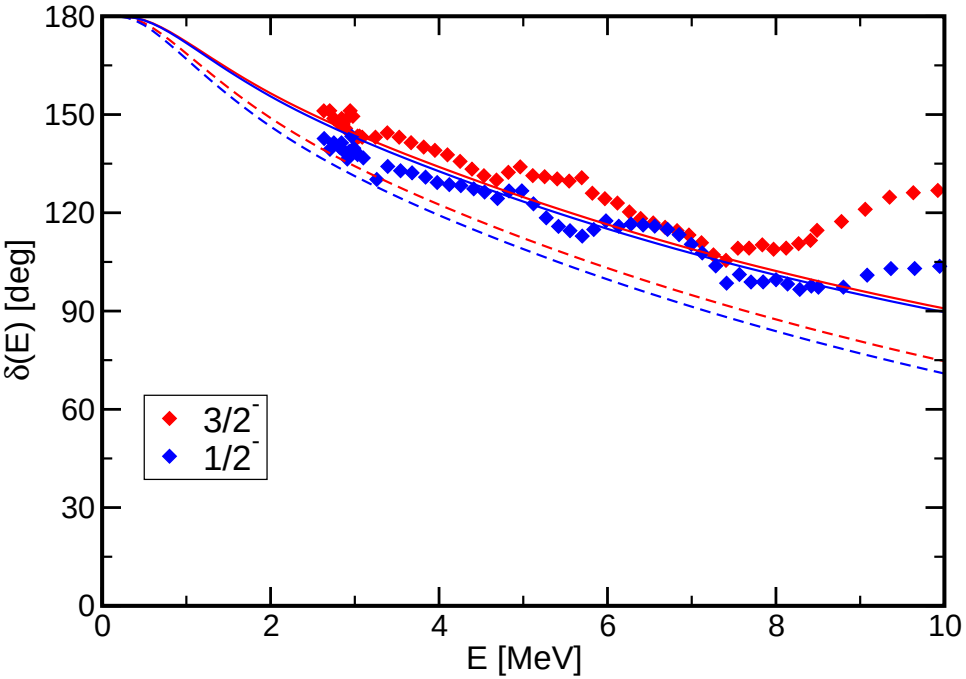
Bound states

		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)

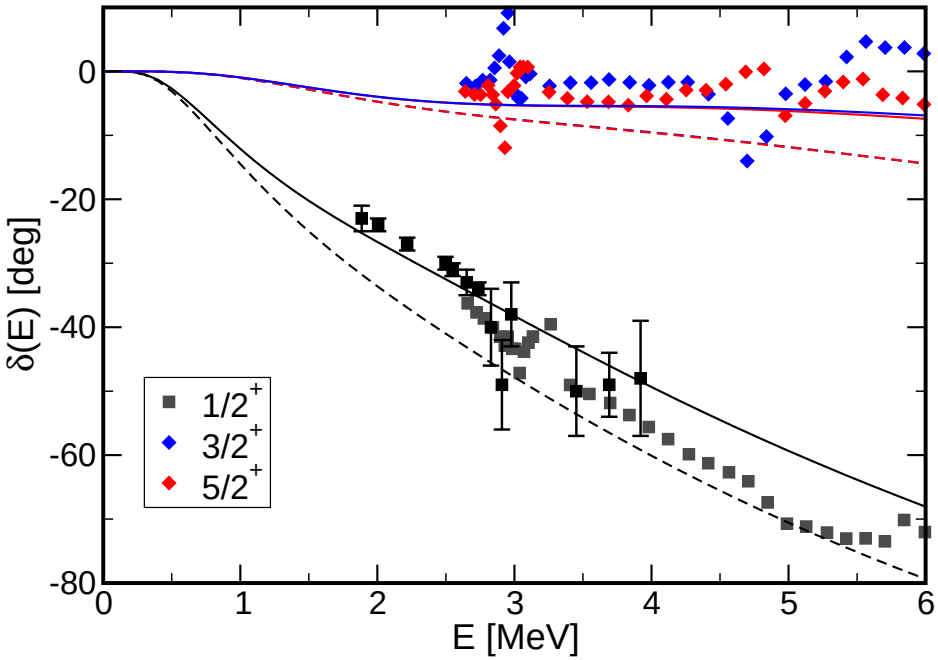


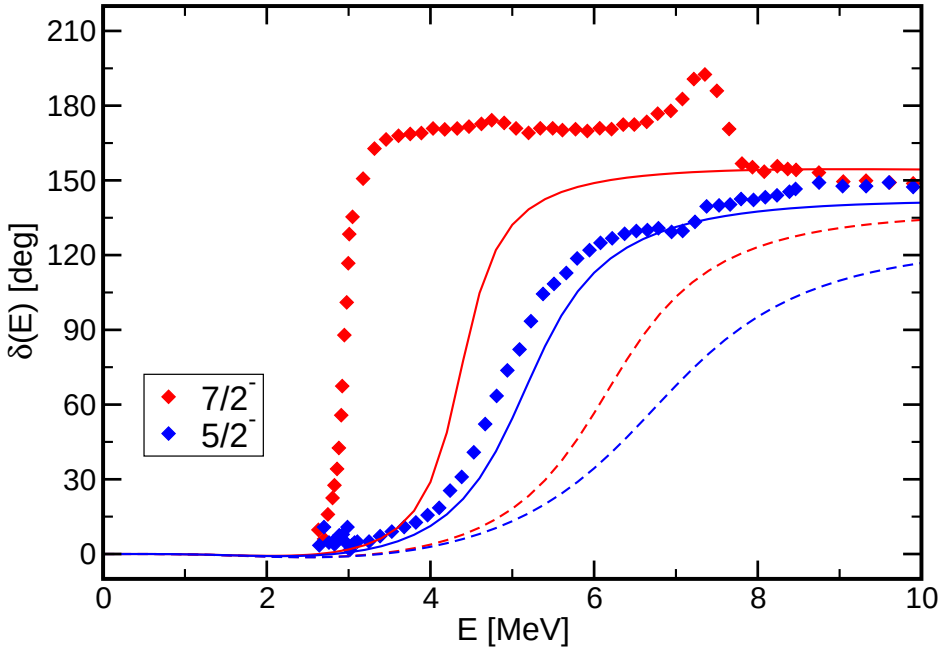
dashed lines – frozen configurations only
solid lines – polarized configurations in interaction region included

- Scattering phase shifts well described, polarization effects important

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

s-, d- and f-wave Scattering States

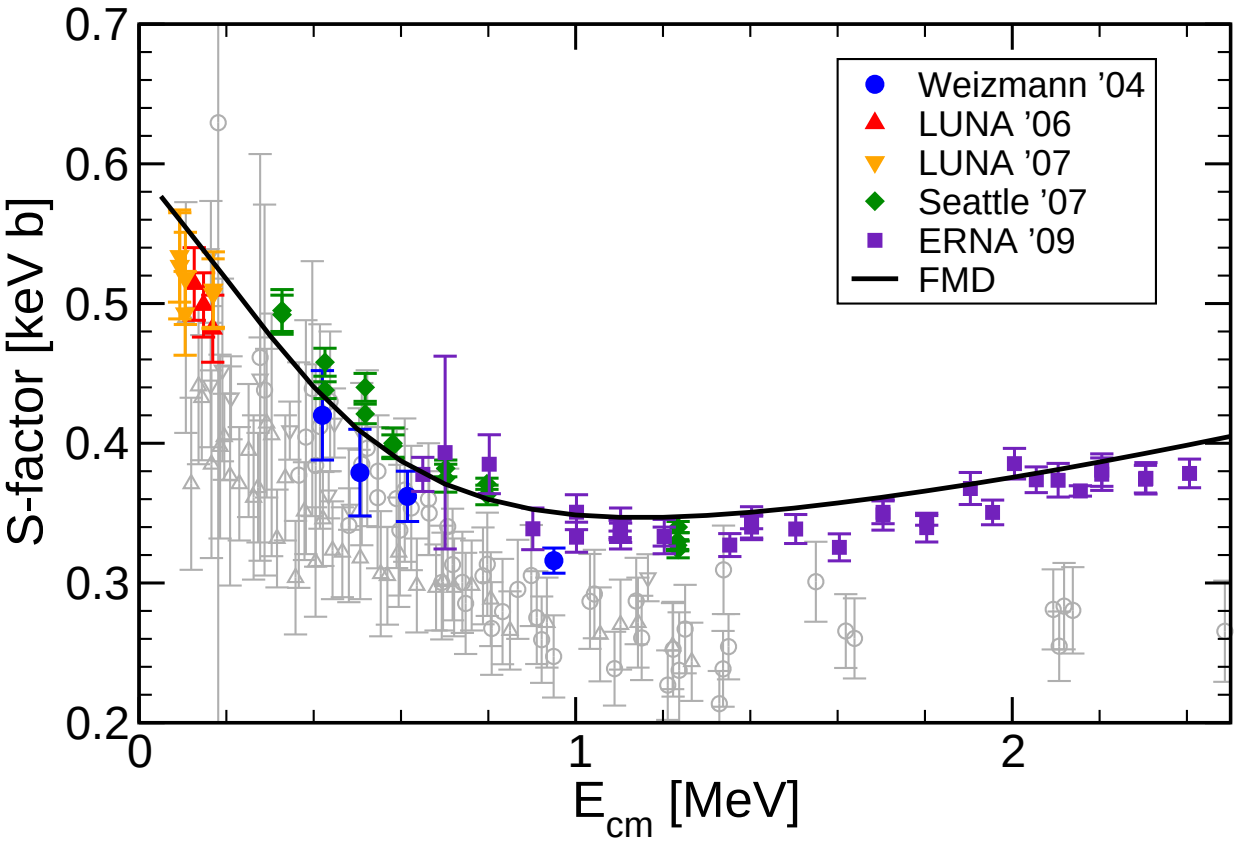




dashed lines – frozen configurations only – solid lines – FMD configurations in interaction region included

- 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

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



S-factor:

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

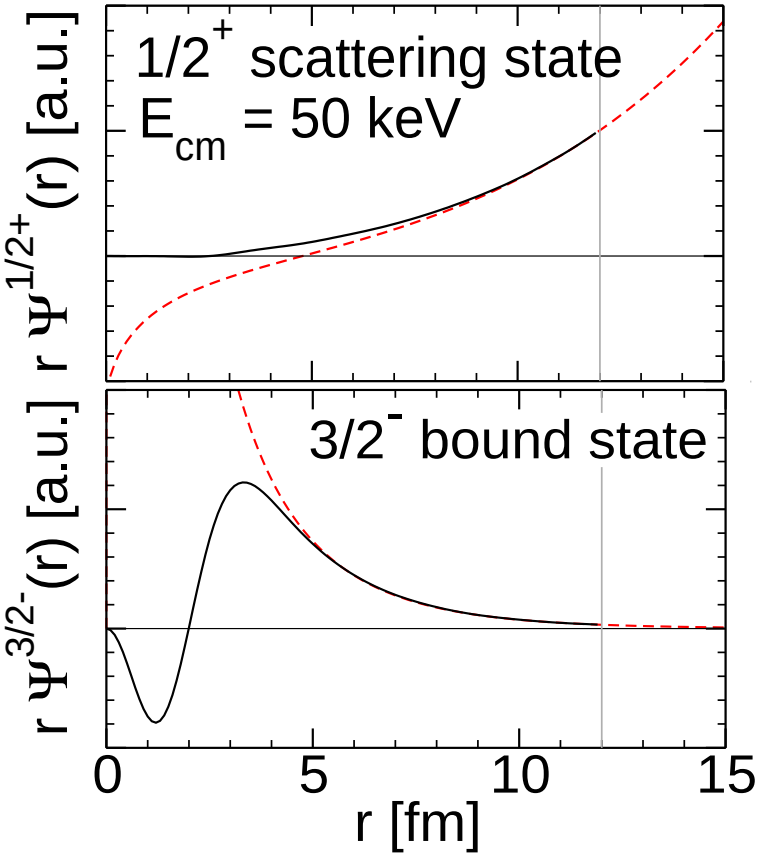
$$\eta = \frac{\mu Z_1 Z_2 e^2}{k}$$

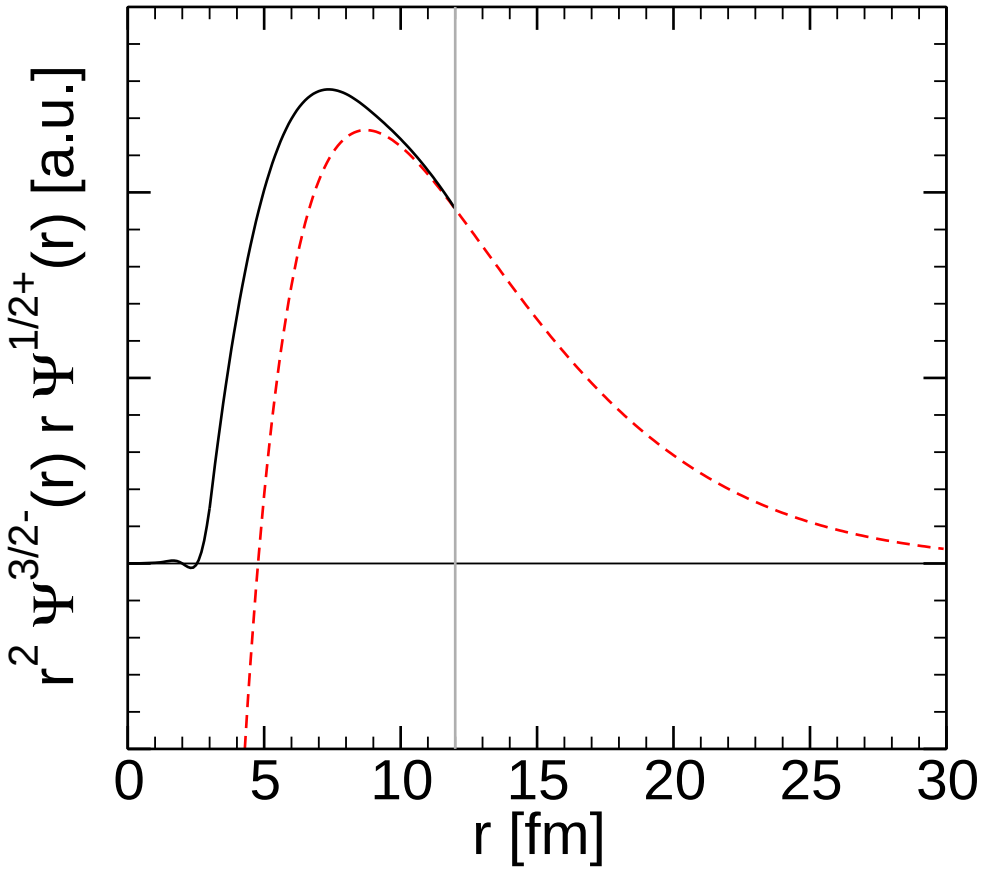
Nara Singh *et al.*, PRL **93**, 262503 (2004)
Bemmerer *et al.*, PRL **97**, 122502 (2006)
Confortola *et al.*, PRC **75**, 065803 (2007)
Brown *et al.*, PRC **76**, 055801 (2007)
Di Leva *et al.*, PRL **102**, 232502 (2009)

- 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

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

Overlap Functions and Dipole Matrixelements

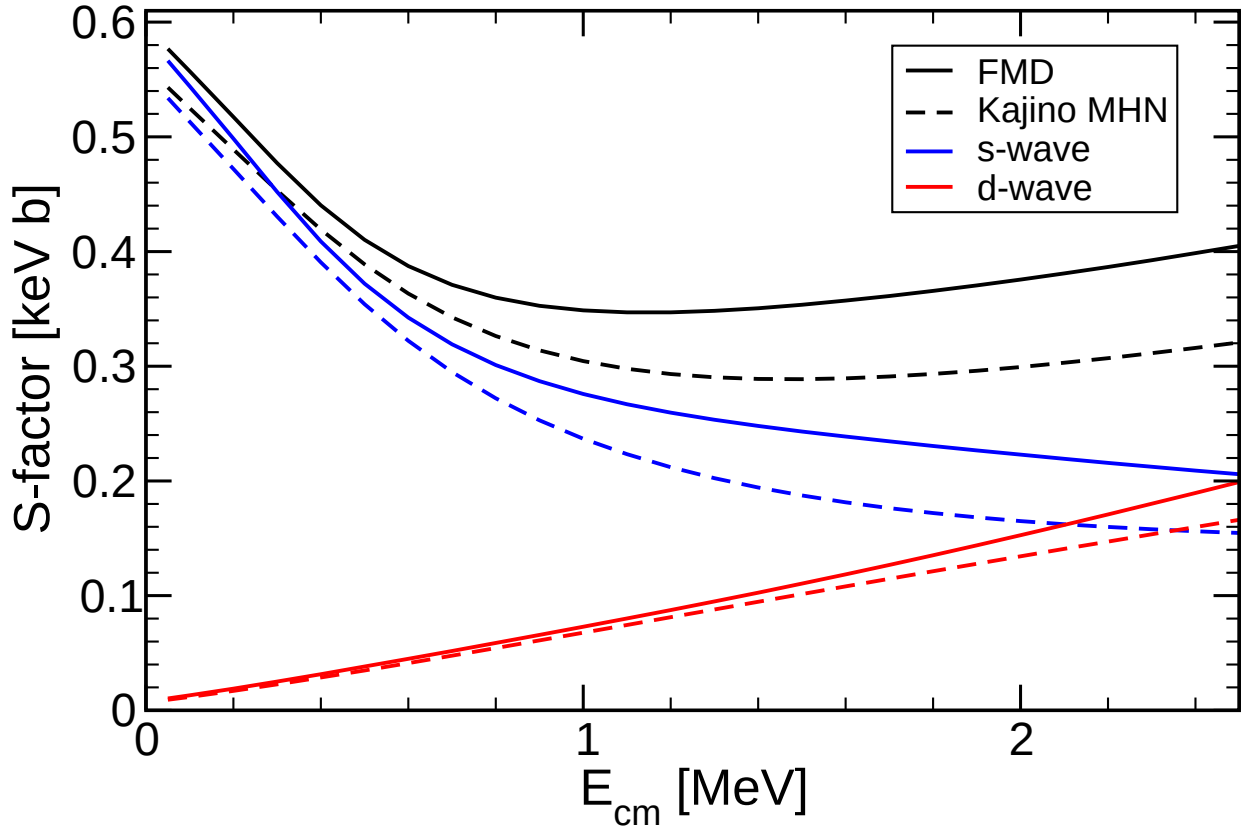




- Overlap functions from projection on RGM-cluster states
- Coulomb and Whittaker functions matched at channel radius a=12 fm
- Dipole matrix elements calculated from overlap functions reproduce full calculation within 2%
- cross section depends significantly on internal part of wave function, description as an “external” capture is too simplified

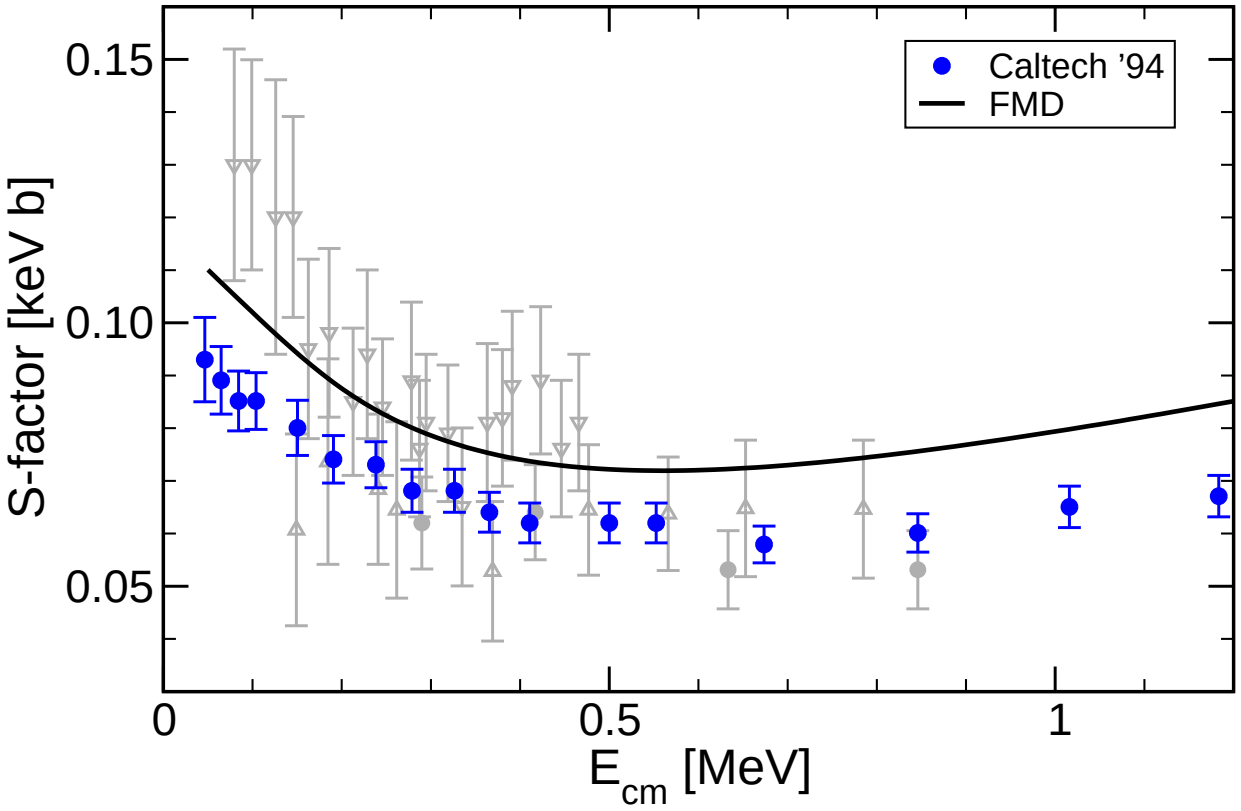
^{3}He(α,γ)^{7}Be

Energy dependence of the S-Factor



- low-energy *S*-factor dominated by *s*-wave capture
- at 2.5 MeV equal contributions of *s*- and *d*-wave capture
- FMD results differ from Kajino results mainly with respect to *s*-wave capture
- related to short-range part of wave functions ?

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



S-factor:

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

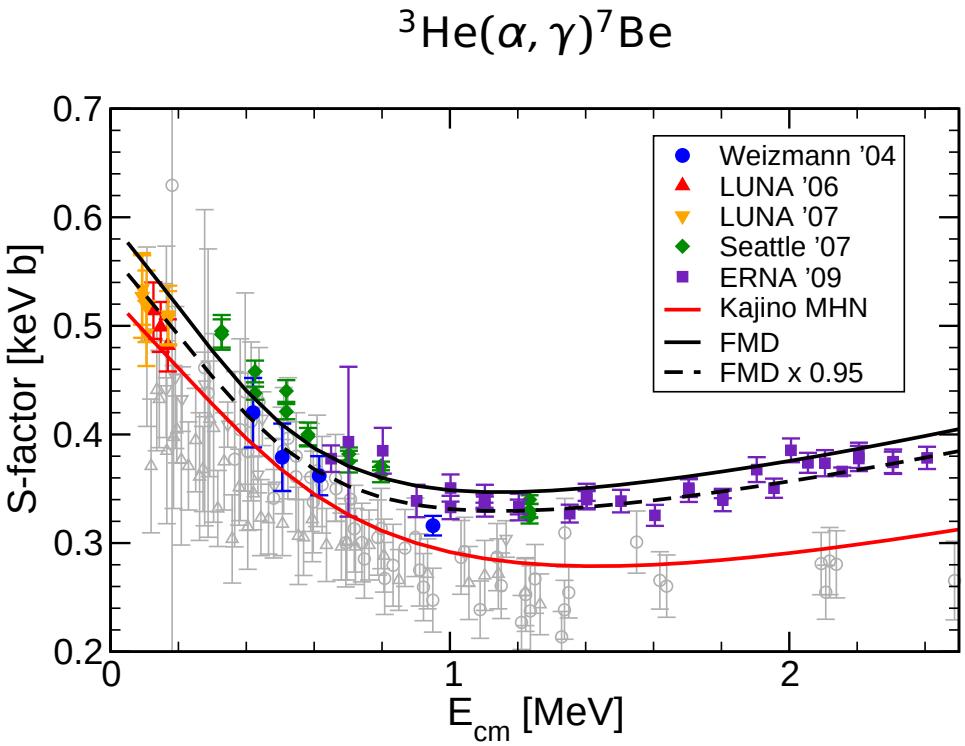
$$\eta = \frac{\mu Z_1 Z_2 e^2}{k}$$

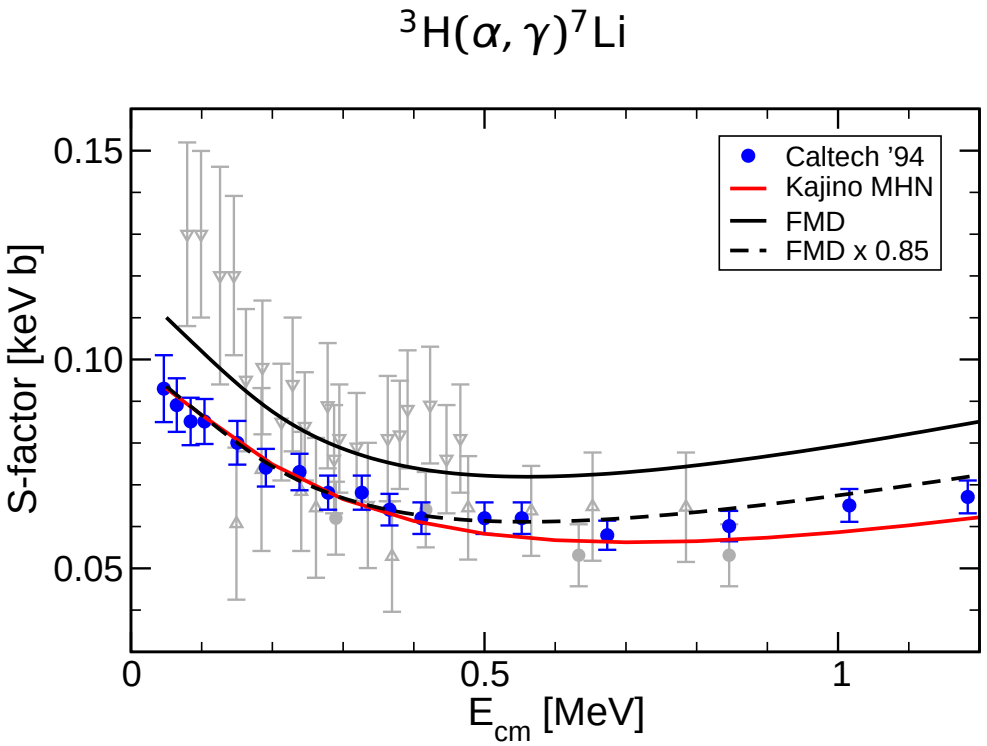
Brune *et al.*, PRC **50**, 2205 (1994)

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

$^3He(\alpha,\gamma)^7Be$ and $^3H(\alpha,\gamma)^7Li$ S-Factors consistent ?





- FMD calculation agrees with normalization and energy dependence of $^3He(\alpha,\gamma)^7Be$ data
- FMD calculation agrees with energy dependence but not normalization of $^3H(\alpha,\gamma)^7Li$ data
- similar inconsistency observed in other models

Summary

Effective interaction and many-body approach

- explicit inclusion of short-range central and tensor in the UCOM approach provides realistic low-momentum interaction
- FMD basis allows to describe frozen cluster configurations and polarized configurations in the interaction region

^{3}He(α,γ)^{7}Be Radiative Capture

- Bound states and scattering states wave functions
- *S*-factor: energy dependence and normalization agrees with data
- Overlap functions, dipole matrix elements
- ^{3}He(α,γ)^{7}Be and ^{3}H(α,γ)^{7}Li data inconsistent ?

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

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