

# Nuclear Clustering in Bound and Continuum States in Fermionic Molecular Dynamics



Hans Feldmeier & Thomas Neff

GSI Darmstadt

GANIL Topical Meeting  
Caen, 9 - 13 Oct. 2017



# Overview



**Many-Body Approach:  
Fermionic Molecular Dynamics**

**Applications:**

**Cluster structures in ground states of  $^{17}\text{Ne}$  -  $^{22}\text{Ne}$  isotopes**

**Cluster states of  $^{12}\text{C}$  in the continuum**

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

$\mathcal{H}_{\text{low-}k}$  Hilbert space:  
**Fermionic Molecular Dynamics**

• •

**FMD many-body wave functions**

**Restore symmetries by projections**

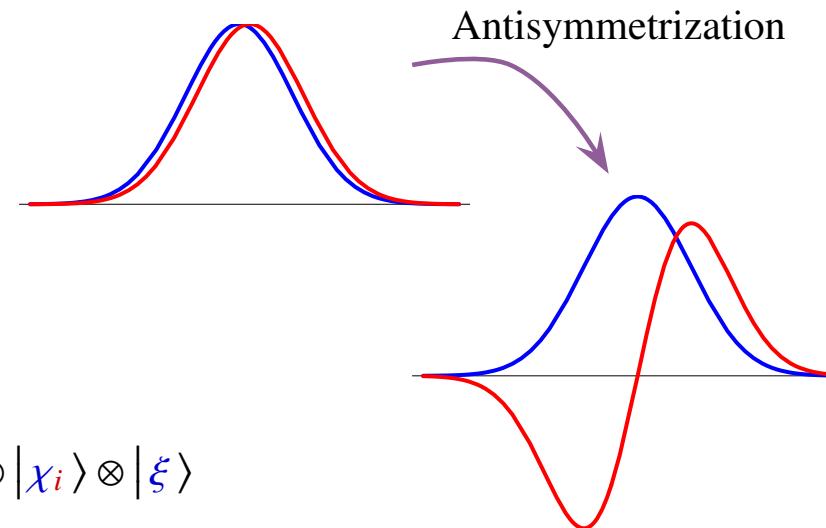
**Variation After Projection (VAP)**

**Configuration mixing**

**Fermionic**

Slater determinant

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

➡ antisymmetrized  $A$ -body state**Molecular**  
single-particle states

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

➡ Gaussian wave-packets in phase-space,  
spin is free, isospin is fixed

➡ Hilbert space contains  
shell-model, clusters, halos,  
scattering states

**Dynamics in many-body Hilbert space**spanned by one or several non-orthogonal  $|\mathcal{Q}^{(a)}\rangle$ 

$$|\Psi; J^\pi M\rangle = \sum_{a,K} \tilde{P}_{MK'}^{J^\pi} \tilde{P}_{\sim}^{\vec{P}=0} |\mathcal{Q}^{(a)}\rangle \cdot \psi_{aK}$$

variational principle →  $\mathcal{Q}^{(a)} = \{q_\nu^{(a)}, \nu=1 \cdots A\}, \psi_{aK}$

# Multi-Configuration Mixing 1

► most general projected state for multi-configuration calculations

$$|\Psi; J^\pi M\rangle = \sum_{aK} \tilde{P}^\pi \tilde{P}_{MK}^J \tilde{P}^{\vec{P}=0} |\mathcal{Q}^{(a)}\rangle \cdot \psi_{aK}$$

► **Task:** find a set of **intrinsic** states  $\left\{ |\mathcal{Q}^{(a)}\rangle, a = 1, \dots, N \right\}$  that describe the physical situation well

# Multi-Configuration Mixing 1

► most general projected state for multi-configuration calculations

$$|\Psi; J^\pi M\rangle = \sum_{aK} \tilde{P}^\pi \tilde{P}_{MK}^J \tilde{P}^{\vec{P}=0} |\mathcal{Q}^{(a)}\rangle \cdot \psi_{aK}$$

► Task: find a set of **intrinsic** states  $\left\{ |\mathcal{Q}^{(a)}\rangle, a = 1, \dots, N \right\}$  that describe the physical situation well

## Variation after projection

Minimize energy  $\frac{\langle \mathcal{Q}^{(a)} | \tilde{H} \tilde{P} | \mathcal{Q}^{(a)} \rangle}{\langle \mathcal{Q}^{(a)} | \tilde{P} | \mathcal{Q}^{(a)} \rangle} = \min$  under constraint  $\frac{\langle \mathcal{Q}^{(a)} | \tilde{A} \tilde{P} | \mathcal{Q}^{(a)} \rangle}{\langle \mathcal{Q}^{(a)} | \tilde{P} | \mathcal{Q}^{(a)} \rangle} = a \Rightarrow \mathcal{Q}^{(a)}$

$\tilde{A}$  = radius, quadrupole moment,  $LS$ , etc.

## Add particles or clusters

Combine already found states  $|\mathcal{Q}_{A_1+A_2}\rangle = \mathcal{A} \left( |\mathcal{Q}_{A_1}\rangle \otimes |\mathcal{Q}_{A_2}\rangle \right)$

# Multi-Configuration Mixing 2

## Many-body Hilbert space

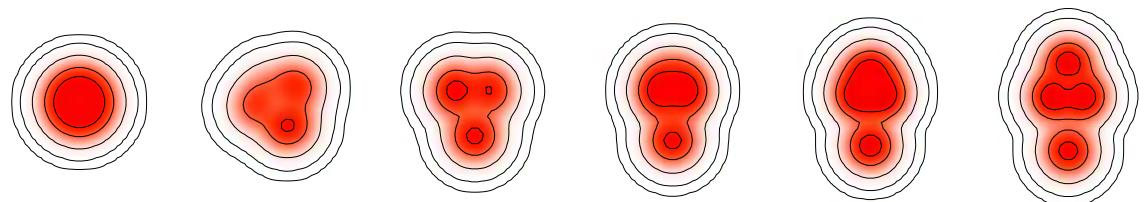
non-orthogonal many-body basis

$$\left\{ \tilde{P}^{\pi} \tilde{P}_{MK}^J \tilde{P}^{\vec{P}=0} | \mathcal{Q}^{(a)} \rangle, a = 1, \dots, N \right\}$$

spans many-body Hilbert space

$^{16}\text{O}$  one-body densities of intrinsic  $|\mathcal{Q}^{(a)}\rangle$

constraints on quadrupole (octupole) moment squeeze out  $\alpha$ -particle



# Multi-Configuration Mixing 2

## Many-body Hilbert space

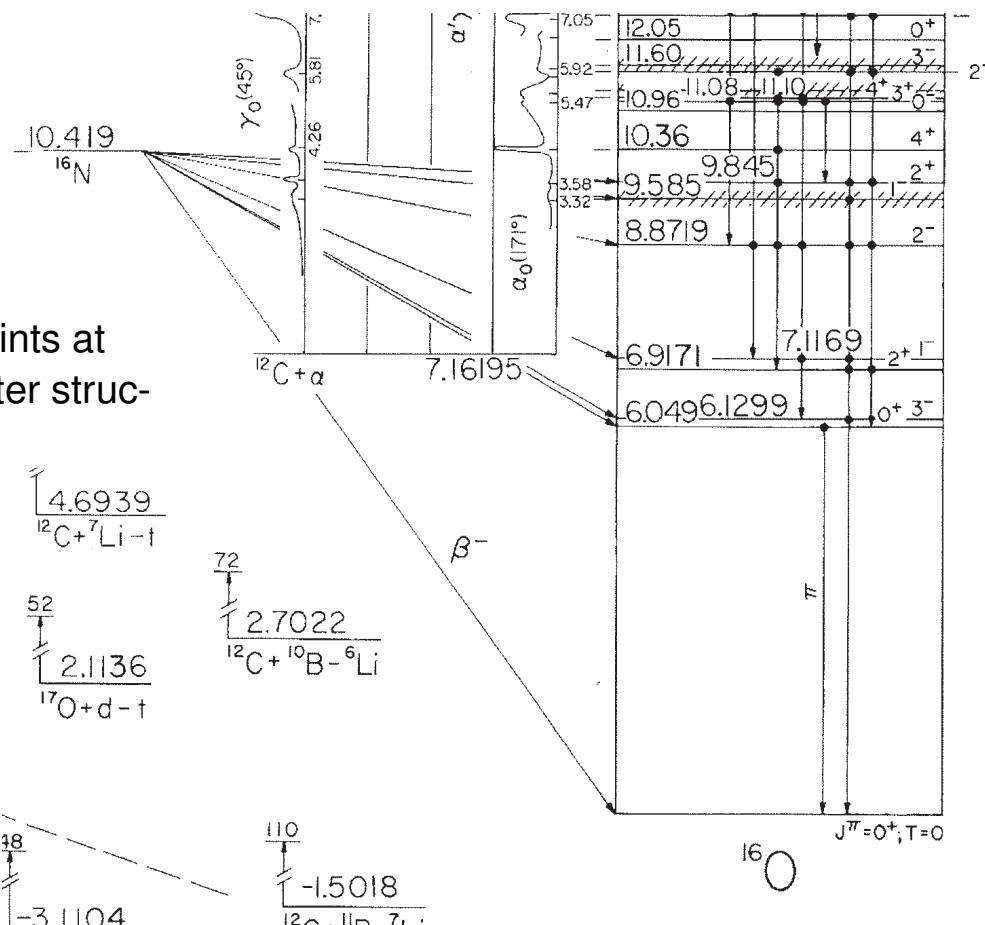
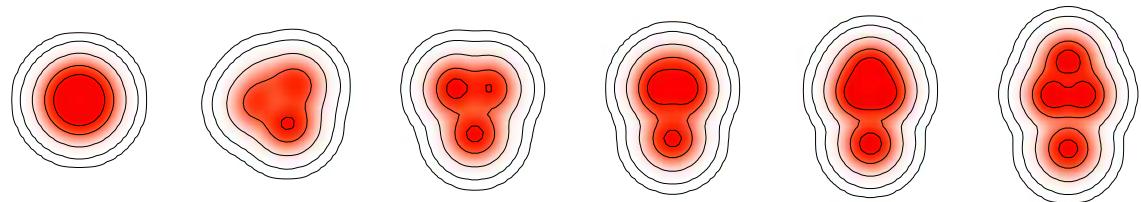
non-orthogonal many-body basis

$$\left\{ P_{\sim}^{\pi} P_{MK\sim}^J P_{\sim}^{\vec{P}=0} |Q^{(a)}\rangle, a = 1, \dots, N \right\}$$

spans many-body Hilbert space

${}^{16}\text{O}$  one-body densities of intrinsic  $|Q^{(a)}\rangle$

constraints on quadrupole (octupole) moment squeeze out  $\alpha$ -particle



threshold  ${}^{12}\text{C} + \alpha$  hints at corresponding cluster structures in  ${}^{16}\text{O}$

# Multi-Configuration Mixing 2

## Many-body Hilbert space

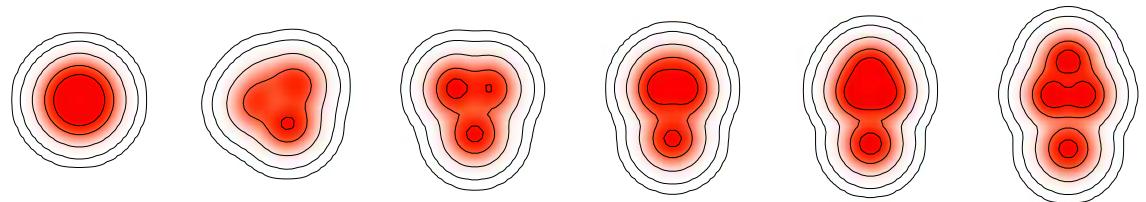
non-orthogonal many-body basis

$$\left\{ \tilde{P}^\pi \tilde{P}_{MK}^J \tilde{P}^{\vec{P}=0} | \mathcal{Q}^{(a)} \rangle, a = 1, \dots, N \right\}$$

spans many-body Hilbert space

$^{16}\text{O}$  one-body densities of intrinsic  $| \mathcal{Q}^{(a)} \rangle$

constraints on quadrupole (octupole) moment squeeze out  $\alpha$ -particle



## Multi-configuration calculation

$$\tilde{H} | J^\pi M, n \rangle = E_n^{J^\pi} | J^\pi M, n \rangle$$

► **diagonalization** of Hamiltonian in this set of non-orthogonal projected intrinsic states provides energy levels  $E_n^{J^\pi}$  and eigenstates  $| J^\pi M, n \rangle$

$$| J^\pi M, n \rangle = \sum_{bK'} \tilde{P}^\pi \tilde{P}_{MK'}^J \tilde{P}^{\vec{P}=0} | \mathcal{Q}^{(b)} \rangle \cdot c_{bK'}^{(n)}$$

- contain **all** nuclear structure information: radii, em & weak transitions, charge & matter distributions, correlations, etc
- Hamiltonian  $\tilde{H}$  decides which basis states contribute to eigenstate

# Neon Isotopes $^{17}\text{Ne}$ - $^{22}\text{Ne}$



## Structure

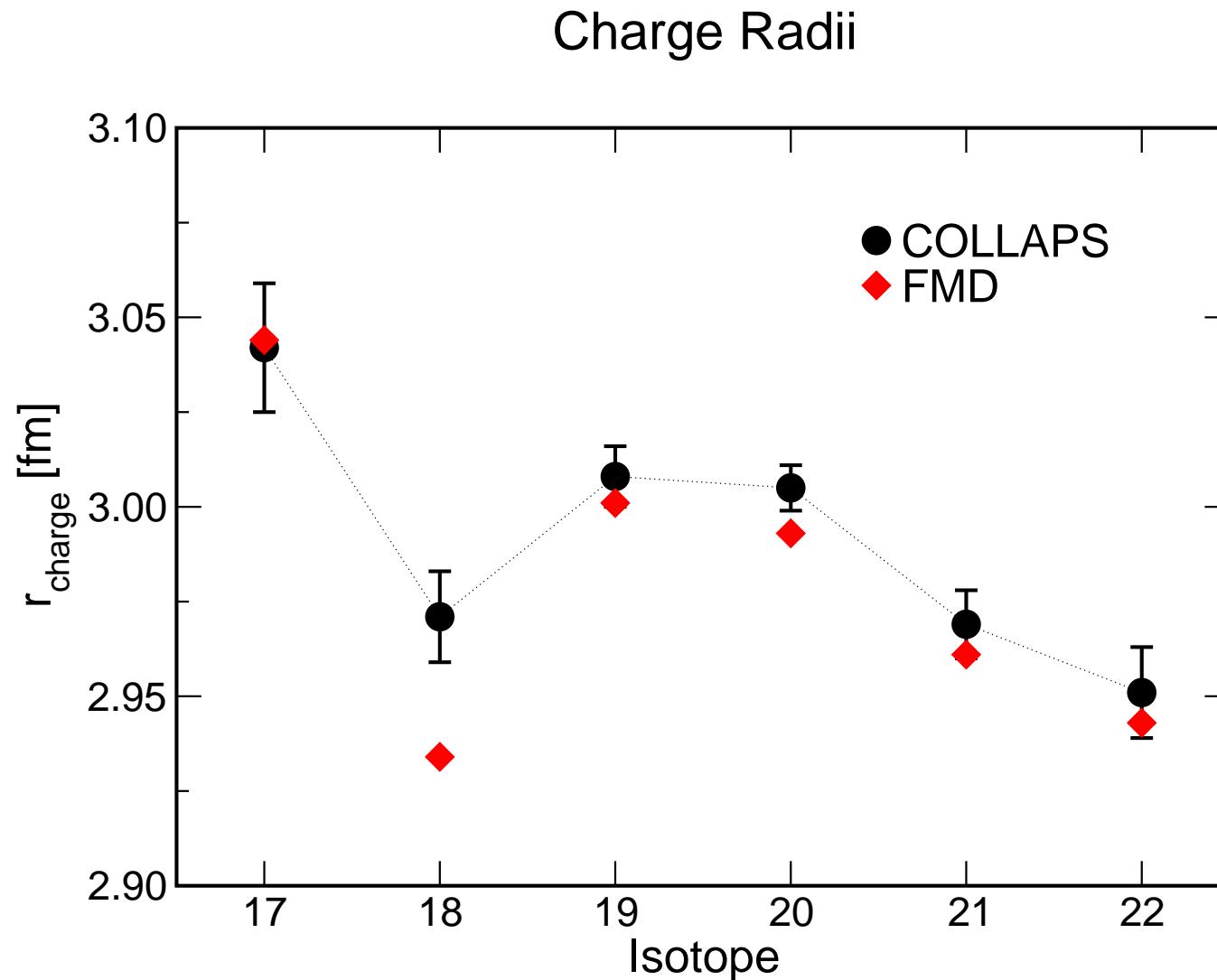
- $s^2/d^2$  competition in  $^{17}\text{Ne}$  and  $^{18}\text{Ne}$
- $^3\text{He}$  and  $^4\text{He}$  cluster admixtures

## Observables

- » Charge Radii
- » Matter Radii
- » Electromagnetic transitions
- » Rotational bands

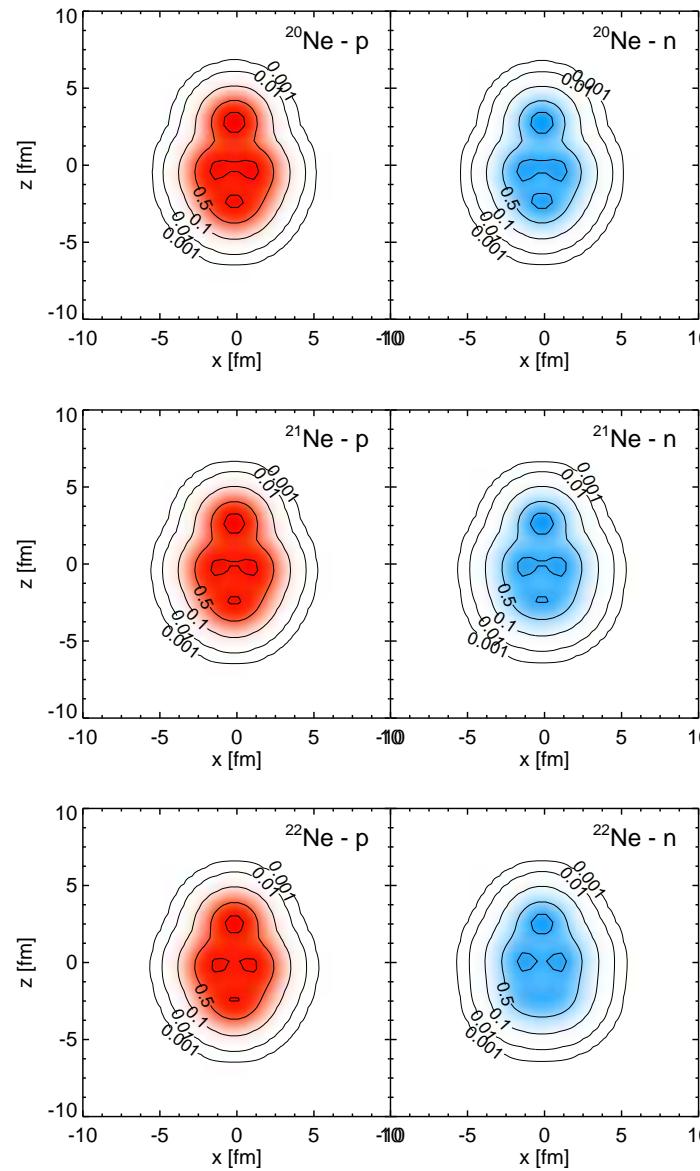
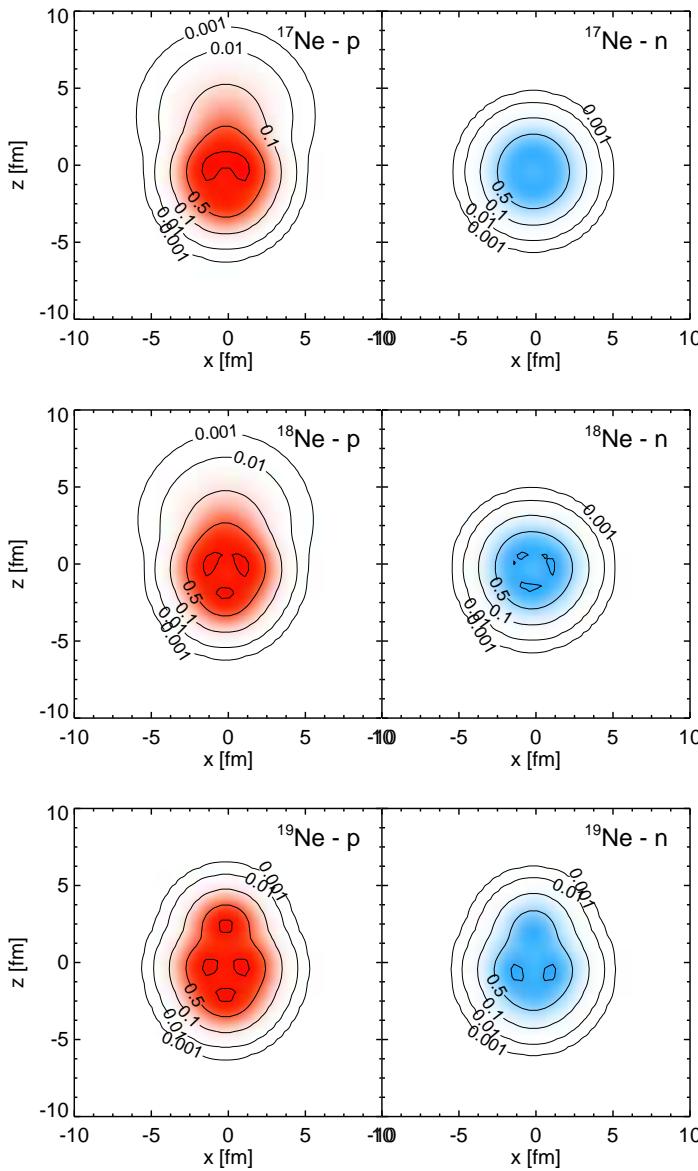
- Neon Isotopes

- Charge radii decrease with mass number ?



W. Geithner, T. Neff *et al.*, Phys. Rev. Lett. **101**, 252502 (2008)

- Neon Isotopes
- Calculation



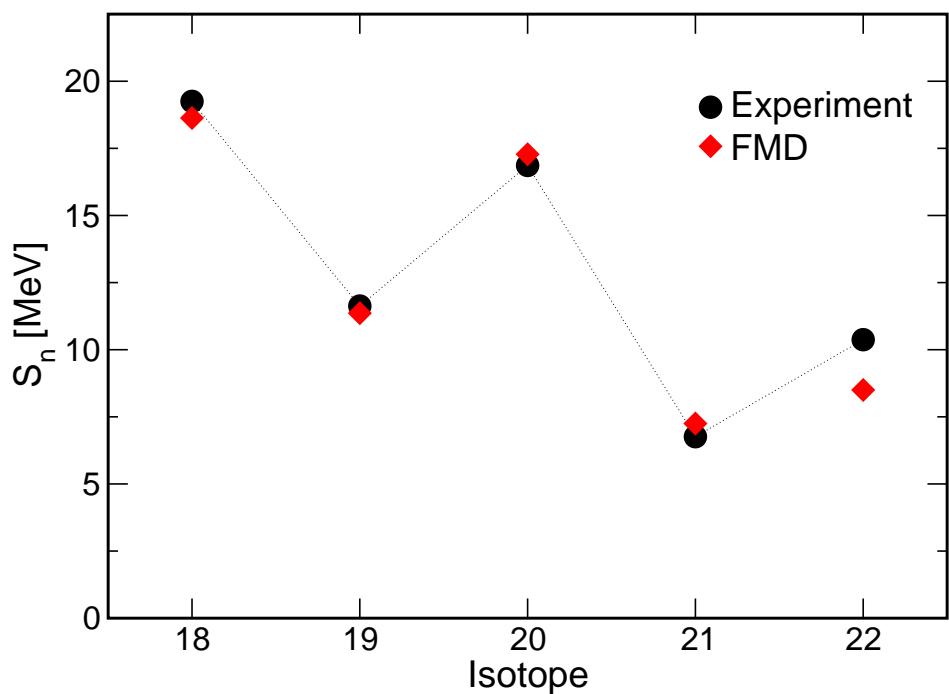
- $^{15,16}\text{O} + "s^2"$  and  $^{15,16}\text{O} + "d^2"$  are minima in  $^{17,18}\text{Ne}$
- explicit cluster configurations:  
 $^{17}\text{Ne}$ :  $^{14}\text{O} + ^3\text{He}$   
 $^{18}\text{Ne}$ :  $^{14}\text{O} + ^4\text{He}$   
 $^{19}\text{Ne}$ :  $^{16}\text{O} + ^3\text{He}$  &  
 $^{15}\text{O} + ^4\text{He}$   
 $^{20}\text{Ne}$ :  $^{16}\text{O} + ^4\text{He}$   
 $^{21}\text{Ne}$ : " $^{17}\text{O}" + ^4\text{He}$   
 $^{22}\text{Ne}$ : " $^{18}\text{O}" + ^4\text{He}$

proton/neutron densities of dominant intrinsic FMD configuration

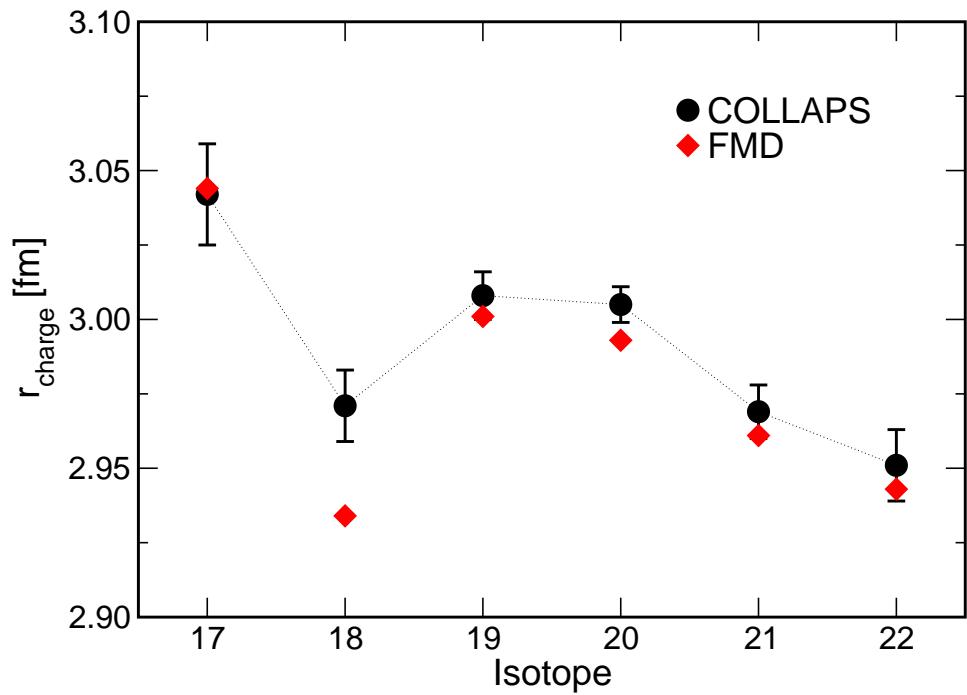
- Neon Isotopes

# Energies and Charge Radii

Separation Energies

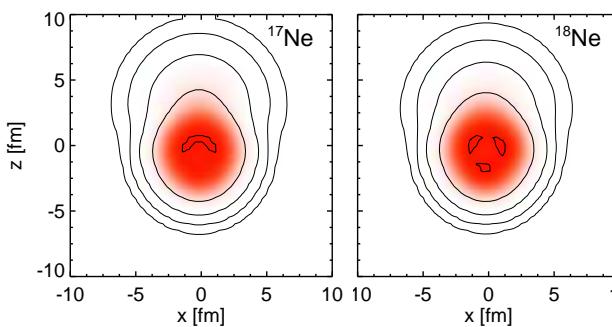


Charge Radii

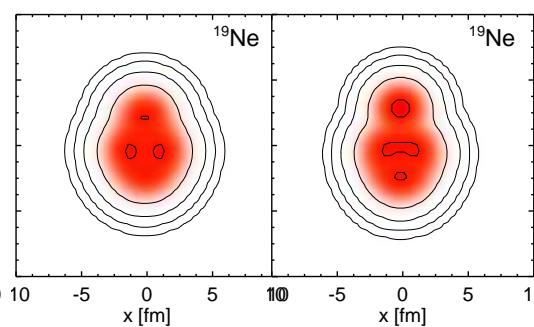


W. Geithner, T. Neff *et al.*, Phys. Rev. Lett. **101**, 252502 (2008)

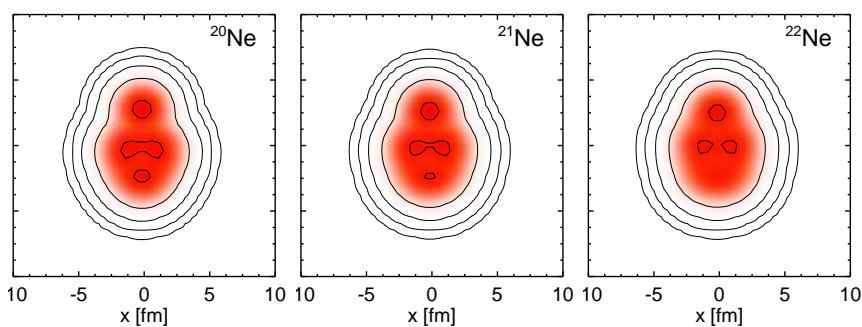
$^{17,18}\text{Ne}$ :  $s^2/d^2$  admixture



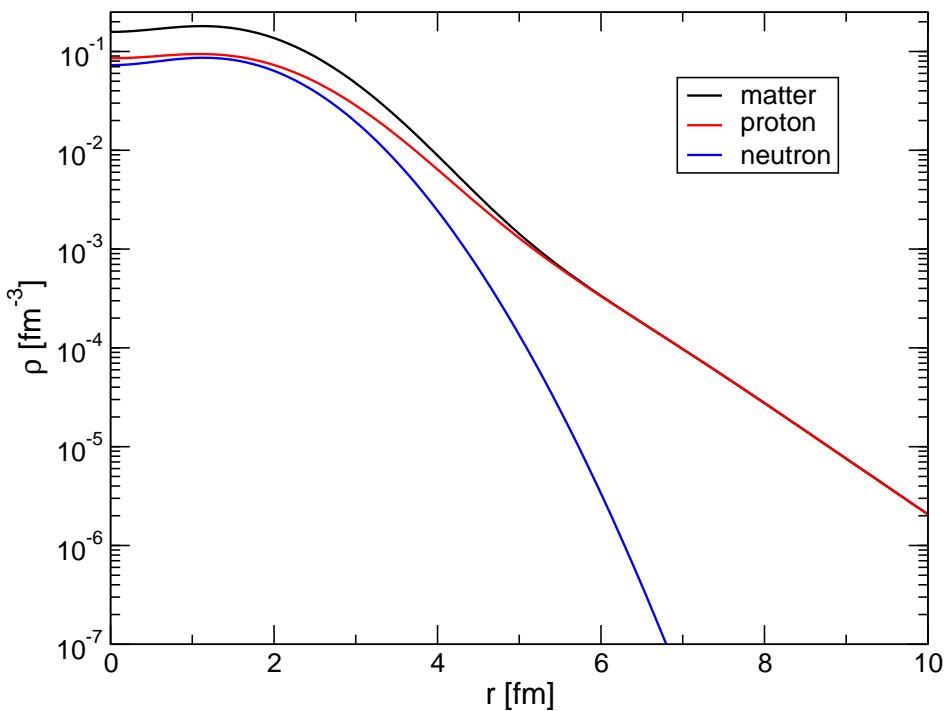
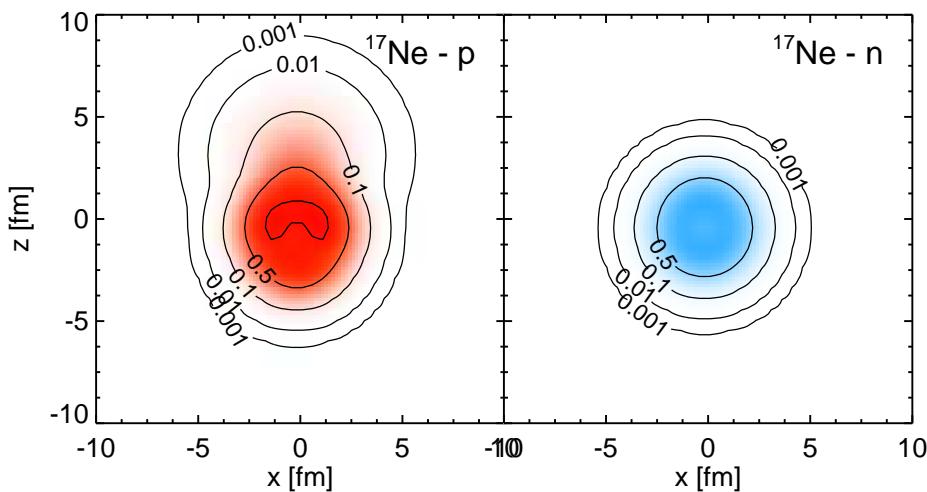
$^{19}\text{Ne}$ :  $^3\text{He}, \alpha$  clustering



$^{20-22}\text{Ne}$ :  $\alpha$  clustering



- Neon Isotopes
- $^{17}\text{Ne}$  Halo ?



	FMD	Experiment
$r_{\text{ch}}[\text{fm}]$	3.04	$3.042(21)$
$r_{\text{mat}}[\text{fm}]$	2.75	$2.75(7)^1$
$B(E2; \frac{1}{2}^- \rightarrow \frac{3}{2}^-)[e^2 \text{fm}^4]$	76.7	$66^{+18}_{-25}^2$
$B(E2; \frac{1}{2}^- \rightarrow \frac{5}{2}^-)[e^2 \text{fm}^4]$	119.8	$124(18)^2$
occupancy $s^2$	42%	
occupancy $d^2$	55%	

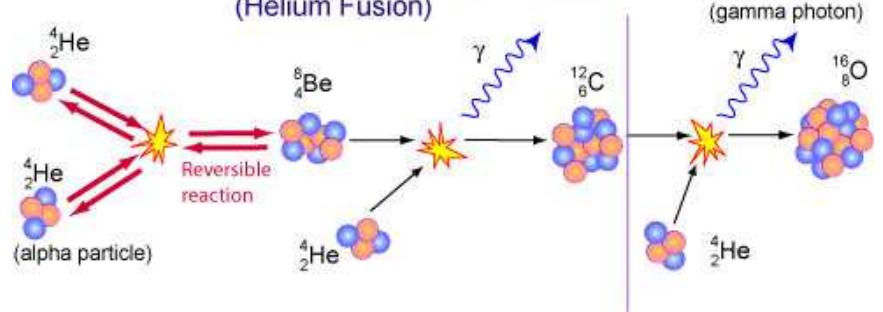
- proton skin  $r_p - r_n = 0.45$  fm
- 40% probability to find a proton at  $r > 5$  fm
- similar results are obtained in a three-body model

L. Grigorenko *et al.*, Phys. Rev. C **71**, 051604 (2005)

<sup>1</sup> A. Ozawa *et al.*, Nuc. Phys. **A693**, 32 (2001)

<sup>2</sup> M. J. Chromik *et al.*, Phys. Rev. C **66**, 024313 (2002)

## The Triple Alpha Process (Helium Fusion)



## Cluster States in $^{12}\text{C}$

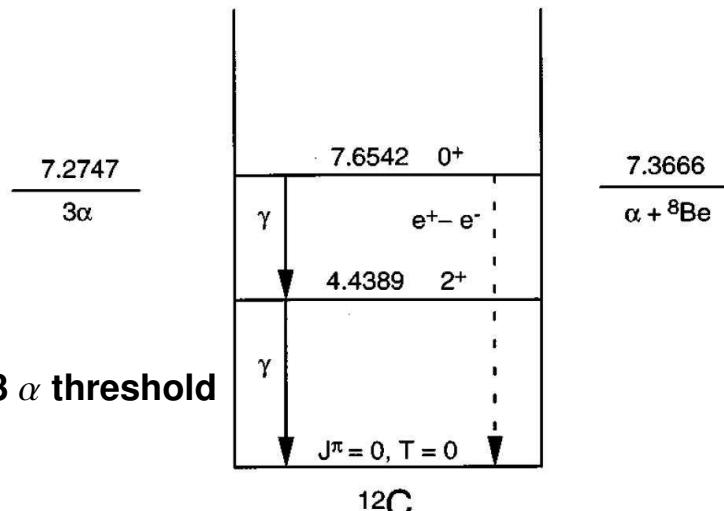


## Astrophysical Motivation

- Helium burning:  
triple alpha-reaction

## Structure

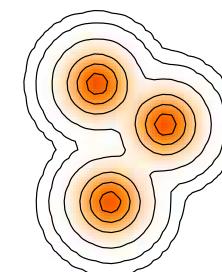
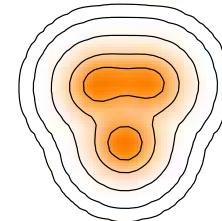
- Hoyle state sharp resonance close to  $3\alpha$  threshold  
prototype of loosely bound  $\alpha$ -particles
- Other  $2^+$ ,  $3^-$  states close to threshold  
also "Hoyle-like"?
- Including  $\alpha+^8\text{Be}$  continuum gives widths of cluster states



- Cluster States in  $^{12}\text{C}$
- Fermionic Molecular Dynamics

## Many-Body Hilbert Space

- spanned by 227 non-orthogonal 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  $\alpha$ -cluster configurations, "triangles"
- ➡ all projected on parity, angular momentum  $J^\pi$  and linear c.m. momentum  $\vec{P}_{cm} = 0$



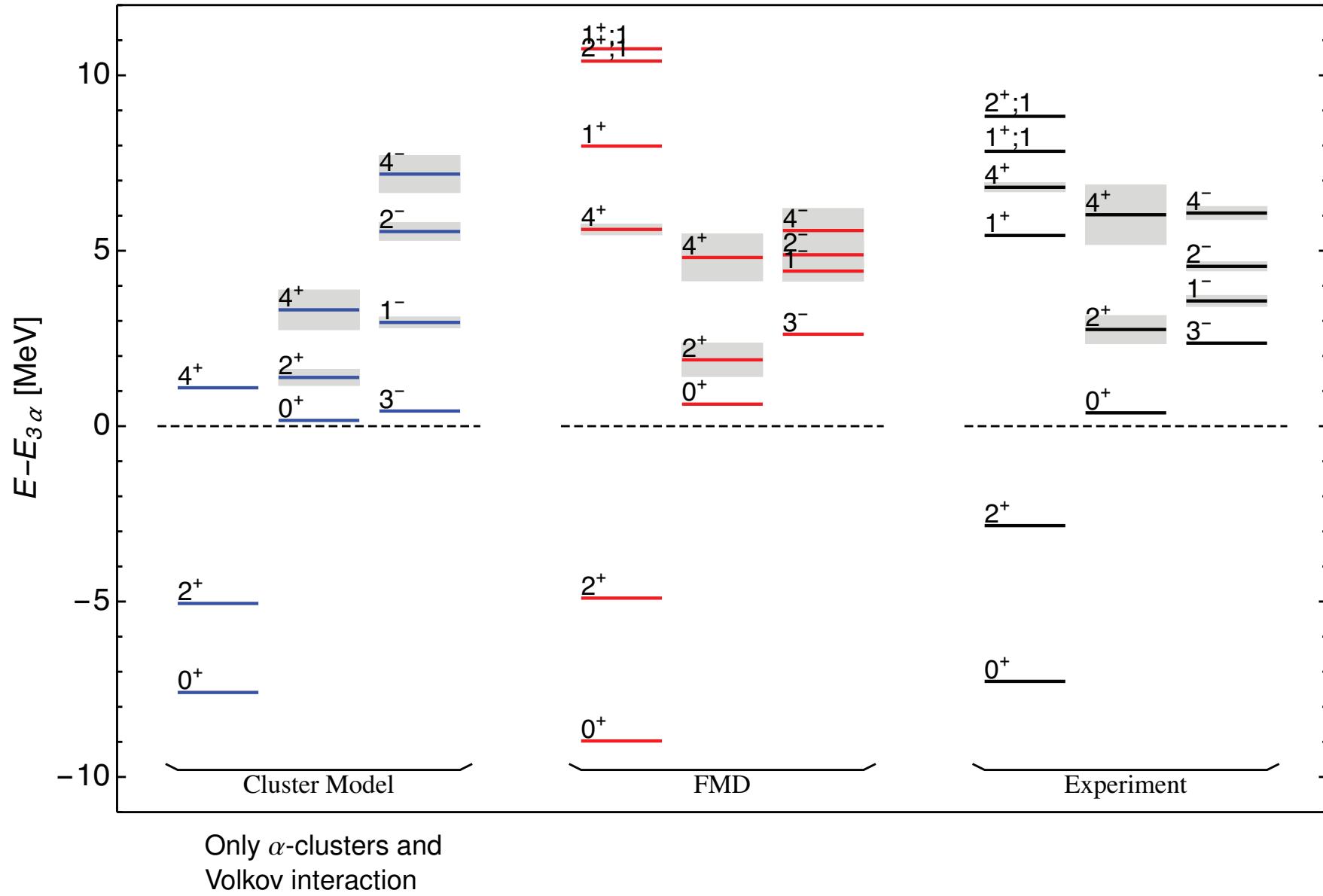
## Interaction

- $\tilde{H} = \tilde{T} + \tilde{V}_{\text{NN}}^{\text{eff}}$
- $\tilde{V}_{\text{NN}}^{\text{eff}}$  = UCOM interaction (ab initio) with two-body correction term fitted to doubly-magic nuclei (to make up for 3N forces)
- not tuned for  $\alpha$ - $\alpha$  scattering or  $^{12}\text{C}$  properties

## Many-Body Schrödinger Equation

- Solve  $\tilde{H} |J^\pi M, n\rangle = E_n^{J^\pi} |J^\pi M, n\rangle$  numerically

- Cluster States in  $^{12}\text{C}$
- Spectrum



- Cluster States in  $^{12}\text{C}$

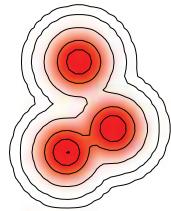
# Important Configurations (intrinsic densities)

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

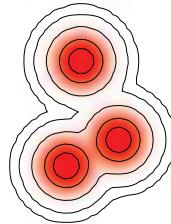


$$|\langle \cdot | 0_1^+ \rangle| = 0.94$$

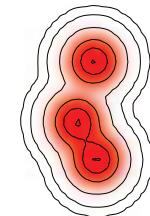
$$|\langle \cdot | 2_1^+ \rangle| = 0.93$$



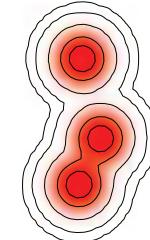
$$|\langle \cdot | 0_2^+ \rangle| = 0.64$$



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



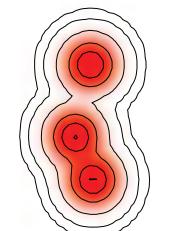
$$|\langle \cdot | 0_2^+ \rangle| = 0.57$$



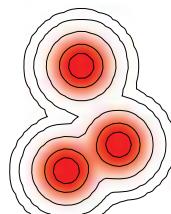
$$|\langle \cdot | 0_2^+ \rangle| = 0.45$$



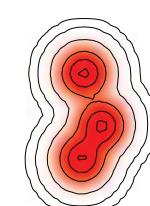
$$|\langle \cdot | 3_1^- \rangle| = 0.91$$



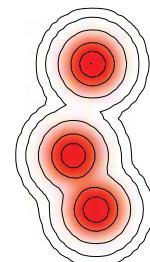
$$|\langle \cdot | 2_2^+ \rangle| = 0.50$$



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



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



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

$|0_2^+\rangle, |2_2^+\rangle$  loosely bound, gas-like states,  
 $|3_1^-\rangle$  more compact

FMD basis states are not orthogonal!

- Cluster States in  $^{12}\text{C}$

# More Hoyle like states ?

Energies [MeV]	Exp	FMD
$E(0_1^+)$	-92.16	-92.64
$E^*(2_1^+)$	4.44	5.31
$E(3\alpha)$	-84.89	-83.59
$E(0_2^+) - E(3\alpha)$	0.38	0.43
$E(2_2^+) - E(3\alpha)$	2.76(11)	2.77

Radii [fm]	Exp	FMD
$r_{\text{charge}}(0_1^+)$	2.47(2)	2.53
$r(0_1^+)$		2.39
$r(2_1^+)$		2.50
$r(0_2^+)$ Hoyle state		<b>3.38</b>
$r(2_2^+)$ Hoyle like		<b>4.43</b>

Transitions [fm $^2$ ] or [e $^2$ fm $^4$ ]	Exp	FMD
$M(E0, 0_1^+ \rightarrow 0_2^+)$	5.4(2)	6.53
$B(E2, 2_1^+ \rightarrow 0_1^+)$	7.6(4)	8.69
$B(E2, 2_1^+ \rightarrow 0_2^+)$	2.6(4)	3.83
$B(E2, 2_2^+ \rightarrow 0_1^+)$	0.73(13)	0.46

Energies in MeV, radii in fm =  $10^{-15}$  m

experimental situation for  $0_3^+$  and  $2_2^+$  states under investigation

$2_2^+$  resonance at 1.8 MeV above threshold included in NACRE compilation

• Cluster States in  $^{12}\text{C}$

# More Hoyle like states ?

Energies [MeV]	Exp	FMD
$E(0_1^+)$	-92.16	-92.64
$E^*(2_1^+)$	4.44	5.31
$E(3\alpha)$	-84.89	-83.59
$E(0_2^+) - E(3\alpha)$	0.38	0.43
$E(2_2^+) - E(3\alpha)$	2.76(11)	2.77

Radii [fm]	Exp	FMD
$r_{\text{charge}}(0_1^+)$	2.47(2)	2.53
$r(0_1^+)$		2.39
$r(2_1^+)$		2.50
$r(0_2^+)$ Hoyle state		<b>3.38</b>
$r(2_2^+)$ Hoyle like		<b>4.43</b>

Transitions [ $\text{fm}^2$ ] or [ $\text{e}^2\text{fm}^4$ ]	Exp	FMD
$M(E0, 0_1^+ \rightarrow 0_2^+)$	5.4(2)	6.53
$B(E2, 2_1^+ \rightarrow 0_1^+)$	7.6(4)	8.69
$B(E2, 2_1^+ \rightarrow 0_2^+)$	2.6(4)	3.83
$B(E2, 2_2^+ \rightarrow 0_1^+)$	0.73(13)	0.46

Energies in MeV, radii in fm =  $10^{-15}$  m

experimental situation for  $0_3^+$  and  $2_2^+$  states under investigation

$2_2^+$  resonance at 1.8 MeV above threshold included in NACRE compilation

calculated in bound state approximation  
 ➡ include  $^8\text{Be} + ^4\text{He}$  continuum for two-body decay width

# Scattering and Resonances



## Procedure

- FMD Hilbert space should contain besides bound states, also resonances and scattering states
- Implement appropriate boundary conditions
- ➡ Phase shifts, resonance widths, capture cross section

## Results

- $^{12}\text{C}$  widths of Hoyle state and others in vicinity of threshold
- $^3\text{He}(\alpha, \gamma)^7\text{Be}$  reaction

# Many-Body Hilbert Space for Scattering and Resonances

## Localized FMD states can represent many-body scattering states

- asymptotic states product of Hamiltonian eigenstates  $(\mathcal{A}|{}^3\text{He}, -D_i/2\rangle \otimes |{}^4\text{He}, +D_i/2\rangle)$
- FMD states for compound system in the interaction region  $(|{}^7\text{Be}\rangle, |{}^7\text{Be}^*\rangle \dots)$

scattering state:

$$|\text{atom} \rangle + \dots +$$

interaction region

$$|\text{dimer} \rangle + \dots +$$

$$|\text{atom} - D_i - \text{atom} \rangle + \dots$$

asymptotic

## Boundary conditions

- matching to the Coulomb solution of two point-like nuclei
- phase shifts for scattering or widths of resonances

- boundary condition Coulomb scattering solutions

$$\langle r | \Psi, [I_a I_b] I_c \ell \rangle \xrightarrow{r \rightarrow \infty} F_\ell(kr) + \tan(\delta_\ell(\mathbf{k})) G_\ell(kr), \quad k = +\sqrt{2\mu E}$$

phase shift  $\delta(E)$

- boundary condition outgoing wave only, Gamov state

$$\langle r | \Psi, [I_a I_b] I_c \ell \rangle \xrightarrow{r \rightarrow \infty} iF_\ell(\mathbf{k}r) + G_\ell(\mathbf{k}r), \quad \mathbf{k} = +\sqrt{2\mu Z}$$

complex eigenvalue  $Z = E - i\Gamma/2$ , width of resonance  $\Gamma$

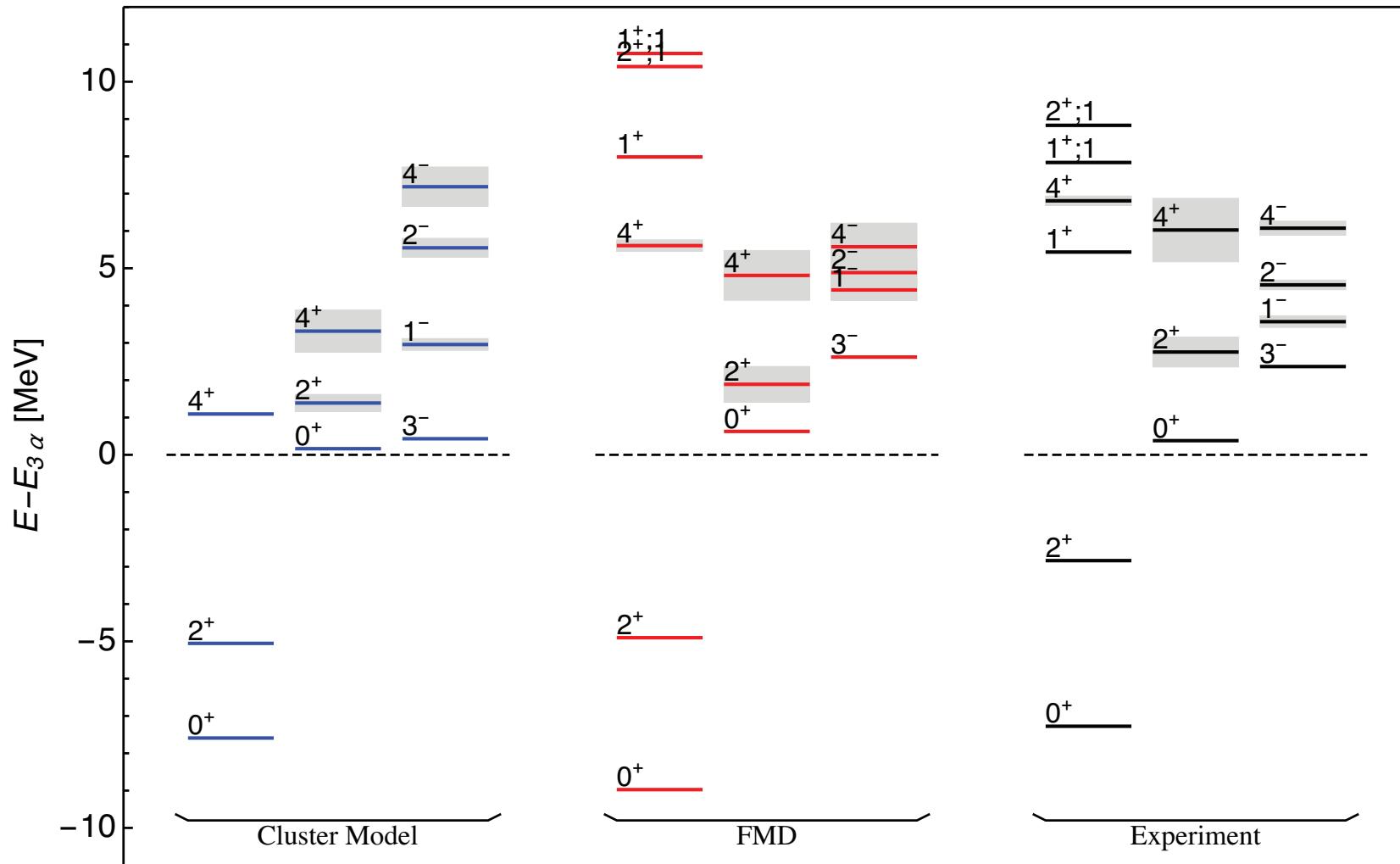
- Cluster States in  $^{12}\text{C}$

# Spectrum and Widths

Gamov states with outgoing  $^8\text{Be} + ^4\text{He}$

$^8\text{Be}$  states with  $I_a = 0, 2$ , and  $^4\text{He}$  with  $I_b = 0$

relative motion  $\ell = 0, 1, 2, 3, 4 \Rightarrow$  coupled channels



# $^3\text{He}(\alpha,\gamma)^7\text{Be}$ radiative capture one of the key reactions in the solar pp-chains

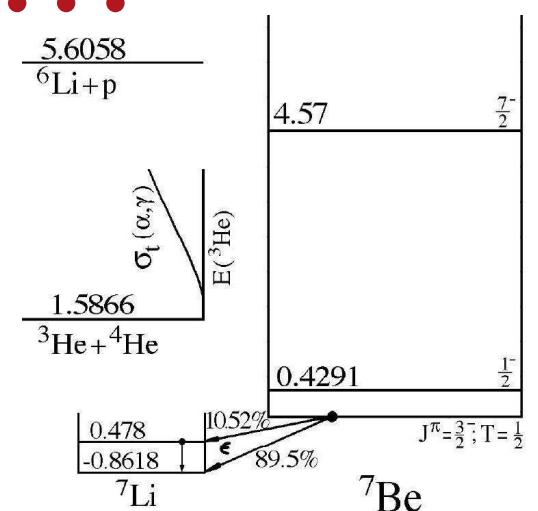
• • • • • • • • • • • • • • • • • • • •

Effective Nucleon-Nucleon interaction  $V_{\text{NN}}^{\text{eff}}$ :

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

Many-Body Approach:

Fermionic Molecular Dynamics



## Many-Body Hilbert Space:

### Frozen configurations

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

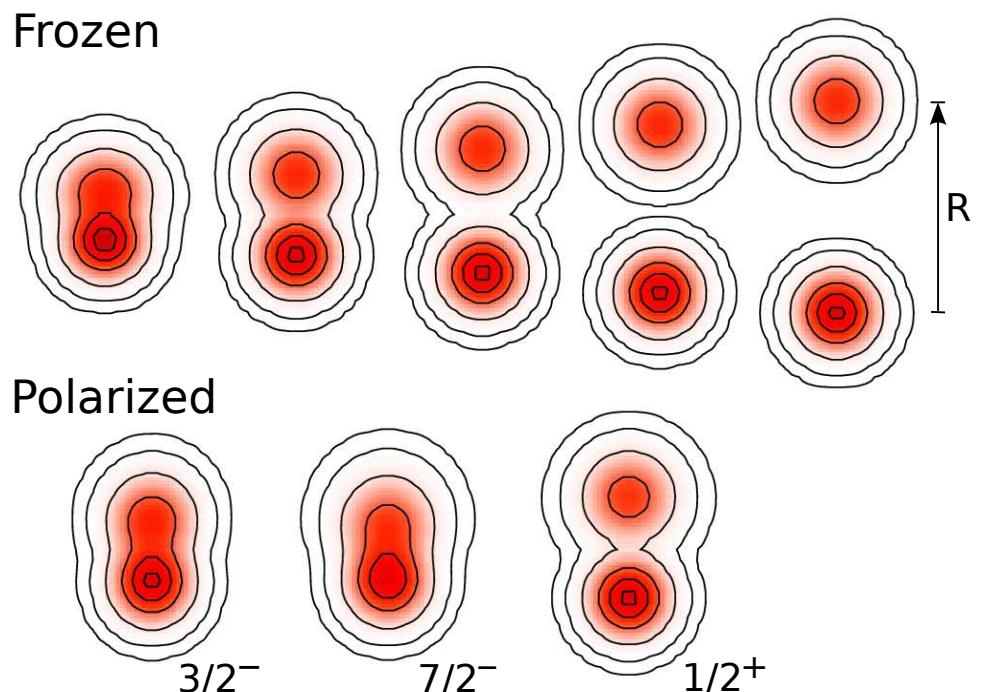
### Polarized configurations

- FMD wave functions obtained by 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



# Bound and Scattering States

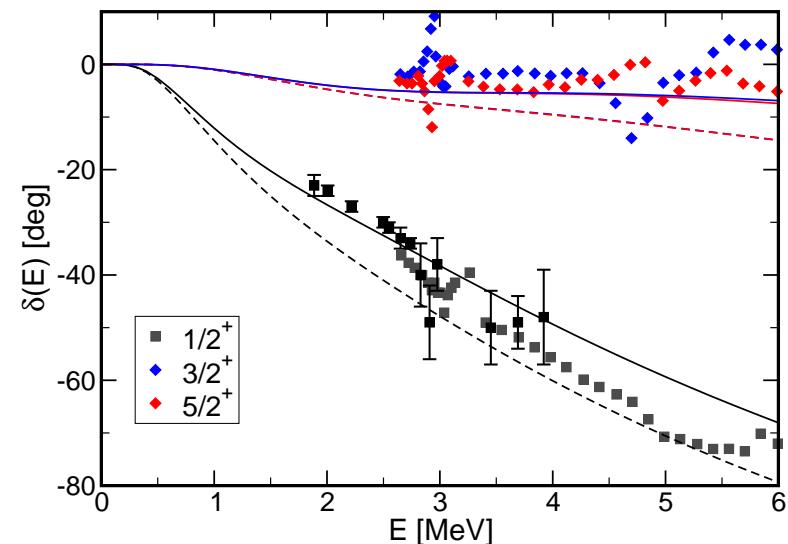
## Bound states

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

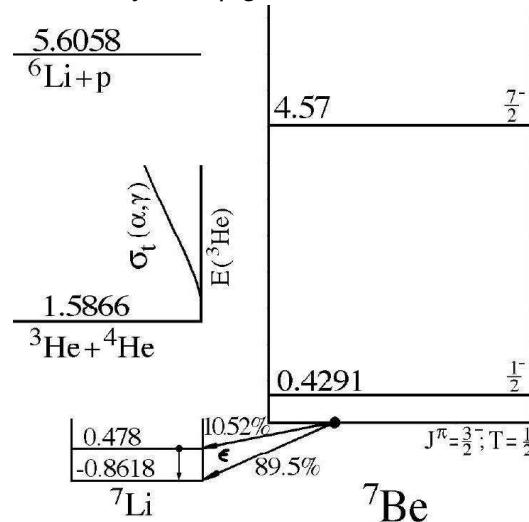
- centroid of bound state energies and phase shifts well described if polarized configurations included
- tail of wave functions important, astrophysical capture happens mainly outside contact
- bound-, scattering states, electromagnetic transition from scattering to bound states, all calculated consistently within same microscopic model

## Microscopic treatment of scattering problem in 7-body Hilbert space

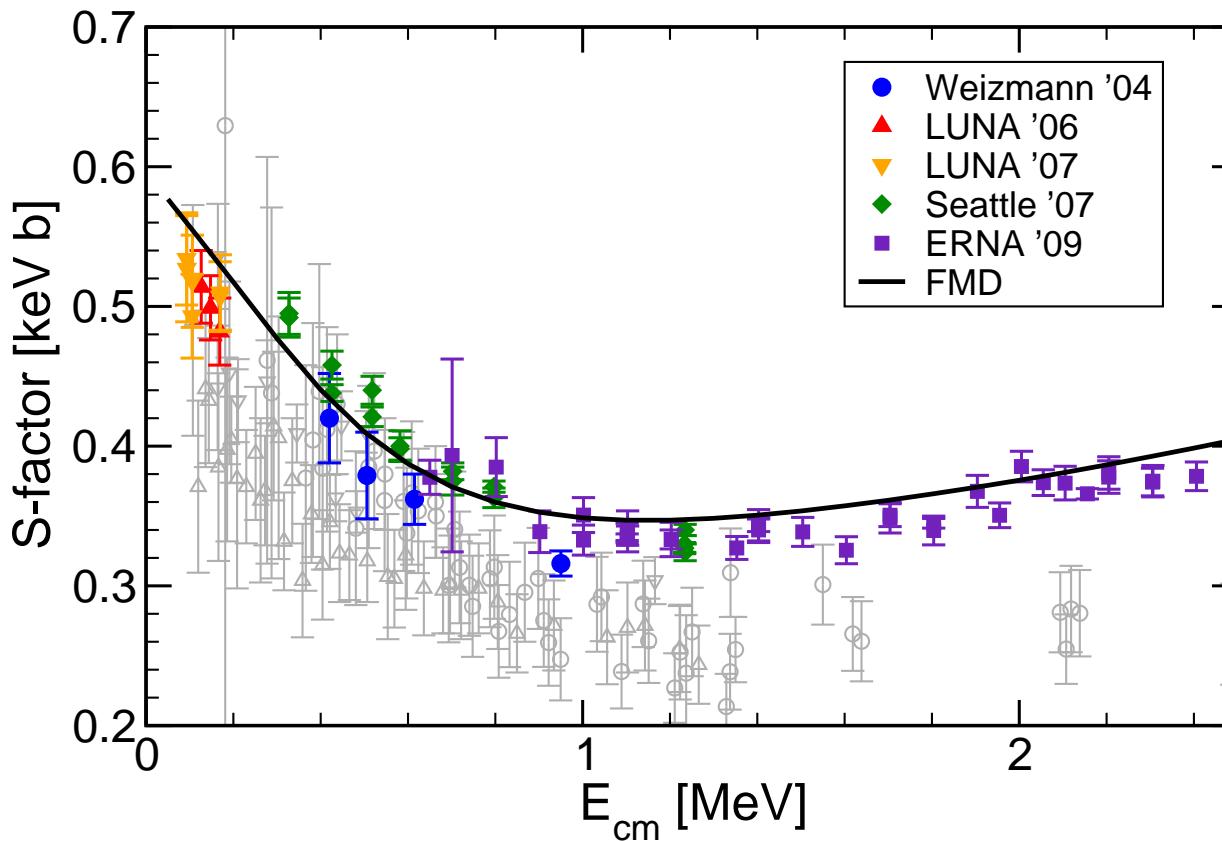
## Scattering states



dashed lines – frozen configurations only  
 solid lines – polarized configurations in interaction region included  
 (phase shift analysis: Spiger and Tombrello, PR **163**, 964 (1967))



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



**S-factor:**

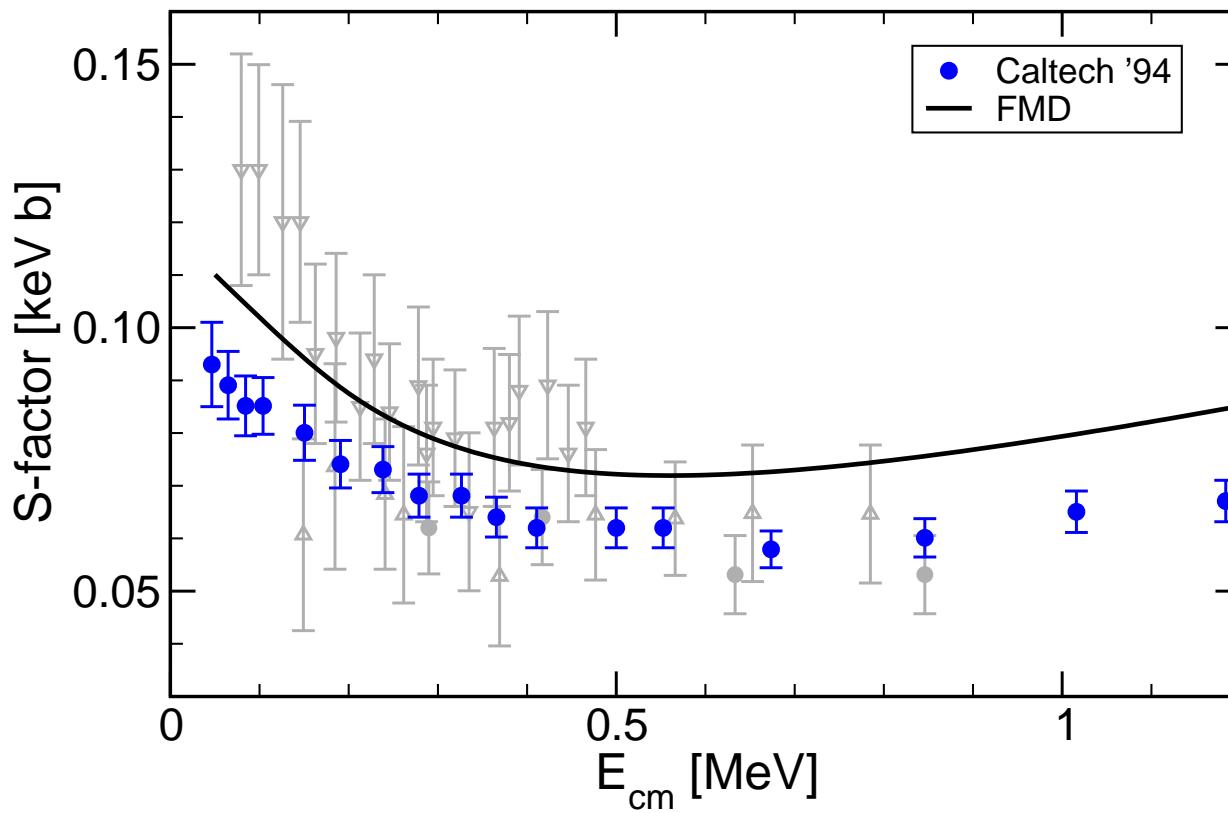
$$S(E) = \sigma(E)E \exp\{2\pi\eta\}$$

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

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

- $^3\text{H}(\alpha, \gamma)^7\text{Li}$
- 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  $^3\text{He}(\alpha, \gamma)^7\text{Be}$
- $^7\text{Li}$  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%

# Summary

## Fermionic Molecular Dynamics

- Microscopic many-body approach using Gaussian wave-packets
- Many-body Hilbert space contains shell model and cluster configurations, halos, scattering states, resonances in many-body continuum
- Many-body Schrödinger equation solved with softened AV18 interaction

## Cluster and Halo Structures in Ne Isotopes

- Two-proton halo in  $^{17}\text{Ne}$
- Changing cluster structures in Ne isotopes explain unconventional behavior of charge radii

## Shell model and cluster states in $^{12}\text{C}$

- Consistent description of ground state band and Hoyle state

## Continuum

- Width of resonances in  $^{12}\text{C}$  vicinity of  $3\alpha$  threshold
  - $^3\text{He}(\alpha, \gamma)^7\text{Be}$  radiative capture  
Consistent model: bound states, resonance and scattering wave functions, and e.m. transitions
- ➡ S-Factor: energy dependence and normalization

**Task:** Improve interaction, add 3-body,  
improve many-body Hilbert space for better accommodation of spin-orbit correlations