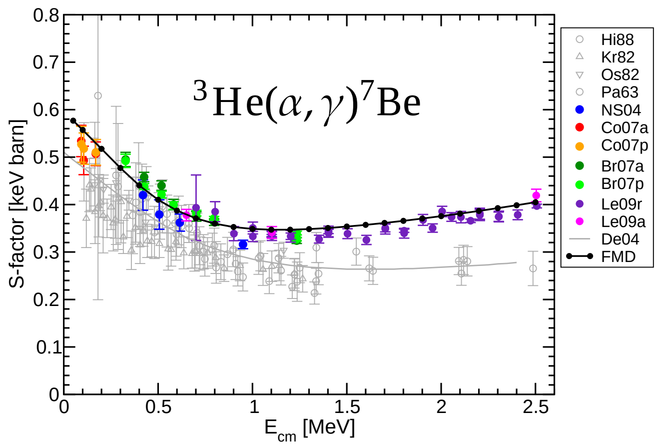
Towards Microscopic Ab Initio Calculations of Astrophysical S-Factors



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GSI

precise cross section important for
solar neutrinos & primordial ^7Li

Modern Nuclear Structure – Ab Initio

Ab Initio : from the beginning, without additional assumptions or special models

”beginning”

- c.m. positions and spins of nucleons $(\mathbf{r}_i, \sigma_i, \tau_i)$ as degrees of freedom
  $\Longrightarrow$ many-body state $\left|\widehat{\Psi}\right\rangle \epsilon \mathcal{H}$ Hilbert space
- interactions among nucleons approximated by potentials $\Longrightarrow V_{\text{NN}} + V_{\text{NNN}}$
  ”realistic” V_{NN} describes NN phase shifts and deuteron

Realistic NN-Potentials

QCD motivated

- symmetries, meson-exchange picture
- chiral effective field theory

short-range phenomenology

- short-range parametrisation or “contact” terms

experimental two-body data

- scattering phase-shifts & deuteron properties reproduced with high precision

supplementary three-nucleon force

- adjusted to data of light nuclei

Argonne V18

CD Bonn

Nijmegen I/II

Chiral N3LO

Argonne V18 +
Illinois 2

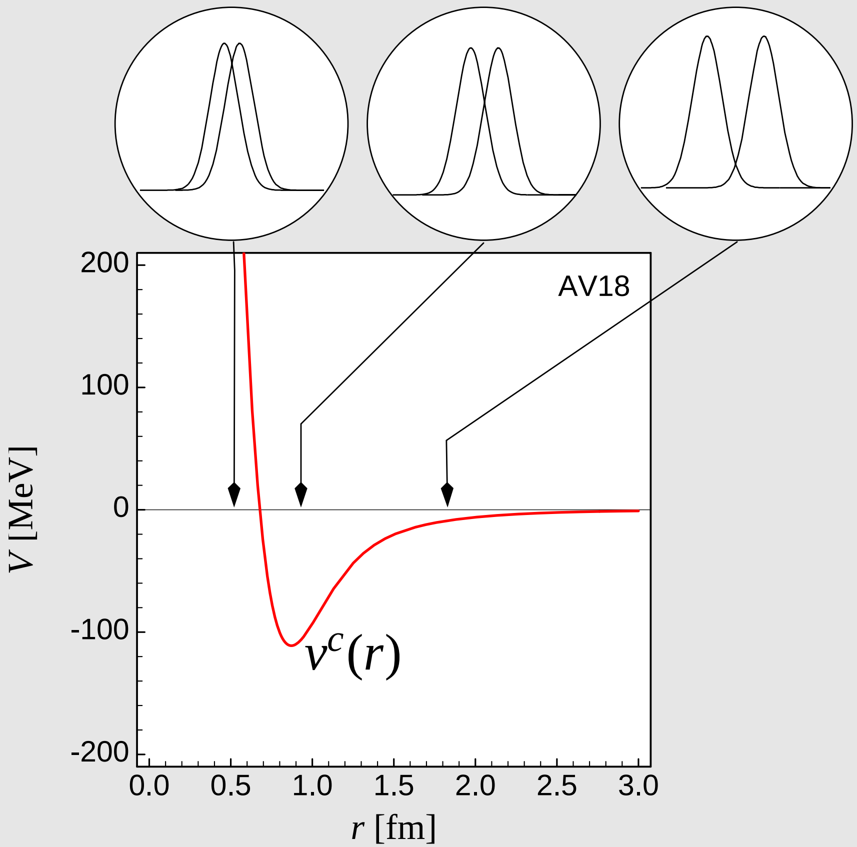
Chiral N3LO +
N2LO

Potential and Nucleon Size

Nucleons are not pointlike !

Proton charge radius $\sqrt{\langle r^2 \rangle_e} = 0.86\ \mathrm{fm}$

Proton charge distribution and S=0, T=1 Potential



- proton size not small compared to interaction range
- half-density overlap at max attraction, average NN-distance

  $1.8\ \mathrm{fm} \approx 2\sqrt{\langle r^2 \rangle_e}$
- V_{NN} not elementary
  more like atom-atom potential
- expect three-body forces

Modern Nuclear Structure – Ab Initio

Ab initio treatment: solve many-body quantum problem

- $\underset{\sim}{H} \left| \widehat{\Psi}_n \right\rangle = E_n \left| \widehat{\Psi}_n \right\rangle$ with $\underset{\sim}{H} = \underset{\sim}{T} + \underset{\sim}{V}_{\text{NN}} + \underset{\sim}{V}_{\text{NNN}}$
- observables: energies E_n, moments $\left\langle \widehat{\Psi}_n \middle| \underset{\sim}{A} \middle| \widehat{\Psi}_n \right\rangle$, transitions $\left| \left\langle \widehat{\Psi}_k \middle| \underset{\sim}{A} \middle| \widehat{\Psi}_n \right\rangle \right|^2$ to be confronted with data

HOWEVER

Modern Nuclear Structure – Ab Initio

HOWEVER, there are conceptional problems

- realistic $\underset{\sim}{V}_{\text{NN}}$ not unique !
  different phase-shift equivalent $\underset{\sim}{V}_{\text{NN}}, \underset{\sim}{V}'_{\text{NN}}, \underset{\sim}{V}''_{\text{NN}}$ describe equally well the 2-body system
- $\underset{\sim}{V}_{\text{NN}} + \underset{\sim}{V}_{\text{NNN}} \Longleftrightarrow \underset{\sim}{V}'_{\text{NN}} + \underset{\sim}{V}'_{\text{NNN}}$
  each NN-interaction needs its NNN-part to describe equally well the 3-body system

➨ in nuclear structure theory there is not the one genuine NN or NNN force

and there are technical problems

- $\underset{\sim}{H} \left| \widehat{\Psi}_n \right\rangle = E_n \left| \widehat{\Psi}_n \right\rangle$ cannot be solved numerically for larger mass numbers

Solution: treat short-range correlations by effective interactions

- Approximation: Hilbert space $\mathcal{H} = \mathcal{H}_{\text{low-}k} \oplus \mathcal{H}_{\text{high-}k}$

  $\underset{\sim}{H}^{\text{eff}} \left| \Psi_n \right\rangle = E_n \left| \Psi_n \right\rangle$ with $\left| \Psi_n \right\rangle \epsilon \, \mathcal{H}_{\text{low-}k}$

- Unitary transformation $\left| \widehat{\Psi}_n \right\rangle = \underset{\sim}{U} \left| \Psi_n \right\rangle$ such that

  $\underset{\sim}{H}^{\text{eff}} = \underset{\sim}{U}^{\dagger} \underset{\sim}{H} \underset{\sim}{U}$ does not connect $\mathcal{H}_{\text{low-}k}$ with $\mathcal{H}_{\text{high-}k}$

  many-body forces appear $\underset{\sim}{H}^{\text{eff}} = \underset{\sim}{T} + \underset{\sim}{V}^{\text{eff}}_{\text{NN}} + \underset{\sim}{V}^{\text{eff}}_{\text{NNN}} + \underset{\sim}{V}^{\text{eff}}_{\text{NNNN}} + \underset{\sim}{V}^{\text{eff}}_{\text{NNNNN}} + \cdots$

- Unitary Correlation Operator Method (UCOM) is used in the following

  UCOM is phase shift equivalent and minimizes effects from 3-body forces

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

FMD many-body wave functions

Restore symmetries by projections

Variation After Projection (VAP)

Configuration mixing

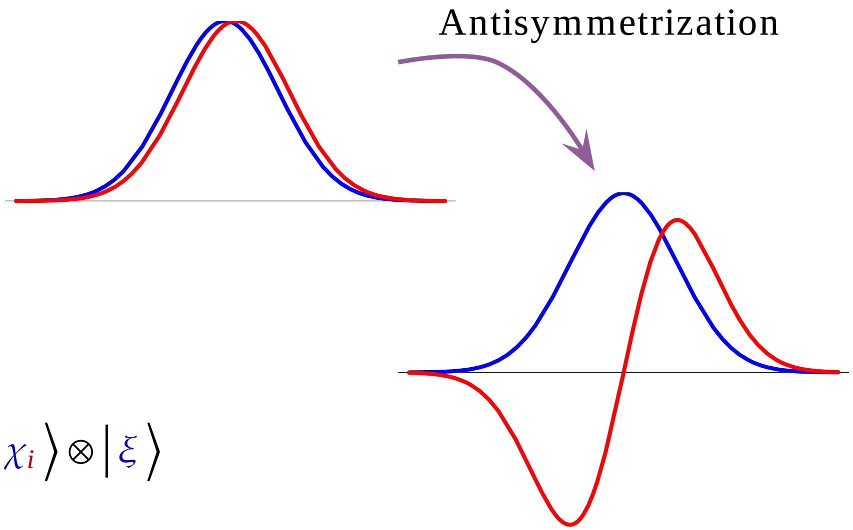
FMD Many-Body Hilbert Space

Fermionic

Slater determinant

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

➨ antisymmetrized A-body state



Molecular

single-particle states

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

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

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

Dynamics in Hilbert space

spanned by one or several non-orthogonal $\left| Q^{(a)} \right\rangle$

$$\left| \Psi; J^\pi M \right\rangle = \sum_{a,K} c_{aK}\, \underset{\sim}{P}^{J^\pi}_{MK'}\, \underset{\sim}{P}^{\mathbf{P}=0} \left| Q^{(a)} \right\rangle$$

variational principle $\rightarrow$ $Q^{(a)} = \{ q_\nu^{(a)}, \nu = 1 \cdots A \},\ c_{aK}$

Multi-Configuration Mixing

- most general projected state for multi-configuration calculations

$$\left| \Psi; J^\pi M \right\rangle = \sum_{aK} c_{aK} \, \underset{\sim}{P}^\pi \underset{\sim}{P}^J_{MK} \underset{\sim}{P}^{\mathbf{P}=0} \left| Q^{(a)} \right\rangle$$

- task: find set of intrinsic states $\left\{ \left| Q^{(a)} \right\rangle, a = 1, \ldots, N \right\}$ that describe the physics well

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Multi-configuration calculations

- **diagonalize** Hamiltonian in this set of non-orthogonal projected intrinsic states

$$\underset{\sim}{H}^{\text{eff}} \left| J^\pi M, n \right\rangle = E_n^{J\pi} \left| J^\pi M, n \right\rangle ; \qquad \left| J^\pi M, n \right\rangle = \sum_{aK} c_{aK}^{(n)} \, \underset{\sim}{P}^{\pi} \underset{\sim}{P}^{J}_{MK'} \underset{\sim}{P}^{\mathbf{P}=0} \left| Q^{(a)} \right\rangle$$

- obtain coefficients $c_{aK}^{(n)}$
- bound states: energy levels $E_n^{J\pi}$ and many-body eigenstates $\left| J^\pi M, n \right\rangle$
- scattering states: for given energy E and boundary conditions
  many-body scattering state $\left| J^\pi M, E \right\rangle$ and phase shifts

Reactions

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

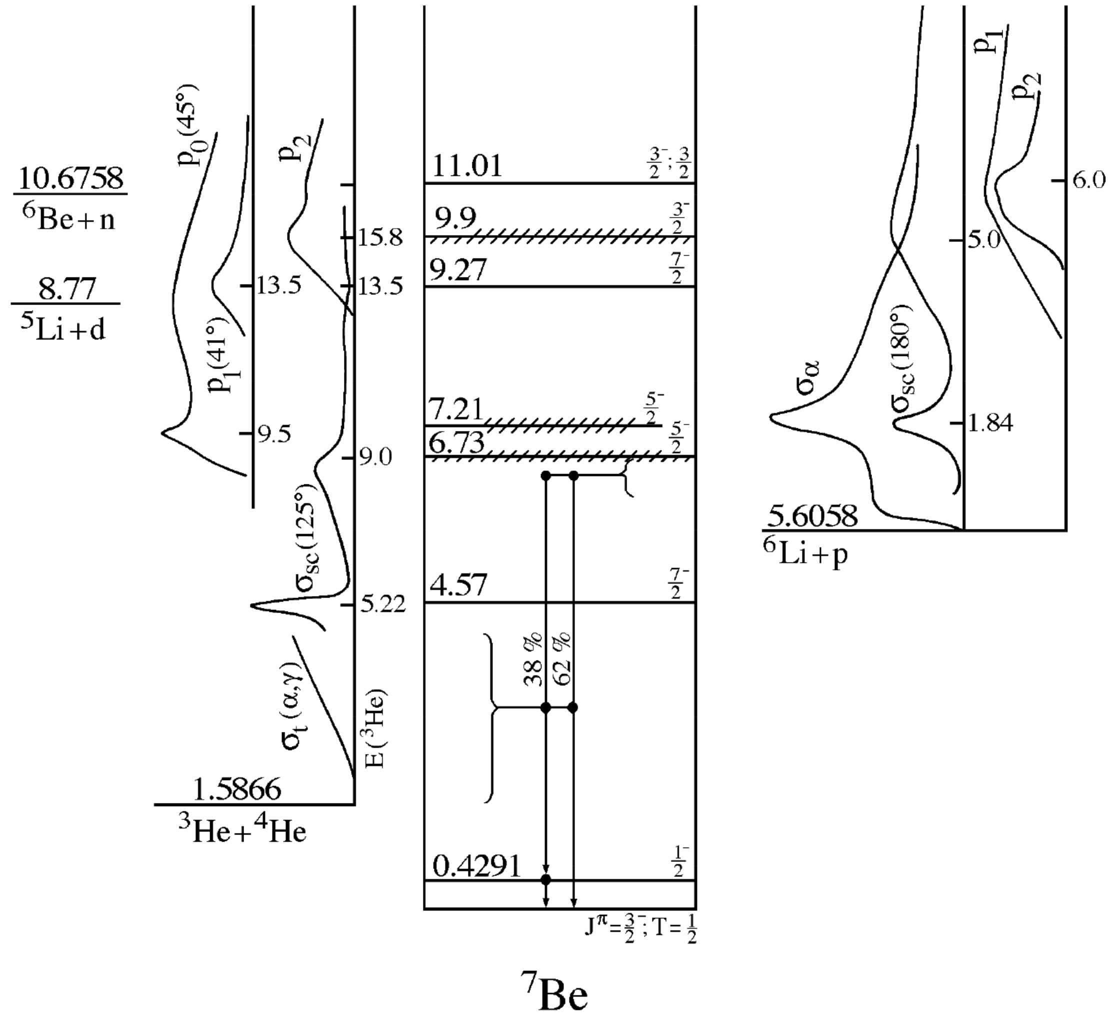
$^{3}\mathrm{He}(\alpha,\gamma)^{7}\mathrm{Be}$ reaction

^{7}Be **Bound States, Resonances, Thresholds**

Open Channels:

$^3He + \alpha \longrightarrow {}^6Li + p$

$^3He + \alpha \longrightarrow {}^7Be + \gamma + \gamma$
$^3He + \alpha \longrightarrow {}^7Be + \gamma$
$^3He + \alpha \longrightarrow {}^3He + \alpha$

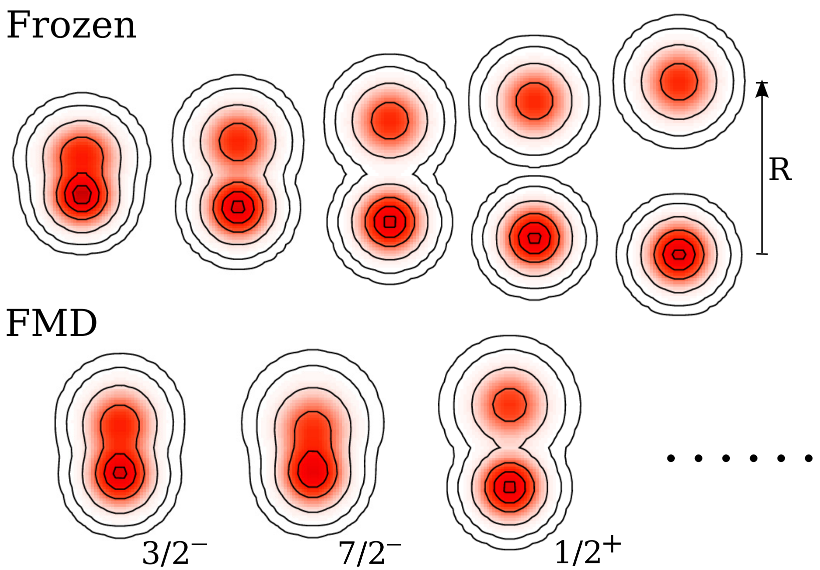


^{7}Be Many-Body Bound & Scattering States

Localized FMD states can represent many-body scattering states

➨ asymptotic states: product of “Frozen” FMD states $\mathcal{A}\left[\left| {}^3\mathrm{He};\ \frac{M_2}{M}R \right\rangle \otimes \left| {}^4\mathrm{He};\ -\frac{M_1}{M}R \right\rangle \right]$

Many-body Hilbert space:



Boundary conditions

- matching to the Coulomb solution of two point-like nuclei at distance $r = a$ (not trivial, $r \neq R$)

➨ phase shifts for scattering

➨ compact states: VAP “FMD” $3/2^-, 1/2^-$, resonance $7/2^-$

➨ polarized states: VAP with constraint on $\sqrt{< r^2 >} = 1, 2, \ldots, 5$ fm

All states together span Hilbert space in which Hamiltonian is diagonalized

$^{3}\text{He} - {}^{4}\text{He}$ phase shifts

- boundary condition Coulomb scattering solutions $\quad (k = +\sqrt{2\mu E})$

RGM channel state $\quad \left|\Phi(r)\right\rangle = \mathcal{A}\left[\,\left|kr,\ell\right\rangle_{rel} \otimes \left|{}^{3}\text{He};\tfrac{1}{2}^{+}\right\rangle_{intr} \otimes \left|{}^{4}\text{He};0^{+}\right\rangle_{intr}\right]^{J\pi}$

$\left\langle\Phi(r)\middle|\Psi,[\ell\ \tfrac{1}{2}^{+}]\,J^{\pi},E\right\rangle \xrightarrow{r\to\infty} \frac{1}{r}\left(F_{\ell}(kr) + \tan\left(\delta_{\ell}^{J\pi}(k)\right) G_{\ell}(kr)\right) \implies$ phase shifts $\delta(E)$

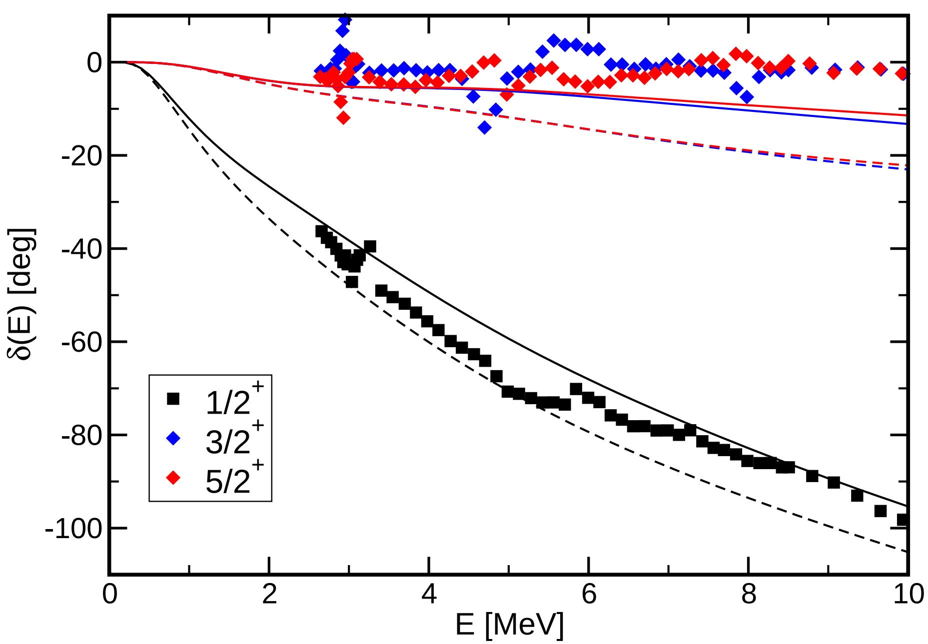
$^3\mathrm{He} - {}^4\mathrm{He}$ phase shifts

- boundary condition Coulomb scattering solutions $\quad (k = + \sqrt{2\mu E})$

RGM channel state $\quad \left| \Phi(r) \right\rangle = \mathcal{A} \left[\left| kr, \ell \right\rangle_{rel} \otimes \left| {}^3\mathrm{He}; \tfrac{1}{2}^+ \right\rangle_{intr} \otimes \left| {}^4\mathrm{He}; 0^+ \right\rangle_{intr} \right]^{J^\pi}$

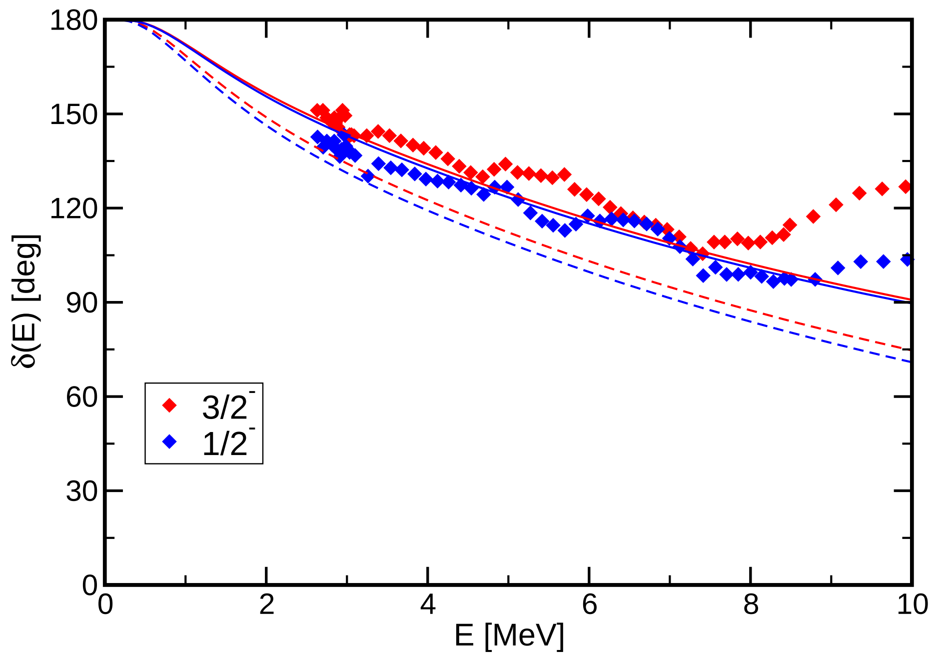
$$\left\langle \Phi(r) \middle| \Psi, [\ell \; \tfrac{1}{2}^+] \, J^\pi, E \right\rangle \xrightarrow{r\to\infty} \frac{1}{r} \left(F_\ell(kr) + \tan\left(\delta_\ell^{J\pi}(k)\right) G_\ell(kr) \right) \implies \text{phase shifts } \delta(E)$$

positive parity



dashed: frozen states only

negative parity



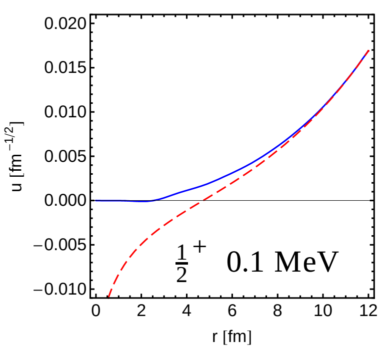
Spectroscopic amplitudes $\left\langle \Phi(r) \middle| \Psi \right\rangle$

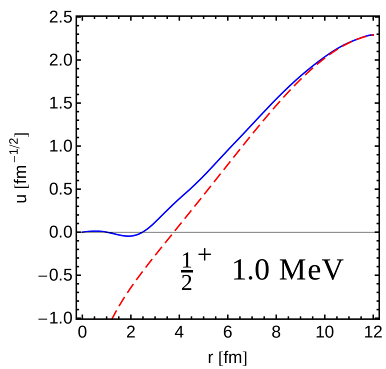
$\hat{\psi}(r) = \int dr' r'^2 \; N^{1/2}(r,r') \left\langle \Phi(r') \middle| \Psi \right\rangle$ "wave function" (for large spectroscopic factors)

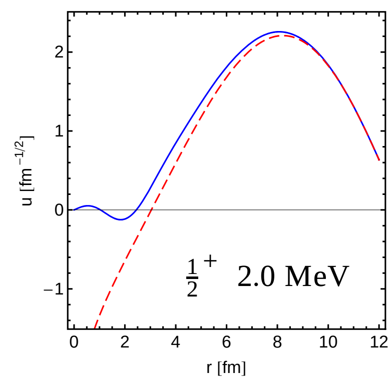
$N(r,r') = \left\langle \Phi(r) \middle| \Phi(r') \right\rangle$ RGM norm kernel

$\hat{\psi}(r \to \infty) \Longrightarrow$ Coulomb scattering state with phase shift

$\Longrightarrow$ Whittaker function for bound state







scattering state $^3\mathrm{He} + {}^4\mathrm{He}$

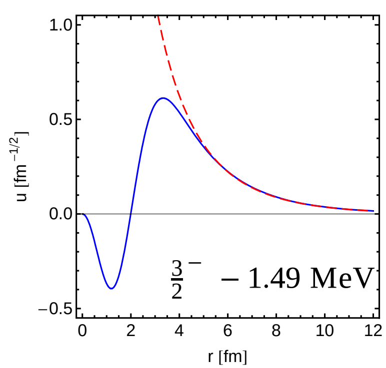
$r\,\hat{\psi}(r), \quad \ell = 0$

interior is Pauli forbidden

2 nodes

$r \to \infty$ Coulomb scattering with phase shift - - - - - -

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



ground state $^7\mathrm{Be}$

$r\,\hat{\psi}(r), \quad \ell = 1$

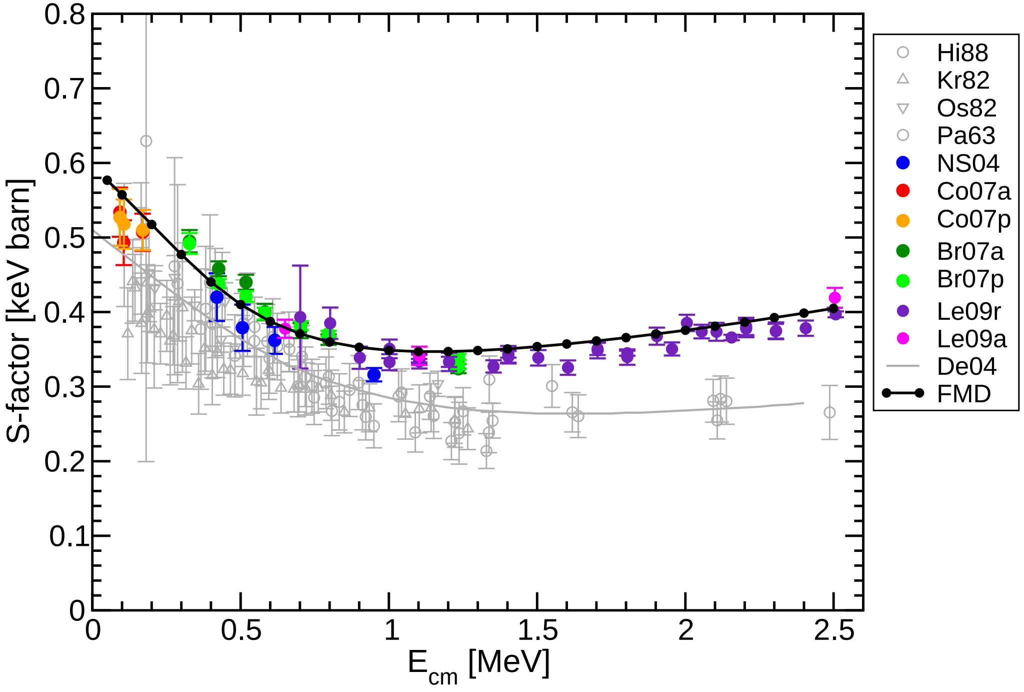
p-state

$r \to \infty$ Whittaker - - - - - -

S-Factor of Radiative Capture $^3\mathrm{He}(\alpha,\gamma)^7\mathrm{Be}$

- Capture from $1/2^+$, $3/2^+$ and $5/2^+$ scattering states into $3/2^-$ and $1/2^-$ bound states

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



$$S(E) = \sigma(E) E \exp\left(2\pi \frac{Z_1 Z_2 e^2}{\sqrt{2E/\mu}}\right)$$

First
ab-inito microscopic calculation based on realistic NN force

Thomas Neff to be published

New data

LUNA, Seattle, Weizmann, ERNA

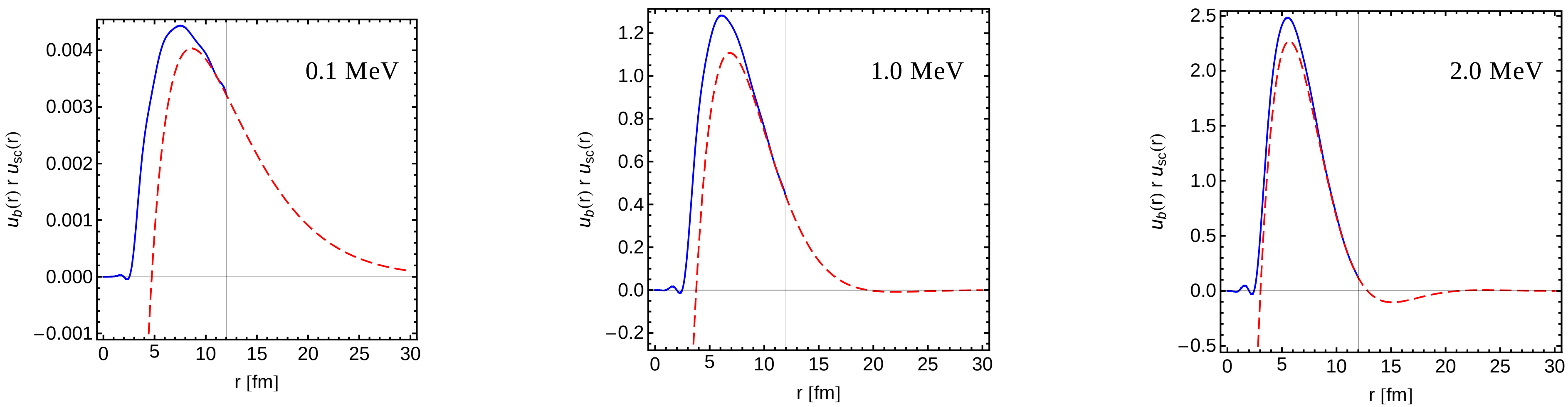
R-matrix fit to old data (—)

Descouvement et al. (2004)

Dipole matrix elements

$^3\text{He} + {}^4\text{He} \rightarrow {}^7\text{Be} + \gamma$ contribution from partial wave $\left[\ell = 0, \frac{1}{2}\right]^{\frac{1}{2}^+} \rightarrow J^\pi = \frac{3}{2}^-$ ground state

energy dependence
dipole strength $r\hat{\psi}^{\frac{1}{2}^+}(r) \cdot r \cdot r\hat{\psi}^{\frac{3}{2}^-}(r)$:

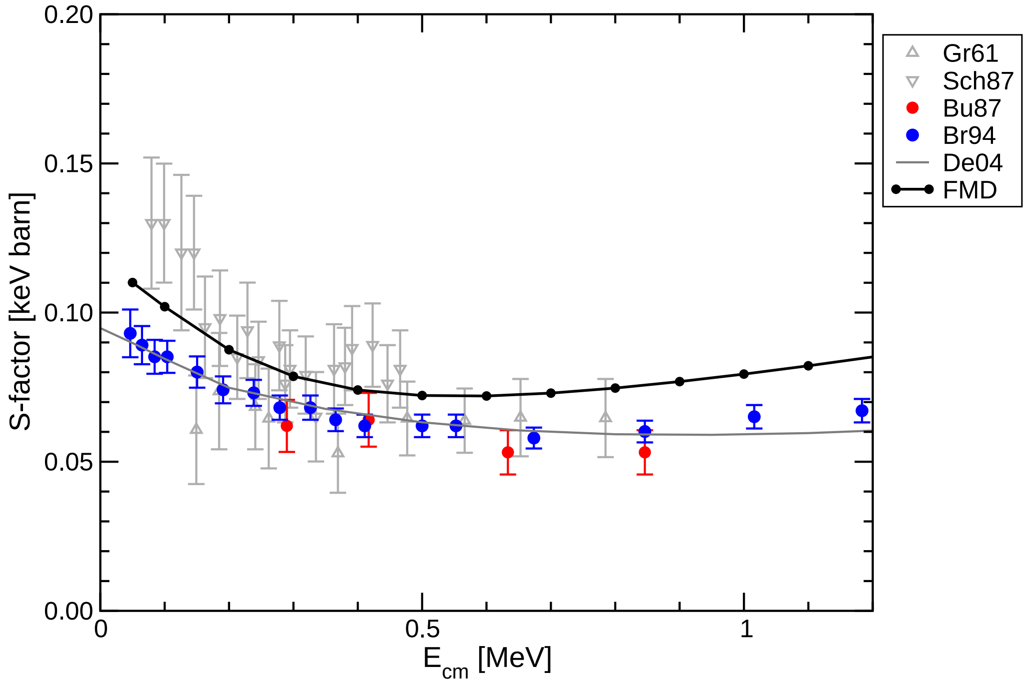


At low energies large fraction of capture happens outside nuclear interaction region

S-Factor of Radiative Capture $^3\mathrm{H}(\alpha,\gamma)^7\mathrm{Li}$

- Capture from $1/2^+$, $3/2^+$ and $5/2^+$ scattering states into $3/2^-$ and $1/2^-$ bound states

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



First
ab-inito microscopic calculation
with realistic NN force

Thomas Neff to be published

Data
Caltec, Warsaw
fit (—)

$$S(E) = \sigma(E) E \exp\left(2\pi \frac{Z_1 Z_2 e^2}{\sqrt{2E/\mu}}\right)$$

$^3\mathrm{H}(\alpha,\gamma)^7\mathrm{Li}$ not consistent with $^3\mathrm{He}(\alpha,\gamma)^7\mathrm{Be}$?

Summary

Ab initio microscopic many-body description
unified approach for nuclear structure and reactions

- Realistic NN-force transformed to H^{eff} with **U**nitary **C**orrelation **O**perator **M**ethod

  Fermionic **M**olecur **D**ynamics many-body Hilbert space for bound and scattering states

  No adjustable parameters

- Good description of many observations in light nuclei

  Halos and clustering, Hoyle state, borromean He isotopes, 2 proton halo,
  energies, formfactors, radii, el. magn. & weak transitions, spectroscopic factors, . . .

- Reproduction of new S-factor data for $^3\mathrm{He}(\alpha,\gamma)^7\mathrm{Be}$ energy dependence & absolute value
  but not for $^3\mathrm{H}(\alpha,\gamma)^7\mathrm{Li}$ absolute value 15% too high ?

To do: Understand why other (simpler) models fail
Improve H^{eff}