Microscopic calculation of the $^3\text{He}(\alpha, \gamma)^7\text{Be}$ reaction rate using realistic interactions

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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
  • $^3\text{He}(\alpha,\gamma)^7\text{Be}$ vs. $^3\text{H}(\alpha,\gamma)^7\text{Li}$
Motivation

• $^3\text{He}(\alpha,\gamma)^7\text{Be}$ one of the key reactions in the solar pp-chains
• in competition with the $^3\text{He}(^3\text{He},2p)^4\text{He}$ reaction it determines production of $^7\text{Be}$ and $^8\text{B}$ neutrinos

What is needed?

• $^7\text{Be}$ bound state energies
• $^7\text{Be}$ bound state wave functions, ANC
• $^3\text{He}$-$^4\text{He}$ scattering states
• dipole matrix elements between bound and scattering states
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
- ANC$s$ calculated from \textit{ab initio} wave functions (Nollett 2001, Navratil et al. 2007)


- 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
Argonne V18 (T=0)
spins aligned parallel or perpendicular to the relative distance vector

- strong repulsive core: nucleons can not get closer than \( \approx 0.5 \text{ fm} \)
  ➤ **central correlations**

- strong dependence on the orientation of the spins due to the tensor force
  ➤ **tensor correlations**
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 \( \approx 0.5 \text{ fm} \)
  - **central correlations**

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

\( V_{NN} \) [MeV]

\( r_{12} \) [fm]
**Unitary Correlation Operator Method**

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

\[ \tilde{C} = \tilde{C}_\Omega \tilde{C}_r = \exp[-i \sum_{i<j} g_{\Omega,ij}] \exp[-i \sum_{i<j} g_{r,ij}] \, , \, \tilde{C}^\dagger \tilde{C} = 1 \]

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

**Correlated Operators**
- correlated operators will have contributions in higher cluster orders

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

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

**Correlated Interaction**

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

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Correlated 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

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

- Effective interaction

$^3S_1$ bare

$^3S_1$ correlated

$^3D_1$ bare

$^3D_1$ correlated

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

correlated interaction is more attractive at low momenta

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

Effective interaction

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$^{3}S_1$ correlated

correlated interaction is more attractive at low momenta

$^{3}S_1 - ^{3}D_1$ correlated

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

similar to $V_{low-k, SRG}$

**Fermionic Molecular Dynamics**

**Fermionic**

Slater determinant

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

- antisymmetrized $A$-body state

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

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Molecular
single-particle states

\[ \langle x | q \rangle = \exp \left\{ -\frac{(x - b)^2}{2a} \right\} \otimes |\chi^\uparrow, \chi^\downarrow\rangle \otimes |\xi\rangle \]

- Gaussian wave-packets in phase-space (complex parameter \( b \) encodes mean position and mean momentum), spin is free, isospin is fixed
- width \( a \) is an independent variational parameter for each wave packet

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FMD basis contains harmonic oscillator shell model and Brink-type cluster configurations

Feldmeier, Schnack, Rev. Mod. Phys. 72 (2000) 655
**Many-body approach**

**Restoration of Symmetries**

**Projection**

- mean-field may break symmetries of Hamiltonian
- restore inversion, translational and rotational symmetry by projection on parity, linear and angular momentum

\[
\begin{align*}
P^\pi &= \frac{1}{2} (1 + \pi \Pi) \\

P^I_{MK} &= \frac{2J + 1}{8\pi^2} \int d^3 \Omega \, D^I_{MK} (\Omega) \, \hat{R}(\Omega) \\

P^P &= \frac{1}{(2\pi)^3} \int d^3 X \, \exp\{-i(P - \hat{P}) \cdot X\}
\end{align*}
\]
Many-body approach

Restoration of Symmetries

Projection

• mean-field may break symmetries of Hamiltonian
• restore inversion, translational and rotational symmetry by projection on parity, linear and angular momentum

Variation After Projection (VAP)

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

• 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

\[ P_{\pi} = \frac{1}{2} (1 + \pi \Pi) \]

\[ P_{MK}^J = \frac{2J + 1}{8\pi^2} \int d^3\Omega \, D_{MK}^J (\Omega)^* R(\Omega) \]

\[ P^P = \frac{1}{(2\pi)^3} \int d^3X \, \exp \{ -i(P - P) \cdot X \} \]
Many-body approach

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Multiconfiguration Mixing

- diagonalize Hamiltonian in a set of projected intrinsic states

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

\[ \sum_{K'\beta} \langle Q^{(a)} | H P_{\pi}^{J\pi} P_P^P = 0 \left| Q^{(b)} \right\rangle \cdot c_{K'\beta}^\alpha = \right. \]

\[ E_{n}^{J\pi\alpha} \sum_{K'\beta} \langle Q^{(a)} | P_{\pi}^{J\pi} P_P^P = 0 \left| Q^{(b)} \right\rangle \cdot c_{K'\beta}^\alpha = \]

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Frozen configurations

- antisymmetrized wave function built with $^{4}\text{He}$ and $^{3}\text{He}$ FMD clusters up to channel radius $\alpha=12$ 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
  Baye, Heenen, Descouvemont
### Bound states

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

- Centroid of bound state energies well described if polarized configurations included
- Tail of wave functions tested by charge radii and quadrupole moments
- Scattering phase shifts well described, polarization effects important

**Phase shift analysis:**

Spiger and Tombrello, PR 163, 964 (1967)

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Dashed lines – frozen configurations only
Solid lines – polarized configurations in interaction region included
\[ ^3\text{He}(\alpha, \gamma)^7\text{Be} \]

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

- polarization effects important
- \( s- \) and \( d- \) wave scattering phase shifts well described
- \( 7/2^- \) resonance too high, \( 5/2^- \) resonance roughly right, consistent with no-core shell model calculations
$S$-factor:

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

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

• 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

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)
Overlap functions from projection on RGM-cluster states
- Coulomb and Whittaker functions matched at channel radius $\alpha=12$ 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
**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%
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?
S-Factors consistent?

\[ ^3\text{He}(\alpha, \gamma)^7\text{Be} \text{ and } ^3\text{H}(\alpha, \gamma)^7\text{Li} \]

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

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

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

Microscopic Calculation of the $^3\text{He}(\alpha,\gamma)^7\text{Be}$ and $^3\text{H}(\alpha,\gamma)^7\text{Li}$ Capture Cross Sections Using Realistic Interactions

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