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

Thomas Neff, Hans Feldmeier, and Karlheinz Langanke
GSI Helmholtzzentrum für Schwerionenforschung GmbH, Planckstraße 1, 64291 Darmstadt, Germany
E-mail: t.neff@gsi.de

Abstract. The radiative capture cross sections for the $^3\text{He}(\alpha,\gamma)^7\text{Be}$ and the $^3\text{H}(\alpha,\gamma)^7\text{Li}$ reactions are calculated in the fully microscopic fermionic molecular dynamics approach. A realistic effective interaction derived in the unitary correlation operator method is employed. The model space consists of frozen cluster configurations at large distances and polarized configurations, obtained by variation of the many-body wave functions, in the interaction region. These polarized configurations are essential for the description of the $^7\text{Be}$ and $^7\text{Li}$ bound states and for the $S$- and $D$-wave scattering phase shifts. The calculated capture cross section agrees with both the normalization and the energy dependence of the modern $^3\text{He}(\alpha,\gamma)^7\text{Be}$ data. In case of the $^3\text{H}(\alpha,\gamma)^7\text{Li}$ reaction the energy dependence of the most recent data is described well but the normalization is larger by about 15% compared to experiment.

1. Introduction
The $^3\text{He}(\alpha,\gamma)^7\text{Be}$ reaction is one of the key reactions in the solar proton-proton chains [1, 2] and determines the production of the solar $^7\text{Be}$ and $^8\text{B}$ neutrinos. In recent years the capture cross section has been remeasured by a number of groups [3, 4, 5, 6, 7]. The new data improve significantly on older results but are still not able to reach the low energies relevant for solar burning.

From the theoretical side this reaction has been studied over the years using simple potential models where $^3\text{He}$ and $^4\text{He}$ are treated as point-like particles interacting via an effective nucleus-nucleus potential, e.g., [8] or microscopic cluster models, e.g., [9, 10] where the $^7\text{Be}$ bound and scattering states are built from microscopic $^3\text{He}$ and $^4\text{He}$ clusters interacting via an effective nucleon-nucleon interaction. Ab-initio calculations using variational Monte Carlo [11] and no-core shell model wave functions [12] were used to calculate asymptotic normalization coefficients but relied on potential models for the scattering states and the calculation of the capture cross sections. In [13] we presented the first consistent calculation of the capture cross section using a realistic effective interaction.

2. Effective Interaction
Starting from the realistic Argonne V18 interaction [14] we derive an effective low-momentum interaction using the unitary correlation operator method (UCOM). The basic idea of the UCOM approach is to explicitly include short-range central and tensor correlations into the many-body state by means of a unitary operator [15, 16, 17]. The correlation operators can also be mapped...
on the Hamiltonian to define a correlated interaction which not only contains two-body but also higher order contributions. In our applications we only consider the two-body part of the correlated Hamiltonian. This effective two-body interaction gives the same phase shifts as the original interaction but behaves differently in many-body systems. No-core shell model calculations show that the two-body UCOM interaction gives a good description of \( s \)- and light \( p \)-shell nuclei [17].

3. Many-Body Approach

We employ fermionic molecular dynamics (FMD) as our many-body approach. FMD uses Slater determinants

\[
|Q\rangle = A \{ |q_1\rangle \otimes \ldots \otimes |q_A\rangle \}
\]

as intrinsic many-body basis states. The single-particle states are Gaussian wave-packets

\[
\langle \vec{x}|q_k\rangle = \exp \left\{ -\frac{(\vec{x} - \vec{b}_k)^2}{2a_k} \right\} \otimes |\chi_k^\uparrow, \chi_k^\downarrow \rangle \otimes |\xi_k\rangle ,
\]

where the complex parameters \( \vec{b}_k \) encode the mean positions and momenta of the wave-packets and \( a_k \) their widths. The spins can assume any direction, isospin is \( \pm 1 \) denoting a proton or a neutron. The wave-packet basis is very flexible – it contains harmonic oscillator shell model and Brink-type cluster states as special limiting cases. To restore the symmetries of the Hamiltonian the intrinsic basis states are projected on parity, angular momentum and total linear momentum. The total linear momentum projection is necessary to decouple the internal motion of the clusters from their relative motion and the total center-of-mass motion.

For the \( ^3\text{He}(\alpha,\gamma)^7\text{Be} \) reaction we divide the model space into two regions. In the external region bound and scattering states are described by \( ^3\text{He} \) and \( ^4\text{He} \) clusters in their FMD ground states. These microscopic wave functions can also be expressed with resonating group (RGM) wave functions. This allows us include the boundary conditions for bound and scattering states by matching to Whittaker and Coulomb functions at the channel radius (\( a=12 \) fm) employing the microscopic \( R \)-matrix method developed by the Brussels group [18]. In the interaction region we include additional FMD many-body configurations that are obtained by variation after parity and angular momentum projection on spin-parity \( 1/2^+, 3/2^+, 5/2^+ \) and \( 3/2^-, 1/2^-, 7/2^-, 5/2^- \). With this procedure we generate polarized cluster configurations. Furthermore a constraint on the radius of the intrinsic states is used to vary the distance between the (polarized) clusters. In Fig. 1 density distributions for some selected frozen and polarized configurations are shown.

4. Results

Up to energies of about 2.5 MeV only the capture from the \( S \)- and \( D \)-wave scattering states into the \( 3/2^- \) and \( 1/2^- \) bound states has to be considered. Using only the frozen configurations \( ^7\text{Be} \)

---

**Figure 1.** Left: Frozen configurations with \( ^3\text{He} \) and \( ^4\text{He} \) clusters in their ground states. Right: Polarized configurations obtained by variation after parity and angular momentum projection.
is only bound by 200 keV. Including the polarized configurations the $3/2^-$ state is bound by 1.49 MeV and the $1/2^-$ state by 1.31 MeV with respect to the cluster threshold. The splitting between the two states is too small compared to the experimental value of 430 keV. This is related to a deficiency of our two-body interaction – additional spin-orbit strength is assumed to be coming from three-body forces. Fortunately the centroid energy agrees nicely with the experimental value. It turns out that the capture cross section depends strongly on the centroid energy but only very weakly on the splitting. Of great importance for the dipole matrix element and therefore for the capture cross section is an accurate description of the tail of the bound state wave functions. The charge radius is an observable that is sensitive to this tail and the calculated value of 2.67 fm agrees well with the experimental value of 2.647(17) fm [19].

In Fig. 2 we compare the calculated phase shifts for the $S$, $D$- and $F$-waves with the phase shifts extracted from the scattering data [20, 21]. There is a noticeably change in the calculations going from the model space containing only the frozen configurations to the full FMD model space. In case of the $S$- and $D$-wave phase shifts we find a good agreement with the experimental data. For the $F$-waves the full calculation agrees reasonable well for the $5/2^-$ resonance but the $7/2^-$ resonance is about 1.5 MeV too high in energy. This again reflects a missing spin-orbit strength of the effective interaction. For the capture cross section this is only relevant at energies above 3 MeV where $F$-wave capture will contribute.

The total cross section for $^3\text{He}(\alpha,\gamma)^7\text{Be}$ capture in form of the astrophysical $S$-factor is shown in the left part of Fig. 3. It agrees very well with the recent experimental data both in absolute normalization and in the energy dependence. Comparing our results for example with the microscopic cluster model calculations by Kajino [10] we find that the biggest differences are found in the $S$-wave contribution to the capture cross section. Our results also deviate from the empirical correlation between radius or quadrupole moment of the $^7\text{Be}$ ground state with the $S$-factor at zero energy that was found in the microscopic cluster model using different phenomenological interactions.

The $A$-body bound and scattering state wave functions can be analyzed in terms of overlap functions where the full microscopic wave function is projected on the subspace of cluster configurations. If one takes antisymmetrization between the clusters into account properly (by folding with the square-root of the RGM norm kernel) these overlap functions can be interpreted as the relative wave functions of point-like $^3\text{He}$ and $^4\text{He}$ clusters. It is interesting that the overlap functions deviate from the Whittaker and Coulomb functions, that describe the asymptotic behavior of the cluster motion for bound and scattering states, up to distances...
of about 9 fm. These deviations from the asymptotic behavior are even more pronounced in the dipole matrix elements. The dipole matrix elements calculated from the overlap functions agree with the matrix elements from the microscopic wave functions within 2%. They have sizable contributions already for distances as small as 3 fm and deviate significantly from matrix elements calculated from the asymptotic Whittaker and Coulomb functions up to 10 fm. It is therefore not really justified to treat the reaction as a pure external capture picture.

As our model successfully describes the $^3\text{He}(\alpha,\gamma)^7\text{Be}$ reaction we expect that it should also work well for the isospin-mirror reaction $^3\text{H}(\alpha,\gamma)^7\text{Li}$. Indeed we find a good agreement for the ground state properties of $^7\text{Li}$ and the phase shifts for $^3\text{H}^4\text{He}$ scattering. For the capture cross section shown in the right part of Fig. 3 we observe that the calculated cross section has the same energy dependence as the data by Brune et al. but the absolute normalization is about 15% larger.

References

[1] Adelberger E G et al. 1998 Rev. Mod. Phys. 70 1265
[2] Adelberger E G et al. 2011 Rev. Mod. Phys. 83 195
[3] Nara Singh B S, Hass M, Nir-El Y and Haquin G 2004 Phys. Rev. Lett. 93 262503
[4] Bemmerer D et al. 2006 Phys. Rev. Lett. 97 122502
[5] Confortola F et al. 2007 Phys. Rev. C 75 065803
[6] Brown T A D et al. 2007 Phys. Rev. C 76 055801
[7] Di Leva A et al. 2009 Phys. Rev. Lett. 102 232502
[8] Kim B T, Izumoto T and Nagatani K 1981 Phys. Rev. C 23 33
[9] Langanke K 1986 Nucl. Phys. A457 351
[10] Kajino T 1986 Nucl. Phys. A460 559
[11] Nollett K M 2001 Phys. Rev. C63 054002
[12] Navrátil P, Gueorguiev V G, Vary J P, Ormand W E and Nogga A 2007 Phys. Rev. Lett. 99 042501
[13] Neff T 2011 Phys. Rev. Lett. 106 042502
[14] Wiringa R B, Stoks V G J and Schiavilla R 1995 Phys. Rev. C 51 38
[15] Feldmeier H, Neff T, Roth R and Schmack J 1998 Nucl. Phys. A632 61
[16] Neff T and Feldmeier H 2003 Nucl. Phys. A713 311
[17] Roth R, Neff T and Feldmeier H 2010 Prog. Part. Nucl. Phys. 65 50
[18] Descouvemont P and Baye D 2010 Rep. Prog. Phys. 73 036301
[19] Nörtershäuser W et al. 2009 Phys. Rev. Lett. 102 062503
[20] Boykin W R, Baker S D and Hardy D M 1972 Nucl. Phys. A195 241
[21] Spiger R J and Tombrello T A 1967 Phys. Rev. 163 964
[22] Brune C R, Kavanagh R W and Rolfs C 1994 Phys. Rev. C 50 2205