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

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Abstract. The cross sections for the $^3$He$(\alpha,\gamma)^7$Be and the $^3$H$(\alpha,\gamma)^7$Li radiative capture reactions are calculated in the fully microscopic Fermionic Molecular Dynamics approach using a realistic effective interaction obtained in the Unitary Correlation Operator Method. The model space is divided in an external region where bound and scattering states are described by antisymmetrized products of $^4$He and $^3$He/$^3$H ground states and an internal region where additional many-body wave functions obtained by variation after parity and angular momentum projection enlarge the Hilbert space. These additional configurations, representing polarized cluster configurations, are necessary for a successful description of the bound and scattering states. The calculated $S$-factor for the $^3$He$(\alpha,\gamma)^7$Be reaction is in good agreement with recent experimental data both in absolute normalization and energy dependence. In case of the isospin mirror reaction $^3$H$(\alpha,\gamma)^7$Li the calculated $S$-factor is larger than the experimental data by about 15%. Dipole matrix elements are analyzed in terms of overlap functions calculated from the $A$-body wave functions.

1. Introduction
The $^3$He$(\alpha,\gamma)^7$Be radiative capture reaction plays an important role in the solar proton-proton chains and determines the production of $^7$Be and $^8$B neutrinos [1, 2]. Together with the $^3$H$(\alpha,\gamma)^7$Li reaction it is the main source for the uncertainty in the primordial $^7$Li production [3]. In recent years lots of experimental efforts went into remeasuring the cross reaction [4, 5, 6, 7, 8]. However it is still not possible to reach the low energies relevant for solar burning.

From the theory side this reaction has been investigated using simple potential models where $^3$He and $^4$He are treated as point-like particles interacting via an effective nucleus-nucleus potential, e.g., [9] or microscopic cluster models, e.g., [10, 11] where the $^7$Be bound and scattering states are constructed from microscopic $^3$He and $^4$He clusters interacting via an effective nucleon-nucleon interaction. Ab-initio calculations using variational Monte Carlo [12] and no-core shell model wave functions [13] were used to calculate asymptotic normalization coefficients for the bound states but relied on potential models for the scattering states and the calculation of the capture cross sections. In [14] we presented the first calculation of the capture cross section using fully microscopic wave functions and a realistic effective interaction.

2. Unitary Correlation Operator Method
Starting from the realistic Argonne V18 interaction [15] 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 [16, 17, 18]. 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. However, the UCOM interaction is defined as the two-body part the correlated Hamiltonian. It provides 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 [18].

3. Fermionic Molecular Dynamics

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

$$|Q⟩ = \mathcal{A}\{|q_1⟩ \otimes \ldots \otimes |q_A⟩\}$$

(1)
as intrinsic many-body basis states. The single-particle states are Gaussian wave-packets

$$⟨\vec{x}|q_k⟩ = \frac{(\vec{x} - \vec{b}_k)^2}{2a_k} \otimes |\chi^+_k, \chi^-_k⟩ \otimes |ξ_k⟩,$$

(2)

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 ±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 decouples the internal motion of the clusters from their relative motion and the total center-of-mass motion.

For the $^3\text{He}(α,γ)^7\text{Be}$ 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 rewritten as resonating group (RGM) wave functions. Using that boundary conditions for bound and scattering states can be included 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 [19]. In the interaction region 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 $3/2^-, 1/2^-, 7/2^-, 5/2^-$ are included. Furthermore a constraint on the radius of the intrinsic states is used to vary the distance between the clusters. By that polarized cluster configurations are generated.

4. Capture Cross Section

Up to energies of about 2.5 MeV only the capture from $S$- and $D$-wave scattering states into the $3/2^-$ and $1/2^-$ bound states has to be considered. The addition of polarized configurations is essential — using the frozen configurations only, $^7\text{Be}$ is 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 the two-body interaction — additional spin-orbit strength is assumed to be coming from three-body forces. Fortunately it turns out that the capture cross section depends strongly on the centroid energy, which is reproduced nicely, but only very weakly on the splitting. The calculated charge radius of 2.67 fm agrees well with the experimental value of 2.647(17) fm [20]. This is important as the dipole matrix element and therefore for the capture cross section depends on an accurate description of the tail of the wave function.

In Fig. 1 we compare the calculated phase shifts for the $S$-, $D$- and $P$-waves with the phase shifts extracted from the scattering data [21, 22]. There is a noticeably change in the results
Figure 1. $^4\text{He}^3\text{He}$ scattering phase shifts. Dashed lines show results using only frozen configurations, solid lines show results with full FMD model space. Left: S- and D-wave phase shifts. Right: P-wave phase shifts. Experimental results are from [21] and [22].

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. Also the P-wave phase shifts are essentially in good agreement with experiment, with the exception of the splitting.

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. 2. It agrees very well with the recent experimental data both in absolute normalization and in the energy dependence. On the right side of Fig. 2 we show the results for the isospin mirror reaction $^3\text{H}(\alpha,\gamma)^7\text{Li}$. Whereas the energy dependence of the calculated S-factor agrees very well with the data the absolute cross section is larger then the data by Brune et al. by about 15%. The uncertainty of the cross section with respect to the effective interaction will be addressed in a future publication.

In the left part of Fig. 3 the S- and D-wave contributions to the total S-factor are shown. If we compare our results for example with the microscopic cluster model calculations by Kajino [11] we find that the biggest differences are found in the S-wave contribution. 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.

Figure 2. Left: S-factor for the $^3\text{He}(\alpha,\gamma)^7\text{Be}$ reaction. Recent experimental data [4, 5, 6, 7, 8] are shown as colored symbols, older data as gray symbols. Right: S-factor for the $^3\text{H}(\alpha,\gamma)^7\text{Li}$ reaction. Most recent data [23] is shown as colored symbols, older data as gray symbols.
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 strength. The dipole matrix element calculated from the overlap functions as shown in the right part of Fig. 3 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 in a pure external capture picture.

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