Theoretical Study of the $d(d,p)^3$H and $d(d,n)^3$He Processes at Low Energies

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We present a theoretical study of the processes $d(d,p)^3$H and $d(d,n)^3$He at energies of interest for energy production and for big-bang nucleosynthesis. We accurately solve the four body scattering problem using the *ab initio* hyperspherical harmonics method, starting from nuclear Hamiltonians which include modern two- and three-nucleon interactions, derived in chiral effective field theory. We report results for the astrophysical S factor, the quintet suppression factor, and various single and double polarized observables. A first estimate of the theoretical uncertainty for all these quantities is provided by varying the cutoff parameter used to regularize the chiral interactions at high momentum.

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Introduction.—The fusion reactions $d(d,p)^3$H and $d(d,n)^3$He are critical processes for our understanding of big-bang nucleosynthesis (BBN) and for new designs of fusion reactors. In fact, the uncertainties in the prediction of the deuteron abundance [D/H] in BBN models is currently dominated by the lack of precise knowledge of the astrophysical S factor $S(E)$ of these processes [1,2]. Therefore, accurate calculations of $S(E)$ could be very helpful in reducing the uncertainty of the [D/H] estimate.

Moreover, it has been speculated that the rate of $d(d,p)^3$H and $d(d,n)^3$He would be reduced preparing the initial deuterons with parallel spins (i.e., being in the "quintet" spin state) [3,4]. This is referred as the quintet suppression. The interest on this suppression is related to the construction of "neutron lean reactors" with a $d+{}^3$He plasma, which would produce energy via the reaction $d+{}^3\mathrm{He}\to p+{}^4$He. However, the neutrons from the process $d+d\to n+{}^3$He would be always present. Hence, the interest in the use of polarized fuel [5] and in the quintet suppression. Naively, the suppression of the $\vec{d}(\vec{d},n)^3$He [and of $\vec{d}(\vec{d},p)^3$H] rate is expected when one assumes the capture to take place in S wave. Then, the process would require a spin flip to produce either a ^{3}H or ^{3}He nucleus, a process generally suppressed. However, this argument does not take into account the presence of the deuteron D state or the possible capture in P and D waves, whose importance has been already established also at low energy [4]. The suppression factor of the reaction rate when the two deuterons are in the total spin $S=2$ quintet state with respect to the unpolarized case is referred as the quintet suppression factor (QSF). No experimental study of the QSF has been reported so far. From the theoretical point of view, different predictions for the QSF have been reported, all at variance between each other [6]. The most accurate calculations predict a mild rate reduction using a polarized beam of laboratory energy above 50 keV, and even a rate increase at lower energy (i.e., QSF >1) [7]. Clearly, further studies are necessary to better clarify this issue.

Another advantage advocated for the use of polarized fuels in reactors is related to the possibility of handling the emission directions of reaction products, in particular the neutrons [5]. This could have an important impact on cost and safety of future fusion reactors, having the possibility to design fusion chambers where less parts of the walls are bombarded by neutrons [4]. The PolFusion experiment is currently being designed to study these processes using polarized deuterons for beam and target [8,9].

The $d(d,n)^3$He reaction is also used as a source of neutrons, subsequently employed to produce innovative medical radioisotopes. For example, the SORGENTINA-RF project [10] has been designed to use these neutrons to produce ^{99}Mo from the stable isotope ^{100}Mo, via the reaction ^{100}Mo$(n,2n)^{99}$Mo. From ^{99}Mo is then possible to produce ^{99m}Tc, a radio tracer used in single photon emission computed tomography. Again, it is important to know accurately the corresponding $d(d,n)^3$He cross section in the energy range more relevant for this application.

The general spin formalism for the scattering of two (identical) spin-one particles can be found in Ref. [4]. There are one unpolarized cross section, one vector analyzing power, three tensor analyzing powers, and 19 correlation coefficients. For future reference, we consider the case of a deuteron beam of energy T_d (in the laboratory system), impinging on a deuteron target at rest. The energy of interest for energy production is in the range $T_d=10$–50 keV, while for BBN $T_d=100\div400$ keV.

For the production of ^{99}Mo, a beam energy in the range $T_d = 200$–300 keV is considered optimal.

The total cross section (or, equivalently, the astrophysical S factor) has been studied with great detail, in view of its importance for BBN and energy production. The most recent measurements are reported in Refs. [11–20]. However, as discussed earlier, the different sets of data show a fairly large scatter [2]. The $d(d,n)^3$He astrophysical S factor has been experimentally investigated also using laser induced fusion in plasmas [21]. The unpolarized differential cross section measurements reported in the literature are somewhat older (and with a gap around $T_d \sim 200$ keV) [13,22–26]. Noticeably, there exist a few accurate measurements of vector and tensor analyzing observables below $T_d < 100$ keV. In particular, very precise data for the tensor analyzing powers $A_{zz,0}$ and $A_{xx,0} - A_{yy,0}$ for both reactions $d(d,p)^3$H and $d(d,n)^3$He have been reported [27]. Moreover, precise measurements of the $d(d,p)^3$H iT_{11}, T_{20}, T_{21}, and T_{22} observables have been performed at the Tandem Accelerator Center at Tsukuba [28]. In all these cases, only the deuterons in the beam were polarized. The already cited PolFusion experiment is planned to measure double-polarized observables, in particular $A_{z,z}$ and $A_{zz,zz}$ [9].

The study of these processes demands accurate solution of the four nucleon scattering problem, as S, P, and D waves have been found to give important contributions, at low energy as well [4]. The importance of P and D waves may be understood by taking into account the large extension of the deuteron wave functions (still sizable at interparticle distances of 6 fm). Therefore, the two entrance particles will interact also at a relatively large impact parameter.

From the theoretical side, there are a few accurate calculations reported in literature, such as those obtained from the solution of the Faddeev-Yakubovsky (FY) equations [7,29] and using the correlated Gaussian method [30,31]. Other calculations can be found in Refs. [32–35]. Moreover, accurate calculations of the ^{3}H$(d,n)^4$He fusion have been also obtained by means of the no-core shell model method [36].

In the present Letter, we study these processes using the hyperspherical harmonics (HH) expansion method [37,38]. The potentials considered in this study are the chiral nucleon-nucleon (NN) interactions derived at next-to-next-to-next-to-leading order (N3LO) by Entem and Machleidt [39,40], with cutoff $\Lambda = 500$ and 600 MeV. We include in the Hamiltonian also a chiral three-nucleon (3N) interaction, derived at next-to-next-to leading order (N2LO) in Refs. [41,42]. The two free parameters in this N2LO 3N potential, denoted usually as c_D and c_E, have been fixed in order to reproduce the experimental values of the $A = 3$ binding energies and the Gamow-Teller matrix element (GTME) of the tritium β decay [43–46]. Such interactions will be labeled as N3LO500/N2LO500 and N3LO600/N2LO600.

We report here the results obtained for a selected set of observables and compare them with the available experimental data and other theoretical calculations. We also provide a first estimate of the associated theoretical uncertainty from the difference of the results using the two adopted values of the cutoff Λ. Strictly speaking, such a procedure yields only a lower bound on the theoretical uncertainty [47]. However, we are confident that the reported theoretical uncertainty, reflecting our incomplete knowledge of the nuclear dynamics, be of the correct order of magnitude. In the future we plan to perform a better estimate of this uncertainty following the procedure of Refs. [48–50].

The Letter is organized as follows. In Section *Theoretical analysis* a brief description of the method is given, while in Section *Results* the results of the calculations are reported and compared with a selected set of available experimental data. The conclusions and the perspectives of this approach will be given in Section *Conclusions*.

Theoretical analysis.—In the following, we will denote with the index γ a particular clusterization $A + B$ of the four-nucleon system in the asymptotic region. More specifically, $\gamma = 1,\ 2,\ 3$ will correspond to the $p + {}^3$H, $n + {}^3$He, and $d + d$ clusterization, respectively. Please note that at the energies considered here, all these three asymptotic channels are open, while breakup channels are closed. Let us consider a scattering state with total angular momentum quantum number JJ_z, and parity π. The wave function $\Psi_{\gamma LS,JJ_z}$ describing a state with incoming clusters γ in a relative orbital angular momentum L and channel spin S [note that $\pi \equiv (-)^L$] can be written as

$$\Psi_{\gamma LS,JJ_z} = \Psi^C_{\gamma LS,JJ_z} + \Psi^A_{\gamma LS,JJ_z}, \tag{1}$$

where the core part $\Psi^C_{\gamma LS,JJ_z}$ vanishes in the limit of large inter-cluster separations, and hence describes the system where the particles are close to each other and their mutual interactions are strong. We compute $\Psi^C_{\gamma LS,JJ_z}$ by expanding it over the HH basis [37,38]. On the other hand, $\Psi^A_{\gamma LS,JJ_z}$ describes the wave function in the asymptotic regions, where the mutual interaction between the clusters is negligible (except for the long-range Coulomb interaction). In the asymptotic region therefore the wave functions $\Psi_{\gamma LS,JJ_z}$ reduce to $\Psi^A_{\gamma LS,JJ_z}$, which must be the appropriate asymptotic solution of the Schrödinger equation. The functions $\Psi^A_{\gamma LS,JJ_z}$ depend on the T-matrix elements (TMEs) ${}^JT^{\gamma,\gamma'}_{LS,L'S'}$, which are the amplitudes for the transition between the initial state γ, L, S to the final state γ', L', S' for the wave with the specified value of J. Clearly, we are interested in the terms ${}^JT^{\gamma=3,\gamma'=1}_{LS,L'S'}$ and ${}^JT^{\gamma=3,\gamma'=2}_{LS,L'S'}$. Full detail of the procedure adopted to determine $\Psi^C_{\gamma LS,JJ_z}$ and the TMEs is reported in Refs. [37,38].

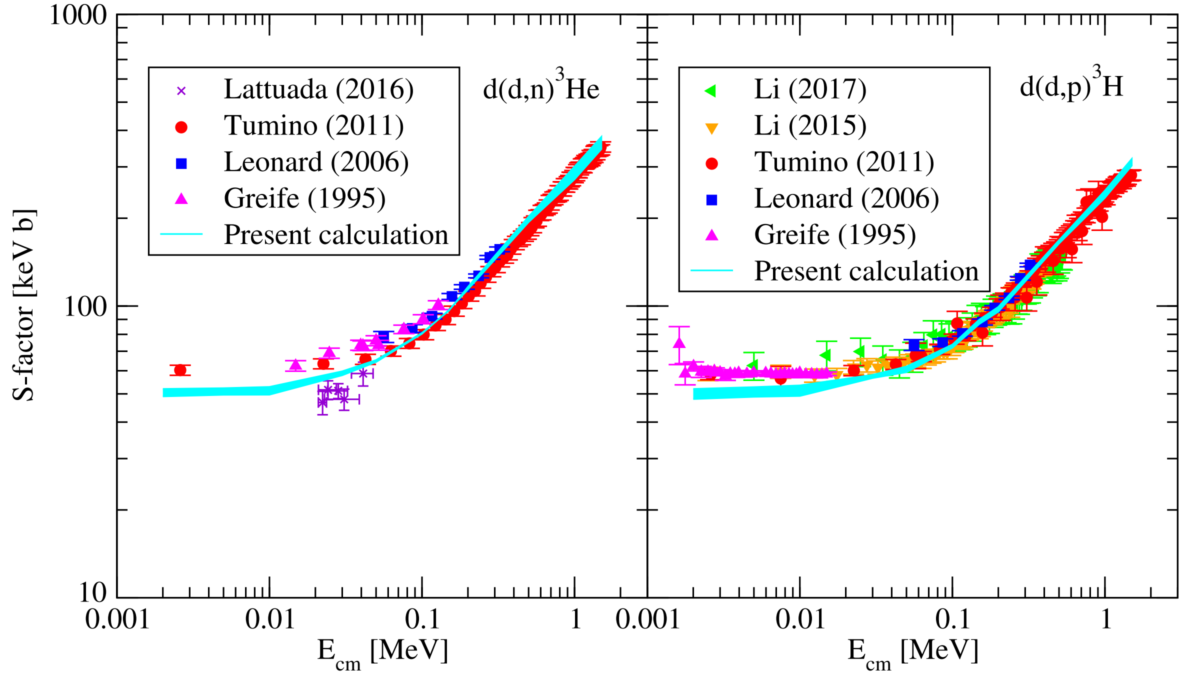

FIG. 1. The astrophysical S factor for the processes $d(d,n)^3$He (left panel) and $d(d,p)^3$H (right panel) calculated with the N3LO500/N2LO500 and N3LO600/N2LO600 interactions. The width of the bands reflects the spread of theoretical results using $\Lambda = 500$ or 600 MeV cutoff values. See the main text for more details. The experimental values are from Refs. [14,15,18–21].

Results.—First of all, let us consider the unpolarized total cross section, which is simply given by

$$\sigma^{(\gamma')} = \frac{1}{9}\frac{4\pi}{q_3^2}\sum_{J,LS,L'S'}(2J+1)|{}^J T^{(3,\gamma')}_{LS,L'S'}|^2, \qquad (2)$$

where q_3 is the relative momentum between the two deuterons and $\gamma' = 1$ (2) for the $d(d,p)^3$H [$d(d,n)^3$He] reaction. We have calculated it including all waves up to $L = 4$. At $T_d < 100$ keV, the dominant contributions comes from the $L = 0$ TMEs, ${}^0T^{(3,\gamma')}_{00,00}$ and ${}^2T^{(3,\gamma')}_{02,2S}$, with $S = 0$, 1 (the TME ${}^2T^{(3,\gamma')}_{02,21}$ gives the largest contribution). However, there is also a sizable contribution from the TME ${}^1T^{(3,\gamma')}_{11,11}$, which, as the energy increases ($T_d > 100$ keV) becomes dominant. Other $L = 1$ TMEs contribute only marginally, while the $L \geq 2$ TMEs are much smaller and become sizable only at $T_d \geq 1$ MeV.

From the total cross section, we have calculated the astrophysical S factor, defined as $S^{(\gamma)}(E_{cm}) = E_{cm}\sigma^{(\gamma)}e^{2\pi\eta}$, where $E_{cm} = T_d/2 \equiv q^2/2m$, m being the nucleon mass and $\eta = me^2/q$ the Sommerfeld parameter. The calculated S factors $S^{(\gamma)}(E)$ for $\gamma = 1$, 2 are reported in Fig. 1, where they are compared with recent experimental data [15,18,21]. The calculations have been performed using the N3LO500/N2LO500 and N3LO600/N2LO600 interactions and the results are shown as bands, their width reflecting the spread of theoretical results using $\Lambda = 500$ or 600 MeV cutoff values. As it can be seen from the figure, the calculations correctly reproduce the energy dependence of the data. The astrophysical S factor for $d(d,n)^3$He results to be larger than that of $d(d,p)^3$H for $E_{cm} > 0.1$ MeV. The calculations are well in agreement with the data of Ref. [18], while the data of Ref. [15] are slightly underpredicted, especially at low energy.

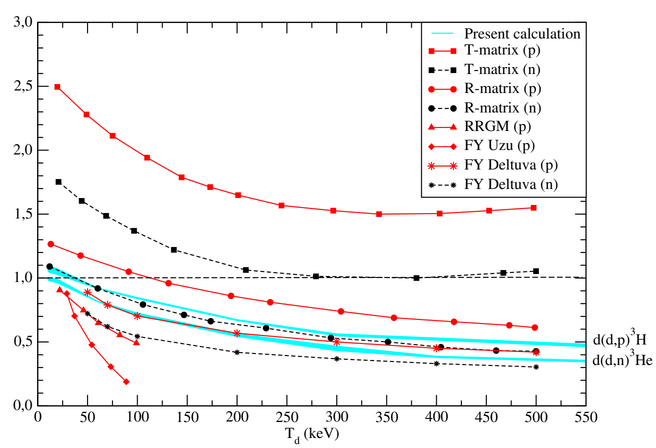

FIG. 2. The QSF for the processes $d(d,n)^3$He and $d(d,p)^3$H shown as bands, in analogy of Fig. 1. We report also the results obtained with other theoretical approaches: T matrix [51]; R matrix [27]; RRGM [32,33]; FY Uzu [35]; FY Deltuva [7]. The red solid [black dashed] lines connecting the red [black] symbols denote the QSF calculated in the literature for the $d(d,p)^3$H [$d(d,n)^3$He] reaction.

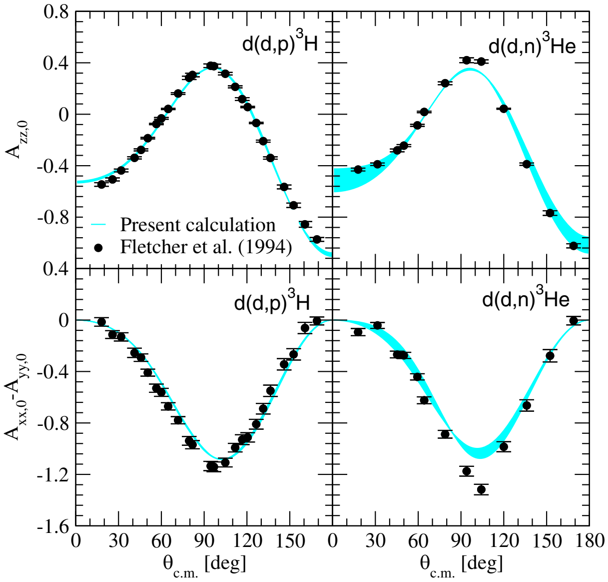

FIG. 3. The observables $A_{zz,0}$ and $A_{xx,0} - A_{yy,0}$ for the $\vec{d}(d,p)^3$H and $\vec{d}(d,n)^3$He processes at $T_d = 21$ keV. The (cyan) bands show the results of the present calculations. The experimental values are taken from Ref. [27].

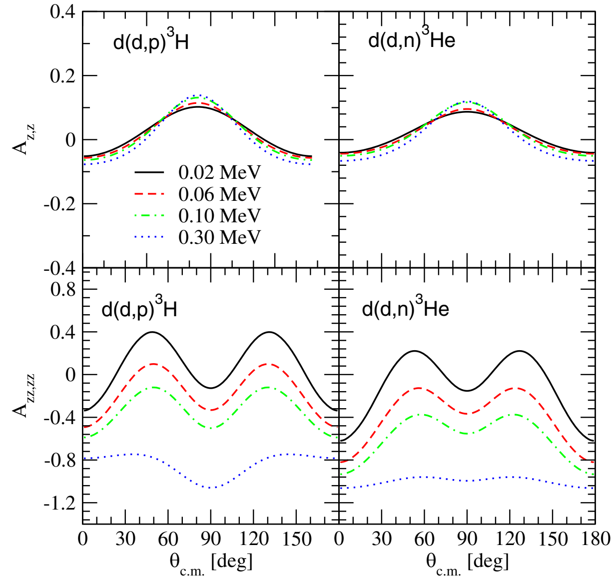

FIG. 4. The polarization observables $A_{z,z}$ and $A_{zz,zz}$ calculated for the $\vec{d}(\vec{d},p)^3$H and $\vec{d}(\vec{d},n)^3$He processes at various laboratory energies. The calculations have been performed for the N3LO500/N2LO500 interaction. The associated theoretical error is of the order of 5%.

Next we consider the QSF. We compute $\sigma_{11}^{(\gamma)}$ as the total cross section for both deuterons polarized along the beam direction. Then, QSF $= \sigma_{11}^{(\gamma)}/\sigma^{(\gamma)}$. We report the calculated QSF in Fig. 2, together with other theoretical estimates obtained using various methods [7,15,32,33,35,51]. As it can be seen, our calculations agree fairly well with the results of the FY calculation of Ref. [7] and with those obtained from the R-matrix analysis reported in Ref. [15]. Therefore, the trend with energy appears to be well consolidated: the QSF is close to unity at small energies and then slowly decreases. At $T_d = 1$ MeV (not shown in the figure), it reaches a sort of plateau. These findings are at variance, however, with what was found by other analyses [32,33,35,51].

The calculated unpolarized differential cross sections up to $T_d < 1$ MeV, are generally in good agreement with the experimental data [13,22–24]. More interesting is the comparison with the measured polarization observables below $T_d < 100$ KeV. For example, we report in Fig. 3, the comparison between our theoretical results and the observables measured at $T_d = 21$ keV in Ref. [27]. The results of our calculations are again shown as bands and they turn out to be in good agreement with these experimental data.

We have performed other comparisons with the available experimental data in this range of energies and a good agreement between theory and measurements has always been found. We are therefore confident of the accuracy of the calculations and we can make (sound) predictions for other observables. For example, in Fig. 4, we show the prediction for the observables $A_{z,z}$ and $A_{zz,zz}$, which will be studied in the near future by the experiment PolFusion [9]. The error estimated from the variation of the cutoff in these cases is of the order of 5%.

Conclusions.—In this Letter, we have studied the $d(d,p)^3$H and $d(d,n)^3$He processes at energies of interest for BBN and for energy production in fusion reactors. The results of the calculations have been presented as bands, being their width a first estimate of the theoretical uncertainty related to our incomplete knowledge of the nuclear dynamics. In practice, the width of the bands reflects the difference between the theoretical results obtained with the two values $\Lambda = 500$ and 600 MeV of the cutoff parameter in the nuclear interaction. By taking into account the width of the bands, we can conclude that the theoretical results and the data well agree. We have also presented predictions for the QSF and for some double-polarized observables, which will be the object of a future campaign of measurements by the PolFusion experiment. The $d(d,p)^3$H [$d(d,n)^3$He] astrophysical S factor at zero energy is estimated to be $S(0) = 50.8 \pm 1.9$ keV b (51.0 ± 1.4 keV b). The analysis of the consequences of these values for the cosmological models is currently underway.

In the future, we plan to perform a better estimate of the theoretical uncertainties, in particular, using the new χEFT interactions derived up to next-to-next-to-next-to-next-to-leading order [52] and the procedure of Refs. [48–50]. We plan also to study the changes in the fusion rates induced by the presence of strong high-frequency electromagnetic fields, as there are suggestions that the Coulomb barrier penetrability could increase significantly in certain configurations [53–55].

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