Improved nuclear reaction network for a reliable estimate of primordial Deuterium yield

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Abstract. A fundamental requisite to get a precise determination of light nuclides primordial abundances is the accurate evaluation of the nuclear reaction rates and corresponding uncertainties. In this paper, I will review the current status of the most important nuclear inputs to deuterium synthesis.

1. Introduction
The first determination of the baryon content of the universe dates to what is considered one of the pillars of the hot Big Bang model, that is Big Bang Nucleosynthesis (BBN). Nowadays, however, the unprecedented accurate determination of the baryonic energy fraction from the Planck experiment on Cosmic Microwave Background radiation (CMB) [1], \( \omega_b \equiv \Omega_b h^2 = 0.02242 \pm 0.00014 \), implies that BBN, in its minimal configuration, is essentially a parameter free model and, as such, has become a high precision tool for investigating beyond standard model physics in the early universe. However, the precision and reliability of BBN predictions relies on an accurate evaluation of the nuclear reaction rates entering the BBN network, requiring therefore a careful study of the available data and/or of the theoretical predictions.

In this paper, I focus on the prediction by BBN of deuterium abundance, whose astrophysical determination has now reached a percent accuracy, \( ^2\text{H}/\text{H}= (2.527 \pm 0.030) \times 10^{-5} \) at 68\% of C.L. [2]. In contrast to the situation present few years ago, all the most recent BBN analysis (see for example [3], [4], or [5]) agree that now the largest contribution to the error on primordial \(^2\text{H}/\text{H}\) comes from the uncertainty of the most influential nuclear reaction rates for deuterium yield: the \(^2\text{H}(p, \gamma)^3\text{He}\) radiative capture and the deuteron-deuteron transfer reactions, \(d(d, p)^3\text{H}\) and \(d(d, n)^3\text{He}\), from now on \(R_2\), \(R_3\), and \(R_4\). This circumstance has motivated a revision of all these reactions, with the inclusion of new data (for the complete analysis see [6]) in such a way to determine their implications on cosmological predictions.

2. Nuclear network: from experiment to rate prediction
For charged particle induced reactions, nuclear reaction rates as function of the temperature can be obtained by integration of the astrophysical factors, \(S(E)\). For every single reaction these functions, in absence of a specific theoretical model, have to be fitted from data collected in different nuclear physics experiments, commonly covering only limited energy ranges that are in whole or in part not overlapping. The key question is that these experiments have typically...
different normalization errors, related to detection efficiency, ion beam current measurement, target thickness, etc., which in some cases are not even estimated. Since there are no well-defined theoretical prescriptions on this matter, in the literature several authors use different approaches to data analysis, which often lead to slightly different outcomes.

As shown in [7], when data sets are affected by different normalization errors, \( \chi^2 \) minimization using the covariance matrix produces a negative bias that systematically underestimates the physical quantities giving more weight to data sets affected by larger systematics, provided they have instead a smaller statistical error. The \( \chi^2 \) implemented in this work, as originally in [8], is the most natural generalization of the solution suggested in [7],

\[
\chi^2(a_i, \omega_k) = \sum_{i_k} \frac{(S_{th}(E_{i_k}, a_i) - \omega_k S_{i_k})^2}{\omega_{k}^2 \sigma^2_{i_k}} + \sum_{k} \frac{(\omega_k - 1)^2}{\epsilon_k^2} \equiv \chi^2_{\text{stat}} + \chi^2_{\text{norm}}. \tag{1}
\]

In this expression the (unknown) quantities determined by the \( \chi^2 \) minimization are the coefficients in a polynomial expansion of the \( S \)-factor, \( a_i \), and the multiplicative normalization constants (one for each experiment), \( \omega_k \). Moreover, \( E_{i_k}, S_{i_k}, \sigma_{i_k}, \) and \( \epsilon_k \) are the (center of mass) energy, \( S \)-factor, statistical uncertainty, and (relative) normalization uncertainty of the \( i \)-th data point of the \( k \)-th data set, respectively, while \( S_{th}(E_{i_k}, a_i) \) is the theoretical function evaluated at \( E_{i_k} \). If only a total error \( \sigma_{i_k}^{\text{tot}} \) is available for the data points of a certain experiment, that error is used instead of \( \sigma_{i_k} \), and the normalization uncertainty, \( \epsilon_k \), is estimated as \( \max[\sigma_{i_k}^{\text{tot}}/S_{i_k}] \).

The polynomial expansion employed in the first term, \( \chi^2_{\text{stat}} \), is justified by the fact that, apart from resonance contributions, the \( S \)-factor is a smooth function of energy. The number of \( a_i \) parameters, i.e. the polynomial degree of \( S \), is chosen by increasing it until the minimum of the reduced \( \chi^2 \) stabilizes; typically, polynomials of 2-th or 3-th degree are a satisfying choice. The second term, \( \chi^2_{\text{norm}} \), links the data normalization factor \( \omega_k \) for each data set to the experimental estimate of the corresponding uncertainty, \( \epsilon_k \). Note that all experimental points, \( S_{i_k} \), of the same data sets are correlated by sharing the same normalization, \( \omega_k \), and that the contribution of the penalty factor, \( \chi^2_{\text{norm}} \), does not allow \( (\omega_k - 1) \) to be greater than the estimated or quoted normalization errors, \( \epsilon_k \).

The authors in [5] use, instead, a standard \( \chi^2 \) expression,

\[
\chi^2(\alpha_k) = \sum_{i_k} \frac{[S_{i_k} - \alpha_k S_{th}(E_{i_k})]^2}{\sigma^2_{i_k}}, \tag{2}
\]

where the fitting functions, \( S_{th}(E) \), come from nuclear reaction models, and the single free parameters of the fit are the normalization constants, \( \alpha_k \), one for each data set. Then, the global normalization for a given reaction measured in multiple data sets is given by the weighted average of the \( \alpha_k \). The same procedure for calculating the global normalization of a reaction is employed by [9], where the fitting functions, \( S_{th}(E) \), are the NACRE-II [10] theoretical \( S \)-factors.

Besides the analysis method, a possible source of disagreement among different authors lies in the data selection. In particular, in [5] a strict data selection was made, excluding from the fit all experiments for which the systematic uncertainty was not quoted or too large. A further data selection was made to exclude all data points falling outside the energy validity range of the theoretical model or with energy dependence different from the theoretical expectation.

While the use of a theoretical prejudice is advisable for discriminating among data which can be invalidated by systematics, excluding points with larger errors at the aim of reducing the uncertainties is not a good strategy, even because one expects that the more precise data will dominate the \( \chi^2 \) minimization. Guided by this attitude, we then include in our analysis the data on deuteron-deuteron transfer reactions measured via the Trojan Horse method [11], which had been excluded by the authors of [5].
The results of our fitting procedure are compared to the other findings in figures 1 and 2, where we show the ratio with our benchmark calculation of the rates of [12] (PArthENoPE1.0), of [9] (Cyburt 2016), and of [5] (Pitrou 2018). Note that in PArthENoPE1.0 the p(n, γ)²H rate from [13] was implemented, while here we consider the ab initio determination of [4]. From the plots a 3% (7%) maximum difference in \( R_3 \) (\( R_4 \)) is induced by the different analysis methods and data selection, while the 15% (8%) difference between \( R_2 \) values corresponds to our use of the rate in [4] instead of [13] ([14]).

In order to make the comparison among the values of deuterium yield obtained with the different rates, we have updated accordingly [15] the numerical code PArthENoPE [16]. To comply with previous analyses, we adopt \( \omega_b = 0.02225 \pm 0.00016 \) (as in table II of [9]) and \( \tau_n = (879.4 \pm 0.6) \) s, while leaving a standard number of relativistic degrees of freedom \( N_{\text{eff}} = 3.045 \) during BBN. Table 1 compares our results, when varying the rate used for \( R_2 \), with the ones of Pitrou et al. (2018) [5] and Cyburt et al. (2016) [9]. While there is a nice agreement with deuterium obtained in [9], a 2.4% difference is found between our finding and the one in [5]. Note the excellent agreement with the experimental measurement, \( ^2\text{H}/\text{H} = (2.527 \pm 0.030) \times 10^{-5} \) [2], of the deuterium prediction by PArthENoPE2.1 with \( R_2 \) of [14].

Table 1. Values of \((^2\text{H}/\text{H})\cdot10^5\) obtained by different groups by varying the rate used for \( R_2 \).

| \( R_2 \)       | this work | Pitrou et al. (2018) [5] | Cyburt et al. (2016) [9] |
|-----------------|-----------|--------------------------|--------------------------|
| Marcucci et al. (2005) [14] | 2.52 ± 0.07 | 2.459 ± 0.036             |
| Adelberger et al. (2011) [13] | 2.58 ± 0.07 |                          | 2.579                   |
| Marcucci et al. (2015) [4] | 2.45 ± 0.07 |                          |                         |

Figure 1. Ratios between different \( R_3 \) (left plot) and \( R_4 \) (right plot) rates and their benchmark values obtained in this work (see text) as a function of the temperature in \( 10^9 \) K.

Figure 2. Ratios between different \( R_2 \) rates and its benchmark values obtained in this work (see text) as a function of the temperature in \( 10^9 \) K.
Figure 3. Likelihood contours (68, 95 and 99% C.L.) in the $\omega_b$-$N_{\text{eff}}$ plane (see text).

We now want to determine the implications of these results on the determination of cosmological parameters in $\Lambda$-CDM scenario. At this aim, we compare our theoretical results with the above deuterium astrophysical measurement [2], $^2\text{H}/\text{H}=(2.527\pm0.030)\times10^{-5}$, and the $^4\text{He}$ mass fraction of [17], $Y_p=0.2446\pm0.0029$. We perform two likelihood analyses with $\omega_b$ and $N_{\text{eff}}$ as free parameters. In one case we consider only deuterium from BBN with a gaussian prior on the baryon density corresponding to the Planck result of Ref. [1], $\omega_b = 0.02242 \pm 0.00014$, (solid red curves in figure 3). In the second case we consider both $^2\text{H}/\text{H}$ and $Y_p$ and no prior on the baryon density (dashed blue curves in figure 3). We show the likelihood contours (68, 95 and 99% C.L.) in the $\omega_b$-$N_{\text{eff}}$ plane for the two cases corresponding to $R_2$ of [14] (left plot) and [4] (right plot). By marginalizing the likelihoods over $\omega_b$ we obtain $N_{\text{eff}} = 3.04 \pm 0.12$ and $N_{\text{eff}} = 3.28 \pm 0.12$, respectively, for the two $R_2$ determinations. We can observe that $R_2$ of [14] is consistent with a standard scenario, while the one of [4] results in a slight tension between the “only” BBN and BBN+CMB $N_{\text{eff}}$. In conclusion, the new data expected from the LUNA experiment [18] on $^2\text{H}(p, \gamma)^{3}\text{He}$ process will be crucial in shedding light on this issue.

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