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Revisiting proton-proton fusion in chiral effective field theory

Bijaya Acharya[a],[1,†] Laura Elisa Marcucci,[2,3,‡] and Lucas Platter[4,1,§]

[1] *Physics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA*

[2] *Department of Physics "E. Fermi", University of Pisa, Pisa, I-56127, Italy*

[3] *Istituto Nazionale di Fisica Nucleare, Sezione di Pisa, Pisa, I-56127, Italy*

[4] *Department of Physics and Astronomy, University of Tennessee, Knoxville, TN 37996, USA*

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Abstract

We calculate the S-factor for proton-proton fusion using chiral effective field theory interactions and currents. By performing order-by-order calculations with a variety of chiral interactions that are regularized and calibrated in different ways, we assess the uncertainty in the S-factor from the truncation of the effective field theory expansion and from the sensitivity of the S-factor to the short-distance axial current determined from three- and four-nucleon observables. We find that $S(0) = (4.100 \pm 0.024(\mathrm{syst}) \pm 0.013(\mathrm{stat}) \pm 0.008(g_A)) \times 10^{-23}$ MeV fm^2, where the three uncertainties arise, respectively, from the truncation of the effective field theory expansion, use of the two-nucleon axial current fit to few-nucleon observables and variation of the axial coupling constant within the recommended range. The increased value of $S(0)$ compared to previous calculations is mainly driven by an increase in the recommended value for the axial coupling constant and is in agreement with a recent analysis based on pionless effective field theory.

[a] Corresponding author.

[†] bid@ornl.gov

[‡] laura.elisa.marcucci@unipi.it

[§] lplatter@utk.edu

I. INTRODUCTION

Nuclear reaction rates are among the main sources of systematic uncertainty in stellar evolution models [1]. The proton-proton (pp) fusion reaction is the rate-determining step of the pp chains that power the Sun and lighter stars. Available experimental techniques are not able to directly measure the rate of this process with sufficient precision at energies relevant for stellar burning, and values predicted by nuclear theory provide critical inputs to astrophysical simulations [2]. More reliable calculations of this reaction rate can shed further light on the inconsistencies in observed solar data such as those that exist between spectroscopic determinations of solar abundances and helioseismology [3, 4]. In concert with improvements in other physics inputs such as radiative opacities, rigorous constraints on this rate can also help us use solar data as a powerful probe of new physics [5].

The calculations of this process were traditionally performed using potential models [6–9]. Over the last few decades, methods based on effective field theory (EFT) techniques [10] that allow us to obtain theoretical predictions with reliable uncertainty estimates, have been employed. EFTs provide a simplified yet rigorous description of the process under study using only those degrees of freedom that are relevant at low energies. The calculations are organized as systematic expansions in the ratio of the typical momentum scale Q of the process to a large momentum scale Λ_b, beyond with the EFT expansion breaks down. The undetermined parameters—the so-called low-energy constants (LECs)—that appear up to a given order in this Q/Λ_b expansion are first fixed, e.g., by fitting to experimental data, and then predictive calculations are performed for other observables. The first applications of EFT to the pp fusion process were based on hybrid approaches [11, 12] that employed wave functions obtained from phenomenological nuclear potentials along with the nuclear electroweak current operators derived in chiral EFT, which employs pions and nucleons as dynamical degrees of freedom. Complete chiral EFT calculations, using potentials and currents both derived consistently within the chiral EFT framework, have been carried out, first in Ref. [13] and then in Ref. [14]. However, as discussed further below, these calculations require important updates and corrections.

Over the past few decades, a number of studies have also been performed in pionless EFT, which uses nucleons as the only dynamical degrees of freedom [15–20]. At energies relevant for astrophysics, the process lies well within the domain of convergence of pionless EFT. In this approach, the pp fusion rate can be calculated with a small number of parameters. The uncertainties have traditionally been dominated by the limitation of experiments and Lattice QCD to sufficiently constrain the LEC $L_{1,A}$ that parametrizes the short-distance two-body axial current [21, 22]. By performing next-to-leading-order calculations of relevant three-body observables, a recent pionless EFT work [19] has quoted the value $S(0) = (4.14 \pm 0.01 \pm 0.005 \pm 0.06) \times 10^{-23})$ MeV fm^2, where the three uncertainties arise, respectively, from the experimental errors on the nucleon axial coupling and the tritium β decay rate, and the theory uncertainty of pionless EFT.

The goal of this work is to present a state-of-the-art calculation of the pp fusion cross section in chiral EFT. In addition to correcting [23] the erroneous treatment of the relationship between the three-nucleon force parameter c_D and the two-nucleon axial current parameter $\hat{d}_R$, we also improve and expand upon the work of Ref. [14] by using recently developed chiral EFT interactions [24, 25], and by accounting for uncertainty sources not previously considered in Ref. [14]. We also review and update the work of Ref. [13] by taking particular care of the convergence [26] in the expansion basis used to calculate the nuclear wave functions, as well as the range of the integration in the axial current matrix element, by also correcting the c_D-$\hat{d}_R$ relation, and by using the most recent values for the fundamental constants, which leads to a reassessment of the Gamow-Teller matrix element of tritium β-decay. The same nuclear interaction of Ref. [13] is implemented, limiting the present study to the case of cutoff $\Lambda = 500$ MeV. This calculation also allows us to perform a benchmark study between the approaches used in Ref. [14] and the one of Ref. [13]. The two approaches will be labelled LS and VM, respectively, since the former used the Lippmann-Schwinger equation to solve the two-body problem, while the latter used a variational method [27] as discussed below.

The paper is organized as follows: we outline the theoretical framework in Section II, present our results in Section III, and conclude with a summary and outlook in Section IV.

II. THE S-FACTOR

The astrophysical S-factor $S(E)$ at the pp center-of-mass energy E is defined as

$$S(E) = \sigma(E)\, E\, e^{2\pi\eta}\,, \tag{1}$$

where $\eta = \sqrt{m_p/E}\,\alpha/2$ is the Sommerfeld parameter, m_p is the proton mass, $\alpha = 1/137.036$ is the fine-structure constant, and $\sigma(E)$ is the pp fusion cross section at energy E, which can be written as

$$\sigma(E) = \int \frac{\mathrm{d}^3 p_e}{(2\pi)^3} \frac{\mathrm{d}^3 p_\nu}{(2\pi)^3} \frac{1}{2E_e} \frac{1}{2E_\nu}\, 2\pi\delta\left(E + 2m_p - m_d - \frac{q^2}{2m_d} - E_e - E_\nu\right)$$
$$\frac{1}{v_{rel}}\, F(Z, E_e)\, \frac{1}{4} \sum |\langle f|\hat{H}_W|i\rangle|^2 \,. \tag{2}$$

Here $p_{e,\nu}$ are the positron and neutrino momenta, $E_{e,\nu}$ their energies, m_d is the deuteron mass, v_{rel} is the pp relative velocity, and q is the momentum of the recoiling deuteron. The function $F(Z, E_e)$ accounts for the distortion of the positron wave function due to the Coulomb field of the deuteron. Its classical expression, which can be found in Ref. [28], needs to be augmented with radiative corrections. We enhance $F(Z, E_e)$ by 1.62% to account for the γW box diagram involving one nucleon, which has been explicitly evaluated in Ref. [29], and ignore the diagram involving both nucleons, which has not yet been calculated. The summation in Eq. (2) runs over the spin projections of all the initial- and the final-state particles. The initial state $|i\rangle$ and the final state $|f\rangle$ are products of leptonic and nuclear states and the weak interaction Hamiltonian $\hat{H}_W$ can be written in terms of the leptonic weak current j^μ and the nuclear weak current J^μ as

$$\hat{H}_W = \frac{G_V}{\sqrt{2}} \int \mathrm{d}^3 x \left[j^\mu(\mathbf{x}) J_\mu{}^\dagger(\mathbf{x}) + \text{h.c.} \right] , \tag{3}$$

where G_V is the vector coupling constant. Unless otherwise stated, the calculations presented below adopt the value $1.149589 \times 10^{-11}\,\mathrm{MeV}^{-2}$, that corresponds to the CKM matrix element $V_{ud} = 0.9737$ and the process independent radiative corrections $\Delta_R^V = 0.02454$ as obtained in a recent reanalysis of the superallowed beta decay rates [30] (see Ref. [31] for a direct computation in Lattice QCD and Ref. [32] for a prediction with minimal phenomenological input).

The matrix element of the leptonic weak current operator j^μ between the leptonic wave functions can be obtained from Dirac algebra and we refer the reader to Refs. [13, 14] for details of the derivation of the matrix elements of the nuclear weak current operator J^μ between the nuclear wave functions. In particular, we regularize the currents using the same Gaussian regulators that were used in Refs. [13, 14]. The incoming pp system can be considered exclusively in an s-wave, as it has been shown that higher partial-wave channels are suppressed by several orders of magnitude (see Ref. [20] and also the erratum of Ref. [13]). Then, the leading contribution to J^μ comes from the one-body (1B) Gamow-Teller (GT) operator and the leading two-body (2B) corrections occur at $\mathcal{O}\left([Q/\Lambda_b]^3\right)$ relative to 1B, which correspond to next-to-next-to-leading order (NNLO) in the chiral expansion. It should be noted that these differ slightly from the currents used in Ref. [13]: besides the leading-order GT 1B contribution, relativistic $1/m_N^2$ corrections to the 1B GT term, where m_N is the nucleon mass, were also included since they are $\mathcal{O}\left([Q/\Lambda_b]^2\right)$ in the power counting adopted in that work. In order to facilitate comparison with Ref. [13], we retain these terms in our updates to the study of Ref. [13] (model D discussed below) although they are small. The 2B current we use are the same as the ones used in Refs. [13, 14], but with the corrected [23] relation (see also Refs. [33, 34]) to the three-nucleon force parameter c_D as discussed in Sec. II A. Unless otherwise stated, we use the latest Particle Data Group (PDG) recommended value of the axial coupling constant $g_A = 1.2754 \pm 0.0013$ [35] in the current operator in the calculations presented below.

The nuclear wave functions are calculated either by solving the Lippmann-Schwinger (LS) equations as in Ref. [14], or by applying the variational method (VM) of Refs. [13, 27]. The chiral EFT Hamiltonians include nuclear as well as electromagnetic potentials. In this work, relativistic and radiative corrections to the Coulomb interaction, discussed in Ref. [36], are included explicitly in the calculation of the wave function, as in Ref. [13]. This is in contrast to Ref. [14], where we first calculated $S(E)$ using pp wave functions with nuclear plus Coulomb interaction and applied a phenomenological correction to take such higher-order electromagnetic effects into account. Finally, in Ref. [14], we used in Eq. (2) the deuteron mass m_d obtained from the calculated value of the binding energy, which gave a negligible numerical error since all of the interactions used in Ref. [14] were fit to the experimental ^{2}H binding energy. As we discuss below, since some of the interactions we use in this work do not reproduce this energy very well, we use the experimental value of $m_d = 1875.61294257$ MeV [37] instead. Note that for the interaction models which properly reproduce the ^{2}H binding energy, the theoretical and experimental value of m_d obviously coincide to sufficient precision.

A. Relationship between the axial current and the the three-nucleon force

The axial 2B current contains a counterterm $\hat{d}_R$ that needs to be fixed before predictive calculations of $S(E)$ can be performed. This LEC has not yet been determined from $A < 3$ observables. In chiral EFT, fitting to $A > 2$ data involves the relationship between $\hat{d}_R$, the πN LECs $c_{3,4}$ and the pion-exchange part of the $3N$ force parameter c_D:

$$\hat{d}_R = -\frac{m_N}{4g_A\Lambda_\chi}c_D + \frac{m_N}{3}c_3 + \frac{2m_N}{3}c_4 + \frac{1}{6}\,, \tag{4}$$

where $\Lambda_\chi \approx 700$ MeV is the breakdown scale of chiral perturbation theory. With $c_{3,4}$ values constrained by πN and/or NN data, the LEC $\hat{d}_R$ (or c_D) can then be obtained by fitting it, along with the contact $3N$ force parameter c_E, to observables such as ^{3}H β decay rate and binding energy.

Following the suggestion of Ref. [38], Eq. (4) was first derived in Ref. [33], albeit with an incorrect factor in front of the c_D term (the factor -1/4 was missing). This error, which propagated widely in the literature and also entered the results of Refs. [13, 14], was first corrected by Ref. [23]. The corrected relation was used by Ref. [39] to compute $S(0)$. The value $S(0) = 4.058 \times 10^{-23}$MeV fm^2 quoted by Ref. [39] was obtained using ^{3}H β decay rate to constrain $\hat{d}_R$, with a set of chiral interactions not explored in this work. Note that the main goal of Ref. [39] was to compute the muon-deuteron capture rate $\Gamma_{\mu d}$ and not $S(E)$—no sources of theory errors on $S(0)$ were thoroughly examined other than the uncertainty in the $\Gamma_{\mu d} - S(0)$ correlation due to nucleon axial form factor.

Eq. (4) also enables us to constrain the axial current from strong-interaction observables. Therefore, different sets of experimental observables have been used, e.g., Ref. [40] used ^{4}He binding energy and elastic ^{4}He-n scattering data whereas Ref. [41] used ^{3}H binding energy and elastic ^{3}H-n scattering data.

III. RESULTS

We now present our results for $S(E)$ obtained using various chiral EFT interactions: (i) model A which uses wave functions obtained by solving the Lippmann-Schwinger equation using a modern potential that is well adapted to EFT truncation studies because it is formulated at different orders, (ii) model B which uses the interactions of Ref. [36] with the updated fits [39] to account for the corrected c_D-$\hat{d}_R$ relation, (iii) model C where the

Model	Method	$1/m_N^2$ currents	g_A	c_D	B(^{2}H)
A	LS	excluded	1.2754	-1.626	2.22038
B	LS	excluded	1.2754	see text	$2.224^{(+0)}_{(-1)}$ [36]
C	LS	excluded	1.2724	-0.0047	2.18553
D	VM	included	1.2754	see Table III	2.22458

TABLE I. Main features of the four models adopted in this work. In particular, for each model we indicate whether the $1/m_N^2$ one-body currents are included, and we provide the adopted values for the single-nucleon axial coupling constant g_A, the LEC c_D, and the calculated deuteron binding energy B(^{2}H) in MeV.

statistical uncertainty of fitting c_D to few-body observables has been studied in detail, and (iv) model D which uses the variational method of Refs. [13, 27] along with interactions of Ref. [42], which requires a new fit of c_D. In Table I, we summarize the salient features of these four models.

A. Model A: the SMS-RS predictions

Table II shows the threshold values and energy-derivatives of $S(E)$ calculated using the SMS-RS potential of Ref. [24] at regulator cutoff $\Lambda = 500$ MeV and the LS equations as in Ref. [14]. In contrast to older momentum-space chiral interactions [42–47] that employed the conventional non-local Gaussian regulators along with an additional spectral function regularization [48] in the two-pion exchange diagrams, the potential of Ref. [24] uses a "semi-local" regularization scheme which consists of a local regulator for the pion-exchange parts and non-local Gaussian regulator for the contact parts of the NN interaction in order to preserve the long-range parts that are unambiguously determined in chiral EFT. The subleading πN LECs in this potential have been fixed to the precise values obtained from a Roy-Steiner analysis [49] of the πN scattering data. The nucleon-nucleon (NN) LECs in the SMS-RS potential have been fit to mutually consistent np and pp scattering data of the Granada 2013 database [50]. In the 2B current, we use $\hat{d}_R$ given by Eq. (4) with the value of $c_D = -1.626$ obtained in Ref. [41] by fitting to Nd scattering cross section data; however,

Order	$S(0)$ [MeV fm^2]	$S'(0)/S(0)$ [MeV^{-1}]	$S''(0)/S(0)$ [MeV^{-2}]	$S'''(0)/S(0)$ [MeV^{-3}]
LO	4.143 $\times 10^{-23}$	10.75	306.75	-5150
NLO	4.094 $\times 10^{-23}$	10.81	312.78	-5370
NNLO	4.100 $\times 10^{-23}$	10.83	313.72	-5382

TABLE II. The threshold S-factor $S(0)$, and the first and second derivatives of the S-factor at threshold divided by $S(0)$ in units of MeV fm^2, MeV^{-1}, MeV^{-2} and MeV^{-3}, respectively, at different orders of the chiral EFT expansion for both the nuclear interaction and current. The SMS-RS interaction is used.

we note that the theoretical uncertainties in the estimation of c_D were not explored in that reference. It should be remarked that, thanks to the availability of the SMS-RS potential at various orders in the EFT expansion, it is possible to perform an order-by-order calculation consistently for both potential and current. This is different from the study of Ref. [13], where the nuclear interaction order was fixed at N3LO, while the different orders were considered only for the chiral expansion of the axial current.

We evaluate $S(E)$ in the energy interval $E = [1, 30]$ keV and fit a polynomial in E to obtain the threshold S-factor $S(0)$ and its derivatives. The extracted values depend on the degree of the fitted polynomial. We obtained stable values, particularly for $S(0)$ and $S'(0)$, for third, fourth and fifth degree polynomials. Unless otherwise stated, we quote values from cubic fits.

We assess the uncertainty of the S-factor due to the EFT truncation by following the method described in Refs. [51, 52]. We first express the S-factor as

$$S(0) = S_{\rm LO} \sum_{n=0}^{3} c_n \left(\frac{Q}{\Lambda_b}\right)^n , \tag{5}$$

where $S_{\rm LO}$ denotes the leading order (LO) result for the S-factor given in Table II, Q denotes the inherent momentum scale of the problem, and Λ_b is the breakdown scale. An estimate of the truncation error is then obtained by calculating $(Q/\Lambda_b)^4 \max(|c_0|, |c_2|, |c_3|)$. Using the order-by-order results of Table II to obtain the expansion coefficients c_n, the pion mass for the momentum scale Q and a conservative estimate of $\Lambda_b = 500$ MeV, we obtain an uncertainty 0.024×10^{-23} MeV fm^2 for the SMS-RS interaction, leading to the prediction $S(0) = (4.100 \pm 0.024(\text{syst})) \times 10^{-23}$ MeV fm^2. Here we have used the label "syst" to emphasize that is is an estimate of the systematic uncertainty from the truncation of the

EFT expansion. We note that this estimate has been found to roughly correspond to a 68% Bayesian credible interval for a particular choice of Bayesian priors for the expansion coefficients c_n [51].

B. Model B: the NNLOsim updates

In Ref. [14], we employed the NNLOsim family of 42 interactions [36] to assess the uncertainty in the pp fusion rate due to the statistical uncertainties in the LECs, the systematic uncertainty due to the chiral EFT cutoff dependence, and the systematic variations in the database used to calibrate the NN interaction. At each of the 7 different cutoff values $\Lambda = [450, 475, 500, 525, 550, 575, 600]$ MeV, the 26 LECs in the NN and πN sectors were simultaneously fit to 6 different pools of input data, leading to 42 interactions. Specifically, the input data consisted of NN scattering data at different truncations of the maximum scattering energy $T_{\rm lab}^{\rm max}$, πN cross sections, the binding energies and charge radii of ^{2,3}H and ^{3}He, the one-body quadrupole moment of ^{2}H, as well as the comparative β-decay half-life of ^{3}H. The NNLOsim interactions have been refit [39] to account for the update in the c_D-$\hat{d}_R$ relation given in Eq. (4) [23], which enters the calculation of the ^{3}H GT matrix element fit to tritium β-decay. The resulting values of c_D for this model are roughly uniformly distributed between -2 and 2. We obtain 4.091×10^{-23} MeV fm^2 for the average $S(0)$ value for the refitted NNLOsim interactions. This is an upward revision, by about 1.1%, partly driven by the refitting of c_D but mainly by the change in the g_A value recommended by the PDG [35], from the result $S(0) = 4.047^{+0.024}_{-0.032} \times 10^{-23}$ MeV fm^2 obtained in Ref. [14], where the quoted uncertainty mainly reflected the sensitivity of the S-factor to input data used to calibrate the LECs of the EFT and to the short-distance behavior of the NN interactions. While a full reanalysis of the uncertainty estimates of Ref. [14] is beyond the scope of this work, we note that $S(0)$ spans the range $4.081{\times}10^{-23}$ to $4.095\ {\times}10^{-23}$ MeV fm^2 for the 42 interactions. Unlike Ref. [14], this range does not include the statistical fitting errors of the LECs. It is also instructive to compare the EFT truncation uncertainty obtained above using SMS-RS interaction to a similar estimate using one of the 42 interactions from the NNLOsim family. To this end, we choose the interaction with $T_{\rm lab}^{\rm max} = 290$ MeV and $\Lambda = 500$ MeV, and obtain 13.537×10^{-23}, 4.869×10^{-23} and 4.092×10^{-23} MeV fm^2 for $S(0)$ at LO, NLO and NNLO. Using the procedure discussed above to assess the EFT truncation error, we obtain $S(0) = (4.092 \pm 0.178(\text{syst})) \times 10^{-23}$ MeV fm^2. We note that this large uncertainty is a result of the LO value being rather large because the deuteron properties are not well reproduced by this interaction at this order. We therefore consider the estimate of the systematic EFT truncation error obtained from the SMS-RS interaction to be more reliable for this problem.

C. Model C: uncertainty in calibrating the axial contact current from few-body observables

An additional uncertainty that has not been included in the SMS-RS result quoted above, $S(0) = (4.100 \pm 0.019(\text{syst})) \times 10^{-23}$ MeV fm^2, is the uncertainty arising from the axial 2B contact current with $\hat{d}_R$ determined using Eq. (4). To estimate this, we consider the Bayesian posterior probability distribution function (PDF) of c_D-c_E obtained by Ref. [25]. In that study, as in the SMS-RS interaction, the πN LECs were fixed to central values determined by the Roy-Steiner analysis in Ref. [49]. The NN LECs at LO, NLO, and NNLO were then fixed by performing a new fit to the np and pp scattering data with $T_{\text{lab}}^{\text{max}} = 290$ MeV gathered from the Granada 2013 database [50] as well as the empirical nn effective range parameters. Constraints on c_D and c_E were obtained from fitting to binding energies of ^{3}H and ^{4}He, the charge radius of ^{4}He, and the GT matrix element of the ^{3}H extracted from tritium β-decay followed by marginalization of all other parameters with both the uncertainty of the chiral EFT Hamiltonian and the uncertainties in the experimental measurements taken into account. The experimental value of the ^{3}H β decay half life (1129.6 ± 3) s [55] adopted by Ref. [25] corresponds to our Fit-2 discussed below.

It was found that, at the older PDG value of $g_A = 1.2724$ [53], the joint PDF of c_D-c_E was well described by a multivariate t-distribution $t_\nu(m, S)$ with $\nu \approx 2.8$ degrees of freedom, a mean vector $m = [-0.0047, -0.1892]$ and a scale matrix of

$$S = \begin{bmatrix} 0.250 & 0.043 \\ 0.043 & 0.008 \end{bmatrix} \tag{6}$$

at one standard deviation (1σ). At least for the energy range considered in this work, $S(E)$ has approximately linear dependence on the values of c_D within the 1σ range for this joint PDF. The uncertainty on $S(E)$ can therefore be very well approximated by sampling c_D from its marginal t-distribution, which spans the approximate 1σ range $c_D \in [-0.615, 0.615]$, and computing $S(E)$ at the 1σ margins. This gives $S(0) = (4.155 \pm 0.013(\mathrm{stat})) \times 10^{-23}$ MeV fm^2. Here we used the label "stat" to indicate that this is an estimate of the statistical uncertainty from the c_D probability distribution. The rather large $S(0)$, in spite of the smaller value of 1.2724 adopted for g_A, is a result of slow convergence of the deuteron properties in this EFT expansion up through NNLO. This indicates that the fitting procedure adopted for this interaction results in large EFT truncation error even at NNLO for extreme low-energy observables. Nevertheless, we consider the quoted uncertainty from c_D variation to be a reasonable estimate of the uncertainty in $S(0)$ from fitting the two-body contact axial current to few-body observables.

D. Model D: updates to Idaho-N3LO results

We now turn our attention to the study of the *pp* fusion performed using the VM to calculate the deuteron and *pp* wave functions as in Ref. [13] from the Idaho-N3LO potential with $\Lambda = 500$ MeV [42]. With respect to Ref. [13], we have put particular attention to the convergence on the basis expansion for the deuteron wave function, and on the integration range used to calculate the transition operator matrix element. In particular, we have verified that not only the deuteron binding energy, but also the asymptotic normalization constants and the so-called D/S-state ratio $\eta = A_D/A_S$ are well reproduced. Furthermore, we have verified that the integral range of $r_{max} = 50$ fm is sufficient to reach convergence of the results. In fact, by going from $r_{max} = 50$ fm to $r_{max} = 60$ fm, the change in $S(0)$ is beyond the third decimal digit. Therefore, the results we are going to present are at convergence at least up to the the third decimal digit of $S(0)$. We note that such an accuracy was not the primary goal of the work of Ref. [13], where the results were obtained with a theoretical accuracy of the order of 1%.

In order to use the most recent values for the fundamental constants entering the calculations, we, first of all, update the value for the experimental GT matrix element in tritium β-decay $\langle GT_{exp}\rangle$. Note that $\langle GT_{exp}\rangle$ and the $A = 3$ binding energies were the observables of choice used to fix the LEC c_D, and consequently $\hat{d}_R$, and the LEC c_E, that parametrizes the three-nucleon contact interaction entering at NNLO (see, for instance, Ref. [27]). The

	$\langle GT_{exp}\rangle$	c_D
Fit-1	0.9488 ± 0.0019	0.1836–0.7680
Fit-2	0.9514 ± 0.0019	0.3830–0.9690
Fit-3	0.9501 ± 0.0024	0.2833–0.8685

TABLE III. Values for $\langle GT_{exp}\rangle$ as obtained using three different values for $ft_{^3\mathrm{H}}$, 1134.6 ± 3.1 s labelled Fit-1, 1129.6 ± 3 s labelled Fit-2, and 1132.1 ± 4.3 labelled Fit-3, respectively. The corresponding ranges for the LEC c_D obtained using the Idaho-N3LO potential with $\Lambda = 500$ MeV are also listed.

GT matrix element is defined as

$$\langle GT\rangle^2 = \left[\frac{2ft_{0^+\to 0^+}}{ft_{^3\mathrm{H}}} - \langle F\rangle^2\right]\frac{1}{f\,g_A^2}\ , \tag{7}$$

where g_A is the single-nucleon axial coupling constant, $f = f_A/f_V = 1.00529$ is the ratio of the axial and vector Fermi functions, $ft_{^3\mathrm{H}}$ and $ft_{0^+\to 0^+}$ are the ft-values for tritium β-decay and for superallowed $0^+ \to 0^+$ transitions. From $\langle GT\rangle$, we define $\langle GT_{exp}\rangle$ as $\langle GT_{exp}\rangle = \langle GT\rangle/\sqrt{3}$. With this definition, $\langle GT_{exp}\rangle$ is related to the reduced matrix element of the electric dipole axial operator E_1 used in Refs. [25, 33] via the relation $\langle GT_{exp}\rangle = \sqrt{\pi}E_1/g_A$. In the present calculation, we have used $g_A = 1.2754 \pm 0.0013$, according to the PDG, and $ft_{0^+\to 0^+} = (3072.24 \pm 1.85)$ s, according to Ref. [30]. This value is consistent with the value of G_V used in Eq. (3). Furthermore, we have used $\langle F\rangle^2 = 0.99967$, as it was obtained in Refs. [27] with the Idaho-N3LO potentials. This value is quite different from the one obtained using the phenomenological AV18/UIX interaction model, and used for instance in Ref. [9], $\langle F\rangle^2 = 0.9987$. However, we have verified that the impact on $\langle GT_{exp}\rangle$ of this different $\langle F\rangle^2$ is negligible. Finally, we have adopted for $ft_{^3\mathrm{H}}$ three different values: (1134.6 ± 3.1) s as obtained in Ref. [54], (1129.6 ± 3) s as obtained in Ref. [55] and adopted by Model C above, and (1132.1 ± 4.3) s as used already in Ref. [27] and obtained averaging these two values and summing the errors in quadrature. The $\langle GT_{exp}\rangle$ obtained with these three values for $ft_{^3\mathrm{H}}$ will be labelled Fit-1, Fit-2 and Fit-3, respectively. The three values for $\langle GT_{exp}\rangle$, together with their uncertainties arising from the experimental errors on g_A, $ft_{0^+\to 0^+}$ and $ft_{^3\mathrm{H}}$, are listed in Table III. In the table, we report also the corresponding ranges for c_D obtained, as mentioned above, with the fitting procedure of Ref. [27]. With the new values for the LEC c_D, or equivalently $\hat{d}_R$, we present in Table IV the results

	Method	$1/m_N^2$ currents	$S(0)$	$S'(0)/S(0)$	$S''(0)/S(0)$	$S'''(0)/S(0)$
Fit-1	VM	included	4.115(4)	10.60	347.1	-6908
	LS	excluded	4.101(4)	10.83	313.8	-5382
Fit-2	VM	included	4.118(4)	10.60	347.1	-6907
	LS	excluded	4.104(4)	10.83	313.8	-5381
Fit-3	VM	included	4.117(4)	10.60	347.1	-6908
	LS	excluded	4.104(4)	10.83	313.8	-5382

TABLE IV. Values for the zero-energy astrophysical S-factor $S(0)$ (in 10^{-23} MeV fm^2), its first, second and third derivatives $S'(0)/S(0)$ (in MeV^{-1}), $S''(0)/S(0)$ (in MeV^{-2}) and $S'''(0)/S(0)$ (in MeV^{-3}) obtained with the Idaho-N3LO potential with $\Lambda = 500$ MeV, using the variational method (VM) of Ref. [13], or the Lippmann-Schwinger (LS) equation as in Ref. [14]. The results labelled Fit-1, Fit-2, and Fit-3 are obtained consistently with the values of c_D listed in Table III. The numbers in parentheses are the theoretical error arising from the range of c_D values allowed for each fitting procedure. For $S'(0)/S(0)$ these errors are beyond the quoted digits.

for the zero-energy astrophysical S-factor $S(0)$, and its first, second and third derivatives, $S'(0)/S(0)$, $S''(0)/S(0)$ and $S'''(0)/S(0)$. We list in the table also the results obtained with the same constants and the same potential using the LS equation and the axial current of Ref. [14]. By inspecting the values in the table, we can conclude that (i) the VM and LS calculations are in very good agreement as the small differences are consistent with the anticipated size of the relativistic corrections to the GT 1B operator which were neglected in the LS calculations but were retained in the VM calculations; (ii) the dependence on the adopted value for $ft_{^3\mathrm{H}}$ is very weak; (iii) the theoretical uncertainty arising from the range of c_D values allowed for each fitting procedure, and therefore ultimately related to the experimental error on $\langle GT_{exp}\rangle$, is extremely small for $S(0)$ and $S''(0)/S(0)$, and beyond the second decimal digit for $S'(0)/S(0)$; (iv) the calculated $S(0)$ is in excellent agreement with the $S(0)$ value obtained with the SMS-RS and NNLOsim interactions. (v) The value for $S(0)$ is $\sim 2.2\%$ larger than the value of Ref. [13]. The difference arises from the improved convergence of the nuclear wave functions adopted in this work, as well as from the increased values for the single-nucleon axial coupling constant g_A.

IV. SUMMARY AND OUTLOOK

We calculated the proton-proton fusion rate using various chiral interactions: the Idaho-N3LO interaction at regulator cutoff of 500 MeV [42], the NNLOsim family of 42 interactions fit at 7 different regulator cutoffs to 6 different pools of input data, and two additional sets of interactions—one non-local [25] and another "semi-local" [24]—in which the pion-nucleon coupling constants are fixed to precise values determined from Roy-Steiner analysis. We obtained an estimate for the uncertainty from the truncation of the EFT expansion and also assessed the uncertainty from fixing the LEC $\hat{d}_R$ in the two-body axial current using c_D fitted to $A \geq 3$ data. Furthermore, by using the Idaho-N3LO potential, we have performed a benchmark calculation between the two different approaches first applied to the pp reaction in Refs. [13] and [14]. We have used recent values of the fundamental constants and have used the corrected relationship between the axial current LEC $\hat{d}_R$ and the three-body force parameter c_D.

The threshold S-factor $S(0)$ obtained from the various EFT interactions indicate an upward revision from the recommendation made by Ref. [2]. It is remarkable that the S-factor value obtained using the SMS-RS interactions [24] is in excellent agreement with the NNLOsim result although its c_D value was obtained without fitting to electroweak data. We also show that variation in c_D within the 68% Bayesian credible interval obtained from the joint $c_D - c_E$ distribution calculated in Ref. [25] translates to an uncertainty of 0.013 MeV fm^2 in $S(0)$, which is smaller than the uncertainty of 0.019 MeV fm^2 stemming from the truncation of the chiral expansion in the SMS-RS potential. We do note, however, that the potential of Ref. [25] underbinds the deuteron at all orders (by about 75% at LO, 15% at NLO and 1% at NNLO) which causes $S(E)$ to be overpredicted, even with just one-body current. We encounter this issue also at LO and NLO in the NNLOsim interactions, which again impacts the extraction of truncation error. This highlights the importance of ensuring that the low-energy properties of the NN system, e.g. the binding energy and the asymptotic normalization coefficient of the deuteron, are reasonably well reproduced while fitting the LECs of chiral EFT. Given the difficulty in assessing the truncation error of the EFT expansion due to slow order-by-order convergence in the non-local chiral interactions used in this work, we consider the central value obtained using the SMS-RS interaction to be more reliable and the corresponding truncation error estimate to be better calibrated.

Combining the systematic EFT truncation error with the statistical uncertainty that arises from the PDF of c_D and the range obtained by varying g_A within the PDG recommendation of 1.2754 ± 0.0013, we recommend

$$S(0) = (4.100 \pm 0.024(\mathrm{syst}) \pm 0.013(\mathrm{stat}) \pm 0.008(g_A)) \times 10^{-23}\ \mathrm{MeV\,fm}^2\,. \tag{8}$$

Note that this value is consistent with the ones obtained using the NNLOsim and Idaho-N3LO interactions, and with the value $S(0) = (4.14 \pm 0.01 \pm 0.005 \pm 0.06) \times 10^{-23}$ MeV fm^2 recently obtained by De-Leon and Gazit in Pionless EFT [19]. Furthermore, we find with the SMS-RS potential $S'(0)/S(0)$ and $S''(0)/S(0)$ values of 10.83 MeV^{-1} and 313.72 MeV^{-2}, respectively. The values of these energy derivatives of $S(E)$ depend on the interaction used, calculation method and degree of the fitted polynomial. We refrain from performing a detailed analysis of uncertainties for them as they are not relevant at currently achievable precision in the energy range of interest for solar conditions.

Finally, we would like to remark that the S-factor is not accurately predicted by the chiral EFT interactions of Refs. [25, 36] at low chiral orders if the deuteron bound-state properties are not adequately reproduced. This highlights the importance of calibrating the interactions by fitting to experimental data using strategies that also lead to systematic convergence pattern for very low-energy observables such as *pp* fusion at solar conditions. Bayesian model mixing between chiral and pionless EFT to ensure that the deuteron and the *pp* effective-range parameters are well reproduced appears to be a promising strategy for reliably predicting solar *pp* fusion rate. Furthermore, we believe that a thorough study of the *pp* fusion reaction should be performed using the largest possible variety of chiral EFT interactions, local or non-local, regularized in co-ordinate or momentum space, with or without the inclusion of Δ-isobar degrees of freedom, possibly available a different chiral orders, as, for instance, those of Refs. [47, 56–58]. Such a study is beyond the scope of this work, but is definitely highly recommended. Work along this line, on the footsteps of Refs. [59, 60], is currently underway.

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