Complex-energy analysis of the proton-proton fusion

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(Dated: February 7, 2019)

A novel analysis of the astrophysical $S$ factor of the proton-proton weak capture ($p + p \rightarrow ^2\text{H} + e^+ + \nu_e$) is performed on a large energy range covering solar-core and early Universe temperatures. The measurement of $S$ being physically unachievable, its value relies on the theoretical calculation of the matrix element $\Lambda$. Surprisingly, $\Lambda$ reaches a maximum near 0.13 MeV that has been unexplained until now. To address this issue, a model-independent parametrization of $\Lambda$ valid up to about 5 MeV is established on the basis of recent effective-range functions. It provides an insight into the relationship between the maximum of $\Lambda$ and the proton-proton resonance pole at $(-140 - 467)\text{ keV}$ from analytic continuation. In addition, this parametrization leads to an accurate evaluation of the derivatives of $\Lambda$, and hence of $S$, at zero energy. These derivatives are crucial for stellar nucleosynthesis.

The proton-proton fusion reaction ($p + p \rightarrow ^2\text{H} + e^+ + \nu_e$), also known as the proton-proton weak capture, is a fundamental process in nuclear astrophysics. It is the starting point of the proton-proton chain for stellar nucleosynthesis in hydrogen-burning stars. It also determines the deuterium abundance in the early Universe. Its cross section $\sigma(E)$ is usually expressed in terms of the astrophysical factor $S(E)$ at the two-proton center-of-mass energy $E$. Unfortunately, this cross section is so small at typical astrophysical temperature ($E \lesssim 0.01 \text{ MeV}$), that a reliable measurement cannot be achieved with enough statistics, even above the Coulomb barrier (about 0.2 MeV). A theoretical prediction of $S$ is therefore required.

The first calculation of $S$ at zero energy was proposed by Bethe and Critchfield [1]. They also introduced the dimensionless weak capture matrix element $\Lambda$ at zero angular momentum from which $S$ is deduced. Thereafter, the accuracy of $S(0)$ was improved by Salpeter [2] and Bahcall and his coworkers [3] using effective-range theory. In the 1990s, several authors calculated $S(0)$ from the nucleon-nucleon wave functions computed in potential models [4, 5]. More recently, systematic computations of $S(0)$ were performed in pionless effective field theory from next-to-leading order (NLO) of the momentum expansion [6, 7] up to N$^4$LO [8]. In parallel, efforts were made in chiral effective field theory to reduce the uncertainty on $S(0)$ by adding two-body corrections to the Gamow-Teller operator adjusted with data for tritium $\beta$-decay [9–13]. As the uncertainty on $S(0)$ has diminished since early works, the small contribution of its energy derivatives $S'(0)$ and $S''(0)$ has become important for stellar astrophysics [12, 14–16]. In this regard, Adelberger et al. recommended a calculation of $S''(0)$ to be undertaken [14].

The calculation of these derivatives raises the question of whether the matrix element $\Lambda$ is analytic in the neighborhood of zero energy. Such an analysis of $\Lambda$ is still missing in the literature. Yet, some peculiarities of the proton-proton scattering are known. In 1980, Kok highlighted the presence of a sub-threshold resonance pole at about $(-140 - 467)\text{ keV}$ in the $^1S_0$ channel [17]. Up to a complex phase, this pole lies in an energy range corresponding to early Universe temperatures below the nucleosynthesis freeze-out point ($E \lesssim 1 \text{ MeV}$) [18]. In addition, the derivatives of $\Lambda$ are likely to be affected by the relative closeness of this pole. The purpose of this work is to determine a novel model-independent parametrization of $\Lambda$, valid on a large energy range, and able to impose constraints on its series expansion at $E = 0$. The parametrization must also describe the pole at $(-140 - 467)\text{ keV}$. To do so, we resort to a recently introduced effective-range function (ERF), namely the $\Delta$ function [19–21], which has only been considered useful for heavier systems until now [22]. This approach is motivated by the efficiency of the ERWs at describing the energy-dependent shape of the proton-proton wave function up to a few MeVs. Finally, we verify our results with the nucleon-nucleon wave functions computed in different potential models, namely Av18 [23], Reid93 [24], and NijmBF [24].

In the present context, it is convenient to define the astrophysical factor as $S(E) = (e^{2\pi\eta} - 1)E\sigma(E)$ [25] where $\eta = 1/(a_Bk)$ is the Sommerfeld parameter, $a_B = \hbar c/(am_n c^2/2) = 57.6398 \text{ fm}$ the proton-proton Bohr radius, and $k$ the wave number corresponding to $E$. After integrating out the emitted leptons, the astrophysical factor as

$S(E) = \frac{12m_n c^2 (\lambda g)^2}{\pi a_B b^3} F(E + Q)|\Lambda(E)|^2 , \hspace{1cm} (1)$

where $\lambda = 1.2724(23)$ is the weak axial/vector ratio, $g = G_F |V_{ud}| (m_n c^2)^2/(\hbar c)^3 = 2.96707(64) \cdot 10^{-12}$ is the dimensionless weak coupling constant for neutrons, $G_F$ is the Fermi constant of muon decay, and $V_{ud}$ is the first element of the CKM quark mixing matrix [18]. The other constants are the deuteron binding wave number $b = \sqrt{2m_{\text{pn}} B_d}/\hbar = 0.231606 \text{ fm}^{-1}$ [3, 14], the
proton-neutron reduced mass \( m_{pn} = m_p m_n / (m_p + m_n) \), and the deuteron binding energy \( B_d = 2.22457 \) MeV. All the fundamental constants are taken from Ref. [18]. The currently recommended value of \( S(0) \) is \( 4.01(4) \cdot 10^{-23} \) MeV fm\(^2\) [14].

The function \( F \) is the Fermi phase-space integral which accounts for the electric repulsion of the emitted positron in a relativistic framework. It also depends on the released energy \( Q = 2m_p c^2 - m_d c^2 - m_e c^2 = 0.42036(17) \) MeV. The expression of \( F \) is extensively discussed in Refs. [27–29], and accurate numerical values are given in the Supplemental Material [25]. This function globally increases as \( \mathcal{O}(E^2) \), so that it dominates the \( \mathcal{O}(E^{-2}) \) behavior of \( \Lambda^2 \).

Lastly, the dimensionless matrix element \( \Lambda(E) \) in Eq. (1) is defined as [2, 3]

\[
\Lambda(E) = \frac{a_B b^{3/2}}{\sqrt{8}} \frac{2\eta}{C_{\eta,0}} \int_0^\infty u_{d,0}(r) u_{pp,0}(E, r) \, dr ,
\]

where \( C_{\eta,0} = \sqrt{2\pi \eta / (\eta^2 \pi - 1)} \) is the Coulomb normalization coefficient. The functions \( u_{d,0} \) and \( u_{pp,0} \) are the radial S-wave \( (\ell = 0) \) components of the deuteron and the proton-proton wave functions, respectively. The contribution from higher-order partial waves can be neglected in the low-energy approximation.

Most of the energy dependence in Eq. (2) comes from the proton-proton wave function \( u_{pp} \). This function is normalized such that it tends to a sine wave of unit amplitude for \( r \to \infty \). This asymptotic regime is already reached for \( r \gtrsim 2 \) fm. Since the spatial extent of the deuteron is much larger than 2 fm, it is relevant [2, 3] to calculate (2) with the asymptotic behavior [25]

\[
u_{pp,0}(r) \xrightarrow{r \to \infty} \frac{C_{\eta,0}}{2\eta} \frac{a_B}{|\Delta_{0}^{+}(E)|} \left( \frac{\kappa_0}{2} \Phi_{0\eta,0} + \Psi_{0\eta,0} \right) .
\]

The functions \( \Phi_{0\eta,\ell} \) and \( \Psi_{0\eta,\ell} \) are the modified Coulomb functions recently introduced in Ref. [30]. In contrast to the standard functions \( F_{0\eta,\ell} \) and \( G_{0\eta,\ell} \), they are free of singularity at zero energy. This property is crucial in the analysis of \( \Lambda \) at complex energy, especially near \( E = 0 \). In Eq. (3), \( \kappa_0 \) is the standard ERF of the proton-proton \( ^1S_0 \) scattering. Its first-order expansion in \( E \) provides an accurate parametrization of the phase shift \( \delta_0 \) at relatively low energy \( (E \lesssim 5 \text{ MeV}) \)

\[
kappa_0(E) = \frac{2}{a_B} \left( \pi \cot \delta_0 / e^{2\pi \eta} - 1 \right) + g_0 \simeq \frac{-1}{a_B} + \frac{r_0 m_p}{2 \hbar^2} E ,
\]

where \( g_0 = [\psi(i\eta) + \psi(-i\eta)] / 2 \ln \eta \) is the Bethe function and \( \psi(z) = \Gamma'(z) / \Gamma(z) \) [20, 31]. The parameters \( a_0 \) and \( r_0 \) are respectively the scattering length and the effective range. The modulus of the modified ERF \( \Delta_0^{+} \) [20, 32] also appears in Eq. (3). This phase-shift-dependent function is related to \( \kappa_0 \) by

\[
\Delta_0^{+}(E) = \left( \frac{a_B}{2} \kappa_0 - g_0 \right) - \frac{i\pi}{e^{2\pi \eta} - 1} ,
\]

However, in contrast to \( \kappa_0 \), the function \( \Delta_0^{+} \) is singular at \( E = 0 \) mostly because of \( g_0 \). The bracket in Eq. (5) is also called the \( \Delta_0 \) function in Ref. [20]. All these ERFs are depicted in Fig. 1.

FIG. 1. Effective-range functions of the proton-proton \(^1S_0\) scattering for the Reid93 potential [24]. The other potential models provide very close curves at this scale.

Since \( u_{d,0}(r) \) asymptotically behaves as \( A e^{-b r} \) for \( r \gtrsim 2 \) fm, the integral (2) approximately reduces to the Laplace transforms of \( \Phi_{0\eta,0} \) and \( \Psi_{0\eta,0} \). Using \( x = br \), the Laplace transform of \( \Phi_{0\eta,0} \) is exactly given by [25]

\[
\phi_0(\epsilon) = \int_0^\infty e^{-x} \Phi_{0\eta,0}(x\sqrt{\epsilon}) \, dx = \frac{\epsilon \exp(|\arctan \sqrt{\epsilon}|)}{1 + \epsilon} ,
\]

where \( \epsilon = k^2 / b^2 = E / B \) is the reduced proton energy, and \( B = 2m_p B_d / m_n \) is the deuteron binding energy corrected for the neutron-proton mass difference. The dimensionless constant \( \chi = 2 / (a_B b) = 0.149816 \) in Eq. (6) is due to Bahcall and May [3].

The Laplace transform of \( \Psi_{0\eta,0} \) cannot be obtained in a simple form. However, it can be shown that, as far as \( \chi \) is small before 1, the following approximation holds for \( E \lesssim 5 \) MeV [25]

\[
\psi_0(\epsilon) \simeq \int_0^\infty e^{-x} \Psi_{0\eta,0}(x\sqrt{\epsilon}) \, dx \simeq \gamma \phi_0(\epsilon) ,
\]

where \( \gamma = \Gamma(-1, \chi) = 4.28065 \) and \( \Gamma(a, z) \) denotes the upper incomplete gamma function. Therefore, combining Eqs. (3), (6), and (7) into Eq. (2), we get

\[
\Lambda(E) = \frac{\exp(|\arctan \sqrt{\epsilon}|)}{|\Delta_0^{+}(E)| (1 + \epsilon)} L(\epsilon) ,
\]

where we have introduced the function \( L \) that is expected to be a quasi-linear function of the energy, as it is related to \( \kappa_0 \) [25]. However, Eq. (3) does not describe the short-range deformation of the wave functions due to the
nuclear potential. Nevertheless, even when accounting for this short-range behavior, $L$ remains a quasi-linear function, as shown in Fig. 2 and further discussed in the Supplemental Material [23]. From the linear fitting of $L$ on $[300, 600]$ keV in the potential models, we get

$$L(\epsilon) = L_0 + L_1 \epsilon = 8.42(1) + 0.55(1) \epsilon .$$  

(9)

The uncertainties are due to the discrepancy between the potential models. The function $L$ of Eq. (9) is compared to the results from potential models in Fig. 2. The actual curve of $L$ deviates from a straight line because of the short-range behavior of the wave functions. Despite this deviation, it turns out that $L$ is accurate by less than 2% error below 5 MeV, and is especially good below 1 MeV. This adequacy confirms the validity of the parametrization (8).

The matrix element $\Lambda$ computed in the Reid93 potential is depicted in Fig. 3. The curves obtained in other potentials, along with the result (8), are indistinguishable at this scale. These curves are quite rarely shown in the literature [33]. At zero energy, we find the important value for stellar nucleosynthesis $\Lambda^2(0) = 7.034(33)$, which is consistent with Ref. [14] but limited to potential models. Using Eq. (1) and the numerical value $F(Q) = 0.14215(2)$ from [29] plus 1.62% to account for radiative corrections [12–15, 29], the corresponding value of $S(0)$ is $3.95(3) \times 10^{-23}$ MeV fm$^2$.

Remarkably, $\Lambda$ reaches a maximum near 130 keV, that corresponds, through Eq. (8), to the minimum of $|\Delta^+_0|$ seen in Fig. 1. The actual origin of this maximum is revealed by the continuation of $\Lambda$ to complex energies, as provided by Eq. (8). The analytic continuation of $\Lambda^2$ based on Eqs. (8) and (9) is shown in Figs. 4 and 5. Note that the curve along the positive real semi-axis in Fig. 4 corresponds to Fig. 3. The deuteron bound state pole in Fig. 4 is due to $(1 + \epsilon)^{-1}$ in Eq. (8).

Furthermore, in contrast to $\Lambda$, the function $L$ is holomorphic in the neighborhood of $E = 0$, because of the properties of the modified Coulomb functions $\Psi_{3/2, 0}$ and $\Psi_{1/2, 0}$ in the limit $E \to 0$ [20, 30]. Therefore, it follows from Eq. (8) that any singularity of $|\Delta^+_0|^{-1}$ is reflected on $\Lambda$. In this regard, it can be shown that $|\Delta^+_0|^{-1}$ has two poles at $(-140 \pm 467i)$ keV, that are interpreted as the proton-proton $1S_0$ resonance poles [17, 20]. In Fig. 4, only one of them is visible because the plot is restricted to the upper half-plane ($\text{Im} E \geq 0$).

The function $|\Delta^+_0|^{-1}$ also possesses a branch cut along the negative real semi-axis due to the logarithm in the Bethe function $g_0$ in Eq. (5). Being on the boundary of the plots, the branch cut cannot be seen either in Figs. 4 or 5. More detailed top views are given in the Supplemental Material [25].

In addition, $|\Delta^+_0|^{-1}$ is responsible for the accumulation of poles and zeros shown in Fig. 5. These singularities originate from the terms $\psi(\pm in)$ in the Bethe function $g_0$. The pole-zero pattern is repeated each $E = -\text{Ry} / n^2$ for $n = 1, 2, 3, \ldots$, where $\text{Ry} = a^2 m_p c^2 / 4 = 12.4911$ keV denotes the nuclear Rydberg energy of the proton-proton system. Such a structure can be understood as a set of virtual states generated by the Coulomb potential between the protons.

These considerations about the analytic properties of $\Lambda$ have two major consequences. First, the maximum of $\Lambda$ is directly related to the Coulomb potential. Especially, one sees in Fig. 4 that it results from a saddle point between the conjugated resonance poles and the low-energy Coulomb singularities.

Second, $\Lambda$ is not analytic at $E = 0$ due to $\Delta^+_0$ in Eq. (8). Therefore, its series expansion is not expected.
to converge over a nonzero energy range around $E = 0$. The common way of extracting the derivatives of $\Lambda$ would be to use polynomial extrapolation from data on a finite energy interval. However, such a method is not accurate due to the non-negligible influence of the interval itself [12, 16].

One way to address this issue is to expand $\Lambda$ in power series directly from Eq. (8) taking advantage of the flatness of $L$ at low energy. Using Eq. (8) and the asymptotic expansion of the Bethe function $g_0$ [17, 20], we find that the logarithmic derivative of $\Lambda$ at $E = 0$ mostly depends on the effective-range parameters

$$\frac{\Lambda'(0)}{\Lambda(0)} = \frac{|\alpha_0|}{2\hbar^2} \left( \frac{a_B}{3} - r_0 \right) - \frac{3 + \chi}{3B} + \frac{L_1}{BL_0}.$$  

The prime over $\Lambda$ refers to the derivative with respect to $E$. This novel result was not obtained by Bahcall and May, although its numerical value is given in their paper [3]. From the effective range $r_0 = 2.77(1)$ fm computed in different potential models [23, 24], and from $L_0$ and $L_1$ in Eq. (9), the result (10) yields

$$\Lambda'(0) = \frac{1.106(2)}{\text{MeV}} + \frac{0.1981(1)}{\text{MeV}} \left( |\alpha_0| - 7.815 \text{ fm} \right),$$  

around the scattering length $\alpha_0 = -7.815(9)$ fm. The central value $1.106(3)$ MeV$^{-1}$ is compatible with Refs. [3, 15].

It turns out that the term $L_1/L_0$ in Eq. (10), which contains the short-range behavior of the wave functions, only contributes to about 2.6%. Therefore, the uncertainty of $L_1/L_0$ marginally affects the overall uncertainty of $\Lambda'(0)/\Lambda(0)$, which is primarily due to the effective-range parameters $\alpha_0$ and $r_0$.

It is worth noting that Eq. (8) now determines all the derivatives of $\Lambda$ at $E = 0$. Indeed, the higher-order derivatives of $L$ are negligible in the expansion of $\Lambda$ compared to the other terms. The reason is that the derivatives of $\Lambda$ are dominated by $\Delta_0$. In particular, the second derivative of $\Lambda$ can also be calculated analytically from Eq. (8), as shown in [25]. We have approximately

$$\Lambda''(0) = \frac{32.795(6)}{\text{MeV}^2} + \frac{4.758(2)}{\text{MeV}^2} \left( |\alpha_0| - 7.815 \text{ fm} \right).$$  

The central value $32.80(5)$ MeV$^{-2}$ is in accordance with Ref. [15]. The uncertainty on $\Lambda''(0)/\Lambda(0)$ is mainly due to $\alpha_0 = -7.815(9)$ fm. Similar effective-range constraints can be derived for higher-order derivatives of $\Lambda$ from Eq. (8) using the asymptotic expansion of $\Delta_0$ and $g_0$ [20]. The expected accuracy of this approach does not exceed about 0.2% as it is limited by the uncertainty on $\alpha_0$.

Finally, we deduce the zero-energy derivatives of the astrophysical $S$ factor from Eqs. (11) and (12). Using the numerical values of the Fermi phase-space integral given in [25], we find

$$\frac{S'(0)}{S(0)} = \frac{11.253(3)}{\text{MeV}} + \frac{0.3962(2)}{\text{MeV}} \left( |\alpha_0| - 7.815 \text{ fm} \right),$$  

$$\frac{S''(0)}{S(0)} = \frac{169.51(8)}{\text{MeV}^2} + \frac{17.56(1)}{\text{MeV}^2} \left( |\alpha_0| - 7.815 \text{ fm} \right).$$  

The central values $11.25(1)$ MeV$^{-1}$ and $169.5(3)$ MeV$^{-2}$ are compatible with Refs. [3, 12, 15, 26, 34]. These results are obtained with an unprecedentedly high accuracy. In the literature, most of the uncertainties are due to the polynomial extrapolation of $S(E)$ which is highly sensitive to the chosen energy interval [12, 16]. Our method is based instead on the fitting of $L$, as suggested by the analytic structure of $\Lambda$ at low energy. Consequently, the results (13) are not affected by the uncertainty of $S(0)$.

To conclude, we have derived an accurate parametrization of the energy dependence of the weak capture matrix.
element $\Lambda$ valid up to a few MeVs, that is based on recent effective-range functions [19, 20]. This result provides the analytic continuation of $\Lambda$ to complex energies, and highlights the relationship between its maximum near 0.13 MeV, the broad proton-proton resonance, and the Coulomb sub-threshold singularities. In addition, it leads to a remarkably accurate determination of the logarithmic derivatives of the astrophysical $S$ factor at $E = 0$ in terms of effective-range parameters. Our method bypasses the issue of the energy-range dependence in the polynomial fitting of $S$ by means of the function $L$ that is analytic at low energy. Finally, the new parametrization (8) is appropriate for use in stellar and Big-Bang astrophysics as it covers a large energy range up to the binding energy of the deuteron.

This work was supported by the European Union’s Horizon 2020 (Excellent Science) research and innovation program under Grant Agreement No. 654002.

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SUPPLEMENTAL MATERIAL: COMPLEX-ENERGY ANALYSIS OF THE PROTON-PROTON FUSION

Astrophysical S factor

Before detailing the calculations, we first want to add some comments on the actual definition of the astrophysical S factor used in this paper. For this purpose, we start from the cross section \( \sigma(E) \) found in the framework of proton-proton weak capture [2, 3]

\[
\sigma(E) = \frac{3m_ec^2(\lambda g)^2}{\pi^2E_k} F(E + Q) \int_0^\infty u_d(r) u_{pp}(E, r) \, dr^2,
\]

(14)

where \( k = \sqrt{m_pE}/h \) the proton-proton wave number, \( u_d \) and \( u_{pp} \) are the S-wave components of the deuteron and proton-proton wave functions respectively, and the other notations are the same as in the main text. It turns out that the overlap integral in Eq. (14) vanishes in the zero energy limit \( (E \to 0) \). This vanishing behavior originates from the cancellation of the proton-proton radial wave function \( u_{pp} \) at \( E = 0 \) due to the Coulomb barrier. We will explain more on this cancellation later. This behavior can be factored out of the overlap integral in defining the matrix element \( \Lambda(E) \) as

\[
\left| \int_0^\infty u_d(r) u_{pp}(E, r) \, dr \right|^2 = \frac{2k^2}{b^2} |C_{\eta,0}|^2 |\Lambda(E)|^2 ,
\]

(15)

where \( |C_{\eta,0}|^2 = 2\pi\eta/(e^{2\pi\eta} - 1) \) is the Coulomb normalization coefficient, and \( \eta = 1/(abk) \) is the Sommerfeld parameter. In contrast to the overlap integral, \( \Lambda(E) \) has a finite limit at \( E = 0 \). In this way, the cross section (14) becomes after some simplifications

\[
\sigma(E) = \frac{1}{(e^{2\pi\eta} - 1)E} \frac{12m_ec^2(\lambda g)^2}{\pi a_Bb^3} F(E + Q) |\Lambda(E)|^2 .
\]

(16)

This expression (16) undoubtedly suggests the most natural definition of the astrophysical S factor, that is

\[
S(E) = (e^{2\pi\eta} - 1) E \sigma(E) .
\]

(17)

This definition (17) of \( S \) is assumed in this work. Strictly speaking, the definition (17) does not reduce to the original definition due to Salpeter [2]

\[
S_{std}(E) = e^{2\pi\eta} E \sigma(E) ,
\]

(18)

and nowadays considered as standard in stellar astrophysics. This subtlety is not mentioned in Bahcall’s and May’s paper [3]. In Sec. II of their paper, they obtained the same \( S \) as in this work, which assumes Eq. (17), even though they actually defined \( S \) by Eq. (18).

On the other hand, at sufficiently low energy, the definitions (17) and (18) coincide. We notice indeed that the approximation \( e^{2\pi\eta} - 1 \simeq e^{2\pi\eta} \) is valid by less than 1% for

\[
E \leq \left( \frac{2\pi}{\ln(100)} \right)^2 \text{Ry} \simeq 1.86 \text{ Ry} ,
\]

(19)

where Ry is the nuclear Rydberg energy which is equal to \( \alpha^2m_ec^2/4 = 12.4911 \text{ keV} \) in the proton-proton system. Since we consider energies much higher than the Rydberg energy in this work, the definition (17) is preferred. Thus, we understand Eq. (18) as the low-energy approximation of the definition (17).

Finally, it should be noted that the definition (17) does not affect any of the values \( S(0) \), \( S'(0) \), and \( S''(0) \) presented in the main text compared to \( S_{std} \). Indeed, the relative error between the two definitions

\[
\frac{S_{std} - S}{S_{std}} = e^{-2\pi\eta} ,
\]

(20)

displays an essential singularity at \( E = 0 \) which cancels all its derivatives in the limit \( E \to 0 \). Therefore, the derivatives of \( S \) at \( E = 0 \) obtained in this work are necessarily equal to the derivatives of \( S_{std} \) at \( E = 0 \).

Fermi phase-space integral

When calculating the proton-proton weak capture cross section, we are led to integrate the Dirac delta of energy-momentum conservation over the momenta of the three outgoing particles: the deuteron, the positron, and the electronic neutrino. The resulting integral is known as the Fermi phase-space integral and reads [15, 27, 28]

\[
F(E + Q) = \int_1^\infty \bar{P}(w) \sqrt{w^2 - 1} (\bar{w} - w)^2 \, dw ,
\]

(21)

as long as the recoil of the deuteron is neglected. The released energy \( Q = 2m_pc^2 - m_dc^2 - m_ec^2 \) is found to be 0.420236(17) MeV with the masses from Ref. [18]. The variable \( w \) in Eq. (21) is the positron energy divided by its mass. With this notation, \( \sqrt{w^2 - 1} \) is to be understood as the positron momentum divided by its mass. From energy conservation, the upper bound denoted as \( \bar{w} \) is equal to \( (E + Q + m_ec^2)/(m_e c^2) \). It means that the Fermi integral \( F \) also depends on the proton-proton energy \( E \). The purpose of this section is to calculate the low-energy dependence of \( F \) on \( E \).

The Coulomb factor \( P \) in Eq. (21), accounting for the distortion of the positron wave function in the electric field of the deuteron, is given by [15, 27, 28]

\[
P(w) = 2(1 + \nu) \left( 2\rho\sqrt{w^2 - 1} \right)^{-2(1-\nu)} \frac{|\Gamma(\nu + i\eta_c)|^2}{e^{\pi\eta_c}\Gamma(2\nu + 1)^2} ,
\]

(22)
where $\nu$ is equal to $\sqrt{1 - \alpha^2}$ with the fine-structure constant $\alpha \simeq 1/137.036$, and $\rho = R \alpha m_e^2/(\hbar c)$ is the dimensionless radius of the deuteron. In the following calculations, we will assume $R = 2.14$ fm [15]. In Eq. (22), the Sommerfeld parameter of the emitted positron $\eta_e = \alpha \omega/\sqrt{w^2 - 1}$ must be positive, as it is repelled by the nucleus. Conversely, in a $\beta^-$ decay, the Sommerfeld parameter $\eta$ should take a minus sign. It should be noted that in the nonrelativistic limit ($\nu = 1$), the Coulomb distortion factor $P(w)$ becomes

$$P(w) = |C_{\eta, 0}|^2 = \frac{2\pi \eta_c}{e^{2\pi \eta - 1}}.$$

(23)

The Fermi integral (21) cannot be analytically calculated in a simple form. However, very efficient approximations exist. One way is to expand the Coulomb factor (22) in series of the fine-structure constant $\alpha$. We find

$$P(w) = 1 - \frac{\alpha \pi w}{\sqrt{w^2 - 1}} + \alpha^2 \left[ \frac{\pi^2}{3} \left( \frac{w}{\sqrt{w^2 - 1}} \right)^2 \right.$$

$$\left. + \frac{11}{4} - \gamma - \ln(2\rho) \right] + O(\alpha^3),$$

where $\gamma = 0.5772\ldots$ is the Euler-Mascheroni constant. In this work, we limit ourselves to the order $\alpha^2$, as it is enough to obtain at least five decimal places in the final results. The same approach is followed in Ref. [28] up to $\alpha^3$. Now, we just have to calculate one Fermi integral for each term in the expansion (24). The advantage is that the integrals of the form

$$f_p(\bar{w}) = \int_1^{\bar{w}} \left( \frac{w}{\sqrt{w^2 - 1}} \right)^p \frac{w}{\sqrt{w^2 - 1}} (\bar{w} - w)^2 \, dw,$$

(25)

which will come into play, can be expressed in terms of elementary functions for $p \in \mathbb{Z}$. Such expressions can be obtained by expanding the last factor $(\bar{w} - w)^2$ in Eq. (25). The results read for $p = 0$

$$f_0(\bar{w}) = \left( \frac{\bar{w}^4}{30} - \frac{3\bar{w}^2}{20} - \frac{2}{15} \right) \sqrt{\bar{w}^2 - 1}$$

$$+ \frac{\bar{w}}{4} \ln \left( \bar{w} + \sqrt{\bar{w}^2 - 1} \right),$$

(26)

for $p = 1$

$$f_1(\bar{w}) = \frac{\bar{w}^5}{30} - \frac{\bar{w}^3}{3} + \frac{\bar{w}}{2} - \frac{1}{5},$$

(27)

and for $p = 2$

$$f_2(\bar{w}) = \left( \frac{\bar{w}^4}{30} + \frac{11\bar{w}^2}{60} + \frac{8}{15} \right) \sqrt{\bar{w}^2 - 1}$$

$$- \frac{3\bar{w}}{4} \ln \left( \bar{w} + \sqrt{\bar{w}^2 - 1} \right).$$

(28)

We notice that, according to Eqs. (26), (27), and (28), the Fermi integral is expected to behave as $O(E^5)$ at relatively large energy $(E \gg m_e c^2)$.

The factor $\sqrt{w^2 - 1}$ in the logarithmic term of expansion (24) can be neglected because it remains of the order of 1 except at large proton-proton energies $(E \gg m_e c^2)$. Therefore, using Eq. (25), the Fermi integral (21) is approximated by

$$F(E + Q) \simeq f_0(\bar{w}) - \alpha \pi f_1(\bar{w})$$

$$+ \alpha^2 \left[ \frac{\pi^2}{3} f_2(\bar{w}) + \left( \frac{11}{4} - \gamma - \ln(2\rho) \right) \right] f_0(\bar{w}).$$

(29)

This expression allows us to find at least five decimal places without requiring numerical integration. Another advantage is the computation of the derivatives of the Fermi integrals with respect to $E$. In this work, we need the first two derivatives of $F(E+Q)$ at zero proton energy $(E = 0)$. This can be easily achieved with the derivatives of $f_p(\bar{w})$ with respect to $\bar{w}$ that are obtained directly from Eqs. (26), (27), and (28). The derivatives of $F(E+Q)$ with respect to $E$ have thus essentially the same expressions as Eq. (29) by replacing $f_p(\bar{w})$ with the derivatives with respect to $\bar{w}$, denoted as $f_p^{(n)}(\bar{w})$.

Note the change of variable $\partial_p^n F = (m_e c^2)^{-n} \partial_p^n F$ in the manipulation. The numerical values of the functions $f_p(\bar{w})$ and their derivatives with respect to $\bar{w}$ at $E = 0$. The upper index $n$ is the order of the derivatives.


tabular
| n = 0 | n = 1 | n = 2 |
|---|---|---|
| $f_0^{(n)}(2) = 0.14827(2)$ | $f_0^{(1)}(2) = 0.68187(8)$ | $f_0^{(2)}(2) = 2.3574(2)$ |
| $f_1^{(n)}(1) = 0.27415(4)$ | $f_1^{(1)}(1) = 1.1233(1)$ | $f_1^{(2)}(1) = 3.3682(2)$ |
| $f_2^{(n)}(0) = 0.64955(7)$ | $f_2^{(1)}(0) = 2.2505(2)$ | $f_2^{(2)}(0) = 5.4045(3)$ |

TABLE I. Numerical values of the functions $f_p(\bar{w})$ and their derivatives with respect to $\bar{w}$ at $E = 0$. The upper index $n$ is the order of the derivatives.

These results have also been checked by numerical integration in Wolfram Mathematica. The uncertainties in Tab. I and Eq. (30) come from the released energy $Q$. Finally, the low-energy behavior of the Fermi integral can be written as

$$\left( \frac{F(E + Q)}{F(Q)} \right) = 1 + \frac{F'(Q)}{F(Q)} E + \frac{F''(Q)}{F(Q)} E^2 + O(E^3),$$

(31)

with the numerical values of Eq. (30), it should be noted that the third derivative of the Fermi function (21) with respect to $E$ is devoid of integral and can be expressed exactly in terms of $P(\bar{w})$.
We have
\[ \frac{d^3F}{dE^3}(E+Q) = \frac{2}{(me^2)^3} P(\bar{w}) \bar{w} \sqrt{\bar{w}^2 - 1}, \]  
(32)
from which we easily find the numerical value \( F^{(3)}(Q) = 40.498(2) \text{ MeV}^{-3} \) at \( E = 0 \). Our approach avoids using numerical derivatives, as they are ill-conditioned in finite precision arithmetic, especially for high-order derivatives. This also ensures the accuracy of the results (30).

### Parametrization of the nucleon wave functions

The following sections present the detailed calculation of the proton-proton weak capture matrix element \( \Lambda(E) \) in the \( \ell = 0 \) channel. The calculations are partly inspired by Bahcall’s and May’s first estimate of \( \Lambda(0) \) based on the far-field asymptotic behavior of the nucleon wave functions [3]. Here we account for the internal structure of the nucleon wave functions. These structures have some influence on the energy dependence of \( \Lambda(E) \). Following this approach, we obtain a very accurate formulation of \( \Lambda(E) \) that is valid from zero energy up to a few MeVs.

One efficient way of including the short-range contribution in \( \Lambda \) is to use analytical forms of the nucleon wave functions. This method was used by many authors, especially to approximate the deuteron wave function on the basis of a series of exponential functions. Such approximations are known as Hulthén-type wave functions [35–39].

Here, we propose to start the calculation from the following original approximation of the \(^3S_1\) bound state of the deuteron:
\[ u_{d,0}(r) = A (1 - e^{-s_d r})^{\nu_d} e^{-\nu_d r}. \]  
(33)
The shape parameters \( s_d \) and \( \nu_d \) are fitted to the deuteron wave function. The normalization coefficient \( A \) is found to be 0.8850(5) fm\(^{-1/2}\) using three different potential models: Argonne-v18 (Av18) [23], Reid93 [24], and NijmII [24]. It is worth noting that \( A \) is related to the shape parameters \( s_d \) and \( \nu_d \) in Eq. (33) by the normalization condition
\[ A = \sqrt{N_S \frac{2b(2\nu_d + 2s_d - 1)}{\Gamma(2\nu_d + 1)\Gamma(2s_d - 1)}}. \]  
(34)
where \( N_S \) is the S-state probability given by \( \langle u_{d,0}|u_{d,0} \rangle = 94.30(6)\% \) for the three potential models (Av18, Reid93, NijmII). The fitted values of the shape parameters subject to the constraint (34) are shown in Tab. II. As one can see in Fig. 6(a), the approximation (33) of the deuteron wave function is remarkably accurate. The root-mean-square deviation from the Reid93 \(^3S_1\) wave function is about 0.015. This accuracy is good enough for our needs.

![Fig. 6. Comparison between the analytical approximations (solid black) of the nucleons wave functions, and the wave functions computed in the Reid93 [24] potential (dotted red).](image)

The same kind of parametrization can be applied to the proton-proton wave function:
\[ u_{pp,\ell}(r) = (1 - e^{-s_p r})^{\nu_p} (F_{\eta,\ell} \cos \delta_{\ell} + G_{\eta,\ell} \sin \delta_{\ell}), \]  
(35)
where \( \eta = 1/(a_0 k) \) is the Sommerfeld parameter, \( F_{\eta,\ell}(kr) \) and \( G_{\eta,\ell}(kr) \) are the standard Coulomb wave functions [40], and \( \delta_{\ell} \) is the proton-proton phase shift. In contrast to the deuteron wave function, this wave function depends on the energy of the incoming protons. Therefore, the shape parameters \( s_p \) and \( \nu_p \) are likely to vary with the energy. However, we will neglect these variations on the considered energy range because of the great depth of the nuclear potentials. The fitted values of the shape parameters are shown in Tab. II for different potential models.

![Table II. Shape parameters in different potential models for the S-state two-nucleons wave functions.](image)
Regularization of the proton-proton wave function

One issue of the proton-proton wave function is its strongly vanishing behavior when the energy decreases. The proton-proton wave function, such as given by Eq. (35), tends to zero as \( \eta^{-1/2} e^{-\pi \eta} \). This behavior is due to the asymptotic normalization of the Coulomb wave functions \( F_{\eta,\ell} \) and \( G_{\eta,\ell} \) that are constrained to sine wave of unit amplitude. This cancellation should be prevented by an adequate coefficient. In order to find this coefficient, we rewrite the Coulomb wave functions \( F_{\eta,\ell} \) and \( G_{\eta,\ell} \) of Eq. (35) in terms of the modified Coulomb functions \( \Phi_{\eta,\ell} \) and \( \Psi_{\eta,\ell} \) introduced in Refs. [19, 20]. Contrary to the standard Coulomb functions, these functions have the advantage of being analytic in the complex plane of the energy. In particular, they tend towards nonzero functions of \( r/\ell \) at zero energy. The function \( \Phi_{\eta,\ell} \) is related to \( F_{\eta,\ell} \) by [30]

\[
F_{\eta,\ell}(kr) = \frac{C_{\eta,\ell} \Gamma(2\ell + 2)}{(2\eta)^{\ell+1}} \Phi_{\eta,\ell}(kr),
\]

where \( C_{\eta,\ell} \) is the Coulomb normalization coefficient that reads [30, 40]

\[
C_{\eta,\ell} = \frac{2^{2\ell} \sqrt{\Gamma(\ell + 1 + i\eta)} \Gamma(\ell + 1 - i\eta)}{\Gamma(2\ell + 2) e^{\eta\pi/2}}.
\]

The function \( G_{\eta,\ell} \) can be expressed in terms of \( \Phi_{\eta,\ell} \) and \( \Psi_{\eta,\ell} \) as [30]

\[
G_{\eta,\ell} = \frac{C_{\eta,\ell} \Gamma(2\ell + 2)}{(2\eta)^{\ell+1}} \frac{e^{2\pi \eta} - 1}{\pi} \left( \Psi_{\eta,\ell} + g_{\eta,\ell} \Phi_{\eta,\ell} \right).
\]

In Eq. (38), the function \( w_{\eta,\ell} \) is defined by

\[
w_{\eta,\ell} = \frac{\ell!}{\ell+1} \left( 1 + \frac{j^2}{\eta^2} \right),
\]

and the Bethe function \( g_{\eta,\ell} \) by

\[
g_{\eta,\ell} = \frac{\psi(\ell + 1 + i\eta) + \psi(\ell + 1 - i\eta)}{2} - \ln \eta.
\]

Combining Eqs. (36) and (38), the asymptotic behavior of the proton-proton wave function becomes

\[
F_{\eta,\ell} \cos \delta_\ell + G_{\eta,\ell} \sin \delta_\ell = \frac{C_{\eta,\ell} \Gamma(2\ell + 2)}{|\Delta_\ell^+| (2\eta)^{\ell+1}} \left( \frac{\ell!^2 a_B^{2\ell+1}}{2w_{\eta,\ell}} \zeta_\ell + \frac{\Psi_{\eta,\ell}}{w_{\eta,\ell}} \right),
\]

where \( \zeta_\ell \) is the standard Coulomb-modified effective-range function defined by

\[
\zeta_\ell(E) = \frac{2w_{\eta,\ell}}{\ell!^2 a_B^{2\ell+1}} (\Delta_\ell + g_{\eta,\ell}),
\]

with the alternate effective-range function \( \Delta_\ell \) recently introduced in Refs. [19, 20]

\[
\Delta_\ell(E) = \frac{\pi \cot \delta_\ell}{e^{2\pi \eta} - 1}.
\]

In contrast to \( \Delta_\ell \), the function \( \zeta_\ell \) is analytic in the neighborhood of the zero-energy point.

In Eq. (41), \( |\Delta_\ell^+| \) is the modulus of the function

\[
\Delta_\ell^+(E) = \frac{\pi (\cot \delta_\ell - 1)}{e^{2\pi \eta} - 1}.
\]

In practical computation, \( \Delta_\ell^+ \) can be evaluated from the knowledge of the effective-range function \( \zeta_\ell \). The square modulus of \( \Delta_\ell^+ \) can be expressed as

\[
|\Delta_\ell^+|^2 = \left( \frac{\ell!^2 a_B^{2\ell+1}}{2w_{\eta,\ell}} \zeta_\ell - g_{\eta,\ell} \right)^2 + \left( \frac{\pi}{e^{2\pi \eta} - 1} \right)^2,
\]

as it will also appear in the parametrization of \( \lambda \). The expression (45) is the analytic continuation of \( |\Delta_\ell^+|^2 \) to the complex plane of the energy.

Finally, we deduce the adequate normalization of the overlap integral from the prefactor in Eq. (41)

\[
I_\ell(E) = \frac{(2\eta)^{\ell+1}}{C_{\eta,\ell} \Gamma(2\ell + 2)} \int_0^\infty u_{\delta,\ell} u_{\ell pp,\ell} \, dr.
\]

This definition tends to a nonzero constant at zero energy for any partial wave \( \ell \), but it is still not analytic at this point because of the Coulomb singularities of \( |\Delta_\ell^+| \) in Eq. (41). It should be noted that \( I_\ell(E) \) is related to the dimensionless matrix element \( \Lambda_\ell \) by a constant factor:

\[
\Lambda_\ell(E) = \frac{a_B b^{3/2} I_\ell(E)}{\sqrt{8}}.
\]

The approximate wave functions (33) and (35) allow us to analytically calculate the overlap integral (46). Since the short-range part of the radial wave functions expands in a series of exponentials, the calculation of Eq. (46) splits into a series of Laplace transforms of the modified Coulomb functions

\[
I_\ell = \frac{A/b}{|\Delta_\ell^+|} \sum_{i,j} c_{i,j} \left( \frac{\ell!^2 a_B^{2\ell+1}}{2w_{\eta,\ell}} \zeta_\ell \phi_{\beta_{i,\ell}} + \psi_{\beta_{i,\ell}} \Phi_{\eta,\ell} \right),
\]

where \( \phi_{\beta_{i,\ell}} \) and \( \psi_{\beta_{i,\ell}} \) are the Laplace transforms of the modified Coulomb functions

\[
\phi_{\beta,\ell}(\epsilon) = \int_0^\infty \frac{e^{-\beta x} \Phi_{\eta,\ell}(x\sqrt{\epsilon}) \, dx}{x},
\]

and

\[
\psi_{\beta,\ell}(\epsilon) = \int_0^\infty \frac{e^{-\beta x} \Psi_{\eta,\ell}(x\sqrt{\epsilon}) \, dx}{x}.
\]
In the main text, the index $\beta$ has been omitted on $\phi_{\beta,\ell}$ and $\psi_{\beta,\ell}$ when evaluated at $\beta = 1$. In Eqs. (49) and (50), we have used the dimensionless quantities $x = br$ and $\epsilon = k^2/b^2 = E/B$ with

$$B = \frac{2m_n}{m_p + m_n} B_d ,$$

where $m_n$ and $m_p$ are the neutron and the proton mass respectively, and $B_d = 2.22457$ MeV is the binding energy of the deuteron $[18]$. The integer indices $\nu$ and $\ell$ in the expansion (48) run over the terms of the binomial expansion of $(1 - e^{-x})^\nu_0$ and $(1 - e^{-x})^\nu_1$ respectively. The variable $\beta_{i,\ell}$ takes the values $\beta_{i,\ell} = 1 + i\delta_d + j\delta_p$, and the corresponding coefficient is

$$c_{i,\ell} = (-1)^{i+j} \left( \frac{\nu_d}{i} \right) \left( \frac{\nu_p}{j} \right) .$$

In this way, we just have to calculate the Laplace transforms (49) and (50).

**Regular Coulomb integral**

In this section, we present the derivation of the Laplace transform of $\Phi_{\eta,\ell}$. As shown in Ref. [30], the Coulomb function $\Phi_{\eta,\ell}$ in Eq. (49) is given by

$$\Phi_{\eta,\ell}(kr) = (x)x^{\ell+1} e^{i\kappa x} M_{\ell+1+2i\nu}(-2i\kappa x) ,$$

where $\kappa = k/b = \sqrt{\epsilon}$ is the dimensionless wave number, and $\chi = 2/(\alpha B_0)$ is the Bahcall and May constant [3]. The regularized confluent hypergeometric function in Eq. (53) is defined by the series [40]

$$M(a; z) = \frac{1}{\Gamma(b)} F_1(a; z) = \sum_{n=0}^{\infty} \frac{(a)_n}{(b+n)!} z^n ,$$

where $(a)_n = \Gamma(a+n)/\Gamma(a)$ is the Pochhammer symbol. The division by $\Gamma(b)$ in Eq. (54) eliminates the singularities of $1 F_1(a; z)$ at $b \in \mathbb{Z}_{\leq 0}$ [40]. Using the definition (53), the regular Coulomb integral (49) expands as follows

$$\phi_{\beta,\ell} = \chi^{\ell+1} \sum_{n=0}^{\infty} \frac{(\ell + 1 + i\eta)_n(-2i\kappa)^n}{\Gamma(2\ell + 2 + n)!} \int_0^\infty e^{-(\beta-i\kappa)x} x^{n+\ell+1} dx .$$

All the remaining integrals in Eq. (55) are given by

$$\int_0^\infty e^{-(\beta-i\kappa)x} x^{n+\ell+1} dx = \frac{\Gamma(n + \ell + 2)}{(\beta - i\kappa)^{n+\ell+2}} .$$

One notices that the combination of Eqs. (55) and (56) leads to the Gauss hypergeometric function $2 F_1$, or more specifically to its regularized version $[40]

$$F(a,b; z) = \frac{1}{\Gamma(c)} 2 F_1(a,b; z) = \sum_{n=0}^{\infty} \frac{(a)_n(b)_n}{(c)_n n!} z^n .$$

Using the definition (57) in Eq. (55), we obtain the following result:

$$\phi_{\beta,\ell}(\epsilon) = \frac{\chi^{\ell+1} \Gamma(\ell + 2)}{(\beta - i\kappa)^{\ell+2}} E\left(\frac{\ell+2,\ell+1+i\eta; -2i\kappa}{\beta - i\kappa} \right) .$$

Remarkably, this result is considerably simplified in the special case $\ell = 0$. Indeed, the hypergeometric function in Eq. (58) is then of the form $2 F_1(a,b; z)$, which reduces to $(1 - z)^{-b}$ [40] because of the simplification in the series (57). From Eq. (58), one finds

$$\phi_{\beta,0}(\epsilon) = \frac{\chi}{\beta^2 + \kappa^2} e^{2\eta \arctan(\kappa/\beta)} .$$

This useful result is at the basis of the parametrization of $\Lambda(E)$ proposed in this paper.

**Irregular Coulomb integral**

Now, we calculate the Laplace transform (50) of $\Psi_{\eta,\ell}$. This calculation is significantly less straightforward than for $\Phi_{\eta,\ell}$, because it does not reduce to elementary functions for $\ell = 0$. The Coulomb function $\Psi_{\eta,\ell}$ is defined in Ref. [30] as

$$\Psi_{\eta,\ell}(\rho) = w_{\eta\ell} \rho \Phi(\ell + 1 \pm i\eta) (2\rho)^{\ell+1} e^{\pm i\rho U(\ell; (\ell+1)\rho; \mp 2\eta)} - w_{\eta\ell} h_{\ell}^\pm \Phi_{\eta,\ell}(\rho) ,$$

where the choice of the upper or lower sign is immaterial. In Eq. (60), $U(\ell; z)$ is the Tricomi confluent hypergeometric function, and the Bethe functions $h_{\ell}^\pm$ are defined as

$$h_{\ell}^\pm = \frac{\psi(\ell + 1 \pm i\eta) + \psi(-\ell \pm i\eta) - \ln(\pm i\eta)}{2} .$$

The subtraction by $w_{\eta\ell} h_{\ell}^\pm \Phi_{\eta,\ell} \Phi_{\eta,\ell}$ in Eq. (60) is intended to compensate for the singularities of $U(\ell; z)$ in the complex plane of the energy. This operation makes $\Psi_{\eta,\ell}(kr)$ regular for $k \in \mathbb{C}$ [30].

Performing the direct integration of Eq. (60) by means of the integral representation of $U(\ell; z)$ [40] leads to

$$\psi_{\beta,\ell} = \frac{\Gamma(\ell+1+i\eta) \Gamma(\ell+2) \Gamma(1-\ell)}{2i\eta} E\left(\frac{\ell+2,\ell+1+i\eta; \beta \pm i\kappa}{\beta \pm i\kappa} \right) - w_{\eta\ell} h_{\ell}^\pm \Phi_{\beta,\ell} \Phi_{\beta,\ell} .$$

Note that, this function is not finite for partial waves higher than $S$ ($\ell > 0$) due to the vertical asymptote of $\Psi_{\eta,\ell}(kr)$ at $r = 0$. When $\ell = 0$, the hypergeometric function in the above equation can be efficiently computed from its continued fraction expansion.

The expression (62) is quite difficult to analyze at low energy because the hypergeometric function shows an essential singularity at $\epsilon = 0$. Although this singularity is
compensated by $w_{nℓ}h_{mℓ}^+\phi_{β,ℓ}$, it prevents the hypergeometric function from having a convergent low-energy expansion. This is why we propose to determine a suitable approximation to Eq. (62) from another approach.

It turns out that the function $Ψ_{η,ℓ}$ is related to the regular Coulomb function $Φ_{η,ℓ}$. We have shown in Ref. [30] that $Ψ_{η,ℓ}$ obeys the following connection formula

$$Ψ_{η,ℓ} = w_{nℓ}^+\frac{ϕ_{η,ℓ}}{2} + \frac{1}{2} \frac{ϕ_{η,−ℓ−1}}{2} ,$$

(63)

where the dots refer to derivatives with respect to $ℓ$. This useful property is preserved by the Laplace transforms (49) and (50). Therefore, the function $ψ_{β,ℓ}(ℓ)$ can be calculated from derivatives of $ϕ_{β,ℓ}(ℓ)$ as follows [30]

$$\frac{ψ_{β,ℓ}}{w_{nℓ}ϕ_{β,ℓ}} = \left( \frac{ψ_{β,ℓ}}{ϕ_{β,ℓ}} + \frac{ϕ_{β,−ℓ−1}}{ϕ_{β,−ℓ−1}} \right) .$$

(64)

However, in order to calculate the derivatives in Eq. (64), we need to use the general expression (58) valid of $ϕ_{β,ℓ}$ for all $ℓ \in \mathbb{C}$. In this regard, we have found convenient to approximate the hypergeometric function by its low-energy confluent limit

$$F\left( \ell+2, \ell+1+iη, \frac{−2η}{β−ι} \right) = M\left( \ell+2, \frac{χ}{β} \right) + \mathcal{O}(κ^2) .$$

(65)

The approximation (65) could be improved at $κ = 0$ by the confluence expansion (20a) in Ref. [41]. However, this expansion converges so slowly for $κ > 1$ that we will not use it here. The advantage of the approximation (65) is the consistency with Bahcall’s and May’s results in the zero-energy limit. It is useful in our calculation to rewrite the confluent hypergeometric function in Eq. (65) in terms of the regular Coulomb function

$$M\left( \ell+2, \frac{χ}{β} \right) = (β/χ)^{ℓ+1} e^{χ/2β} Φ_{−1,ℓ}(iχ/2β) .$$

(66)

The approximation of $ϕ_{β,ℓ}$ for $ℓ \ll 1$ is thus given by

$$ϕ_{β,ℓ} \simeq \frac{β^{ℓ+1}Γ(ℓ+2)}{√{β^2 + κ^2}^ℓ} e^{2η\arctan(κ/β)} e^{−χ/2β} Φ_{−1,ℓ}(iχ/2β) .$$

(67)

From Eq. (58) to Eq. (67), we have taken the modulus of the factor $(β−ικ)^{-ℓ−2}$ because $ϕ_{β,ℓ}$ should still remain a positive real function after the approximation (65). The logarithmic derivative of $ϕ_{β,ℓ}$ with respect to $ℓ$ can be easily calculated from Eq. (67):

$$\frac{ϕ_{β,ℓ}}{ϕ_{β,ℓ}} \simeq ψ(ℓ+2) − ln \sqrt{1 + κ^2/β^2} + Φ_{−1,ℓ}(iχ/2β)/Φ_{−1,ℓ}(iχ/2β) .$$

(68)

We neglect the logarithmic term in Eq. (68) because it is irrelevant in the $O(κ^2)$ approximation of Eq. (65). Combining two expressions (68) evaluated at $ℓ$ and $−ℓ−1$ in Eq. (64), we get

$$\frac{ψ_{β,ℓ}}{w_{nℓ}ϕ_{β,ℓ}} \simeq \frac{ψ(ℓ+2) + ψ(1−ℓ)}{2} + \frac{Ψ_{−1,ℓ}(iχ/2β)}{w_{−1,ℓ}Ψ_{−1,ℓ}(iχ/2β)} .$$

(69)

This relation can be simplified further by means of the definition (60) of $Ψ_{η,ℓ}$ with the plus sign. Finally, after the elimination of the digamma functions with Eq. (61), we obtain

$$\frac{ψ_{β,ℓ}}{w_{nℓ}ϕ_{β,ℓ}} \simeq Γ(1−ℓ) U\left( ℓ+2; χ/β \right) .$$

(70)

In the special case of interest $ℓ = 0$, this result can be written as

$$\frac{ψ_{β,0}}{ϕ_{β,0}} \simeq Γ(−1, χ/β) ,$$

(71)

where $Γ(a, z)$ is the upper incomplete gamma function defined by

$$Γ(a, z) = \int_z^∞ t^{a−1} e^{−t} dt .$$

(72)

When $β = 1$ and $χ ≃ 0.149816$, the ratio (71) evaluates to about 4.28065. The incomplete gamma function in Eq. (71) can also be related to the exponential integral $E_1(z) = Γ(0, z)$ as done in Bahcall’s and May’s work [3]:

$$Γ(−1, z) = \frac{e^{−z}}{z} − E_1(z) .$$

(73)

Bahcall, however, limited his calculation to zero energy, in contrast to the property (71) valid up to a few MeVs.

![Graph](image-url)

FIG. 7. Comparison between the Coulomb integrals $ϕ_{β,ℓ}(ℓ)$ and $ψ_{β,ℓ}(ℓ)$ for $β = 1$, $χ = 2/(ηab) ≃ 0.149816$, and $ℓ = 0$. Panel (a) shows $ψ_{1,0}(ℓ)$ and $Γ(−1, χ)ϕ_{1,0}(ℓ)$, and panel (b) depicts the relative error between $ψ_{1,0}$ computed from Eq. (62) and the approximation (71).

Furthermore, the novel result (71) means that $ψ_{β,0}$ is nearly proportional to $ϕ_{β,0}$ on a large energy range. The accuracy of this property is graphically tested in
Fig. 7. As we can see, the relative error of the estimate at \( \epsilon = 1 \), that corresponds to \( E = B \), is only 2.9%.

The overall accuracy of the approximation (71) over a few MeVs is primarily due to the smallness of \( \chi \) before 1 (\( \chi \approx 0.149816 \)). In fact, it can be shown that both \( \psi_{\beta,0} \) and \( \Gamma(-1, \chi/\beta)\phi_{\beta,0} \) have the same neutral-charge limit:

\[
\lim_{\chi \to 0} \psi_{\beta,0} = \lim_{\chi \to 0} \Gamma(-1, \chi/\beta)\phi_{\beta,0} = \frac{\beta}{\beta^2 + \epsilon}.
\] (74)

Therefore, the property (71) tends to be exact for \( \chi \to 0 \), but also for \( \beta \to \infty \). These observations have important consequences in the parametrization of the weak capture matrix element that follows.

**Linearized overlap integral**

Now, using results (59) and (71), we can calculate the overlap integral \( I_0 \) from Eq. (48). As a reminder, the expression (48) comes from the expansion of the nucleon wave functions over a series of decaying exponentials. It is useful to separate the first term of this expansion (\( \beta_{\beta,0} = 1 \)) because it corresponds to the contribution of the asymptotic part of the nucleon wave functions. One thus expects this contribution to be larger than the short-range part of the wave functions [3]. We find convenient to introduce an energy-dependent function, denoted \( C \), which gathers all the contributions of the short-range part of the wave functions:

\[
C = - \sum_{i,j \neq 0,0} c_{i,j} \left[ \frac{ab}{2} \chi \Phi_{i,j}(\chi) \right] \phi_{\beta_{i,j},0}(\epsilon).
\] (75)

The minus sign before the series of Eq. (75) makes \( C \) a positive function. Consequently, the expansion (48) can be rewritten as

\[
I_0 = \frac{A/b}{\Delta_0^+} \left[ \left( \frac{ab}{2} \chi \Phi_{1,0}(\gamma) \right) \phi_{1,0}(\epsilon) - C(\epsilon) \right],
\] (76)

where \( \gamma = \Gamma(-1, \chi) \simeq 4.28065 \) is independent of the energy. Using Eq. (47), expression (76) directly translates in terms of the standard matrix element:

\[
\Lambda = \frac{A/\sqrt{2b}}{\chi |\Delta_0^+|} \left[ \left( \frac{ab}{2} \chi \Phi_{1,0}(\gamma) \right) \phi_{1,0}(\epsilon) - C(\epsilon) \right].
\] (77)

The shape parameters of the nucleon wave functions in Tab. II provide an estimation of \( C \). At zero energy, we get from Eq. (75) the estimate \( C(0) \approx 0.253 \). The full curve of \( C \) built on Eq. (75) is shown as curve (a) in Fig. 8. It turns out to be a relatively poor estimate in comparison with the actual function \( C \) computed for different potential models from the inversion of Eq. (76), and depicted as curve (b) in Fig. 8. At zero energy, we find \( C(0) = 0.260(1) \); the error being due to the uncertainty on potential models. It should be noted that Bahcall and May originally obtained remarkably good estimates of \( A \) and \( C(0) \) from effective-range theory [3]

\[
\left\{ \begin{array}{l}
A \simeq \frac{2b}{\sqrt{1 - br_{pp}}} \approx 0.883(2) \text{ fm}^{-1/2}, \\
C(0) \approx \frac{b(r_{pp} + r_{pp})}{4} \approx 0.262(1).
\end{array} \right.
\] (78)

In Eq. (78), we have used the numerical values of the proton-proton \( ^1S_0 \) effective range \( r_{pp} = 2.77(1) \) fm and the proton-neutron \( ^3S_1 \) effective range \( r_{pn} = 1.75(1) \) fm from Table XIV in Ref. [42].

![Fig. 8. Correction function \( C \) up to 10 MeV for different potential models. The curves (a) depict the linear behavior of \( C \) predicted by Eq. (75) using the fitted nucleon wave functions of Tab. II. The curves (b) show the numerical computation of \( C \) from the inversion of Eq. (77).](image)

Although they are quite close, one notices a discrepancy of shape between the curves (a) and (b) in Fig. 8. The curve (b) rather quickly deviates from a straight line, in contrast to curve (a). This discrepancy is due to the limitation of the assumption in Eq. (35) that the short-range part of the proton-proton wave function, i.e., the shaping factor \((1 - e^{-s_{pp}r})\nu_r\), does not depend on the energy. This assumption is already broken beyond about 2 MeV, as the curve (b) deviates from a straight line. A possible fix would be to make this factor dependent on the energy, but it would involve the use of a specific potential model. Such an approach is beyond the scope of the model-independent analysis achieved in this paper.

From Eq. (77), we establish an expression of \( \Lambda \) that is more convenient to practical applications

\[
\Lambda = \frac{\phi_{1,0}(\epsilon)}{\chi |\Delta_0^+|} L(\epsilon),
\] (79)
where the function $L(\epsilon)$ can be related to $C(\epsilon)$ with

$$L(\epsilon) = \frac{A}{\sqrt{2b}} \left[ \frac{a_B}{2} \zeta_0 + \gamma - \frac{C(\epsilon)(1 + \epsilon)}{\chi \exp\left(\frac{\arctan \sqrt{\epsilon}}{\sqrt{\epsilon}}\right)} \right],$$  \hspace{1cm} (80)

using the result (59). It is worth noting that the function $L(\epsilon)$ is pretty close to a smoothly varying straight line, as discussed in the main text. Indeed, the three terms in the square brackets of Eq. (80) display very linear behaviors over a large energy range, at least up to 2 MeV. Surprisingly, this very important feature is practically independent from our first guess (35) about the proton-proton wave function. Therefore, we deduce that the function $L(\epsilon)$ is appropriate to model fitting over a large energy range.

The analytic continuation of $\Lambda^2$ to complex energies based on Eq. (79) is shown in Fig. 9. Note that, in addition to Coulomb singularities, the function $\Delta^+_0$ also brings a branch cut running along the negative real semi-axis due to the logarithm of the Bethe function $g_{\eta, \epsilon}$ in Eq. (45). This branch cut makes $\Lambda$ complex at negative energy, although it is real at positive energy.

**Zero-energy expansion of the overlap integral**

Furthermore, the result (80) allows us to calculate the zero-energy values of $\Lambda$ and $\Delta$. Using $A = 0.8850(5)$ fm$^{-1/2}$ and $C(0) = 0.260(1)$ computed previously in potential models, we find

$$L(0) = \frac{A}{\sqrt{2b}} \left[ \frac{-a_B}{2\alpha_0} + \gamma - \frac{C(0)}{\chi e^\chi} \right] = 8.42(1).$$  \hspace{1cm} (81)

If we set $\epsilon \to 0$ in Eq. (79), we get

$$\Lambda(0) = \frac{2 |\alpha_0|}{a_B} e^\chi L(0) = 2.652(6),$$  \hspace{1cm} (82)

or in other words $\Lambda^2(0) = 7.034(33)$, which is consistent with Ref. [14]. The uncertainty in Eq. (82) is due to the discrepancy of the scattering length $\alpha_0$ among the potential models. This discrepancy also affects the uncertainty on $L(0)$ in Eq. (81). The quantity (82) is very important at solar energies ($E < 10$ keV), since $\Lambda$ is nearly constant in this range.

Another important consequence of the result (79) is the accurate description of the low-energy behavior of $\Lambda$. This result provides a constraint on the derivatives of $\Lambda$ with respect to the energy, especially the first derivative at zero energy: $\Lambda'(0)$. This value plays a significant role in the proton-proton fusion at solar energies [14]. From Eq. (79), the logarithmic derivative of $\Lambda$ can be easily calculated

$$\frac{d \ln \Lambda}{dE} = \frac{d \ln \phi_{1,0}}{dE} - \frac{d \ln \Delta_0}{dE} + \frac{d \ln L}{dE},$$  \hspace{1cm} (83)

where the function $|\Delta^+_0|$ has been replaced by $\Delta_0$ because they share the same asymptotic expansion at $E = 0$. This is due to the fact that the term $(e^{\pi \eta} - 1)^{-2}$ in Eq. (45) is negligible since all of its derivatives are zero. The first terms in the asymptotic expansion of $\Delta_0$ are

$$\Delta_0 = \frac{a_B}{2} \zeta_0 - \left( \frac{E}{12 \text{Ry}} + \frac{E^2}{120 \text{Ry}^2} + \mathcal{O}(E^3) \right),$$  \hspace{1cm} (84)

where the nuclear Rydberg energy of the two-proton system. However, it should be noted that this expansion does not converge at $E = 0$ because of the Coulomb singularities in $\Delta_0$. It remains nevertheless valid for $E \ll \text{Ry}$ [20, 21]. In addition, the expansion of the regular Coulomb integral is given by

$$\phi_{1,0} = \chi e^\chi \left( 1 - \frac{3 + \chi}{3} \epsilon + \frac{90 + 48 \chi + 5 \chi^2}{90} \epsilon^2 - \mathcal{O}(\epsilon^3) \right).$$  \hspace{1cm} (85)

Combining these results in Eq. (83) leads to

$$\frac{\Lambda'(0)}{\Lambda(0)} = \frac{|\alpha_0|}{2|\alpha_0|} \left( \frac{a_B}{3} - r_0 \right) - \frac{3 + \chi}{3B} + \frac{L'(0)}{B L(0)} \simeq \frac{1}{B} \left( \frac{2 |\alpha_0| (a_B - 3r_0)}{3(a_B \chi)^2} - 1 - \frac{\chi}{3} + \frac{L'(0)}{L(0)} \right).$$  \hspace{1cm} (86)
Here, the prime over \( \Lambda \) denotes the derivative with respect to \( E \), and the prime over \( L \) denotes the derivative with respect to \( \epsilon \). From potential models, we obtain the value \( L'(0) = 0.55(1) \). The second line in Eq. (86) derives from the approximation \( B \simeq (\hbar b)^2/m_p \) neglecting the neutron-proton mass difference. It means that the main contribution is predicted by the experimental values \( a_0 \) and \( B \), in addition to the effective-range parameters \( \alpha_0 \) and \( r_0 \).

Replacing all the quantities in Eq. (86) with their numerical values, except for \( \alpha_0 \) and \( r_0 \), allows us to study the influence of the effective-range parameters. We get in unit MeV\(^{-1}\n\)

\[
\frac{\Lambda'(0)}{\Lambda(0)} = -0.4423(6) + (0.23149 - 0.01205r_0)|\alpha_0|, \quad (87)
\]

where \( \alpha_0 \) and \( r_0 \) are expressed in fm. It should be noted that, according to Eq. (80), \( L(0) \) and \( L'(0) \) also depend on effective-range parameters. In this regard, the expansion (87) is incomplete. However, it is not possible to extract the full dependence of \( L \) in the effective-range parameters since it would require to modify the potential models accordingly.

Besides, one notices in Eq. (87) that the uncertainty of the effective range \( r_0 \) only marginally affects the result. Therefore, it is useful to re-express Eq. (87) in the neighborhood of \( |\alpha_0| = 7.815 \) fm with \( r_0 = 2.77(1) \) fm. We obtain the following result in unit MeV\(^{-1}\) presented in the main text

\[
\frac{\Lambda'(0)}{\Lambda(0)} = 1.106(2) + 0.1981(1)(|\alpha_0| - 7.815), \quad (88)
\]

where \( \alpha_0 \) is expressed in fm. Finally, using \( |\alpha_0| = 7.815(9) \) fm, we find from Eq. (88) the central value

\[
\frac{\Lambda'(0)}{\Lambda(0)} = 1.106(3) \text{ MeV}^{-1}. \quad (89)
\]

The uncertainty in Eq. (89) is slightly increased because of the uncertainty on \((|\alpha_0| - 7.815)\), that is 0.009.

If we perform the fitting directly on \( \Lambda \) over the interval \( E \in [1, 2] \) keV, we find the result \( \Lambda'(0)/\Lambda(0) = 1.108(2) \text{ MeV}^{-1} \), where the central value has been slightly shifted up compared to Eq. (89). This shift is likely due to the non-analytic behavior of \( \Lambda(E) \) at \( E = 0 \). In fact, we notice a suspiciously large dependence of \( \Lambda'(0) \) on the energy interval chosen for the fitting, as pointed out in Ref. [16]. The overestimation of \( \Lambda'(0) \) seems to go along with the positive curvature of \( \Lambda \) at \( E = 0 \). A great advantage of the analytical result (86) is that it is not biased by the Coulomb singularities in \( \Lambda \), in contrast to the direct polynomial extrapolation of \( \Lambda \). It should be noted that it will be also the case for higher-order derivatives of \( \Lambda \).

The logarithmic derivative of the \( S \) factor at \( E = 0 \) can also be computed from Eq. (89). Knowing that \( S(E) \) is proportional to \( F(E + Q)|\Lambda(E)|^2 \) where \( F(E + Q) \) is the Fermi phase-space integral, the logarithmic derivative reads [26]

\[
\frac{S'(0)}{S(0)} = \frac{F'(Q)}{F(Q)} + 2\frac{\Lambda'(0)}{\Lambda(0)}. \quad (90)
\]

Using the previously computed numerical value of the logarithmic derivative of the Fermi integral \( F'(Q)/F(Q) = 9.0413(3) \text{ MeV}^{-1} \) from Eq. (30), we get the result

\[
\frac{S'(0)}{S(0)} = 11.253(3) + 0.3962(2)(|\alpha_0| - 7.815), \quad (91)
\]

in unit MeV\(^{-1}\) shown in the main text. The central value is 11.25(1) MeV\(^{-1}\).

The second derivatives of \( \Lambda \) and \( S \) can also be calculated in the same way as before. After some calculations, we obtain the following expression

\[
\frac{\Lambda''(0)}{\Lambda(0)} = \frac{\phi_{1,0}''}{B^2\phi_{1,0}} - \frac{\Delta_0''}{\Delta_0} + \frac{L''}{B^2L} + 2\left(\frac{\Delta_0'}{\Delta_0}\right)^2
\]

\[
- 2\frac{\phi_{1,0}L'}{B\phi_{1,0}L} + 2\frac{\phi_{1,0}'L'}{B^2\phi_{1,0}L} - 2\frac{L\Delta_0'}{BL\Delta_0}, \quad (92)
\]

where the primes refer to derivatives with respect to \( E \), except for \( \phi_{1,0}(\epsilon) \) and \( L(\epsilon) \), as previously. All the functions in Eq. (92) are implicitly evaluated at \( E = 0 \). It turns out that the second derivative \( \Lambda''(0) \) can be neglected, as it contributes to only 0.01\%, far below the uncertainty of the other terms. The terms of Eq. (92) containing \( \Delta_0 \) and its derivatives are dominating the others, especially the term \(-\Delta_0''/\Delta_0\) which is about equal to 29 MeV\(^{-2}\). Inserting the expansion of \( \phi_{1,0} \) and \( \Delta_0 \) at \( E = 0 \) into Eq. (92), but without replacing the effective-range parameters \( \alpha_0 \) and \( r_0 \) by their numerical value for now, we find the expression in unit MeV\(^{-2}\)

\[
\frac{\Lambda''(0)}{\Lambda(0)} = 0.4051(5) + (3.5017(3) + 0.01066(1)r_0)|\alpha_0|
\]

\[
+ (0.32737 - 0.01704r_0)^2|\alpha_0|^2, \quad (93)
\]

where \( \alpha_0 \) and \( r_0 \) are expressed in fm. The last term in Eq. (93) comes from the term \((\Delta_0'/:\Delta_0)^2\) in Eq. (92). The uncertainties in this term are negligible, as it solely depends on accurately known physical quantities (\( h, \alpha, \) and \( m_p \)).

As previously, if we focus on the neighborhood of \( |\alpha_0| = 7.815 \) fm assuming \( r_0 = 2.77(1) \) fm, we get from Eq. (93) the expression in unit MeV\(^{-2}\) presented in the main text

\[
\frac{\Lambda''(0)}{\Lambda(0)} = 32.795(6) + 4.758(2)(|\alpha_0| - 7.815), \quad (94)
\]
where $\alpha_0$ is expressed in fm. Note that the remainder term in Eq. (94) is $0.0785(1) (|\alpha_0| - 7.815)^2$ in unit MeV$^{-2}$. Using $|\alpha_0| = 7.815(9)$ fm, we obtain the result

$$\frac{\Lambda'(0)}{\Lambda(0)} = 32.80(5) \text{ MeV}^{-2}, \quad (95)$$

where the uncertainty is mainly due to $\alpha_0$, as one can notice from Eq. (94). This result is considerably more accurate than what we get from direct fitting on $\Lambda$. In fact, the direct computation of the second derivative of $\Lambda$ depends too much on the energy interval chosen for the fitting, hence degrading its accuracy. Finally, the result (95) directly leads to the accurate value of the second derivative of the $S$ factor at zero energy

$$\frac{S''(0)}{S(0)} = \frac{F''(Q)}{F(Q)} + 4 \frac{F'(Q)}{F(Q)} \frac{\Lambda'(0)}{\Lambda(0)} + 2 \left( \frac{\Lambda'(0)}{\Lambda(0)} \right)^2 + 2 \frac{\Lambda''(0)}{\Lambda(0)}. \quad (96)$$

Using the numerical values of the Fermi integral $F'(Q)/F(Q) = 9.0413(3) \text{ MeV}^{-1}$ and $F''(Q)/F(Q) = 61.479(5) \text{ MeV}^{-2}$ from Eq. (30), we obtain the result in unit MeV$^{-2}$

$$\frac{S''(0)}{S(0)} = 169.51(8) + 17.56(1) (|\alpha_0| - 7.815), \quad (97)$$

presented in the main text. The remainder term is $0.2355(3) (|\alpha_0| - 7.815)^2$ in unit MeV$^{-2}$. The central value is found to be $169.5(3) \text{ MeV}^{-2}$.

To conclude, it is remarkable that so many physical features about the proton-proton weak capture reaction are embedded in the single parametrization (79). This parametrization allows us not only to cover up a large energy range ($|E| \lesssim 5 \text{ MeV}$) with a limited number of parameters ($L(0), L'(0)$), but also to accurately calculate the derivatives of $\Lambda$ at $E = 0$ without the numerical bias of the Coulomb singularities.