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Reaction-rate function of proton-deuteron radiative capture within potential model

Dao Nhut Anh[1,†], **Do Huy Tho**[1] **and Nguyen Le Anh**[2]

[1]*Ho Chi Minh City University of Education, 280 An Duong Vuong, District 5, Ho Chi Minh City, Vietnam*

[2]*Department of Physics, Ho Chi Minh City University of Education, 280 An Duong Vuong, District 5, Ho Chi Minh City, Vietnam*

E-mail: [†]daonhutanh2004@gmail.com

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Abstract. *The proton-deuteron (pD) radiative capture reaction is a key process in primordial nucleosynthesis, requiring precise inputs for the reaction rate, cross section, and astrophysical S-factor. In this study, the S-factor and reaction rate are calculated using a phenomenological potential model, incorporating both electric dipole ($E1$) and magnetic dipole ($M1$) transitions. The results show good agreement with recent experimental data. In addition, an approximate polynomial expression for the reaction-rate function is provided to facilitate its application in nucleosynthesis calculations.*

Keywords: radiative capture; potential model; proton-deuteron; astrophysical S-factor.

Classification numbers: 25.40.Lw; 12.39.Pn.

1. Introduction

Big Bang nucleosynthesis (BBN) refers to the production of the first light nuclei shortly after the Big Bang. The high temperatures and dense baryon matter of the early universe dictated the rates of nuclear reactions, shaping the abundance of light elements [1]. The synthesis of these elements is sensitive to variations in nuclear cross sections and astrophysical S-factors, highlighting their importance in accurately modeling nucleosynthesis [2]. Therefore, precise calculations of these quantities are essential to understanding the conditions and outcomes of BBN [3].

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The reaction D$(p,\gamma)^3$He, commonly referred to as pD radiative capture, plays an important role in BBN. The abundance of deuterium becomes an important indicator for cosmological parameters [3, 4]. It has attracted significant global attention from both theoretical and observational perspectives [5]. In the theoretical calculation, the radiative capture is modeled as an electromagnetic transition between a continuum state and a bound state. In our recent works [6,7], the astrophysical S-factors and reaction rates for the pD radiative capture were calculated using a phenomenological potential model, considering both electric dipole ($E1$) and magnetic dipole ($M1$) transitions. The theoretical results from this model show good agreement with experimental data. While the $E1$ transition predominantly contributes to the S-factor, its role alone cannot account for the observed enhancement at very low energies [6]. Consequently, the role of the $M1$ transition was investigated, highlighting its significant contribution, particularly in the low-energy regime [7].

This study revisits the pD radiative capture reaction within potential model, aiming to provide a reliable S-factor and accurate reaction rates. Based on numerical results, an approximate polynomial expression for the reaction-rate function, $R(T)$, is derived. This expression provides a practical tool for abundance calculations using publicly available codes [8]. The primary objective is to present the coefficients of the nuclear reaction-rate function for accurate primordial deuterium abundance calculations.

2. Potential model

2.1. Cross section and astrophysical S factor

The astrophysical S-factor is introduced to simplify the analysis of nuclear reaction cross sections at low energies, where the Coulomb barrier strongly influences the reaction dynamics. The energy-dependent astrophysical S-factor is defined as

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

where η is the energy-dependent Sommerfeld parameter. The pD radiative capture cross section, which includes contributions from both $E1$ and $M1$ transitions, is expressed as

$$\sigma(E) = \frac{16\pi}{9}\frac{k_\gamma^3}{\hbar}\sqrt{\frac{\mu}{2E}}\frac{1}{(2s+1)(2I+1)} \times (|M_{E1}|^2 + |M_{M1}|^2), \tag{2}$$

where E and μ are the energy and reduced mass of the pD system, respectively, and k_γ is the wave number of emitted photon. The spins of deuteron target I and incident proton s remain unchanged within the potential model. The calculation of the cross section in Eq. (2) relies on the matrix elements of electromagnetic transitions ($|M_{E1}|$ and $|M_{M1}|$), which involve the overlap between the scattering-state wave function (describing the collision of two nuclei) and the bound-state wave function (representing the fused nucleus). The matrix elements are detailed in previous works [7, 9].

The system is treated as a two-body problem, where an inert deuteron core captures a proton into a single-particle state. The matrix elements of the transitions can be simplified by the calculation of the single-particle reduced matrix element, in which the single-particle wave functions are key inputs for calculating the matrix elements of electromagnetic transitions from the scattering states to the bound state. The single-particle wave functions are obtained by solving the radial Schrödinger equation for bound and scattering states. The potentials serve as inputs

for these equations, providing the framework for the calculation of wave functions essential to determining the cross section and S-factor.

2.2. Phenomenological potentials

The potential includes contributions from the nuclear potential and the Coulomb potential

$$V(r) = V_{\text{cent.}}(r) + V_{\text{s.o.}}(r)(\vec{\ell}\cdot\vec{\sigma}) + V_{\text{Coul.}}(r). \tag{3}$$

The nuclear potential can be decomposed into the nuclear central and the spin-orbit terms

$$V_{\text{cent.}}(r) = V_0[1+\exp((r-R_0)/a_0)]^{-1}, \tag{4}$$

$$V_{\text{s.o.}}(r) = \frac{2}{r}\frac{d}{dr}V_{\text{S}}[1+\exp((r-R_0)/a_0)]^{-1}, \tag{5}$$

where R_0 and a_0 are the radius and diffuseness of the Woods-Saxon form in fm, respectively. The form of the Woods-Saxon potential is used with $R_0 = 2.31$ fm and $a_0 = 0.37$ fm, as adopted from Refs. [6, 7]. The V_0 and V_{S} are the depths of the nuclear central potential and spin-orbit potential in MeV, respectively. The spin-orbit coupling strength is set to $V_{\text{S}} = 5$ MeV [7]. This work only adjusts the potential depth V_0 to simultaneously reproduce the binding energy and pD scattering. Finally, the Coulomb potential is of a uniformly charged sphere

$$V_{\text{Coul.}}(r) = \begin{cases} (3-r^2/R_0^2)e^2/(2R_0), & r < R_0 \\ e^2/r, & r \geq R_0 \end{cases}. \tag{6}$$

2.3. Reaction-rate function

After calculating the S-factor, the average reaction rate at temperature T is

$$R(T) = \sqrt{\frac{8}{\pi\mu}}\frac{N_A}{(k_BT)^{3/2}}\int \exp\left[-\frac{E}{k_BT} - 2\pi\eta(E)\right] S(E)\,dE, \tag{7}$$

where N_A and k_B are the Avogadro and Boltzmann constants, respectively. The integration is computed numerically using the Gaussian quadrature method. Additionally, the reaction-rate function can be approximated in polynomial form as

$$R_{\text{ana}}(T) \approx \exp\left(\frac{a_0}{T^{1/3}}\right)\sum_{i=1}^{18} a_i T^{(i-3)/3}, \tag{8}$$

where the coefficients a_i can be determined using optimization algorithms provided by the SciPy library. The value of reduced χ^2 for the fit is calculated as

$$\chi^2 = \frac{1}{N-p}\sum_{i=1}^{N}\left[\frac{R_{\text{ana}}(T_i) - R_{\text{num}}(T_i)}{R_{\text{ana}}(T_i)}\right]^2, \tag{9}$$

where $R_{\text{num}}(T_i)$ is the numerically calculated reaction rate, N is the number of data points, and p is the number of fitted parameters.

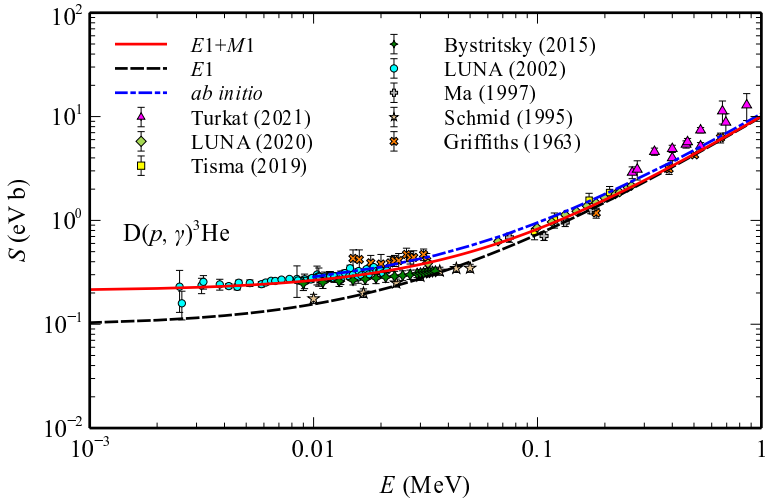

Fig. 1. Calculated and experimental astrophysical S-factors for the pD radiative capture reaction.

3. Result and discussions

For the bound state, the ground state of ^{3}He is modeled as a proton coupled to the deuterium core, which has a ground-state spin $I = 1$. In the framework of the shell model, it is conventional to describe approximately ^{3}He as three nucleons occupying the $1s_{1/2}$ states. Consequently, the bound proton is described in the $1s_{1/2}$ state. The binding energy of the proton in the $1s_{1/2}$ state $E_{s_{1/2}} = -5.49$ MeV is equal to the energy released by the reaction. To reproduce this binding energy value, a depth of $V_0 = -32$ MeV for the bound state is extracted.

In the continuum state, the $E1$ transitions originate from scattering p states to the bound $1s_{1/2}$ state, while the $M1$ transitions occur from the scattering s state. As validated in Ref. [7] for both pD radiative capture and elastic scattering, the potential depth of $V_0 = -27$ MeV for scattering was determined to provide the best description.

Figure 1 shows the contribution of both the $E1$ and $M1$ transitions below 1 MeV. The significance of the $M1$ transition was highlighted in the energy region below 100 keV, particularly in its contributions to the astrophysical S-factor and reaction rate, as emphasized in Ref. [7]. At the most relevant energy range for astrophysics [2], the S-factor of $M1$ transition contributed approximately 11%-16% [7]. At 0.01 GK, excluding the $M1$ contribution reduces the reaction rate by approximately 40% compared to the combined $E1 + M1$ contributions. The extrapolated values in the $E1$ and $M1$ transitions are $S_{E1}(0) = 0.098$ eV b and $S_{M1}(0) = 0.113$ eV b. The total extrapolated value of $S(0)$ is 0.211 ± 0.016 eV b. The value of $S(E)$ is in good agreement with the experimental data below 1 MeV [2, 10–16]. Moreover, the S-factor obtained using the potential model in this study aligns closely with modern *ab initio* calculations reported in Ref. [17], as shown in Figure 1.

In this work, the total astrophysical S-factor calculated for energies up to 2 MeV, serves as the upper limit in the integral of Eq. (7). Figure 2 presents the reaction rate for pD radiative capture, with the rates analytically approximated using the formula from Eq. (8). In our calculation, the temperature range extends up to 4 GK with a step size of 10^{-3} GK, resulting in $N = 4000$ data points. The fit involves $p = 19$ parameters, as described by Eq. (8). The reduced χ^2 value of

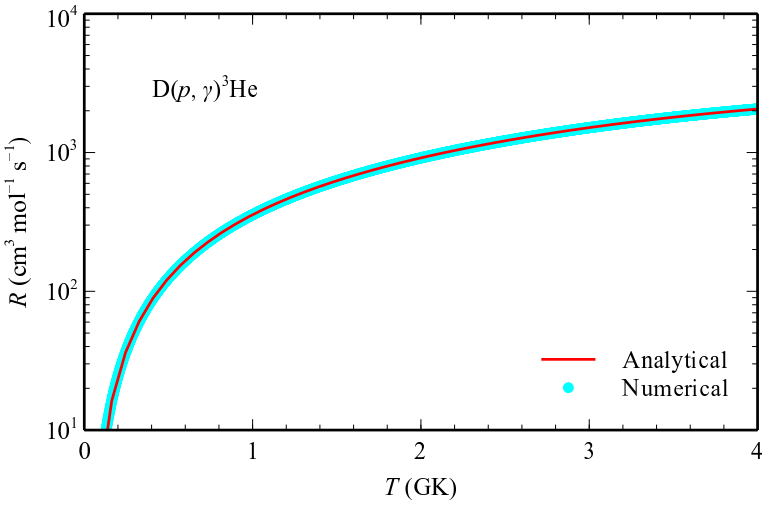

Fig. 2. Reaction rate of the pD radiative capture.

the reaction-rate fit is determined to be 0.00237. All coefficients a_i for the reaction-rate function $R(T)$, listed in Table 1, can be easily incorporated into BBN calculation programs to facilitate accurate computations of primordial deuterium abundances, such as Public Algorithm Evaluating the Nucleosynthesis of Primordial Elements (PArthENoPE) [8].

Table 1. The coefficients a_i used in analytical solution of $R(T)$.

i	a_i	i	a_i
0	0.12	10	−39631.84
1	0.05	11	31486.67
2	−1.47	12	−220.37
3	17.84	13	−13082.87
4	−99.60	14	−86.08
5	178.18	15	11560.20
6	678.37	16	−8987.71
7	−3397.30	17	2901.34
8	1309.70	18	−357.33
9	18048.75		

4. Conclusions

While modern microscopic methods can also address the pD radiative capture problem, this study demonstrates that the potential model offers a simple yet effective framework for analyzing the reaction. From a physics perspective, only one parameter is used in this study: the nuclear central potential depth of the Woods-Saxon form. The reaction rate obtained in this study exhibits

high reliability, with the computed S-factor showing good agreement with experimental data. Furthermore, a reliable polynomial for the pD radiative capture reaction rate is presented, containing 19 coefficients. Based on the coefficients of the reaction-rate function, future work will aim to calculate primordial abundances to more accurately determine the deuterium-hydrogen ratio (D/H) in the BBN calculations.

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Conflict of interest

The authors have no conflicts of interest to declare.

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