

Application of the calculable R -matrix method to study the (p, γ) reaction

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Abstract. *We apply the calculable R -matrix method to determine the (p, γ) cross section. We compare our cross-section calculation for the benchmark $^{12}\text{C}(p, \gamma)^{13}\text{N}$ reaction with results from the widely used FRESKO and RADCAP codes, which use the conventional Numerov method. Our calculations are in good agreement with these codes. Furthermore, we extend the calculable R -matrix method to accommodate non-local potentials.*

Keywords: (p, γ) reaction, calculable R -matrix, local potential, nonlocal potential.

Classification numbers: 25.70.Hi, 21.60.Cs, 24.10.Eq.

1. Introduction

Following the Big Bang, hydrogen constituted over 74% of the universe's baryonic mass. Given this abundance, nuclear reactions involving hydrogen, particularly the (p, γ) reaction at low energies, represent a crucial link in cosmic evolution [1, 2]. For light nuclei, the direct capture mechanism often dominates over compound nucleus formation in (p, γ) reactions at astrophysical energies. These direct capture reactions occur in numerous processes, including Big Bang nucleosynthesis, stellar evolution, and element synthesis across various astrophysical sites [2, 3]. Consequently, accurately determining the cross section for direct proton capture is essential for nuclear astrophysics.

Several theoretical approaches exist to describe the direct capture cross section at low energies near the Coulomb barrier [4]. Two common frameworks are the phenomenological R -matrix

method [5,6] and microscopic models [4]. The phenomenological R -matrix method effectively parameterizes experimental data in terms of resonance properties and the Asymptotic Normalization Coefficient (ANC) of the final bound state. However, its predictive power is limited without available experimental data, especially for reactions involving short-lived unstable nuclei. On the other hand, microscopic models aim to describe the (p, γ) reaction from fundamental nucleon degrees of freedom but involve significant complexity, particularly in fully accounting for the antisymmetrization of the involved nuclear wave functions.

A third widely used approach, adopted in this study, is the potential model [4, 7, 8]. This model offers a balance between phenomenology and microscopic principles. Its flexibility allows adjusting the nuclear potential to fit experimental data while retaining a microscopic connection through the potential itself. Calculating the direct capture cross section within the potential model requires determining the wave functions for the initial scattering state and the final bound state of the proton-nucleus system by solving the Schrödinger equation.

Standard numerical codes for direct capture calculations, such as FRESKO [9] and RADCAP [10], typically employ finite-difference methods like the Numerov algorithm [11] to solve the underlying Schrödinger equation. In this work, we utilize an alternative technique, which is the calculable R -matrix method [5, 12]. This method divides configuration space into internal and external regions. When combined with a Lagrange mesh basis and associated Gauss quadrature [12, 13], the calculable R -matrix method offers significant numerical advantages and simplifies the treatment of the Schrödinger equation.

A key strength of the calculable R -matrix method, particularly with the Lagrange-mesh implementation, is its ability to handle both local and non-local nuclear potentials consistently [5]. This technique was previously employed by Phuc *et al.* [14] to study non-locality effects in the $^{16}\text{O}(p,\gamma)^{17}\text{F}$ and $^{13}\text{C}(p,\gamma)^{14}\text{N}$ DC reactions. In contrast, widely used codes like FRESKO and RADCAP are generally restricted to local potentials. The non-local character of the nucleon-nucleus interaction, primarily stemming from the Pauli exclusion principle and couplings between different reaction channels [15], is physically important. While often approximated by equivalent local potentials, a direct treatment of non-locality is preferable. Methods based on iterative Numerov algorithms have been developed [16] but can encounter convergence difficulties. The calculable R -matrix approach provides a robust non-iterative alternative. We choose the specific $^{12}\text{C}(p,\gamma)^{13}\text{N}$ reaction for the non-local case precisely because it allows for a comparison with previous theoretical work [16], thus providing a crucial test of our method's ability to handle non-locality.

The present work aims to demonstrate the application and reliability of the Lagrange-mesh R -matrix method for calculating (p, γ) cross sections. We first benchmark our implementation against FRESKO and RADCAP using a local potential for the $^{12}\text{C}(p,\gamma)^{13}\text{N}$ reaction. We then extend the calculation to include a non-local Perey-Buck potential for the same reaction, comparing our results with previous findings where possible.

2. Formalism

2.1. The (p, γ) cross section with potential model

In this section, we summarize the formalism for calculating the direct (p, γ) cross section within the potential model. The mechanism of the (p, γ) reaction involves a transition from the

scattering state of the proton-nucleus system to a bound state via gamma emission through an electric transition. Note that in some cases, magnetic transitions may dominate over electric ones. However, this study focuses solely on electric transitions. The cross section for proton capture with gamma emission of multipolarity λ is proportional to the squared modulus of the matrix element between the scattering and bound state wave functions, and is given by [8, 10, 17]

$$\sigma_{\lambda, J_i \rightarrow J_f}(E) = \frac{4\pi(\lambda+1)(2\lambda+1)}{\lambda[(2\lambda+1)!!]^2} \frac{\mu c^2}{(\hbar c)^2} \frac{k_\gamma^{2\lambda+1}}{k^3} C_\lambda^2 \frac{(2J_i+1)(2J_f+1)}{(2S+1)} S_F \times \sum_{l_i, j_i} \left| i^{l_i} (-1)^{j_f+l_f} \hat{j}_i \hat{j}_f \hat{l}_i \begin{Bmatrix} j_i & J_i & S \\ J_f & j_f & \lambda \end{Bmatrix} \begin{Bmatrix} l_i & j_i & \frac{1}{2} \\ j_f & l_f & \lambda \end{Bmatrix} \langle l_i 0, \lambda 0 | l_f 0 \rangle I(k) \right|^2, \quad (1)$$

where $\mu = m_A m_p / (m_A + m_p)$ is the reduced mass of the proton-nucleus system, m_p and m_A are the masses of the proton and the target nucleus, respectively. $C_\lambda = e [m_A^\lambda + Z_A (-m_p)^\lambda] / m_B^\lambda$ is the effective charge, Z_A is the proton number of the target nucleus, m_B is the mass of the nucleus formed after capture, S is the spin of the target. S_F is the spectroscopic factor of the bound state, which characterizes the probability of finding the proton-nucleus A configuration within nucleus B and is often treated as a parameter fitted to experimental data. $j_f = |l_f \pm 1/2|$ and $j_i = |l_i \pm 1/2|$ are the total angular momenta of the proton in the final and initial states, respectively, l_f and l_i are the corresponding orbital angular momenta, and $\hat{j} = \sqrt{2j+1}$. k and k_γ are the wave numbers of the proton with energy E and the emitted photon with energy E_γ .

In Eq. (1), the overlap integral $I(k)$ is defined as

$$I(k) = \int_0^\infty \phi_{n_f l_f j_f}(r) \chi_{l_i j_i}(k, r) r^\lambda dr, \quad (2)$$

where $\chi_{l_i j_i}(E, r)$ is the scattering wave function and $\phi_{n_f l_f j_f}$ is the bound state wave function (n_f is the principal quantum number). For the $A(p, \gamma)B$ reaction at low energies below the Coulomb barrier, the reaction occurs only via the quantum tunneling, and cross section $\sigma(E)$ decreases rapidly with the decreasing energy. For convenience, instead of the reaction cross section, the astrophysical S-factor $S(E)$ is commonly used, defined as

$$S(E) = E \exp(2\pi\eta) \sigma(E), \quad (3)$$

where $\eta = Z_A e^2 / (\hbar v)$ is the Sommerfeld parameter, and v is the relative velocity between the proton and the target. The astrophysical S-factor $S(E)$ and the (p, γ) cross section are considered equivalent, differing only by the energy-dependent factor $E \exp(2\pi\eta)$. However, in nuclear astrophysics, the astrophysical S-factor $S(E)$ is preferred because it directly relates to the reaction rate in stellar environments. Thus, to calculate the direct (p, γ) cross section, we need to determine the overlap integral $I(k)$ in Eq. (2) using the scattering wave function $\chi_{l_i j_i}(E, r)$ and the bound state wave function $\phi_{n_f l_f j_f}$. These two wave functions are obtained by solving the Schrödinger equation for a local proton-nucleus potential (a potential depending only on the distance r between the proton and the center of the nucleus) as follows

$$-\frac{\hbar^2}{2\mu} \left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} \right] \psi_{l_j}(k, r) + [V_L(r) + X_{l_j} V_{SO}(r) + V_C(r)] \psi_{l_j}(k, r) = E \psi_{l_j}(k, r). \quad (4)$$

The solution $\psi_{l_j}(r)$ for $E > 0$ corresponds to the scattering state and is denoted as $\chi_{l_i j_i}(r)$, while for $E < 0$, it corresponds to the bound state, denoted as $\phi_{n_f l_f j_f}(r)$. $X_{l_j} = [j(j+1) - l(l+1) - 3/4]$ is

the spin-orbit coupling coefficient between the proton and the relative orbital angular momentum, $V_L(r)$ and $V_{SO}(r)$ are the central and spin-orbit components of the local potential, respectively. $V_C(r)$ is the Coulomb potential, typically assumed to arise from a uniformly charged sphere with radius $R_C = r_C A^{1/3} = 1.25 A^{1/3}$ (fm).

$$V_C(r) = \begin{cases} \frac{Z_A e^2}{r}, & r > R_C \\ \frac{Z_A e^2}{2R_C} \left(3 - \frac{r^2}{R_C^2}\right), & r \leq R_C. \end{cases} \quad (5)$$

The central component of the local potential is commonly taken to have the phenomenological Woods-Saxon (WS) form, while the spin-orbit potential is often modeled as the derivative of the WS form

$$V_L(r) = -V_L f_c(r), \quad (6)$$

$$V_{SO}(r) = V_{SO} \left(\frac{\hbar}{m_\pi c}\right)^2 \frac{1}{r} \frac{d}{dr} f_{SO}(r), \quad (7)$$

$$\text{with } f_x(r) = \left[1 + \exp\left(\frac{r - R_x}{a_x}\right)\right]^{-1}, \quad x = c, \text{SO}. \quad (8)$$

R_x and a_x are the radius and diffuseness parameters of the WS potential, respectively. $[\hbar/(m_\pi c)]^2 \approx 2 \text{ fm}^2$ is the square of the pion Compton wavelength. Note also that in calculations of the direct (p, γ) cross section, the phenomenological WS potential can be replaced by more microscopic potential models.

In nuclear scattering, the non-locality of the optical potential arises from two primary sources. First, it originates from the antisymmetrization requirement imposed by the Pauli exclusion principle on the system's wave function when the incident proton is exchanged with nucleons in the target [15]. Second, it arises from couplings between the elastic scattering channel and the nonelastic channels. In this process, the nucleus at position \mathbf{r} , after being excited, returns to its ground state at position \mathbf{r}' , contributing to the non-locality of the optical potential. Within a phenomenological framework, the central potential component can be taken in the Perey-Buck (PB) form [18]. The Schrödinger equation then becomes

$$-\frac{\hbar^2}{2\mu} \left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} \right] \psi_{lj}(k, r) + [V_C(r) + X_{lj} V_{SO}(r)] \psi_{lj}(k, r) + \int v_l(r, r') \psi_{lj}(k, r') dr' = E \psi_{lj}(k, r), \quad (9)$$

where

$$v_l(r, r') = U \left(\frac{r+r'}{2}\right) \frac{1}{\pi^{1/2} \beta} \exp\left[-\frac{(r^2+r'^2)}{\beta^2}\right] 2i^l z j_l(-iz), \quad (10)$$

with $U(x) = V_{NL} f_c(x)$ and $z = 2rr'/\beta^2$. β represents the non-locality range. $j_l(x)$ is the spherical Bessel function, and $f_c(x)$ is defined as in Eq. (8) for the local potential. The Schrödinger equation (9) is more general than Eq. (4) because its left-hand side incorporates both local (spin-orbit, Coulomb) and non-local (central) potential terms.

2.2. The Calculable R-matrix Method

As discussed previously, the direct (p, γ) cross section is determined from the scattering and bound wave functions obtained by solving the Schrödinger equation (4) or (9). In this study, we employ the *calculable R-matrix method* to determine these wave functions [5, 14]. The fundamental principle of solving the Schrödinger equation within the *R-matrix framework* involves dividing the configuration space into two regions at a channel radius $r = b$: an internal region ($r \leq b$) and an external region ($r > b$). For the calculable *R-matrix method*, the radius b is chosen to be sufficiently large so that the nuclear potential vanishes in the external region. In the internal region, the wave function is expanded over a basis set $\{\varphi_n\}$ as follows

$$\psi_{lj}^{\text{int}}(r) = \sum_{n=1}^N c_n \varphi_n(r). \quad (11)$$

In the external region $r > b$, the wave function depends on the energy E . If $E > 0$, $\psi_{lj}(r)$ corresponds to the scattering wave function of the initial state, denoted as χ_{lj} . This wave function has the asymptotic form

$$\chi_{lj}^{\text{ext}}(k, r) \equiv \psi_{lj}^{\text{ext}}(r) = [F_{l_i}(kr) \cos \delta_{l_i j_i} + G_{l_i}(kr) \sin \delta_{l_i j_i}] \text{ with } r > b, \quad (12)$$

where $\delta_{l_i j_i}$ is the nuclear phase shift, and F_{l_i} and G_{l_i} are the regular and irregular Coulomb functions, respectively [19]. Conversely, if $E < 0$, $\psi_{lj}(r)$ corresponds to the bound state wave function of the final state, denoted as $\phi_{n_f l_f j_f}(r)$. This wave function has an asymptotic form expressed via the Whittaker function W as [19]

$$\phi_{n_f l_f j_f}^{\text{ext}}(r) \equiv \psi_{lj}^{\text{ext}}(r) = a_{n_f l_f j_f} W_{-\eta, l_f + 1/2}(2\kappa r), \text{ for } r > b. \quad (13)$$

Here, $a_{n_f l_f j_f}$ is the Asymptotic Normalization Coefficient (ANC) of the bound state wave function, and κ is the wave number associated with the bound state energy. The scattering and bound states can be fully determined by calculating the coefficients c_n in (11) by solving the corresponding system of equations.

$$\sum_{n=1}^N C_{in}(E, B) c_n = \frac{\hbar^2}{2\mu} \varphi_i(b) \left. \frac{d\psi_{lj}^{\text{ext}}(r)}{dr} \right|_{r=b}, \quad (14)$$

where the matrix elements $C_{in}(E, B)$ are given by.

$$C_{in}(E, B) = \int \varphi_i(r) \left\{ -\frac{\hbar^2}{2\mu} \left[\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} \right] + V_C(r) + X_{lj} V_{so}(r) - E + \mathcal{L}(B) \right\} \times \varphi_n(r) dr + \int \varphi_i(r) v_l(r, r') \varphi_n(r') dr dr', \quad (15)$$

with $\mathcal{L}(B)$ being the Bloch operator [5, 20].

For the case of the scattering wave function, B is set to 0. Consequently, the internal wave function can be computed from the external wave function as

$$\chi_{lj}^{\text{int}}(k, r) = \frac{\hbar^2}{2\mu b \mathcal{R}_{lj}(E)} \chi_{lj}^{\text{ext}}(k, r)(b) \sum_{j=1} \varphi_j(r) (\mathbf{C}^{-1})_{ij} \varphi_i(b), \quad (16)$$

where the matrix \mathbf{C} with elements defined in (15), and $\mathcal{R}_{lj}(E)$ is defined as follows

$$\mathcal{R}_{lj}(E) = \frac{\hbar^2}{2\mu b} \sum_{i,n=1}^N \varphi_i(b) (\mathbf{C}^{-1})_{in} \varphi_n(b). \quad (17)$$

For the case of the bound wave function, a convenient choice for the boundary parameter B in Eq. (14) is

$$B = S_l(E_B) = 2\kappa b \frac{W'_{-\eta, l+1/2}(2\kappa r)}{W_{-\eta, l+1/2}(2\kappa r)}, \quad (18)$$

where W' denotes the derivative of the Whittaker function with respect to its argument. This choice simplifies the calculations by causing the right-hand side of Eq. (14) to vanish, thereby reducing Eq. (14) to a simpler form

$$\sum_{n=1}^N C_{in}(E, B) c_n = 0, \quad (19)$$

This system of equations resembles a standard eigenvalue problem, and by solving these equations, we obtain

$$\phi_{nlj}^{int} = N_l^{-1/2} \sum_{n=1}^N c_n \varphi_n(r). \quad (20)$$

The factor $N_l^{-1/2}$ appears in Eq. (20) to ensure that the wave function ϕ is normalized to 1. Thus, using the calculable R -matrix method, we can determine both the scattering and bound state wave functions. Subsequently, we can calculate the overlap integral using Eq. (2) and the γ -ray cross section using Eq. (1).

3. Results and discussion

3.1. Calculations with local potential

To verify the reliability of our (p, γ) cross section calculations using the calculable R -matrix method, we compare our results with two widely used codes for direct (p, γ) reactions: FRESKO [9] and RADCAP [10]. The FRESKO code [9], developed by Ian Thompson, is extensively used in nuclear reaction theory studies. The other code, RADCAP [10], was developed by Carlos Bertulani. While less common than FRESKO, RADCAP is specifically designed for (p, γ) reactions, whereas FRESKO applies to various reaction types. Consequently, RADCAP is often considered more user-friendly than FRESKO for this specific purpose. Note that both of these programs can only calculate the (p, γ) cross section using local potentials.

We consider the benchmark case of the $^{12}\text{C}(p, \gamma)^{13}\text{N}$ reaction. This reaction initiates the CNO cycle, which fuses hydrogen into helium in hot stellar environments and plays a crucial role in energy production in massive stars [21]. The reaction is dominated by a single-particle $E1$ transition from the $s_{1/2}$ scattering state to the $1p_{1/2}$ bound ground state of ^{13}N . The ^{13}N ground state is considered to have a configuration of a single proton with $j_b = 1/2$ coupled to a ^{12}C core with spin $S = 0$, and has a binding energy $E_B = -1.943$ MeV. The $^{12}\text{C}(p, \gamma)^{13}\text{N}$ capture cross section exhibits a resonance peak at $E_R \approx 0.422$ MeV, corresponding to the $p+^{12}\text{C}$ scattering system having spin-parity $1/2^+$ [22–24].

To calculate the $^{12}\text{C}(p, \gamma)^{13}\text{N}$ reaction, we use a local central potential of the phenomenological WS form, as described by Eqs. (4), with fixed parameters $R_c = 1.2A^{1/3}$ fm and $a_c = 0.65$

Table 1. Woods-Saxon potential parameters used in describing the $^{12}\text{C}(p, \gamma)^{13}\text{N}$ reaction with different calculation codes. The deviation is calculated relative to the R -matrix result.

Code	$E_R(E_B)$ (MeV)	V_L (MeV)	R_c (fm)	a_c (fm)	Deviation %
Scattering wave function					
R -matrix	0.422	56.78	2.862	0.65	-
FRESCO	0.422	56.79	2.862	0.65	0.18
RADCAP	0.422	57.10	2.862	0.65	0.56
Bound wave function					
R -matrix	-1.943	43.54	2.862	0.65	-
FRESCO	-1.943	43.68	2.862	0.65	0.32
RADCAP	-1.943	43.73	2.862	0.65	0.43

fm. We assume a local spin-orbit potential with parameters set to $V_{SO} = 5$ MeV, $R_{SO} = 1.25A^{1/3}$ fm, and $a_{SO} = 0.65$ fm. Only the depth V_L of the central potential component is varied to reproduce the binding energy $E_B = -1.943$ MeV for the bound state and the resonance energy $E_R \approx 0.422$ MeV for the scattering state. The potential depths obtained from the calculable R -matrix, FRESCO, and RADCAP calculations are presented in Table 1.

Table 1 shows that the potential depths V_L obtained from the three codes are very close. For the scattering wave function, our calculable R -matrix calculation yields $V_L = 56.78$ MeV. The depths from FRESCO and RADCAP are similar, with deviations relative to the R -matrix result being less than 0.6%. Likewise, for the bound wave function, the potential depths from FRESCO and RADCAP differ from the R -matrix result by less than 0.5%.

In addition to the potential depths, the astrophysical S-factor $S(E)$ calculated by the three programs is compared in Fig. 1. To match the experimental data, a spectroscopic factor of $S_F = 0.4$ was used in all three calculations. The difference in the calculated $S(E)$ values among the three programs is less than 1%. With such small discrepancies, the $S(E)$ results from the three codes are virtually indistinguishable on the graph. This outcome confirms the reliability of our (p, γ) cross section calculations based on the calculable R -matrix method.

3.2. Calculations with non-local potential

We have also extended the calculation for the $^{12}\text{C}(p, \gamma)^{13}\text{N}$ reaction to include the non-local potential. Note that current research addressing the non-locality of the potential in the Schrödinger equation for direct (p, γ) reactions primarily relies on iterative methods [16]. However, since the code implementing this iterative approach has not been made public, we cannot directly compare our $S(E)$ calculated using the calculable R -matrix method with the results from Ref. [16]. Therefore, we compare the spectroscopic factor S_F obtained from the two methods. To fit the experimental astrophysical S-factor $S(E)$, our calculation yields $S_F = 0.35$ for the non-local potential case. This value matches the calculation by Tian *et al.* [16]. The calculated $S(E)$ with the non-local potential is presented in Fig. 2 and agrees well with the results of Tian *et al.* (compare with the dashed line in Fig. 2 of Ref. [16]).

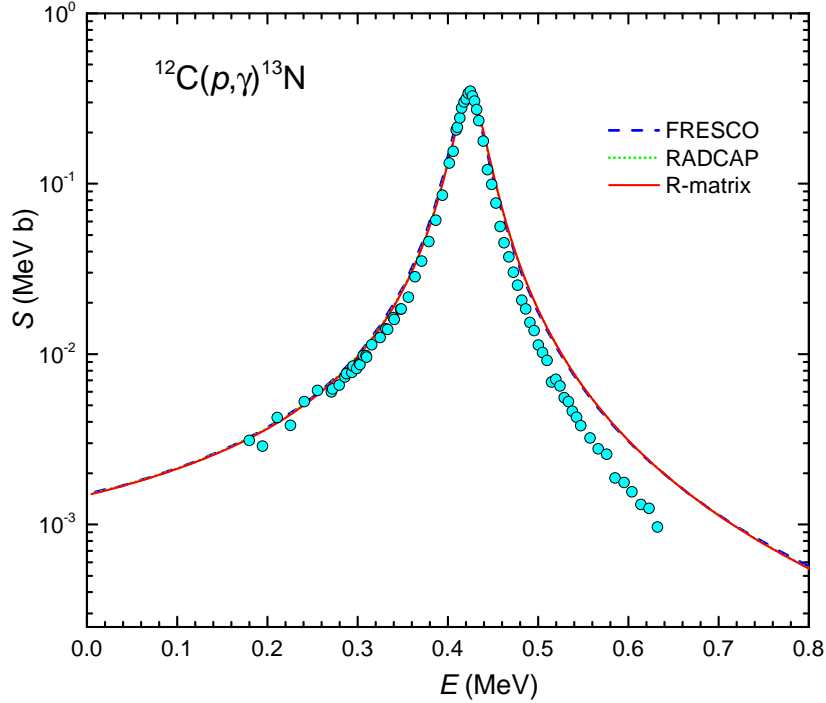


Fig. 1. Astrophysical S -factor for the $^{12}\text{C}(p, \gamma)^{13}\text{N}$ reaction calculated using FRESKO, RADCAP, and the calculable R -matrix method with a local phenomenological Woods-Saxon potential. The calculations were fitted to experimental data using a spectroscopic factor $SF = 0.4$ for all three codes. Experimental data are taken from [23].

4. Conclusions

We have successfully applied the calculable R -matrix method to calculate the (p, γ) cross section. We compared our results for the benchmark $^{12}\text{C}(p, \gamma)^{13}\text{N}$ reaction using a local potential with those from two widely used codes, FRESKO and RADCAP. The potential depths obtained from our method differ from those of FRESKO and RADCAP by less than 0.6%. The calculated astrophysical S -factor $S(E)$ shows excellent agreement with the FRESKO and RADCAP results, with deviations below 1%.

In addition to local potentials, we performed calculations using a non-local potential. Since no publicly available code calculates the (p, γ) cross section with a non-local potential, we compared the spectroscopic factor S_F derived from our calculation with the value reported by Tian *et al.* [16]. The results show perfect agreement between the two methods. The successful application of the R -matrix method to calculate the (p, γ) cross section confirms the reliability of this method for the study of other capture reactions within the CNO cycle. In particular, we plan to investigate the influence of potential non-locality on these reactions in the astrophysically relevant energy range.

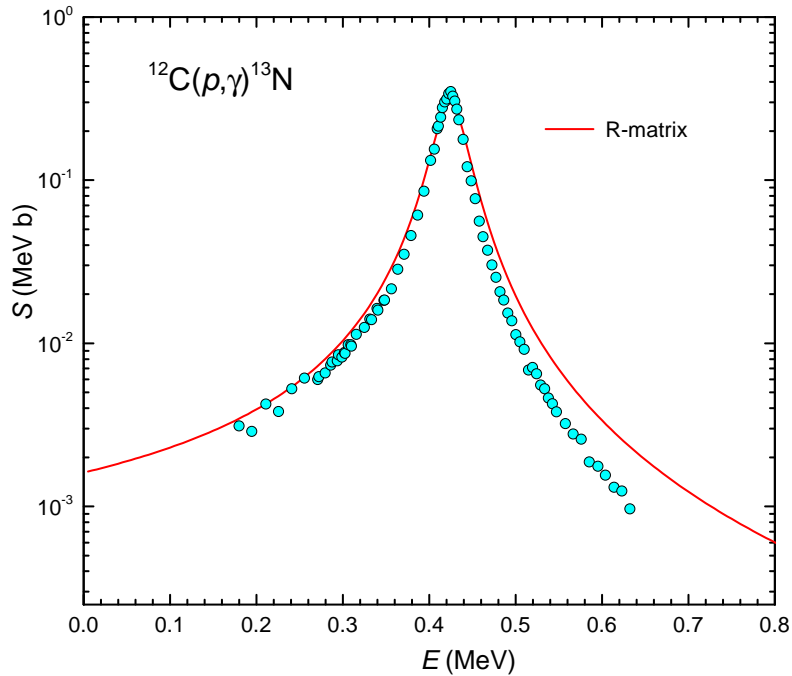


Fig. 2. Astrophysical S-factor for the $^{12}\text{C}(p, \gamma)^{13}\text{N}$ reaction calculated using the calculable R -matrix method with a phenomenological non-local Perey-Buck (PB) potential. The calculation was fitted to experimental data using a spectroscopic factor $SF = 0.35$. Experimental data are taken from [23].

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