

Theoretical analysis of double-differential cross-sections of neutron, proton, deuteron, ^3He , and α for the $p+^6\text{Li}$ reaction

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Abstract

Based on the unified Hauser-Feshbach and exciton model, which can describe the particle emission processes between discrete energy levels with energy, angular momentum, and parity conservations, a statistical theory of light nucleus reaction (STLN) is developed to calculate the double-differential cross-sections of the outgoing neutron and light charged particles for the proton-induced ^6Li reaction. A significant difference is observed between the $p + ^6\text{Li}$ and $p + ^7\text{Li}$ reactions owing to the discrepancies in the energy-level structures of the targets. The reaction channels, including sequential and simultaneous emission processes, are analyzed in detail. Taking the double-differential cross-sections of the outgoing proton as an example, the influence of contaminations (such as ^1H , ^7Li , ^{12}C , and ^{16}O) on the target is identified in terms of the kinetic energy of the first emitted particles. The optical potential parameters of the proton are obtained by fitting the elastic scattering differential cross-sections. The calculated total double-differential cross-sections of the outgoing proton and deuteron at $E_p = 14$ MeV agree well with the experimental data for different outgoing angles. Simultaneously, the mixed double differential cross-sections of ^3He and α are in good agreement with the measurements. The agreement between the measured data and calculated results indicates that the two-body and three-body breakup reactions need to be considered, and the pre-equilibrium reaction mechanism dominates the reaction processes. Based on the STLN model, a PLUNF code for the $p + ^6\text{Li}$ reaction is developed to obtain an ENDF-6-formatted file of the double-differential cross-sections of the nucleon and light composite charged particles.

Full Text

Preamble

Theoretical analysis of double-differential cross-sections of neutron, proton, deuteron, ^3He , and α for the $p+^6\text{Li}$ reaction*

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Based on the unified Hauser-Feshbach and exciton model, which can describe particle emission processes between discrete energy levels with conservation of energy, angular momentum, and parity, we have developed a statistical theory of light nucleus reaction (STLN) to calculate the double-differential cross-sections of outgoing neutrons and light charged particles for proton-induced reactions on ^6Li . A significant difference is observed between the $p + ^6\text{Li}$ and $p + ^7\text{Li}$ reactions due to discrepancies in the energy-level structures of the target nuclei. The reaction channels, including both sequential and simultaneous emission processes, are analyzed in detail. Using the double-differential cross-sections of outgoing protons as an example, we identify the influence of target contaminants (such as ^1H , ^7Li , ^{12}C , and ^{16}O) based on the kinetic energy of the first emitted particles. The optical potential parameters for protons are obtained by fitting elastic scattering differential cross-sections. The calculated total double-differential cross-sections for outgoing protons and deuterons at $E_p = 14$ MeV agree well with experimental data at various emission angles. Simultaneously, the mixed double-differential cross-sections for ^3He and α particles are in good agreement with measurements. This agreement indicates that both two-body and three-body breakup reactions must be considered, and that the pre-equilibrium reaction mechanism dominates the reaction processes. Based on the STLN model, we have developed a PLUNF code for the $p + ^6\text{Li}$ reaction to generate an ENDF-6-formatted file of double-differential cross-sections for nucleons and light composite charged particles.

Keywords: Statistical theory of light nucleus reaction, $p + ^6\text{Li}$ reaction, Light composite charged particle, Double-differential cross-sections, Two-body breakup, Three-body breakup

INTRODUCTION

Nuclear data—including cross-sections for all reaction channels, differential cross-sections, and double-differential cross-sections—for nucleon-induced reactions on ${}^6\text{Li}$, ${}^7\text{Li}$ are important for various applications such as compact accelerator-driven neutron sources and the International Fusion Materials Irradiation Facility (IFMIF), as discussed in Refs. [1–7]. A lithium-glass scintillator containing natural lithium is used as a small-angle neutron scattering spectrometer (SANS) for materials research at the China Spallation Neutron Source (CSNS) to satisfy both neutron detection efficiency and gamma elimination requirements [8]. In molten salt fast reactors (MSFRs), ${}^7\text{Li}$ enrichment and ${}^6\text{Li}$ inventory are important influencing factors [9]. In recent years, lithium has received considerable attention in astrophysics because it can lead to a better understanding of the evolution and formation of the universe. The standard big-bang nucleosynthesis (BBN) theory overestimates primordial ${}^7\text{Li}$ abundance by a factor of approximately three to four, a discrepancy known as the cosmological lithium problem [10]. The reaction ${}^6\text{Li}(p, \gamma){}^7\text{Be}$ plays an important role in the consumption of ${}^6\text{Li}$ and the formation of ${}^7\text{Be}$, which eventually decays into ${}^7\text{Li}$ at the end of big-bang nucleosynthesis [11]. In the atmospheres of approximately 1% of giant stars, there exists an anomalous elevation in lithium abundance that directly contradicts expectations from conventional stellar evolution models. Studying an extremely Li-rich giant (possibly newly enriched) and its evolutionary stage is therefore important [12]. Furthermore, in-depth investigation of nucleon- ${}^6, {}^7\text{Li}$ reactions will enhance our understanding of 1p-shell light nuclear reactions [13–15].

Although ${}^6\text{Li}$ and ${}^7\text{Li}$ differ by only one neutron, they exhibit significant differences. The natural abundance of ${}^6\text{Li}$ is only 7.5%, whereas that of ${}^7\text{Li}$ is as high as 92.5%. The energy levels of ${}^6\text{Li}$ and ${}^7\text{Li}$ differ both in terms of their energies and widths. Additionally, every energy level of the ${}^6\text{Li}$ nucleus has a spin that is an even multiple of $1/2$, whereas the spin of the ${}^7\text{Li}$ nucleus is an odd multiple of $1/2$ [16]. ${}^6\text{Li}$ is easily captured by neutrons, producing ${}^7\text{Li}$ and high-energy gamma rays, whereas ${}^7\text{Li}$ is more likely to undergo α decay. Moreover, the capture cross-section of ${}^6\text{Li}$ is smaller than that of ${}^7\text{Li}$ in the thermal neutron energy range, making ${}^6\text{Li}$ a common material for slow neutron shielding in certain nuclear applications. Differences in the energy-level diagrams of ${}^6\text{Li}$ and ${}^7\text{Li}$ can lead to variations in their decay properties and the particles emitted from individual levels [1–6]. Therefore, the results of $n+{}^6, {}^7\text{Li}$ reactions are significantly different, as shown both experimentally and theoretically [1, 2, 7]. In our previous study, we successfully predicted the double-differential cross-sections of charged particles for the $p+{}^7\text{Li}$ reaction using the statistical theory of light nucleus reaction (STLN) model [15]. On this basis, we obtained an ENDF-6-formatted file of the double-differential cross-section. File-6 (the file of double-differential cross-sections) is one of the important files in the nuclear reaction database, recommended when the energy and angular distributions of emitted particles must be coupled, when it is important to provide a concurrent

description of neutron scattering and particle emission, when so many reaction channels are open that it is difficult to provide separate reactions, or when accurate distributions of charged particles or residual nuclei are required for particle transport, heat deposition, or radiation damage calculations [17]. However, there are still no publications describing the double-differential cross-sections of outgoing particles for the $p+6\text{Li}$ reaction.

Quantitatively describing all physical quantities is challenging because of the limited availability of comprehensive experimental data for the $p+6\text{Li}$ reaction. For the $p+6\text{Li}$ reaction, only a small number of experimental partial cross-sections exist for the (p, γ) , (p, el) , and $(p, 3\text{He})$ channels [18–20]. Furthermore, numerous elastic scattering angular distributions have been measured at various incident energies [20, 21]. Fortunately, the double-differential cross-sections of outgoing protons, deuterons, and the mixture of 3He and α for the $p+6\text{Li}$ reaction were measured in 1989 and 1991 [22, 23], making it possible to validate theoretical calculations. Evaluated partial cross-sections for (p, el) , $(p, 3\text{He})$, and (p, x) are available in nuclear reaction databases such as ENDF/B-VIII.0 [24] and JENDL-5 [25]. However, the double-differential cross-sections of outgoing neutrons and charged particles were not included in these databases because the effects of secondary particle emission processes between discrete levels and cluster separations in light nuclear reactions have not been considered. In ENDF/B-VIII.0, the cross-sections of (p, el) , $(p, 3\text{He})$, and (p, x) were derived from R-matrix analysis [24, 26], while in JENDL-5, multichannel R-matrix fitting was used to evaluate experimental data in the incident proton energy range from 10 keV to 3 MeV. The CCONE code [25] was employed to calculate the differential cross-sections of emitted particles in the incident proton energy range from 3 to 200 MeV. Subsequently, proton-induced reactions on $6,7\text{Li}$ were also calculated using the CDCC method in 2013 [5], but the double-differential cross-sections of outgoing protons, deuterons, and tritons were not provided. A possible reason for this is that sequential secondary particle emission processes were not considered in the CDCC model [6].

This study provides an in-depth analysis of the $p+6\text{Li}$ reaction based on the STLN model with conservation of energy, angular momentum, and parity. The Coulomb barriers of both incident and exit channels are considered for different charged particles. Using an impure target as an example, the influence of contamination is described in terms of kinetic energy. The double-differential cross-sections of total outgoing protons, deuterons, and the mixture of 3He and α are calculated by analyzing reaction channels at different incident energies. The calculated results at $E_p = 14$ MeV agree well with available experimental data.

Section II briefly introduces the theoretical model used in this study. Section III analyzes the reaction channels of the $p + 6\text{Li}$ reaction below 20 MeV in detail. Section IV provides comparisons between calculated results and experimental data along with corresponding analysis. A summary is provided in the final section.

Fig. 1 [Figure 1: see original paper]. Schematic of momentum conservation in nuclear reactions in the laboratory system (LS).

Fig. 2 [Figure 2: see original paper]. (Color online) Measured and calculated total double-differential cross-sections of the outgoing proton for a proton-induced impure ${}^6\text{Li}$ reaction at an angle of 60° and $E_p = 14$ MeV in the laboratory system (LS). Panel (a) shows the experimental data from Ref. [23]. The black narrow bands in panel (b) represent contributions from outgoing protons originating from discrete levels (illustrated from ground state to the fifth energy level as marked) of target ${}^6\text{Li}$ and contaminants (including ${}^1\text{H}$, ${}^7\text{Li}$, ${}^{12}\text{C}$, and ${}^{16}\text{O}$).

II. THEORETICAL DESCRIPTIONS

A. Theoretical Framework

Based on the unified Hauser-Feshbach and exciton model [27], which can describe particle emission processes between discrete energy levels with conservation of energy, angular momentum, and parity, we have developed a statistical theory of light nucleus reaction (STLN) to describe the mechanism of nucleon-induced light nucleus reactions [13, 14]. A considerable amount of experimental data, particularly double-differential cross-sections—such as neutron-induced reactions on ${}^6\text{Li}$ [1], ${}^7\text{Li}$ [2], ${}^9\text{Be}$ [28, 29], ${}^{10}\text{B}$ [30], ${}^{11}\text{B}$ [31], ${}^{12}\text{C}$ [27, 32, 33], ${}^{14}\text{N}$ [34], ${}^{16}\text{O}$ [35, 36], and ${}^{19}\text{F}$ [37], as well as proton-induced reactions on ${}^7\text{Li}$ [15] and ${}^9\text{Be}$ [14, 38]—has been reproduced very well.

The cross-sections of first-emitted particles from the compound nucleus to discrete energy levels of the first residual nuclei can be expressed as:

$$\sigma_{m1,k1}(EL) = \sum_j \sigma_{j\pi} a(EL) \left[\sum_{n=0}^{n_{\max}} P_{j\pi}(n) \frac{W_{j\pi m1,k1}(n, E^*, c m1)}{W_{j\pi T}(n, E^*)} + Q_{j\pi}(n) \frac{W_{j\pi m1,k1}(E^*, c m1)}{W_{j\pi T}(E^*)} \right]$$

where $P_{j\pi}(n)$ is the occupation probability of the n -th exciton state in the $j\pi$ channel (j and π denote the angular momentum and parity in the final state, respectively). $P_{j\pi}(n)$ can be obtained by solving the j -dependent exciton master equation under angular momentum conservation in pre-equilibrium reaction processes [39]. $Q_{j\pi}(n)$ is the occupation probability of the equilibrium state in the $j\pi$ channel. $W_{j\pi m1,k1}(n, E^*, c m1)$ is the emission rate of the first emitted particle $m1$ in the n -th exciton state with outgoing kinetic energy $c m1$ in the center-of-mass system (CMS), and $W_{j\pi T}(n, E^*)$ is the total emission rate in the n -th exciton state. $W_{j\pi m1,k1}(E^*, c m1)$ is the emission rate of the first emitted particle $m1$ in the equilibrium state with outgoing kinetic energy $c m1$, and $W_{j\pi T}(E^*)$ is the total emission rate in the equilibrium state. E^* is the excitation energy of the compound nucleus, and $\sigma_{j\pi} a(EL)$ is the absorption cross-section in the $j\pi$ channel. The first term inside the brackets of Eq. (1) represents the pre-equilibrium process, which is the predominant process in $1p$ -shell light nucleus reactions induced by nucleons. The second term inside the brackets describes the equilibrium process.

The cross-section of the second outgoing particle from discrete energy levels of the first residual nucleus to discrete energy levels of the second residual nucleus can be expressed as:

$$\sigma_{k1 \rightarrow k2}(n, m1, m2) = \sigma_{k1}(n, m1) \cdot R_{k1 \rightarrow k2}(Ek1)$$

where $\sigma_{k1}(n, m1)$ is the cross-section of the first emitted particle $m1$ expressed in Eq. (1), and $R_{k1 \rightarrow k2}(Ek1)$ is the branching ratio of the second outgoing particle $m2$ from the energy level $Ek1$ of the first residual nucleus $M1$ to the energy level $Ek2$ of the second residual nucleus $M2$.

For simultaneous emission processes, for example $a + A \rightarrow b1 + b2 + b3$ (also called a breakup reaction), the total kinetic energy EC in the CMS can be expressed as:

$$EC = (MA / (MA + ma)) EL + Q$$

where ma and MA are the masses of projectile particle a and target A , respectively. EL is the incident energy, and Q is the reaction energy. According to Ohlsen theory [40], the momentum distribution function of particle $b1$ with momentum $k1$ in the CMS is expressed as:

$$f1(k1) = (k1, k2, k3) \delta(\sum_i ki) \delta(\sum_i \epsilon_i - EC) d^3k2 d^3k3$$

where mi denotes the mass of particle bi , and $\epsilon_i = k_i^2 / (2mi)$ denotes the kinetic energy of particle bi in the CMS. The δ functions represent momentum conservation and energy conservation. Assuming the momentum distribution function is constant (uniformly distributed in momentum space), a momentum transformation can be performed:

$$p2 = k2 + k3 \quad p3 = (m2 k3 - m3 k2) / (m2 + m3) \quad q3 = 3(k3 / m3 - k2 / m2)$$

where $3 = m2 m3 / (m2 + m3)$. From these transformations, we obtain:

$$2 d^3k2 = d^3p3 d^3q3$$

Here $M3 = m2 + m3$, $M2 = m2$, and $3 = m2 m3 / (m2 + m3)$. Thus Eq. (4) can be rewritten as:

$$f1(k1) = \delta(p3 + k1) \delta(p3^2 / (2M3) + q3^2 / (23) + 1 - EC) d^3p3 d^3q3$$

After performing double-vector integrations, Eq. (7) can be expressed as:

$$f1(k1) = 2\pi (23)^{3/2} \sqrt{M3 / (M3 + m1)} (EC - 1)^2$$

In terms of isotropic energy spectra in the CMS, as mentioned earlier, the energy spectra of particle $b1$ can be expressed using the momentum distribution function:

$$N1(1) d1 = f1(k1) d^3k1 = f1(k1) 4\pi m1 k1 dk1 = f1(k1) 4\pi m1 \sqrt{(2m1 1)} d1$$

Thus, the energy spectrum of particle b1 with outgoing kinetic energy E_1 or momentum k_1 in the CMS is expressed as:

$$N_1(E_1) = C_3 \sqrt{1 - \max_1 - E_1}$$

where $\max_1 = (M_3 / (m_1 + m_2 + m_3)) E_C$ denotes the maximum outgoing kinetic energy of particle b1. $C_3 = (15 / (8\pi (\max_1)^{5/2}))$ is the normalization constant given by $N_1(E_1) dE_1 = 1$.

Based on the isotropic energy spectra assumption in the CMS for three-body breakup reactions (i.e., the spectra for all azimuthal angles are identical), the double-differential cross-section of particle b1 in the CMS can be expressed as:

$$d^2\sigma / (d\Omega_1 dE_1) = \sigma_{\text{breakup}} (1 / (4\pi)) N_1(E_1)$$

Similarly, the double-differential cross-sections of b2 and b3 can also be expressed in the same form. We use E_C and $d\Omega_C = d\cos\theta_C d\phi_C$ to represent the kinetic energy and azimuthal angle of particle b_i in the CMS, respectively, without loss of generality. Similarly, E_L and $d\Omega_L = d\cos\theta_L d\phi_L$ represent the kinetic energy and azimuthal angle of particle b_i in the laboratory system (LS), respectively. In both measurements and theoretical calculations, $\phi_C = \phi_L$. The following relationship universally exists for double-differential cross-sections in the CMS and LS:

$$d^2\sigma / (d\Omega_L dE_L) = d^2\sigma / (d\Omega_C dE_C) \cdot |(\cos\theta_C, \theta_C) / (\cos\theta_L, \theta_L)|$$

According to the Jacobian determinant of the coordinate transformation, the double-differential cross-section of particle b_i in the laboratory system (LS) is expressed as [41]:

$$d^2\sigma / (d\Omega_L dE_L) = d^2\sigma / (d\Omega_C dE_C) \cdot (E_L / E_C)^{1/2} \cdot (m_a + M_A)^2 / (M_A (m_a + M_A - m_a \sqrt{(E_L / E_C) \cos\theta_L}))$$

with the transformation:

$$E_C = E_L + (m_a^2 / (m_a + M_A)^2) E_L - (2 m_a \sqrt{(E_L / E_C) \cos\theta_L} / (m_a + M_A)) \cos\theta_L$$

Equations (10-13) have been validated in our previous studies, such as $n+6\text{Li} \rightarrow 7\text{Li}^* \rightarrow n + d + \alpha$ [1], $n+7\text{Li} \rightarrow 8\text{Li}^* \rightarrow n + t + \alpha$ [2], and $p+7\text{Li} \rightarrow 8\text{Be}^* \rightarrow p + t + \alpha$ [15].

B. Coulomb Barrier

Fig. 3 [Figure 3: see original paper]. (Color online) Total double-differential cross-sections of the outgoing proton for the $p + 6\text{Li}$ reaction at angles of 20° , 30° , 40° , 50° , 60° , and 70° and $E_p = 14$ MeV in the laboratory system (LS). The black points denote experimental data from Ref. [23]. The red solid lines denote calculated results. The abrupt peaks represent contributions from contaminants such as 1H , 7Li , 12C , and 16O . Different outgoing angles are indicated in the figure.

For charged particle emission, the kinetic energy of the first outgoing charged particle c must be higher than the Coulomb barrier V_{Coul} , i.e., $c > V_{\text{Coul}}$. The reduced penetration factor calculated using the optical model potential must be zero if $c < V_{\text{Coul}}$. Assuming a spherical nucleus [13], V_{Coul} can be approximated as:

$$V_{\text{Coul}} = e^2 Z_{M1} Z_{m1} / r_C (A_{M1}^{1/3} + A_{m1}^{1/3})$$

where Z_{M1} , A_{M1} and Z_{m1} , A_{m1} are the charge and mass numbers of the residual nucleus and first outgoing charged particle, respectively. $r_C = 1.2-1.5$ fm is the charge radius. For the charge radii of the proton, deuteron, triton, ^3He , α , and ^5He , we use experimental data from Ref. [44].

Therefore, the incident energy E_p must satisfy the following equation for open reaction channels:

$$E_p \geq (M_C / M_T) [V_{\text{Coul}} + E_{k1} + B_1 - B_p]$$

where M_C , M_T , and M_1 are the masses of the compound nucleus, target nucleus, and first residual nucleus, respectively, after the first particle is emitted. E_{k1} denotes the excitation energy of the k -th discrete level of the first residual nucleus. B_1 is the binding energy of the first emitted particle in the compound nucleus. B_p is the binding energy of the incident particle in the compound nucleus. Clearly, the Coulomb barrier can significantly affect the open reaction channels.

C. Particle Identification

To conveniently describe the $A(a, b)B$ reaction, we define the following quantities: A , B , a , and b represent the target nucleus, residual nucleus, incident particle, and emitted particle, respectively. The target nucleus A is fixed in the LS, so its kinetic energy and momentum are zero. The Q -value is thus expressed as:

$$Q = E_b + E_B - E_a$$

where E_b , E_B , and E_a are the kinetic energies of b , B , and a in the LS, respectively. A schematic of momentum conservation in nuclear reactions in the LS is shown in Fig. 1, and momentum conservation is expressed as:

$$p_a = p_B + p_b$$

where $p_a = \sqrt{2 m_a E_a}$, $p_b = \sqrt{2 m_b E_b}$, and $p_B = \sqrt{2 m_B E_B}$ are the momenta of a , b , and B in the LS, respectively. Furthermore, m_a , m_b , and m_B are the masses of a , b , and B , respectively.

From Eqs. (16) and (17), the kinetic energy of the first emitted particle b in the LS can be expressed as:

$$E_b = [((A_a A_b E_a)^{1/2} / (A_b + A_B) \cos \theta \pm ((A_B - A_a) / (A_b + A_B) + (A_B A_a / (A_B + A_b)^2) \cos^2 \theta + (A_B / (A_B + A_b)) (Q / E_a))^{1/2}]^2$$

where $Aa = ma / \mu$, $Ab = mb / \mu$, and $AB = mB / \mu$ are the mass numbers of a , b , and B , respectively, with μ being the atomic mass unit.

III. ANALYSIS OF THE REACTION CHANNELS

Fig. 7 [Figure 7: see original paper]. (Color online) Same as Fig. 3, but for outgoing ${}^3\text{He}$ and α particles. The experimental data are from Ref. [22].

For the proton-induced ${}^6\text{Li}$ reaction, the following reaction channels theoretically exist at incident energies $E_p \leq 20$ MeV based on their threshold energies E_{th} :

$p + {}^6\text{Li} \rightarrow {}^7\text{Be}^* \rightarrow - (p, \gamma){}^7\text{Be}$, $Q = +5.606$ MeV, $E_{th} = 0.000$ MeV - $(p, n){}^6\text{Be}$, $Q = -5.071$ MeV, $E_{th} = 5.9206$ MeV - $(p, p){}^6\text{Li}$, $Q = 0.000$ MeV, $E_{th} = 0.000$ MeV - $(p, {}^3\text{He})\alpha$, $Q = +4.019$ MeV, $E_{th} = 0.000$ MeV - $(p, d){}^5\text{Li}$, $Q = -3.442$ MeV, $E_{th} = 4.0187$ MeV - $(p, np){}^5\text{Li}$, $Q = -5.666$ MeV, $E_{th} = 6.6153$ MeV - $(p, pn){}^5\text{Li}$, $Q = -5.666$ MeV, $E_{th} = 6.6153$ MeV - $(p, 2p){}^5\text{He}$, $Q = -4.594$ MeV, $E_{th} = 5.3637$ MeV - $(p, pd){}^4\text{He}$, $Q = -1.475$ MeV, $E_{th} = 1.7221$ MeV - $(p, dp){}^4\text{He}$, $Q = -1.475$ MeV, $E_{th} = 1.7221$ MeV

From Eq. (19), one can see obvious differences compared to the $p+{}^7\text{Li}$ reaction, as shown in Eq. (20) of Ref. [15]. For first-particle emission processes, the $p+{}^6\text{Li}$ reaction lacks the (p, t) and (p, α) channels. For second-particle emission processes, the $p+{}^6\text{Li}$ reaction lacks the $(p, n{}^3\text{He})$, (p, pt) , $(n, 2p)$, $(n, 2d)$, and (n, npd) channels. Furthermore, the threshold energies of the same channels are different.

Considering energy, angular momentum, and parity conservation in particle emission processes, the reaction channels for first-particle emission are:

$p + {}^6\text{Li} \rightarrow {}^7\text{Be}^* \rightarrow - n + {}^6\text{Be}^* (k_1 = \text{gs}, 1) - p + {}^6\text{Li}^* (k_1 = \text{gs}, 1, 2, 3, 4, 5) - d + {}^5\text{Li}^* (k_1 = \text{gs}, 1) - {}^3\text{He} + \alpha$

where k_1 denotes the energy levels of the first residual nuclei M_1 , and gs denotes the ground state. Their energy-level schemes are taken from experimental data in Refs. [16, 45, 46].

For the first-particle emission channel ${}^6\text{Li}(p, n){}^6\text{Be}$, the first residual nucleus ${}^6\text{Be}$ that reaches the first excited level can still emit a proton, leaving the second residual nucleus ${}^5\text{Li}$. Furthermore, the second residual nucleus ${}^5\text{Li}$ can emit a proton and alpha particle through direct two-body breakup, thus contributing to the $(p, n2p\alpha)$ reaction channel.

For the first-particle emission channel ${}^6\text{Li}(p, p){}^6\text{Li}$, the second excited energy level ($E_{k_1=2} = 3.563$ MeV) of the residual nucleus ${}^6\text{Li}$ cannot emit any particle because parity is not conserved; thus, this process contributes only to the inelastic scattering channel. The first and third excited energy levels of ${}^6\text{Li}$ can emit a deuteron, so they contribute to the $(p, pd\alpha)$ reaction channel. If the first residual nucleus ${}^6\text{Li}$ is in the k_1 -th ($k_1 \geq 4$) excited energy level, some levels will emit a proton with the second residual nucleus ${}^5\text{He}$. Furthermore, the second

residual nucleus ${}^5\text{He}$ can emit a neutron and alpha particle through direct two-body breakup, thereby contributing to the $(p, n2p\alpha)$ reaction channel. If the first residual nucleus ${}^6\text{Li}^*$ is in the k_1 -th ($k_1 \geq 4$) excited energy level, some levels can also emit a deuteron, so these processes contribute to the $(p, pd\alpha)$ reaction channel. Therefore, the first-particle emission channel ${}^6\text{Li}(p, p){}^6\text{Li}^*$ can contribute to both the $(p, n2p\alpha)$ and $(p, pd\alpha)$ reaction channels in the final state, in addition to elastic and inelastic channels.

For the first-particle emission channel ${}^6\text{Li}(p, d){}^5\text{Li}$, *the reaction process ${}^5\text{Li} \rightarrow p + \alpha$* occurs as mentioned above, so this channel belongs to the $(p, dp\alpha)$ reaction channel in the final state. For the first outgoing ${}^3\text{He}$ from the compound nucleus to the ground state of the first residual nucleus α , this process contributes only to the $(p, {}^3\text{He})\alpha$ reaction channel.

Based on the analyses of reaction channels discussed above, the total spectra can be determined by summing all partial spectra of the same outgoing particle obtained from every reaction channel. The contributions to the double-differential cross-sections of total emitted protons come from elastic scattering, inelastic scattering, direct three-body breakup, and the $(p, n2p\alpha)$ and $(p, pd\alpha)$ reaction channels. The contributions to the double-differential cross-sections of total emitted deuterons come from $(p, d){}^5\text{Li}$, $(p, pd\alpha)$, and *the direct three-body breakup process ${}^7\text{Be} \rightarrow p + d + \alpha$* . The contributions to the double-differential cross-sections of total emitted alpha particles come only from $(p, {}^3\text{He})\alpha$, $(p, n2p\alpha)$, $(p, pd\alpha)$, and the direct three-body breakup process ${}^7\text{Be}^* \rightarrow p + d + \alpha$. The contribution to the double-differential cross-section of total emitted ${}^3\text{He}$ comes only from the $(p, {}^3\text{He})\alpha$ reaction channel. It is worth mentioning that the experimental double-differential cross-sections represent a mixture of ${}^3\text{He}$ and α because of difficulties encountered in measurement [22].

In conclusion, for the proton-induced ${}^6\text{Li}$ reaction, the following reaction channels exist at incident energies $E_p \leq 20$ MeV:

$p + {}^6\text{Li} \rightarrow {}^7\text{Be}^* \rightarrow -n + {}^6\text{Be}^* (k_1 = \text{gs}, 1) \rightarrow p + {}^5\text{Li}^* \rightarrow p + \alpha (p, n2p\alpha) -$
 $p + {}^6\text{Li}^* (k_1 = \text{gs}, 1, 2, 3, 4, 5) \rightarrow -\text{Compound elastic } (p, p) - p + {}^5\text{He}^* \rightarrow$
 $n + \alpha (p, n2p\alpha) - d + \alpha (p, pd\alpha) - d + {}^5\text{Li}^* (k_1 = \text{gs}, 1) \rightarrow p + \alpha (p, pd\alpha) -$
 ${}^3\text{He} + \alpha (p, {}^3\text{He})\alpha - \text{Direct three-body breakup } (p, pd\alpha)$

IV. CALCULATED RESULTS

The experimental double-differential cross-sections of light charged particles (proton, deuteron, ${}^3\text{He}$, and α) for the $p+{}^6\text{Li}$ reaction were measured in Refs. [22, 23]. Based on the STLN model, we developed a PLUNF code for the $p+{}^6\text{Li}$ reaction to calculate the double-differential cross-sections of outgoing nucleons and light composite charged particles. We performed comparisons between calculations and measurements of double-differential cross-sections for total outgoing protons, deuterons, ${}^3\text{He}$, and alpha particles for the $p+{}^6\text{Li}$ reaction.

Because the target is contaminated by ${}^1\text{H}$, ${}^7\text{Li}$, ${}^{12}\text{C}$, and ${}^{16}\text{O}$, there are addi-

tional contributions to the double-differential cross-sections. Using Eq. (18), we identified the kinetic energies of outgoing protons and their residual nuclei from the ground state to the fifth energy level of pure ${}^6\text{Li}$ and contaminants. For example, for the double-differential cross-sections of outgoing protons at an angle of 60° and $E_p = 14$ MeV in the LS, shown in Fig. 2(a), the black narrow bands in panel (b) represent contributions from outgoing protons originating from discrete levels (illustrated from ground state to the fifth energy level as marked) of target ${}^6\text{Li}$ and contaminants (including ${}^1\text{H}$, ${}^7\text{Li}$, ${}^{12}\text{C}$, and ${}^{16}\text{O}$). From Fig. 2, we see that contributions to the first abrupt peak on the right-hand side come from elastic scattering of protons with ${}^{12}\text{C}$ and ${}^{16}\text{O}$. Contributions to the second peak on the right-hand side come from elastic scattering of protons with ${}^6\text{Li}$ and ${}^7\text{Li}$, and the first inelastic scattering of ${}^7\text{Li}$. The contribution to the third peak on the right-hand side is the pure inelastic scattering of protons with the first excited energy level of ${}^6\text{Li}$. Contributions to the first peak on the left-hand side come from elastic scattering of protons with ${}^1\text{H}$, inelastic scattering of protons from the third to fifth excited energy levels of ${}^{12}\text{C}$, and the fifth excited energy level of ${}^7\text{Li}$. The levels of ${}^7\text{Li}$ exhibit clear differences in their contributions to the double-differential cross-section of outgoing protons compared to those of ${}^6\text{Li}$.

Comparisons of calculated double-differential cross-sections of total outgoing protons with measured data are shown in Figs. 3–5 at an incident proton energy of 14 MeV for outgoing angles of 20° , 30° , 40° , 50° , 60° , 70° , 80° , 90° , 100° , 110° , 120° , 130° , 140° , 150° , 160° , and 165° . The black points represent experimental data from Ref. [23], and the red solid lines denote calculated total double-differential cross-sections of outgoing protons. We see that calculated results agree well with measurements, except for some peaks contaminated by elastic and inelastic scattering from ${}^1\text{H}$, ${}^7\text{Li}$, ${}^{12}\text{C}$, and ${}^{16}\text{O}$, as reported in Ref. [23]. Using the calculated double-differential cross-sections of outgoing protons at 60° and $E_p = 14$ MeV as an example, the partial spectra are shown in Fig. 6. The yellow dash-dotted line denotes partial spectra of protons emitted from direct three-body breakup through ${}^7\text{Be}^* \rightarrow p+d+\alpha$. The pink dash-dotted lines denote partial spectra of the first outgoing proton from the compound nucleus to the ground state and fifth excited energy levels of the first residual nucleus, ${}^6\text{Li}$. *The green dash-dotted line represents the contribution from the reaction channel $(p, np){}^5\text{Li} \rightarrow (p, n2p)\alpha$ from the first excited energy level of ${}^6\text{Be}^*$ to the first excited energy level of ${}^5\text{Li}$, which can break up into $d+\alpha$.* The brown dash-dotted lines denote partial spectra of the second outgoing proton from the fourth and fifth excited energy levels of ${}^6\text{Li}$ to the ground state of ${}^5\text{He}$. The purple dash-dotted lines denote partial spectra of the second outgoing proton from the ground state and first excited energy levels of ${}^5\text{Li}$ to the ground state of ${}^4\text{He}$.

As the target is contaminated by ${}^1\text{H}$, ${}^7\text{Li}$, ${}^{12}\text{C}$, and ${}^{16}\text{O}$, there are additional contributions to the double-differential cross-sections besides those from the target nucleus ${}^6\text{Li}$. The energy levels of contaminants contribute more to lower outgoing energy regions as the emission angle increases, resulting in theoretical

underestimations of outgoing protons in these regions.

The calculated double-differential cross-sections of total outgoing deuterons for the $p+6\text{Li}$ reaction at 14 MeV are compared with experimental data obtained at angles of 20° , 30° , 40° , 50° , 60° , 70° , 80° , 90° , 100° , 110° , 120° , 130° , 140° , 150° , 160° , and 165° , as shown in Figs. 9–11. The black points represent experimental data from Ref. [22], and the red solid lines denote calculated total double-differential cross-sections of outgoing deuterons. Figure 12 [Figure 12: see original paper] shows partial double-differential cross-sections of outgoing deuterons at an angle of 60° and $E_p = 14$ MeV in the LS. The yellow dash-dotted line denotes partial spectra of deuterons emitted from direct three-body breakup through $7\text{Be}^* \rightarrow p+d+\alpha$. The green dash-dotted lines denote partial spectra of the first outgoing deuteron from the compound nucleus to the ground state and first excited energy level of the first residual nucleus, 5Li . *The pink dash-dotted lines denote the second outgoing deuteron from the first and third-fifth excited energy levels of 6Li to the ground state of 4He .*

The calculated double-differential cross-sections of total outgoing 3He and α for the $p+6\text{Li}$ reaction at 14 MeV are compared with experimental data obtained at angles of 10° , 20° , 30° , 40° , 50° , 60° , 70° , 80° , 90° , 100° , 110° , and 120° , as shown in Figs. 7–8. The black points represent experimental data from Ref. [22], and the red solid lines denote calculated total double-differential cross-sections. The calculated results agree well with measurements. From Fig. 13 [Figure 13: see original paper], we see that the yellow dash-dotted line denotes partial spectra of α particles emitted from direct three-body breakup through $7\text{Be}^* \rightarrow p+d+\alpha$. The green dash-dotted line denotes the contribution from the reaction channel $(p, np)5\text{Li}^* \rightarrow (p, n2p)\alpha$ from the first excited energy level of 6Be^* to the first excited energy level of 5Li , *which can break up into $d+\alpha$.* *The pink dash-dotted lines denote the second outgoing α from the first and third-fifth excited energy levels of 6Li to the ground state of 4He .* The blue dash-dotted lines denote partial spectra of the first outgoing 3He from the compound nucleus to the ground state of the first residual nucleus α . We see that the first and second peaks on the right-hand side are the differential cross-sections of outgoing 3He and α for $p+6\text{Li}$, respectively. In particular, $p+6\text{Li} \rightarrow 3\text{He} + \alpha$ is different from secondary particle emission because it has no threshold. It is worth mentioning that the peaks are marked incorrectly in Figs. 7–8 of Ref. [22].

As an example, Fig. 14 shows predicted total and partial spectra of the outgoing neutron for the $p+6\text{Li}$ reaction at 14 MeV and an angle of 60° . The red line shows the total double-differential cross-section of the outgoing neutron. The green dash-dotted lines denote partial spectra of the first outgoing neutron from the compound nucleus to the ground state and first excited energy level of the first residual nucleus, 6Be . *The brown dash-dotted lines denote the contribution from the reaction $(p, 2p)5\text{He} \rightarrow (p, n2p)\alpha$ from the fourth and fifth excited energy levels of 5He to the ground state of α .*

However, the threshold energies of composite charged particles such as deuteron and triton (except 3He and α for the $p+6\text{Li}$ reaction) are usually higher than

those of protons for both the target and contaminants. Furthermore, the Coulomb barriers for these outgoing composite charged particles are higher than those for protons; therefore, the impact of contaminants is greatly reduced. These factors hinder accurate measurement of these composite charged particles, particularly at larger emission angles. Thus, it is reasonable to assume that theoretical calculations are slightly higher than measurements for large outgoing angles.

V. SUMMARY

The STLN model [39, 47, 48] has been improved to calculate the double-differential cross-sections of outgoing neutrons, protons, deuterons, ^3He , and alpha particles for the $p+^6\text{Li}$ reaction. Emission processes between discrete energy levels with conservation of energy, angular momentum, and parity are strictly considered. The results show that the pre-equilibrium emission process is the dominant reaction mechanism for 1p-shell light nucleus reactions and that calculated double-differential cross-sections are sensitive to the energy, spin, and parity of discrete levels for both target and residual nuclei. Recoil effects are also considered due to the light mass of 1p-shell nuclei. A PLUNF code has been developed based on the STLN model to obtain an ENDF-6-formatted file of double-differential cross-sections for nucleons and light composite charged particles for the $p+^6\text{Li}$ reaction. The calculated results agree well with existing measurements of outgoing protons, deuterons, ^3He , and alpha particles.

AUTHOR CONTRIBUTIONS

All authors contributed to the study conception and design. Material preparation, data collection, and analysis were performed by Xiao-Jun Sun, Fang-Lei Zou, and Jing-Shang Zhang. The first draft of the manuscript was written by Xiao-Jun Sun and Fang-Lei Zou, and all authors commented on previous versions of the manuscript. All authors read and approved the final manuscript.

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CONFLICT OF INTEREST

The authors declare that they have no competing interests.

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