Comprehensive study of nuclear reactions in muon catalyzed fusion: I. dtμ system

M. Kamimura

Meson Science Laboratory, RIKEN Nishina Center, RIKEN, Wako 351-0198, Japan

Y. Kin

Department of Chemistry, Tohoku University, Sendai, 980-8578, Japan

T. Yamashita

Institute for Excellence in Higher Education Division of Developmental Research in Education Programs, Tohoku University, Sendai, 980-8576, Japan

and Department of Chemistry, Tohoku University, Sendai, 980-8578, Japan

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Muon catalyzed fusion (μCF) has recently regained considerable research interest owing to several new developments and applications. In this regard, we have performed a comprehensive study of the most important fusion reaction, namely (dμ)n→α+n+μ+17.6 MeV or (μn)n→α+n+17.6 MeV. For the first time, the coupled-channels Schrödinger equation for the reaction is solved, satisfying the boundary condition for the muonic molecule (dμ)n→α, as the initial state and the outgoing wave in the αμ channel. We employ the dμ- and αn-channel coupled three-body model. All the nuclear interactions, the d-μ and α-n potentials, and the dτ-αn channel-coupling nonlocal tensor potential are chosen to reproduce the observed low-energy (1–300 keV) astrophysical S-factor of the reaction d+τ→α+n+17.6 MeV, as well as the total cross section of the α+n reaction at the corresponding energies. The resultant dτμ fusion rate is 1.03×10^{12}s^{-1}. Substituting the obtained total wave function into the T-matrix based on the Lippmann-Schwinger equation, we have derived absolute values of the reaction rates going to the individual bound and continuum states of the outgoing α-μ pair. Using these reaction rates, we obtain the initial α-μ sticking probability \( \omega_0^2 \approx 0.857\% \), which is \( \sim 7\% \) smaller than the literature values (\( \sim 0.91–0.93\% \)), and it is not inconsistent with the most recent observations (2001) at high D/T densities. The origin of the \( \sim 7\%-\)reduction of \( \omega_0^2 \) is that we have employed the outgoing α-n D wave and the dt-αn coupling tensor force. We also calculate the absolute values for the momentum and energy spectra of the muon emitted during the fusion process. The most important result is that the peak energy is 1.1 keV although the mean energy is 9.5 keV owing to the long higher-energy tail. This is a useful result for the ongoing experimental project to realize the generation of an ultra-slow negative muon beam by utilizing the μCF for various applications e.g., a scanning negative muon microscope and an injection source for the muon collider.

I. INTRODUCTION

In the mixture of deuterium (D) and tritium (T), an injected negatively charged muon (μ) forms a muonic molecule with a deuteron (d) and a triton (t), namely, dtμ. Since the mass of a muon is 207 times heavier than that of an electron, the nuclear wave functions of d and t overlap inside the dtμ molecule, which instantly results in an intramolecular nuclear fusion reaction d+t→α+n+17.6 MeV. After this reaction, the muon becomes free and can facilitate another fusion reaction (Fig. 1). This cyclic reaction is called muon catalyzed fusion (μCF).

The μCF has been dedicatedly studied since 1947 [1, 2], and is reviewed in Refs. [3, 4]. Among various isotopic species of muonic molecules (ppμ, pdμ, dtμ, dμ and τμ), the dtμ has attracted particular attention in μCF with the expectation that it may be exploited as a future energy source.

Efficiency of the μCF has been discussed in the literature as following: As seen in Fig. 1. the muon emitted after the d-t fusion sticks to the α particle with a probability, \( \omega_0^2 \), and is lost from the cycle due to spending its lifetime (\( \tau_\mu = 2.2 \times 10^{-6} \) s) as a coupled entity, although the muon is reactivated (stripped) with a probability R during the collision of an (μn) ion with the D/T mixture. The net loss-probability \( \omega_0^2 \phi = \omega_0^2 (1-R) \) is called effective sticking probability, whereas \( \omega_0^2 \phi \) is referred to as initial sticking probability. The number of fusion events, \( Y_1 \), catalyzed by one muon is essentially represented as

\[
Y_1 \approx \left( \omega_0^2 + \frac{\lambda_0}{\lambda_\alpha \phi} \right)^{-1}
\]

where \( \lambda_0 = 1/\tau_\mu = 0.455 \times 10^6 \) s\(^{-1} \), \( \lambda_\alpha \) is a cycle rate, and \( \phi \) is a target density relative to the liquid hydrogen (4.25 \times 10^{22} \text{ atoms cm}^{-3} \). A typical parameter set of \( \omega_0^2 \phi \approx 0.5\% \) and \( \lambda_\alpha \sim 1.1 \times 10^6 \) s\(^{-1} \) at \( \phi = 1.25 \) results in \( Y_1 \sim 120 \), which produces \sim 2.1 GeV per a muon. A literature reported \( Y_1 \sim 150 \) which was the highest value known so far, and results in \sim 2.6 GeV, whereas \sim 5 GeV of energy is required to generate a muon in accelerator; the efficiency of μCF for energy production is approximately half that required to achieve a scientific break-even. If \( \omega_0^2 \phi \) is omitted in Eq. (1.1), \( Y_1 \sim 300 \) cycles is obtained. On the other hand, if we omit \( \lambda_0/\lambda_\alpha \phi \) from Eq. (1.1), we have \( Y_1 \sim 200 \). Therefore, the low efficiency of the μCF comes from both parameters of \( \omega_0^2 \phi \) and \( \lambda_\alpha \); it is desirable to examine \( \omega_0^2 \phi \), R and \( \lambda_\alpha \) carefully.
Although the fusion yield $Y_t$ as well as the fundamental parameters $\omega_c^0$, $R$ and $\lambda_c$ have been often investigated in liquid/solid targets thus far, such a cold target $\mu$CF would not be realistic as a practical energy source due to the low thermal efficiency of the Carnot cycle. The experimental knowledge of $\mu$CF at high-temperature conditions, however, is limited.

The $\mu$CF has recently regained considerable interest owing to several new developments and applications. They are grouped into the following two types:

I) To realize the production of energy by the $\mu$CF using the high-temperature gas target of the D/T mixture with high thermal efficiency.

II) To realize an ultra-slow negative muon beam by utilizing the $\mu$CF for various applications e.g., a scanning negative muon microscope and an injection source for the muon collider.

They are explained as follows:

Type I): The $\mu$CF kinetics model in high-temperature gas targets is re-examined, including the excited (resonant) muonic molecules and fusion in-flight processes [10–13]. Recent improvements in the energy resolution of X-ray detectors facilitate the examination of the dynamics of muon atomic processes [14–16], and may allow for the detection of the resonance states of muonic molecules during the $\mu$CF cycle. An intense muon beam [17] also creates the upgraded conditions required to explore these $\mu$CF fundamental studies. In parallel to the re-examination of the $\mu$CF kinetics model, there is a new proposal to strongly reduce the $\alpha$-$\mu$ sticking probability by boosting the negative muon stripping using resonance radio-frequency acceleration of $(\alpha\mu)^+$ ions in a spatially located D/T mixture gas stream [18]. In addition to studies on the $\mu$CF as possible energy sources, the 14.1 MeV neutron has been considered as a source for the mitigation of long-lived fission products (LLFPs) with nuclear transmutation [19]. Since the mitigation of LLFPs requires a well-defined condition for a neutron beam, $\mu$CF-based monochromatic neutrons would be more suitable than those from a nuclear reactor and/or spallation neutron sources.

Type II): In general, muon beams generated by accelerators have $\sim$ MeV kinetic energies. At present, the negative muon beam, with a size of a few tens of millimeters, has proven to be suitable for non-destructive elemental analysis [20, 22] in various research fields such as archeology, earth-and-planetary science, and industry. In contrast to the accelerator-based muon beam, the mean kinetic energy of the muon released after the $\mu$CF reaction is $\sim$ 10 keV since the $dt\mu$ molecule nearly takes the $(^3\text{He}\mu)_1$ configuration at the instant of the fusion reaction. Therefore, the $\mu$CF can be utilized as a means for beam cooling [23–27]. Recently, the aim has been to produce a negative muon beam by reducing the beam size to an order of 10 $\mu$m using a set of beam optics, by utilizing the muons emitted by the $\mu$CF. This beam is called an ultra-slow negative muon beam [23–25], which will facilitate various applications such as a scanning negative muon microscope, as well as an injection source for a muon collider [25]. The scanning negative muon microscope that can utilize characteristic muonic X-rays will allow for three-dimensional analysis of elements and isotopes. Owing to the high penetrability of muon, such a microscope can be applied to biological samples under the atmospheric environment. Experiments for direct observation of the muon released after the $\mu$CF using a layered hydrogen thin disk target are in progress [23–27, 29–31].

Here, we note that two of the present authors (Y.K. and T.Y.) have contributed to the aforementioned studies of Type I in Refs. [10–13] and Type II in Refs. [29–31]. The purpose of the present paper is that considering the latest developments regarding the new $\mu$CF applications, we thoroughly investigate the mechanism of the nuclear reaction

$$
(dt\mu)_{J,\nu=0} \rightarrow \alpha + n + \mu + 17.6 \text{ MeV} \tag{1.2}
$$

by employing a sophisticated framework that has not been explored in the literature work on this reaction. The reaction (1.2) is the most important among the muon catalyzed nuclear reactions, but it has a complicated struc-
The reaction (1.2) was calculated using approximate models (cf. Secs. 7 and 8) and in the sophisticated methods. Another reason is that such a precise calculation of the reaction has not been required in previous CF studies; the required quantities were the total fusion rate \( \lambda_f = \Gamma / \hbar \) and the \( \alpha \mu \) initial sticking probability \( \omega_{\alpha \mu}^0 \), which were calculated using approximate models (cf. Secs. 7 and 8 of the CF review paper [5]), for example, in Ref. [32, 33] by one of the present authors (M.K.) (see Secs. II A and VB).

For the new situation of \( \mu \) CF mentioned in Types I and II, it is desirable to precisely calculate the following quantities of the reaction (1.2):

a) Reaction rates, in absolute values, going to the individual bound and continuum states of the outgoing \( \alpha \mu \) pair, together with the \( \alpha \mu \) sticking probability \( \omega_{\alpha \mu}^0 \) based on those reaction rates.

b) Momentum and energy spectra, in absolute values, of the muon emitted by the fusion reaction.

To calculate these quantities and conduct additional analyses, we employ the \( dt\mu \)- and \( an\mu \)-channel coupled three-body model and perform the following:

i) We first determine all the nuclear interactions (the \( dt \) and \( an \) potentials and the \( dt-an \) channel coupling potential) to reproduce the observed astrophysical S-factor of the reaction

\[
d + t \rightarrow \alpha + n + 17.6 \text{ MeV} \quad (1.3)
\]

at the low-energies of \( 1 - 300 \) keV [42] as well as the total cross section of the \( \alpha + n \) reaction at the corresponding energies [43] (see Sec. II B).

ii) We solve a coupled-channels three-body Schrödinger equation on the Jacobi coordinates in Fig. 3 satisfying the boundary condition to have the muonic molecular bound state \( (dt\mu)_\text{even} \) as the initial state (as the source term of Schrödinger equation) and the outgoing wave in the \( an\mu \) channel with the 17.6-MeV D-state \( \alpha-n \) relative motion based on the observation (see Sec. III).

iii) We calculate the quantities a) and b) by substituting the obtained total wave function into the \( T \)-matrix elements for a) and b) based on the Lippmann-Schwinger equation [44] (see Secs. IV, V and VI).

The reliability of these calculations shall be carefully examined as follows: The total fusion rate \( \lambda_f \) (the number of fusions per second) is calculated in the three different prescriptions:

A) \( \lambda_f \) from the \( S \)-matrix of the asymptotic amplitude of the total wave function solved using the coupled-channels Schrödinger equation (see Sec. III).

B) \( \lambda_f \) from the \( T \)-matrix calculation of the reaction rates mentioned in item a) (see Sec. V).

C) \( \lambda_f \) from the \( T \)-matrix calculation of the muon spectra mentioned in item b) (see Sec. VI).

If our total wave function is the exact rigorous solution of the coupled-channels Schrödinger equation, the fusion rates \( \lambda_f \) obtained by A)-C) should be equal according to the Lippmann-Schwinger equation that is equivalent to the Schrödinger equation. However, since the function space employed in our total wave function is not complete, the resultant \( \lambda_f \) are not equal, but they should be consistent with each other. This check of \( \lambda_f \) is one of the highlights of the present paper.

The authors possess their own three methods to solve the present coupled-channels three-body Schrödinger equation. Namely, the Kohn-type variational method for the reactions between composite particles [45], the Gaussian expansion method (GEM) for few-body systems [32, 46, 47] here for describing the \( (dt\mu) \) molecule nonadiabatically, and the continuum-discretized coupled-channels (CDCC) method [48, 50] here for discretizing the \( \alpha \mu \) and \( \alpha-n \) continuum states.

This paper is organized as follows. In Sec. II we will determine all the nuclear interactions used in this work to reproduce the observed S-factor of the reaction (1.3) and the total cross section of the \( \alpha + n \) reaction. In Sec. III we solve the coupled-channels Schrödinger equation for the reaction (1.2). Section IV is devoted to providing an overview of the \( T \)-matrix framework based on the Lippmann-Schwinger equation. In Sec. V, based on the \( T \)-matrix calculation, we derive the reaction rates going to the \( \alpha \mu \) bound and continuum states. In Sec. VI, we also derive the momentum and energy spectra of the muon ejected from the fusion reaction. Finally, a summary is given in Sec. VII.

FIG. 3: All the sets of Jacobi coordinates in the \( dt\mu \) system (\( c = 1, 2 \) and 3) and in the \( an\mu \) system (\( c = 4, 5 \) and 6).
II. NUCLEAR INTERACTIONS FOR LOW-ENERGY

\[ \text{d} + \text{t} \rightarrow \alpha + \text{n} \text{ REACTION} \]

To investigate the mechanism of the \( \mu \)CF reaction \[1,2\] based on the \( d\mu \)- and \( \alpha\mu \)-channels coupled three-body model, it is necessary to use the nuclear interactions (the \( d\)-t and \( \alpha\)-n potentials and the \( dt\text{-an} \) channel-coupling potential) that reproduce the observed low-energy cross section (astrophysical \( S \)-factor) of the reaction \[1,3\] as well as the total cross section of the \( \alpha + n \) reaction at the corresponding energies.

We shall determine the interactions in Sec. IIB, but before doing so, our previous work \[32,33\] that involved the analysis of the data using the \( d\)-t optical-potential model and the calculated the fusion rate \( \lambda_f \) of the \( d\mu \) molecule (similar work in Ref. \[34\]) will be briefly examined in Sec. IIA.

A. \( d\text{-t} \) optical-potential model

A summary of the observed \( S \)-factor is shown in Fig. 4, which was taken from Ref. \[42\]. In the energy region of this figure, the \( d\)-t channel has a spin-parity \( I = \frac{1}{2}^+ \) with a \( S \)-wave relative motion and spin \( \frac{1}{2} \). In Ref. \[33\], we assumed the following shape of the \( d\)-t optical potential:

\[
V(r) = V_0/(1 + e^{(r-R_0)/a}) \\
W(r) = W_0/(1 + e^{(r-R_0)/a}) \\
V_C(r) = \left\{ \begin{array}{ll}
\frac{\pi}{k^2} \left( \frac{r}{R_c} \right) & (r < R_c) \\
\frac{\pi}{k^2} & (r \geq R_c)
\end{array} \right.
\]

for the real, imaginary and Coulomb components, respectively, where \( r \) is the \( d\)-t relative distance.

We have solved the Schrödinger equation for \( d\text{-t} \) scattering using the optical potential and derived the \( S \)-matrix element \( S(E) \), where \( E \) is the c.m. energy of the \( d\)-t relative motion. In the energy region of Fig. 4, only the \( \alpha\)-n channel is open, except for the incoming channel. Therefore, the absorption cross section becomes the cross section of the reaction \[1,3\] as

\[
\sigma_{dt\rightarrow an}(E) = \frac{2I + 1}{(2I_d + 1)(2I_t + 1)} \frac{\pi}{k^2} (1 - |S(E)|^2),
\]

where \( I_d = 1, I_t = 1/2 \) and \( k = \sqrt{2\mu_{dt}E}/\hbar \). The astrophysical \( S \)-factor \( S(E) \) is derived from the cross section as

\[
\sigma_{dt\rightarrow an}(E) = S(E) e^{-2\eta(E)/E},
\]

where \( \eta(E) \) is the Sommerfeld parameter.

We include the \( d\)-t potential in the nonadiabatic three-body calculation of the \( (d\mu)_{f\nu} \) molecular bound states (cf. Sec. IIIA for the calculation method \[32,33\]). The fusion rate \( \lambda_f \) was derived from the imaginary part \( E_{imag} = -\Gamma/2 \) of the eigenenergy \( E_{\nu} \) as \( \lambda_f = \Gamma/\hbar \).

Since there is no \( d\text{-t} \) elastic-scattering information for \( E \lesssim 100 \text{ keV} \[60\] to show the nuclear-interaction effect, it is impossible to determine a unique function of the optical-model potential based on the \( S \)-factor of Fig. 4. Therefore, in Ref. \[33\], we examined five types of optical potentials to demonstrate that the exact form of the potential is not essential for calculating the fusion rate (namely, energy width of the muonic molecule) and the \( \alpha\)-\( \mu \) sticking probability. We confirmed this assertion numerically. For example, for the \( (d\mu)_{f\nu=0} \) state, we had \( \Gamma = (0.800 - 0.842) \text{ meV} \) and the resultant \( \lambda_f = (1.22 - 1.28) \times 10^{12} \text{ s}^{-1} \) for the five cases; in

![FIG. 4: Observed S-factor S(E) of the \( d + t \rightarrow \alpha + n \) reaction with respect to the c.m. energy E of the incoming d-t wave. This figure is taken from a review paper \[42\] that summarizes the original data from HE55 \[51\], AR52 \[52\], Co52 \[53\], AR54 \[54\], Ga56 \[55\], BA57 \[56\], KO66 \[57\], JA84 \[58\] and BR87 \[59\]. The data are fitted \[43\] using the function \( S(E) = (26 - 0.361E + 248E^2)/(1 + ((E - 0.0479)/0.0392)^2) \) MeV b (here, \( E \) in MeV) in the black curve.]

![FIG. 5: Calculated S-factor S(E) for the \( d + t \rightarrow \alpha + n \) reaction based on the \( d\text{-t} \) optical-potential model. The observed data are represented by the black curve, which is the same as the black curve in Fig. 4. The blue and green dotted curves are obtained by changing the depth of the real-part potential to examine the contributions of the resonance peak and the low-energy tail relative to the \( d\mu \) fusion rate (see text).]
other words, all the sets of the potentials and the inside wave functions that yield nearly the same information (astrophysical S-factor) regarding the outside wave functions generate almost the same fusion rate of the \(dtu\) molecule. The same is the case with the \(\alpha - \mu\) sticking probability (c.f. Sec. VB) \(\omega_{S}^{0} = 0.921 - 0.929\%\) for the five potentials \([33]\).

Therefore, we here employ the "type B" potential as the representative of the five potentials, type A to E \([33]\). The parameters of type B are given as \(V_{0} = -38.01\) MeV, \(R_{0} = 3.0\) fm, \(a = 0.5\) fm, \(W_{0} = -0.30\) MeV, \(R_{t} = R_{0}\), \(a_{t} = 0.5\) fm and \(R_{0} = W_{0}\) (\(W_{0}\) is slightly changed to improve the agreement with the data for \(E \leq 10\) keV).

In Fig. 5 the red curve shows the calculated S-factor \(S(E)\), whereas the the observed \(S(E)\) is represented by the black curve, which is the same as the black curve in Fig. 4. The calculated result agrees well with the observations.

We then employed this interaction in the \(dtu\) three-body calculation of the ground state \((J = \nu = 0)\) of \(dtu\) molecule. The resultant fusion rate \(\lambda_{t}\) is given as

\[
\lambda_{t} = 1.15 \times 10^{12} \text{ s}^{-1}. \tag{2.6}
\]

This value is consistent with the fusion rate obtained in literature calculations using the optical-potential model \([33, 34]\) and the \(R\)-matrix method \([32, 41]\).

It is interesting to know whether the dominant contribution to the fusion rate \(\lambda_{t}\) originates from the large resonance peak or the low-energy tail. To investigate this phenomenon, we obtained the blue and green dotted curves in Fig. 4 by changing the potential parameter \(V_{0} (-39.05\) and \(-37.20\) MeV, respectively). Although the peak height is several times different between the two dotted curves, the calculated fusion rates \(\lambda_{t}\) differ by only \(\sim 10\%\) from each other. This implies that the resonance tail (below \(E \sim 10\) keV), not the resonance peak, is effective in determining the fusion rate. This supports the literature calculations of the \(dtu\) fusion rate using the observed information of the reaction \([15]\) at \(E \rightarrow 0\) only (cf. Table 8 of the \(\mu\)CF review paper \([5]\)).

Since the present optical-potential method for deriving the \(dtu\) fusion rate \(\lambda_{t}\) is natural and reasonable, we expect that the much more sophisticated calculations of \(\lambda_{t}\) in this work will yield results that are not inconsistent with the above value of \(\lambda_{t}\).

**B. \(dt\alpha\)-coupled-channels model**

Next, we investigate the astrophysical S-factor \(S(E)\) by solving the \(dt\) and \(\alpha\)-n channels coupled Schrödinger equation \([13]\). Considering that a similar framework for channel coupling will also be used in the study of \(\mu\)CF reaction \([12]\), we apply the same coordinates \(r_{3}\) and \(r_{4}\) in Fig. 5 to the \(dt\) and \(\alpha\)-\(n\) relative coordinates, respectively, in this subsection.

The total wave function of the system has spin-parity \(I = \frac{3}{2}^{+}\) in the energy region of the resonance and below. It is known that the \(dt\) channel has \(S\)-wave and spin \(\frac{1}{2}\) and the \(\alpha\)-\(n\) channel has \(D\)-wave with spin \(\frac{3}{2}\) coupled to \(I = \frac{3}{2}^{+}\). Let \(E\) denote the c.m. energy of the \(dt\) relative motion. The total wave function is written as

\[
\Phi_{\frac{3}{2}M}(E) = \phi_{0}(r_{3}) \hat{\varphi}_{\frac{3}{2}M}(dt) + \left[\psi_{2}(r_{4}) \hat{\chi}_{\frac{3}{2}M}(an)\right]_{\frac{3}{2}M}, \tag{2.7}
\]

which has an asymptotic behavior

\[
\phi_{0}(r_{3}) \rightarrow \infty \quad U_{0}^{(\mu)}(k_{3},r_{3}) - S_{0}^{(dt)}U_{0}^{(\alpha)}(k_{3},r_{3}), \tag{2.8}
\]

\[
\psi_{2}(r_{4}) \rightarrow - \sqrt{V_{3}^{2}} S_{2}^{(dt,an)} U_{2}^{(\alpha)}(k_{4},r_{4}), \tag{2.9}
\]

where \(k_{3}(k_{4})\) and \(V_{3}(V_{4})\) are the wave number and the velocity of relative motion along \(rf_{3}(r_{4})\), respectively, and \(U_{L}^{(\alpha)}(k,r)\) is the Coulomb function given by

\[
U_{L}^{(\alpha)}(k,r) = G_{L}(k,r) \mp iF_{L}(k,r). \tag{2.10}
\]

We assume that the \(S\) and \(D\)-state wave functions are coupled to each other by the following tensor force, which is nonlocal between \(r_{3}\) and \(r_{4}\):

\[
V_{T}^{(dt,an)}(r_{3},r_{4}) = v_{T}^{(dt,an)}(r_{3},r_{4}) \left[\hat{V}_{2}(r_{3}) S_{2}(dt,an)\right]_{00}, \tag{2.11}
\]

\[
v_{T}^{(dt,an)}(r_{3},r_{4}) = v_{T}^{(dt,an)}(r_{3},r_{4}) e^{\mu r_{3}} e^{\mu r_{4}} - \mu \overline{R}_{i}, \tag{2.12}
\]

\[
S_{2}(dt,an) = r_{3} + r_{4}. \tag{2.13}
\]

In Eq. (2.11), \(S_{2}(dt,an)\) is a spin-tensor operator composed of spins of \(dt\) and \(\alpha\)-\(n\)-pairs. However, it is not necessary to know the explicit form of \(S_{2}(dt,an)\) in the present work, as will be explained in the paragraph below Eq. (2.20).

The coupled-channels Schrödinger equation required to solve \(\phi_{0}(r_{3})\) and \(\psi_{2}(r_{4})\) is written as

\[
\begin{align*}
(H_{dt} - E)\phi_{0}(r_{3}) & = -V_{T}^{(dt)} \left[\psi_{2}(r_{4}) \hat{\chi}_{\frac{3}{2}M}(an)\right]_{\frac{3}{2}M}, \tag{2.13} \\
(H_{an} - (E + Q)) \psi_{2}(r_{4}) & = -V_{T}^{(dt)} \phi_{0}(r_{3}) \hat{\chi}_{\frac{3}{2}M}(dt), \tag{2.14}
\end{align*}
\]

where \(Q = 17.589\) MeV and

\[
\begin{align*}
H_{dt} & = T_{r_{3}} + V_{T}^{(NN)}(r_{3}) + V_{T}^{(C)}(r_{3}), \tag{2.15} \\
H_{an} & = T_{r_{4}} + V_{T}^{(NN)}(r_{4}), \tag{2.16} \\
V_{T}^{(dt,an)} & = \int d r_{3} V_{T}^{(dt,an)}(r_{3},r_{4}). \tag{2.17}
\end{align*}
\]

The coupled-channels Schrödinger equation \([2.13, 2.14]\) with the scattering boundary condition \([2.8, 2.9]\) can be accurately solved by using the couple-channels Kohn-type variational method for composite-particle reactions that was proposed by one of the authors (M.K.) \([15]\) and has been employed in the literature in three-body transfer reactions such
as \((d\mu)_{1s} + t \rightarrow (\mu)_{1s} + d\) and \(^{16}\text{O} + d \rightarrow ^{17}\text{O} + n\) [61, 63].

The method is explained in detail in Ref. [45] together with sample calculations; especially, see Secs. 2.2, 2.4 and 5.1 as the basic aspects for use of the method.

The reaction cross section \(\sigma_{dt-an}\) is given by

\[
\sigma_{dt-an}(E) = \frac{2I + 1}{(2I + 1)(2I + 1)} \frac{\pi}{k^2} |S_{2}(dt, an)|^2, 
\]

and the \(S\)-factor \(S(E)\) is derived from Eq. (2.5).

When the matrix element of the tensor force is calculated, the spin part \(S_0^{(T)}\) is factored out as follows:

\[
\langle \phi_2(r_3) \chi_2(\alpha n) \rangle \left| V_{an,dt}^{(T)} \right| \langle \phi_0(r_3) \chi_2(\alpha n) \rangle \left| \right. 
= v_0^{(T)} S_0^{(T)} 
\times \langle \phi_2(r_3) \rangle | f_{34}^2 \exp(-\alpha r_1^2 - \mu r_3^2) | Y_2 r_3 \rangle \langle \phi_0(r_3) \rangle, 
\]

where

\[
S_0^{(T)} = \frac{1}{\sqrt{10}} \langle \chi_2(\alpha n) \rangle \left| S_2 dt, an \chi_2(\alpha n) \rangle \right| \right. 
\]

The R.H.S. of Eqs. (2.19) and (2.20) are independent of \(m\) and \(m_\mu\), respectively, and hence, the L.H.S. of Eqs. (2.19) does not depend on \(M\).

In our phenomenological manner of searching for the tensor force required to reproduce the experimental data of \(S(E)\), it is not necessary to know \(S_0^{(T)}\) (namely, to know \(S_2\)) since it is sufficient to search for the optimum value of the product \(v_0^{(T)} S_0^{(T)}\). It is to be noted that for the investigations of Secs. III, V and VI, we verified that the same \(v_0^{(T)} S_0^{(T)}\) is factored out when calculating the three-body matrix elements of the tensor force and the \(T\)-matrix elements due to the same force. Consequently, we can treat the tensor force consistently throughout the present work without knowing the explicit forms of \(S_2 dt, an \) and \(S_0^{(T)}\).

The \(d+t\) potential \(V_{dt}^{(N)}(r_3)\) is the same as \(V(r)\) in Sec. IIA, Eq. (2.11), except for \(v_0\) which is tuned slightly to reproduce the observed data, whereas the imaginary part \(v_0\) is not necessary. \(V_{dt}^{(C)}(r)\) is the same as Eq. (2.3). As the \(a+n\) potential \(V_{an}^{(N)}(r_3)\), we employ the Kanada-Kaneko \(a+n\) potential [64, 65] (see Fig. 6), which is derived based on an equivalent local potential to the nonlocal kernel of the microscopic resonating group method for the \(a+n\) system, and is often used in the \(a\)-cluster-model calculations of light nuclei [65]. We then fix the potential as \(V_{an}^{(N)}(r)\) throughout this work.

For the tensor force (2.11), we fix \(\mu' = 1/(6.0\text{fm})^2\) and tune \(\mu\) around \(1/(1.6\text{fm})^2\) and \(v_0^{(T)} S_0^{(T)}\). The optimized three potential parameters are \(\mu = 1/(1.6\text{fm})^2\) and \(v_0^{(T)} S_0^{(T)} = 5.43\text{MeV fm}^{-3}\) and \(v_0 = -37.2\text{MeV}\). The shape of the potentials \(V_{dt}^{(N)}(r_3)\) and \(V_{an}^{(N)}(r_3)\) are illustrated in Fig. 6.

The calculated \(S(E)\) using the optimized interactions is given in Fig. 7 by the red curve. The black curve represents the observed data and is the same curve as that in Figs. 4 and 5. The agreement with the data has the same good quality as in Fig. 5 for the optical-potential model.

**FIG. 6:** The optimised nuclear \(d+t\) potential \(V_{dt}^{N(r)}\) (the dashed curve) and the Kanada-Kaneko \(a+n\) potential \(V_{an}^{N(r)}\) [64, 65] for the even-parity case (the solid curve).

**FIG. 7:** Calculated \(S\)-factor \(S(E)\) of the \(d + t \rightarrow a + n\) reaction as represented by the red curve based on the \(dt-an\) coupled-channels method. The black curve represents the observed data associated with the black curve in Fig. 4.

We now discuss the observed total cross section \(\sigma_T(E_n)\) of the \(a + n\) reaction [43] given in Fig. 8. The data should be explained by our calculation simultaneously as the \(S\)-factor \(S(E)\) of the \(d + t \rightarrow a + n\) reaction. The total cross section of the \(I = \frac{1}{2}^+\) state can be expressed using our model as:

\[
\sigma_T(E_n) = \sigma_{\text{elastic}}(E_n) + \sigma_{\text{reaction}}(E_n) = \frac{4\pi}{k^2} |1 - \text{Re}(S^{(an)}_{2})|, 
\]

which is given by

\[
\sigma_{\text{elastic}}(E_n) = \frac{2\pi}{k^2} |S^{(an)}_{2}|^2, 
\]

\[
\sigma_{\text{reaction}}(E_n) = \frac{2\pi}{k^2} |S^{(an,dt)}_{2}|^2. 
\]
FIG. 8: The total cross section \( \sigma_T(E_n) \) of the \( \alpha + n \) reaction based on the observation [43] and the present calculation (the red curve), where \( E_n \) is the neutron incident energy. The dotted line denotes the background cross section based on partial waves other than the \( D_{1/2}^\pi \) wave [43, 66]. The calculated red curve for the \( I = \frac{1}{2}^- \) state is piled on the background dotted line. The peak at \( E_n \approx 22.1 \text{ MeV} \) corresponds to the peak in Fig. 7 for the \( d+t \) channel. The \( d+t \) threshold \((E = 0)\) corresponds to \( E_n = 22.03 \text{ MeV} \) (at the red arrow) in the \( \alpha-n \) channel.

and the unitarity

\[
|S_{2}^{(\alpha n)}|^2 + |S_{2}^{(\alpha n,dt)}|^2 = 1. \tag{2.24}
\]

The \( S \)-matrix elements are determined by the asymptotic behavior, similarly to Eqs. (2.8) and (2.9).

\[
\begin{align*}
\mathcal{S}_{0}^{(\alpha n)}(r_3) & \rightarrow -\frac{\sqrt{v_3}}{v_3} S_{2}^{(\alpha n,dt)} U_{0}^{(\pi)}(k_3, r_3), \\
\mathcal{S}_{2}^{(\alpha n)}(r_4) & \rightarrow U_{2}^{(\pi)}(k_4, r_4) - S_{2}^{(\alpha n)} U_{2}^{(\pi)}(k_4, r_4). \tag{2.25}
\end{align*}
\]

Recall that when tuning the potential parameters to reproduce the \( S \)-factor \( S(E) \) in Fig. 7, we fixed the \( \alpha-n \) potential \( V_{\alpha n}^{(N)}(r_4) \) and did not include the observed \( \alpha + n \) data for fitting. Therefore, it is impressive to see in Fig. 8 that our result (the red curve) agrees well with the data.

However, this is not unexpected because of the following reason: The reaction \( d + t \rightarrow \alpha + n \) in Fig. 4 is known as one of the most strongly channel-coupled reactions in nuclear physics [67, 68]. Actually, at the peak, our calculation shows \( |S_{2}^{(\alpha n,dt)}| \approx 1 \) and \( S_{0}^{(\alpha n)} \approx 0 \). Accordingly, we see that at the peak of the \( \alpha + n \) reaction, \( |S_{2}^{(\alpha n,dt)}| = |S_{2}^{(\alpha n,dt)}| \approx 1 \) and \( S_{0}^{(\alpha n)} \approx 0 \) and hence \( \sigma_T(I = \frac{1}{2}^-) \approx 4\pi/k_4^2 = 0.19 \text{ b} \) with \( k_4 = 0.824 \text{ fm}^{-1} \). This is the peak value of \( \sigma_T(I = \frac{1}{2}^-) \) of the calculation (observation) in Fig. 8. It is asserted that even if we employ another \( \alpha-n \) potential instead of the above \( V_{\alpha n}^{(N)}(r_4) \), the same situation will be repeated as long as the observed data of the \( d + t \rightarrow \alpha + n \) reaction are reproduced using the replaced \( \alpha-n \) potential.

In the following sections on the study of the reaction \( \alpha + n \), we shall use the same set of potentials that was determined using the coupled-channels calculation in this subsection.

III. COUPLED-CHANNELS SCHÖDINGER EQUATION FOR \( dt\mu \) FUSION REACTION

In this section, we formulate and solve the Schrödinger equation for the fusion reaction \( \alpha + n \) using the nuclear interactions that were determined in the previous section and satisfying the boundary condition for the muonic molecule \((dt\mu)_{J=0}^{(n)}\) as the initial state and the outgoing wave in the \( an\mu \) channel. We first divide the fusion decay process into the following two steps:

Step 1) Construction of the nonadiabatic wave function of the initial \((dt\mu)_{J=0}^{(n)}\) state using the Coulomb potentials only. We denote the wave function as \( \Phi_0^{(C)}(dt\mu) \), while the eigenenergy as \( E_{00} \) that is given by

\[
E_{00} = -0.003030 \text{ MeV} \tag{3.1}
\]

with respect to the \( d + t + \mu \) threshold (cf. Fig. 2).

Step 2) Decay of the \((dt\mu)_{J=0}^{(n)}\) state (now, a Feshbach resonance after the nuclear interactions are switched on) into the outgoing wave due to the nuclear \( d-t, \alpha-n \) and \( dt-an \) interactions. The kinetic energy of the outgoing wave with the wave number \( k_4 \) is given by

\[
\frac{\hbar^2}{2\mu_{\alpha+n}} k_4^2 = E_{00} + Q, \quad Q = 17.589 \text{ MeV}. \tag{3.2}
\]

By employing the Step-1 wave function \( \Phi_0^{(C)}(dt\mu) \) as the fixed source term of the coupled-channels Schrödinger equation, it becomes possible to impose the outgoing-wave boundary condition upon the \( an\mu \) channel with no incoming wave for the entire system. The symbol \( (\cdot) \) placed on the top of \( \Phi_0^{(C)}(dt\mu) \) is to show ‘given’ before solving the Schrödinger equation of Step 2. \( \Phi_0^{(C)}(dt\mu) \) will be calculated in Sec. IIIA.

The total angular momentum of the enewhole system is \( \frac{1}{2} \) with its z-component \( M \) similarly to the \( dt-an \) case in Sec. IIB (muon spin is neglected). We then describe the total wave function in term of the three parts based on the aforementioned two steps as follows:

\[
|\Psi^{(+)}_{M}(E)\rangle = \Psi^{(C)}_{M}(dt\mu) + \Psi^{(N)}_{M}(dt\mu) + \Psi^{(+)}_{M}(an\mu), \tag{3.3}
\]

with

\[
\begin{align*}
\Psi^{(C)}_{M}(dt\mu) & = \Phi_0^{(C)}(dt\mu) \chi^{(C)}_{M}(dt), \tag{3.4} \\
\Psi^{(N)}_{M}(dt\mu) & = \Phi_0^{(N)}(dt\mu) \chi^{(N)}_{M}(dt), \tag{3.5} \\
\Psi^{(+)}_{M}(an\mu) & = \left[ \Phi_2^{(+)}(an\mu) \chi^{(C)}_{M}(an) \right]_{M}. \tag{3.6}
\end{align*}
\]

Here, \( \Phi_0^{(C)}, \Phi_0^{(N)} \) and \( \Phi_2^{(+)} \) are spatially \( S-, S- \) and \( D-wave \) functions, respectively. The spin functions \( \chi_{M}^{(C)}(dt) \) and \( \chi_{M}^{(N)}(an) \) were introduced in Eq. (2.20). However, the explicit form of the spin functions is not necessary because the phenomenological spin-tensor operator \( S_{2}(dt, an) \) and its matrix element \( s^{(2)}_{0} \) of Eq. (2.20) are used.
In Eq. (3.3), the first component $\Psi^{(C)}_{\frac{3}{2}M}(dt\mu)$ becomes the source term of the coupled-channels Schrödinger equation. The second component $\Psi^{(N)}_{\frac{3}{2}M}(dt\mu)$ is introduced to describe the $d$-$t$ relative motion due to the nuclear interactions, and the third term $\Psi^{(+)}_{\frac{3}{2}M}(an\mu)$ is for the $an\mu$ channel, which should satisfy the outgoing-wave boundary condition.

The coupled-channels Schrödinger equation required to solve $\Psi^{(N)}_{\frac{3}{2}M}(dt\mu)$ and $\Psi^{(+)}_{\frac{3}{2}M}(an\mu)$ can be written as

\begin{equation}
\begin{aligned}
(H_{dt\mu} - E_{00})(\Psi^{(C)}_{\frac{3}{2}M}(dt\mu) + \Psi^{(N)}_{\frac{3}{2}M}(dt\mu)) &= -V^{(T)}_{dt,an\mu}(\Psi^{(+)}_{\frac{3}{2}M}(an\mu)),
\end{aligned}
\end{equation}

\begin{equation}
\begin{aligned}
(H_{an\mu} - (E_{00} + Q))(\Psi^{(+)}_{\frac{3}{2}M}(an\mu)) &= -V^{(T)}_{an,dt}(\Psi^{(C)}_{\frac{3}{2}M}(dt\mu) + \Psi^{(N)}_{\frac{3}{2}M}(dt\mu)).
\end{aligned}
\end{equation}

where

\begin{equation}
\begin{aligned}
H_{dt\mu} &= T_{c} + T_{R} + V^{(C)}_{dt}(r_{1}) + V^{(C)}_{dt}(r_{2}) + V^{(C)}_{an}(r_{3}) + V^{(C)}_{an}(r_{4}),
H_{an\mu} &= T_{c} + T_{R} + V^{(N)}_{an}(r_{3}) + V^{(C)}_{an}(r_{4}),
V^{(T)}_{dt,an\mu} &= \int dr_{1} V^{(T)}_{dt}(r_{1}, r_{3}), V^{(T)}_{an,dt}.
\end{aligned}
\end{equation}

This is an extension of the Schrödinger equation (2.13)-(2.14) of the $dt \rightarrow an$ problem to the $dt\mu \rightarrow an\mu$ problem. All the nuclear interactions used were determined in Sec. IIB. It should be noted that the contribution from the nuclear interactions to the energy of the $dt\mu$ molecule is on the order of $10^{-3}$ eV [32,40], which is negligible in $E_{00}$ in the present reaction calculation. Also, it is not necessary to consider the back-coupling change of the source amplitude $\Psi^{(C)}_{\frac{3}{2}M}(dt\mu)$ due to $\Psi^{(N)}_{\frac{3}{2}M}(dt\mu)$, although the coupling between $\Psi^{(N)}_{\frac{3}{2}M}(dt\mu)$ and $\Psi^{(+)}_{\frac{3}{2}M}(an\mu)$ is strong.

The most difficult aspect when solving the coupled-channels three-body Schrödinger equation (3.7), (3.8) is the imposition of the outgoing-wave condition on $\Psi^{(+)}_{\frac{3}{2}M}(an\mu)$. To address this problem, we analyze the structure of the nuclear component $\Psi^{(N)}_{\frac{3}{2}M}(dt\mu)$ in Sec. IIB and propose an appropriate method in Sec. IIC. The solution of the Schrödinger equation is presented in Sec. IID, together with an evaluation of the validity of the proposed boundary-condition method.

A. Solution of source term $\Psi^{(C)}_{\frac{3}{2}M}(dt\mu)$ using GEM

In Step 1), we calculate $\Phi^{(C)}_{0}(dt\mu)$ of Eq. (3.4) and its energy $E_{00}$ by solving the Coulomb-three-body Schrödinger equation

\begin{equation}
(H^{0}_{dt\mu} - E_{00})\Phi^{(C)}_{0}(dt\mu) = 0,
\end{equation}

where $H^{0}_{dt\mu}$ is given by Eq. (3.9) omitting the nuclear potential $V^{(N)}_{dt\mu}(r_{1})$. The spins of $d$ and $t$ are neglected in the formulation in this subsection. Since, we study fusion decay starting from one $dt\mu$ molecule, we normalize $\Phi^{(C)}_{0}(dt\mu)$ as

\begin{equation}
\langle \Phi^{(C)}_{0}(dt\mu) | \Phi^{(C)}_{0}(dt\mu) \rangle = 1.
\end{equation}

We solve Eq. (3.12) by using the Gaussian expansion method (GEM) for few-body systems. This method was proposed by one of the present authors (M.K.) to accurately solve the $dt\mu$ molecule [32]; one of the most precise values in the literature was obtained for the energy of the very shallow $(dt\mu)_{2\pi=1}$ state. The method was then applied to the high accuracy calculation of the three-nucleon bound states [46] with a realistic $NN$ force; numerous applications for various types of few-body systems have been summarized in review papers [47,69,71].

The Coulomb three-body wave function $\Phi^{(C)}_{0}(dt\mu)$ is described as a sum of the amplitudes of three rearrangement channels $c = 1, 2$ and 3 (cf. Fig. [3])

\begin{equation}
\Phi^{(C)}_{0}(dt\mu) = \Phi^{(1)}_{IM}(r_{1}, R_{1}) + \Phi^{(2)}_{IM}(r_{2}, R_{2}) + \Phi^{(3)}_{IM}(r_{3}, R_{3}).
\end{equation}

Each amplitude is expanded in terms of the Gaussian basis functions of the Jacobi coordinates $r_{c}$ and $R_{c}$:

\begin{equation}
\Phi^{(c)}_{IM}(r_{c}, R_{c}) = \sum_{n_{l_{c}}, n_{L_{c}}} A^{(c)}_{n_{l_{c}}, n_{L_{c}}}(r_{c}) \psi_{N,L}(R_{c}),
\end{equation}

where $c = 1, 2, 3$.

\begin{equation}
\psi_{N,L}(R_{c}) = N_{d} R_{c}^{-L_{c}} e^{-\nu_{N} R_{c}^{2}}, \quad (N = 1 - N_{max}),
\end{equation}

where $N_{d}$ and $N_{L}$ are the normalization constants:

\begin{equation}
N_{d} = \left( \frac{2^{l_{c} + 3/2}(2 \nu_{N})^{l_{c} + 3/2}}{\sqrt{\pi} (2l_{c} + 1!!)} \right)^{1/2}, \quad N_{L} = \left( \frac{2^{l_{c} + 3/2}(2 \nu_{N})^{l_{c} + 3/2}}{\sqrt{\pi} (2L_{c} + 1!!)} \right)^{1/2}.
\end{equation}

The Gaussian ranges are postulated to lie in geometric progression:

\begin{equation}
\nu_{N} = 1/r_{N}^{2}, \quad \nu_{N} = 1/r_{N}^{2}, \quad (N = 1 - N_{max}),
\end{equation}

\begin{equation}
\lambda_{N} = 1/R_{N}^{2}, \quad \lambda_{N} = 1/R_{N}^{2}, \quad (N = 1 - N_{max}).
\end{equation}

$l_{c}$ and $L_{c}$ are restricted to $0 \leq l_{c} \leq l_{max}$ and $|l_{c} - L_{c}| \leq L_{c} \leq l_{max}$. The eigenenergies $E_{00}$ and coefficients $A^{(c)}_{n_{l_{c}}, n_{L_{c}}}$ are determined by the Rayleigh-Ritz variational principle. In the precise calculation [32] of the eigenenergies of the $(dt\mu)_{2\pi}$ molecule, we took $l_{max} = 4$, but $l_{max} = 1$ is sufficient in the present fusion reaction problem. The Gaussian-basis parameters employed are listed in Table [1]. Although the large-size calculation [32] of the $J = 0$ state with $l_{max} = 4$ gave an eigenenergy of $-319.14$ eV with respect to the $(\mu\beta d)$ threshold, the case of $l_{max} = 1$ (0) results in $-319.12 (-317.22)$ eV; $l_{max} = 1$ is sufficient in the
which gives rise to the following advantage: the overlap of functions cause of the following: i) The basis functions are densely set
basis functions. The 'geometric progression' works well be-
very wide function space facilitates the ease of optimization
the exponential-decay solid line in Fig. 9, and many example
short-range structure and long-range asymptotic behavior (cf.
expect that coupling among the entire basis functions occurs
round easily performed. Since the computation time required to cal-
in the GEM review papers [47, 69–71]).

| c  | l_0 | nmax | r_1  | rmax  | L_0 | Nmax | R_1  | Rmax |
|----|-----|------|------|-------|-----|-------|------|-------|
| 1  | 0   | 20   | 5    | 1500  | 0   | 15    | 20   | 1500  |
| 2  | 0   | 20   | 5    | 1500  | 0   | 15    | 20   | 1500  |
| 3  | 0   | 20   | 5    | 1000  | 0   | 15    | 10   | 1500  |
| 1  | 1   | 10   | 20   | 1000  | 1   | 10    | 50   | 1500  |
| 2  | 1   | 10   | 20   | 1000  | 1   | 10    | 50   | 1500  |
| 3  | 1   | 10   | 20   | 1000  | 1   | 10    | 50   | 1000  |
| 3  | 0   | 20   | 0.5  | 20    | 0   | 15    | 10   | 1500  |

reaction calculations (the digits below 1 eV does not affect the results). We then take (cf. Fig. 2)
\[ E_{00} = -0.003030 \text{ MeV}. \] (3.23)

Here, we emphasize the advantages of utilizing the GEM basis functions. The 'geometric progression' works well be-
cause of the following: i) The basis functions are densely set in the internal region, which is suitable for short-range correlations. ii) The norm-overlap matrix elements of the basis functions \( \phi_{n}(r) \) of (3.14) with (3.21) have the relation
\[ \langle \phi_{n} | \phi_{n+k} \rangle = \left[ 2n^2/(1 + a^2k^2) \right]^{3/2}, \] (3.24)
which gives rise to the following advantage: the overlap of \( \phi_{n} \) with the \( k \)-th neighbor \( \phi_{n+k} \) is independent of \( n \) and decreases gradually, from unity, with increasing \( k \). We then ex-
pect that coupling among the entire basis functions occurs smoothly and coherently to simultaneously describe both the short-range structure and long-range asymptotic behavior (cf. the exponential-decay solid line in Fig. 2) and many examples in the GEM review papers [47, 69–71].

Another advantage of utilizing Gaussian ranges in a geo-
metric progression is that the number of the nonlinear variational parameters are so small that their optimization can be easily performed. Since the computation time required to cal-
culate the Hamiltonian matrix elements with the Gaussian ba-
is set is very short, we can take an appropriately large number (even more than enough) of basis functions. The use of this very wide function space facilitates the ease of optimization of the Gaussian ranges using round numbers such as those presented in Table I. The GEM calculation is transparent in the sense that all the nonlinear variational parameters can be explicitly reported in a small table such as Table I.

When utilizing the GEM, the total wave function of a few-body bound state is expanded in terms of the Gaussian basis functions of the Jacobi coordinates for all the rearrangement channels such as in Eqs. (3.14)-(3.15). This multi-channel representation makes the function space much wider than that spanned by single-channel basis functions.

### B. Structure of \( \Psi^{(N)} (d\mu) \) for nuclear interactions

In this subsection, we investigate the structure of the spatial part \( \Phi_0^{(N)}(d\mu) \) of \( \Psi^{(N)} (d\mu) \) in Eq. (3.23) with the coupling to the \( \alpha \mu \) channel switched off. \( \Phi_0^{(N)}(d\mu) \) describes the motion of the \( d\mu \) system when \( d \) and \( t \) are moving in the nu-
clear interaction region. Using this result, we shall propose a method for imposing the outgoing-wave boundary condition on \( \Psi^{(N)} (d\mu) \) in Sec. IIIIC.

\( \Phi_0^{(N)}(d\mu) \) is written as a function of the Jacobi coordinates \((r_3, R_3)\) in channel \( e = 3 \) (cf. Fig. 3) as
\[ \Phi_0^{(N)}(r_3, R_3) \equiv \Phi_0^{(N)}(d\mu). \] (3.25)

The simplest assumption on it may be
\[ \Phi_0^{(N)}(r_3, R_3) \approx \varphi^{(3He)}(r_3) \Phi_0^{(He)}(R_3), \] (3.26)
which is known as an approximate shape of the \( d\mu \) system just before the \( d-t \) fusion occurs. Here, \( \varphi^{(3He)}(r_3) \approx \delta(r_3) \) denotes the \( ^3\text{He} \) nucleus and \( \Phi_0^{(He)}(R_3) \) represents the \( (\text{He} \mu)_{11} \) atom which is illustrated in Fig. 6 by the dotted line.

Sec. IIIIB aims to demonstrate that the \( \Phi_0^{(N)}(r_3, R_3) \) of the present work is well approximated by the product form
\[ \Phi_0^{(N)}(r_3, R_3) = \Phi_0^{(N)}(r_3, 0) \Phi_0^{(N)}(0, R_3)/\Phi_0^{(N)}(0, 0), \] (3.27)
by solving the Schrödinger equation (3.7) where the R.H.S. is set to be null and \( \Psi_{GEM}^{(N)}(d\mu) \) is treated as the fixed source term. The product form (3.27) is on account of the fact that the realistic \( d-t \) system is also located in a small region of \( r_3 \) due to the nuclear \( d-t \) potential, whereas the muon is distributed far away. Eq. (3.27) will be a key point when we consider how to impose the outgoing boundary condition on \( \Psi^{(N)} (d\mu) \).

We expand the unknown function \( \Phi^{(N)}(r_3, R_3) \) in terms of the Gaussian basis functions in the same way as Eqs. (3.14)-(3.22):
\[ \Phi^{(N)}(r_3, R_3) = \sum_{nN} B_{nN} \phi_{n,t=0}(r_3) \psi_{N,L=0}(R_3), \] (3.28)
\[ \phi_{n,t=0}(r_3) = N_0 e^{-\lambda N^2} Y_{00}(\hat{r}_3), \] (3.29)
\[ \psi_{N,L}(R_3) = N_0 e^{-\lambda L^2} R_0^2 Y_{00}(\hat{R}_3), \] (3.30)
where the Gaussian-basis parameters with \( l = L = 0 \) are given in the geometric progression in the last line of Table I which are suitable for correlating with the nuclear interactions. The bases with \( l = L > 0 \) are not employed for the nuclear-interaction region since they have negligible contributions. The coefficients \( \{B_{nN} ; n = 1 \rightarrow n_{max}, N = 1 \rightarrow N_{max}\} \) are solved based on the linear equations
\[ \langle \phi_{n,t=0} \psi_{N,L} | H_{d\mu} - E_{00} | \phi_{n,t=0} \psi_{N,L} \rangle = -\langle \phi_{n,t=0} \psi_{N,L} | H_{d\mu} - E_{00} | \Phi_0^{(C)}(d\mu) \rangle, \] (3.31)
The wave function for \( \Phi \) at \( r_3 = 0 \) is represented by the solid curve, whereas the dotted curve represents the wave function of the \( ^{3}\text{He}\mu \) atom, normalized to \( \Phi_0(0, R_3) \) at \( R_3 = 0 \) for comparison. The solid curve is well simulated by the function \( e^{-R_3/a} \) with \( a = 154 \text{ fm} \); this will be used in Eqs. (5.21) and (5.22).

where \( \Phi^{(C)}_0(d\mu) \) and \( E_{00} \) were already given in Sec. IIIA.

To observe the structure of \( \Phi_0^{(N)}(r_3, R_3) \) obtained, we first plot \( \Phi_0^{(N)}(0, R_3) \) in Fig. 9 using the solid curve. The dotted curve is the wave function of the \( ^{3}\text{He}\mu \) atom, normalized to \( \Phi_0^{(N)}(0, R_3) \) at \( R_3 = 0 \) for comparison. The less-steep slope of the solid curve indicates that the charge density of the \( d\)-pair along \( r_3 \) spreads into the nuclear-interaction region. The r.m.s. radius \( \langle R_3^2 \rangle^{1/2} \) of the solid- and dotted-curve wave functions are 260 and 227 fm, respectively. The exponential-like decay of the solid curve is well described up to \( R_3 \sim 1700 \text{ fm} \) by the solid black, the dotted red and the dotted green curves, respectively. However, they overlap with each other within the thickness of the curves. Thus, we conclude the following, independent of \( a \):

\[
\Phi_0^{(N)}(r_3, a)/\Phi_0^{(N)}(0, a) = \Phi_0^{(N)}(r_3, 0)/\Phi_0^{(N)}(0, 0),
\]  

which indicates, after the replacement of \( a \) by \( R_3 \),

\[
\Phi_0^{(N)}(r_3, R_3)/\Phi_0^{(N)}(0, R_3) = \Phi_0^{(N)}(r_3, 0)/\Phi_0^{(N)}(0, 0).
\]

This is just Eq. (3.32), more generally,

\[
\Phi_0^{(N)}(r_3, a)/\Phi_0^{(N)}(0, a) = \Phi_0^{(N)}(r_3, 0)/\Phi_0^{(N)}(0, 0),
\]

for any \( a \) and \( b \).

The expression (3.32) indicates that just before the fusion reaction occurs, the wave functions of the \( d\)-\( \mu \) relative motion and the \( (d\)-\( \mu \) relative motion are given by \( \Psi_0^{(N)}(r_3, 0) \) and \( \Phi_0^{(N)}(0, R_3) \), respectively, and are independent of each other. This is an important point when we consider the outgoing boundary condition of the \( \alpha n\mu \) wave function \( \Phi^{(+)}_{2m}(\alpha n\mu) \) in the next subsection.

### C. Outgoing boundary condition on \( \Phi^{(+)}_{2m}(\alpha n\mu) \)

Now, the problem is how to impose the outgoing-wave boundary condition on the three-body \( \alpha n\mu \) channel with the kinetic energy of 17.6 MeV. We note that the \( d\)-\( \mu \) and \( \alpha n \) pairs couple to each other via the interaction \( V_{\text{d}_{\alpha n}}^{(T)} \) of Eq. (3.11) independently of the muon coordinate \( R_4(= R_3) \). Therefore, we assume that the spatial component of the \( \alpha n\mu \) wave function, \( \Phi^{(+)}_{2m}(\alpha n\mu) \) in Eq. (3.6), is proportional to the \( \Phi^{(N)}_0(0, R_4) = \Phi^{(N)}_0(b, R_3) \Phi^{(N)}_0(0, 0)/\Phi^{(N)}_0(0, b) \) for the muon motion: namely,

\[
\Phi^{(+)}_{2m}(\alpha n\mu) = \varphi_{2m}(r_3) \Phi^{(N)}_0(0, R_3).
\]

This assumption should be carefully examined since no attention is paid to the effect of the \( \alpha\mu \) Coulomb force although the force is much smaller than the nuclear interactions considered here. It will be shown later that the effect is sufficiently small and is recovered, as a correction, in the calculation of the fusion rate \( \lambda_4 \) in Sec. VIB and the muon spectrum in Sec. VIC using the \( T \)-matrix based on the Lippmann-Schwinger equation.

The three-types of wave-function amplitudes in Eqs. (3.4)- (3.6) are rewritten as

\[
\Psi^{(C)}_{2m}(d\mu) = \Phi^{(C)}_0(d\mu) X^{\mu}_M(dt),
\]
\[ \Psi^{(N)}_{\pm M}(dt\mu) = \sum_{nN} A_{nN} \phi_{n0}(r_3) \psi_{N0}(R_3) \chi^{\pm M}_{\pm}(dt), \quad (3.37) \]
\[ \Psi^{(+)(an\mu)}_{\pm M} = \left[ \phi^{(+)}_{\pm}(r_4) \chi_{\pm}(am) \right]_{\pm M} \Phi^{(N)}_0 (0, R_4), \quad (3.38) \]

where the Gaussian basis functions \( \phi_{n0}(r_3) \) and \( \psi_{N0}(R_3) \) are the same as those in Eqs. (3.29)-(3.30). The coefficients \( A_{nN} \) and the function \( \phi^{(+)}_{\pm}(r_4) \) can be solved using the Schrödinger equation (3.7)-(3.8), whereas \( \Phi^{(0)}_0 (0) \) is the given source-term function.

We rewrite \( \phi^{(+)}_{\pm}(r_4) \) as
\[ \phi^{(+)}_{2m}(k_4, r_4) = \frac{u^{(+)}_{2m}(k_4, r_4)}{r_4} Y_{2m}(r_4) \quad (3.39) \]
and explicitly impose the outgoing boundary condition on \( u^{(+)}_{2m}(k_4, r_4) \) as
\[ u^{(+)}_{2m}(k_4, r_4) \rightarrow S_2 e^{i\delta r_4}. \quad (3.40) \]

where the momentum \( k_4 \) between \( \alpha \) and \( n \) is given in Eq. (3.36). The amplitude \( S_2 \) of the outgoing wave (3.40) is slightly different from the usual definition of \( S \)-matrix in the scattering with an incoming wave. In the present case, the dimension of \( S_2 \) is \( L^1 \) owing to the dimension \( L^{-3} \) of the initial \((dt\mu)\) bound state \( \Phi^{(N)}_0 (dt\mu) \) in Eq. (3.36).

The flux of the \( \alpha-n \) relative motion at \( r_4 \rightarrow \infty \) into the full direction \((4\pi) \) st in a unit time is given as (note \( r_4 = k_4 \))
\[ v_4 N_\mu \int \left| S_2 Y_2(k_4)|\chi_2(\alpha n)\right|^2 \, dk_4 = v_4 N_\mu |S_2|^2, \quad (3.41) \]
where \( v_4 = \hbar k/\mu r_4 \) is the velocity of the \( \alpha-n \) relative motion, and \( N_\mu \) is given by
\[ N_\mu = \int \left| \Phi^{(0)}_0 (0, R_4) \right|^2 \, dR_4, \quad (3.42) \]
which indicates the probability of finding the muon anywhere when the \( \alpha-n \) distance \( r_4 = 0 \). The R.H.S. of Eq. (3.41) is the fusion rate, namely, the number of \( \alpha-n \) pair (number of muon) outgoing from one \((dt\mu)\) molecule:
\[ \lambda_\mu = v_4 N_\mu |S_2|^2. \quad (3.43) \]

Recall that, at the end of Sec. IIA, we expected that the calculations of \( \lambda_\mu \) in the present work to generate results that are not inconsistent with \( \lambda_\mu \) in (2.6) given by the optical-potential model.

### D. Results

The coupled-channels Schrödinger equation (3.7)-(3.8) with the outgoing boundary condition (3.40) can be precisely solved by using the coupled-channels Kohn-type variational method for composite-particle scattering [45], which was used in Sec. IIB.

---

**FIG. 11:** The \( \alpha-n \) outgoing wave function \( u^{(+)}_{2m}(k_4, r_4) \). The real (imaginary) part is represented by the solid (dotted) curve.

The outgoing \( D \)-wave function \( u^{(+)}_{2m}(k_4, r_4) \) is obtained as in Fig. 11 together with
\[ S_2 = (0.5934 + 0.1985 i) \text{ fm}. \quad (3.44) \]
Therefore, using \( |S_2|^2 = 3.915 \times 10^2 \text{ fm} \), \( v_4 = 6.50 \times 10^{22} \text{ fm s}^{-1} \) and \( N_\mu = 4.045 \times 10^{-11} \text{ fm}^{-3} \) in Eq. (3.42), the calculated fusion rate is given as
\[ \lambda_\mu = 1.03 \times 10^{12} \text{ s}^{-1}. \quad (3.45) \]

It is striking that the fusion rates (3.45) and (2.6) are consistent with each other although the calculational methods are quite different. However, this is reasonable since the optical-potential model is a phenomenological substitute in which the coupling between the \( d-t \) and the \( \alpha-n \) channels is represented by the imaginary part of the potential.

Next, we examine the spatial component of \( \Phi^{(N)}_0 (dt\mu) \) in Eq. (3.37), namely
\[ \Phi^{(N)}_0 (r_3, R_3) \equiv \sum_{nN} A_{nN} \phi_{n0}(r_3) \psi_{N0}(R_3), \quad (3.46) \]
which was obtained by solving the coupled-channels Schrödinger equation (3.7)-(3.8). We compare this \( \Phi^{(N)}_0 (r_3, R_3) \) with \( \Phi^{(0)}_0 (r_3, R_3) \) in Eq. (3.27) which was previously derived from Eqs. (3.28)-(3.30) without the coupling to the \( an \mu \) channel, as was illustrated in Figs. 9 and 10.

We first verify that the new \( \Phi^{(N)}_0 (r_3, R_3) \) can also be described, similarly to Eq. (3.27), in the product form
\[ \Phi^{(N)}_0 (r_3, R_3) = \Phi^{(0)}_0 (r_3, 0) \Phi^{(N)}_0 (0, R_3)/\Phi^{(0)}_0 (0, 0). \quad (3.47) \]

In the same manner as Figs. 9 and 10, we represent \( \Phi^{(N)}_0 (0, R_3) \) and \( \Phi^{(0)}_0 (r_3, 0) \) in Figs. 12 and 13 as the red solid curves for the real part and the dotted red curves for the imaginary part. The solid black curves represent the previous \( \Phi^{(N)}_0 (0, R_3) \) and \( \Phi^{(0)}_0 (r_3, 0) \) in Figs. 9 and 10 respectively.

Based on these figures, we find the relation
\[ \Phi^{(N)}_0 (r_3, R_3) \sim (1.7 + 0.6 i) \Phi^{(0)}_0 (r_3, R_3). \quad (3.48) \]
pling is enhanced by \( \sim 3 \) for comparison. It should be noted that in the calculation of \( d \) and \( T \) interactions are considered. The black solid curve for \( \rho^{(N)}(r_3) \) represents the case for which the \( dt-an \) coupling is switched off.

The red curve shows \( \tilde{\rho}^{(N)}(r_3) \) for the \( d-t \) relative motion when all the nuclear interactions are considered. The black solid curve for \( \rho^{(N)}(r_3) \) represents the case for which the \( dt-an \) coupling is switched off.

where the integration over the muon-coordinate \( R_3 \) is performed. \( \tilde{\Phi}_0^{(C)}(r_3, R_3) \) is the same as \( \Phi_0^{(C)}(d\mu) \) in Eq. \( \text{(3.36)} \), but transformed to the function of \( (r_3, R_3) \). By the normalization of \( \tilde{\Phi}_0^{(C)}(d\mu) \) in Eq. \( \text{(3.12)} \), we have

In Fig. 14, \( \tilde{\rho}^{(C)}(r_3) \) multiplied by 100 is illustrated by the dashed curve for \( r_3 < 10 \) fm, whereas the inserted figure shows \( \tilde{\rho}^{(C)}(r_3) \) for the entire region. The red curve gives \( \tilde{\rho}^{(N)}(r_3) \) for the \( d-t \) relative motion when all the nuclear interactions are employed, whereas the black solid curve for \( \rho^{(N)}(r_3) \) is the case for which \( dt-an \) coupling is switched off. The red curve is 3.25 times enhanced compared to the black-sold curve owing to the \( dt-an \) coupling; this factor corresponds to the square of the absolute value of the numerical factor in the R.H.S. of Eq. \( \text{(3.33)} \). It should be emphasized that \( \tilde{\rho}^{(C)}(r_3) \) is significantly smaller than \( \tilde{\rho}^{(N)}(r_3) \) in the nuclear interaction region. Therefore, \( \tilde{\Phi}_0^{(C)}(r_3, R_3) \) is expected to play a minor role compared to \( \tilde{\Phi}_0^{(N)}(r_3, R_3) \) in the estimation of the \( \alpha-\mu \) sticking and the
ejected muon’s spectrum after the fusion; this will be discussed in detail in Secs. V and VI.

IV. USE OF LIPPmann-Schwinger EQUATION FOR $dt\mu$ FUSION REACTION

A. $T$-matrix element

In this section, we propose the use of the Lippmann-Schwinger equation [44] as another method for studying the fusion reaction (1.2), in particular, to calculate the initial sticking of a muon to an $\alpha$ particle and the momentum and energy spectra of the emitted muon, respectively in Secs. V and VI.

Let’s suppose that the reaction from a plain-wave initial $\alpha$-channel is outgoing to the final $\beta$-channels assuming the following wave functions:

Total wave function : $\Psi^{(+)}_\alpha(E_\alpha)$,
Initial $\alpha$-channel wave function : $e^{iK_\alpha\cdot R_\alpha}\phi_\alpha(\xi_\alpha)$,
Asymptotic form of final $\beta$-channel wave function :

$$f_{\beta\alpha}(\Omega_\beta) = \frac{e^{iK_\alpha\cdot R_\beta}}{R_\beta} \phi_\beta(\xi_\beta),$$

where $\phi_\alpha(\xi_\alpha)$ and $\phi_\beta(\xi_\beta)$ are ortho-normalized intrinsic wave functions of the $\alpha$- and $\beta$-channels, respectively, and $f_{\beta\alpha}(\Omega_\beta)$ is the scattering amplitude to be determined.

One can calculate the transition matrix elements $T_{\beta\alpha}$ from the well-known integral formula [44, 72] based on the Lippmann-Schwinger equation as

$$T_{\beta\alpha} = \langle e^{iK_\alpha\cdot R_\alpha}\phi_\alpha(\xi_\alpha) | V_\beta | \Psi^{(+)}_\alpha(E_\alpha) \rangle,$$  

(4.1)

where $V_\beta$ is the interaction in the $\beta$-channel. Using this $T_{\beta\alpha}$, the $\beta$-channel asymptotic form of the total wave function $\Psi^{(+)}_\alpha(E_\alpha)$ is written as

$$\langle \phi_\beta(\xi_\beta) | \Psi^{(+)}_\alpha(E_\alpha) \rangle \xrightarrow{R_\beta \to \infty} \frac{\mu_{R_\beta}}{2\pi \hbar^2} T_{\beta\alpha} e^{iK_\alpha\cdot R_\beta} R_\beta,$$  

(4.2)

where $\mu_{R_\beta}$ is the reduced mass associated with $R_\beta$. Therefore, we have

$$f_{\beta\alpha}(\Omega_\beta) = -\frac{\mu_{R_\beta}}{2\pi \hbar^2} T_{\beta\alpha}.$$

(4.3)

The reaction cross section $\sigma_{\beta\alpha}$ is usually defined by the flux of the outgoing wave with a velocity $v_\beta = (\hbar K_\beta/\mu_{R_\beta})$ into the full direction (4sr) in a unit time divided by the flux of the incident wave ($= v_\alpha$) as

$$\sigma_{\beta\alpha} = \frac{v_\beta}{v_\alpha} \int |f_{\beta\alpha}(\Omega_\beta)|^2 \, d\Omega_\beta,$$

(4.4)

$$= \frac{v_\beta}{v_\alpha} \frac{\mu_{R_\beta}}{2\pi \hbar^2} \int |T_{\beta\alpha}|^2 \, d\Omega_\beta.$$

(4.4)

The preceding expressions are exact provided that the total wave function $\Psi^{(+)}_\alpha(E_\alpha)$ is rigorously exact. However, for typical reaction calculations, $\Psi^{(+)}_\alpha(E_\alpha)$ in Eq. (4.1) is replaced by an approximate wave function.

In the present fusion reaction (1.2), however, the initial $\alpha$-channel is not the plain wave $e^{iK_\alpha\cdot R_\alpha}\phi_\alpha(\xi_\alpha)$, but the $dt\mu$ bound state $\tilde{\Phi}^{(C)}_{Z_M}(dt\mu)$ in Eq. (3.3). Therefore, in Eq. (4.4), we omit the incoming-channel information and replace the total wave function by our $\Psi^{(+)}_\beta(E)$ of Eq. (3.3), and introduce the ‘reaction rate’, $r_{\beta\alpha}$, as

$$r_{\beta\alpha} = v_\beta \frac{\mu_{R_\beta}}{2\pi \hbar^2} \int |T_{\beta\alpha}|^2 \, d\Omega_\beta.$$

(4.5)

Since the initial-state wave function $\tilde{\Phi}^{(C)}_{Z_M}(dt\mu)$ is normalized to unity (namely, starting with one molecule), $r_{\beta\alpha}$ represents the number (probability) of a molecule decaying into the $\beta$ channel per unit time. Therefore, the sum of $r_{\beta\alpha}$ over $\beta$ becomes the fusion rate $\lambda_\alpha$:

$$\lambda_\alpha = \sum_\beta r_{\beta\alpha}.$$

(4.6)

Note that we call $r_{\beta\alpha}$ the reaction rate and $\lambda_\alpha$ the fusion rate throughout this work.

The definition of reaction rate $r_{\beta\alpha}$ is applied to the study of $\alpha$-$\mu$ sticking in Sec. V and to the momentum and energy spectra of the emitted muon in Sec. VI. In these applications, alternatively-defined fusion rates $\lambda_\alpha$ using $r_{\beta\alpha}$ are calculated; these two types of additional fusion rates should be consistent with the values already obtained using Eqs. (4.6) and (3.35), which will be a significant test of the reliability of the presented calculations.

B. Discretization of two-body continuum states

In the definition of the $T$-matrix (4.1), $\phi_\beta(\xi_\beta)$ are treated as ortho-normalized states. As the $\beta$-channel intrinsic states, however, we will consider the $\alpha$-$\mu$ continuum states associated with $r_\alpha$ (Sec. V) and the $\alpha$-$n$ continuum states associated with $r_4$ (Sec. VI).

It is difficult to directly treat the continuum states in the $T$-matrix calculation. Instead, we discretize these states and construct the ortho-normalized discretized continuum states, such as $\phi_{l\mu}(r_\alpha)$ using $i$ to number the discretized states; we then consider their convergence back to the continuum. This discretization is performed by employing the CDCC (Continuum-Discertized-Coupled Channels) method that was developed by one of the present authors (M.K.) and his collaborators (for example, see review papers [48, 50]) for the study of projectile-breakup reactions. At present, this is one of the standard methods for investigating various reactions using light- and heavy-ion projectiles.

The discretization of continuum states is performed as follows (cf. Fig. 15): Let $\phi_{l\mu}(k, r)$ denote $k$-continuum states with angular-momentum $lm$ that satisfies the Schrödinger equation

$$\left[-\frac{\hbar^2}{2\mu_r} \nabla_r^2 + V(r) - \varepsilon \right] \phi_{l\mu}(k, r) = 0, \quad \varepsilon = \frac{\hbar^2 k^2}{2\mu_r}.$$

(4.7)
Each continuum-discretized wave function $\phi_{ilm}(r)$ is taken based on the interval $\Delta k_i = k_{i-1} - k_i$ ($i = 1, ..., N$); usually, $\Delta k_i$ is taken to be independent of $i$. We then take an average of the continuum wave functions in each momentum bin as

$$\bar{\phi}_{ilm}(r) = \frac{1}{\sqrt{\Delta k_i}} \int_{k_{i-1}}^{k_i} \phi_{ilm}(k, r) dk, \quad (i = 1, ..., N)$$

(4.8)

where the integration is performed numerically with the required accuracy.

Since $\phi_{ilm}(k, r)$ is normalized as

$$\langle \phi_{ilm}(k, r) | \phi_{ilm}(k', r) \rangle = \delta(k - k'),$$

(4.9)

the discretized-continuum wave functions $\bar{\phi}_{ilm}(r)$ have the ortho-normal relation

$$\langle \bar{\phi}_{ilm}(r) | \bar{\phi}_{il'm}(r) \rangle = \delta_{ii'}.$$  

(4.10)

Namely, $\bar{\phi}_{ilm}(r)$ becomes an $L^2$-integrable function because of the cancelation between the asymptotic (oscillating) amplitudes of $\phi_{ilm}(k, r)$ during the $k$-integration. A typical example of such a damping in the asymptotic region by averaging oscillating functions is as follows:

$$\int_{k_i}^{k_i + \Delta k_i} \sin kr \, dk = \frac{2}{\Delta k_i} \sin \frac{k_i}{2} \sin \left( k_i + \frac{\Delta k_i}{2} \right).$$

(4.11)

Each $\bar{\phi}_{ilm}$ can be regarded as if it were a discrete excited-state wave function with energy $\epsilon_{il}$ given by the expectation value of the Hamiltonian as

$$\bar{\epsilon}_i = -\frac{\hbar^2}{2\mu} \frac{k_i^2}{2} = \left( k_i + k_{i-1} \right)^2 + \frac{\Delta k_i^2}{12}.$$  

(5.3)

Therefore, we can treat the $T$-matrix elements of three-body break-up systems similar to those of ‘two-body’ systems with many ‘discrete excited’ states.

Convergence of the calculated reaction rates with respect to $\Delta k_i \to 0$ is discussed in Sec. V (cf. Fig. 16); see Refs. [48–50] for additional details about this type of convergence.

V. Muon sticking to a particle

After the fusion reaction (1.2) takes place, the emitted muon sticks to the $\alpha$-particle or goes to the $\alpha$-$\mu$ continuum states. The probability that this muon sticks to the bound state is referred to as the initial sticking probability, $\omega_{0\alpha}$, and is one of the most important parameters for determining fusion efficiency, since this muon is not available for further $\mu$CF cycles. However, as summarized in a previously published review paper [3], the $\alpha$-$\mu$ sticking is not yet completely understood.

In this section, we study the muon sticking problem in a much more sophisticated manner than that in the literature. We derive, for the first time, absolute values of the reaction (1.2) going to the $\alpha$-$\mu$ bound and continuum states. This is performed by calculating the $T$-matrix (4.1) for the reaction rate (4.5), in which the exact total wave function $\Psi^{(+)}_{\alpha}(E_\alpha)$ is approximated by $\Psi^{(+)\alpha}(E)$ of Eq. (3.3) that was already obtained by solving the Schrödinger equation (3.2)–(3.3).

A. $T$-matrix calculation of fusion rate

We calculate the $T$-matrix (4.1) for the reaction rate (4.5) of the fusion reaction

$$(d\mu)_{l=0} \rightarrow (\alpha\mu)_{nl} + n + 17.6 \text{ MeV}$$

(5.1)

$$\gamma (\alpha\mu)_{nl} + n + 17.6 \text{ MeV},$$

where $(\alpha\mu)_{nl}$ denotes the $n$-th $(\alpha\mu)$ bound state with $l$ presented by $\phi_{ilm}(r)$ with the eigenenergy $\epsilon_{nl}$, whereas $(\alpha\mu)_{nl}$ describes the $i$-th discretized $\alpha$-$\mu$ continuum state that is obtained by discretizing $\phi_{ilm}(k, r)$ into $[\bar{\epsilon}_i, \bar{\phi}_{ilm}(r), i = 1, ..., N]$ by performing Eqs. (4.8) and (4.12) (cf. Fig. 15). We take $l = 0$ to 25, $N = 200$ and the maximum momentum $h k_N = 10 \text{ MeV}/c$ ($\epsilon_N \approx 487 \text{ keV}$) in this section.

In $T$-matrix (4.1), we replace the exact total wave function $\Psi^{(+)}_{\alpha}(E_\alpha)$ by $\Phi^{(+)\alpha}(E)$ that was given in Sec. III as the sum of the three components (cf. Eq. (3.3)):

$$\Psi^{(+)\alpha}(E) = \Psi^{(C)}_{\alpha\mu}(d\mu) + \Psi^{(N)}_{\mu \alpha}(d\mu) + \Psi^{(+\alpha)}_{\alpha\mu}(\alpha\mu).$$

(5.2)

Correspondingly, we divide the $T$-matrix (4.1) into three parts employing channel $c = 5$ with the Jacobi coordinates $(r_5, R_5)$ as

$$T^{(C)}_{nl,mm} = \langle e^{K_5, R_5} \bar{\phi}_{ilm}(r_5)k_{\epsilon_{nl}}(n) | V^{(C)}_{\alpha\mu, \alpha\mu, \nu\alpha, \nu\alpha}(\mu \alpha) \rangle,$$

$$T^{(N)}_{nl,mm} = \langle e^{K_5, R_5} \bar{\phi}_{ilm}(r_5)k_{\epsilon_{nl}}(n) | V^{(N)}_{\mu \alpha, \alpha\mu, \nu\alpha, \nu\alpha}(\mu \alpha) \rangle,$$

$$T^{(+\alpha)}_{nl,mm} = \langle e^{K_5, R_5} \bar{\phi}_{ilm}(r_5)k_{\epsilon_{nl}}(n) | V^{(+\alpha)}_{\alpha\mu, \alpha\mu, \nu\alpha, \nu\alpha}(\mu \alpha) \rangle,$$

(5.3)

for the $\alpha$-$\mu$ bound states $\phi_{ilm}(r_5)$ with the energy $\epsilon_{nl}$, and

$$\bar{T}^{(C)}_{nl,mm} = \langle e^{K_5, R_5} \bar{\phi}_{ilm}(r_5)k_{\epsilon_{nl}}(n) | V^{(C)}_{\alpha\mu, \alpha\mu, \nu\alpha, \nu\alpha}(\mu \alpha) \rangle,$$

$$\bar{T}^{(N)}_{nl,mm} = \langle e^{K_5, R_5} \bar{\phi}_{ilm}(r_5)k_{\epsilon_{nl}}(n) | V^{(N)}_{\mu \alpha, \alpha\mu, \nu\alpha, \nu\alpha}(\mu \alpha) \rangle,$$

$$\bar{T}^{(+\alpha)}_{nl,mm} = \langle e^{K_5, R_5} \bar{\phi}_{ilm}(r_5)k_{\epsilon_{nl}}(n) | V^{(+\alpha)}_{\alpha\mu, \alpha\mu, \nu\alpha, \nu\alpha}(\mu \alpha) \rangle,$$

(5.4)
for the $\alpha$-$\mu$ discretized continuum states $\widetilde{\phi}_{\text{lin}}(r_5)$ with $\varepsilon_{il}$. In Eqs. (5.3) and (5.4), the plain-wave momenta $K_s$ and $K_i$ are determined, respectively, as

$$\frac{\hbar^2}{2M_s}K_s^2 = E_{00} + Q - \varepsilon_{nl},$$  \hspace{1cm} (5.5)

$$\frac{\hbar^2}{2M_i}K_i^2 = E_{00} + Q - \varepsilon_{il}, \quad \varepsilon_{il} = \frac{\hbar^2}{2\mu_5}k_i^2,$$ \hspace{1cm} (5.6)

where $E_{00} = -0.003030$ MeV and $Q = 17.589$ MeV (cf. Fig. 2). The reaction rate (4.5) is written as

$$r_{nl} = v_{nl}\left(\frac{\mu_{R_s}}{2\pi\hbar^2}\right)^2 \times \sum_{m,m_i} \int \left| T_{nl,m,m_i}^{(C)} + T_{nl,m,m_i}^{(N)} + T_{nl,m,m_i}^{(+)\dagger}\right|^2 d\vec{K}_s,$$ \hspace{1cm} (5.7)

$$\tilde{r}_{il} = v_{il}\left(\frac{\mu_{R_i}}{2\pi\hbar^2}\right)^2 \times \sum_{m,m_i} \int \left| T_{il,m,m_i}^{(C)} + T_{il,m,m_i}^{(N)} + T_{il,m,m_i}^{(+)\dagger}\right|^2 d\vec{K}_i,$$ \hspace{1cm} (5.8)

respectively, for the bound state $(nl)$ and for the discretized continuum state $(il)$. $v_{nl} = \hbar K_n/\mu_{R_s}$ is the velocity of the $(\alpha\mu)n$ relative motion associated with $R_s$, and similarly for $v_{il} = \hbar K_i/\mu_{R_i}$. Since the reaction rates $r_{nl}(\tilde{r}_{il})$ do not depend on the $M$ ($s$-component of the total angular momentum $\frac{1}{2}$), it is not necessary to take the average with respect to $M$.

The components of the $T$-matrix elements are explicitly expressed to identify the dominant contribution to the reaction rates $r_{nl}(\tilde{r}_{il})$. This is a new approach for analyzing the initial sticking probability $\omega_{il}^2$ in Sec. VB.

We then transform the summation $\sum_i \tilde{r}_{il}$ into the integration of a smooth continuum function $r_l(k)$ of $k$ as

$$\sum_i \tilde{r}_{il} = \sum_i \int \frac{dK_i}{dK} \tilde{r}_{il} dk \rightarrow \int_0^{K_i} \left| r_l(k) \right|^2 dk = \equiv r_{l}^{\text{cont}}.$$ \hspace{1cm} (5.9)

A test of this procedure is illustrated in Fig. 16 for the case of $l = 0$. The step function denotes the constant strength $\tilde{r}_{il}/dk$ within each momentum bin $i$. The bin-width $dk$ in the red step function is 40% of that in the blue one. The black curve, $r_l(k)$, is obtained by smoothing the step function for which the bin-width is 10% of that in the blue one. It is observed that the procedure (5.9) works well.

The calculated reaction rates $r_l(k)$ are shown in Fig. 17 for angular momenta $l$ between $\alpha$ and $\mu$. The dotted black curve represents the summed rates $\sum_{l=0}^{25} r_l(k)$ multiplied by $\frac{1}{4}$. We see that the peak of the dotted curve is at $\hbar k \sim 4.3$ MeV/c ($\epsilon \sim 88$ keV). This is understood as follows: With the kinetic energy 3.5 MeV (with speed $v_{\alpha}/c = 0.043$), the $\alpha$ particle escapes from the muon cloud which has approximately the $(^5\text{He})_1s$ wave function of $R_s$. Conversely, the muon cloud is moving with respect to the $\alpha$ particle with the same speed $v_{\mu}/c$, namely $\hbar k \sim 4.3$ MeV/c. The width of the peak of the dotted curve corresponds to the width of the momentum distribution within the muon cloud.

Furthermore, the reason why so many angular momenta $l$ appear in $r_l(k)$ in Fig. 18 is as follows: In the $T$-matrix elements (5.4), the component $\left| V[\Psi(1\mu)] \right|$ is composed of very short-range functions of $r_s$ and long-range functions of $R_i$. Therefore, many angular momenta $l$ are necessary to expand this unique function of $(r_s, R_i)$ in terms of the functions $e^{i\vec{K}_s \cdot \vec{r}_s}, \tilde{\phi}_{\text{lin}}(r_5)$ on the different Jacobi coordinates $(r_5, R_i)$.

For comparison with $r_{l}^{\text{cont}}$ in Eq. (5.9), we introduce

$$j_{l}^{\text{bound}} = \sum_n r_{nl},$$ \hspace{1cm} (5.10)

for the transition to all the $\alpha$-$\mu$ bound states with $l$. Figure 18 illustrates how $j_{l}^{\text{bound}}$ and $r_{l}^{\text{cont}}$ depend on the angular momentum $l$ of $0 \leq l \leq 25$. $j_{l}^{\text{bound}}$ are given by the red circles and $r_{l}^{\text{cont}}$ by the black ones. The rates $j_{l}^{\text{bound}}$ decrease quickly with increasing $l$, whereas $r_{l}^{\text{cont}}$ changes slowly with respect to $l$. The ratio ($\sim 1\%$) of the strength of the red-circle group to that of the black-circle group is the essence of the initial $\alpha$-$\mu$ sticking probability, which is discussed in the next subsection.

Finally, we define the fusion rates to all the bound states and to all the continuum states, respectively as

$$\lambda_{l}^{\text{bound}} = \sum_{l=0}^{5} j_{l}^{\text{bound}},$$ \hspace{1cm} (5.11)

$$\lambda_{l}^{\text{cont}} = \sum_{l=0}^{25} r_{l}^{\text{cont}},$$ \hspace{1cm} (5.12)

and the sum of them as

$$\lambda_{l} = \lambda_{l}^{\text{bound}} + \lambda_{l}^{\text{cont}}.$$ \hspace{1cm} (5.13)

This $\lambda_{l}$ is the fusion rate of the reaction (1.2) defined by using the $T$-matrix in channel $c = 5$.

FIG. 16: Convergence of the reaction rates $r_l(k)$ going to the $\alpha$-$\mu$ continuum states in Eq. (5.9) with respect to the momentum-bin size $dk \rightarrow 0$ in the case of $l = 0$. 

[Image: FIG. 16]
Another important result in Table III is that the contribution to the fusion rates from $T^{(C)}$ is much smaller than that from $T^{(N)}$; this was expected from Fig. 14 since $\tilde{\rho}^{(C)}(r_1)$ is much smaller than $\tilde{\rho}^{(N)}(r_1)$ in the nuclear interaction region. This will be referred to in the next subsection for the $\alpha$-$\mu$ sticking probability $\omega_0^\alpha$.

**B. Initial sticking probability $\omega_0^\alpha$**

The absolute values of the fusion rates $\lambda_{\text{cont.}}^\alpha$ and $\lambda_{\text{bound}}^\alpha$ have been explicitly calculated in the present three-body reaction calculation. This requires a change in the way of discussing the $\alpha$-$\mu$ sticking, as will be emphasized later.

Now, it is possible to calculate the initial muon-sticking probability by the definition

$$\omega_0^\alpha = \frac{\lambda_{\text{bound}}^\alpha}{\lambda_{\text{bound}}^\alpha + \lambda_{\text{cont.}}^\alpha} \tag{5.15}$$

that is based on the original idea for $\omega_0^\alpha$ (cf., for example, Eq. (192) in Ref. 9), employing the nuclear interactions that reproduce the observation quantities in Figs. 7 and 8.

Before discussing our calculation of $\omega_0^\alpha$, we review the essential point of previously reported studies on the $\alpha$-$\mu$ sticking probability according to the review papers of $\mu$CF [11, 3]. Since the sudden approximation was used in the literature to define $\omega_0^\alpha$, we first derive the same representation of their $\omega_0^\alpha$ using our framework. We start from our definition (5.15) and make the following approximations i) to v):

i) In the $T$-matrix elements (5.3) and (5.4), the $\alpha\mu$ outgoing wave $\Psi^{(+)}_{\alpha\mu}(\alpha\mu)$ is excluded from the total wave function $\Psi^{(+)}_{\alpha\mu}(E)$ of (5.2). Omitting the spin component, the total $d\mu$ wave function is represented by the $\Phi_{d\mu}(r_3, R_3)$ that is obtained by diagonalizing the $d\mu$ Hamiltonian with the full use of the $d\mu$ GEM basis functions in Eqs. (3.15) and (3.28); all the Jacobi coordinates are transformed into $(r_1, R_3)$.

ii) In Eqs. (5.3) and (5.4), the $dt$-$an$ transition interaction (5.11), $V^\text{an,dt}$, is replaced as

$$\int dr_3 V^\text{an,dt}_3(r_3, r_4) \to V_\delta \int dr_3 \delta(r_3) \delta(r_4), \tag{5.16}$$

which is the essence of the sudden approximation.

iii) The momentum $K_a$ of the plain wave $e^{-iK_a \cdot R_3}$ is fixed to $K$ given by $\hbar^2 K^2/2\mu_{R_3} = 17.589$ MeV.

iv) Thus, the $T$-matrix elements and the fusion rates are given by

$$T_{nlm} = \langle e^{iK_a \cdot R_3} \phi_{nlm}(r_3) | V_\delta \int dr_3 \delta(r_3) \delta(r_4) | \phi_{nlm}(r_3) \rangle \times \Phi_{d\mu}(r_3, R_3) \rangle_{r_3, R_3}, \tag{5.17}$$

$$\lambda_{\text{bound}}^\alpha = 2\pi \int \left( \frac{\mu_{R_3}}{2\pi \hbar^2} \right)^2 \sum_{nlm} |T_{nlm}|^2, \tag{5.18}$$

$$\lambda_{\text{cont.}} = 2\pi \int \left( \frac{\mu_{R_3}}{2\pi \hbar^2} \right)^2 V_\delta \langle \Phi_{d\mu}(0, r_3) \Phi_{d\mu}(0, R_3) \rangle_{r_3}. \tag{5.19}$$
TABLE II: Fusion rates $\lambda^\text{cont}_t$ and $\lambda^\text{bound}_t$ of the reaction $(d\mu)_J \to (\alpha\mu)_J$, for $(\alpha\mu)_J + n$ or $(\alpha\mu)_J + n$, respectively, and their sum $\lambda_t$, defined by Eqs. (5.11)-(5.13) on the Jacobi-coordinate channel $c = 5$. Contribution to them from the full $T$-matrix and from the individual $T$-matrix elements $T^{(N)}$, $T^{(C)}$ and $T^{(\lambda)}$ are listed. The initial sticking probability $\omega^S_0$ is given in the last line. Since the contribution from $T^{(C)}$ and $T^{(\lambda)}$ are minor, $\omega^S_0$ is not calculated there.

| $T$-matrix type | $|T^{(C)} + T^{(N)} + T^{(\lambda)}|^2$ | $|T^{(C)}|^2$ | $|T^{(N)}|^2$ | $|T^{(\lambda)}|^2$ |
|-----------------|-------------------------------------|----------------|----------------|----------------|
| $\lambda_t$ (s$^{-1}$) | 8.05 \times 10^{11} | 3.70 \times 10^{10} | 7.73 \times 10^{11} | 1.18 \times 10^{13} |
| $\lambda^\text{cont}_t$ (s$^{-1}$) | 7.98 \times 10^{11} | 3.67 \times 10^{10} | 7.66 \times 10^{11} | 1.17 \times 10^{13} |
| $\lambda^\text{bound}_t$ (s$^{-1}$) | 6.90 \times 10^{9} | 3.14 \times 10^{10} | 6.63 \times 10^{9} | 9.41 \times 10^{8} |
| $\omega^S_0$ (%) | 0.857 | — | (0.857) | — |

where $q = \frac{e\mu}{m_\mu R}$ and $v = \hbar K/\mu R$. The completeness of the $\alpha-\mu$ basis functions $\{\phi_{nlm}(\mathbf{r}_5), \phi_{nlm}(\mathbf{r}_5)\}$ is used to derive $\lambda_t$. v) Finally, the sticking probability $\omega^0_S$ defined by (5.15) is approximated by $\tilde{\omega}^0_S$ as

$$
\tilde{\omega}^0_S = \frac{\sum_{nlm} |\langle \Phi_{nlm}(\mathbf{r}_5) | \Phi_{nlm}(\mathbf{r}_5) \rangle|^2}{\langle \Phi_{nlm}(\mathbf{r}_5) | \Phi_{nlm}(\mathbf{r}_5) \rangle^2},
$$

(5.20)

where no calculation is performed on the absolute values of $\lambda^\text{bound}_t$, $\lambda^\text{cont}_t$ and $\lambda_t$, since the $dt-an$ coupling interaction $V_t \int \text{d}r_4 \delta(|\mathbf{r}_4| \delta(|\mathbf{r}_4|)$ is not appropriate for the purpose.

We see that Eq. (5.20) is the same as the previous expression for $\omega^0_S$ under the sudden approximation (for example, see Eq. (207) of Ref. [5] and Eq. (36) of Ref. [4]). Most of the literature calculations gave values in the region of

$$
\tilde{\omega}^0_S \approx 0.88 - 0.89%
$$

(5.21)

without nuclear d-t interactions (see the lines for 'Theory: Coulombic problem' in Table 10 of the $\mu$CF review paper [5]). Similarly, with the nuclear d-t,

$$
\tilde{\omega}^0_S \approx 0.91 - 0.93%
$$

(5.22)

were obtained by the optical-potential model [33, 35] and the R-matrix method [36-41] (in Refs. [39, 41], an internuclear distance $a_{dt} = 0.51$ fm was taken in place of $a_{dt} = 0$ in Eq. (5.20)). One of the present authors (M.K.) [33] participated in those calculations.

However, it should be noted that there is a serious problem in the discussion of $\tilde{\omega}^S_0$ in the case of (5.21) with the Coulomb force only for $\Phi_{dt}(\mathbf{r}_4, \mathbf{r}_5)$). This problem occurs because attention was not paid to the absolute values of $\lambda^\text{bound}_t$ and $\lambda^\text{cont}_t$. This is made clear in Table III for $\lambda^\text{bound}_t$ and $\lambda^\text{cont}_t$ together with their contributions from the three types of $T$-matrix, namely, $T^{(C)}$, $T^{(N)}$ and $T^{(\lambda)}$. The column $|T^{(C)}|^2$ is responsible for the calculation of (5.21). We see that the contribution from $T^{(C)}$ to $\lambda^\text{cont}_t$ and $\lambda^\text{bound}_t$ is much smaller than that from $T^{(N)}$; this is known from Fig. 13 since $\tilde{\rho}^{(C)}(\mathbf{r}_5)$ is much smaller than $\tilde{\rho}^{(N)}(\mathbf{r}_5)$ in the nuclear interaction region.

Therefore, we say that such a calculation of $\tilde{\omega}^0_S$ using the minor components of $\lambda^\text{cont}_t$ and $\lambda^\text{bound}_t$ is not so meaningful (although it is useful when comparing the accuracy of the employed calculation methods with each other). In this sense, we placed the symbol ‘—’ in the column of $|T^{(C)}|^2$ in the last line for $\omega^S_0$, and similarly in the column of $|T^{(\lambda)}|^2$. We also note that the statement “the additional effect of the nuclear force to the sticking probability” is not appropriate since $T^{(N)}$ dominantly contributes to $\lambda_t$ (Table III), not additionally.

Our final result on the initial sticking probability is, as shown in the full $T$-matrix column of Table III

$$
\omega^S_0 \approx 0.857% \quad \text{(present)},
$$

(5.23)

which is reduced by ~7% from the value in (5.22). The origin of this reduction will be discussed in the next-to-last paragraph of Sec. VC.

Table III lists the result of the calculation of the muon initial sticking probability $\omega^0_S(\%)$ of the $(d\mu)_J \to (\alpha\mu)_J + n$ state together with the $(\alpha\mu)_J$-n components. The last column is shown, only for reference, and is from our previous result in Ref. [33] based on the sudden approximation (5.20), in which the d-t nuclear interaction is included but the $\alpha-n$ channel is not considered.

C. Effective sticking probability $\omega^S_{\text{eff}}$

Finally, we discuss the effective sticking probability $\omega^S_{\text{eff}}$ that is defined as

$$
\omega^S_{\text{eff}} = \omega^S_0 (1 - R),
$$

(5.24)

where $R$ is the muon reactivation coefficient that expresses the probability that the muon is shaken off from the $(\alpha\mu)_J$ state during slowing down from the initial kinetic energy 3.5 MeV. The effective sticking $\omega^S_{\text{eff}}$ is the most crucial parameter in the $\mu$CF cycle because it sets a limit on the maximum possible fusion output per muon.

Regarding the sticking problem, we understand as follows from Secs. 8.4-8.6 of the $\mu$CF review paper [5] (1992): Using $R = 0.287$ (for a low density $\phi = 0.17$ of Ref. [73], the theoretical values of $\omega^S_0 \approx 0.91 - 0.93\%$ in (5.22) result in $\omega^S_{\text{eff}} \sim 0.66\%$, which is 10% larger than the experimental
TABLE III: The initial $\alpha$-$\mu$ sticking probability $\omega_0^S$ (%) of the $(d\mu)_{r=0}$ state together with the $(\alpha\mu)_{r=0}$-components. The present wave function includes the any channel with D-wave $\alpha$-$n$ relative motion. The last column is shown for reference only and is from our previous result [5], which employed the sudden approximation [6]. The $d$-$t$ nuclear interaction was included but the any channel was not considered.

| $J = \nu = 0$ | Present | Ref. [33] | Ref. [33] |
|---------------|---------|-----------|-----------|
| $\Psi_0^{(s)}$ (any) | $\alpha$-$n$ D wave | No $\alpha$-$n$ wave | (sudden approx.) |
| $\lambda_0(s^{-1})$ | $8.05 \times 10^{-2}$ | – | – |
| $\lambda_0^{\text{bound}}(s^{-1})$ | $6.90 \times 10^{-10}$ | – | – |
| $\omega_0^S(\%)$ | 0.857 | 0.9261 | |
| 1s | 0.6583 | 0.7141 | |
| 2s | 0.0950 | 0.1021 | |
| 2p | 0.0233 | 0.0248 | |
| 3s | 0.0289 | 0.0310 | |
| 3p | 0.0084 | 0.0089 | |
| 3d | 0.0002 | 0.0002 | |
| 4s | 0.0123 | 0.0132 | |
| 4p | 0.0038 | 0.0040 | |
| 4d + 4f | 0.0001 | 0.0001 | |
| 5s | 0.0063 | 0.0068 | |
| all others | 0.0204 | 0.0208 | |

value $\omega_0^S = 0.59 \pm 0.07$% ($\phi = 0.175$) at PSI [74] (1991). Ref. [5] states that the 10% difference is large enough to motivate further studies, because it may be a signal that the sticking problem is not yet completely understood.

In 2001, the final (last) precise experimental data on $\omega_0^S$ were reported from RIKEN-RAL [7] and PSI [75] at high densities ($\phi = 1.2 - 1.4$). The results showed that

$$\omega_0^S = \begin{cases} 
0.532 \pm 0.030\% & \text{(Liquid [7])} \\
0.515 \pm 0.030\% & \text{(Solid [7])} \\
0.505 \pm 0.029\% & \text{(Liquid [75])} 
\end{cases}$$

(5.25)

We derive our $\omega_0^S$ with the use of $\omega_0^S = 0.857$% in (5.24) and $R = 0.35$ [73, 76, 78] for high densities (density dependence seems to be very small for $\phi \sim 1.2 - 1.5$ in Table VI of Ref. [73]). We obtain

$$\omega_0^S = 0.557\% \quad \text{(present),}$$

(5.26)

which is not inconsistent with the observed values illustrated in Fig. 19 whereas the $\omega_0^S \approx 0.91 - 0.93$% by the previous work gives $\omega_0^S = 0.60$%.

To consider the most important origin of the change to $\omega_0^S = 0.857$% in (5.24) from $0.91 - 0.93$% in (5.22), we perform an additional calculation in which the $\alpha$-$n$ outgoing D-wave is replaced by S-wave. This is performed only for a reference calculation since this change contradicts the obser-

![FIG. 19: Comparison of the calculated effective sticking probability $\omega_0^S$ with the observed values based on from the precise high-density experiments EXP1 [7], EXP2 [7] and EXP3 [75] in 2001. CAL1 is given by the previous work with $\omega_0^S = 0.91 - 0.93$% [33, 35, 41], and CAL2 is owing to the present result with $\omega_0^S = 0.857$% of (5.24), with the definition $\omega_0^S = \omega_0^S(1 - R)$ taking the reactivation coefficient as $R = 0.35$ for high densities [73, 74, 78].

vation that the outgoing $\alpha$-$n$ channel with $I^\pi = 3^+$ has D-wave angular momentum.

We consider the following nonlocal central-force coupling, instead of the tensor force $V_{\text{t-n}, \text{cont}}^{(T)}(r_1, r_4)$ in Eq. (2.11):

$$V_{\text{t-n}, \text{cont}}^{(S)}(r_3, r_4) = v_0^{(S)} e^{-\mu r_3^2 - \mu R_i^2}$$

(5.27)

with $\mu = 1/(1.0 \text{ fm})^2$, $\mu' = 1/(6.0 \text{ fm})^2$ and $v_0^{(S)} = 0.81$ MeV fm$^{-3}$ with a slight change to $V_0 = -38.05$ MeV in the $d$-$t$ potential. The quality of the fitting to the observed $S$-factors is almost the same as the red curve in Fig. 7.

We have obtained $\lambda_0 = 8.87 \times 10^{-11}$ s$^{-1}$ by solving the coupled-channels Schrödinger equation (3.3) - (3.5) and $\lambda_0 = 7.56 \times 10^{-11}$ s$^{-1}$ by calculating the $T$-matrix elements (5.3) and (5.4); this result is not unreasonable. As for the $\alpha$-$\mu$ sticking problem, we see the change as follows:

$$\lambda_0, S\text{-wave} = 7.09 \times 10^{-9} \text{ s}^{-1} \rightarrow \lambda_0, D\text{-wave} = 6.90 \times 10^{-9} \text{ s}^{-1}$$

$$\lambda_0, S\text{-wave} = 7.49 \times 10^{-11} \text{ s}^{-1} \rightarrow \lambda_0, D\text{-wave} = 7.98 \times 10^{-11} \text{ s}^{-1},$$

which gives the change of $\omega_0^S = \lambda_{0, \text{bound}}^{\text{S-wave}} / (A_{0, \text{bound}}^{\text{S-wave}} + A_{0, \text{cont}}^{\text{S-wave}})$ from 0.938% (S-wave) to 0.857% (D-wave). Furthermore, we see that the former number of $\omega_0^S = \lambda_{0, \text{bound}}^{\text{D-wave}} / (A_{0, \text{bound}}^{\text{D-wave}} + A_{0, \text{cont}}^{\text{D-wave}})$ is expected. Because we employed the $\alpha$-$n$ D-wave in the outgoing channel by taking the tensor-force coupling between the $d$-$t$ and $\alpha$-$n$ channels.

For more progress on the theoretical investigation of the effective sticking probability $\omega_0^S$, further development of the study on the reactivation coefficient $R$ is expected. Our result on the absolute values of the transition rates to the individual $(\alpha\mu)$ bound and continuum states will be useful.
VI. MOMENTUM AND ENERGY SPECTRA OF EMITTED MUON

In this section we calculate the momentum and energy spectra (in absolute values) of the emitted muon after the $dt\mu$ fusion of $(\alpha n)$.

It is often stated that '10-keV' muons are emitted during the reaction. However, it should be noted that 10 keV is the 'average' of the muon kinetic energy in the $(He\mu)_3$ atom wherein the muon momentum distribution has a long higher-momentum tail. If one considers the utilization of such muons, for example, as the source of an ultra-slow negative muon beam [23–25, 25–31], it is important to determine the momentum and energy spectra of the released muon.

We calculate the muon spectra using the $T$-matrix procedure in Sec. VIB and the total wave function that was already obtained in Sec. III as the sum of three components:

$$\Psi^T_M(E) = \Psi^C_M(dt\mu) + \Psi^N_M(dt\mu) + \Psi^{(+)}_M(\alpha n\mu).$$

(6.1)

Correspondingly, as in Sec. VA, we divide the $T$-matrix (4.1) into three components on the Jacobi coordinates $(r_4, R_4)$ in channel $c = 4$ (cf. Fig. 3) as

$$T^{(C)}_{ilm, nm} = \langle e^{-\overline{K}}, R_4 | \phi_{ilm}(r_4) \chi^{m_1}(n) | V^{(T)}_{mt,dr} | \Psi^C_M(dt\mu) \rangle,$$

$$T^{(N)}_{ilm, nm} = \langle e^{-\overline{K}}, R_4 | \phi_{ilm}(r_4) \chi^{m_1}(n) | V^{(N)}_{mt,dr} | \Psi^N_M(dt\mu) \rangle,$$

$$T^{(+)}_{ilm, nm} = \langle e^{-\overline{K}}, R_4 | \phi_{ilm}(r_4) \chi^{m_1}(n) | V^{(+)}_{mt,dr} | \Psi^{(+)}_M(\alpha n\mu) \rangle,$$

(6.2)

where $\phi_{ilm}(r_4)$ $(i = 1 - N)$ is the discretized $\alpha n$ continuum state with energy $\varepsilon_i$, and $e^{-\overline{K}}, R_4$ is the associated $(\alpha n)$-muon plane wave, satisfying the energy conservation

$$\varepsilon_i + \varepsilon_i = E_{00} + Q \quad (i = 0 - N).$$

(6.3)

with $E_{00} = -0.003030$ MeV and $Q = 17.589$ MeV. The third component $T^{(+)}$ of (6.2) estimates the effect of the Coulomb potential $V_{\alpha}(r_3)$ on the $T$-matrix; check of this point was claimed in the last paragraph of Sec. III.

For simplicity, in this section, we refer to $\overline{K}, K_4$, or $K$ as 'muon momentum'; more precisely, it is the momentum of the relative motion between the muon and the $\alpha n$ pair.

A. Discretization of continuum states

Referring to Fig. 20 we explain how to construct $\phi_{ilm}(r_4)$ and $e^{-\overline{K}}, R_4$. We start by assuming an appropriate upper limit of the muon momentum $K_N$ at the top of the left end of the figure, whereas the minimum momentum is $K_0 = 0$. We then divide the muon momentum space $[K_0, K_N]$ into $N$ bins $(K_i, i = 0 - N)$ with equal intervals $\Delta K$. Correspondingly, we divide the momentum space $[k_N, k_0]$ of the $\alpha n$ relative motion on the right half of the figure into $N$ bins $(k_i, i = 0 - N)$ where the energy conservation is kept as

$$E_i + \varepsilon_i = E_{00} + Q \quad (i = 0 - N).$$

(6.4)

B. $T$-matrix calculation of fusion rate

The reaction rate for a muon emitted to the discretized continuum state $(\alpha n)_{i\mu}$ is written as

$$r_{i\mu} = \frac{v_{\alpha} \left( \frac{\mu K_4}{2 \pi \hbar^2} \right)^2}{2 \pi \kappa^2} \times \sum_{m,m'} \int |T^{(C)}_{ilm, nm} + T^{(N)}_{ilm, nm} + T^{(+)}_{ilm, nm}| \frac{1}{2 \overline{K}} d\overline{K},$$

(6.6)

where $v_{\alpha} = \hbar \overline{K}/\mu R_4$ is the velocity of the $(\alpha n)_{i\mu}$ relative motion. Since the reaction rate $r_{i\mu}$ does not depend on the $M$ ($z$-component of the total angular momentum $\overline{K}$), it is not necessary to take the average with respect to $K$. The sum of the transition rates

$$\lambda_{\mu} = \sum_{i\mu} r_{i\mu},$$

(6.7)

is the fusion rate of the reaction (1.2) using the $T$-matrix based on channel $c = 4$. This $\lambda_{\mu}$ is compared with the $\lambda_{\mu}$ obtained in Secs. IIA, IID, and VA using different prescriptions.
TABLE IV: Fusion rate \( \lambda_t \) defined by (6.7) and individual rates \( \lambda^{(C)}_t \), \( \lambda^{(N)}_t \) and \( \lambda^{(s)}_t \) defined by (6.12)- (6.13), respectively, on the Jacobi-coordinate channel \( c = 4 \).

| T-matrix type | \( [T^{(C)} + T^{(N)} + T^{(s)}]^2 \) | \( \lambda^{(C)}_t \) dMeV | \( \lambda^{(N)}_t \) dMeV | \( \lambda^{(s)}_t \) dMeV |
|---------------|---------------------------------|-----------------|-----------------|-----------------|
| Fusion rate (s\(^{-1}\)) | \( 1.15 \times 10^{12} \) | \( 4.58 \times 10^8 \) | \( 1.04 \times 10^{12} \) | \( 1.80 \times 10^{11} \) |

To investigate the role of the three types of T-matrix elements in Eq. (6.6), we calculate the individual reaction rates

\[
\lambda^{(C)}_t = \nu_l \left( \frac{\mu R_s}{2\pi \hbar^2} \right)^2 \sum_{m,m_1} |T_{il,mm_1}|^2 dK_{il}, \quad (6.8)
\]

\[
\lambda^{(N)}_t = \nu_l \left( \frac{\mu R_s}{2\pi \hbar^2} \right)^2 \sum_{m,m_1} |T_{il,mm_1}|^2 dK_{il}, \quad (6.9)
\]

\[
\lambda^{(s)}_t = \nu_l \left( \frac{\mu R_s}{2\pi \hbar^2} \right)^2 \sum_{m,m_1} |T_{il,mm_1}|^2 dK_{il}. \quad (6.10)
\]

Individual fusion rates \( \lambda^{(C)}_t \), \( \lambda^{(N)}_t \) and \( \lambda^{(s)}_t \) are given in the same way assimilating to Eq. (6.7) by

\[
\lambda^{(C)}_t = \sum_{il} \lambda^{(C)}_{il}, \quad (6.11)
\]

\[
\lambda^{(N)}_t = \sum_{il} \lambda^{(N)}_{il}, \quad (6.12)
\]

\[
\lambda^{(s)}_t = \sum_{il} \lambda^{(s)}_{il}. \quad (6.13)
\]

We take \( N = 200 \) as the number of momentum bins to discretize the continuum states in Fig. 24 setting \( \hbar K_N = 6.0 \) MeV/c (\( E_N = 175 \) keV). This is more than enough for calculating the fusion rate \( \lambda_t \) but it is taken for another purpose to derive the muon momentum spectrum as a continuous function of \( K \), starting from the reaction rates \( \rho_{ij} \) (\( i = 1, ..., N \)).

In the calculation of the \( \lambda^{(C)}_t \) and \( \lambda^{(N)}_t \), the contribution from the final states \( \phi_{fin}(r_t) \) with \( l \neq 2 \) is negligible under the present condition Eq. (3.35) and Eq. (3.40), but the approximation is recovered in the aforementioned T-matrix calculation based on the Lippmann-Schwinger equation.

It should be noted that, in some cases, the calculation of T-matrix elements for the Coulomb force between the continuum states is hindered by a problem in the integration up to the infinity. However, this issue is circumvented in the present work since we employ the discretization of the continuum states then smooth it as done in Eq. (5.9) and Fig. 16.

C. Muon spectrum

The main purpose of this Sec. VI is to calculate the muon momentum and energy spectra as continuous functions of \( K \) and the kinetic energy \( E \), respectively. Here, \( K(E) \) is the momentum (kinetic energy) of the \( (an)\mu \) relative motion associated with \( R_s \), whereas the muon momentum \( K_\mu \) (kinetic energy \( E_\mu \)) measured from the center of mass of the \( (an)\mu \) system is given by

\[
K_\mu = K, \quad E_\mu = \gamma E, \quad (6.15)
\]

with \( \gamma = \frac{m_a + m_m}{m_a + m_m + m_\mu} = 0.9779 \). We note that the center of mass of the \( (an)\mu \) is almost at rest in the laboratory system since the \( (dt)\mu \) molecule is also almost at rest at the time of the fusion reaction (1.2).

The momentum spectra \( r(K) \) and \( r^{(N)}(K) \) can be obtained, by smoothing \( r_{il} \) and \( r^{(N)}_{il} \) (cf. Fig. 15) respectively, as

\[
\lambda_t = \sum_{il} \left( \frac{\rho_{il}}{\partial K} \right) dK \int_{0}^{K_N} r(K) dK, \quad (6.16)
\]

\[
\lambda^{(N)}_t = \sum_{il} \left( \frac{\rho^{(N)}_{il}}{\partial K} \right) dK \int_{0}^{K_N} r^{(N)}(K) dK, \quad (6.17)
\]

and similarly for \( r^{(C)}(K) \) and \( r^{(s)}(K) \).

The energy spectra \( \bar{r}(E) \) and \( r^{(N)}(E) \) are derived, with the use of \( E = \hbar^2 K^2 / 2m_\mu \), by

\[
\bar{r}(E) dE = r(K) dK, \quad (6.18)
\]

\[
r^{(N)}(E) dE = r^{(N)}(K) dK, \quad (6.19)
\]
FIG. 21: Momentum spectrum of the muon emitted by the $d\mu$ fusion. The red and black curves denote $r(K)$ and $r^{(N)}(K)$ defined in (6.16) and (6.17), respectively. The dotted curve shows $r^{(N)}_{\text{AD}}(K)$ by the adiabatic approximation for $r^{(N)}(K)$ (see text); $r^{(N)}_{\text{AD}}(K)$ is normalized to $r^{(N)}(K)$ so that the same $K$-integrated values, $\lambda_t^{(N)} = 1.04 \times 10^{12}$ s$^{-1}$ is given.

FIG. 22: Energy spectrum of the muon emitted during the $d\mu$ fusion. The red and black curves denote $\tilde{r}(E)$ and $\tilde{r}^{(N)}(E)$ defined in (6.18) and (6.19), respectively. The peak position is at $E = 1.1$ keV in the two cases. The dotted curve shows $\tilde{r}^{(N)}(E)$ obtained using the adiabatic approximation for $\tilde{r}^{(N)}(E)$ (see text); $\tilde{r}^{(N)}_{\text{AD}}(E)$ is normalized to $\tilde{r}^{(N)}(E)$ so that the same $E$-integrated values, $\lambda_t^{(N)} = 1.04 \times 10^{12}$ s$^{-1}$ is given.

and similarly for $\tilde{r}^{(C)}(E)$ and $\tilde{r}^{(+)}(E)$.

The calculated momentum spectrum $r(K)$ is illustrated in Fig. 21 by the red curve in units of s$^{-1}$(MeV/c)$^{-1}$, whereas $r^{(N)}(K)$ is represented by the black curve. The energy spectrum $\tilde{r}(E)$ is shown in Fig. 22 by the red curve in units of s$^{-1}$(keV)$^{-1}$, whereas $\tilde{r}^{(N)}(E)$ is represented by the black curve.

The difference between the red and black curves in Figs. 21 and 22 originates from the $\alpha$–$\mu$ Coulomb-force contribution $T^{(C)}$ in Eq. (6.6) as mentioned in the next-to-last paragraph of Sec. VIB. The contribution from $T^{(C)}$ is minor. The effect of $T^{(+)}$ is small at low energies but becomes relatively large at high energies, which is seen in Fig. 23 for the log scale, in the dotted green curve derived based on only $|T^{(+)}/2$. As shown in Fig. 22 and Table V, the peak of the energy spectrum is located at $E = 1.1$ keV both for $\tilde{r}(E)$ and $\tilde{r}^{(N)}(E)$. Since the spectrum has a long high-energy tail, the average energy is 9.5 keV (8.5 keV for $\tilde{r}(E)\tilde{r}^{(N)}(E)$). Therefore, ‘muons with 1-keV peak energy and 10-keV average energy’ are emitted by the $d\mu$ fusion. This result (more precisely, Figs. 21 and 22 will be useful for the ongoing experimental project to realize an ultra-slow negative muon beam using the $\mu$CF reaction (1.2), they used

TABLE V: Property of the energy spectrum of muon emitted from $d\mu$ fusion. The red and black curves denote $\tilde{r}(E)$ and $\tilde{r}^{(N)}(E)$, and the adiabatic approximation $\tilde{r}^{(N)}_{\text{AD}}(E)$ which gives no absolute value (cf. Fig. 23).

| Muon energy spectrum | Peak energy (keV) | Average energy (keV) | Peak strength (s · keV)$^{-1}$ |
|----------------------|------------------|----------------------|-------------------------------|
| Present, $\tilde{r}(E)$ | 1.1 | 9.5 | $1.60 \times 10^{11}$ |
| Present, $\tilde{r}^{(N)}(E)$ | 1.1 | 8.5 | $1.47 \times 10^{11}$ |
| Adiabatic, $\tilde{r}^{(N)}_{\text{AD}}(E)$ | 1.6 | 10.9 | – |
the calculated muon energy spectrum in Fig. 1 of Ref. [79], wherein the spectrum was represented by a shape that was set to unity at \( E = 0 \). The definition of this energy spectrum is different from our energy spectrum \( \bar{\Phi}(E) (= 0 \text{ at } E = 0) \) that is represented in absolute value and \( \int_{0}^{\infty} \bar{\Phi}(E) dE \) gives the fusion rate \( \lambda_E = 1.15 \times 10^{12} \text{ s}^{-1} \). The role of the alpha Coulomb force, discussed in Ref. [79] by using their convoy-muon approximation, is included in our formulation via the \( T \)-matrix in (6.1) (cf. the next-to-last paragraph of Sec. VIB).

For the sake of the observation of the muon energy spectrum, we present a cumulative distribution function, \( P(E_\alpha) \), associated with the muon energy spectrum \( \bar{\Phi}(E) \), defined by

\[
P(E_\alpha) = \int_{0}^{E_\alpha} \bar{\Phi}(E) dE \leq 1 , \tag{6.20}
\]

which is illustrated by the red curve in Fig. 24. The dotted black curve is for \( P(E_\alpha) \) calculated with the adiabatic approximation, namely using \( \bar{\Phi}^{(N)}(E) \) instead of \( \bar{\Phi}(E) \) in Eq. (6.20). Here, absolute value of the energy spectrum is not concerned.

The red curve indicates that 24 % of the emitted muon is in the region \( 0 < E < 2 \text{ keV} \) and 35 % is in \( 0 < E < 3 \text{ keV} \), and hence 11 % is from \( 2 < E < 3 \text{ keV} \), whereas the muon having \( 0 < E < 4.7 \text{ keV} \) is 50 % and the one with \( 0 < E < 10 \text{ keV} \) amounts to 75 %. The curve reaches 99 % when \( E_\alpha = 80 \text{ keV} \).

![Cumulative distribution function](image)

**FIG. 24:** Cumulative distribution function \( P(E_\alpha) \) associated with the muon energy spectrum \( \bar{\Phi}(E) \). \( P(E_\alpha) \) is defined by Eq. (6.20). The red curve is derived by integrating \( \bar{\Phi}(E) \) of Fig. 22 whereas the dotted curve is given by using \( \bar{\Phi}^{(N)}(E) \) instead of \( \bar{\Phi}(E) \).

It is found that the ‘shape’ of the two black curves for \( r^{(N)}(K) \) and \( \bar{\Phi}^{(N)}(E) \) in Figs. 21 and 22 respectively, are well simulated by simple functions as

\[
r^{(N)}(K) \propto \frac{K^2}{(1 + K^2 a^2)^4}, \tag{6.21}
\]

\[
\bar{\Phi}^{(N)}(E) \propto \frac{K}{(1 + K^2 a^2)^4}, \quad E = \hbar^2 K^2 / 2 \mu R_4 \tag{6.22}
\]

with \( a = 154 \text{ fm} \) (this number appeared in Fig. 9). The reason is as follows: Using the property (3.27) of \( \Phi^{(N)}_0(r_4, R_4) \), we can represent the \( T \)-matrix (6.2), without the spin part, as

\[
T^{(N)}_{il, im} = \langle \phi^{(N)}_{il}(r_4) | V^{(T)}(r_4, r_3) | \Phi^{(N)}_0(r_3, 0) \rangle_{r_3, r_4} \times \langle \phi^{(N)}_{il}(r_4) | \Phi^{(N)}_0(0, R_4) \rangle_{R_4} / \Phi^{(N)}_0(0, 0). \tag{6.23}
\]

Taking \( E_N \approx 0.2 \text{ MeV} \ll Q \) and the relations (cf. Fig. 20)

\[
Q - E_N \leq e_i \leq Q \quad \text{(namely, } e_i \approx Q, k_i \approx k_0) \tag{6.24}
\]

together with Eqs. (6.4)-(6.5), we can derive

\[
\Delta k_i \approx \mu_e K_i \Delta K \approx K_i. \tag{6.25}
\]

We then obtain, in the interaction region of \( V^{(T)}(r_4, r_3) \),

\[
\bar{\Phi}^{(N)}_{il}(r_4) = \frac{1}{\sqrt{4 \pi i}} \int_{K_i}^{K_i - 1} \bar{\Phi}^{(N)}_{il}(k, r_4) dk 
\approx \sqrt{4 \pi i} \phi^{(N)}_{il}(k_0, r_4) \approx \sqrt{4 \pi i} \phi^{(N)}_{il}(k_0, r_4) \tag{6.26}
\]

Substituting this \( \bar{\Phi}^{(N)}_{il}(r_4) \) into Eq. (6.23) and smoothing \( K_i \) to \( K_0 \), we finally obtain (note \( v_\alpha \approx K_i \))

\[
r^{(N)}(K) \propto K^2 \int \langle e^{K R_4} | \Phi^{(N)}_0(0, R_4) \rangle |^2 dK. \tag{6.27}
\]

As shown in Fig. 9 (note \( R_4 = R_3 \)), the function form of \( \Phi^{(N)}_0(0, R_4) \) is well represented by \( e^{-R_4/a} \) with \( a = 154 \text{ fm} \). Putting this function form into Eq. (6.27), we immediately obtain Eq. (6.21). From Eq. (6.21) together with Eq. (6.19), we have Eq. (6.22). We found that both the simulated functions well reproduce the corresponding black solid curves in Figs. 21 and 22 within the width of the curves under the normalization at the peaks.

Finally, we discuss the muon momentum and energy spectra if we take the adiabatic approximation for the \( d-t \) relative motion just before the fusion reaction occurs. In this case, the wave function of the \((d-t)\mu\) relative motion is simply given by \( e^{-R_4/a} \) with \( a = 131 \text{ fm} \) (namely, the 1s wave function of the He\(^\mu \) atom as seen in Fig. 9), which has the mean kinetic energy of 10.9 keV. Based on the preceding discussion, the ‘shape’ of the muon momentum spectrum, \( r^{(N)}_{AD}(K) \), is given by Eq. (6.21) with \( a = a_0 \); similarly for the muon energy spectrum, \( \bar{\Phi}^{(N)}_{AD}(E) \), given by Eq. (6.22). The spectra are illustrated in Figs. 21 and 22 by the dotted curves that are normalized, as explained in the figure captions. It should be noted that, in both figures, the peak of the dotted curve has higher energy and broader width than the solid black curve (cf. Table V).
VII. SUMMARY

Recently, the study of muon catalyzed fusion has regained significant interest owing to several new developments and applications as explained in the Introduction. In this regard, we have comprehensively examined the fusion reaction \( (dt\mu)_{s=0} \rightarrow \alpha + \mu + n \) or \( (\alpha\mu)_{n} + n \), by employing the \( dt\mu - \) and \( any\mu - \) channel coupled three-body model. For the first time, we have solved the coupled-channels Schrödinger equation (3.7)–(3.8) under the boundary condition whereby the muonic molecular bound state \( (dt\mu)_{s=0} \) is the initial state and the outgoing wave in the \( any\mu \) channel. The total wave function of \( (\alpha\mu)_{n} \) is composed of the three components \( \Psi^{(C)}(dt\mu) + \Psi^{(N)}(dt\mu) + \Psi^{(f)}(\alpha\mu) \). Here, \( \Psi^{(C)}(dt\mu) \) is the given function employed to nonadiabatically describe the \( (dt\mu)_{s=0} \) initial molecular state with only the Coulomb force, and is treated as the source term of the Schrödinger equation. \( \Psi^{(N)}(dt\mu) \) is the additional \( dt\mu \) wave function required to correlate with the nuclear interactions. \( \Psi^{(f)}(\alpha\mu) \) is the outgoing wave function of the \( any\mu \) channel.

We take the \( d-t \) and \( \alpha-n \) nuclear potentials together with the nonlocal tensor force to couple the \( S \)-wave \( d-t \) channel and the \( D \)-wave \( \alpha-n \) channel. They are then determined to reproduce the observed low-energy \( S \)-factor, \( S(E) \), of the reaction \( d + t \rightarrow \alpha + n + 17.6 \text{ MeV} \) for \( E = 1-300 \text{ keV} \) (Fig. 1). Use of the determined interactions simultaneously accounts for the \( -n + nth \text{ total cross section} \). Applying the obtained total wave function to the \( T \)-matrix framework based on the Lippmann-Schwinger equation, we have investigated the reaction rates going to the individual \( \alpha-\mu \) bound states and the continuum states together with the \( \alpha-\mu \) sticking probability. We also studied the momentum and energy spectra of the muon emitted via the fusion reaction.

The main conclusions are summarized as follows.

i) From the calculated \( S \)-matrix of the outgoing wave, we have derived the fusion rate \( \lambda_{f} = 1.03 \times 10^{2} \text{s}^{-1} \). This is consistent with the previously obtained values, for example, by utilizing the \( d-t \) optical-potential model [33–55] and the \( R \)-matrix method [64–44]. The total wave function obtained is precisely analyzed using Figs. 1T–14.

ii) By performing the \( T \)-matrix calculation on the Jacobi-coordinate channel \( c = 5 \) (Fig. 3) with the use of the total wave function obtained in i), we have calculated the \textit{absolute} values of the fusion rate \( \lambda_{f}^{\text{bound}} = 6.90 \times 10^{9} \text{s}^{-1} \) to the \( (\alpha\mu)_{n} \) states and \( \lambda_{f}^{\text{cont}} = 7.98 \times 10^{11} \text{s}^{-1} \) to the \( (\alpha\mu)_{n} \) states, giving their sum as \( \lambda_{f} = 8.05 \times 10^{11} \text{s}^{-1} \). We derive the \( \alpha-\mu \) initial sticking probability \( \omega_{s}^{\alpha\mu} \) to the \( (\alpha\mu)_{n} \) states, according to the definition by the original idea for this phenomenon; that is, we have \( \omega_{s}^{\alpha\mu} = \lambda_{f}^{\text{bound}} / (\lambda_{f}^{\text{cont}} + \lambda_{f}^{\text{bound}}) = 0.857\% \). This is smaller by \( \sim 7\% \) than the literature result \( \omega_{s}^{\alpha\mu} \approx 0.91 - 0.93\% \) based on the sudden approximation including the nuclear \( d-t \) potential.

iii) Our additional calculation considering \( dt\alpha-n \) coupling with a \textit{central} nonlocal-potential gives \( \omega_{s}^{\alpha\mu} = 0.938\% \). Therefore, the origin of the aforementioned \( \sim 7\% \)-reduction is because we employed the \( D \)-wave \( \alpha-n \) relative motion and the \( dt\alpha \) channel coupling with the nonlocal tensor force. This \( \omega_{s}^{\alpha\mu} = 0.857\% \) corresponds, with the reactivation coefficient \( R = 0.35 \) [73–76], to \( \omega_{s}^{\alpha\mu} = (1 - R) \omega_{s}^{\alpha\mu} = 0.557\% \) which is not inconsistent with the previously reported experimental values (Fig. 19). For further progress on the study of \( \omega_{s}^{\alpha\mu} \), development on the calculation of \( R \) is expected. Our result on the absolute values of the transition rates to the individual \( \alpha-\mu \) bound and continuum states (Fig. 17) will be useful.

iv) In the aforementioned \( T \)-matrix calculation of \( \lambda_{f}^{\text{cont}} \) and their sum \( \lambda_{f} \), we have found that \( \Psi^{(N)}(dt\mu) \) dominantly contributed to the fusion rates, whereas \( \Psi^{(C)}(dt\mu) \) and \( \Psi^{(f)}(\alpha\mu) \) play a minor role (Table II). We then conclude that the calculation of the initial sticking \( \omega_{s}^{\alpha\mu} \), using \( \Psi^{(C)}(dt\mu) \) only is not meaningful and that the statement “the additional effect of the nuclear force to the sticking probability” is not appropriate since \( \Psi^{(N)}(dt\mu) \) dominantly contributes to the fusion rate \( \lambda_{f} \).

v) We have performed another \( T \)-matrix calculation to derive \textit{absolute} values for the momentum and energy spectra of the muon emitted during the fusion process (Figs. 21 and 22). The most important conclusion is that the ‘peak’ energy of the muon energy spectrum is 1.1 keV, whereas the ‘mean’ energy is 9.5 keV (Table V) owing to the long higher-energy tail. This result will be useful to the new ongoing experimental project to realize an ultra-slow-negative muon beam by utilizing the fusion reactions in the \( dt\mu \) molecule as well as in the \( dd\mu \) one, and for a variety of applications e.g. a scanning negative muon microscope and an injection source for the muon collider. It is shown that the ‘shape’ of the momentum and energy spectra can be simulated by simple functions (6.21) and (6.22). The \( T \)-matrix calculation for the channel \( c = 4 \) (Fig. 3) gives \( \lambda_{f} = 1.15 \times 10^{12} \text{s}^{-1} \).

vi) We have reported three numbers for the fusion rate \( \lambda_{f} \) of the \( dt\mu \) molecule that are calculated using very different methods. The values are consistent with each other but not \textit{equal}. This is because the solution of the Schrödinger equation (3.7)–(3.8) used in the \( T \)-matrix calculations is not rigorously exact. However, before this situation can be improved, we shall proceed to the detailed study of the nuclear reaction in the \( dd\mu \) fusion because of its urgent importance, as indicated in item v).

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