Muon transfer and elastic scattering in $t + d\mu$ collisions at low energies

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Muon transfer and elastic scattering in low-energy collisions of $t + d\mu(1s)$ are studied by the hyperspherical coupled-channel method in which many closed channels are explicitly coupled to obtain converged cross sections. A hybrid procedure of the diabatic-by-sector and the traditional adiabatic-basis-expansion methods is developed for solving a large set of coupled equations influenced by the nearly singular nature of couplings induced by numerous avoided crossings. It is shown that the adiabatic states belonging to the $n = 2$ excited states in the separated-atom limit contribute significantly to the muon transfer. The discrepancy between the previous hyperspherical calculation of Fukuda *et al.* [Phys. Rev. A **41**, 145, (1990)] and other existing theoretical calculations has been resolved by taking into account the couplings with these excited states.

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I. INTRODUCTION

Muon transfer between hydrogen isotopes in thermal-energy collisions

$$t + d\mu(1s) \rightarrow t\mu(1s) + d \tag{1}$$

plays an important role as a trigger process in the chain cycle of the muon catalyzed fusion (μCF) [1]. Although this process is similar to the electron transfer in low-energy ion-atom collisions, there exists a distinct difference owing to the heavy mass of the leptonic particle. The standard perturbed stationary method, in which the electronic states of the diatomic molecule of the fixed nuclei are used as basis functions for the expansion, breaks down since it does not explicitly take into account the finitude of the nucleon masses and hence does not satisfy the correct boundary conditions of the entrance and the exit channels in the sense that the ground-state energies of the atoms $d\mu$ and $t\mu$ are degenerate in this representation. Their precise binding energies differ by 48 eV, which is much larger than the kinetic energy of the projectile in a thermal energy region. A large number of adiabatic basis functions, including continuum states, is needed for the expansion to remedy this defect in the framework of the traditional adiabatic-state expansion [2].

Kobayashi *et al.* [3] developed an alternative type of adiabatic basis expansion in which molecular states are constructed in Jacobi coordinates and the boundary conditions are fulfilled exactly. Kamimura applied the Kohn-Hulthen-Kato-type variational method using Gaussian basis functions [4]. These two methods gave cross sections consistent with each other. Another approach that is also formulated in Jacobi coordinates is the hyperspherical coupled-channel (HSCC) method. In this method, the two sets of Jacobi coordinates of the entrance and the exit channels are unified into a six-dimensional spherical space. Fukuda *et al.* [5] applied the HSCC method to the process (1) and obtained transfer cross sections smaller than those of the two aforementioned methods by a factor of 2. The problem of which value is closer to the real cross section has been unsettled.

Recently the present authors successfully applied the HSCC method to positronium formation from a hydrogen atom [6]. We have demonstrated that the formation cross sections agree well with other elaborate variational calculations and the hyperspherical approach is a powerful and reliable tool for rearrangement collisions of Coulomb three-body systems. The physical situation of the positronium formation process is somewhat different from that of the system (1). One particle is lighter than the other two by only one order of magnitude in the system (1), while one particle is heavier than the other two by three orders of magnitude in the positronium formation. However, the validity of the hyperspherical representation is not expected to be worse for the system (1). The HSCC method is hopeful for general rearrangement collisions since it has a conspicuous merit that the coupled differential equations do not have a nonlocal potential. The clarification of the discrepancy between the HSCC calculation and the others is required not only for the importance in the application to the μCF, but also for the understanding of the mechanism of rearrangement collisions.

II. THEORY

We denote the internal coordinates of $d\mu$ and $t\mu$ by $\mathbf{r}_T$ and $\mathbf{r}_P$ and the position vectors of the triton and the deuteron measured from the centers of mass of the atoms $d\mu$ and $t\mu$ by $\mathbf{R}_T$ and $\mathbf{R}_P$, respectively. The hyperradius ρ is related to the Jacobi coordinates as follows:

$$\nu\rho^2 = \nu_T R_T^2 + m_T r_T^2 = \nu_P R_P^2 + m_P r_P^2, \tag{2}$$

where ν is an arbitrary parameter that is a dimension of mass, m_T and m_P are the reduced masses of the atoms $d\mu$ and $t\mu$, and ν_T and ν_P are the reduced masses for the relative motion in the initial and the final channels, respectively,

$$m_T = \frac{M_d m_\mu}{M_d + m_\mu}, \tag{3}$$

$$m_P = \frac{M_t m_\mu}{M_t + m_\mu}, \tag{4}$$

$$\nu_T = \frac{(M_d + m_\mu)M_t}{M_d + M_t + m_\mu}, \tag{5}$$

and

$$\nu_P = \frac{(M_t + m_\mu)M_d}{M_d + M_t + m_\mu}. \tag{6}$$

In the above equations, M_d, M_t, and m_μ are the masses of a deuteron, a triton, and a muon, respectively. Hereafter, unless stated explicitly otherwise, we use the reduced muon atomic unit (m.a.u.) in which the reduced mass

$$m = \frac{(M_d + M_t)m_\mu}{M_d + M_t + m_\mu} \tag{7}$$

is set to unity in place of the electron mass in addition to $\hbar = e = 1$. The scale of the length is smaller and the scale of the energy is larger, by a factor of 200, than those of the ordinary atomic unit. After separating the center-of-mass motion of the total system, the Hamiltonian of the collision system is written as [6]

$$H = -\frac{1}{2\nu}\left(\frac{d^2}{d\rho^2} + \frac{5}{\rho}\frac{d}{d\rho}\right) + h_{\rm ad}(\rho, \Omega) \tag{8}$$

with

$$h_{\rm ad} = \frac{\mathbf{\Lambda}^2}{2\nu\rho^2} + V(\rho, \Omega), \tag{9}$$

where $\mathbf{\Lambda}$ is the five-dimensional grand-angular-momentum operator and the variable Ω represents the set of five angular variables in the hyperspherical space. The arbitrary parameter ν is chosen to be the reduced mass between d and t, namely,

$$\nu = \frac{M_d M_t}{M_d + M_t} \tag{10}$$

in the practical calculations. $V(\rho, \Omega)$ is the sum of the Coulomb interactions among the three particles and the adiabatic Hamiltonian $h_{\rm ad}$ contains ρ as a parameter. The adiabatic basis functions are the eigenfunctions of $h_{\rm ad}$

$$h_{\rm ad}\varphi_i = \left(U_i(\rho) - \frac{15}{8\mu\rho^2}\right)\varphi_i. \tag{11}$$

We have obtained the eigenvalues and the eigenfunctions of the above equation by diagonalizing the adiabatic Hamiltonian at each ρ in terms of Sturmian orbitals. We do not mix the hyperspherical harmonics, which are the eigenfunctions of the grand-angular-momentum operator Λ^2, with the trial functions in the present calculations since it turned out that their contribution is small for the system $d\mu + t$.

In a previous study of positronium formation [6] the scattering equation

$$(H - E)\Psi(\rho, \Omega) = 0 \tag{12}$$

was solved by utilizing the diabatic-by-sector method [7] to overcome the numerical difficulty caused by sharply peaked nonadiabatic couplings in the vicinity of avoided crossing points of the adiabatic potential curves. In this method, the entire region of ρ is divided into a large number of small sectors and the scattering wave function is expanded in terms of basis functions that are diabatic locally in each sector. The diabatic basis functions were chosen to be the eigenfunctions of the adiabatic Hamiltonian $h_{\rm ad}(\rho, \Omega)$ at a *fixed* point ρ_k in each sector

$$\Psi = \sum_i \frac{F_i^k(\rho)}{\rho^{5/2}}\varphi_i(\rho_k, \Omega). \tag{13}$$

As stated above the diabatic-by-sector method has a merit that the coupled equations can be solved easily even when nonadiabatic couplings among the adiabatic potential curves are nearly singular, but it also has a peculiarity that the couplings among the basis states decrease less rapidly with the increase of the hyperradius ρ than the ordinary nonadiabatic couplings. The leading term of the coupling matrix elements in the diabatic-by-sector representation behaves asymptotically as $1/\rho^2$. The slow decay of the couplings sometimes brings about difficulty in accurate numerical solution of the coupled equations when the collision energy is extremely small. The traditional adiabatic treatment is more suitable for thermal energy collisions if no avoided crossing occurs.

Figures 1 and 2 show the adiabatic potential curves for the total angular momenta $J = 0$ and 1. The lowest curve corresponds to the final channel and the next curve to the initial channels. Noting that there is no avoided crossing between these two main channels, we have adopted a hybrid scheme in which the ordinary adiabatic representation is used for states that have no avoided crossing with others, while the locally diabatic representation is used for the other states

$$\phi_i^k(\rho, \Omega) = \begin{cases} \varphi_i(\rho, \Omega) & \text{if } \varphi_i \text{ has no avoided crossing} \\ \varphi_i(\rho_k, \Omega) & \text{otherwise.} \end{cases} \tag{14}$$

The representation of each state is chosen independently in each sector. The adiabatic representation is used in

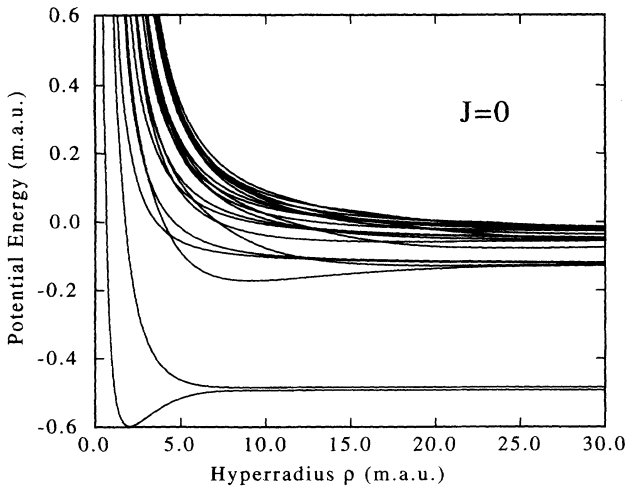

FIG. 1. The adiabatic potential curves in the hyperspherical coordinate representation for J=0. The scales are given in muon atomic units.

some sectors and the diabatic representation is used in the other sectors for the same level. The adiabatic representation is used throughout the entire region only for the two lowest levels. Substitution of the expansion

$$\Psi^k = \sum_i \frac{F_i^k(\rho)}{\rho^{5/2}} \phi_i^k(\rho, \Omega) \tag{15}$$

into the scattering equation (12) gives a set of coupled equations in matrix representation for each sector

$$\left(-\frac{1}{2\nu}\frac{d^2}{d\rho^2} - E\right)\mathbf{F}^k = (S^k)^{-1}\left(-U^k + \frac{1}{\nu}P^k\frac{d}{d\rho} + \frac{1}{2\nu}Q^k\right)\mathbf{F}^k \tag{16}$$

with

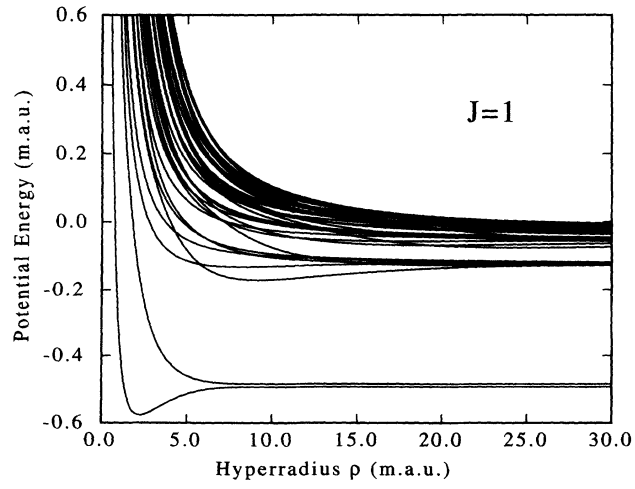

FIG. 2. The same as Fig. 1, but for $J = 1$.

$$S_{ij}^k = \langle \phi_i^k | \phi_j^k \rangle, \tag{17}$$

$$P_{ij}^k = \left\langle \phi_i^k \left| \frac{d}{d\rho}\phi_j^k \right. \right\rangle, \tag{18}$$

$$Q_{ij}^k = \left\langle \phi_i^k \left| \frac{d^2}{d\rho^2}\phi_j^k \right. \right\rangle, \tag{19}$$

$$U_{ij}^k = \left\langle \phi_i^k \left| h_{ad} + \frac{15}{8\nu\rho^2} \right| \phi_j^k \right\rangle. \tag{20}$$

Here $\mathbf{F}^k$ is a column vector whose ith component is the function $F_i^k(\rho)$. The overlap matrix S is diagonal in the subspace of the adiabatic states $\varphi_i(\rho, \Omega)$ and in that of the diabatic states $\varphi_i(\rho_k, \Omega)$. The solution in the interval around ρ_k is matched to the solution in the adjacent sector around the next point ρ_{k+1} at the boundary $\rho_m = (\rho_k + \rho_{k+1})/2$ by requiring that the wave functions and their derivatives are smoothly connected.

The solution is propagated up to the outermost boundary $\rho = \rho_{\text{end}}$, where the hyperspherical representation is projected onto the Jacobi representation before the reactance matrix K is extracted from the asymptotic form of the scattering wave function. The procedure for extracting the reactance matrix and cross sections is similar to that in a previous paper [6].

III. RESULTS AND DISCUSSION

The eigenstates of the adiabatic Hamiltonian h_{ad} are calculated for the total angular momenta J=0 and 1 by the variational method. After the diagonalization, all the states associated with the n=1 – 4 states of the $d\mu$ and $t\mu$ atoms for $\rho \to \infty$ are used for the expansion of Eq. (13). The coupled equations are solved up to $\rho_{\text{end}} = 500$ m.a.u., which is sufficiently large to obtain an accurate T matrix even for the highest exited states belonging to $n = 4$. The cross sections do not change shifting for the point ρ_{end} farther.

We show how the cross sections of the muon transfer (1) and the elastic scattering

$$t + d\mu(1s) \to t + d\mu(1s) \tag{21}$$

converge with increasing basis functions for $J = 0$ in Table I. The HSCC cross sections of Fukuda *et al.* are also presented for comparison. The present calculation of the smallest set in which only the two lowest levels ($n = 1$) are coupled is essentially the same as theirs except for one point. Fukuda *et al.* did not employ the matching procedure in which the solutions in the hyperspherical coordinates are projected onto those in the Jacobi representation. We do not specify other causes for the difference between the two calculations. In any case, it is evident from Table I that the calculation does not converge if only the two lowest levels are included for the expansion. The transfer cross sections increase considerably by adding the couplings with the states of $n = 2$ for all the collision energies shown here. They do not change much for increasing the basis functions further

TABLE I. Convergence of the elastic and transfer cross sections for $J = 0$ in units of 10^{-20} cm^2. The labels of the states mean that all the states with the principal quantum number n and below in the separated-atom limit are coupled fully in the calculations. E is the center-of-mass collision energy in eV.

E	Process	$n = 1$	$n = 2$	$n = 3$	$n = 4$
0.001	elastic	1.82	1.65	1.64	1.63
		1.7[a]			
	transfer	8.57	13.6	14.0	14.2
		9.1[a]			
0.01	elastic	2.39	2.19	2.17	2.15
		2.3[a]			
	transfer	2.69	4.25	4.40	4.44
		2.9[a]			
0.1	elastic	4.43	4.16	4.13	4.12
	transfer	0.819	1.29	1.34	1.35

[a] Fukuda, Ishihara, and Hara [5].

up to $n = 4$. By contrast, the change of the elastic cross sections is not so drastic for going from $n = 1$ to $n = 2$. The elastic scattering proceeds more adiabatically since it enters and exits along the same potential curve. Table II shows the convergence behavior of the cross sections for $J = 1$. In this case the convergence is faster than in the case of $J = 0$ both for the transfer and the elastic scatterings. The elastic cross sections have converged for the $n = 1$ set while transfer cross sections change by 10% for adding the couplings with the $n = 2$ states. We do not present the elastic cross sections of $J = 1$ for the lowest energy since they are too small to be calculated accurately. We give a rough estimate of 4×10^{-24} cm^2 for the elastic cross section at $E = 0.001$ eV.

In Table III we compare the present cross sections with other theoretical calculations. The agreement of the present results with others is generally excellent. Among them our cross sections are very close to the results of the multichannel adiabatic representation [2] at all the energies listed in the table. The disagreement of the previous HSCC results reported by Fukuda *et al.* [5] has been resolved satisfactorily by the consideration of the couplings with the excited channels.

Although agreement is improved significantly, it may not be easy to understand intuitively the large contribution of the excited states. The adiabatic energy levels of the excited states are well separated from the two lowest levels as shown in Figs. 1 and 2. It is to be noted that the process (1) is entirely a nonadiabatic transition

TABLE II. Convergence of the elastic and transfer cross sections for $J = 1$ in units of 10^{-20} cm^2. $a[b]$ denotes $a \times 10^b$. Other notations are the same as in Table I.

E	Process	$n = 1$	$n = 2$	$n = 3$	$n = 4$
0.001	transfer	4.09[-2]	3.66[-2]	3.58[-2]	3.56[-2]
0.01	elastic	1.19[-2]	1.20[-2]	1.20[-2]	1.20[-2]
	transfer	1.29[-1]	1.16[-1]	1.13[-1]	1.12[-3]
0.1	elastic	8.44[-2]	8.56[-2]	8.59[-2]	8.60[-2]
	transfer	4.06[-1]	3.63[-1]	3.55[-1]	3.53[-1]

TABLE III. Comparison with other theoretical cross sections. Cross sections are given in units of 10^{-20} cm^2. Notations are the same as in Table I.

E	Method	Elastic		Transfer	
		$J = 0$	$J = 1$	$J = 0$	$J = 1$
0.001	present	1.63		14.2	3.56[-2]
	Ka[a]			16.	3.6[-2]
	KIT[b]	2.0		16.0	
	MAR[c]	1.56		13.5	
0.01	present	2.15	1.20[-2]	4.44	1.12[-1]
	Ka			5.1	1.1[-1]
	KIT	2.13		4.9	
	MAR	2.13	1.22[-2]	4.25	1.13[-1]
0.1	present	4.12	8.60[-2]	1.35	3.53[-1]
	Ka			1.6	3.6[-1]
	MAR	4.15	9.32[-2]	1.30	3.54[-1]

[a] Kamimura [4].
[b] Kobayashi, Ishihara, and Toshima [3].
[c] Chiccoli *et al.* [2].

between levels which have no crossing point. The energy splitting between the initial and the final states is 48 eV, which is much larger than the collision energy. The nonadiabatic transition between the lowest two levels occurs gradually over a wide range of ρ and it can be affected even by the weakly coupled higher levels. The fact that the transfer cross sections are larger than the elastic cross sections below 0.01 eV indicates the importance of nonadiabatic couplings in the collision system of $t + d\mu$. It is also helpful for the understanding to mention that a huge number of basis functions is needed, including continuum states, to get convergence for the calculations of Chiccoli *et al.* [2], who used the traditional Born-Oppenheimer adiabatic states representation.

We have studied the scatterings of an idealized three-body system in this paper. In the practical situation of the muon catalyzed fusion, however, the collisions occur with molecules D_2 or DT and the present results are not directly related to those in the fusion experiments. Among the modifications needed for the realistic problems, the screening effect by the target electrons is the most important. According to a previous study [8], the elastic cross sections are greatly changed below 0.1 eV, while the effect is much smaller for the transfer cross sections. We leave the problem of the electron screening and the molecular structure to a future study.

IV. SUMMARY

We have executed large-scale coupled-channel calculations based on the hyperspherical-coordinate representation for the collisions of $t + d\mu$ increasing the number of basis functions until convergence is achieved. It was found that the couplings with excited levels have to be taken into account for the muon transfer and good agreement was obtained for both the elastic and transfer cross sections with other existing theoretical studies. An alternative numerical procedure that possesses both the mer-

its of the traditional adiabatic-base expansion and the diabatic-by-sector methods has been proposed for solving a large set of coupled differential equations for thermal energy collisions. It was confirmed that the HSCC method is a useful and reliable method for rearrangement collisions of Coulomb three-body systems.

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