Hyperspherical calculations of low-energy rearrangement processes in $dt\mu$

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The results of accurate hyperspherical calculations of the reaction $d\mu(n_i)+t\rightarrow t\mu(n_f)+d$ between states of the $n_i=n_f=1$ and $n_i=n_f=2$ manifolds for zero total angular momentum of the collision system are reported. A parametrization of the threshold behavior of the ground-to-ground–state muon transfer cross section in the spirit of the effective range theory is discussed. [S1050-2947(99)05311-1]

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I. INTRODUCTION

In this Brief Report we consider the reaction

$$d\mu(n_i)+t\rightarrow t\mu(n_f)+d+\Delta E \tag{1}$$

for zero total angular momentum of the collision system, $L=0$. This reaction has been attracting much theoretical effort during the past decade [1–13] due to its role in muon-catalyzed fusion [14]. In the course of our recent study, whose brief account has appeared in Ref. [15], in order to test the proposed new method of calculating the cumulative reaction probability we have also performed ''standard'' calculations of the scattering matrix for a $dt\mu$ system for energies up to the $n=6$ threshold. These results were left beyond Ref. [15] and will be partly reported here. In slow collisions, which are of main interest for applications, quasiresonance processes characterized by small values of the energy defect ΔE occur most efficiently. This is the case for $n_i=n_f\equiv n$ when

$$\Delta E=E_{d\mu(n)}-E_{t\mu(n)}=\frac{m_{t\mu}-m_{d\mu}}{2n^2}\approx\frac{0.85\times10^{-2}}{n^2}, \tag{2}$$

where $E_{d\mu(n)}$ and $E_{t\mu(n)}$ are the bound-state energies of the pairs $d\mu$ and $t\mu$, respectively, and $m_{d\mu}$ and $m_{t\mu}$ are the corresponding reduced masses. Muonic atomic units $|e|=\hbar=m_\mu=1$ (μa.u.) are used throughout the paper unless explicitly stated otherwise. Here we consider only reaction (1) between states of the $n_i=n_f=1$ and $n_i=n_f=2$ manifolds. Also, we analyze the threshold behavior of the ground-to-ground–state muon transfer cross section.

II. METHOD OF CALCULATIONS

Skipping details of the present numerical procedure, we just name its most important elements. We used the hyperspherical method [16,17] implemented in terms of hyperspherical elliptic coordinates [18] with the nonadiabatic coupling treated by means of the slow/smooth variable discretization method [19] in combination with the $\mathcal{R}$-matrix propagation technique of Ref. [20]. This approach provides high accuracy of hyperspherical adiabatic potentials and channel functions and fast convergence of the results with respect to the number of coupled channels and the parameters controlling solution of the radial part of the problem. It has proven to be very efficient and accurate in studying various three-body Coulomb systems [18,19,21,22,15] as well as in applications to chemical reactions [23,24]. Given the $\mathcal{R}$ matrix at the matching surface, the scattering matrix was extracted by applying a two-dimensional matching procedure similar to that used in [25,26], as described in [23]. The lack of convergence of the scattering matrix, as the matching radius R_m is increased, is the main source of numerical errors. The convergence is fast for scattering between states of the $n=1$ manifold, but becomes progressively slower for processes involving higher states, especially in the near-threshold regions. This is due to a strong dipole coupling between channels converging to the $n\geqslant2$ thresholds [12] not accounted for by the asymptotic form of the wave function used here. (It should be emphasized that the cumulative reaction probability is invariant under unitary transformations mixing asymptotic states separately in each arrangement and is not affected by this problem, as was demonstrated in [15]). Several sophisticated methods to remedy this problem are known, however in the present calculations we resorted to the simple act of increasing R_m, which is quite feasible for calculating scattering between states of the $n=1$ and $n=2$ manifolds.

The results reported below were obtained with 100 coupled hyperspherical adiabatic channels and the matching applied at $R_m=800$. The hyperradius R in our approach is defined by

$$R=\sqrt{m_d r_d^2+m_t r_t^2+m_\mu r_\mu^2}, \tag{3}$$

where $\mathbf{r}_d$, $\mathbf{r}_t$, and $\mathbf{r}_\mu$ give the positions of the particles in the center-of-mass frame. For heavy-light-heavy systems at negative total energies, the wave function is localized in the region of configuration space where the hyperradius is close to the length of the mass-scaled Jacobi vector joining the two heavy particles. For $dt\mu$ this means the following approximate relation:

$$R\approx\sqrt{m_{dt}}r_{dt}\approx3.26r_{dt}, \tag{4}$$

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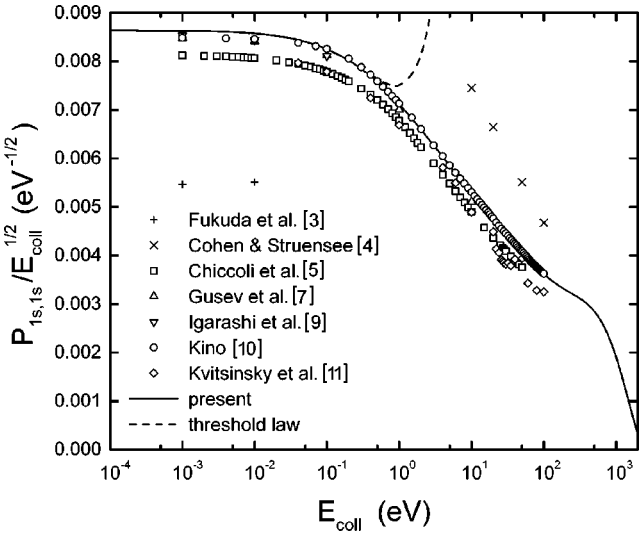

FIG. 1. Comparison of different calculations of reaction (1) between the $n_i=n_f=1$ states. $P_{1s,1s}$ is the reaction probability, $E_{\rm coll}=E-E_{d\mu(n=1)}$ is the collision energy in the initial state. Pluses — Ref. [3], crosses — Ref. [4], squares — Ref. [5], upper triangles — Ref. [7], lower triangles — Ref. [9], circles — Ref. [10], diamonds — Ref. [11], solid line — present results, dashed line — threshold behavior according to Eq. (10).

where $r_{dt}=|\mathbf{r}_d-\mathbf{r}_t|$. The above value of R_m corresponds to $r_{dt}\approx 245$, which is more intuitive. In the following, we shall characterize reaction (1) by the reaction probability $P_{fi}=|S_{fi}|^2$, where S_{fi} is the corresponding element of the scattering matrix. This quantity is related to the muon transfer cross section by

$$[\sigma_{fi}(10^{-20}\ \text{cm}^2)]\approx 52.65\frac{P_{fi}}{[E_{\rm coll}(\text{eV})]}, \tag{5}$$

where $E_{\rm coll}=E-E_{d\mu(n_i)}$ is the collision energy in the initial state and E is the total energy of the system.

III. MUON TRANSFER BETWEEN $n_i=n_f=1$ STATES

This process is of major interest for applications. Our results for energies up to the $n=2$ threshold ($E_{\rm coll}\approx 2000$ eV) are presented by the solid line in Fig. 1 and by the set of numerical data given in Table I. The accuracy of these results is estimated to be better than 1%. In Fig. 1 we also show results of some other accurate calculations reported during the past decade. For comparison purposes in this figure, instead of the reaction probability $P_{1s,1s}$, we plot the ratio $P_{1s,1s}/E_{\rm coll}^{1/2}$ which more explicitly reveals differences between different calculations. The early hyperspherical calculations by Fukuda *et al.* [3] and the improved adiabatic calculations by Cohen and Struensee [4] (we use their results reported in [11]) differ considerably from the present results, especially at low energies. The results by Chiccoli *et al.* [5] are the best obtained using an expansion in terms of the two-center Coulomb basis. These calculations reproduce well the shape of the energy dependence of $P_{1s,1s}$ but give 6% lower values which may be due to difficulties in achieving convergence with respect to the two-center continuum states. More recent hyperspherical calculations by Gusev *et al.* [7] and Igarashi *et al.* [9] demonstrate much improvement on the results of Ref. [3] and agree well with each other giving values of $P_{1s,1s}$ just 1% lower than ours. The results by Kvitsinsky *et al.* [11] obtained by solving Faddeev equations are close to those of Ref. [5], but are less stable, demonstrating irregular behavior at higher energies. Finally, the unpublished results by Kino [10] (also cited in Ref. [11]) obtained by the coupled-rearrangement-channel method of Ref. [6] agree excellently with our results except at very low energies where there is about 1% difference. Such good agreement in a wide energy range between two completely different methods of calculation is a strong argument for confidence in each of them. In the very low energy region $E_{\rm coll}\leqslant 0.01$ eV the results of Ref. [10] agree well with those of Refs. [7] and [9]. However, based on tests of convergence with respect to both the number of coupled channels and the matching radius we believe that the present results are more accurate.

TABLE I. Present results for reaction (1) between $n_i=n_f=1$ states. $P_{1s,1s}$ is the reaction probability, $E_{\rm coll}=E-E_{d\mu(n=1)}$ is the collision energy in the initial state, in eV. $a[b]=a\times 10^b$.

$E_{\rm coll}$	$P_{1s,1s}$	$E_{\rm coll}$	$P_{1s,1s}$
1[−4]	0.8635[−4]	1	0.7120[−2]
2[−4]	0.1221[−3]	2	0.9326[−2]
5[−4]	0.1930[−3]	5	0.1308[−1]
1[−3]	0.2728[−3]	10	0.1673[−1]
2[−3]	0.3856[−3]	20	0.2126[−1]
5[−3]	0.6083[−3]	50	0.2880[−1]
1[−2]	0.8574[−3]	100	0.3618[−1]
2[−2]	0.1205[−2]	200	0.4653[−1]
5[−2]	0.1879[−2]	500	0.6369[−1]
1[−1]	0.2608[−2]	1000	0.6034[−1]
2[−1]	0.3586[−2]	1500	0.3804[−1]
5[−1]	0.5353[−2]	1900	0.1870[−1]

IV. MUON TRANSFER BETWEEN $n_i=n_f=2$ STATES

Reaction (1) between states of higher manifolds plays an important role in the kinetics of muon-catalyzed fusion [8,13]. The present $L=0$ calculations for this case are of somewhat academic interest since higher partial waves are expected to contribute significantly. However they do represent a necessary first step. Our results for reaction (1) between the $n_i=n_f=2$ states for energies up to the $n=3$ threshold ($E_{\rm coll}\approx 360$ eV) are shown in Fig. 2 and a set of representative numerical data is given in Table II. We estimate these results to be accurate within a few percent, although the error may grow closer to the threshold. We are not aware of any other published numerical results for these reactions.

V. PARAMETRIZATION

Now we discuss a parametrization of the ground-to-ground–state muon transfer cross section at low collision energy. It is well known that the first two terms in the threshold behavior of a reaction cross section can be written in the form [27]

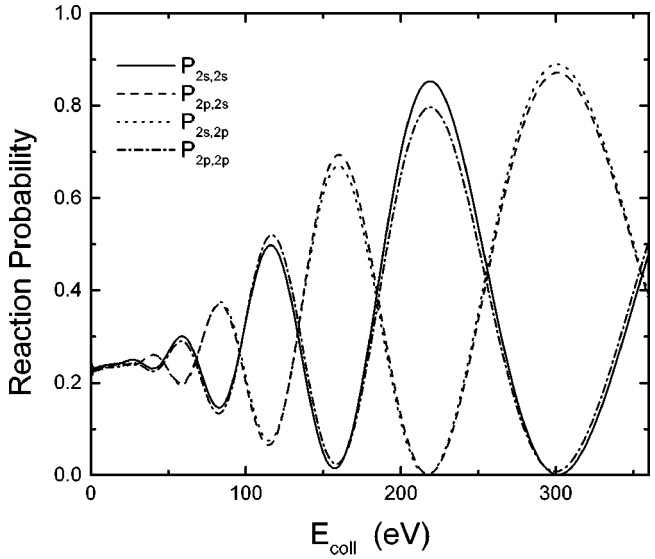

FIG. 2. Present results for reaction (1) between states of the $n_i=n_f=2$ manifold. P_{fi} is the reaction probability, $E_{\rm coll}=E-E_{d\mu(n=2)}$ is the collision energy in the initial state.

$$\sigma_{fi}|_{k\to 0}=\frac{4\pi|a''|}{k}[1-2|a''|k], \tag{6}$$

where k is the wave number of relative motion of initial fragments and $a''<0$ is defined by the ''scattering length'' $a=a'+ia''$. The latter can be introduced in a multichannel problem in the standard way as a characteristic of low-energy elastic scattering,

$$S_{ii}|_{k\to 0}=1-2iak, \tag{7}$$

but is complex in the presence of other open channels. The $1/k$ behavior of the leading term in Eq. (6) is known as the $1/v$ Bethe law. It is valid when the potential energy $V(r)$ of interaction between initial fragments vanishes faster than $1/r^2$. The fact that the second term in Eq. (6) can be expressed in terms of the same coefficient $|a''|$ was first realized by Shapiro [28]. Equation (6) holds if $V(r)$ vanishes faster than $1/r^3$. The interaction between $d\mu(n=1)$ and t at large distances r between their centers of mass is described by a polarization potential [29]

$$V(r)|_{r\to\infty}=-\frac{\alpha}{2r^4}+O(1/r^6), \tag{8}$$

where $\alpha=9/(2m_{d\mu}^3)\approx 5.304$ is the electric polarizability of $d\mu(n=1)$. It turns out that in this case one can write down one more term in Eq. (6) without introducing a new coefficient. Indeed, for elastic scattering by potential (8) further terms in Eq. (7) are given by [30]

$$S_{ii}=1-2iak-2\left(a^2+\frac{i\pi}{3}\beta\right)k^2-\frac{8i}{3}\beta a k^3\ln k+O(k^3), \tag{9}$$

where $\beta=m_{t,d\mu}\alpha\approx 58.32$ and $m_{t,d\mu}\approx 10.00$ is the reduced mass of t and $d\mu$. From this and the condition of unitarity of the scattering matrix $|S_{ii}|^2+|S_{fi}|^2=1$ we obtain

$$\sigma_{fi}=\frac{4\pi|a''|}{k}\left[1-2|a''|k+\frac{4}{3}\beta k^2\ln k+O(k^2)\right]. \tag{10}$$

To find the next term in this expansion would require introducing a new coefficient related to a complex ''effective range.''

To compare Eq. (10) with the present results we have attempted to fit the numerical values of the reaction cross section between the $n_i=n_f=1$ states by

$$[\sigma_{1s,1s}(10^{-20}\ \text{cm}^2)]=\frac{c_1}{x}+c_2+c_3x\ln x+c_4x, \tag{11}$$

where

$$x\equiv\sqrt{[E_{\rm coll}(\text{eV})]}\approx 16.00[k(\mu\text{a.u.})]. \tag{12}$$

We considered several intervals of collision energy $E_{\rm coll}$ with the maximum values ranging from 0.1 eV to 1 eV; in all the cases the first term in Eq. (11) is dominant. First, we found that the coefficient c_1 comes out stably and has the value $c_1=0.4546$, which means that $|a''|=0.034\,53\ \mu$a.u. From Eq. (10) then follows that $c_2=-0.001\,963$ and $c_3=0.1382$. Next, our fitting analysis certainly confirms the presence of the logarithmic term in Eq. (11), since with this term dropped the coefficient c_4 becomes strongly dependent on the interval of fitting. However we found that it is difficult to numerically disentangle the terms $\sim x\ln x$ and $\sim x$. So we have fixed c_3 to the value that follows from Eq. (10) and thus obtained $c_2^{\rm fit}=0.0068$ and $c_4^{\rm fit}=-0.0669$. The coefficient $c_2^{\rm fit}$ is about three times larger than that predicted by Eq. (10) and has the opposite sign. However this coefficient is small; the contribution from the term $\sim x$ is less than 1% over the considered interval of $E_{\rm coll}$, so this discrepancy might be due to an inaccuracy of our numerical results. Equation (11) with

TABLE II. Present results for reaction (1) between states of the $n_i=n_f=2$ manifold. P_{fi} is the reaction probability, $E_{\rm coll}=E-E_{d\mu(n=2)}$ is the collision energy in the initial state, in eV.

$E_{\rm coll}$	$P_{2s,2s}$	$P_{2p,2s}$	$P_{2s,2p}$	$P_{2p,2p}$
20	0.2435	0.2404	0.2398	0.2366
40	0.2310	0.2602	0.2602	0.2250
60	0.2996	0.2008	0.1970	0.2890
80	0.1513	0.3626	0.3649	0.1377
100	0.3332	0.2008	0.2130	0.3359
120	0.4862	0.0882	0.0946	0.5116
140	0.1862	0.4524	0.4411	0.2147
160	0.0192	0.6937	0.6695	0.0254
180	0.2973	0.4827	0.4586	0.2716
200	0.6986	0.1293	0.1158	0.6490
220	0.8527	0.0045	0.0047	0.7959
240	0.6905	0.1809	0.1925	0.6419
260	0.3751	0.5008	0.5189	0.3440
280	0.1068	0.7685	0.7884	0.0956
300	0.0013	0.8712	0.8894	0.0074
320	0.0700	0.7989	0.8139	0.0887
340	0.2563	0.6089	0.6199	0.2818
360	0.4812	0.3794	0.3869	0.5087

either c_2 or $c_2^{\rm fit}$ used describes our results with an error less than 1% for $E_{\rm coll}<0.5$ eV and less than 5% for $E_{\rm coll}<1$ eV. Corresponding results for the ratio $P_{1s,1s}/E_{\rm coll}^{1/2}$ are shown by the dashed line in Fig. 1. A more stringent test of the threshold law (10) for the present reaction requires numerical results of accuracy better than 0.1% over the interval $E_{\rm coll}=0.01-1$ eV.

VI. CONCLUSIONS

The calculations reported here reveal the following qualitative features of reaction (1). (i) The reaction between $n_i=n_f=1$ states is suppressed as compared to that between $n_i=n_f=2$ states: the maximum probability of the former is about 0.07 while that of the latter is close to 1. (ii) The probabilities P_{fi} of reactions between $n_i=n_f=2$ states oscillate as functions of energy. (iii) There is an approximate degeneracy: $P_{2s,2s}$ is close to $P_{2p,2p}$ and $P_{2s,2p}$ is close to $P_{2p,2s}$. These features result from interference effects in the reaction dynamics and can be explained in terms of semiclassical theory or by a model analysis [31]. These go beyond the scope of this work. Besides the numerical results we presented an analysis of the threshold behavior of the reaction between ground states. Equation (10) giving an analytical expression for the reaction cross section in terms of a single parameter $|a''|$ yields a good accuracy in the most interesting energy range for applications $E_{\rm coll}\leqslant 1$ eV and can be used in muon-catalyzed fusion kinetics calculations. Upon appropriate redefinition of β, this equation applies to a wide class of rearrangement processes in collisions between a charged particle and a neutral polarizable target having no permanent dipole and quadrupole moments.

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