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Three-body muon-transfer collisions from hydrogen isotope to He^{2+} and Li^{3+} ions

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Abstract. The muon transfer rates from hydrogen isotpes (p, d) to $^{3,4}He^{2+}$ and $^{6,7}Li^{3+}$ ions are calculated in the hyperspherical close coupling method. Well converged results are obtained. The present rates are comparable to those of exsisting calculations for He^{2+}, while they are much larger for Li^{3+}. The parameters for resonances near the $(H\mu)_{1s}$ threshold are also calculated.

PACS. 36.10 Dr Positronium, muonium, muonic atoms and molecules

1 Introduction

The muon transfer process of negative muons (μ) from hydrogen isotopes (H = p, or d) to elements of charge $Z > 1$ is important in the catalyzed fusion (μCF) [1–3]. There are two models for the muon transfer mechanism [2,4–6], namely, the direct transfer

$$H\mu + Z \to Z\mu + H, \tag{1}$$

and the molecular transfer

$$H\mu + Z \to H\mu Z \to Z\mu + H \tag{2}$$

where the metastable $H\mu Z$ molecule is formed as an intermediate state and its decay leads to the muon transfer. The process (2) is much faster than that of (1) for He [2, 4]. The process (1) is expected to be more important for higher Z [2]. However, the rate for the process (1) may not be accurate even in the Coulomb three-body treatment. In this work, we calculate reliable muon transfer rates for the collisions of $^{3,4}He^{2+} + (H\mu)_{1s}$ and $^{6,7}Li^{3+} + (H\mu)_{1s}$ using the hyperspherical close coupling (HSCC) method, which is a powerful tool to study bound states and scattering states of three-body systems [7]. The study of such collisions is also interesting as an example of rearrangment scattering with Coulomb interaction in the final states [3].

Muon atomic units (m.a.u), where muon mass is set to unity in addition to $\hbar = e = 1$, are used throughout this paper unless otherwise stated.

2 The HSCC method

The HSCC method is described in some details in [8,9]. The internal motion of three particles is described by hyperradius ρ and five angular variable Ω in the hyperspherical coordinates. The total Hamiltonian of the system is written in terms of ρ and Ω as

$$H = -\frac{1}{2M}\left(\frac{d^2}{d\rho^2} + \frac{5}{\rho}\frac{d}{d\rho}\right) + h_{ad}(\rho, \Omega) \tag{3}$$

with

$$h_{ad}(\rho, \Omega) = \frac{\Lambda^2(\Omega)}{2M} + V(\rho, \Omega) \tag{4}$$

where $\Lambda(\Omega)$ is the five-dimensional grand angular momentum operator, V is the sum of Coulomb interactions among three particles, and M is an arbitrary parameter with dimension of mass, which is taken to be reduced mass of heavy nuclei here.

The adiabatic channel functions $\{\varphi(\rho, \Omega)\}$ and the adiabatic potential $U_i(\rho)$ are defined by the eigen-value equation

$$h_{ad}(\rho, \Omega)\varphi_i(\rho, \Omega) = \left(U_i(\rho) - \frac{15}{8M\rho^2}\right)\varphi_i(\rho, \Omega) \tag{5}$$

where ρ is an adiabatic parameter.

In the HSCC method, the scattering wave function is expanded by the product of radial function $F_i(\rho)$ and φ_i as

$$\Psi^{J\Pi}(\rho, \Omega) = \sum_i^N \frac{F_i(\rho)}{\rho^{5/2}}\varphi_i(\rho, \Omega). \tag{6}$$

for each partial wave J and parity Π. Inserting this expansion in the Shrödinger equation $(H - E)\Psi^{J\Pi} = 0$, we have coupled differential equations for $\{F_i\}$

$$\left(-\frac{1}{2M}\frac{d^2}{d\rho^2} + U_i(\rho) - E\right)F_i(\rho) + \sum_j W_{ij}(\rho)F_j(\rho) = 0, \tag{7}$$

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where E is the total energy in the center of mass system and $W_{ij}(\rho)$ represents a non-adiabatic coupling. To obtain the scattering matrix, the wave function in Eq. (6) is matched with the scattering boundary conditions in the Jacobi coordinates at sufficiently large ρ. Since the system has an arrangement of a charged particle and hydrogenic atom (ion) in the asymptotic region, the dipole representation [10] is appropriate as channels in the Jacobi coordinates.

3 Results

The HSCC calculations are carried out for partial waves $J = 0 - 4$ both in $He^{2+} + H\mu$ and in $Li^{3+} + H\mu$ collisions. Two basis sets are adopted in each collision, namely, basis sets A and B for He^{2+} and basis sets C and D for Li^{3+}. We couple the channels leading to $He^{2+} + (H\mu)_{n=1}$ and $H^+ + (He\mu)^+_{n=1-3}$ for $\rho \to \infty$ in basis set A, and similarly, $He^{2+} + (H\mu)_{n=1}$ and $H^+ + (He\mu)^+_{n=1-4}$ in basis set B, $Li^{3+} + (H\mu)_{n=1}$ and $H^+ + (Li\mu)^{2+}_{n=1-3}$ in basis set C, and $Li^{3+} + (H\mu)_{n=1}$ and $H^+ + (Li\mu)^{2+}_{n=1-4}$ in basis set D.

The muon transfer rate is defined by $\lambda = N_0 v \sigma$, where $N_0 (= 4.25 \times 10^2\ /\mathrm{cm}^3)$ is the liquid-hydrogen density, v is the collision velocity, and σ is the muon-transfer cross section.

3.1 $^{3,4}He^{2+} + (^{1,2}H\mu)_{1s}$ collisions

The S-wave adiabatic potential curves for the $^3He^{2+} + p\mu$ system are shown in Fig. 1. Each potential curve converges to the atomic energy of $(p\mu)$ or $(He\mu)^+$ as $\rho \to \infty$, and the corresponding adiabatic channel function describes the fragmentaion into $He^{2+} + (p\mu)$ or $p + (He\mu)^+$. The potential curve corresponding to the initial channel, $He^{2+} + (p\mu)_{n=1}$, are close to those leading to $p + (He\mu)^+_{n=2}$. The coupling of $(He\mu)^+_{n=2}$ channels with $(p\mu)_{n=1}$ channel is considerable for $\rho < 15$. However, the transfer to $(He\mu)^+_{n=2}$ channels is less probable at low energies owing to the Coulomb repulsion between H^+ and He^+. Thus, the muon transfer into low-lying $(He\mu)^+_{n=1}$ state is dominant at low energies.

The summed muon-transfer rates up to $J = 4$ and their partial-wave contributions are depicted in Fig. 2 for the center-of-mass collision energy $0.001 \le E_c \le 100$ in eV. The calculations of basis sets A and B give similar results, and the convergence is good for the basis set. S-wave is dominant for low collision energy and the contribution from higher partial wave becomes large with increasing energy. The muon transfer of $(He\mu)_{n=2}$ becomes important for $E_c > 10$ eV in $p\mu$ target. Though it is negligible for $E_c \le 100$ ev in $d\mu$ target, it comes to contribute for $E_c \gg 100$ eV.

The obtained muon transfer rates are compared in Table 1 with those of other works involving the perturbed stationary state (PSS) calculation [1], the semiclassical calculation [6], and the Faddeev-Hahn-type calculation [3], in which the muon transfer rate is treated as direct muon transfer. The molecular transfer rate of Kravtsov *et al.* [4] is included in Table 1. At 0.04 eV, the molecular transfer rate is about one (two) order(s) of magnitude larger than the present rate for $p\mu$ ($d\mu$) traget. The rate in the PSS calculation is fairly close to the present at $E_c = 0.04$ eV, bu the agreement with the semiclassical and the Faddeev-Hahn-type calculations is not good. The disagreement is worse for the $d\mu$ target than for the $p\mu$ target.

The resonance structures are seen in the D-wave contribution for the $^{3,4}He^{2+} + p\mu$ collision in Fig. 2(a) and (b). Figures 3 (a) and (b) give the rate in resonance region and adiabatic potentials of the initial channel for the $^4He^{2+} + (p\mu)_{1s}$ collision. The adiabatic potentials of $^4He^{2+} + (p\mu)_{1s}$ channel support Feshbach resonances in $J = 0$ and 1, and a shape resonance in $J = 2$. For D-wave resonance in the $^4He^{2+} + p\mu$ system, the resonance energy and width are $E_c = 0.182$ eV and 7×10^{-4} eV, respectively, with the basis set B. The resonance parameter is derived by fitting the eigen phase sum to the Breit-Wigner formula with a linear background. Resonances near the the $(H\mu)_{n=1}$ threshold in the $^{3,4}He^{2+} + ^{1,2}H\mu$ systems are summarized in Table 2, where the values of Belyaev *et al.* [11] are included for comparison. The calculations for resonances below the $(H\mu)_{n=1}$ threshold are treated in several works, which are found in [11]. The present results are consistent with those of Belyaev *et al.*

3.2 $^{6,7}Li^{3+} + (^{1,2}H\mu)_{1s}$ collisions

The S-wave adiabatic potential curves for the $^6Li^{3+} + p\mu$ system are shown in Fig. 4 as an example of $Li^{3+} + H\mu$ systems. The muon transfer into $(Li\mu)_{n=2}$ is predominat at low energy collisions. The potential curves which describe fragmentation $p + (Li\mu)^{2+}_{n=3}$ are repulsive, and the muon transfer into $(Li\mu)_{n=3}$ is suppressed at low energies. The contribution of transfer to states with $n = 1$ and $n = 3$ is negligible for $E_c \le 100$ eV, but the transition to the $n = 3$ states is expected to be important for higher energies.

The muon transfer rates for the $^{6,7}Li^{3+} + (^{1,2}H\mu)_{1s}$ collisions are shown in Fig. 5. The rates in two basis sets C and D agree well, which shows good convergence with respect to the basis set. It seems better to include higher partial-wave contribution for $E_c > 10$ eV in $d\mu$ target. The energy dependence of muon transfer rate is more similar for $^6Li^{3+}$ and $^6Li^{3+}$ than for $^3He^{2+}$ and $^4He^{2+}$ in $p\mu$ target or $d\mu$ target, since the reduced mass of system is closer for heavier ions. The peak structures are seen for $J = 2$ in $p\mu$ target (Fig. 4(a), (b)) and for $J = 3$ in $d\mu$ target (Fig. 4(c), (d)). The peak widths are comparable to the collision energy.

The rates for muon transfer are tabulated in Table. 3, which includes the results of the Faddeev-Hahn-type calculation by Sultanov and Adhikari [3] and the molecular muon transfer rates calculated by Kravtsov *et al.* [5]. The present rates are much larger than those of the Faddeev-Hahn-type calculation and of the molecular transformation, and indicating that the direct muon transfer is important in the muon transfer to Li.

The potential curves for $Li^{3+} + (H\mu)_{1s}$ channel support resonances in low partial waves. The resonance parameters

are tabulated in Table 4. The present calculation gives deeper resonance energies than the work of Kravtsov *et al.* [12]. The widths are broader for Li ions than those of He ions. The larger width is consistent with larger cross section for Li than that for He, since the resonances below the $(\mathrm{H}\mu)_{1s}$ threshold mainly decay through couplings with $\mathrm{H}^+ + (\mathrm{He}\mu)^+_{n=1}$ channels for He and with $\mathrm{H}^+ + (\mathrm{Li}\mu)^{2+}_{n=2}$ channels for Li.

4 Summary

The HSCC method is applied to calculate the three-body muon transfer rate in the $\mathrm{He}^{2+}+(\mathrm{H}\mu)_{1s}$ and $\mathrm{Li}^{3+}+(\mathrm{H}\mu)_{1s}$ collisions, where electrons in atoms are neglected. The present calculation shows good convergence with respect to the basis set, and it seems reliable.

The transfer to $(\mathrm{He}\mu)^+_{n=1}$ is dominant at lower energies in the He^{2+} collision. The present transfer rate is within the same order as those calculated in the three body treatment. The molecular transfer is roughly estimated to be 10 times faster than the direct transfer in the $\mathrm{He}+p\mu$ system and 100 times faster in the $\mathrm{He}+d\mu$ system.

For the case of Li^{3+} impact, $(\mathrm{Li}\mu)^{2+}$ is formed in the $n=2$ states for $E_c \leq 100$ eV. The present transfer rates are about fifty times as large as those calculated with the Faddeev-Hahn-type calculation [3]. The molecular transfer rates [5] are three orders of magnitude smaller than the present rates.

It is theoretically desirable to treat the direct and molecular transfer processes coherently with considering electrons.

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Figure captions

Fig.1 The S wave adiabatic potential curves of $^3\mathrm{He}^{2+}+p\mu$ system. The asymptotic fragmentation described by corresponding adiabatic channel function is indicated as $p+(\mathrm{He}\mu)^+_n$ or $\mathrm{He}^{2+}+(p\mu)_n$. The notation $\epsilon_{p\mu}$ denotes the atomic energy of $(p\mu)_{1s}$.

Fig. 2 The muon transfer rates for the $\mathrm{He}^{2+}+(\mathrm{H}\mu)_{1s}$ collisions.
Partial wave rate calculated with basis set B: $J=0$ (dashed curve), $J=1$ (dot-dashed curve), $J=2$ (dot-dot-dashed curve), $J=3$ (dotted curve), $J=4$ (solid curve).
Summed rate for $J=0-4$: transfer to $(\mathrm{He}\mu)^+_{n=1}$ calculated with basis set B (bold solid curve), transfer to $(\mathrm{He}\mu)^+_{n=1,2}$ calculated with basis set B (bold dashed curve), transfer to $(\mathrm{He}\mu)^+_{n=1,2}$ calculated with basis set A (circles).
The transfer rate to $n=2$ states is negligibly small in the $^{3,4}\mathrm{He}^{2+}+(d\mu)_{1s}$ collisions in the figure.

Fig. 3 (a) The muon transfer rate for energies near the D-wave resonance in the $^4\mathrm{He}^{2+}+(p\mu)_{1s}$ collision. (b) The adiabatic potential curves converging to the energy of $(p\mu)_{1s}$ for the $^4\mathrm{He}^{2+}+p\mu$ system. The potential curves are for $J=0-3$ from the bottom.

Fig. 4 The S wave adiabatic potential curves of $^6\mathrm{Li}^{3+}+p\mu$ system. The asymptotic fragmentation described by corresponding adiabatic channel function is indicated as $p+(\mathrm{Li}\mu)^{2+}_n$ or $\mathrm{Li}^{3+}+(p\mu)_n$. The notation $\epsilon_{p\mu}$ denotes the atomic energy of $(p\mu)_{1s}$.

Fig. 5 The muon transfer rates for the $\mathrm{Li}^{3+}+(\mathrm{H}\mu)_{1s}$ collisions.
Partial wave rate calculated with basis set D: $J=0$ (dashed curve), $J=1$ (dot-dashed curve), $J=2$ (dot-dot-dashed curve), $J=3$ (dotted curve), $J=4$ (solid curve).
Summed rate for $J=0-4$: basis set C (circle), basis set D (bold solid curve).

Table 1. Comparison of muon transfer rate (10^6/s) in the $He^{2+} + (H\mu)_{1s}$ collision at center-of-mass collision energy E_c.

	$^3He^{2+}$	$^4He^{2+}$	$^3He^{2+}$	$^4He^{2+}$
E_c (eV)	$p\mu$		$d\mu$	
0.001	8.18[a]	8.04[a]	1.98[a]	5.30[a]
0.004	8.13[a]	7.98[a]	1.94[a]	4.52[a]
	110	59	258	552
0.01	8.04[a]	7.86[a]	1.87[a]	3.52[a]
0.04	7.70[a]	7.54[a]	1.60[a]	1.74[a]
	91[b]	48[b]	162[b]	218[b]
	6.3[c]	5.5[c]	1.3[c]	1.0[c]
	10.9[d]	10.7[d]	9.6[d]	9.6[d]
	8.4[e]	6.8[e]	5.2[e]	5.0[e]
0.1	7.25[a]	9.60[a]	1.27[a]	0.92[a]
	82[b]	42[b]	126[b]	134[b]
	8.3[e]		5.1[e]	
0.4	6.19[a]	11.6[a]	0.76[a]	0.34[a]
1.0	5.56[a]	7.11[a]	0.59[a]	0.22[a]
	8.1[e]		4.7[e]	
4.0	6.84[a]	5.53[a]	0.62[a]	0.20[a]
10.0	16.0[a]	4.96[a]	0.68[a]	0.22[a]

[a] Present calculation with basis set A.
[b] Molecular transfer rate of Kravtsov *et al.* [4].
[c] Matveenko and Ponomarev [1].
[d] Czaplinski *et al.* [6].
[e] Sultanov and Adhikari [3].

Table 2. Resonances associated with $(H\mu)_{1s}$ threshold of the $He^{2+} + H\mu$ system. Each resonance is expressed as (E_r, Γ) in eV, where E_r is the resonance energy measured from the $(H\mu)_{1s}$ threshold and Γ is the width. $x[y] = x \times 10^y$.

Partial wave	$^3He^{2+} + p\mu$	$^4He^{2+} + p\mu$
$J = 0$	$(-73.70, 5.6[-3])^a$	$(-81.69, 3.9[-3])^a$
	$(-72.76, 6.4[-3])^b$	$(-80.64, 4.7[-3])^b$
$J = 1$	$(-41.73, 2.8[-3])^a$	$(-50.51, 2.2[-3])^a$
	$(-38.82, 3.1[-3])^b$	$(-47.45, 2.5[-3])^b$
$J = 2$	$(7.2, 1.9)^a$	$(0.205, 7.9[-4])^a$
	$(7.2, 1.9)^c$	$(0.181, 6.7[-4])^c$
	$^3He^{2+} + d\mu$	$^4He^{2+} + d\mu$
$J = 0$	$(-70.90, 3.5[-4])^a$	$(-79.36, 9.9[-5])^a$
	$(-69.37, 1.9[-4])^b$	$(-77.49, 4.8[-5])^b$
$J = 1$	$(-48.33, 3.8[-4])^a$	$(-58.14, 1.3[-4])^a$
	$(-46.31, 2.1[-4])^b$	$(-55.74, 7.9[-5])^b$
$J = 2$	$(-9.46, 1.7[-4])^a$	$(-20.48, 9.5[-5])^a$
	$(-7.11, 1.2[-4])^b$	$(-17.49, 6.9[-5])^b$
$J = 3$	$(30.4, 20)^a$	$(20.5, 8.1)^a$
	$(30.0, 20)^c$	$(20.3, 7.8)^c$

[a] Present calculation with basis set A.
[b] Belyaev *et al.* [11].
[c] Present calculation with basis set B.

Table 3. Comparison of muon transfer rate (10^8/s) for the $Li^{3+} + (H\mu)_{1s}$ collisions at center-of-mass collision energy E_c. $x[y] = x^y$

	$^6Li^{2+}$	$^7Li^{2+}$	$^6Li^{3+}$	$^7Li^{3+}$
E_c (eV)	$p\mu$		$d\mu$	
0.001	9.95[a]	9.57[a]	1.50[a]	1.21[a]
0.004	9.84[a]	9.45[a]	1.42[a]	1.11[a]
	0.01[c]	3.4[−3][c]	6.6[−4][c]	1.65[−3][c]
0.01	9.67[a]	9.25[a]	1.28[a]	0.96[a]
0.04	9.15[a]	8.67[a]	0.95[a]	0.63[a]
			1.9[−2][b]	1.6[−2][b]
	9.0[−3][c]	3.0[−3][c]	4.7[−4][c]	1.0[−3][c]
0.1	8.82[a]	8.21[a]	0.71[a]	0.43[a]
			1.9[−2][b]	1.6[−2][b]
	7.8[−3][c]	2.6[−3][c]	3.6[−4][c]	7.2[−4][c]
0.4	9.30[a]	8.35[a]	0.68	0.36[a]
1.0	10.7[a]	9.59[a]	1.02[a]	0.50[a]
			1.2[−2][b]	1.2[−2][b]
	2.2[−3][c]	6.5[−4][c]	2.3[−4][c]	3.1[−4]
4.0	22.1[a]	30.3[a]	1.43[a]	0.80[a]
10.0	30.1[a]	25.8[a]	2.41[a]	2.46[a]

[a] Present calculation with basis set B.
[b] Sultanov and Adhikari [3].
[c] Molecular muon transfer rate of Kravtsov *et al.* [5].

Table 4. Resonances associated with $(H\mu)_{1s}$ threshold of the Li^{3+}+Hμ system. Each resonance is expressed as (E_r, Γ) in eV, where E_r is the resonance energy measured from the $(H\mu)_{1s}$ threshold and Γ is the width. $x[y] = x \times 10^y$.

Partial wave	$^6Li^{3+} + p\mu$	$^7Li^{3+} + p\mu$
$J = 0$	$(-18.4, 0.25)^a$	$(-19.3, 0.23)^a$
	$(-17.6, —)^b$	$(-18.5, —)^b$
$J = 1$	$(-8.4, 0.17)^a$	$(-9.3, 0.16)^a$
	$(-6.96, —)^b$	$(-7.9, —)^b$
$J = 2$	$(5.78, 4.6)^a$	$(5.15, 3.6)^a$
	$^6Li^{3+} + d\mu$	$^7Li^{3+} + d\mu$
$J = 0$	$(-20.25, 1.4[-2])^a$	$(-21.40, 6.7[-3])^a$
	$(-19.8, —)^b$	$(-21.0, —)^b$
$J = 1$	$(-13.52, 1.7[-2])^a$	$(-14.76, 1.0[-2])^a$
	$(-12.9, —)^b$	$(-14.1, —)^b$
$J = 2$	$(-1.62, 1.5[-2])^a$	$(-2.87, 1.2[-2])^a$
	$(-0.84, —)^b$	$(-2.02, —)^b$
$J = 3$	$(10.0, 7.0)^a$	$(9.98, 7.0)^a$

[a] Present calculation with basis set C.
[b] Kravtsov *et al.* [12].