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Semiclassical approach to the three-body muon-transfer collisions

R.A. Sultanov[1,2,a], W. Sandhas[1], and V.B. Belyaev[3]

[1] Physikalisches Institut, Universität Bonn, 53115 Bonn, Germany
[2] Instituto de Fisica Teorica, UNESP, Rua Pamplona 145, 01405-900 Sao Paulo SP, Brazil
[3] Laboratory of Theoretical Physics, JINR, 141980 Dubna, Russia

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Abstract. Muon-transfer rates in collisions of hydrogen-like atoms $(p\mu^-)$ or $(d\mu^-)$ with light nuclei t, ^{3}He, ^{4}He, ^{6}Li or ^{7}Li, are calculated in a semiclassical approximation to the Faddeev-Hahn equations. The two nuclei involved are treated classically, while the motion of the muon in their Coulomb field is considered from the quantum mechanical point of view. The experimentally observed strong dependence on the charge of the nuclei is reproduced.

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

1 Introduction

The motion of negative muons in hydrogen media with admixtures of elements A of charge $Z > 2$ shows a peculiar behavior [1,2]. Opposite to the smooth Z-dependence predicted by the Landau-Zener formula, the experimental muon transfer rates in processes like $(p\mu^-) + A \to p + (A\mu^-)$ depend in a complicated manner on the charge Z. The measured isotropy effects, *e.g.* the ratio of the transitions $(p\mu^-) + \mathrm{Ne} \to p + (\mathrm{Ne}\mu^-)$ and $(d\mu^-) + \mathrm{Ne} \to d + (\mathrm{Ne}\mu^-)$, differ also considerably from the Landau-Zener predictions. Another phenomenon which has not yet found a satisfactory theoretical explanation is the time distribution of the γ-production occurring in such transition processes [3]. In what follows we develop a method for solving these problems, which is based on detailed few-body equations rather than the effective potential treatment employed in alternative investigations.

Coulombic three-body systems with two heavy and one light particle are considered traditionally within the framework of the Born-Oppenheimer approximation. For muon transfer processes, Faddeev-type equations [4], especially the modified version proposed by Hahn [5], appear to be better suited. They are formulated for appropriately chosen wave-function components which show the correct physical asymptotics. Our method for describing rearrangement processes

$$2 + (1,3) \to (2,3) + 1 \tag{1}$$

with one light particle 3 of charge $Z_3 = -1$ and two heavy particles 1 and 2 of charges $Z_1 = 1$ and $Z_2 = 1, 2, 3, ...$, is based on a semiclassical approximation to such Faddeev-Hahn (FH) equations [6]. These equations are treated by means of an adequate coupled channel expansion.

In the following section we develop the formalism. The results obtained for the collision of hydrogen-like systems $(h\mu^-) = (p\mu^-)$ or $(d\mu^-)$ with light ions t^+, $^3\mathrm{He}^{++}$, $^4\mathrm{He}^{++}$, $^6\mathrm{Li}^{+++}$ or $^7\mathrm{Li}^{+++}$ are given in Section 3. Fairly good agreement with quantum mechanical calculations is found for processes involving t^+ and He^{++}. This justifies to apply our semiclassical approach also to processes of higher charge, like Li^{+++}, for which no fully satisfactory quantum mechanical calculations exist. As an additional test of the method, calculations for the charge exchange scattering of protons off electronic hydrogen atoms are also performed.

In the muonic case the units are $e = \hbar = m_\mu = 1$, in the electronic case we use $e = \hbar = m_e = 1$.

2 Formalism

Written as integro-differential equations, the Faddeev equations [4] read

$$\left(i\frac{\partial}{\partial t} - H_0 - V_{jk}\right)|\Psi_l\rangle = V_{jk}\left(|\Psi_j\rangle + |\Psi_k\rangle\right). \tag{2}$$

Here H_0 is the kinetic energy operator of the three particles,

$$H_0 = -\frac{1}{2\mu_{jk}}\Delta_{\mathbf{r}_{jk}} + \frac{1}{2M_l}\Delta_{\mathbf{R}_l}\ , \tag{3}$$

$\mathbf{r}_{jk}$ and $\mathbf{R}_l$ are the Jacobi coordinates, μ_{jk} and M_l the corresponding reduced masses, V_{jk} the two-body potentials.

[a] e-mail: sultanov@ift.unesp.br

As mentioned above we consider particle 3 to be the light one, *i.e.*,

$$\frac{m_3}{m_1} \ll 1, \qquad \frac{m_3}{m_2} \ll 1. \tag{4}$$

Then, the heavy particles 1 and 2 can be considered as moving along classical trajectories $\mathbf{R}_1(t)$ and $\mathbf{R}_2(t)$. For the treatment of this situation we employ, instead of the three Faddeev equations, the two coupled FH equations [6,7]

$$\left(i\frac{\partial}{\partial t} - \frac{p_r^2}{2\mu_1} - V_{13}(\mathbf{x}) - \frac{Z_2Z_3}{R(t)}\right)\Psi_1(\mathbf{r},\mathbf{R}(t),t) = \left(V_{13}(\mathbf{x}) - \frac{Z_1Z_3}{R(t)}\right)\Psi_2(\mathbf{r},\mathbf{R}(t),t)$$

$$\left(i\frac{\partial}{\partial t} - \frac{p_r^2}{2\mu_2} - V_{23}(\mathbf{y}) - \frac{Z_1Z_3}{R(t)}\right)\Psi_2(\mathbf{r},\mathbf{R}(t),t) = \left(V_{23}(\mathbf{y}) - \frac{Z_2Z_3}{R(t)}\right)\Psi_1(\mathbf{r},\mathbf{R}(t),t). \tag{5}$$

Here, $\mathbf{R}(t)$ is the relative vector between particles 1 and 2, its time dependence being determined according to classical mechanics. The motion of the light particle 3 is treated quantum mechanically, $\mathbf{p}_r = \boldsymbol{\nabla}_r/i$ is the momentum operator corresponding to the relative variable $\mathbf{r}$ between particle 3 and the center of mass of particles 1 and 2. The relative vectors in the (13) and (23) subsystems are denoted by $\mathbf{x}$ and $\mathbf{y}$, respectively, and the corresponding reduced masses are given by

$$\begin{aligned}\mu_1 &= m_1m_3/(m_1+m_3),\\ \mu_2 &= m_2m_3/(m_2+m_3).\end{aligned} \tag{6}$$

To solve equations (5), we expand the wave function components $\Psi_k(\mathbf{r},\mathbf{R}(t),t)$ into the solutions $\Phi_n^{k3}(\mathbf{r},\mathbf{R}(t),t)$ of the respective subsystem Schrödinger equations

$$\left(i\frac{\partial}{\partial t} - \frac{p_r^2}{2\mu_k} - V_{k3}(\mathbf{r}-\mathbf{R}_k(t))\right)\Phi_n^{k3}(\mathbf{r},\mathbf{R}_k(t),t) = 0\ . \tag{7}$$

That is, we write

$$\Psi_k(\mathbf{r},\mathbf{R}(t),t) = \left(\sum + \int\right)_n C_n^k(\mathbf{R}(t),t)\Phi_n^{k3}(\mathbf{r},\mathbf{R}(t),t), \tag{8}$$

the summation (integration) running over the whole discrete and continuous spectrum.

For a constant velocity $\dot{\mathbf{R}}_k(t) = \boldsymbol{v}_k$ one finds

$$\Phi_n^{k3}(\mathbf{r},\mathbf{R}(t),t) = e^{i\mu_k\boldsymbol{v}_k\cdot\mathbf{r} - i(E_n^{k3}+\frac{\mu_k}{2}v_k^2)t}\varphi_n^{k3}(\mathbf{r}-\mathbf{R}_k(t)), \tag{9}$$

the functions φ_n^{k3} being given by

$$\left(-\frac{1}{2\mu_k}\Delta_{\mathbf{x}} + V_{k3}(\mathbf{x})\right)\varphi_n^{k3}(\mathbf{x}) = E_n^{k3}\varphi_n^{k3}(\mathbf{x})\ . \tag{10}$$

Inserting the expansion (8) into (5), we obtain for the coefficients C_n^k a set of coupled equations [6,7]

$$i\frac{\partial C_n^1(\mathbf{R}(t),t)}{\partial t} = \left(\sum + \int\right)_m \mathcal{W}_{nm}^{12}(R(t),t)\gamma_{nm}^{12}(t)C_m^2(\mathbf{R}(t),t)$$

$$i\frac{\partial C_m^2(\mathbf{R}(t),t)}{\partial t} = \left(\sum + \int\right)_n \mathcal{W}_{mn}^{21}(R(t),t)\gamma_{nm}^{12*}(t)C_n^1(\mathbf{R}(t),t)\ , \tag{11}$$

where

$$\begin{aligned}\gamma_{nm}^{(jk)}(t) &= e^{i(E_n^{j3}-E_m^{k3}+\Delta\epsilon)t},\\ E_n^{j3} &= -\mu_jZ_j^2/2n^2,\\ j &\neq k = 1,2.\end{aligned} \tag{12}$$

The matrix elements $\mathcal{W}_{nm}^{jk}(R(t),t)$ are obtained by sandwiching the potentials in equation (5) between the channel functions (9),

$$\mathcal{W}_{nm}^{jk}(R(t),t) = \left\langle e^{i\mu_j\boldsymbol{v}_j\cdot\mathbf{r}-i\frac{\mu_j}{2}v_j^2t}\varphi_n^{j3}(\mathbf{r}-\mathbf{R}_j(t))\middle| V_{j3}(\mathbf{r}-\mathbf{R}_j(t)) - \frac{Z_jZ_3}{R(t)}\middle| e^{i\mu_k\boldsymbol{v}_k\cdot\mathbf{r}-i\frac{\mu_k}{2}v_k^2t}\varphi_m^{k3}(\mathbf{r}-\mathbf{R}_k(t))\right\rangle\ . \tag{13}$$

Equations (5) are to be solved under the initial condition

$$\begin{aligned}\Psi_1(\mathbf{r},\mathbf{R}(t),t) &\underset{t\to-\infty}{\sim} \Phi_{1s}^{13}(\mathbf{r},\mathbf{R}(t),t),\\ \Psi_2(\mathbf{r},\mathbf{R}(t),t) &\underset{t\to-\infty}{\sim} 0\ ,\end{aligned} \tag{14}$$

which implies for the coefficients $C_n^j(\mathbf{R}(t),t)$

$$\begin{aligned}C_n^1(\mathbf{R}(t),t) &\underset{t\to-\infty}{\sim} \delta_{n1},\\ C_n^2(\mathbf{R}(t),t) &\underset{t\to-\infty}{\sim} 0\ .\end{aligned} \tag{15}$$

For low-energies, say below 20 eV, the relative nuclear velocities are practically zero in the respective muon-atomic unities. The exponential factor in equation (9), hence, can be replaced by unity and the matrix elements (13) simplify to

$$\mathcal{W}_{nm}^{jk}(R(t)) = \int d^3r\varphi_n^{j3^*}(\mathbf{r}-\mathbf{R}_j(t)) \times \left(V_{j3}(\mathbf{r}-\mathbf{R}_j(t)) - \frac{Z_jZ_3}{R(t)}\right)\varphi_m^{k3}(\mathbf{r}-\mathbf{R}_k(t))\ . \tag{16}$$

In order to obtain the capture probabilities $|C_n^2(t\sim\infty)|^2$ we, thus, have to solve the system of coupled ordinary differential equations (11), its ingredients and initial conditions being given by equations (12, 15, 16).

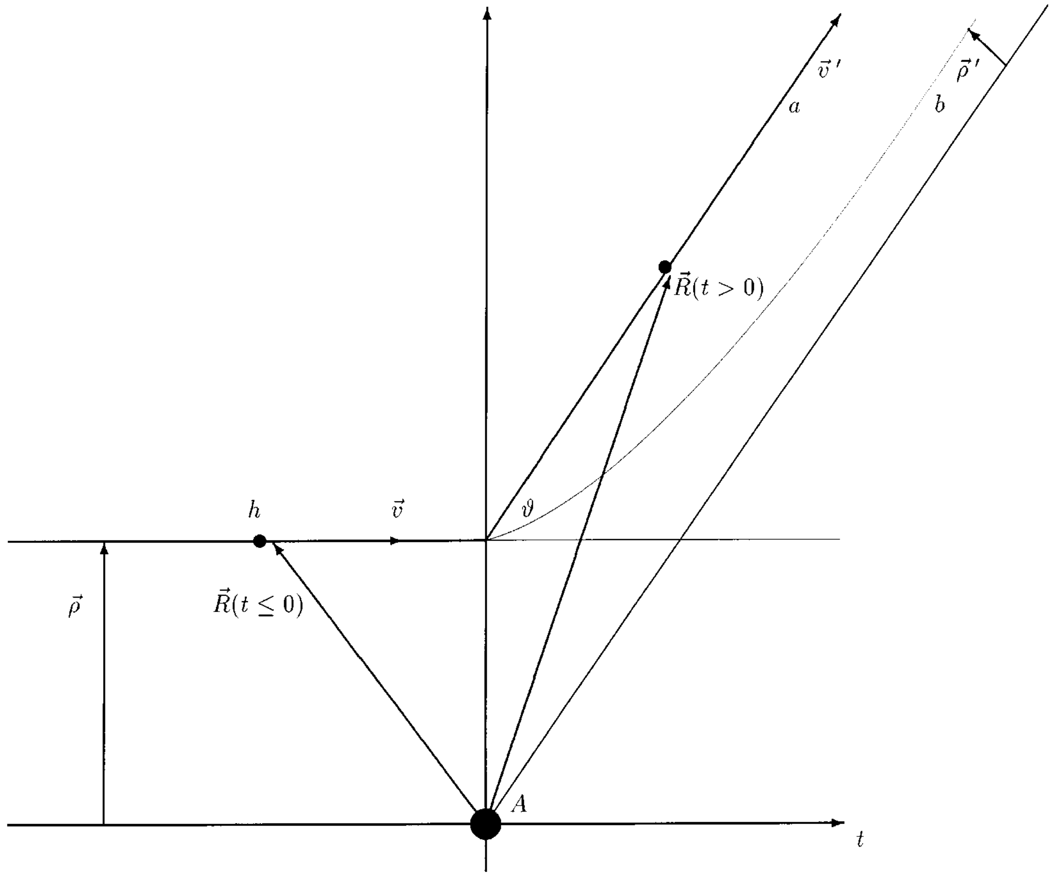

Fig. 1. The relative positions of the heavy particles h and A before and after collision: the straight line a is an approximate trajectory, b is the real one.

The trajectories of the heavy particles will be chosen as straight lines, $\mathbf{R}(t) = \boldsymbol{\rho} + \mathbf{v}t$ for $t \leq 0$ and $\mathbf{R}(t) = \boldsymbol{\rho} + \mathbf{v}\,'t$ for $t > 0$, with $\boldsymbol{\rho}$ being the impact parameter, $\mathbf{v}$ and $\mathbf{v}\,'$ the velocities before and after the collision, respectively. Taking them as asymptotes to the actual motion, the angle between their directions, *i.e.* between $\mathbf{v}$ and $\mathbf{v}\,'$, is the deflection angle ϑ. Moreover,

$$v = \sqrt{2E/M_1}, \tag{17}$$

$$v\,' = \sqrt{2(E + \Delta E)/M_2}, \tag{18}$$

where E is the CM collision energy,

$$\Delta E = E_n^{13} - E_m^{23} \tag{19}$$

and

$$M_1 = \frac{(m_3 + m_1)m_2}{m_1 + m_2 + m_3}, \quad M_2 = \frac{(m_3 + m_2)m_1}{m_1 + m_2 + m_3}\,\cdot \tag{20}$$

To choose the trajectory before the collision as a straight line is justified because of the neutrality and the small size of the incident hydrogen-like atom $(h\mu^-)$. To choose a straight trajectory also after the charge exchange process is, of course, an approximation to the real hyperbolic curve (see Fig. 1) [7].

From the definition of $\mathbf{R}(t)$ we infer

$$R(t) = \sqrt{\rho^2 + v^2t^2}, \qquad \text{for } t \leq 0 \tag{21}$$

and

$$R(t) = \sqrt{\rho^2 + v\,'^2t^2 - 2\rho v\,'t\sin\vartheta}, \quad \text{for } t > 0. \tag{22}$$

The angle ϑ is determined according to classical mechanics (see Fig. 1),

$$\vartheta = \pi/2 - \int_{r_{min}}^{\infty} \frac{\rho\,'/r^2dr}{\sqrt{1 - \rho\,'^2/r^2 - U(r)/T_{kin}}}, \tag{23}$$

with the final-state impact parameter $\rho\,'$ being given, due to angular momentum conservation, by

$$\rho\,' = \frac{M_1v}{M_2v\,'}\rho. \tag{24}$$

$U(r)$ is the screened Coulomb potential between $h = p^+$ or d^+ and $(A\mu^-)$,

$$U(r) = (Z_2 - 1)/r + (1/r + Z_2\mu_2)e^{-2Z_2\mu_2 r}. \quad (25)$$

The lower bound r_{min} of the integral is obtained as a root of

$$1 - \frac{\rho'^2}{r_{min}^2} - \frac{U(r_{min})}{T_{kin}} = 0, \quad (26)$$

where

$$T_{kin} = \frac{M_2 v'^2}{2} \quad (27)$$

represents the kinetic energy of the outgoing fragments in the center-of-mass system. Note that the angle in (23) is half the one given in [8] since the Coulomb-like potential (25) acts only during the time after the collision.

When solving the resulting coupled set of equations for the expansion coefficients, it is seen that its solutions $C_n^k(\mathbf{R}(t), t)$ tend towards an asymptotic value $C_n^2(\rho)$ which depends, of course, on the impact parameter ρ. The cross-section of process (1) is given by

$$\sigma_{tr}^n = 2\pi \int_0^{+\infty} |C_n^2(\rho)|^2 \rho d\rho. \quad (28)$$

3 Results

In this section we present cross-sections σ_{tr} and muon transfer rates λ_{tr} calculated within the above formalism for processes of the type

$$(h\mu^-)_{1s} + A \to (A\mu^-)_{1s} + h, \quad (29)$$

where $h = p^+$ or d^+ and $A = t^+$, $^3\mathrm{He}^{++}$, $^4\mathrm{He}^{++}$, $^6\mathrm{Li}^{+++}$ or $^7\mathrm{Li}^{+++}$. We restrict ourselves to a two-level approximation by choosing in the relevant close-coupling expansion only the hydrogen-like ground states $(h\mu^-)_{1s}$ and $(A\mu^-)_{1s}$. The transfer rate is defined by

$$\lambda_{tr} = \sigma_{tr} v N_0, \quad (30)$$

with v being the relative velocity of the incident fragments and N_0 the liquid-hydrogen density chosen here as 4.25×10^{22} cm^{-3}.

In Table 1 we compare our cross-sections $\sigma_{tr}/10^{-20}$ cm^2 for the case $h = d^+$ and $A = t^+$ at various collision energies E with those of reference [9]. For the muon transfer rate of this process at $E = 0.04$ eV we find $\lambda_{tr} = 3.70 \times 10^8$ s^{-1}. Measurements of this value range from $\lambda_{tr}^{exp} = 2.8 \times 10^8$ s^{-1} [10] to $\lambda_{tr}^{exp} = 3.5 \times 10^8$ s^{-1} [11].

The rates λ_{tr} $/10^6$ s^{-1} for $h = p^+$ or d^+ and $A = {}^3\mathrm{He}^{++}$, $^4\mathrm{He}^{++}$, $^6\mathrm{Li}^{+++}$ or $^7\mathrm{Li}^{+++}$ at $E = 0.04$ eV are presented in Table 2 together with the $^3\mathrm{He}^{++}$ and $^4\mathrm{He}^{++}$ results of [12].

Figure 2 shows our $d\mu + t \to t\mu + d$ cross-sections compared with variational calculations [13] which are generally considered to be most accurate. It is seen that the shapes of the curves agree fairly well over a wide energy range.

Table 1. Cross-sections $\sigma_{tr}/10^{-20}$ cm^2 for $t + (d\mu) \to (t\mu) + d$.

E(eV)	our results	[9]
5.0	3.40	2.87
3.0	3.17	2.12
2.0	3.12	1.76
1.0	3.05	1.43
0.1	3.16	2.00
0.04	3.50	2.94

Table 2. Muon transfer rates $\lambda_{tr}/10^6$ s^{-1} at low energy $E = 0.04$ eV.

	$^3\mathrm{He}^{++}$	[12]
p^+	7.25	6.3
d^+	4.77	1.3
	$^4\mathrm{He}^{++}$	[12]
p^+	6.65	5.5
d^+	4.17	1.0
	$^6\mathrm{Li}^{+++}$	$^7\mathrm{Li}^{+++}$
p^+	1.72	1.67
d^+	1.01	0.96

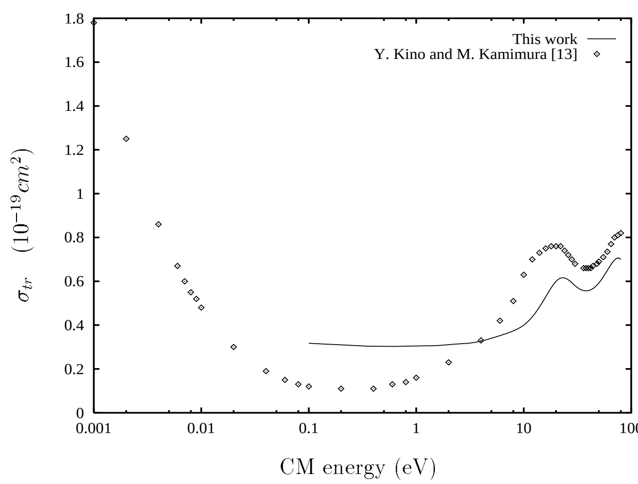

Fig. 2. Cross-section of the reaction $d\mu + t \to t\mu + d$.

All these comparisons demonstrate the efficiency of our semiclassical treatment for atoms of charge $Z = 1$ or 2. Its application to processes involving higher charges, therefore, is expected to be also justified. Our ^{6}Li or ^{7}Li calculations represent first examples for such an extension.

As a further test of our method, we have also calculated the low-energy charge exchange scattering of protons by hydrogen atoms

$$p_1 + (p_2, e) \to (p_1, e) + p_2. \quad (31)$$

In Table 3 our results are compared with calculations

Table 3. Cross-sections $\sigma_{ex}/10^{-15}$ cm^2 for charge exchange scattering of protons by hydrogen atoms.

E(eV)	our results	[14]
10.0	3.73	
5.0	4.10	3.72
1.0	4.95	4.54
0.22	5.60	5.18

based on the Born-Oppenheimer approximation [14]. The agreement is again quite satisfactory.

Calculations involving nuclei of higher charge, and a full quantum mechanical treatment are in progress.

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