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SEMICLASSICAL APPROACH TO THREE-BODY MUON-TRANSFER COLLISIONS

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Muon-transfer rates in collisions of hydrogenlike atoms ($p\mu^-$) or ($d\mu^-$) with light nuclei t , ^3He , ^4He , ^6Li or ^7Li 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.

The investigation has been performed at the Bogoliubov Laboratory of Theoretical Physics, JINR.

Трехчастичная перезарядка мюонов в полуклассическом подходе

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В рамках полуклассического приближения к уравнениям Фаддеева—Ханна рассмотрен процесс перезарядки мюонов при столкновении ($p\mu^-$) и ($d\mu^-$) с легкими ядрами t , ^3He , ^4He , ^6Li , ^7Li . В данном подходе тяжелые частицы рассматриваются движущимися по классическим траекториям, в то время как мюон описывается как квантовая частица. Установленная экспериментально сильная зависимость сечения перезарядки от заряда ядра воспроизведена в данных расчетах.

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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 $(p\mu^-) + A \rightarrow p + (A\mu^-)$ depend in a complicated manner on the charge Z . The measured isotope effects, e.g., the ratio of the transitions $(p\mu^-) + \text{Ne} \rightarrow p + (\text{Ne}\mu^-)$ and $(d\mu^-) + \text{Ne} \rightarrow d + (\text{Ne}\mu^-)$, differ also considerably from the Landau–Zener predictions. Another phenomenon which has not yet found a satisfactory theoretical explanation is the

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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 wavefunction components which show the correct physical asymptotics. Our method for describing rearrangement processes



with one light particle 3 of charge $Z_3 = -1$ and two heavy particles 1 and 2 of charges $Z_1 = 1$ and $Z_2 = 1, 2, 3, \dots$, 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 hydrogenlike systems $(h\mu^-) = (p\mu^-)$ or $(d\mu^-)$ with light ions t^+ , ${}^3\text{He}^{++}$, ${}^4\text{He}^{++}$, ${}^6\text{Li}^{+++}$ or ${}^7\text{Li}^{+++}$ are given in Sec.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

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

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

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

\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.

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

$$\frac{m_3}{m_1} \ll 1, \quad \frac{m_3}{m_2} \ll 1. \quad (4)$$

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]

$$\left(i \frac{\partial}{\partial t} - \frac{p_r^2}{2\mu_1} - V_{13}(\mathbf{x}) - \frac{Z_2 Z_3}{R(t)} \right) \Psi_1(\mathbf{r}, \mathbf{R}(t), t) = \left(V_{13}(\mathbf{x}) - \frac{Z_1 Z_3}{R(t)} \right) \Psi_2(\mathbf{r}, \mathbf{R}(t), t),$$

$$\left(i \frac{\partial}{\partial t} - \frac{p_r^2}{2\mu_2} - V_{23}(\mathbf{y}) - \frac{Z_1 Z_3}{R(t)} \right) \Psi_2(\mathbf{r}, \mathbf{R}(t), t) = \left(V_{23}(\mathbf{y}) - \frac{Z_2 Z_3}{R(t)} \right) \Psi_1(\mathbf{r}, \mathbf{R}(t), t). \quad (5)$$

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, $\mathbf{p}_r = \nabla_r / i$ 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

$$\mu_1 = m_1 m_3 / (m_1 + m_3), \quad \mu_2 = m_2 m_3 / (m_2 + m_3). \quad (6)$$

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

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

That is, we write

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

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

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

$$\Phi_n^{k3}(\mathbf{r}, \mathbf{R}(t), t) = e^{i\mu_k \mathbf{v}_k \cdot \mathbf{r} - i(E_n^{k3} + \mu_k v_k^2 / 2)t} \phi_n^{k3}(\mathbf{r} - \mathbf{R}_k(t)), \quad (9)$$

the functions ϕ_n^{k3} being given by

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

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

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

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

where

$$\gamma_{nm}^{(jk)}(t) = e^{i(E_n^{j3} - E_m^{k3} + \Delta\varepsilon)t}, \quad E_n^{j3} = -\mu_j Z_j^2 / 2n^2, \quad j \neq k = 1, 2. \quad (12)$$

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

$$\mathcal{W}_{nm}^{jk}(R(t), t) = \langle e^{i\mu_j \mathbf{v}_j \cdot \mathbf{r} - i\mu_j v_j^2 t / 2} \phi_n^{j3}(\mathbf{r} - \mathbf{R}_j(t)) \left| V_{j3}(\mathbf{r} - \mathbf{R}_j(t)) - \frac{Z_j Z_3}{R(t)} \right| e^{i\mu_k \mathbf{v}_k \cdot \mathbf{r} - i\mu_k v_k^2 t / 2} \phi_m^{k3}(\mathbf{r} - \mathbf{R}_k(t)) \rangle. \quad (13)$$

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

$$\Psi_1(\mathbf{r}, \mathbf{R}(t), t) \underset{t \rightarrow -\infty}{\sim} \Phi_{1s}^{13}(\mathbf{r}, \mathbf{R}(t), t), \quad \Psi_2(\mathbf{r}, \mathbf{R}(t), t) \underset{t \rightarrow -\infty}{\sim} 0, \quad (14)$$

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

$$C_n^1(\mathbf{R}(t), t) \underset{t \rightarrow -\infty}{\sim} \delta_{n1}, \quad C_n^2(\mathbf{R}(t), t) \underset{t \rightarrow -\infty}{\sim} 0. \quad (15)$$

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

$$\mathcal{W}_{nm}^{jk}(\mathbf{R}(t)) = \int d^3r \phi_n^{j3*}(\mathbf{r} - \mathbf{R}_j(t)) \left(V_{j3}(\mathbf{r} - \mathbf{R}_j(t)) - \frac{Z_j Z_3}{R(t)} \right) \phi_m^{k3}(\mathbf{r} - \mathbf{R}_k(t)). \quad (16)$$

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 (12), (15) and (16).

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,

$$v = \sqrt{2E/M_1}, \quad (17)$$

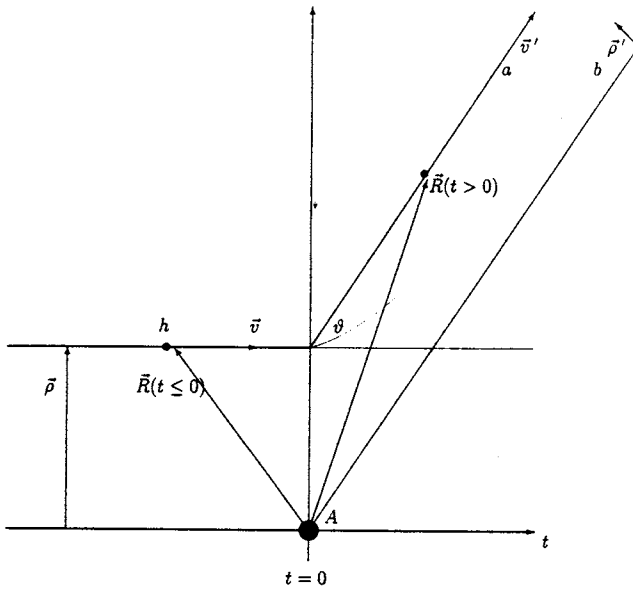


Fig.1. The relative positions of the heavy particles h and A before and after collision: the straight line a is an approximate trajectory, b is the real one

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

where E is the CM collision energy,

$$\Delta E = E_n^{13} - E_m^{23} \quad (19)$$

and

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

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

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

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

and

$$R(t) = \sqrt{\rho^2 + v^2 t^2 - 2\rho v t \sin \vartheta}. \quad (22)$$

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

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

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

$$\rho' = \frac{M_1 v}{M_2 v'} \rho. \quad (24)$$

$U(r)$ 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

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

where

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

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 [7] 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



where $h = p^+$ or d^+ and $A = t^+$, ${}^3\text{He}^{++}$, ${}^4\text{He}^{++}$, ${}^6\text{Li}^{+++}$ or ${}^7\text{Li}^{+++}$. We restrict ourselves to a two-level approximation by choosing in the relevant close-coupling expansion only the hydrogenlike 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 $4.25 \times 10^{22} \text{ cm}^{-3}$.

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

The rates $\lambda_{tr}/10^6 \text{ sec}^{-1}$ for $h = p^+$ or d^+ and $A = {}^3\text{He}^{++}$, ${}^4\text{He}^{++}$, ${}^6\text{Li}^{+++}$ or ${}^7\text{Li}^{+++}$ at $E = 0.04 \text{ eV}$ are presented in Table 2 together with the ${}^3\text{He}^{++}$ and ${}^4\text{He}^{++}$ results of [11]. Experimentally p^+ the rates are about twice as big as the d^+ rates. Our results are consistent with this observation, while the corresponding ratio in [11] is definitely too high.

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

E (eV)	Our results	[8]	E (eV)	Our results	[8]
5.0	3.40	2.87	1.0	3.05	1.43
3.0	3.17	2.12	0.1	3.16	2.00
2.0	3.12	1.76	0.04	3.50	2.94

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

	${}^3\text{He}^{++}$	[11]	${}^4\text{He}^{++}$	[11]	${}^6\text{Li}^{+++}$	${}^7\text{Li}^{+++}$
p^+	7.25	6.3	6.65	5.5	1.72	1.67
d^+	4.77	1.3	4.17	1.0	1.01	0.96

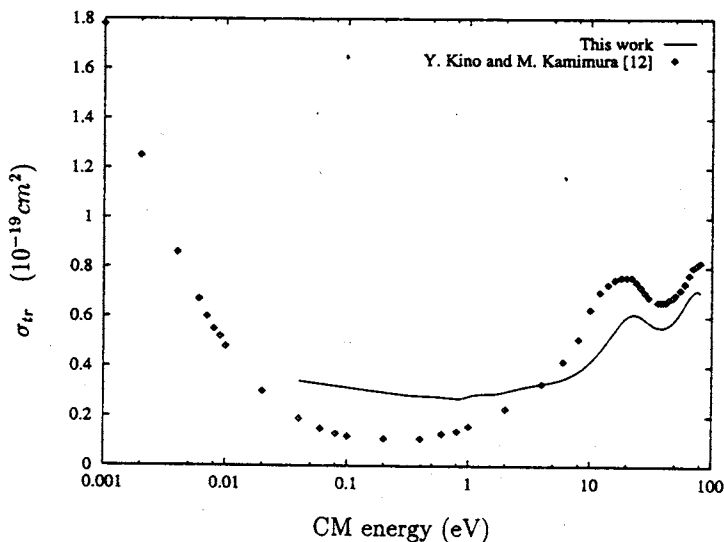


Fig.2. Cross section of the reaction $d\mu + t \rightarrow t\mu + d$

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

E (eV)	Our results	[13]	E (eV)	Our results	[13]
10.0	3.73		1.0	4.95	4.54
5.0	4.10	3.72	0.22	5.60	5.18

Figure 2 shows our $d\mu + t \rightarrow t\mu + d$ cross sections compared with variational calculations [12] 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.

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 ${}^6\text{Li}$ or ${}^7\text{Li}$ 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



In Table 3 our results are compared with calculations based on the Born–Oppenheimer approximation [13]. 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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