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# MUON TRANSFER RATES IN COLLISIONS
# OF HYDROGEN ISOTOPE MESIC ATOMS
# ON "BARE" NUCLEI.
# MULTICHANNEL ADIABATIC APPROACH

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## Introduction

Low-energy collision problem of Coulomb three-body system with comparable masses plays an important role in description of muonic atom diffusion during $\mu CF$ cycle. Because of the smallness of a mesic atom with respect to the electron structure of molecules in a hygrogen isotope mixture it is possible to neglect the electron screening effects in the first order of approximation and to consider the scattering of mesic atoms on *bare* nuclei. In this case the following reactions are available:
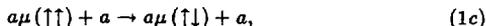
a) elastic scattering

$$a\mu + b \rightarrow a\mu + b, \tag{1a}$$

b) isotope exchange

$$a\mu + b \rightarrow b\mu + a, \tag{1b}$$

c) spin-flip

$$a\mu(\uparrow\uparrow) + a \rightarrow a\mu(\uparrow\downarrow) + a, \tag{1c}$$

where $a$ and $b$ denote hydrogen isotope nuclei $p$, $d$ and $t$. It is clear now that the stage starting from the formation of a mesic atom and ending in the mesic molecule formation, where the above-mentiond collisions occur, demands a precise theoretical investigation[1]. The scope of this study is restricted to the consideration of reactions involving atoms in their ground states.

From the numerical point of view, the most difficult and challenging problem in mesic atomic scattering is an isotope exchange reaction. The muon-nucleus mass ratio is signifi-

cantly greater than that of an ordinary atom, so the standard adiabatic two-level approximation cannot provide sufficient accuracy of a three-body wave function. On the other hand, the great magnitude of isotope splitting in energy levels of mesic atoms involved into the reaction makes direct numerical methods rather complicate due to a difference in energy scales (see Fig.1) for upper (colliding energy $\sim$0.04eV) and lower ($\sim 50 \div 200$eV) channels (isotopic energy splitting for mesic molecules $p\mu$, $d\mu$ and $t\mu$ is shown in Table 1). The period of oscillation for these two open channels differs by the several orders of magnitude one from another.

**Table 1.** Isotopic energy splitting

|  | $\Delta E_{\text{iso}}(\text{eV})$ |
|---|---|
| $E_{d\mu} - E_{p\mu}$ | 134.709 |
| $E_{t\mu} - E_{p\mu}$ | 182.751 |
| $E_{t\mu} - E_{d\mu}$ | 48.042 |

This paper presents the multi-level adiabatic calculation of the muon transfer rates. We consider the convergence of the computed figures with respect to the number of states that ensured us that the high accuracy results are achieved. It is perfectly seen that the contribution of the continuous spectrum into the charge transfer rate are of significant amount to be neglected. The convergence analysis allows us to demand that these new calculated results are most accurate up to date. The described method was successfully applied to compose the Atlas of elastic and inelastic cross sections of asymmetric mesic atomic processes[2]. It can be regarded as a further extension of our multi-level adiabatic approach given in Ref. 3 and Ref. 4 to the asymmetrical case of mesic atomic collisions.

For very low incident energies (0.001–0.01eV) the cross section of charge transfer process becomes sensitive to the influence of the molecular structure. To achieve the demanded

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accuracy in this case we have to take into consideration the electron screening and other molecular effects. These corrections were carried out and are now available in Ref. 5.

## 1. Multichannel adiabatic expansion

After separating of the center-of-mass motion, the nonrelativistic Hamiltonian of a three-particle system can be written in Jacobian coordinates ($e = \hbar = m_e = 1$)

$$
\begin{aligned}
H = -\frac{1}{2M_{ab}}\Delta_{\mathbf{R}} - \frac{1}{2m_{ab}}\Delta_{\mathbf{r}} - \frac{1}{r_a} - \frac{1}{r_b} + \frac{1}{R}, \\
M_{ab}^{-1} = M_a^{-1} + M_b^{-1}, \\
m_{ab}^{-1} = m_\mu^{-1} + (M_a + M_b)^{-1},
\end{aligned}
\tag{2}
$$

where $\mathbf{R}$ is the position vector of nucleus $a$ relative to nucleus $b$ with the masses $M_a$ and $M_b$, $\mathbf{r}$ is the position vector of the muon with mass $m_\mu$ relative to the center of mass of the nuclei, $r_a$ and $r_b$ are the relative muon nucleus distances.

The multichannel adiabatic approach is based on an expansion of the three-body wave function $\Psi(\mathbf{r}, \mathbf{R})$ in terms of the states of the discrete and continuous spectra of the two-center problem[6]:

$$
\begin{aligned}
\left\{ -\frac{1}{2}\Delta_{\mathbf{r}} - \frac{1}{r_a} - \frac{1}{r_b} \right\} \phi_j(\mathbf{r}; R) = E_j(R)\, \phi_j(\mathbf{r}; R), \\
\left\{ -\frac{1}{2}\Delta_{\mathbf{r}} - \frac{1}{r_a} - \frac{1}{r_b} \right\} \phi_c(\mathbf{r}; R, k) = (k^2/2)\, \phi_c(\mathbf{r}; R, k),
\end{aligned}
\tag{3a}
$$

where variables can be separated in spheroidal coordinates:

$$
\xi = (r_a + r_b)/R, \quad \eta = (r_b - r_a)/R, \quad \varphi = \arctan x/y.
$$

Functions $\phi_j$ and $\phi_c$ are numbered by respective sets $j = \{\tau q m\}$ and $c = \{q m\}$ of spheroidal quantum numbers

$$
\begin{aligned}
\phi_j(\mathbf{r}) = \Pi_\tau^{(m)}(\xi)\, \Xi_q^{(m)}(\eta) \exp im\varphi, \\
\phi_c(\mathbf{r}; k) = \Pi^{(m)}(\xi; k)\, \Xi_q^{(m)}(\eta; k) \exp im\varphi,
\end{aligned}
\tag{3b}
$$

where $\tau$ and $q$ are equal to the number of nodes of corresponding Coulomb spheroidal radial and angular functions[7]. It is worthy to note that oddness of a quantum number $q$ defines symmetry (with respect to inversion: $\mathbf{r} \to -\mathbf{r}$) of solutions and after transformation:

$$
\psi_{ia} = \frac{1}{\sqrt{2}} \left( \phi_{\tau,2k,m} + \phi_{\tau,2k+1,m} \right), \qquad \psi_{ib} = \frac{1}{\sqrt{2}} \left( \phi_{\tau,2k,m} - \phi_{\tau,2k+1,m} \right),
$$

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in the limit of $R \to \infty$ the wave functions become respectively the states of $(a, e)$ and $(b, e)$ atoms in parabolic coordinates[7]. In another limit case of $R \to 0$ the wave functions can be described by the states of the helium ion $He_\infty^+$ with the spherical quantum numbers: $N = \tau + q + m$, $l = q + m$ and $m$.

To describe the rotational movement of nuclei we make use of Wigner $D$-functions which define a wave function with a certain total angular momentum $J$, its projection $M$ onto $z$-axis and spatial parity $\lambda$ ($P_\lambda$: $\Psi(r, R) = \lambda \Psi(-r, -R)$),

$$
\begin{aligned}
\Psi_M^{J\lambda}(\mathbf{R}, \mathbf{r}) = \sum_{j'm} \psi_{j'm}(\gamma \mathbf{r}; R) R^{-1} \chi_{j'm}(R) \mathcal{D}_{Mm}^{J\lambda}(\Phi, \Theta, 0) + \\
+ \sum_{c'm} \int_k dk \psi_{c'm}(\gamma \mathbf{r}; R, k) R^{-1} \chi_{c'm}(R; k) \mathcal{D}_{Mm}^{J\lambda}(\Phi, \Theta, 0),
\end{aligned}
\tag{4}
$$

]

where $\Phi$ and $\Theta$ are polar angles of $\mathbf{R}$ and $\mathcal{D}_{Mm}^{J\lambda}(\Phi, \Theta, \varphi)$ are symmetrized $D$-functions (see Ref. 6 or Ref. 8). The two-center problem (3) is formulated in terms of electronic movement around nuclei of infinite mass. The scaling factor $\gamma$ converts the solutions of (3) to muonic measures. So the value $\gamma_a = (M_a + m_\mu)/(M_a m_\mu)$ provides a muonic wave function which for $R \to \infty$ transfers simply to a state of $a\mu$ atom. The use of $\gamma_a$ leads to the correst energy threshold in an $a\mu + b$ channel.

Substitution of the expansion (4) into the Schrödinger three-body equation and averaging over the light particle motion ($\mathbf{r}$) and angular coordinates ($\Phi, \Theta$) gives the system of coupled radial equations for the amplitudes $\chi_i$ describing the relative motion of the nuclei:

$$
\begin{aligned}
\frac{d^2}{dR^2} \chi_i(R) + \left[ 2M\varepsilon - \frac{J(J+1)}{R^2} \right] \chi_i(R) - \sum_j U_{ij}(R) \chi_j(R) \\
- \sum_j \int_k dk \, U_{ij}(R, k) \chi_j(R, k) = 0,
\end{aligned}
\tag{5}
$$

where $M = M_{ab}/m_{a\mu} = M_{ab}(M_a + m_\mu)/(m_\mu M_a)$ is the reduced mass of the system and $\varepsilon$ is an incident energy of colliding particles in the body-frame coordinates. The matrix elements $U_{ij}(R)$ are effective potentials of the problem,

$$
U_{ij}(R) = 2Q_{ij}(R) \frac{d}{dR} + \left[ \frac{dQ_{ij}}{dR}(R) + H_{ij}(R) \right],
$$

which obey the symmetry conditions

$$
Q_{ij} = -Q_{ji}, \qquad H_{ij} = H_{ji},
$$

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The effective potentials were calculated and tabulated in works[9,10] within the range of $R = 0.1 \div 100$ for the discrete and continuous spectra respectively. For $R \ll 1$ and $R \gg 1$ analytical expressions of potentials are available[11,6].

## 2. Formulation of the scattering problem

The disadvantages of the two-level adiabatic PSS method (keeping only two ground states of expansion (4)) are well known (see, for example, Ref. 12). It gives incorrect isotope splitting between energy thresholds of channels $a\mu + b$ and $b\mu + a$, what follows from the fact that the adiabatic wave function in the limit of $b\mu + a$ dissociation is the same as for the $a\mu$ atom. Several attempts were made to overcome this difficulty in a framework of two-level approximation. We point out on two most recent investigations dealing with muonic atom scattering problem[13,14].

Another serious objection is an improper mass of compound particles involved into reaction. Indeed, the reduced mass $M = M_{ab}/m_{a\mu}$ of the reaction $(m_{a\mu}^{-1} = M_a^{-1} + m_\mu^{-1})$ is the same for both channels $a\mu + b$ and $b\mu + a$ and differs from their genuine values

$$\mathcal{M}_a = \left[ M_b \left( M_a + m_\mu \right) / \left( M_a + M_b + m_\mu \right) \right] / m_{a\mu}$$

and

$$\mathcal{M}_b = \left[ M_a \left( M_b + m_\mu \right) / \left( M_a + M_b + m_\mu \right) \right] / m_{b\mu}.$$

This fault rises from the strong coupling of the states by the velocity-dependent potential $Q\left(R\right) d/dR$ which doesn't vanish at the infinity. That can be easily seen with the use of the asymptotic expansion of $a\mu + b$ channel solution

$$\Psi\left(\mathbf{R}, \mathbf{r}\right) = \sum_i \psi_{ia}\left(\mathbf{r}_a\right) \chi_a\left(\mathbf{R}\right), \qquad \mathbf{r}_a = \mathbf{r} + \frac{M_b}{M_a + M_b}\mathbf{R}.$$

After inserting it into the Schrödinger equation

$$\left\{ -\frac{1}{2M_{ab}}\Delta_{\mathbf{R}} - \frac{1}{2m_{a\mu}}\Delta_{\mathbf{r}} - \frac{1}{M_a}\nabla_{\mathbf{R}}\nabla_{\mathbf{r}_a} + V\left(R, r_a, r_b\right) \right\}\Psi = \varepsilon\Psi,$$

we get

$$Q^{(a)}\left(\infty\right) = \langle\psi_{ia}|\frac{M_{ab}}{M}\nabla_{\mathbf{r}_a}|\psi_{ja}\rangle.$$

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The roots of this effect are based on the translation of the Jacoby vector $\mathbf{R_a}$ of the system $(a\mu) - b$ which correctly describes the relative motion of two compound particles, and in terms of which the scattering problem is formulated into the internuclear vector $\mathbf{R} = \mathbf{R_a} + p_a\mathbf{r_a}$ (see Fig.2). In this case an asymptotic solution transforms

$$\Psi^{(\pm)}\left(\mathbf{R_a}, \mathbf{r_a}\right) \sim \exp\left(\pm i k \mathbf{R_a}\right)\psi_{ia}\left(\mathbf{r_a}\right) = \exp\left(\pm i k \mathbf{R}\right)\bar{\psi}_{ia}^{\pm}\left(\mathbf{r_a}\right),$$

where

$$\bar{\psi}_{ia}^{\pm}\left(\mathbf{r_a}\right) = \exp\left(\mp i p_a \mathbf{k} \mathbf{r_a}\right)\psi_{ia}\left(\mathbf{r_a}\right),$$

and $p_a = m_\mu/\left(m_\mu + M_a\right)$ is a translational parameter. Bates and McCarroll have suggested simply to include this translational factor into the trial function of the expansion[15] in order to avoid this spurious mass transformation. But it leads to an energy dependent correction to the effective potentials.

Instead of that, the successive usage of the multichannel approach provides solutions of the scattering problem which converge to the genuine solution of the original three-body problem. Indeed, the scattering states $\bar{\psi}_{ia}$, $\bar{\psi}_{ib}$ of both atoms can be approximated with any given accuracy by the complete basis set of adiabatic states (3), so any sufficiently large finite basis set provides an equation which has correct (within the given accuracy) thresholds and masses of compound particles.

Let us introduce here the functions

$$\Psi_{i\sigma}^{(\pm)}\left(\mathbf{R}, \mathbf{r}\right) = \Psi_{i\sigma}^{(\pm)}\left(\mathbf{R}_\sigma, \mathbf{r}_\sigma\right) = e^{\pm k_i R_\sigma} R^{-1}\psi_{i\sigma}\left(\mathbf{r}_\sigma\right)\mathcal{D}_{Mm}^{J\lambda}\left(\Phi, \Theta, 0\right) =$$
$$= \sum_{j\rho}\chi_{j\rho}^{\pm|i\sigma\rangle}\left(R\right)R^{-1}\psi_{j\rho}\left(\mathbf{r}_\rho\right)\mathcal{D}_{Mm}^{J\lambda}\left(\Phi, \Theta, 0\right),$$

where $\sigma, \rho = \{a, b\}$ are indexes of dissociation channels and

$$\chi_{j\rho}^{\pm|i\sigma\rangle}\left(R\right) = \langle\psi_{j\rho}\mathcal{D}_{Mm'}^{J\lambda}|\exp\left(\mp i p_\sigma \mathbf{k}_i \mathbf{r}_\sigma\right)\psi_{i\sigma}\mathcal{D}_{Mm}^{J\lambda}\rangle\, e^{\pm i k_i R}$$

are components of the radial wave function. In what follows we assume that the wave numbers $k_j$ for open channels are real and positive. In terms of this functions we can define asymptotic boundary condition for the scattering problem

$$\Psi^{(i)}\left(\mathbf{R}, \mathbf{r}\right) \sim v_i^{-1/2}\Psi_i^{(-)}\left(\mathbf{R}, \mathbf{r}\right) - \sum_{j=1}^{m} S_{ij}v_j^{-1/2}\Psi_j^{(+)}\left(\mathbf{R}, \mathbf{r}\right), \tag{6}$$

where $v_j = \hbar k_i/m_i$ are velocities of incident and scattered particles of different channels, $m$ is the number of open channels and quantities $S_{ij}$ define the $S$-matrix of the reaction. The asymptotic states of adiabatic expansion contain the states of isolated atom described in parabolic quantum numbers and having the mixture of rotational states with respect to the nucleus-atom orbital momentum. That is why we don't use the constant phase shifts of partial waves in expressions of asymptotic functions. From the other side, they can be easily included directly into the $S$-matrix of the reaction after calculations.

The wave functions $\Psi^{(\pm)}$ expressed in terms of expansion (4) provide the multicomponent asymptotical boundary condition for the radial Schrödinger equation (5)

$$\chi^{(i)}(R) \sim \sum_j v_j^{-1/2} \left\{ \mathbf{c}^{(j)} e^{-ik_j R} \delta_{ij} - \mathbf{d}^{(j)} e^{ik_j R} S_{ij} \right\}, \tag{7}$$

and

$$c_l^{(j)} = d_l^{(j)^*} = \langle \psi_l \mathcal{D}_{Mm'}^{J\lambda} | e^{ip_j \mathbf{k}_j \mathbf{r}_j} \psi_j \mathcal{D}_{Mm}^{J\lambda} \rangle$$

that reduces the initial scattering problem to the solution of the infinite system of second order differential equations with linear boundary conditions at $R = 0$ (where $\chi_i(0) = 0$) and in the infinity. Thus, so far we made no any approximation assumption, then Eq. (5) with Eq. (7) provides the exact solution of the problem.

Truncation of the system of equations (5) to some finite $N$-component set gives slightly different values of the wave number $k_i^{(N)}$ and vectors $\mathbf{c}^{(i,N)}$ and $\mathbf{d}^{(i,N)}$ if we demand that asymptotic solution should satisfy the truncated asymptotic equation

$$\left\{ -\frac{d^2}{dR^2} + 2Q^{(N)}(\infty)\frac{d}{dR} + H^{(N)}(\infty) - 2M\varepsilon \right\} \chi^{\pm|i)}(R) = 0.$$

The asymptotic solution has a form $\chi^{+|i)}(R) \sim \mathbf{d}^{(i)} \exp ik_i R$, thus, inserting it into the last equation we can obtain these quantities as non-zero solutions of the following algebraic equation

$$\left[ k_i^2 + 2ik_i Q^{(N)}(\infty) + H^{(N)}(\infty) - 2M\varepsilon \right] \mathbf{d}^{(i)} = 0, \tag{8}$$

where we have one parameter free to determine a solution uniquely. We can define

$$d_i^{(i)} = \langle \psi_i \mathcal{D}_{Mm}^{J\lambda} | e^{\mp ip_i \mathbf{k}_i \mathbf{r}_i} \psi_i \mathcal{D}_{Mm}^{J\lambda} \rangle. \tag{9}$$

The only undefined values now are the velocity coefficients in Eq. (6) which have the meaning of the factors making the flows of particles of incoming and outgoing waves balanced.

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To calculate the number of particles incoming and outgoing the region of interaction we make use of the density operator of particle flux[16]

$$v_i^{(N)} = -i \oint_S dS \left[ - (\chi^* \nabla_{\mathbf{R}} \chi - \chi \nabla_{\mathbf{R}} \chi^*) + (\chi^* Q \chi - \chi Q \chi^*) \right],$$

where $S$ is the spherical surface of constant radius $R$ bounded the interaction region. For the stationary asymptotic solutions $\chi^{+|i)}(R) \sim \mathbf{d}^{(i,N)} \exp(ik_i R)$ we get

$$v_i^{(N)} = \|\chi^{+|i)}\|_Q^2 = \left| k_i \|\mathbf{d}^{(i,N)}\|^2 - i \left( \mathbf{d}^{(i,N)}, Q\mathbf{d}^{(i,N)} \right) \right|.$$

This sequence of definitions allows us to build new boundary conditions for the truncated system of radial Schrödinger equations:

$$\chi^{(i,N)}(R) \sim \sum_{j=1}^{m} \left[ v_j^{(N)} \right]^{-1/2} \left\{ \mathbf{c}^{(j,N)} e^{-ik_j R} \delta_{ij} - \mathbf{d}^{(j,N)} e^{ik_j R} S_{ij}^{(N)} \right\}, \tag{10}$$

which are from the one side self-consistent (by means of the truncated asymptotic solution) and from the other side closely related to the one of the original three-body problem. The completeness of the adiabatic basis allows us to assert that these quantities describing the asymptotic wave function of the truncated system converge to their correct values as the number of states of expansion (4) will be increased.

Some problems will arise with involving into consideration of continuous spectrum due to inasymptotic behaviour of continuous spectrum states. We could refer our readers to Ref. 17 where a detailed and complete discussion of how to overcome this problem is presented.

For numerical calculations it is more convenient to use real functions with real boundary conditions. To achieve that we can perform asymptotic solutions in a form of "standing waves"

$$\chi_i^{(1)} = \frac{1}{2i} \left( \chi^{+|i)} - \chi^{-|i)} \right),$$
$$\chi_i^{(2)} = \frac{1}{2} \left( \chi^{+|i)} + \chi^{-|i)} \right).$$

For these functions a common asymptotic solution can be expressed in terms of the reactance matrix $K$:

$$\chi(i) \sim \chi_i^{(1)} - \sum_{j=1}^{m} K_{ij} \chi_j^{(2)}, \tag{11}$$

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and it is well known that matrix $K$ is real and symmetric[18]. The $S$-matrix can be expressed

$$S = (I + iK)(I - iK)^{-1},$$

where the identity matrix $I$ is used.

For the case of the muon transfer from the ground states (the reaction (1b)) we have two open channels and the partial cross sections $\sigma_{ab}^J$ are calculated by the formulas

$$\sigma_{ab}^J = \frac{\pi}{k_a^2}(2J + 1)|S_{ab}^J|^2,$$

where $k_a$ is the wave number of the incident channel $(a\mu) + b$ and the total cross section is simply a sum of all partial cross sections

$$\sigma_{ab} = \sum_J \sigma_{ab}^J.$$

## 3. Results

The method we have expounded above was applied to the calculation of the cross sections of the reaction (1b) and the rates of muon transfer from a lighter to a heavier nucleus in a liquid hydrogen mixture. In the calculations we made use of the set of physical constants that is collected in Table 2.

The following model of interaction was taken into consideration (see Fig.3): the complete set of potentials connecting the states of the first three shells of the discrete spectrum, then potentials connecting the states of the first shell with the fourth shell of the discrete spectrum and with the set of shells of continuous spectrum. These shells consist of the states of two-body problem as follows:

discrete spectrum:

1-st shell: $1s\sigma - 2p\sigma$ (when $R \to 0$) or $1s$ (when $R \to \infty$);

2-nd shell: $2s\sigma - 3p\sigma, 3d\sigma - 4f\sigma, 2p\pi - 3d\pi$ (when $R \to 0$) or $2s, 2p_0, 2p_1$ (when $R \to \infty$);

3-d shell: $3s\sigma - 4p\sigma, 4d\sigma - 5f\sigma, 5g\sigma - 6h\sigma, 3p\pi - 4d\pi, 4f\pi - 5g\pi, 3d\delta - 4f\delta$ (when $R \to 0$)
or $3s, 3p_0, 3p_1, 3d_0, 3d_1, 3d_2$ (when $R \to \infty$)...

continuous spectrum:

1-st shell: $s\sigma - p\sigma, p\pi - d\pi$ (when $R \to 0$);

2-nd shell: $d\sigma - f\sigma, f\pi - g\pi$ (when $R \to 0$);

3-d shell: $g\sigma - h\sigma, h\pi - i\pi$ (when $R \to 0$)...

The other potentials can be neglected in a view of the adiabatic smallness of their influence on the final result.

To get rid of the integral part of the radial Schrödinger equation (5) we have discretized the continuous spectrum parameter $k \to k_\alpha = 0.1\,(0.1)\,3.0\,(0.5)\,10$ (44 points for every state $(lm)$) and have used the Simpson quadrature rule for an approximation of the last term in Eq. (5). The method of the numerical integration of a finite component radial equation with the boundary conditions (10) is described in Ref. 19.

Table 3 shows the convergence of the method for the special case of $S$-wave scattering of atom $d\mu$ on $t$ for different values of incident energy. We deliberately regard the case of the $S$-wave scattering because it yields the major contribution into the total cross section within the range of thermal energies in $\mu CF$. Practical calculation also depends on some other parameters like a step $h$ of the difference scheme of the numerical integration or a point $R_{as}$ which divides the space into an interaction domain and an asymptotic region or $R_c$ (see Ref. 17) defining the origin of asymptotic corrections of continuous spectrum and so on. We have carefully investigated these potential sources of numerical errors and come to conclusion that our results with four significant figures presented in Table 3 do not depend on variations of $R_{as}$ and $R_c$ and the error of numerical integration of the system which includes four shells of discrete and five shells of continuous spectra is about $10^{-4}$. So this investigation shows that our results presented in the paper are the most accurate up to the date and we estimate the error bounds of about 2% for $d\mu + t \to t\mu + d$ reaction and $\sim 3\%$ for $p\mu + d \to d\mu + p$ and $p\mu + t \to t\mu + p$.

Tables 4 and 5 summarize results of our calculations presenting the cross sections of the considered reactions and the transfer rate in the liquid hydrogen mixture. To calculate the transfer rate of the muon we make use of the formula

$$\lambda = \sigma_{ab} v N_0,$$

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where $N_0 = 4.25 \times 10^{22} \text{cm}^{-3}$ is the liquid hydrogen density and $v$ is the velocity of the incident atom (in the center-of-mass coordinates)

$$v = \sqrt{\frac{2\varepsilon}{M_{(a\mu)b}}} \, (\text{cm/s}) = c \sqrt{\frac{2\varepsilon \, (\text{eV})}{\left[M_{(a\mu)b}c^2\right](\text{eV})}}, \qquad M_{(a\mu)b} = \frac{(M_a + m_\mu) \, M_b}{M_a + M_b + m_\mu},$$

where $c = 2.9979 \times 10^{10} \, (\text{cm/s})$, $m_e c^2 = 0.511003 \times 10^6 \, (\text{eV})$.

## 4. Conclusions and perspectives

As we mention in introduction, the obtained results should be corrected within the range of low energies by taking into account the molecular structure of hydrogen isotope molecules $H_2$, $D_2$ and so on. This work involves rather different calculational technique to be included here and was carried out elsewhere[5]. This last reference contains also detailed comparison of our results with the different previous calculations. We would like to point out that the major part of these calculations has been used in the adiabatic *two-level* approximation or some of its modifications. The earliest multi-level investigations of these reactions could be found in Ref. 4 and Ref. 20. We think that these accurate results will give new impulse to the development of the theory describing time-dependent diffusion processes of mesic atoms in hydrogen isotope mixture.

The other reaction having a great effect on mesic atom diffusion is the charge transfer process from the excited states:

$$(a\mu)_n + b \rightarrow (b\mu)_n + a, \qquad n \geq 2.$$
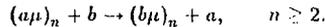
It is not sufficient for this problem to keep only pure Coulombic interaction which leads to degeneracy of energy levels in atomic states and to $\sim 1/\varepsilon$ threshold behaviour of charge transfer cross section. We also need to take into account the vacuum polarization and hyperfine structure corrections for getting relevant results. This perspective work is in progress now.
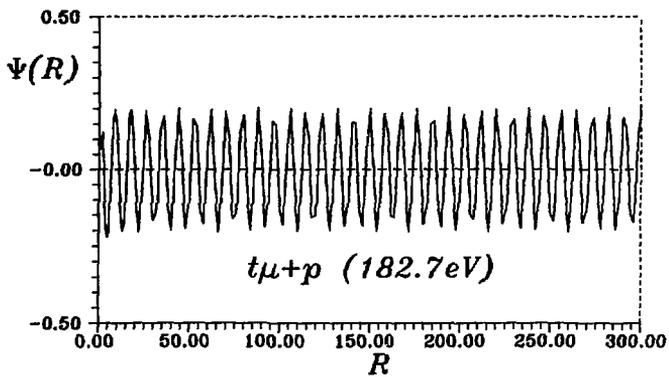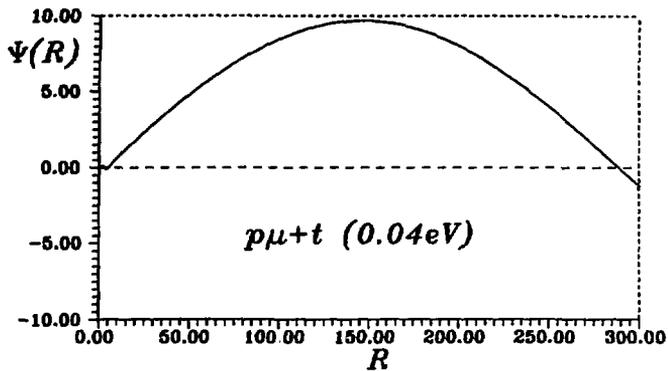
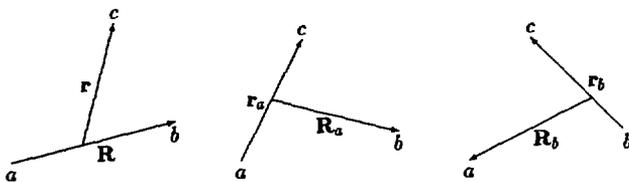Fig.1 Elastic and inelastic channel wave functions in the reaction $p\mu + t \rightarrow t\mu + p$.



Fig.2 Different definitions of the three-body Jacoby coordinates.

**Table 2.** Masses (in $m_e$), Rydberg energy (in eV) and ground state energies of mesic atoms (in eV)

|  | $E_{a\mu}(eV)$ |
|---|---|
| $m_p = 1836.1515$ | $E_{p\mu} = 2528.517$ |
| $m_d = 3670.481$ | $E_{d\mu} = 2663.226$ |
| $m_t = 5496.918$ | $E_{t\mu} = 2711.268$ |
| $m_\mu = 206.7686$ |  |
| $Ry = 13.6058041$ |  |

**Table 3.** Convergence of the charge transfer cross section $\sigma_{dt}$ $(10^{-20} \text{cm}^2)$ for $S$-wave $d\mu + t \rightarrow t\mu + d$ scattering and different incident energies (in brackets the number of channels is shown)

| number of shells | | 0.01eV | 0.04eV | 0.1eV |
|---|---|---|---|---|
| discrete spectrum | continuous spectrum |  |  |  |
| 1 [2] | – | 1.209 | 0.596 | 0.369 |
| 2 [6] | – | 3.215 | 1.583 | 0.980 |
| 3 [12] | – | 3.440 | 1.694 | 1.047 |
| 4 [20] | – | 3.498 | 1.722 | 1.065 |
| 4 [20] | 1 [+88] | 3.998 | 1.965 | 1.217 |
| 4 [20] | 2 [+176] | 4.129 | 2.029 | 1.257 |
| 4 [20] | 3 [+264] | 4.375 | 2.148 | 1.329 |
| 4 [20] | 4 [+352] | 4.381 | 2.154 | 1.333 |
| 4 [20] | 5 [+440] | 4.376 | 2.150 | 1.329 |

**Table 4.** A summary of cross section results $\sigma_{ab}$ $(10^{-20} \text{cm}^2)$ for the low energy scattering of hydrogen isotope mesic atoms

| $\varepsilon(eV)$ | $p\mu + d \rightarrow d\mu + p$ | $p\mu + t \rightarrow t\mu + p$ | $d\mu + t \rightarrow t\mu + d$ |
|---|---|---|---|
| 0.001 | 723.8 | 347.0 | 13.94 |
| 0.01 | 226.7 | 109.1 | 4.490 |
| 0.04 | 111.6 | 54.10 | 2.380 |
| 0.1 | 69.45 | 33.97 | 1.693 |
| 0.4 | 33.78 | 17.16 | 1.376 |
| 1.0 | 21.51 | 11.64 | 1.646 |
| 10.0 | 9.467 | 6.842 | 6.817 |
| 50.0 | 6.374 | 4.649 | 5.256 |
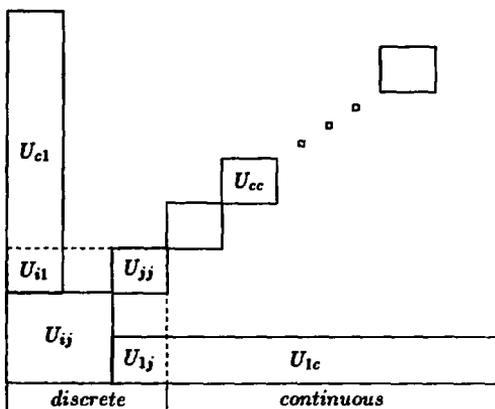
**Fig.3** The scheme of effective potentials taken into account in adiabatic calculations.

**Table 5.** A summary of results for low energy isotope exchange rates of hydrogen isotope mesic atoms $\lambda = \sigma_{ab} v N_0 \left(10^9 \text{s}^{-1}\right)$

| $\varepsilon$(eV) | $p\mu + d \rightarrow d\mu + p$ | $p\mu + t \rightarrow t\mu + p$ | $d\mu + t \rightarrow t\mu + d$ |
|---|---|---|---|
| 0.001 | 15.9 | 7.17 | 0.233 |
| 0.01 | 15.8 | 7.13 | 0.238 |
| 0.04 | 15.5 | 7.07 | 0.252 |
| 0.1 | 15.3 | 7.02 | 0.283 |
| 0.4 | 14.9 | 7.09 | 0.460 |
| 1.0 | 15.0 | 7.61 | 0.871 |
| 10.0 | 20.9 | 14.1 | 11.4 |
| 50.0 | 31.4 | 21.5 | 19.7 |

## References

1. L.I. Ponomarev, Contemporary Physics, **31** (1991)219.

2. C. Chiccoli *et al.*, Muon Catalysed Fusion, **7** (1992)87.

3. V.S. Melezhik, L.I. Ponomarev and M.P. Faifman, Sov. Phys. JETP, **58** (1983)254; V.S. Melezhik, J. Comp. Phys., **65** (1986)1; V.S. Melezhik, Muon Catalyzed Fusion, **2** (1988)117.

4. V.S. Melezhik and J. Wozniak, Phys. Lett. A,**116** (1986) 370; L. Bracci *et al.*, Phys. Lett. A, **134** (1989)435; L.Bracci *et al.*, Muon Catalyzed Fusion, **5/6** (1990)21; L.Bracci *et al.*, Muon Catalyzed Fusion, **4** (1989)247.

5. A. Adamczak *et al.*, Phys. Lett. B, 285 (1992)319.

6. S.I. Vinitsky and L.I. Ponomarev, Sov. J. Part. Nucl., **21** (1982)557.

7. I.V. Komarov, L.I. Ponomarev and S.Yu. Slavyanov, *Spheroidal and Coulomb Spheroidal Functions*, (Nauka, Moscow, 1976).

8. V.I.Korobov, I.V. Pusynin and S.I. Vinitsky, Muon Catalysed Fusion, **7** (1992)63.

9. L.I. Ponomarev, T.P. Puzynina, N.F. Truskova, J. Phys. B, **11** (1978)3861.

10. D.I. Abramov, V. Gusev, Preprint IHEP, 84-148, Protvino, 1984; D.I. Abramov and V.V. Gusev, J. Phys. B, **23** (1990)1467.

11. M.P. Faifman, L.I. Ponomarev, S.I. Vinitsky, J. Phys. B, **9** (1976)2255.

12. J.B. Delos, Rev. Mod. Phys., **53** (1981)287.

13. M. Bubak and M.P. Faifman, Preprint JINR E4-87-464, Dubna, 1987.

14. J.S. Cohen and M. Struensee, Phys. Rev. A, **43** (1991) 3460; J.S. Cohen, ibid., 43 (1991)4668.

15. D.R. Bates, R. McCarroll, Proc. R. Soc. A, **245** (1958)175.

16. V.I. Korobov, Preprint JINR, E4-92-356, Dubna; Submitted to J. Phys B.

17. L. Bracci *et al.* Il Nuovo Cimento, **105** (1990) 459.

18. A.I. Bas', Ja.B. Zel'dovich, A.M. Perelomov, *Scattering, Reactions and Decays in Nonrelativistic Quantum Mechanics*, (Nauka, Moscow, 1971).

19. V.I. Korobov, Preprint JINR, E11-92-357, Dubna; Submitted to J. Comp. Phys..

20. M. Kamimura, Muon Catalyzed Fusion, **3** (1988)335.

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Коробов В.И., Мележик В.С., Пономарев Л.И.                E4-92-358
Скорость перезарядки мюона в столкновениях
мезоатомов изотопов водорода на "голых" ядрах.
Многоканальный адиабатический подход

Численная схема решения проблемы медленных столкновений
в рамках адиабатического подхода задачи трех тел применяется
для вычисления скоростей перезарядки мюона в столкновениях
атомов изотопов водорода на голых ядрах. Показывается, что мно-
гоканальный адиабатический подход позволяет достичь высокой
точности ($\sim$ 3%) в вычислениях сечений процессов перезарядки,
которая является наилучшей в настоящее время. Метод применим
в широком диапазоне энергий (0.001 — 50 эВ), представляющих
интерес для анализа экспериментов мюонного катализа.

Korobov V.I., Melezhik V.S., Ponomarev L.I.                E4-92-358
Muon Transfer Rates in Collisions of Hydrogen Isotope
Mesic Atoms on "Bare" Nuclei.
Multichannel Adiabatic Approach

A numerical scheme for solving the problem of slow collisions in
the three-body adiabatic approach is applied for calculation of muon
transfer rates in collisions of hydrogen isotope atoms on bare nuclei.
It is demonstrated that the multichannel adiabatic approach allows one
to reach high accuracy results ( $\sim$ 3%) estimating the cross sections of
charge transfer processes which are the best ones up to date. The me-
thod is appliable in a wide range of energies (0.001 — 50 eV) which is
of interest for analysis of muon catalysed fusion experiments.

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