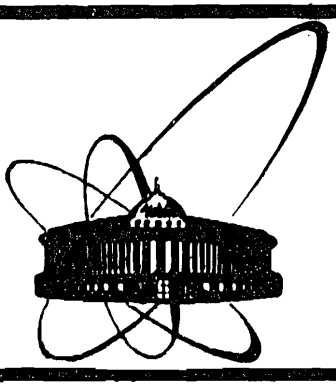

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LOW ENERGY SCATTERING OF MUONIC HYDROGEN ON HYDROGEN MOLECULES

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1. Cross sections of muonic hydrogen scattering are needed in the kinetic of muon catalyzed fusion [1] and in the measurements of muon nuclear capture rate by proton in a gaseous hydrogen [2]. To obtain these cross sections we use the elastic cross sections of muonic hydrogen scattering on nuclei of hydrogen isotopes [3] calculated in the framework of the adiabatic representation [4]. Effects of bonding of hydrogen nuclei in the molecule have been discussed in [5] and more precisely in [6] following the Fermi approach [7]. It has been shown in [8] and [9] that the electron screening is significant for muonic hydrogen scattering on hydrogen atoms at collision energies below 1 eV. Therefore, this effect should also be included in calculations of scattering on molecules. Moreover, an influence of the resonant formation of $dd\mu$ and $dt\mu$ muonic molecules on the discussed cross sections should be estimated.

2. Let us consider the scattering of a muonic atom $(a\mu)$ on a molecule consisting of nuclei b and c and of two electrons, where a,b,c denote any hydrogen isotopes. Let the masses of the muon and the nuclei be m_μ, M_a, M_b, M_c, respectively. The reduced mass of $(a\mu)$ equals m_a. It is assumed that an interaction of $(a\mu)$ and the molecule is described by the potential

$$V(\vec{r},\vec{R}) = V_n(\vec{r},\vec{R}) + V_e(\vec{r},\vec{R}). \qquad (1)$$

The vector $\vec{r}$ connects the centres of mass of both the systems and $\vec{R} = \vec{r}_c - \vec{r}_b$, where $\vec{r}_c$ and $\vec{r}_b$ are the positions of nuclei b,c. The $(a\mu)$ – nuclei interaction is given, according to the Fermi method [7] by the potential V_n ($\hbar = e = m_a = 1$)

$$V_n(\vec{r},\vec{R}) = \frac{2\pi}{\mu_b}\lambda_b\delta(\vec{r}-\vec{r}_b) + \frac{2\pi}{\mu_c}\lambda_c(\vec{r}-\vec{r}_c), \qquad (2)$$

where μ_b, μ_c are the reduced masses for $(a\mu)$ scattering on the nuclei b,c and λ_b, λ_c are the scattering lengths for elastic collisions of $(a\mu)$ with the nuclei b and c, respectively. The term V_e in /1/ represents an effective potential of $(a\mu)$ interaction with the electrons. It is obtained by averaging a potential [9]

$$U(r_1,r_2)=\sum_{i=1,2}\left[-\varkappa_\mu(1+\frac{1}{r_i})\exp(-2r_i)-\frac{2}{3}\frac{m_e}{r_i^4}\sum_{n\neq 0}|\langle n|\vec{x}|0\rangle|^2 g_n(r_i)\frac{1}{\gamma_n^2}\right], \quad (3)$$

$g_n(r_i)=1-(1+\gamma_n r_i)\exp(-\gamma_n r_i)$, $\gamma_n=\left[2m_e(E_{\mu n}-E_{\mu 0})\right]^{\frac{1}{2}}$, $\varkappa_\mu=(M_a-m_\mu)/(M_a+m_\mu)$ with an electronic ground state wave function Ψ_e of the hydrogen molecule /10/

$$\Psi_e=\left[2(1+S^2)\right]^{-\frac{1}{2}}\left[\varphi(\varrho_{1b})\varphi(\varrho_{2c})+\varphi(\varrho_{1c})\varphi(\varrho_{2b})\right], \quad (4)$$

$S=e^{-w}(1+w+\frac{1}{3}w^2)$, $w=\alpha R/a_e$, $\varphi(\varrho_{ib,c})=(\alpha/\pi^3 a_e^3)^{\frac{1}{2}}\exp(-\alpha\varrho_{ib,c}/a_e)$, $i=1,2$,

where r_i is a distance between the $(a\mu)$ centre of mass and the i-th electron, $\vec{x}$ is an internal vector of $(a\mu)$, ϱ_{ib}, ϱ_{ic} are the distances between the electrons and the respective nuclei b,c. The Bohr radius of hydrogen atom and the electron mass are denoted by a_e and m_e ($a_e\approx m_e^{-1}\approx 200$ in muonic atomic units). The matrix elements $\langle n|\vec{x}|0\rangle$ are calculated for the ground state $|0\rangle$ with energy $E_{\mu 0}$ and excited states $|n\rangle$ with energies $E_{\mu n}$ of $(a\mu)$. Averaging (3) with (4) one obtains

$$V_e(\vec{r},\vec{R})=-\frac{C\alpha^3}{a_e^3(1+S^2)}\left[\exp\left(-\frac{2\alpha|\vec{r}+\beta\vec{R}|}{a_e}\right)+\exp\left(-\frac{2\alpha|\vec{r}-\beta'\vec{R}|}{a_e}\right)+\right. \quad (5)$$
$$\left.+2S\exp\left(-\frac{\alpha|\vec{r}+\beta\vec{R}|+\alpha|\vec{r}-\beta'\vec{R}|}{a_e}\right)\right], \quad C=-2\left[\varkappa_\mu+4.20m_e^{1/2}\right], \quad \beta=\frac{M_c}{M_b+M_c}, \quad \beta'=1-\beta.$$

Since the electron screening is the most significant for collision energies ε lower than the energy ω of excitation of vibrational levels ($\omega\approx 0.35$ eV), the hydrogen molecule is assumed to be a rigid rotator. Therefore, in our calculations the internuclear distance R has fixed equilibrium value R=1.4a and the corresponding variational parameter α equals to 1.32 /10/. An amplitude for $(a\mu)$ scattering on the molecule, connected with any change of an initial rotational quantum number K, is given in the first Born approximation by the formula

$$f(\vec{p}',K';\vec{p},K)=f_n(\vec{p}',K';\vec{p},K)+f_e(\vec{p}',K';\vec{p},K)=-\frac{m}{2\pi}\int Y^*_{K'M'_K}\left(\frac{\vec{R}}{R}\right)V(\vec{q},\vec{R})Y_{KM_K}\left(\frac{\vec{R}}{R}\right)d\Omega_R, \quad (6)$$

$$V(\vec{q},\vec{R})=V_n(\vec{q},\vec{R})+V_e(\vec{q},\vec{R}), \qquad V_n(\vec{q},\vec{R})=\int V_n(\vec{r},\vec{R})\exp(i\vec{q}\cdot\vec{r})d^3r, \quad (7)$$

$$V_e(\vec{q},\vec{R})=\int V_e(\vec{r},\vec{R})\exp(i\vec{q}\cdot\vec{r})d^3r, \quad \vec{q}=\vec{p}-\vec{p}', \quad m^{-1}=(M_a+m_\mu)^{-1}+(M_b+M_c)^{-1}, \quad (8)$$

where $\vec{p},K$, M_K and $\vec{p}',K'$, M'_K are the momenta and the rotational quantum

numbers of initial and final states, respectively, and Y_{KM_K} are the spherical functions of a solid angle Ω_R. Inserting (2) and (5) into (7) one obtains

$$V_n(\vec{q},\vec{R})=2\pi\frac{\lambda_b}{\mu_b}\exp(i\beta\vec{q}\cdot\vec{R})+2\pi\frac{\lambda_c}{\mu_c}\exp(-i\beta'\vec{q}\cdot\vec{R}), \quad (9)$$

$$V_e(\vec{q},\vec{R})=-\frac{\pi C}{a_e^3(1+S^2)}\left\{\left[A(\zeta)+\exp(iw\zeta)F(\zeta)\right]\exp(i\beta\vec{q}\cdot\vec{R})+A(\zeta)\exp(-i\beta'\vec{q}\cdot\vec{R})\right\}, \quad (10)$$

where

$$\zeta=\frac{qa_e}{2\alpha}, \qquad A(\zeta)=(1+\zeta^2)^{-2}, \quad (11)$$

$$F(\zeta)=S\exp(-w)\left\{A(\zeta)\left[\left(w+1+(w-1)\zeta^2\right)\frac{\sin w\zeta}{\zeta}+(w+2+w\zeta^2)\cos w\zeta\right]+\right. \quad (12)$$
$$\left.+\frac{1}{\zeta^2}\left[w^2h(\zeta)-(w-1)\frac{\sin w\zeta}{\zeta}-w\cos w\zeta\right]\right\}, \quad h(\zeta)=\zeta^{-1}\exp(w)\int_w^\infty\frac{dz}{z}\exp(-z)\sin\zeta z.$$

The total cross section of $(a\mu)$ scattering on the molecule for given initial K is

$$\sigma^{mol}(\varepsilon)=\sigma_n^{mol}+\sigma_e^{mol}+\Delta\sigma=\frac{1}{2K+1}\sum_{M_K;K',M'_K}|f(\vec{p}',K';\vec{p},K)|^2\frac{p'}{p}\delta(\varepsilon'+\varepsilon_{K'}-\varepsilon-\varepsilon_K)d^3p, \quad (13)$$

where

$$\varepsilon'=p'^2/2m, \quad \varepsilon=p^2/2m, \quad \varepsilon_{K'}=BK'(K'+1), \quad \varepsilon_K=BK(K+1), \quad B=\frac{1}{2R^2}\left(\frac{1}{M_b}+\frac{1}{M_c}\right)\sim 10^{-2}\text{eV}.$$

The nuclear term σ_n^{mol} in (13), connected with $|f_n|^2$, has been estimated in /6/ under the condition $\varepsilon\gg B(K'\gg K\gg 1)$. For $B\ll\varepsilon\lesssim\omega$ it equals

$$\sigma_n^{mol}(\varepsilon)=C_F^b\sigma_n^b(\varepsilon)+C_F^c\sigma_n^c(\varepsilon), \quad (14)$$

where σ_n^b, σ_n^c are the cross sections for $(a\mu)$ scattering on single nuclei b and c, respectively, and C_F^b, C_F^c are coefficients depending on a given combination of hydrogen isotopes. The pure electronic term σ_e^{mol}, describing $(a\mu)$ scattering on the potential (5), and the interference term $\Delta\sigma$ are calculated in this paper. Since the electronic amplitude V_e decreases rapidly for $q\gtrsim 2\alpha/a_e$ ($\zeta\gtrsim 1$) and inelastic processes are connected with a dimensionless momentum transfer ζ of an order of 1 one should expect that the elastic scattering ($K'=K$) gives a main contribution to σ_e^{mol}. The elastic cross sections are described, by virtue of (9), (10) and (13), by the formulae

$$\sigma_e^{mol}(\zeta_0)=\sigma_e^{mol}(0)\,G_0(\zeta_0)\,,\quad \zeta_0=\frac{pae}{2\alpha}\,,\quad \sigma_e^{mol}(0)=4\pi m^2c^2,$$

$$G_0(\zeta_0)=\frac{1}{8(1+S^2)^2\zeta_0^2}\int_0^{2\zeta_0}|T_0(\zeta)|^2\zeta\,d\zeta\;\longrightarrow 1\,,\ (\zeta_0\to 0)\,, \tag{15}$$

$$T_0(\zeta)=A(\zeta)\left[j_0(2\beta w\zeta)+j_0(2\beta' w\zeta)\right]+F(\zeta)\,j_0(2\beta' w\zeta)\exp(iw\zeta),\quad j_0(\zeta)=\frac{\sin\zeta}{\zeta},$$

$$\Delta\sigma(\zeta_0)=-2\sigma_e^{mol}(0)\left[\frac{\lambda_b}{\mu_b c}\,G_1^b(\zeta_0)+\frac{\lambda_c}{\mu_c c}\,G_1^c(\zeta_0)\right],\quad G_1^b\to 1,\ G_1^c\to 1,\ (\zeta_0\to 0), \tag{16}$$

$$G_1^b(\zeta_0)=\frac{1}{4(1+S^2)\zeta_0^2}\int_0^{2\zeta_0} j_0(2\beta w\zeta)\,\mathrm{Re}\,T_0(\zeta)\,\zeta\,d\zeta,\quad G_1^c(\zeta_0)=\frac{1}{4(1+S^2)\zeta_0^2}\int_0^{2\zeta_0} j_0(2\beta' w\zeta)\,\mathrm{Re}\,T_0(\zeta)\,\zeta\,d\zeta.$$

In particular, for the homogeneous molecules ($\beta=\beta'=0.5$, $\lambda_b=\lambda_c=\lambda$, $G_1^b=G_1^c=G_1$, $C_F^b=C_F^c=C_F$) and for $\zeta_0\gtrsim 0.75$ ($\varepsilon\gtrsim 0.02$ eV)

$$G_0(\zeta_0)=0.051/\zeta_0^2\,,\quad G_1(\zeta_0)=0.075/\zeta_0^2\,. \tag{17}$$

Thus, the total cross section σ^{mol} at collision energies $B\ll\varepsilon\lesssim\omega$ can be written in the form

$$\sigma^{mol}(\varepsilon)=2C_F\sigma_n(\varepsilon)+\frac{0.176}{m a_e^2}\left(1-5.96\,\frac{\lambda}{\mu c}\right)\sigma_e^{mol}(0)\,\frac{1}{\varepsilon}\,. \tag{18}$$

The inelastic cross sections, connected with the transitions $K\to K'=K+1$, give a contribution to σ_e^{mol} less than few per cent. For example, $\sigma_e^{mol}(\zeta_0)$ for the reaction $d\mu+D_2$ $(K=0)\longrightarrow d\mu+D_2$ $(K'=1)$ equals to $0.00077\,\sigma_e^{mol}(0)/\zeta_0^2$ in the region $\varepsilon\gtrsim 0.02$ eV. On the other hand, $\sigma_e^{mol}(\zeta_0)$ for the process $d\mu+D_2$ $(K=1)\to d\mu+D_2$ $(K'=0)$ is governed by $0.001\,\sigma_e^{mol}(0)/\zeta_0$ law at $\zeta_0\to 0$. It is of the order of $\sigma_e^{mol}(0)$ at $\zeta_0\sim 10^{-3}$ ($\varepsilon\sim 10^{-7}$ eV). However, after averaging over the Boltzmannian distribution of collision energies ε it gives a negligible contribution to the averaged σ_e^{mol} . Some results of our calculations for the homogeneous molecule are presented in the Table.

3. A resonant mechanism of formation of muonic molecules $dd\mu$ and $dt\mu$ leads to additional resonant corrections σ_r^{mol} to the considered cross sections given by the Breit-Wigner formula

$$\sigma_r^{mol}(\varepsilon)=\frac{\pi}{k^2}\sum_{K',K''}\frac{\Gamma^e_{K''K}\,\Gamma^e_{K''K'}}{(\varepsilon-\varepsilon^r_{K''K})^2+\frac{1}{4}\,\Gamma^2_{K''}} \tag{19}$$

Table. Cross sections of scattering of muonic hydrogen

Process	Cross section $[10^{-20}\ cm^2]$	Collision Energy [eV] 0.04	0.10	0.25
$d\mu(\uparrow\downarrow)+D_2$ *	σ_n	17.5	19.3	21.7
	σ^{mol}	35.8	43.5	50.5
$d\mu(\uparrow\uparrow)+D_2$ *	σ_n	17.6	19.6	21.7
	σ^{mol}	36.3	44.3	51.1
$d\mu(\uparrow\downarrow)+D_2$	σ_n	19.9	21.7	23.9
	σ^{mol}	38.5	48.3	56.1
$j=3/2$	$\sigma_e^{mol}+\Delta\sigma$	-10.2	-5.0	-2.4
$t\mu+D_2$	σ_n	16.0	19.4	27.2
	σ^{mol}	43.0	48.7	67.8
	$\sigma_e^{mol}+\Delta\sigma$	2.1	-1.0	-1.9
$t\mu(\uparrow\downarrow)+T_2$	σ_n	0.62	1.25	1.67
	σ^{mol}	49.0	20.6	10.8
$j=1/2$	$\sigma_e^{mol}+\Delta\sigma$	47.5	17.6	6.7

* averaged over the total spin j of the nuclei a , b or c and the muon.

where $\Gamma^e_{K''K}$, $\Gamma^e_{K''K'}$ are the partial widths of resonances [12] , $\varepsilon^r_{K''K}$ are the resonance energies, $\Gamma_{K''}$ is the sum of partial widths of all the channels including the nuclear fusion [13] and deexcitation [14] of the muonic molecules. Our estimations, using the results of [12,13,14] show that σ_r^{mol} averaged over the Maxwellian distribution of collision energies give a contribution of an order of 1 % to the averaged nonresonant σ^{mol}. This result is caused by very small widths (10^{-3} – 10^{-4} eV) of the resonances.

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Низкоэнергетическое рассеяние мезоатомов водорода на молекулах водорода

Вычислены сечения низкоэнергетического рассеяния мезоатомов водорода на молекулах изотопов водорода. Учтено влияние электронного экранирования и образования мезомолекул на сечения упругого рассеяния мезоатомов. Сечения этих процессов вычислены при энергиях столкновения $\varepsilon \gtrsim 0{,}04$ эВ. Показано, что при энергиях < 1 эВ электронное экранирование существенно влияет на процессы упругого рассеяния мезоатомов, его влияние на неупругие процессы переворота спина мезоатома и перезарядки существенно меньше.

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Low Energy Scattering of Muonic Hydrogen on Hydrogen Molecules

Influence of electron screening and muonic molecule formation on low energy scattering of muonic hydrogen on molecules of hydrogen isotopes is estimated. Cross sections of these processes at collision energies $\varepsilon \gtrsim 0.04$ eV are calculated.

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

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