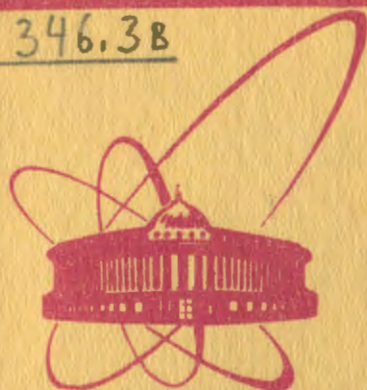


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ОБЪЕДИНЕННЫЙ  
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$\mu$  -CAPTURE  
AND ORTHO-PARA TRANSITIONS  
IN MESIC MOLECULE  $PP\mu$

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## 1. Introduction

The reaction of  $\mu^-$ -capture by hydrogen nuclei



is important for determining the weak interaction constants ( see reviews /1,2/. This fact has first been indicated in refs. /3,4/ .

These papers also pointed out a strong dependence of reaction (1) on mutual muon and nuclear spin orientation, which was then thoroughly investigated in refs. /5/ .

It is well known that the  $\mu^-$ -mesic atom is formed in the singlet (total spin  $F=0$ ) and triplet ( $F=1$ )  $1s$ -states with the probabilities  $1/4$  and  $3/4$ , respectively. The calculated rates of  $\mu^-$ -capture (1) in these two states are strongly different /6/ :  $\Lambda_s = 659 \text{ s}^{-1}$ ,  $\Lambda_t = 14.6 \text{ s}^{-1}$  and much lesser than the decay rate of a free muon  $\lambda_0 = 0.455 \cdot 10^6 \text{ s}^{-1}$ .

The observed rate of  $\mu^-$ -capture  $\Lambda_\mu$  in hydrogen depends on the rates of different mesic atomic and mesic molecular processes (their scheme is shown in fig.1) and on the experimental

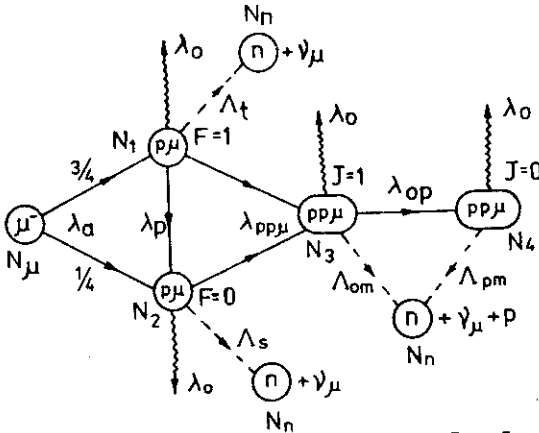


Fig.1. Scheme of mesic atomic and mesic molecular processes accompanying  $\mu^-$ -capture by hydrogen nuclei.

conditions, in particular on the relative hydrogen density  $\varphi = N/N_0$ , where  $N_0 = 4.25 \cdot 10^{22} \text{ cm}^{-3}$  is the density of liquid hydrogen, and  $N$  is the experimental density of hydrogen.

All the rates of mesic molecular processes are proportional to  $\varphi$ :

$$\lambda_\alpha = \lambda_\alpha^0 \varphi, \lambda_p = \lambda_p^0 \varphi, \lambda_{pp\mu} = \lambda_{pp\mu}^0 \varphi \text{ where } \lambda_\alpha^0 \approx 10^{11} \text{ s}^{-1},$$

$$\lambda_p^0 \approx 1.7 \cdot 10^{10} \text{ s}^{-1}, \lambda_{pp\mu}^0 \approx 2.2 \cdot 10^6 \text{ s}^{-1} / 7, 8/.$$

The observed rates vary considerably with  $\varphi$  :

a) At  $\varphi < 10^{-5}$ , when  $\lambda_p \ll \lambda_0$ , the statistical population of the hyperfine structure of levels (h.f.s.) of the  $p\mu$ -mesic atoms is conserved and the rate of  $\mu$ -capture is given by

$$\Lambda_\mu = \frac{1}{4} \Lambda_s + \frac{3}{4} \Lambda_t \approx \frac{1}{4} \Lambda_s \quad (2)$$

b) If  $10^{-4} < \varphi < 10^{-2}$ , then  $\lambda_p \gg \lambda_0$  and  $\lambda_{pp\mu} \ll \lambda_0$ . Under these conditions as has first been shown in ref. /9/, the process

$p\mu(F=1)+p \rightarrow p\mu(F=0)+p$  leads to the total depolarization of spins of the  $p\mu$ -mesic atoms, but one can still neglect the formation of the  $pp\mu$ -molecules; therefore the rate of  $\mu$ -capture is equal to  $\Lambda_\mu \approx \Lambda_s$ , i.e., four times as large as the value in (2a), which corresponds to the statistical population of levels of the hyperfine structure of  $p\mu$  atoms /9/. The experiments /10,11/ confirm this prediction in accordance with the (V-A) theory of weak interaction /4/.

c) At  $\varphi \sim 1$  the  $\lambda_{pp\mu} \gg \lambda_0$  condition is fulfilled and reaction (1) proceeds from the bound state of the  $pp\mu$  mesic molecule. As has been shown in ref. /12/, the  $pp\mu$  mesic molecule is formed in the rotational excited orthostate with orbital momentum

$J=1$  and total nuclear spin  $I=1$ . In the nonrelativistic approximation the electromagnetic ortho-para transitions ( $J=1$ ,  $I=1$ )  $\rightarrow$  ( $J=0$ ,  $I=0$ ) from the excited orthostate of the

$pp\mu$ -mesic molecule to the ground parastate are strictly forbidden by the selection rule  $\Delta I=0$  /12/. In the absence of the ortho-para transitions, i.e., when  $\lambda_{op} \ll \lambda_0$ , the rate  $\Lambda_{om}$  of  $\mu$ -capture in the  $pp\mu$ -mesic molecule is three times as large as the rate (2a) /12/ :  $\Lambda_{om} \approx \frac{3}{4} \Lambda_s$ . Taking into account also the difference in the wave functions of the  $pp\mu$  mesic molecule and  $p\mu$  mesic atom, the rate  $\Lambda_{om}$  in the

orthostate of the  $pp\mu$  mesic molecule can be represented in the form /13/ :

$$\Lambda_{\mu} \approx \Lambda_{om} = 2\gamma_0 \left( \frac{3}{4} \Lambda_s + \frac{1}{4} \Lambda_t \right), \quad (2')$$

where  $\gamma_0$  is the ratio of the  $\mu^-$  meson density in the proton in the orthostate of the  $pp\mu$  mesic molecule to the  $\mu^-$  density in the  $p\mu$  atom. The experiments performed in liquid hydrogen /14,15/ and in bubble chambers /16/ on the whole confirm formula (20).

Obviously, the validity of formula (20) depends on the value of  $\lambda_{op}$ . It follows from the recent experiments /17/ that  $\lambda_{op} \lesssim 5 \cdot 10^4 s^{-1}$  in accordance with the previous estimates /14,15/ :  $\lambda_{op} \lesssim 0.1 \lambda_0$ , i.e., equation  $\Lambda_{\mu} \approx \Lambda_{om}$  is true with the accuracy  $O(\lambda_{op}/\lambda_0)^{-1}$  only. Hence, for a precise determination of the rates  $\Lambda_s$  and  $\Lambda_t$  from the measurements of  $\Lambda_{\mu}$  in liquid hydrogen, one should first calculate the values of  $\lambda_{op}$  and  $\gamma_0$ .

In this paper we present the calculations of the rate of the ortho-para transition in the  $pp\mu$  mesic molecule on the basis of a relativistic treatment of the three-body system as in refs. /18,19/. The paper also gives the precise calculations of the factors  $\gamma_0$  and  $\gamma_p$  and considers the kinetics of  $\mu^-$  capture at different hydrogen densities.

## 2. Energy Levels and Wave Functions of the $pp\mu$ Mesic Molecule

In the nonrelativistic approximation the bound states of the  $pp\mu$  molecule are specified by the set of quantum numbers /18/

$$\{n_1 n_2 m p, v J m_T, \lambda\}, \quad (3)$$

where  $[n_1 n_2 m p]$  are the parabolic quantum numbers characterizing the motion of  $\mu^-$ -meson around the protons,  $v$  is the vibrational quantum number specifying the relative motion of protons,  $J$  is the total orbital momentum of the three-body system,  $m_T$  is its Z-axis projection,  $\lambda = +(-1)^J$  is the to-

tal parity of the three-body system, and  $p$  is the parity with respect to the inversion of  $\mu^-$ -meson coordinates. Most interesting are the states of the  $pp\mu$  mesic molecule which correspond to motion of  $\mu^-$ -meson with zero quantum numbers  $[n_s n_l m p] = [000g]$  and positive parity  $p = g$  (i.e., ground state). Then mesic molecule can be formed either in  $(J=0, v=0)$  or  $(J=1, v=0)$  states with binding energies  $-\epsilon_{J,v}$  (reckoned from the energy level  $E_a = -2528.52$  eV of the ground state of the  $p\mu$  mesic atom)  $\epsilon_{0,0} = -253$  eV and  $\epsilon_{1,0} = -107$  eV, respectively /20/.

The interaction of proton spins  $\vec{S}_a, \vec{S}_p$  and of  $\mu^-$  meson spin  $\vec{S}_\mu$  with each other and with the orbital momentum  $\vec{J}$  of the system results in a fine and hyperfine splitting of the nonrelativistic energy levels  $\epsilon_{J,v}$  of the mesic molecule  $pp\mu$  /18-19/, which is schematically represented in fig. 2.

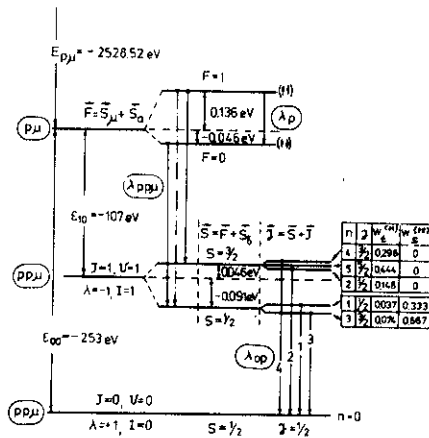


Fig.2. Scheme of h.f.s. energy levels of  $pp\mu$  molecule and ortho-para transitions between them. From the state  $F=0$  of the  $p\mu$ -atom the  $pp\mu$ -molecules are formed only in the states  $n=1$  and  $n=3$ . The rate  $\lambda_{op}$  is practically determined by the ortho-para transitions from these states ( see eqs. (33)-(35)).

Table 1

Main characteristics of stationary states  $|n\rangle$  of the h.f. structure of  $\rho\rho\mu$  mesic molecule

$\varepsilon_{IV}(\text{eV})$	$n$	$J$	$N^{*})$	$J$	$S$	$I$	$\lambda$	$\varepsilon_n(\text{eV})$	$W_S^{(n)}$	$W_T^{(n)}$	$\beta_{\frac{1}{2}0}^{(n)}$	$\beta_{\frac{1}{2}1}^{(n)}$	$\beta_{\frac{3}{2}1}^{(n)}$
$\varepsilon_{00} = -253$	0	1/2	1	0	1/2	0	+	0	1	1	1	0	0
$\varepsilon_{10} = -107$	1	1/2	1	1	1/2	1	-	-0.0905	0.3330	0.0371	0	0.9996	-0.0286
	2	1/2	2	1	3/2	1	-	0.0427	0.0002	0.1481	0	0.0286	0.9996
	3	3/2	1	1	1/2	1	-	-0.0924	0.6667	0.0741	0	0.9999	-0.0095
	4	3/2	2	1	3/2	1	-	0.0468	0.0001	0.2963	0	0.0095	0.9999
	5	5/2	1	1	3/2	1	-	0.0463	0	0.4444	0	0	1

\*) Numeration of states introduced in ref. /19/ .

In this case the states of the  $pp\mu$  mesic molecule are specified by the set of quantum numbers

$$n = \{n_1 n_2 m g, v J S I, j j_z \lambda\}, \quad n_1 = n_2 = m = v = 0, \quad (4)$$

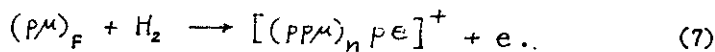
where  $I$ ,  $S$  and  $J$  are the quantum numbers of the total spin of nuclei, total spin and total momentum of the  $pp\mu$  mesic molecule, respectively,

$$\vec{I} = \vec{S}_a + \vec{S}_p, \quad \vec{S} = \vec{I} + \vec{S}_\mu, \quad \vec{J} = \vec{S} + \vec{J} \quad (5)$$

(the quantum numbers  $J$  and  $j$  from the set (4) will be sometimes denoted by the state index  $J = J^{(n)}$ ,  $j = j^{(n)}$ ). According to the Pauli principle the following relation takes place

$$P = \lambda (-1)^I = (-1)^{J+I} \quad (6)$$

In what follows it is convenient to introduce a new numeration  $n$  of the states (4), which is given in tabl. 1 with the energies  $\tilde{E}_n$  of these states (see also fig.2). This table also gives the populations  $W_n(F)$  of these states, which correspond to the formation of the mesic molecule in the state  $n$  in collisions of protons of  $H_2$  molecules with  $p\mu$  mesic atoms in states with a total spin  $F$  /18,19/



In the relativistic case the quantities  $j$ ,  $j_z$  and  $\lambda$  are conserved, while the quantum numbers  $n_1, n_2, m, p, J, S$  and  $I$  are "good" only approximately, since the operators corresponding to them do not commute with the Hamiltonian of the system. Accordingly, the wave function  $\Psi_n(\vec{z}, \vec{R}) = \langle \vec{z}, \vec{R} | n \rangle$  of the  $pp\mu$  mesic molecule in the state  $|n\rangle$  can be represented as an expansion over the adiabatic basis /21/

$$\Psi_n(\vec{z}, \vec{R}) = R^{-1} \sum_{\substack{n_1 n_2 m p \\ J S I}} \varphi_{n_1 n_2 m p}(\xi, \zeta; R) Y_{m J S I}^{j j_z \lambda}(\phi, \theta, \varphi) \chi_{n_1 n_2 m p J S I}^{(n)}(R)$$

(with summation indices  $p, J, I$  obeying eq. (6) ),

$$y_{m_{JSI}}^{JJ\lambda}(\phi, \theta, \psi) = \sum_{m_J=-J}^J \langle S(J_z - m_J) J m_J | (SJ) JJ_z \rangle D_{mm_J}^{J\lambda}(\phi, \theta, \psi) e_{J_z - m_J}^{SI} \quad (8)$$

$$D_{mm_J}^{J\lambda}(\phi, \theta, \psi) = \left\{ \frac{2J+1}{16\pi^2(1+\delta_{m_0})} \right\}^{1/2} \left\{ (-)^m D_{mm_J}^J(\phi, \theta, \psi) + \lambda (-)^J D_{-mm_J}^J(\phi, \theta, \psi) \right\}^{1/2}$$

$$e_{\zeta}^{SI} = \sum_{\zeta_\mu \zeta_a} \langle I(\zeta - \zeta_\mu) S_\mu \zeta_\mu | (I S_\mu) S S \rangle \cdot$$

$$\cdot \langle S_a \zeta_a S_\theta(\zeta - \zeta_\mu - \zeta_a) | (S_a S_\theta) I(\zeta - \zeta_\mu) \rangle \cdot$$

$$\cdot e_{\zeta_\mu}^{S_\mu} e_{\zeta_a}^{S_a} e_{\zeta_\theta}^{S_\theta}, \quad \zeta_\theta = \zeta - \zeta_a - \zeta_\mu$$

$$[\vec{S}^2 - S(S+1)] e_{\zeta}^{SI} = [\vec{I}^2 - I(I+1)] e_{\zeta}^{SI} = (S_z - \zeta) e_{\zeta}^{SI} = 0$$

$$\zeta = \zeta_a + \zeta_\theta + \zeta_\mu$$

Here we use the following notation:

$\varphi_{n_1 n_2 m p}(\xi, \zeta; R)$  are the solutions of the Coulomb two-center problem of quantum mechanics /21/, whose dependence on the angle of rotation  $\psi$  around the axis  $\vec{R}$  is included in the Wigner D-function /22/  $D_{mm_J}^J(\phi, \theta, \psi)$ ;  $\theta$  and  $\phi$  are the spherical coordinates of the vector  $\vec{R}$  connecting the nuclei of the  $pp\mu$  molecule;  $\xi = \frac{z_a + z_\theta}{R}$  and  $\zeta = \frac{z_a - z_\theta}{R}$ , where  $z_a$  and  $z_\theta$  are the distances between  $\mu^-$  meson and protons  $a$  and  $\theta$ ;  $e_{\zeta_\mu}^{S_\mu}$ ,  $e_{\zeta_a}^{S_a}$  and  $e_{\zeta_\theta}^{S_\theta}$  are constant spinors



of spin  $S_\mu$ ,  $S_a$  and  $S_f$ ;  $e^{SI}_{j_a - m_j}$  is a spinor of spin  $S$ , constructed according to the coupling scheme (5);

$\langle S (j_a - m_j) J m_j | (SI) J J_a \rangle$ , etc., are the Clebsch-Gordan coefficients; all the spinors refer to the laboratory system of coordinates in which the vector  $\vec{R}$  is determined.

The wave functions  $\Psi_n(\vec{z}, \vec{R})$  satisfy the Schrödinger equation

$$(H^{nrel} + V^{spin} - \mathcal{E}_n) \Psi_n(\vec{z}, \vec{R}) = 0, \quad (9)$$

where the nonrelativistic Hamiltonian  $H^{nrel} = H^{nrel}(\vec{z}, \vec{R})$  has been determined in ref. /23/,  $V^{spin} = V^{spin}(\vec{z}, \vec{R})$  is the operator of the spin interaction /18/ and  $\mathcal{E}_n$  is the stationary state  $|n\rangle$  energy level reckoned from the nonrelativistic value of  $\mathcal{E}_{J\pi}$  (see tabl. 1).

In what follows all the values will be given in units  $e = \hbar = m_a = 1$ ,  $m_a^{-1} = m_\mu^{-1} + M_p^{-1}$ , where  $m_\mu = 206.769 m_e$

and  $M_p = 1836.152 m_e$  are the  $\mu^-$ -meson and proton masses and  $m_e$  is the electron mass /24/. Let us introduce also an abbreviated index of summation  $j = (n_1 n_2 m p J S I)$ . Hence, equation (9), upon substituting into it expansion (8) and averaging over the coordinates  $\xi, \zeta, \varphi, \theta, \phi$ , gets the form

$$\sum_{j'}^{n_0} \left\{ H_{jj'}^\lambda(R) + V_{jj'}^{j\lambda}(R) - \mathcal{E}_n \delta_{jj'} \right\} R^{-1} \chi_{j'}^{(n)}(R) = 0. \quad (10)$$

The effective potentials of this system of equation

$$H_{jj'}^\lambda(R) = \delta_{JJ'} \delta_{SS'} \delta_{II'} \delta_{m_j m_{j'}} \quad (11)$$

$$\int d\tau d\Omega \mathcal{D}_{mm_j}^{J\lambda}(\phi, \theta, \varphi) \varphi_{n_1 n_2 m p}(\xi, \zeta; R) H^{nrel}(\vec{z}, \vec{R}) \varphi_{n_1' n_2' m' p'}(\xi, \zeta; R) \mathcal{D}_{m m_j}^{J\lambda}(\phi, \theta, \varphi)$$

$$d\tau = \frac{R^3}{8} (\xi^2 - \zeta^2) d\xi d\zeta, \quad d\Omega = \sin\theta d\theta d\phi$$

$$V_{jj'}^{j\lambda}(R) = \int d\Omega d\tau Y_{m'JSI}^{*j\lambda}(\Phi, \Theta, \Psi) \varphi_{n_1 n_2 m p}(\xi, \zeta; R) \cdot \\ \cdot V^{spin}(\vec{z}, \vec{R}) \varphi_{n_1' n_2' m' p'}(\xi, \zeta; R) Y_{m'J'S'I'}^{j\lambda}(\Phi, \Theta, \Psi)$$

have been calculated in refs. /25/ and /18,19/ .

Expansion (8) contains "large" and "small" components. Large components are specified by the values of quantum numbers

$$J = J^{(n)}, \quad I = I^{(n)}, \quad P = g \quad (12)$$

and in the nonrelativistic limit have the form

$$X_{n_1 n_2 m p}^{(n)JSI}(R) \approx X_{n_1 n_2 m g}^{(n)}(R) \beta_{SI}^{(n)} \delta_{pg} \delta_{JJ^{(n)}} \delta_{II^{(n)}} \quad (12a)$$

The functions  $X_{n_1 n_2 m g}^{(n)}(R)$  are determined from the system of equations (10) with the nonrelativistic Hamiltonian  $H_{jj'}^{(n)}(R)$  at  $J = J^{(n)}$ , and the amplitudes  $\beta_{SI}^{(n)}$  are calculated from the secular equation arising after averaging of eq. (10) over the functions  $X_{n_1 n_2 m g}^{(n)}(R)$  /19/ ( see tabl.1).

Small components arise due to relativistic corrections  $V^{spin}$  to the Hamiltonian  $H^{nrel}$  in the nonrelativistic limit they vanish. At least one of the conditions (12a) is not fulfilled for them.

In further calculations we shall keep in expansion (8) only two functions of the adiabatic basis:  $\varphi_g = \varphi_{000g}(\xi, \zeta; R)$  and  $\varphi_u = \varphi_{000u}(\xi, \zeta; R)$  <sup>x)</sup>. Omitting in this expansion the indices  $n_1 = n_2 = m = 0$ , we get the expression

x) Such an approximation provides an accuracy of the calculation of the functions  $X_j^{(n)}(R)$  not worse than 10% in the whole interval of varying  $R$ , that is sufficient for evaluating the ortho-para transitions rate in the  $pp\mu$  mesic molecule with the same accuracy. To calculate  $\gamma_0$  and  $\gamma_p$  with an accuracy of  $\sim 10^{-3}$ , it is sufficient to use  $\sim 20$  functions  $\varphi_j(\xi, \zeta; R)$ .

$$\Psi_n(\vec{r}, \vec{R}) = R^{-1} \sum_{p J S I} \varphi_p(\vec{\xi}, \vec{b}; R) Y_{J S I}^{J J \lambda}(\Phi, \Theta, \varphi) \chi_{p J S I}^{(n)}(R). \quad (8a)$$

Omitting also the arguments of the functions, expansion (8a) can explicitly be written as follows ( $J_z = -J, \dots, J$ )

$$\text{for } n=0 \quad (J^{(n)} = 0, \quad J^{(n)} = \frac{1}{2}) \quad (8b)$$

$$\Psi_n = R^{-1} \left\{ \varphi_g Y_{0 \frac{1}{2} 0}^{\frac{1}{2} J_z^+} \chi_{g 0 \frac{1}{2} 0}^{(n)} + \right. \\ \left. + \varphi_u \left[ Y_{0 \frac{1}{2} 1}^{\frac{1}{2} J_z^+} \chi_{u 0 \frac{1}{2} 1}^{(n)} + Y_{2 \frac{3}{2} 1}^{\frac{1}{2} J_z^+} \chi_{u 2 \frac{3}{2} 1}^{(n)} \right] \right\}$$

$$\text{for } n=1, 2, 3, 4; \quad (J^{(n)} = 1, \quad J^{(1)} = J^{(2)} = \frac{1}{2}, \quad J^{(3)} = J^{(4)} = \frac{3}{2}) \quad (8c)$$

$$\Psi_n = R^{-1} \left\{ \varphi_g \left[ Y_{1 \frac{1}{2} 1}^{J J_z^-} \chi_{g 1 \frac{1}{2} 1}^{(n)} + Y_{1 \frac{3}{2} 1}^{J J_z^-} \chi_{g 1 \frac{3}{2} 1}^{(n)} \right] + \right. \\ \left. + \varphi_u \left[ Y_{1 \frac{1}{2} 0}^{J J_z^-} \chi_{u 1 \frac{1}{2} 0}^{(n)} + (\text{terms with } J=3) \right] \right\}$$

$$\text{for } n=5 \quad (J^{(n)} = 1, \quad J^{(5)} = \frac{5}{2})$$

$$\Psi_n = R^{-1} \left\{ \varphi_g Y_{1 \frac{3}{2} 1}^{\frac{5}{2} J_z^-} \chi_{g 1 \frac{3}{2} 1}^{(n)} + (\text{terms with } J=3) \right\}.$$

Large components  $\chi_g^{(n)} = \chi_{000g}^{(n)}(R)$  are calculated from the equation

$$\left\{ \frac{d^2}{dR^2} + 2M\varepsilon_{Jr} - \frac{J(J+1)}{R^2} - 2M V_g(R) \right\} \chi_g^{(n)}(R) = 0 \quad (13)$$

$$J = J^{(n)}, \quad \chi_g^{(n)}(0) = \chi_g^{(n)}(R_m) = 0, \quad R_m = 20$$

which is the one-level approximation of the system (10)<sup>x</sup>.

Small components are calculated from inhomogeneous equations which are obtained from system (10) in the first perturbation order

<sup>x</sup>The functions determined from this equation differ by  $\sim 1\%$  only from the corresponding functions calculated from the complete system of equations (10) at  $n_0 = 20 / 26$ . Note, that the relativistic corrections to large components (12) do not exceed  $0,1\%$ .

$$\left\{ \frac{d^2}{dR^2} + 2M(\epsilon_{Jv} + \epsilon_n) - \frac{J(J+1)}{R^2} - 2M V_u(R) \right\} \chi_{u J S I}^{(n)}(R) = \quad (14)$$

$$= V_{u J S I}^{(n)}(R) \chi_g^{(n)}(R)$$

$$\chi_{u J S I}^{(n)}(0) = \chi_{u J S I}^{(n)}(R_m) = 0, \quad R_m = 20.$$

In equations (13) and (14) the potentials  $V_g(R)$  and  $V_u(R)$  represent the well-known symmetric and antisymmetric terms of the molecular ion with the diagonal adiabatic corrections to motion of nuclei /23, 26/.

The effective potentials

$$V_{u_0 \frac{1}{2} 1}^{(0)}(R) = V_{u_0 \frac{1}{2} 1, g_0 \frac{1}{2} 0}^{J\lambda}(R) = V_1^{(f)} \quad (15)$$

$$V_{u_2 \frac{3}{2} 1}^{(0)}(R) = V_{u_2 \frac{3}{2} 1, g_0 \frac{1}{2} 0}^{J\lambda}(R) = V_2^{(f)}$$

$$V_{u_1 \frac{1}{2} 0}^{(n)}(R) = V_{u_1 \frac{1}{2} 0, g_1 \frac{1}{2} 1}^{J\lambda}(R) \beta_{\frac{1}{2} 1}^{(n)} + V_{u_1 \frac{1}{2} 0, g_1 \frac{3}{2} 1}^{J\lambda}(R) \beta_{\frac{3}{2} 1}^{(n)} = V_n^{(i)}$$

and the functions  $\chi_{u J S I}^{(n)}(R)$ :  $n = 1, 2, 3, 4.$

$$\chi_{u_0 \frac{1}{2} 1}^{(0)}(R) = \chi_1^{(f)}, \quad \chi_{u_2 \frac{3}{2} 1}^{(0)}(R) = \chi_2^{(f)} \quad (16a)$$

$$\chi_{u_1 \frac{1}{2} 0}^{(n)}(R) = \chi_n^{(i)}, \quad n = 1, 2, 3, 4.$$

are plotted in figs. 3-5. For comparison we also plot the "large" components

$$\chi_g^{(0)}(R) = \chi_0^{(f)} \quad \text{and} \quad \chi_g^{(n)}(R) = \chi_0^{(i)}, \quad n = 1, 2, 3, 4. \quad (16b)$$

The solution of eqs. (13) and (14) was obtained by means of the algorithms /27/ constructed on the basis of the continuous analog of the Newton method /28/. The corresponding boundary value problems were solved in the interval  $R = [0, R_m]$  with step  $\Delta R = 0.1$  with boundary conditions  $\chi_j^{(n)}(0) = \chi_j^{(n)}(R_m) = 0$  at  $R_m = 20$ .

The functions  $\chi_n^{(f)}$  and  $\chi_n^{(i)}$  thus obtained are then used to calculate the rate  $\lambda_{op}$  of ortho-para transition in the  $PP\mu$  mesic molecule.

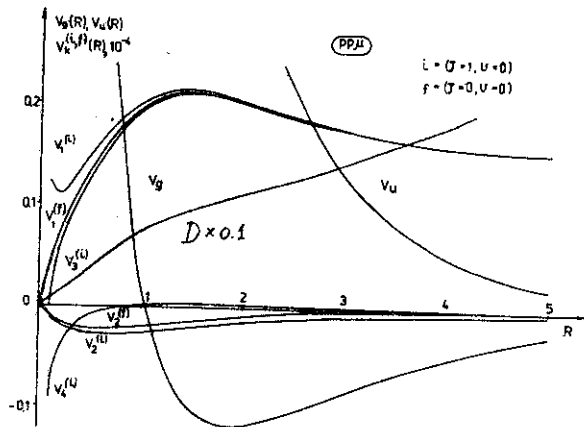


Fig.3. Dipole moment  $D(R)$  and effective potentials in eqs. (13) and (14) for the nonrelativistic ( $V_g \equiv V_g(R)$ ,  $V_u \equiv V_u(R)$ ) and relativistic ( $V_n^{(l)}$ ,  $V_\kappa^{(l)}$ ) three-body problem.

### 3. Calculation of the Rates $\lambda_{op}(F)$ of the Orto-Para Transition in the $pp\mu$ Mesic Molecule

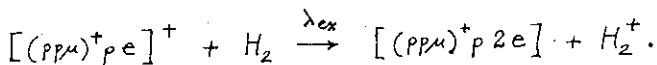
The mesic molecules  $pp\mu$  are formed in reaction (7) in ortho- ( $J=1, I=1$ ) and para- ( $J=0, I=0$ ) states with the rates  $\lambda_{pp\mu}^{ortho/para}$  (at the density  $N_0$  of liquid hydrogen nuclei)

$$\lambda_{pp\mu}^{ortho} = 2.2 \cdot 10^6 \text{ s}^{-1}, \quad \lambda_{pp\mu}^{para} = 0.72 \cdot 10^4 \text{ s}^{-1}$$

respectively.

Following reaction (7) with the rate  $\lambda_{ex}$  there occurs the charge exchange

x) The rate  $\lambda_{pp\mu}^{para}$  is calculated according to the algorithm of ref. /30/. It is determined by the  $E0$ -transition from the  $-S$  scattering states of the system  $p\mu + p$  to the bound state ( $J=0, v=0$ ) of the  $pp\mu$  mesic molecule.



An estimate  $\lambda_{ex} \sim 10^{13} s^{-1}$ , i.e.,  $\lambda_{ex} \gg \lambda_0 \gg \lambda_{op}$  follows from the results of paper /31/ for the analogous reaction  $H_2^+ + H_2 \rightarrow H_2 + H_2^+$ . Thus, the ortho-para transition proceeds in the system  $[(pp\mu)^+ p 2e]$ . In the nonrelativistic limit dipole ortho-para transitions in the  $pp\mu$  mesic molecule from any of the orthostates  $n = 1, 2, 3, 4, 5$  to the ground parastate  $n = 0$  are forbidden by the selection rule

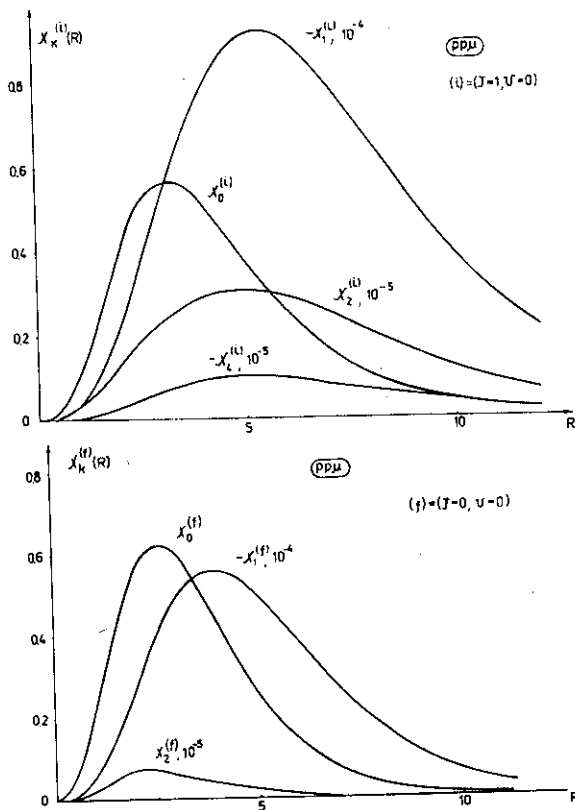
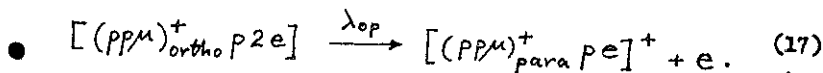


Fig.4.5. "Large" and "small" components of the wave functions (16) describing the relative motion of nuclei in the initial (i) and final (f) states of  $pp\mu$  -molecule.

$\Delta I=0$ . However, as one can see from expansion (8) the value of small components of the excited states  $n=1+4$  coincides with the value  $I$  of the large component of the ground state  $n=0$  and the values of their orbital momentum  $J$  differ by unity (according to formula (6) their parities  $\rho$  and  $\lambda$  also differ). The same relation exists between small components of the ground state  $n=0$  and large components of the excited states  $n = 1, 2, 3, 4$  of the  $pp\mu$  mesic molecule <sup>x)</sup>. Just these "cross" combinations between large and small components of the relativistic wave functions of the  $pp\mu$  mesic molecule allow intense  $KI$ -transitions ( $J=1, I=1$ )  $\rightarrow$   $\rightarrow (J=0, I=0)$  with conversion of an electron according to the scheme in fig.2.



The initial population  $\rho_n$  of the states  $|n\rangle$  of the hyperfine structure of the  $pp\mu$  mesic molecule

$$\rho_n = C_s W_s^{(n)} + C_t W_t^{(n)} \quad (18)$$

is expressed in terms of the concentration  $C_s$  and  $C_t$  of  $p\mu$  mesic atoms in the singlet ( $F=0$ ) and triplet ( $F=1$ ) states, respectively, ( $C_s + C_t = 1$ ) and by the quantities  $W_s^{(n)} = W_n(F=0)$  and  $W_t^{(n)} = W_n(F=1)$ , whose numerical values are given in tabl.1. Here  $W_n(F)$  are nothing but the initial populations of the  $pp\mu$  molecule states  $|n\rangle$  when the latter are formed in collisions of  $H_2$  nuclei with  $p\mu$ -atoms in singlet ( $F=0$ ) or triplet ( $F=1$ )  $1S$ -states /19/.

The rate  $\lambda_{op}$  of the ortho-para transition is determined by the partial rates  $\lambda_{op}^{(n)}$  of transitions from the initial ( $i$ ) states ( $n = 1, 2, 3, 4$ ) to the final one ( $f$ ),  $n=0$  :

$$\lambda_{op} = \sum_{n=1}^4 \rho_n \lambda_{op}^{(n)}. \quad (19)$$

<sup>x)</sup>The dipole transition from the state  $n = 5$  to  $n = 0$  is forbidden by the selection rules  $\Delta J = 0, \pm 1$ ; therefore we shall not consider it in what follows.

The probability  $d\lambda_{op}^{(n)}$  of the ortho-para transition (17) with the emission of an electron with momentum in the interval  $(\vec{q}, \vec{q} + d\vec{q})$  is equal to

$$d\lambda_{op}^{(n)} = \frac{2\pi}{\hbar} \delta(E_f - E_i) d\vec{q} \cdot \frac{1}{2J^{(n)} + 1} \cdot \sum_{J_A^{(n)}} \sum_{J_B^{(n)}} \cdot \quad (20)$$

$$\cdot \sum_{J_A^{(n)}} \sum_{J_B^{(n)}} \left| \int d\vec{R} d\vec{z} d\vec{p} \Psi^{*(f)}(\vec{z}, \vec{R}) \Psi^{*(i)}(\vec{p}) \hat{H}_{int} \Psi^{(i)}(\vec{p}) \Psi^{(f)}(\vec{z}, \vec{R}) \right|^2,$$

where  $\Psi^{(f)}(\vec{z}, \vec{R}) = \Psi_0(\vec{z}, \vec{R})$  and  $\Psi^{(i)}(\vec{z}, \vec{R}) = \Psi_n(\vec{z}, \vec{R})$  are the wave functions of the ground  $n=0$  and excited  $n \neq 0$  states of the  $pp\mu$  mesic molecule, determined by relations (8),  $\mathcal{E}_0$  and  $\mathcal{E}_n$  are their energies reckoned from the nonrelativistic values of the energy  $\mathcal{E}_{IV}$  of states  $|n\rangle$ ,  $E_i = \mathcal{E}_{i0} + \mathcal{E}_n + \mathcal{E}_I$ ,  $E_f = \mathcal{E}_{00} + \mathcal{E}_0 + q^2/2m_e$ , and  $-\mathcal{E}_I = 15.4$  eV is the electron binding energy in the  $H_2$  molecule,  $\vec{q}$  is the momentum of the conversion electron

$$q = \left[ 2m_e (|\mathcal{E}_{00} + \mathcal{E}_0| - |\mathcal{E}_{i0} + \mathcal{E}_n| - |\mathcal{E}_I|) \right]^{1/2} \quad (21)$$

$$\approx \left[ 2m_e (|\mathcal{E}_{00}| - |\mathcal{E}_{i0}| - |\mathcal{E}_I|) \right]^{1/2},$$

$\vec{\rho}$  is the vector connecting the center of mass of the  $pp\mu$  molecule and the electron.

The wave functions of the electron in the initial and final states have the following form, (in units  $e = \hbar = m_e = 1$ )<sup>30/</sup>

$$\Psi^{(i)}(\vec{\rho}) = \left[ \frac{Z_0^3}{2\pi(1+\Delta)} \right]^{1/2} \left( e^{-Z_0 \rho} + e^{-Z_0 |\vec{\rho} - \vec{R}_p|} \right) \quad (22a)$$

$$\Psi^{(f)}(\vec{\rho}) = \frac{3i}{4\pi q} e^{-ib_1 \rho} R_{q1}(\rho) \cos \theta_{q\rho} \quad (22b)$$

$$R_{q1}(\rho) = \frac{2}{3} q^2 \left[ \frac{b_1(1+b_1^2)}{1 - e^{-2b_1^2}} \right]^{1/2} \cdot \rho F(2+ib_1, 4, 2ib_1 \rho), \quad (22c)$$

where  $Z_0$  and  $Z^*$  are the effective charges of the Coulomb centers in the molecular complex  $[(pp\mu)P_2e]$ , which determine the



electron wave functions in the initial and final states, respectively;  $\vec{R}_p$  is the vector connecting the  $pp\mu$  center of mass with the other nucleus of the molecular complex,  $\theta_{q,p}$  is the angle between the vectors  $\vec{q}$  and  $\vec{p}$ . In this paper we use the following values of the electron wave function parameters (22) <sup>/30/</sup>

$$Z_0 = 1.19, \quad R_p = 1.40, \quad \Delta = 0.677, \quad Z^* = 1. \quad (23)$$

The interaction operator describing dipole ortho-para transitions has the form <sup>/30/</sup>

$$\hat{H}_{int} = -e^2 \left(1 + \frac{m_\mu}{m_\mu + 2M_p}\right) \frac{\vec{z} \vec{p}}{\rho^3}. \quad (24)$$

After integrating over the variables  $\vec{p}$ ,  $\vec{z}$ ,  $\vec{R}$  and momentum  $\vec{q}$ , we get the following expression for the rates <sup>x)</sup>

$$\begin{aligned} \lambda_{op}^{(n)} &= \frac{8\pi}{3} \left(\frac{m_e}{m_a}\right)^2 \left(1 + \frac{m_\mu}{m_\mu + 2M_p}\right)^2 \frac{Z_0^3}{1+\Delta} q^{-1} |I(q)|^2 |T_{n0}|^2 \frac{m_e e^4}{\hbar^3} = (25) \\ &= C_q |T_{n0}|^2, \quad C_q = 1.39 \cdot 10^{12} s^{-1}. \end{aligned}$$

Here

$$I(q) = \int_0^\infty d\rho R_{q1}(\rho) e^{-Z_0 \rho} + \frac{1}{2} \int_0^\infty d\rho R_{q1}(\rho) \int_{-1}^1 d \cos \theta_{p,R} e^{-Z_0 |\vec{p} - \vec{R}_p|} \quad (26)$$

$$|T_{n0}|^2 = \frac{1}{2j^{(n)}+1} \sum_{j_z^{(n)}} \sum_{j_z^{(0)}} |M_{n0}|^2 \quad (27a)$$

$$M_{n0} = \int d\vec{R} d\vec{z} \Psi_n^*(\vec{z}, \vec{R}) z_3 \Psi_0(\vec{z}, \vec{R}), \quad (27b)$$

where <sup>xx)</sup>

$$z_3 = \frac{R}{2} \xi \zeta \cos \theta - \frac{R}{2} \sqrt{(\xi^2-1)(1-\zeta^2)} \sin \theta \cos \varphi \quad (28)$$

<sup>x)</sup> The value of  $q^{-1} |I(q)|^2$  is calculated in atomic units, and  $|T_{n0}|^2$  is in units  $e = \hbar = m_a = 1$ .

<sup>xx)</sup> The second term in the r.h. side of eq. (28) can be neglected in the two-level approximation adopted here, as far as its matrix elements between the basis functions (8) vanish for  $m = m' = 0$ .

Using the Wigner-Eckart theorem, we have

$$\bar{M}_{n_0} = \langle j^{(n)} j_{\pm}^{(n)} 1 0 | (j^{(n)} 1) j^{(0)} j_{\pm}^{(0)} \rangle \delta_{j_{\pm}^{(n)} j_{\pm}^{(0)}} \bar{M}_{n_0} \quad (29)$$

and upon substituting this expression into relation (27a), we get

$$\begin{aligned} |\bar{T}_{n_0}|^2 &= \frac{2j^{(0)}+1}{2j^{(n)}+1} \cdot \sum_{j_{\pm}^{(n)}} \left( \begin{array}{c} j^{(n)} \quad 1 \quad j^{(0)} \\ j_{\pm}^{(n)} \quad 0 \quad -j_{\pm}^{(n)} \end{array} \right) |\bar{M}_{n_0}|^2 = \\ &= \frac{2j^{(0)}+1}{2j^{(n)}+1} \frac{1}{3} |\bar{M}_{n_0}|^2 = \frac{2}{3} \frac{1}{2j^{(n)}+1} |\bar{M}_{n_0}|^2, \end{aligned} \quad (30)$$

where  $\left( \begin{array}{c} j^{(n)} \quad 1 \quad j^{(0)} \\ j_{\pm}^{(n)} \quad 0 \quad -j_{\pm}^{(n)} \end{array} \right)$  is  $3j$ -Wigner coefficient [32].

Using explicit expressions (8b) and (8c) for the functions we get

for  $n=1, 2$  ( $j^{(n)} = \frac{1}{2}$ )

$$\begin{aligned} \bar{M}_{n_0} &= -\frac{1}{\sqrt{3}} \int_0^{\infty} dR D(R) \left\{ \chi_{u1\frac{1}{2}0}^{(n)}(R) \chi_{g0\frac{1}{2}0}^{(0)} + \right. \\ &+ \left. \chi_{g1\frac{1}{2}1}^{(n)}(R) \chi_{u0\frac{1}{2}1}^{(0)}(R) - \chi_{g1\frac{3}{2}1}^{(n)}(R) \chi_{u2\frac{3}{2}1}^{(0)}(R) \right\} = \\ &= -\frac{1}{\sqrt{3}} \left\{ D_n + \beta_{\frac{1}{2}1}^{(n)} \bar{D}_1 - \beta_{\frac{3}{2}1}^{(n)} \bar{D}_2 \right\} \end{aligned} \quad (31)$$

for  $n=3, 4$  ( $j^{(n)} = \frac{3}{2}$ )

$$\begin{aligned} \bar{M}_{n_0} &= -\sqrt{\frac{2}{3}} \int_0^{\infty} dR D(R) \left\{ \chi_{u1\frac{1}{2}0}^{(n)}(R) \chi_{g0\frac{1}{2}0}^{(0)} + \right. \\ &+ \left. \chi_{g1\frac{1}{2}1}^{(n)}(R) \chi_{u0\frac{1}{2}1}^{(0)}(R) + \frac{1}{\sqrt{10}} \chi_{g1\frac{3}{2}1}^{(n)}(R) \chi_{u2\frac{3}{2}1}^{(0)}(R) \right\} = \\ &= -\sqrt{\frac{2}{3}} \left\{ D_n + \beta_{\frac{1}{2}1}^{(n)} \bar{D}_1 + \frac{1}{\sqrt{10}} \beta_{\frac{3}{2}1}^{(n)} \bar{D}_2 \right\}. \end{aligned}$$

Here we introduce the notation

$$\begin{aligned} D_n &= \int_0^{\infty} dR \chi_0^{(j)}(R) D(R) \chi_n^{(i)}(R), \quad n=1, 2, 3, 4. \\ \bar{D}_k &= \int_0^{\infty} dR \chi_k^{(j)}(R) D(R) \chi_0^{(i)}(R), \quad k=1, 2. \end{aligned} \quad (32)$$

$$D(R) = \int d\tau \varphi_g(\xi, z; R) \frac{R}{2} \xi z \varphi_u(\xi, z; R).$$

The dipole moment  $D(R)$  presented in fig.3 has been calculated in refs. /25/ and tabulates in ref. /33/. The values of  $D_n$  and  $\bar{D}_k$  calculated by formulae (32) with the wave functions given in figs.4 and 5, are equal to

$$\begin{aligned} D_1 &= -2.5 \cdot 10^{-4} & \bar{D}_1 &= -2.0 \cdot 10^{-4} \\ D_2 &= 9.0 \cdot 10^{-6} & \bar{D}_2 &= 1.5 \cdot 10^{-6} \\ D_3 &= -2.5 \cdot 10^{-4} \\ D_4 &= -2.8 \cdot 10^{-6} \end{aligned} \quad (33)$$

Using the values of the coefficients  $\beta_{SI}^{(n)}$ , given in tabl.1, we finally get

$$\begin{aligned} \bar{M}_{10} &= 2.6 \cdot 10^{-4} & \bar{M}_{20} &= -1.0 \cdot 10^{-6} \\ \bar{M}_{30} &= 3.7 \cdot 10^{-4} & \bar{M}_{40} &= 4.2 \cdot 10^{-6} \end{aligned} \quad (34)$$

Then in accordance with formulae (18), (19), (25) and (30) we get

$$\lambda_{op}^{(1)} \approx \lambda_{op}^{(3)} = 3.2 \cdot 10^4 s^{-1}, \quad \lambda_{op}^{(2)} \approx \lambda_{op}^{(4)} \sim 10^2 s^{-1}. \quad (34a)$$

The rate  $\lambda_{op}$  averaged over the initial distribution  $P_n$  is equal to

$$\lambda_{op} = \sum_{n=1}^4 P_n \lambda_{op}^{(n)} = (C_s \cdot 3.2 \cdot 10^4 + C_t \cdot 0.35 \cdot 10^4) s^{-1}. \quad (35)$$

#### 4. Rates $\Lambda_{om}$ and $\Lambda_{pm}$ of Muon-Capture from Ortho- and Parastates of the $p\bar{p}\mu$ Mesic Molecule

The  $\mu$ -capture rates  $\Lambda_{om}$  and  $\Lambda_{pm}$  from ortho- and parastates of the  $p\bar{p}\mu$  mesic molecule are usually expressed in terms of the rates  $\Lambda_s$  and  $\Lambda_t$  of  $\mu$ -capture from the singlet and triplet states of the  $p\mu$  mesic atom

$$\Lambda_s = \Lambda_- P_a, \quad \Lambda_t = \Lambda_+ P_a, \quad (36)$$

where  $\Lambda_{\pm} = \Lambda_{\sigma}$  are the reaction constants, corresponding to the singlet (-) and triplet (+) states of the  $p\mu$  mesic atom and  $P_a$  is the muon density in the proton in the  $p\mu$ -atom (in units  $e = \hbar = m_a = 1$ )

$$P_a = |\Psi_{1s\sigma_j}(0)|^2 = \frac{1}{\pi} \quad (37)$$

The rates  $\Lambda_{\mu}^{j\nu}$  of  $\mu$ -capture from the state ( $j\nu$ ) of the  $pp\mu$  mesic molecule:  $\Lambda_{om} = \Lambda_{\mu}^{10}$  and  $\Lambda_{pm} = \Lambda_{\mu}^{00}$  are expressed in terms of the constants  $\Lambda_{\sigma}$  by the formulae

$$\Lambda_{om} = 2 \sum_{n=1}^5 \sum_{\sigma} \rho_n \Lambda_{\sigma} P_{n\sigma} \quad (38)$$

$$\Lambda_{pm} = 2 \rho_0 \sum_{\sigma} \Lambda_{\sigma} P_{0\sigma}, \quad (39)$$

where  $\rho_n$  are defined in eq. (18) and

$$P_{n\sigma} = \int d\vec{R} \int d\vec{z} \delta(\vec{z} \pm \frac{\vec{R}}{\lambda}) \Psi_n^*(\vec{z}, \vec{R}) \Pi^{F_{\sigma}} \Psi_n(\vec{z}, \vec{R}) \quad (40)$$

are the muon densities in the proton of the  $pp\mu$  mesic molecule in the state  $|n\rangle$  in the case of parallel ( $F_{\sigma} = F_{+} = S_a + S_{\mu} = 1$ ) or antiparallel ( $F_{\sigma} = F_{-} = S_a - S_{\mu} = 0$ ) spins and

$$\Pi^{F_{\sigma}} = \sum_{F_z = -F_{\sigma}}^{F_{\sigma}} e^{F_{\sigma} F_z} \otimes e^{* F_{\sigma} F_z} \quad (41)$$

is the projector onto states with a fixed value  $F_{\sigma} = S_a + \sigma S_{\mu} = S_a + \frac{\sigma}{2}$ .

Here

$$e_{F_z}^{F_{\sigma}} = \sum_{S_{\mu} = -1/2}^{1/2} \langle S_a (F_z - S_{\mu}) S_{\mu} S_{\mu} | (S_a S_{\mu}) F_{\sigma} F_z \rangle e_{F_z - S_{\mu}}^{S_a} e_{S_{\mu}}^{S_{\mu}} \quad (42)$$

By substituting expansion (8) for the functions  $\Psi_n(\vec{z}, \vec{R})$  into (40), neglecting small components and replacing in (8) the coupling scheme (5) by the scheme

$$\vec{F} = \vec{S}_a + \vec{S}_{\mu}, \quad \vec{S} = \vec{F} + \vec{S}_p, \quad \vec{J} = \vec{S} + \vec{J} \quad (43)$$

we are led to the following expression:

$$P_{n\sigma} = \frac{1}{\pi} Q_{\sigma}^{(n)} \gamma^{J\nu}, \quad Q_{\sigma}^{(n)} = \sum_S \left( \sum_I \beta_{SI}^{(n)} \alpha_{IF_{\sigma}}^S \right)^2 \quad (44)$$

Here

$$\alpha_{IF_{\sigma}}^S = \left( e_{\frac{S}{I}}^{*SI} \cdot e_{\frac{S}{I}}^{SF_{\sigma}} \right) = (-1)^{S_{\sigma} + S_{\mu} + I + F_{\sigma}} \cdot \left\{ (2I+1)(2F_{\sigma}+1) \right\}^{\frac{1}{2}} \begin{Bmatrix} S_a & S_{\sigma} & I \\ S & S_{\mu} & F_{\sigma} \end{Bmatrix} \quad (45)$$

are the coefficients recoupling of schemes (5) and (43),  $\left\{ \begin{matrix} S_a & S_{\sigma} & I \\ S & S_{\mu} & F_{\sigma} \end{matrix} \right\}$  are the  $6j$ -symbols [32] of Wigner,

$$e_{\frac{S}{I}}^{SF_{\sigma}} = \sum_{S_{\sigma} = -S_{\sigma}}^{S_{\sigma}} \langle F_{\sigma}(S-S_{\sigma}) S_{\sigma} S_{\sigma} | (F_{\sigma} S_{\sigma}) S S \rangle e_{\frac{S-S_{\sigma}}{I}}^{F_{\sigma}} e_{\frac{S_{\sigma}}{I}}^{S_{\sigma}} \quad (46)$$

The ratio  $\frac{S_{\sigma}}{\gamma^{J\nu}}$  of  $\mu^-$ -meson densities in the proton in the  $pp\mu$ -molecule and in the  $p\mu$ -atom (the so-called  $\gamma$ -factors of the states  $|n\rangle = |J\nu\rangle$ ) may be expressed in the following way:

$$\gamma^{J\nu} = \frac{1}{2} \int_0^{\infty} dR \left\{ \sum_{n_1 n_2} N_{n_1 n_2 o g}(R) \chi_{n_1 n_2 o g}^{J\nu}(R) \right\}^2 \quad (47)$$

where  $N_{n_1 n_2 o g}(R)$  are the normalization coefficients of the two-center functions, determined by the relations

$$\Psi_{n_1 n_2 o g}(\xi, \zeta; R) = N_{n_1 n_2 o g}(R) \prod_{o n_1}(\xi, R) \sum_{o g}(\zeta; R) \quad (48)$$

$$\prod_{o n_1}(1; R) = \sum_{o n_2 g}(\pm 1; R) = 1$$

$$\int d\tau \left[ \Psi_{n_1 n_2 m p}(\xi, \zeta; R) \right]^2 = 1.$$

When calculating  $\gamma^{J\nu}$  from (47),  $n_1 \leq 3$ ,  $n_2 \leq 3$ , i.e., in expansion (8) for the function  $\Psi_n(\vec{r}, \vec{r}')$ , 20 states of the discrete spectrum of the two-center problem have been used. The contribution of the highest states of the discrete spectrum and of the continuous spectrum of the two-center problem does not exceed  $5 \cdot 10^{-4} / 18$ .

According to our calculations

$$2\gamma_o = 2\gamma^{10} = 1.009 \pm 0.001 \quad (47a)$$

$$2\gamma_p = 2\gamma^{00} = 1.143 \pm 0.001.$$

Table 2

Source	$2\gamma_0$	$2\gamma_p$
Weinberg (1960) /13/ x)	1.165	1.308
Halpern (1964) /34/	$1.01 \pm 0.005$	-
Wessel and Phillipson (1964) /35/	1.000	1.146
Kabir (1966) /36/	$1.01 \pm 0.01$	-
Carter (1966) /37/	-	1.136
Fatterson and Becker (1967) /38/	1.124	1.255
Kolos (1969) /45/	-	1.147
Ferrante et al. (1976) /46/	-	1.161
This paper	$1.009 \pm 0.001$	$1.143 \pm 0.001$

x) Calculated on the basis of the results of ref. /39/ .

In tabl.2 our values of  $\gamma$ -factors are compared with the results of previous papers /34-39/ .

Taking into account the relations (36)-(40) and (44)

$$\Lambda_{om} = \sum_{n=1}^5 \beta_n \Lambda_{om}^{(n)}, \quad \Lambda_{om}^{(n)} = 2\gamma_0 \Lambda^{(n)} \quad (49)$$

$$\Lambda_{pm} = 2\gamma_p \Lambda^{(0)},$$

where

$$\Lambda^{(n)} = \Lambda_s Q_s^{(n)} + \Lambda_t Q_t^{(n)}, \quad n=0, 1, \dots, 5 \quad (50)$$

$$Q_s^{(n)} + Q_t^{(n)} = 1.$$

Using the values of  $\beta_{SI}^{(n)}$  given in table 1 and the coefficients (45) we get

$$\begin{aligned} Q_S^{(0)} &= 0.2500 & Q_S^{(3)} &= 0.7499 \\ Q_S^{(4)} &= 0.7494 & Q_S^{(4)} &= 0.0001 \\ Q_S^{(2)} &= 0.0006 & Q_S^{(5)} &= 0. \end{aligned} \quad (51)$$

Taking into account that the rate of formation of  $pp\mu$  - molecules ( $\lambda_{pp\mu}^0 = 2.2 \cdot 10^6 s^{-1}$ ) is negligibly small in comparison with the rate of transition of  $p\mu$  -atom into the singlet state ( $\lambda_p^0 = 1,7 \cdot 10^{10} s^{-1}$ ) one can assume with an accuracy of  $\sim 10^{-4}$  that  $C_s = 1$ ,  $C_t = 0$ .

Bearing this in mind, we finally have

$$\Lambda_{om} = 0.756 \Lambda_s + 0.253 \Lambda_t \quad (52)$$

$$\Lambda_{pm} = 0.286 \Lambda_s + 0.857 \Lambda_t .$$

Our formulae coincide with an accuracy of  $\sim 10^{-2}$  with the results of Halpern<sup>/34/</sup>

At the values of  $\Lambda_s = 659 s^{-1}$  and  $\Lambda_t = 14.6 s^{-1}$  <sup>/6/</sup> we have from (52)

$$\Lambda_{om} = 502 s^{-1} , \quad \Lambda_{pm} = 201 s^{-1} . \quad (53)$$

Now let us take into account the effect of the ortho-para transitions on the observed value of the  $\mu$  -capture rate  $\Lambda_{\mu}$  in the  $pp\mu$ -molecule.

### 5. Kinetics of $\mu$ -Capture in Hydrogen

The system of equations describing the kinetics of the processes which are schematically given in fig.1, has the form

$$\begin{aligned} -\frac{dN_1}{dt} &= \lambda_1 N_1 , & -\frac{dN_3}{dt} &= \lambda_3 N_3 - \lambda_{pp\mu} (N_1 + N_2) \\ -\frac{dN_2}{dt} &= \lambda_2 N_2 , & -\frac{dN_4}{dt} &= \lambda_4 N_4 - \lambda_{op} N_3 \\ -\frac{dN_n}{dt} &= \Lambda_t N_1 + \Lambda_s N_2 + \Lambda_{om} N_3 + \Lambda_{pm} N_4 \end{aligned} \quad (54a)$$

with the initial conditions

$$N_1(0) = \frac{3}{4} \frac{\lambda_a}{\lambda_0 + \lambda_a} , \quad N_2(0) = \frac{1}{4} \frac{\lambda_a}{\lambda_0 + \lambda_a} , \quad N_3(0) = N_4(0) = N_n(0) = 0 .$$

Here  $N_2$  and  $N_1$  are the numbers of mesic atoms in the singlet and triplet  $1S$ -states, respectively;  $N_3$  and  $N_4$  are the numbers of mesic molecules  $pp\mu$  in the ortho- and para-states  $x$ ,

$N_n$  is the number of neutrons formed in reaction (1), and the following notations are used:

$$\begin{aligned}\lambda_1 &= \lambda_0 + \lambda_p + \lambda_{pp\mu} + \Lambda_t & (54b) \\ \lambda_2 &= \lambda_0 + \lambda_{pp\mu} + \Lambda_s \\ \lambda_3 &= \lambda_0 + \lambda_{op} + \Lambda_{om}, & \lambda_4 &= \lambda_0 + \Lambda_{pm}.\end{aligned}$$

The solution of system (54a) can be represented in an analytical form at any value of  $\varphi = N/N_0$ . The general solution, however, is given by cumbersome formulae, so let us treat some particular cases.

If  $1 \geq \varphi \geq 2 \cdot 10^{-3}$ , i.e., at hydrogen pressure  $P > 1$  atm. the following relations are valid:

$$\begin{aligned}C_s &\approx 1, \quad C_t \approx 0 & (55) \\ \lambda_p &\gg \lambda_{pp\mu}, \lambda_0; & \lambda_a &\gg \lambda_0; \\ \lambda_{op}, \lambda_{pp\mu} &\gg \Lambda_s, \Lambda_t, \Lambda_{om}, \Lambda_{pm}\end{aligned}$$

and the general solution is essentially simplified. The time distribution of neutrons in reaction (1) in this case has the form

$$\begin{aligned}\frac{dN_n}{dt} &= e^{-\lambda_0 t} \left\{ \Lambda_{pm} + \frac{\lambda_{pp\mu} (\Lambda_{om} - \Lambda_{pm})}{\lambda_{pp\mu} - \lambda_{op}} e^{-\lambda_{op} t} + \right. & (56a) \\ &+ \left. \left[ \Lambda_s - \frac{\lambda_{pp\mu}}{\lambda_{pp\mu} - \lambda_{op}} (\Lambda_{om} - \frac{\lambda_{op} \Lambda_{pm}}{\lambda_{pp\mu}}) \right] e^{-\lambda_{pp\mu} t} \right\}\end{aligned}$$

$x$ ) Strictly speaking, instead of one equation for  $N_3 \equiv N_3(t)$  it is necessary to consider five equations ( $n=1, \dots, 5$ )  
 $-\frac{dN_3^{(n)}}{dt} = (\lambda_0 + \lambda_{op}^{(n)} + \Lambda_{om}^{(n)}) N_3^{(n)} - \rho_n \lambda_{pp\mu} (N_1 + N_2)$ , where  $N_3^{(n)} = \rho_n N_3$ .  
 However, according to definitions (19) and (49) and to the normalization relation  $\sum_n \rho_n = 1$  this set is equivalent to the given equation for  $N_3(t)$ .



and the integral yield of neutrons is equal to <sup>x)</sup>

$$N_n(\infty) = \frac{\Lambda_s}{\lambda_o + \lambda_{pp\mu}} + \frac{\Lambda_{om}}{\lambda_o + \lambda_{op}} \cdot \frac{\lambda_{pp\mu}}{\lambda_o + \lambda_{pp\mu}} + \frac{\Lambda_{pm}}{\lambda_o} \cdot \frac{\lambda_{pp\mu}}{\lambda_o + \lambda_{pp\mu}} \cdot \frac{\lambda_{op}}{\lambda_o + \lambda_{op}} \quad (56b)$$

The observed capture rate is equal to

$$\Lambda_\mu = \lambda_o N_n(\infty) = \Lambda_s \cdot \frac{\lambda_o}{\lambda_o + \lambda_{pp\mu}} + \frac{\lambda_{pp\mu}}{\lambda_o + \lambda_{pp\mu}} \cdot \frac{\lambda_o}{\lambda_o + \lambda_{op}} \cdot (\Lambda_{om} + \Lambda_{pm} \cdot \frac{\lambda_{op}}{\lambda_o}) \quad (56c)$$

At the density of liquid hydrogen ( $\varphi=1$ ) when  $\lambda_{pp\mu} \gg \lambda_{op}$  /40/ the time distribution of neutrons from reaction (1) has the form

$$\frac{dN_n}{dt} = e^{-\lambda_o t} \left\{ \Lambda_{pm} + (\Lambda_{om} - \Lambda_{pm}) e^{-\lambda_{op} t} \right\} \quad (57)$$

Using the rates (35), (53) and the value  $\lambda_{pp\mu}^o = 2.5 \cdot 10^6 \text{ s}^{-1}$  averaged over the data of different experiments ( $\lambda_{pp\mu}^o = 2.55 \pm 0.18$  /42/,  $\lambda_{pp\mu}^o = 2.74 \pm 0.25$  /43/,  $\lambda_{pp\mu}^o = 2.34 \pm 0.17$  /44/), we obtain at the density of liquid hydrogen:

$$\Lambda_\mu = 509 \text{ s}^{-1}.$$

## 6. Conclusion

The results obtained in this paper can be used for planning different types of experiments /40/ on  $\mu$ -capture by hydrogen nuclei and for their theoretical analysis /41/.

When calculating the rate  $\lambda_{op}$  the main sources of errors are the choice of the simplest expression (22) for the wave functions describing motion of the bound and conversion electrons and the use of the two-level approximation in expansion (8) over the adiabatic basis. All these errors do not exceed 10% of the obtained value

<sup>x)</sup> Since  $\lambda_{pp\mu}^{\text{para}} / \lambda_{pp\mu}^{\text{ortho}} \approx 3 \cdot 10^{-3}$ , within the accepted approximations (55), we neglected the production of the  $pp\mu$  molecules in the parastate in the reaction (7).

$\lambda_{of} = 3.2 \cdot 10^4 s^{-1}$  and can be removed if necessary. When calculating  $\gamma$ -factors (47a), an expansion over 20 states of the discrete spectrum of the two-center problem was used, that allowed one to find the values of  $\gamma_0$  and  $\gamma_p$  with an accuracy of  $\sim 10^{-3}$ . Note, that the relativistic corrections to the wave functions of the mesic molecule may be  $\sim 10^{-3}$  and should be taken into account in further more precise calculations of  $\gamma$ -factors.

The main sources of errors in determination of the value  $\Lambda_s$  from Eq. (56c) is the uncertainty of the  $\rho\rho\mu$ -formation rate  $\lambda_{\rho\rho\mu}$ , which is known now with the accuracy of about 10%.

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