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QUANTAL CALCULATION OF THE $p\mu(2s) + d \rightarrow d\mu(n=2) + p$ THERMAL REACTION

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1. INTRODUCTION

A unique experiment, which is a part of an experimental program of a precise measurement of the 2s–2p energy difference in muonic hydrogen by laser spectroscopy, has recently been reported [1]. Earlier measurements at SIN [2] proved the absence of a long-lived, i.e., metastable, $p\mu(2s)$ state at 150 and 600 Torr. Now the authors managed to extend the measurements to low densities (< 1 Torr) to diminish the collisional quenching of $p\mu(2s)$ [1].

It was proposed earlier to use the transfer process from the $p\mu(2s)$ to the heavier nuclei as a probe for the presence of the small fraction of muons of $p\mu(2s)$ atoms [3]. This should be reasonable if the transfer process were fast, as it is expected to be in the case of the reaction

$$p\mu(2s) + d \rightarrow d\mu(n=2) + p. \qquad (1)$$

In the energy interval between the thermal (room temperature) energy E_T and 1 eV the motion of the $p\mu$-atom is adiabatic. The adiabatic potential curves together with the matrix elements accounting for the breakdown of the adiabatic picture are now available [4]. Two facts, a large polarizability of the $p\mu(2s)$ state and a charge symmetry of nuclei (gerade-ungerade classification of the adiabatic states [5]) make the process (1) rather fast.

In this paper we first formulate the basic ideas of the adiabatic-state approach to the reaction (1) in the low collision energy interval. We start from the approximation of adiabatic states which include all $p\mu$ ($n=2$) and $d\mu$ ($n=2$) asymptotic states (n-atomic principal quantum number). Only two of these six states apper to be important for the low energy collisions. The equations of the two-state-adiabatic approximation were solved numerically in a pure quantum manner. The effect of two other equations was incorporated analytically in some way. The last two equations (of total six) accounting for the rotational coupling were neglected.

II. ADIABATIC STATES AND POTENTIALS

Three-body problem of proton, deuteron and μ^- with masses m_p, m_d and μ, with center of mass motion separated, has a Hamiltonian

$$H = -\frac{1}{2M}\Delta_{\vec{R}} - \frac{1}{2m}\Delta_{\vec{r}} - \frac{1}{r_p} - \frac{1}{r_d} + \frac{1}{R} \qquad (2)$$

with ($\hbar = e = 1$)

$$\frac{1}{M} = \frac{1}{m_p} + \frac{1}{m_d}, \quad \frac{1}{m} = \frac{1}{\mu} + \frac{1}{m_p + m_d}. \qquad (2a)$$

Here $\vec{r}$ is the position vector of muon with respect to the CM of the nuclei and $\vec{R}$ is the internuclear vector. The distances between muon and heavy particles are given by r_p and r_d.

Next we introduce the adiabatic Hamiltonian h_0, adiabatic states $\phi_\alpha(\vec{r};R)$ and adiabatic potentials $W_\alpha(R)$, all of them depending parametrically on the internuclear distance by Schrödinger equation

$$h_0 \phi_\alpha(\vec{r};R) = W_\alpha(R)\phi_\alpha(\vec{r};R) \qquad (3)$$

with h_0 as a part of H

$$h_0 = -\frac{1}{2m}\Delta_{\vec{r}} - \frac{1}{r_p} - \frac{1}{r_d} + \frac{1}{R}. \qquad (3a)$$

The solution of the original Schrödinger problem

$$H\Psi(\vec{R},\vec{r}) = E\Psi(\vec{R},\vec{r}) \qquad (4)$$

is tried in the form

$$\Psi(\vec{R},\vec{r}) = \sum_\alpha \psi^g_\alpha(\vec{R})\phi^g_\alpha(\vec{r};R) + \sum_\beta \psi^u_\beta(\vec{R})\phi^u_\beta(\vec{r};R). \qquad (5)$$

Here a specific quantum number (g – gerade, u – ungerade) of the adiabatic states is introduced. It accounts for the charge symmetry of the problem (3), where the nuclei do not move, thus being identical.

To meet asymptotical requirements of the process (1), we should examine at least all the solutions $\phi^i_\alpha(\vec{r};R)$ of the adiabatic problem (3) which turn into linear combinations of "muonic hydrogen" wave functions with principal quantum number $n=2$, as R goes to infinity. These are gerade $2s\sigma$, $3d\sigma$, $3d\pi$ states and ungerade $3p\sigma$, $4f\sigma$, $2p\pi$ states in the united atom classification of the adiabatic states /5/. If we take m=1 we have for large R /5/

$$W_{2s\sigma} \approx W_{3p\sigma} \approx -\frac{1}{8} + \frac{3}{R^2} - \frac{6}{R^3} + \dots \qquad (6a)$$

$$W_{3d\sigma} \approx W_{4f\sigma} \approx -\frac{1}{8} - \frac{3}{R^2} - \frac{6}{R^3} + \dots \qquad (6b)$$

$$W_{2p\pi} \approx W_{3d\pi} \approx -\frac{1}{8} + \frac{6}{R^3} + \dots \qquad (6c)$$

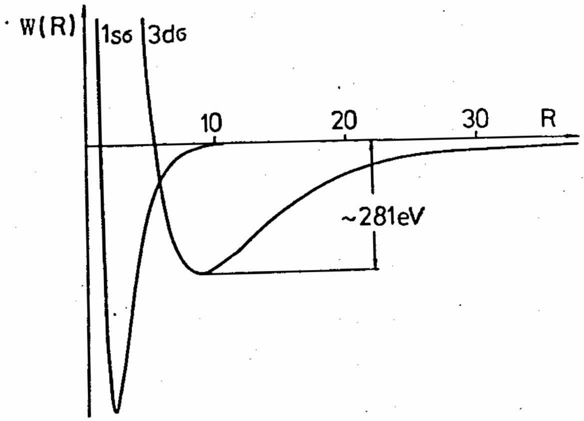

Fig. $W_{3d\sigma}(R)$ adiabatic potential in comparison with the ground $W_{1s\sigma}(R)$ curve. The powerful longrange attraction of $W_{3d\sigma}(R)$, see formulae (6b), makes the reaction (1) fast and unlike of the reaction (7).

The potentials $W_{3d\sigma}$ and $W_{4f\sigma}$ are powerful and attractive as $R \to \infty$, the other four are powerful and repulsive. As far as we are interested in low energy collisions, we can neglect the repulsive states in some reasonable approximation. Actually the $3d\sigma$ potential curve is pictured below, and it is easily seen that the collision energies in the interval $0 < E < 1$ eV are negligible not only in comparison with the depth of the potential but also when compared with the powerful tail of the potential given by (6). This means that in the adiabatic representation only two of six asymptotically adequate states (6) are "open" for low energy reaction (1). In the following we shall have some numerical test of this assumption.

The other potential pictured with the $3d\sigma$ potential is the ground solution of the adiabatic problem (3), the gerade $1s\sigma$ – state potential. It is used (with ungerade $2p\sigma$-state) in the calculation of the processes like /6/

$$p\mu(1s) + d \to d\mu(1s) + p \qquad (7)$$

of the low energy muon transfer from $p\mu$ atom in the ground state. In what follows our consideration will be very similar to that from our earlier paper /6/.

III. EQUATIONS FOR NUCLEAR MOTION

We take solution of the original Schrödinger equation (4) in the form

$$\Psi(\vec{R},\vec{r}) = \psi_1(R)(\phi_g + \phi_u)/\sqrt{2} + \psi_2(R)(\phi_g - \phi_u)/\sqrt{2} \cdot Y_{\ell 0}(\theta,\phi) \qquad (5a)$$

with $\phi_g = \phi_{3d\sigma}$ and $\phi_u = \phi_{4f\sigma}$ which suffices to form pure atomic states from their gerade and ungerade combination as $R \to \infty$. The substitution of this form into equation (4) with further integration over $\vec{r}$-coordinates and partial-wave analysis, produces the system of radial equations

$$\left(\frac{d^2}{dR^2} + k_1^2 - \frac{\ell(\ell+1)}{R^2}\right) X_1 = K_{11} X_1 + K_{12} X_2 + 2 Q_{12} \frac{dX_2}{dR},$$
$$\left(\frac{d^2}{dR^2} + k_2^2 - \frac{\ell(\ell+1)}{R^2}\right) X_2 = K_{22} X_2 + K_{21} X_1 - 2 Q_{12} \frac{dX_1}{dR}, \qquad (8)$$
$$X_i(R) = \psi_i(R)/R.$$

Here
$$K_{11}(R) = M(W_g + W_u) + \frac{1}{2}(K_{gg} + K_{uu} - K_{gu} - K_{ug}),$$
$$K_{12}(R) = M(W_g - W_u) + \frac{1}{2}(K_{gg} - K_{uu} + K_{gu} - K_{ug}),$$
$$K_{21}(R) = M(W_g - W_u) + \frac{1}{2}(K_{gg} - K_{uu} - K_{gu} + K_{ug}), \qquad (9)$$
$$K_{22}(R) = M(W_g + W_u) + \frac{1}{2}(K_{gg} + K_{uu} + K_{gu} + K_{ug}),$$
$$Q_{12}(R) = -Q_{gu}.$$

The adiabatic corrections $K_{gg}, \dots K_{uu}, Q_{gu}$ are defined by the equations
$$K_{ij} = \langle i | -\Delta_{\vec{R}} | j \rangle, \quad Q_{ij} = \frac{\vec{R}}{R} \langle i | -\nabla_{\vec{R}} | j \rangle, \qquad (10)$$
$$i,j = g,u$$
and are now available [4]. Their asymptotic form is known analytically [7]
$$K_{gg} \approx K_{uu} \approx \frac{1}{16}(1+\Delta^2) - \frac{1}{2R^2}(1+3\Delta^2),$$
$$K_{gu} \approx K_{ug} \approx -\left(\frac{1}{8} - \frac{3}{R^2}\right)\Delta, \quad \Delta = \frac{m_d - m_p}{m_d + m_p}. \qquad (11)$$

The matrix element $Q_{gu}(R)$ decreases exponentially as $R \to \infty$. The linear momenta k_1 and k_2 according to equations (9) and (11), are given by
$$k_1^2 = k_2^2 + \Delta/4, \qquad k_2^2 = 2ME. \qquad (12)$$
That is $\Delta/8M$ represents isotopic energy difference, E is CM collision energy. Now we introduce the matrix formulation of the scattering problem (8)
$$L\hat{X} = K\hat{X} + 2Q\hat{X}' \qquad (12a)$$
with L being a free motion operator of the left-hand side of equation (8), and K and Q being two by two matrices whose matrix elements are given by (9). Following Baz et al. [8], we form the regular solution of equation (8a) with an asymptotic behaviour
$$\hat{X} \approx [\hat{\psi}^{(-)} - \psi^{(+)}\hat{S}], \qquad (13)$$

where $\hat{\psi}^{(\pm)}$ are incoming and outcoming spherical waves in the form of diagonal matrices. They are the solutions of the equation
$$L\,\hat{\psi}^{(\pm)} = 0. \qquad (14)$$
Then $\hat{S}$ is a usual S-matrix. An important feature of reaction (1), which makes it totally different from earlier studied reaction (7), is the infinite range character of the potentials involved in the calculation. This follows from equations (6), (9) and (11). The $E_{3d\sigma}$ potential pictured in fig. 1 in comparison with $E_{1s\sigma}$ used for reaction (7) clarifies what we mean. Actually the powerful attractive tail in diagonal matrix elements of matrix K(R) from equation (8a), see formulas (9), forms in the l-th partial wave effective potential (R large)
$$K_{ii}(R) + \frac{\ell(\ell+1)}{R^2} \approx \frac{-6M + \ell(\ell+1)}{R^2} \qquad (15)$$
which appears to be still attractive for $0 \leq \ell < 6$. This means that six partial waves are scattered without repulsive barrier even at $E \to 0$ limit. For $\ell \geq 6$ the potential tail (15) becomes repulsive, i.e., the pair of adiabatic potentials chosen ($3d\sigma$, $4f\sigma$) should be treated in this case on the same footing as the other adiabatic potentials (6a) and (6c) of the $n=2$ family, that is, should be omitted. That is indeed the fact we have experienced in our numerical solution of equation (8a) with the scattering condition (13). We have found that only $\ell < 6$ partial waves contribute to the muon exchange cross-section due to reaction (1) for $E \leq 1$ eV, i.e., in the energy interval under investigation. This circumstance justifies our two-state ansatz introduced earlier.

We should mention two important numerical details. Because of the already mentioned specific attractive character of the channel potentials (15), the bessel functions of the imaginary index should be involved in the calculation for $\ell < 6$ partial waves [9]. This was done in the framework of the two channel phase function method [6].

IV. SPHERICAL AND PARABOLIC HYDROGEN-STATE S-MATRIX

The S-matrix of the previous section is that of the process
$$p\mu(n=2, n_1=0, n_2=1) + d \to d\mu(n=2, n_1=1, n_2=0) + p, \qquad (1a)$$
where n_1 and n_2 are parabolic quantum numbers. This follows from the asymptotic behaviour of the adiabatic $3d\sigma$ and $4f\sigma$ states, which are gerade and ungerade combinations of the (1a) parabolic states. Let us suppose the four state approximation of $3d\sigma$, $4f\sigma$, $2s\sigma$ and $3p\sigma$ adiabatic states introduced

and the scattering problem (8a) with appropriate asymptotic condition of type (13) solved. Then recalling our arguments for the role of the $3d\sigma$ and $4f\sigma$ potentials in the transfer process (1a), we should immediately state that four by four scattering matrix should have a form

$$\hat{S}_4 = \begin{bmatrix} S_{11} & S_{12} & 0 & 0 \\ S_{21} & S_{22} & 0 & 0 \\ 0 & 0 & S_{33} & 0 \\ 0 & 0 & 0 & S_{44} \end{bmatrix} \qquad (16)$$

with the upper left-hand submatrix coinciding with S-matrix of the process (1a). Now what we need is the matrix transformation between parabolic and spherical hydrogenic states /10/. It is simple in our case

$$\begin{pmatrix} 2p \\ 2s \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} n_2=1 \\ n_2=0 \end{pmatrix} . \qquad (17)$$

With the help of (17) S-matrix for the process (1) between spherical states $\bar{S}$ can be expressed in the form

$$\bar{S} = A\hat{S}_4 A^{-1} , \qquad (18)$$

where

$$A = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix} . \qquad (19)$$

This leads to the S-matrix of the process (1)

$$\bar{S} = \frac{1}{2} \begin{bmatrix} S_{11}+S_{33} & S_{12} & S_{11}-S_{33} & S_{12} \\ S_{21} & S_{22}+S_{44} & S_{21} & S_{22}-S_{44} \\ S_{11}-S_{33} & S_{12} & S_{11}+S_{33} & S_{12} \\ S_{21} & S_{22}-S_{44} & S_{21} & S_{22}+S_{44} \end{bmatrix} \qquad (20)$$

in which the column numbering corresponds to the $p\mu(2s)$, $d\mu(2s)$, $p\mu(2p)$ and $d\mu(2p)$ physical state sequence. If follows from (20) that $\sigma^{\ell}_{ex} = \bar{\sigma}^{\ell}\{p\mu(2s)\to d\mu(n=2)\}$, that is the partial cross-section of the reaction (1), is given by

$$\sigma^{\ell}_{ex} = \frac{2\pi}{k_2^2}(2\ell+1)|S^{\ell}_{12}|^2 . \qquad (21)$$

We have introduced index ℓ of the partial matrix element of S-matrix for the first time. It was suppresed in previous consideration for simplicity.

V. RESULTS AND CONCLUDING REMARKS

The Schrödinger equation with the potential

$$V(R) = -\frac{\alpha}{R^2}, \quad \alpha > \frac{1}{4} \qquad (22)$$

has some specific features both for bound solutions /8/ and for the scattering problem /9/. Some of these features are due to the $R\to 0$ singularity whereas the other are caused by the $R\to\infty$ behaviour. We shall list these latter ones: a) Total elastic cross-section does not exist (diverges), b) Scattering parameters become constants as collision energy goes to zero, c) As a result of (b) partial cross-sections exibit const/E threshold law as $E\to 0$, d) Several partial waves should be taken into account in the $E\to 0$ limit if α of (22) is sufficiently large. If summarized, the low energy scattering cross-section should be large and abnormally behaving.

In our case we had to solve a two-channel scattering problem (8) with diagonal matrix elements of the potential energy matrix of type (22). For collision energies $0 < E \le 1$ eV six partial waves proved to make a contribution to the muon transfer cross-section σ_{ex}. These were the partial waves which had satisfied the condition $\alpha > \ell(\ell+1)$ with α-s slightly different for different channels but somewhat greater than 30.0. The const/E law proved to be valid for the muon transfer cross section. Thus

$$\sigma_{ex} = \sum_{\ell=0}^{5} \sigma^{\ell}_{ex} \approx 0.85/E\,(eV) \times 10^{-17}\,cm^2 \qquad (23)$$

which is our main result. This formula can be used in the whole $E_T < E \le 1$ eV energy interval. At $E = 10$ eV $\sigma_{ex} = 0.11\times10^{-17}\,cm^2$, that is the formula (23) still approximately works.

To end the discussion, we give the muon transfer cross-section due to the reaction (7) which has $\bar{\sigma}_{ex} \approx const/\sqrt{E}$ low energy law

$$\bar{\sigma}_{ex} = 0.23/\sqrt{E(eV)} \times 10^{-18}\,cm^2 . \qquad (24)$$

At $E = 10^{-2}$ eV $\sigma_{ex}/\bar{\sigma}_{ex} \approx 400$.

The multichannel problem of the type

$$H(2s) + d \to D(2s) + p, \qquad (25)$$

which coincides with the problem considered in this paper, when electron is substituted by muon, was given some attention in atomic physics. The references can be found in the recent paper[12].

But the pure quantum calculation of the low energy capture of the light particle, when both classical and semiclassical treatment should fail, was given here for the first time.

Our analysis does not take into account the vacuum polarization corrections to the Coulomb interaction[13]. This effect should destroy the const/E law for energies E less than 0.2 eV, that is, for the energies compared with the vacuum polarization splitting of the $p\mu(n=2)$ multiplet.

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