Mesic atom deexcitation via an external Auger process

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The mesic atom deexcitation via an external Auger process on hydrogen molecules (atoms) is considered in a semiclassical approach: relative motion of nuclei is described as a classical process in the potential field, while the motion of the muon and electron is described quantum mechanically. The rates of the hydrogen deexcitation are calculated, beginning from the principal quantum number $n=6$. It is shown that as a result of the Auger transition, mesic atoms can either accelerate up to energies ~ 1 eV or form a bound state (molecule) with a target atom. The decay of such a state via predissociation is characterized by a considerable rate ($\sim 10^{12}$ s^{-1}) and high-energy release (~ 100 eV).

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I. INTRODUCTION

The excited mesic hydrogen atoms are formed when muon beam stops in a hydrogen target. The rate of radiative transitions for highly excited states ($n \gg 1$, n—principal quantum number) is small, so deexcitation in collisions of mesic atom with target molecules becomes important. Immediately after the muon capture onto the atomic state with $n \sim \sqrt{m/m_e}$ (m is the reduced mass of the mesic atom and m_e is the electron mass), the main deexcitation process is a chemical reaction

$$(p\mu)_n + H_2 \rightarrow (p\mu)_{n'} + H + H, \tag{1}$$

where p or H is a nucleus of any hydrogen isotope, and μ denotes a meson (μ^-, π^- or K^-). For $n \lesssim 10$ (for muonic hydrogen), the main deexcitation processes are the Auger ionization of the target molecules, when the energy of the mesic atom transition is taken by the electron of the molecule

$$(p\mu)_n + H_2 \rightarrow (p\mu)_{n'} + H_2^+ + e, \tag{2}$$

and the Coulomb deexcitation, in which the deexcitation energy is shared by the separating nuclei

$$(p\mu)_n + H_2 \rightarrow (p\mu)_{n'} + H_2. \tag{3}$$

At lower states of the mesic atom ($n \leqslant 3$), radiative deexcitation is the most probable. The competition of the deexcitation processes and elastic scattering determines the mesic atom distribution in kinetic energy at each energy level. The energy distribution in the ground state is a very important characteristic for calculation of the kinetics of the muon catalyzed fusion.

The rates of the Coulomb deexcitation were the object of intensive theoretical study during past several years; the calculations were performed in a quasiclassical approach [1–4].

As for the Auger process, its rates were calculated 40 yrs ago in a pioneer work by Leon and Bethe [5]. The process was considered in a Born approximation, the plane waves being used to describe the relative motion of mesic atom and target atom. In later papers Refs. [6,7], classical mechanics and straight-line approximation were used when treating the relative motion. In Refs. [5,6], the states of the mesic atom were characterized by spherical quantum numbers (n, l, m), which were not good quantum numbers for a mesic atom in the field of the nucleus. The authors of Ref. [7] used a parabolic basis, which is more adequate for the problem in question.

It is important that according to the approaches used in all these papers Refs. [5–7], the most of the energy of mesic atom deexcitation was taken away by the ejected electron, kinetic energy of the mesic atom changing negligibly.

The cascade calculations with the available rates of both processes resulted in wrong kinetic-energy distributions in the lower excited states of the mesic atom. For example, in experiment [8], a considerable fraction of the π atoms in the state $n=3$ was observed to have energy as high as 70 eV. Such an observation could be understood if only the Coulomb and the Auger deexcitation rates were comparable with each other. However, according to the calculations, for $n < 10$ the rates of the Coulomb deexcitation are considerably lower than the Auger rates. This is one of the reasons for reconsidering the rates of these processes.

In this paper, we present a calculation of the mesic atom deexcitation via the Auger ionization of the target molecules. We use a semiclassical approach when describing the relative motion of nuclei, declining straight-line approximation and taking into account the effect of interatomic potential on the relative nuclear motion. We begin our consideration from the level $n=6$,[1] since at higher levels, mesic atoms are known to be thermalized quickly as a result of elastic collisions [10].

II. CALCULATION TECHNIQUE

We shall consider mesic atom collision with a hydrogen atom, and calculate the cross section of the reaction

$$(p\mu)_n + H \rightarrow (p\mu)_{n-1} + H^+ + e \tag{4}$$

in slow collisions (the velocity of the nuclei is small compared with muon and electron velocities). We consider only

[1] A preliminary calculation which begins from $n=5$ is presented in Ref. [9].

transitions in which n decreases by 1, since they correspond to the largest reaction rates. A semiclassical approximation is used with classical description of the nuclear motion and quantum-mechanical description of the motion of muon and electron. The cross section is then obtained as

$$\sigma = 2\pi \int_0^\infty \rho d\rho P(\rho), \quad P(\rho) = 1 - \exp\left(- \int_{-\infty}^{+\infty} \Gamma(R) dt \right). \tag{5}$$

Here, $P(\rho)$ is the probability of the Auger ionization of the quasimolecule $(p\mu)_n H$ in the collision with an impact parameter ρ and $\Gamma(R)$ is the frequency of the Auger transitions at the fixed internuclear distance R.

According to calculations, the integral in the exponential (5) is small, so one may use the first two terms in the Taylor expansion of the exponential. Introducing the radial velocity of the nuclei,

$$v_R = dR/dt = v \sqrt{1 - \frac{u_1}{\varepsilon} - \frac{\rho^2}{R^2}}, \tag{6}$$

where $\varepsilon = Mv^2/2$ is the collision energy, v is the velocity, M is the reduced mass of the atoms, and $u_1 = U_1(R) - U_1(\infty)$ is the potential energy of the nuclei in the initial channel (initial term with the account of the Coulomb repulsion between the nuclei and electron screening), one has

$$P(\rho) = 2 \int_{R_0}^\infty \Gamma(R) \frac{dR}{v_R} = \frac{2}{v} \int_{R_0}^\infty \frac{\Gamma(R) dR}{\sqrt{1 - u_1/\varepsilon - \rho^2/R^2}}. \tag{7}$$

R_0 is the minimal distance between the nuclei at given ρ and ε (classical turning point for the motion on the initial term). The factor 2 corresponds to the double passage of the interaction region, one on the way in and the other on the way out.

In a quasiclassical approach, one uses angular momentum L instead of the impact parameter $\rho = (L + 1/2)/p$ (p is the asymptotic momentum of the system in the input channel; atomic units are used with $\hbar = e = m_e = 1$). Then the cross section

$$\sigma = \frac{\pi}{p^2} \sum_{L=0}^{\infty} (2L+1) P(L), \quad p = \sqrt{2M\varepsilon}, \tag{8}$$

$$P(L) = \frac{2}{v} \int_{R_0}^\infty \frac{\Gamma(R) dR}{\sqrt{1 - u_1/\varepsilon - (L+\frac{1}{2})^2/p^2 R^2}}. \tag{9}$$

The calculations with Eqs. (5) and (7), and (8) and (9) give close results (the difference is $\sim 20\%$).

In slow collisions, the frequency of the Auger transitions $\Gamma(R)$ can be calculated in the same way as that for fixed nuclei, since the heavy subsystem does not change its position during the transition in the light system (Franck-Condon principle). The calculations are performed in the perturbation theory, the perturbation that causes the transition to be the interaction between the $p\mu$ atom and electron (Fig. 1):

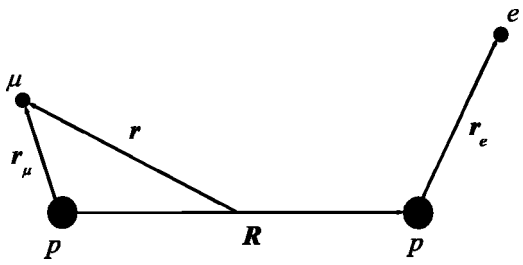

FIG. 1. Coordinate system used in calculations.

$$V = \frac{1}{|\mathbf{R} + \mathbf{r}_e - \mathbf{r}_\mu|} - \frac{1}{|\mathbf{R} + \mathbf{r}_e|}. \tag{10}$$

III. CALCULATION OF $\Gamma(R)$

In the first-order perturbation theory,

$$d\Gamma(R) = 2\pi |V_{fi}|^2 \delta(E_f - E_i) d\nu_f, \tag{11}$$

$$V_{fi} = \langle \Psi_f | V | \Psi_i \rangle. \tag{12}$$

Unperturbed wave functions Ψ_f and Ψ_i are taken as products of the mesic wave function of the problem of two Coulomb centers and one-center electronic wave function:

$$\Psi_i = \Phi_1(\mathbf{r}, R) \psi_{1s}(\mathbf{r}_e), \quad \Psi_f = \Phi_2(\mathbf{r}, R) \psi_{E\ell m}(\mathbf{r}_e). \tag{13}$$

The initial electron is in the ground state of the hydrogen atom. The final state corresponds to the ejected electron with energy $E = k^2/2m_e$, angular momentum ℓ and angular-momentum projection m. Since in the asymptotic region $R \to \infty$, a muon is bound on one proton, and an electron on the other, and we neglect the contribution of the deexcitation process in which the muon is transferred to the other proton, two-center wave functions in the initial and final states are taken as a superposition of symmetric (g) and antisymmetric (u) adiabatic functions, the potentials that determine the motion of the nuclei being taken as half of the sum of those for symmetric and antisymmetric channels:

$$\Phi_1(\mathbf{r}, R) = \frac{1}{\sqrt{2}} (\Phi_{1g} + \Phi_{1u}) \xrightarrow[R \to \infty]{} \varphi_{nj}(\mathbf{r}_\mu),$$

$$\Phi_2(\mathbf{r}, R) = \frac{1}{\sqrt{2}} (\Phi_{2g} + \Phi_{2u}) \xrightarrow[R \to \infty]{} \varphi_{n'j'}(\mathbf{r}_\mu), \tag{14}$$

$$U(R) = \frac{1}{2} [U_g(R) + U_u(R)]. \tag{15}$$

Here n, n' are principal quantum numbers, $j = (n_1 n_2 m)$, $j' = (n_1' n_2' m')$ parabolic quantum numbers, and $\varphi_{nj}(\mathbf{r}_\mu)$ mesic hydrogen wave function in the state $(n n_1 n_2 m)$.

Since even the smallest R in the problem in question is much larger than the dimension of the excited mesic atom, one may use asymptotic functions $\varphi_{nj}(\mathbf{r}_\mu)$ instead of the two-center wave functions $\Phi_i(\mathbf{r}, R)$ when calculating matrix element (12).

Turning to Eq. (11), we observe that

$$E_i = W_1(R) + U_1(R) - I_e, \quad I_e = 13.6 \text{ eV},$$

$$E_f = W_2(R) + U_2(R) + E, \quad E = k^2/2m_e. \tag{16}$$

According to the Franck-Condon principle, the kinetic energy W does not change during the transition: $W_1(R) = W_2(R)$. Then from Eq. (16) and energy conservation $E_f = E_i$, one can find the energy of the emitted electron,

$$\frac{k^2}{2m_e} = U_1(R) - U_2(R) - I_e, \tag{17}$$

which depends on the internuclear distance R at the instance of the emission.

Potential energy of nuclei in the initial (U_1) and final (U_2) channels is the sum of the corresponding molecular term and the Coulomb repulsion of the nuclei, the electron screening correction $\Delta_e(R)$ being included to $U_1(R)$. Strictly speaking, one should take as a perturbation not V, but $V' = V - \Delta_e(R)$ because the interaction of the $p\mu$ atom with the electron is partially taken into account in the potential energy $U_1(R)$. However, the term $\Delta_e(R)$, as well as the second term in Eq. (10) does not contribute to the matrix element V_{fi} because of the orthogonality of the wave functions in the initial and final states.

Since the wave function of the final electron is normalized to the δ function of energy, the final-state interval can be written as $d\nu_f = dE$. To obtain the total rate of the Auger transitions at a given R, one should integrate Eq. (11) over E and sum over ℓ and m:

$$\Gamma(R) = 2\pi \sum_{\ell,m} |V_{fi}|^2, \tag{18}$$

$$V_{fi}^* = \int d\mathbf{r}_\mu d\mathbf{r}_e \varphi_{n'j'}(\mathbf{r}_\mu) \psi_{E\ell m}(\mathbf{r}_e) \times \frac{1}{|\mathbf{R} + \mathbf{r}_e - \mathbf{r}_\mu|} \psi_{1s}(\mathbf{r}_e) \varphi_{nj}^*(\mathbf{r}_\mu). \tag{19}$$

Due to the small mesic atom dimension, one may present Eq. (19) as

$$V_{fi}^* = -\mathbf{D} \cdot \boldsymbol{\nabla}_R Q_{\ell m}(\mathbf{R}), \tag{20}$$

$$\mathbf{D} = \int d\mathbf{r}_\mu \varphi_{n'j'}(\mathbf{r}_\mu) \mathbf{r}_\mu \varphi_{nj}^*(\mathbf{r}_\mu), \tag{21}$$

$$Q_{\ell m}(\mathbf{R}) = \int d\mathbf{r}_e \psi_{E\ell m}(\mathbf{r}_e) \frac{1}{|\mathbf{R} + \mathbf{r}_e|} \psi_{1s}(\mathbf{r}_e). \tag{22}$$

Matrix elements (21) for coordinates x, y, z can be calculated via general formulas given in Ref. [11]. Writing the electron wave functions as

$$\psi_{1s}(\mathbf{r}) = \frac{1}{\sqrt{4\pi}} R_{1s}(r), \quad \psi_{E\ell m}(\mathbf{r}) = R_{E\ell}(r) Y_{\ell m}(\hat{r}), \quad \hat{r} = \frac{\mathbf{r}}{r} \tag{23}$$

and expanding $|\mathbf{R}+\mathbf{r}|$ over spherical functions, one obtains

$$Q_{\ell m}(\mathbf{R}) = \sqrt{4\pi}\, \frac{(-1)^\ell}{2\ell+1} f(R) Y_{\ell m}(\hat{R}), \quad \hat{R} = \frac{\mathbf{R}}{R}, \tag{24}$$

$$f(R) = f_1(R) + f_2(R), \tag{25}$$

$$f_1(R) = \int_0^R dr R_{E\ell} R_{1s} \frac{r^{\ell+2}}{R^{\ell+1}}, \quad f_2(R) = \int_R^\infty dr R_{E\ell} R_{1s} \frac{R^\ell}{r^{\ell-1}}. \tag{26}$$

It is easy to check that

$$\boldsymbol{\nabla}_R Q_{\ell m}(\mathbf{R}) = (-1)^\ell \frac{\sqrt{4\pi}}{R} (a_\ell \mathbf{Y}_{\ell m}^{\ell+1} + b_\ell \mathbf{Y}_{\ell m}^{\ell-1}), \tag{27}$$

$$a_\ell = \sqrt{\frac{\ell+1}{2\ell+1}} f_1(R), \quad b_\ell = \sqrt{\frac{\ell}{2\ell+1}} f_2(R), \tag{28}$$

where $\mathbf{Y}_{\ell m}^{\ell\pm1} = \mathbf{Y}_{\ell m}^{\ell\pm1}(\hat{r})$ are spherical vectors [11].

Inserting Eq. (27) into Eq. (20) and summing the square of the matrix element modulus over m using the formulas from Ref. [12], one has

$$\begin{aligned} \sum_m |V_{fi}|^2 &= \frac{4\pi}{R^2} \sum_m |\mathbf{D} \cdot (a_\ell \mathbf{Y}_{\ell m}^{\ell+1} + b_\ell \mathbf{Y}_{\ell m}^{\ell-1})|^2 \\ &= \frac{4\pi}{R^2} \{ a_\ell^2 [\ell |\mathbf{D}|^2 + (\ell+2) |\mathbf{D} \cdot \mathbf{n}_R|^2] \\ &\quad + b_\ell^2 [(\ell+1) |\mathbf{D}|^2 + (\ell-1) |\mathbf{D} \cdot \mathbf{n}_R|^2] \\ &\quad + 2 a_\ell b_\ell \sqrt{\ell(\ell+1)} (|\mathbf{D}|^2 - 3 |\mathbf{D} \cdot \mathbf{n}_R|^2) \}, \end{aligned}$$

$$\mathbf{n}_R = \frac{\mathbf{R}}{R}. \tag{29}$$

Let us transform the coefficients a_ℓ and b_ℓ (28). Inserting into Eq. (26) $R_{1s} = 2e^{-r}$ and the function $R_{E\ell}$, normalized on the δ function of energy [13],

$$R_{E\ell} = C_{E\ell} (2kr)^\ell e^{-ikr} F(r),$$

$$F(r) = F\left(\frac{i}{k} + \ell + 1, 2\ell + 2, 2ikr \right), \tag{30}$$

$$C_{E\ell} = \frac{2}{(2\ell+1)!} \left(\frac{\Pi_\ell}{1 - \exp} \right)^{1/2}, \quad \Pi_\ell = \prod_{s=1}^{\ell} (s^2 + k^{-2}),$$

$$\Pi_0 = 1, \quad \exp = e^{-2\pi/k}, \tag{31}$$

one obtains the functions $f_{1,2}(R)$:

$$f_1(R)=N_\ell\varphi_{1\ell}(R),\quad f_2(R)=N_\ell\varphi_{2\ell}(R),$$

$$N_\ell=2R(2kR)^\ell C_{E\ell}, \tag{32}$$

$$\varphi_{1\ell}(R)=\int_0^R dr\left(\frac{r}{R}\right)^{2\ell+2} e^{-r-ikr}F(r),$$

$$\varphi_{2\ell}(R)=\int_R^\infty dr\frac{r}{R}e^{-r-ikr}F(r). \tag{33}$$

The final expression for $\Gamma(R)$ becomes then

$$\Gamma(R)=a\left[\frac{1}{2}(|\mathbf{D}|^2-|\mathbf{D}\cdot\mathbf{n}_R|^2)\Gamma_1(R)+|\mathbf{D}\cdot\mathbf{n}_R|^2\Gamma_2(R)\right], \tag{34}$$

where $a=32\pi/3(1-\exp)$,

$$\Gamma_1(R)=\sum_{\ell=0}^{\infty}A_l\frac{\ell(\ell+1)}{2\ell+1}[\varphi_{1\ell}(R)+\varphi_{2\ell}(R)]^2, \tag{35}$$

$$\Gamma_2(R)=\sum_{\ell=0}^{\infty}\frac{A_\ell}{2\ell+1}[(\ell+1)\varphi_{1\ell}(R)-\ell\varphi_{2\ell}(R)]^2, \tag{36}$$

$$A_\ell=\frac{\Pi_\ell(2kR)^{2\ell}}{[(2\ell+1)!]^2}.$$

A much more simpler expression can be obtained for $R\gg1$. In this case, the Coulomb potential $|\mathbf{R}+\mathbf{r}_e|^{-1}$ in Eq. (22) can be expanded in series in r_e/R. The result is

$$Q_{\ell m}(\mathbf{R})=(\mathbf{d}\cdot\boldsymbol{\nabla}_R)\frac{1}{R},\quad \mathbf{d}=\int d\mathbf{r}_e\psi_{E\ell m}\mathbf{r}_e\psi_{1s},$$

$$V_{fi}=\frac{\mathbf{D}\cdot\mathbf{d}-3(\mathbf{D}\cdot\mathbf{n}_R)(\mathbf{d}\cdot\mathbf{n}_R)}{R^3},$$

$$\Gamma(R)=16a(|\mathbf{D}|^2+3|\mathbf{D}\cdot\mathbf{n}_R|^2)\frac{\exp\left(-\frac{4}{k}\arctan k\right)}{(1+k^2)^5}\frac{1}{R^6}. \tag{37}$$

A simple expression for $\Gamma(R)$ may be also obtained when one takes a plane wave for the wave function of the ejected electron (this is justified for $k\gg1$) and the Auger ionization is considered for R of the order of the target atom dimension

$$\Gamma(R)=|\mathbf{D}|^2\frac{16}{3k}e^{-2R}. \tag{38}$$

A comparison of $\Gamma(R)$ calculated with different formulas is given in Table I.

As seen from Table I, in the range $1<R<5$, the difference between the results obtained with accurate Eq. (34) and those obtained in the plane-wave approximation (38) does not exceed 50%. For $R\geqslant10$ the asymptotic formula (37), which takes into account only the dipole-dipole interaction between the atoms, gives quite good results.

TABLE I. Values of $\Gamma(R)$ (in atomic units), calculated with Eqs. (34), (37), and (38) for mesoatomic transition 5040→4030. Here $k\approx1.747$.

R, (a.u.)	Eq. (34)	Eq. (37)	Eq. (38)
0.5	0.74		1.12
1	0.32		0.42
2	7.0×10^{-2}		5.6×10^{-2}
3	1.3×10^{-2}		7.6×10^{-3}
4	1.9×10^{-3}	4.5×10^{-5}	1.0×10^{-3}
5	2.8×10^{-4}	1.2×10^{-5}	1.4×10^{-4}
6	4.8×10^{-5}	3.9×10^{-6}	1.9×10^{-5}
8	1.6×10^{-6}	7.0×10^{-7}	3.4×10^{-7}
10	2.4×10^{-7}	1.8×10^{-7}	6.3×10^{-9}

IV. CALCULATION OF $|\mathbf{D}|^2$

The frequency of the Auger transitions depends on the squared dipole matrix element of the mesic atom,

$$|\mathbf{D}|^2=|\mathbf{r}_{j'j}|^2=|x_{j'j}|^2+|y_{j'j}|^2+|z_{j'j}|^2$$

and on its squared component along the internuclear axis

$$|\mathbf{D}\cdot\mathbf{n}_R|^2=|z_{j'j}|^2.$$

We need to calculate these matrix elements for parabolic states. In parabolic coordinates the matrix elements of coordinates x and z are real, while that of the y coordinate is imaginary with $y_{j'j}=\pm ix_{j'j}$. For this reason

$$|\mathbf{D}|^2=2(x_{j'j})^2+(z_{j'j})^2,\quad |\mathbf{D}\cdot\mathbf{n}_R|^2=(z_{j'j})^2. \tag{39}$$

The most probable deexcitation transitions are those in which the lower states $j'=(n_1'n_2'm')$ differ from the upper one by only one quantum number, this number being by a unit smaller than the upper one. The other matrix elements are smaller by at least an order of magnitude. One should note that there exists a selection rule for magnetic quantum number m: the matrix element of the x coordinate is nonzero only for $m-m'=1$, while the matrix element of the z coordinate is nonzero only for $m'=m$.

V. RESULTS AND DISCUSSION

An important characteristic of the process in question is relative energy of the nuclei after the collision, ε', counted from the final term value at $R\to\infty$. One can find it from the energy conservation:

$$\varepsilon'+U_2(\infty)+\frac{k^2}{2m_e}=\varepsilon+U_1(\infty)-I_e. \tag{40}$$

Taking into account Eq. (17), one has

$$\varepsilon'\equiv\varepsilon'(R)=\varepsilon(R)+u_2(R)-u_1(R),$$

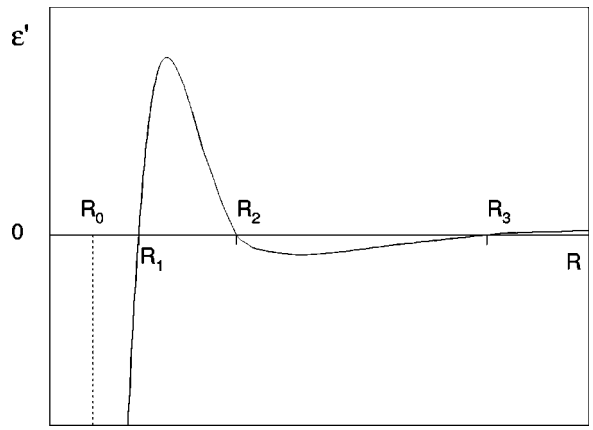

FIG. 2. A sample of the dependence of relative energy of nuclei in the final state on the internuclear distance at which ionization occurred. R_0 is a turning point.

$$u_{1,2}=U_{1,2}(R)-U_{1,2}(\infty). \tag{41}$$

For $R\gtrsim 1$,

$$u_1(R)\approx\frac{\beta}{R^2}S(R),\quad \beta=\frac{3}{2}n(n_1-n_2),$$

$$S(R)=(1+2R+2R^2)e^{-2R}, \tag{42}$$

$$u_2(R)\approx\beta'/R^2,\quad \beta'=\frac{3}{2}n'\,(n_1'-n_2'). \tag{43}$$

So the relative kinetic energy of the nuclei in the final state is a function of the internuclear distance at which the Auger transition occurred. As a result there exists an energy distribution in the final state, the energy ε' may be positive or negative. A typical dependence of ε' on the internuclear distance at which the electron ejection occurred is shown in Fig. 2. Negative ε' means that the nuclei cannot separate infinitely after the collision, i.e., the system is bound.[2]

The total cross section of the Auger ionization summed over the final states and averaged over the initial ones is

$$\sigma_n=\sum_{jj'}P_j\sigma_{jj'},\quad P_j=\frac{2-\delta_{0m}}{n^2}, \tag{44}$$

n is the principal quantum number of the initial mesic atom state. Summing over the quantum number sets j and j' is performed at fixed $n=n_1+n_2+m+1$ and $n'=n-1$. Using the results obtained in Secs. III and IV, we obtain for the sum over the final states,

$$\sigma_j=\sum_{j'}\sigma_{jj'}=\sigma_{n_1,n_1-1}+\sigma_{n_2,n_2-1}+\sigma_{m,m-1}. \tag{45}$$

[2]Menshikov was the first to point out the possibility of the bound-state formation after the Auger transition in the $(p\mu)_n+H_2$ system [13].

Here only those quantum numbers that are left change in the transition,

$$\sigma_{jj'}=\frac{2\pi}{p^2}\sum\,(2L+1)\int_{R_0}^{\infty}\Gamma_{jj'}(R)\frac{dR}{v_R}, \tag{46}$$

$\Gamma_{jj'}(R)$ being determined in Eq. (34) as $\Gamma(R)$.

Let us write the expression for the rate of the Auger ionization process:

$$\lambda_{jj'}=N_0 v\sigma_{jj'},\quad \lambda_n=N_0 v\sigma_n,$$

$$N_0=4.25\times10^{22}\,\mathrm{cm}^{-3}=0.63\times10^{-2}\,\mathrm{a.u.} \tag{47}$$

For the case shown in Fig. 2 the integral over R in Eq. (46) comprises four parts:

$$\int_{R_0}^{\infty}f(R)dR=\left(\int_{R_0}^{R_1}+\int_{R_1}^{R_2}+\int_{R_2}^{R_3}+\int_{R_3}^{\infty}\right)f(R)dR.$$

The first and the last integrals are small (the first due to the smallness of the integration region, the last because $f(R)$ is small for $R>R_3$) and can be omitted. The total ionization cross section can then be expressed as a sum of two parts. One of them (σ^+) determines the probability of the Auger process with infinite motion of the nuclei after the collision (positive kinetic energy of the nuclei, Auger-plus process). The second one (σ^-) determines the probability of the nuclei to occur in the bound state after the electron ejection (negative kinetic energy of the separated atoms, Auger-minus process). So

$$\sigma_{jj'}=\sigma_{jj'}^{+}+\sigma_{jj'}^{-},$$

$$\sigma_{jj'}^{+(-)}=\frac{2\pi}{p^2}\sum\,(2L+1)\int_{R_{1(2)}}^{R_{2(3)}}\Gamma_{jj'}(R)\frac{dR}{v_R}. \tag{48}$$

What is important for the muon catalyzed fusion, as well as for a number of other problems of the mesic atom physics, is an average energy acquired by the nuclei as a result of the Auger transition. For a partial $j\to j'$ transition, this energy for an Auger-plus process is

$$\varepsilon_{jj'}'^{+}=\frac{\sum\,(2L+1)\int_{R_1}^{R_2}\varepsilon'(R)\Gamma_{jj'}(R)\frac{dR}{v_R}}{\sum\,(2L+1)\int_{R_1}^{R_2}\Gamma_{jj'}(R)\frac{dR}{v_R}}. \tag{49}$$

To obtain a corresponding formula for the Auger-minus process, one should change the integration limits in Eq. (49): $R_1\to R_2$, $R_2\to R_3$. The average energy of the nuclei in the $n\to n'$ transition is then

$$\langle\varepsilon_n'^{+}\rangle=\frac{1}{\sigma_n^{+}}\sum_{jj'}P_j\sigma_{jj'}^{+}\varepsilon_{jj'}'^{+}. \tag{50}$$

TABLE II. The rates ($10^{12}\,s^{-1}$) of Auger-plus and Auger-minus processes and average final-state energies (eV) as functions of the collision energy ε.

n	ε	λ_n^+	λ_n^-	$\langle\varepsilon_n'^+\rangle$	$\langle\varepsilon_n'^-\rangle$
	0.005	2.29	3.29	0.78	−0.34
	0.01	2.91	4.02	0.75	−0.37
6	0.04	3.99	4.43	0.70	−0.34
	0.10	5.91	4.48	0.66	−0.35
	1.00	12.5	0.59	1.29	−0.72
	0.005	0.96	1.22	0.96	−0.28
	0.01	1.13	1.43	0.90	−0.24
5	0.04	1.60	1.51	0.82	−0.26
	0.10	2.39	1.46	0.76	−0.25
	1.00	4.50	0.11	1.31	−0.91
	0.005	0.24	0.16	1.00	−0.17
	0.01	0.33	0.23	1.03	−0.18
4	0.04	0.50	0.27	0.91	−0.17
	0.10	0.67	0.23	0.81	−0.16
	1.00	1.05	0.013	1.37	−0.98

The rates $\lambda_n^{\pm}=N_0 v\sigma_n^{\pm}$ and average energies $\langle\varepsilon_n'^+\rangle$, $\langle\varepsilon_n'^-\rangle$ for the transitions $n\to n-1$ ($n=6,5,4$) are given in Table II for various collision energies.

Energy dependence of the total Auger rates $\lambda_n(\varepsilon)$ is shown in Fig. 3, together with the results of paper Ref. [5]. As seen from Fig. 3, the results obtained here are in a good agreement with those of paper Ref. [5] for energies $\varepsilon \geqslant 0.5$ eV. Figure 4 shows the energy dependence of the rate of the Auger-minus process $\lambda_n^-(\varepsilon)$.

The bound state in which the system appeared will decay

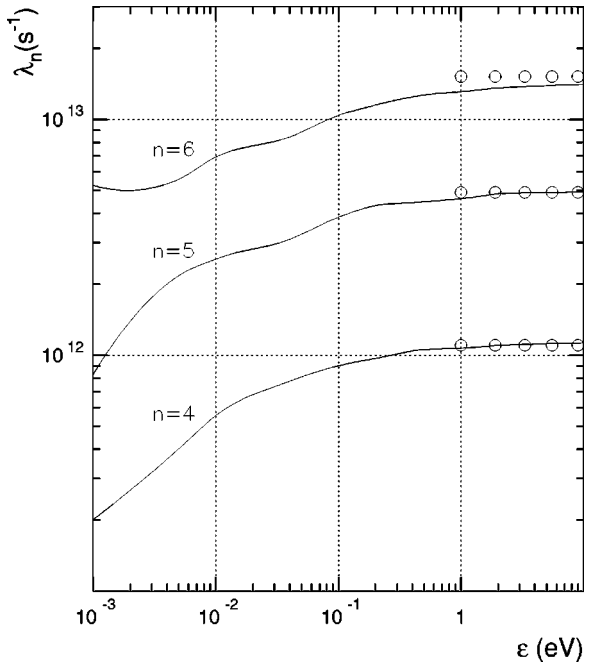

FIG. 3. Energy dependence of the total Auger ionization rates $\lambda_n(\varepsilon)$ (per second) for $n=4$, 5, and 6. The circles show the results of Ref. [5].

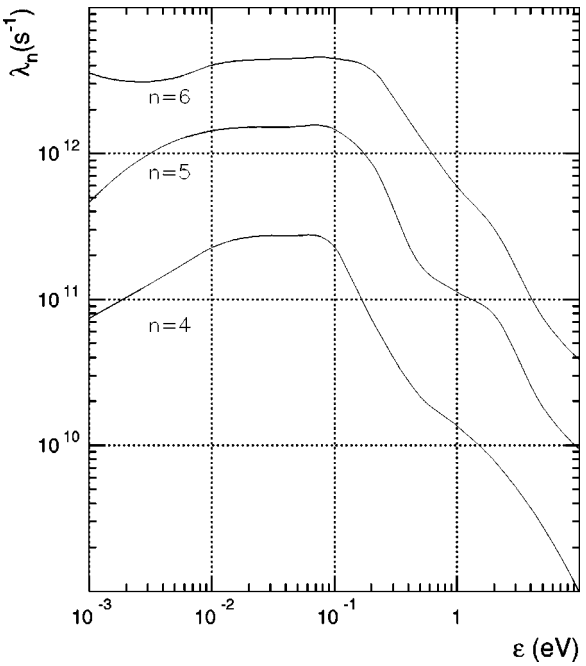

FIG. 4. Energy dependence of the rate of the Auger-minus process $\lambda_n^-(\varepsilon)$ (per second) for $n=4$, 5, and 6.

either via predissociation (Coulomb deexcitation)

$$(p\mu p)_{n'}\to(p\mu)_{n''}+p,\quad n''=n'-1, \tag{51}$$

or via the external Auger ionization

$$(p\mu p)_{n'}+H_2\to(p\mu)_{n''}+H_2^+ +e. \tag{52}$$

If the binding energy of the quasimolecule $(p\mu p)_{n'}$ is smaller than thermal energy, it can decay in quasielastic collisions with target molecules,

$$(p\mu p)_{n'}+H_2\to(p\mu)_{n'}+p+H_2. \tag{53}$$

In this case, the mesic atoms do not accelerate. As a rule, the average binding energy of the quasimolecule amounts to about several tenths eV, so the quasielastic mechanism has low probability.

If the system in the final state represents a quasimolecule comprising the excited mesic atom and hydrogen molecular ion $(p\mu)_{n'}H_2^+$, or $(p\mu p)_{n'}H$, the internal Auger process is also possible. In this case, as it was shown by Menshikov [13], mesic atom acquires some part of the muon energy, accelerating up to energies about 1 eV.

The predissociation process (51) leads to a two-particle decay, in which the deexcitation energy transforms into the kinetic energy of the fragments because of the Coulomb repulsion of nuclei. The predissociation rate can be determined according to the formula [14]

$$\lambda_{pr}=\nu w_{pr},\quad w_{pr}=2e^{-2\delta_{ij}}(1-e^{-2\delta_{ij}}). \tag{54}$$

Here, ν is the oscillation frequency of the quasimolecule, equal to

$$\nu = \left(2 \int_a^b \frac{dR}{v_R} \right)^{-1} \tag{55}$$

(a and b are the turning points of the nuclear motion in the well of the lower term n'), and the Stückelberg parameter δ_{ij} is determined by the formula [15]

$$\delta_{ij} = \left| \mathrm{Im} \int_{\mathrm{Re}R_c}^{R_c} [p_i(R) - p_j(R)] dR \right|, \tag{56}$$

$$p_{i,j}(R) = \sqrt{2M(E' - U_{i,j}(R)) - (L+1/2)^2/R^2},$$

$$E' = \varepsilon' + U_i(\infty),$$

where $p_i(R)$ and $p_j(R)$ are radial momenta of the relative motion of the nuclei in the initial and final channels of reaction (51), respectively. A T-type branch point R_c in the complex plane of internuclear distance R connects the terms $i = [n_1\, n_2\, m\, \lambda]$ and $j = [n_1\, n_2 - 1\, m\, \lambda]$, where n_1, n_2, m—parabolic quantum numbers and $\lambda = (g \text{ or } u)$ is the parity of the term. As a matter of fact, T-type branch points connect pairwise either g states or u states. The real parts $\mathrm{Re}\, R_c$ are practically the same for g and u states for a given set of other quantum numbers, while imaginary parts $\mathrm{Im}\, R_c$ are two times smaller for g terms, as compared with u terms. For this reason, predissociation proceeds with a noticeable probability only from the g states of the lower n' term. After the Auger $n \to n'$ transition, the system in the lower state is described by the wave function $\Psi = (\Psi_g + \Psi_u)/\sqrt{2}$, which is a mixture of g and u states with equal weights. Then one may write

$$\lambda_{pr} = \tfrac{1}{2}\lambda_{pr}^g + \tfrac{1}{2}\lambda_{pr}^u \approx \tfrac{1}{2}\lambda_{pr}^g \approx \nu e^{-2\delta_{ij}} \tag{57}$$

because for the Coulomb deexcitation at low levels ($n' \lesssim 5$), the Stückelberg parameter δ_{ij} is rather large. The predissociation rates $\overline{\lambda}_{pr}$ averaged over all bound states with a given n' were found to be $\sim 10^{10}$–10^{12} s^{-1} for $n' = 3$–5.

The rate of the Auger decay of the weakly bound system $(p\mu p)_{n'}$ can be approximated by the rate of the Auger process $(p\mu)_{n'} + H \to (p\mu)_{n'-1} + H^+ + e$. For target density equal to the liquid hydrogen density (LHD), this rate is comparable with the predissociation rate. However, for usual experimental densities of gaseous targets ($\sim 5\%$ of LHD), the predissociation dominates, since its rate does not depend on the target density, unlike the Auger decay.

So, mesic hydrogen deexcitation via the external Auger process on the hydrogen target could lead to the formation of the bound state of the mesic molecule, which decays very quickly (with the rate of $\sim 10^{11}$–10^{12} s^{-1}) into two heavy particles with high-energy release (~ 100 eV). This circumstance can probably explain the appearance of a large fraction of fast pionic atoms in the low-energy states [8], as well as influence the results of the mesic atom cascade calculations.

[1] L. Bracci and G. Fiorentini, Nuovo Cimento Soc. Ital. Fis., A **43A**, 9 (1978).

[2] A.V. Kravtsov and A.I. Mikhailov, Zh. Eksp. Teor. Fiz. **107**, 1473 (1995) [JETP **80**, 822 (1995)].

[3] L.I. Ponomarev and E.A. Solovyov, Pis'ma Zh. Eksp. Teor. Fiz. **68**, 7 (1998).

[4] A.V. Kravtsov and A.I. Mikhailov, Phys. Rev. A **58**, 4426 (1998).

[5] M. Leon and H.A. Bethe, Phys. Rev. **127**, 636 (1962).

[6] A.P. Bukhvostov and N.P. Popov, Zh. Eksp. Teor. Fiz. **82**, 23 (1982) [Sov. Phys. JETP **55**, 13 (1982)].

[7] G. Ya. Korenman and G.A. Fesenko, in *Proceedings of the Fifth International Workshop on Autoionization Phenomena in Atoms, Dubna, Russia, 1995* (Joint Institute for Nuclear Research, Dubna, 1995).

[8] J.F. Crawford *et al.*, Phys. Lett. B **213**, 391 (1988); Phys. Rev. D **43**, 46 (1991).

[9] A.V. Kravtsov, A.I. Mikhailov, I.A. Mikhailov, and L.I. Ponomarev, Hyperfine Interact. **138**, 103 (2001).

[10] V.V. Gusev, V.P. Popov, and V.N. Pomerantsev, Hyperfine Interact. **119**, 141 (1999).

[11] H.A. Bethe and E.E. Salpeter, *Quantum Mechanics of One-and Two-Electron Atoms* (Springer-Verlag, Berlin, 1957).

[12] D.A. Varshalovich and A.N. Moskalev, and V.K. Khersonskiy, *Quantum Theory of Angular Momentum* (Nauka, Leningrad, 1975).

[13] L.I. Menshikov, Muon Catal. Fusion **2**, 173 (1988).

[14] L.D. Landau and E.M. Lifshits, *Quantum Mechanics* (Nauka, Moscow, 1989).

[15] E.A. Solovyov, Uspekhi Fiz. Nauk **157**, 437 (1989) [Sov. Phys. Usp. **32**, 228 (1989)].