Coulomb deexcitation and isotope exchange of excited mesic hydrogen

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(Received 26 May 1998)

The processes of Coulomb deexcitation and quasiresonant charge exchange have been considered in the framework of the asymptotic theory of the nonadiabatic transitions. The approach used is scrutinized and improved in the light of recent critical statements. The unambiguous agreement between different calculations for energies $\epsilon > 0.5$ eV proves the approximation used to be valid. [S1050-2947(98)08511-4]

PACS number(s): 36.10.Dr, 36.10.Gv

The cascade of the excited mesic hydrogen atom in the mixture of hydrogen isotopes is an interesting problem both in itself and for the muon catalyzed fusion. The most important reactions that determine the main characteristics of mesic atoms after the cascade are Coulomb deexcitation

$$(\mathrm{H}\mu)_n^* + \mathrm{H} \rightarrow (\mathrm{H}\mu)_{n-1}^* + \mathrm{H} \tag{1}$$

and isotope exchange

$$(\mathrm{H}\mu)_n^* + \mathrm{H}' \rightarrow (\mathrm{H}'\mu)_n^* + \mathrm{H}. \tag{2}$$

The acceleration of the excited mesic atoms during cascade transitions has attracted a lot of attention in the last few years [1,2], especially after the experimental observation of ''hot'' pionic atoms [3]. Theoretical analysis of the matter numbers few papers, which are either unable to predict a reaction rate large enough to explain the experiment [4], or are rather out of date [5], i.e., using an approach that is inadequate for the problem. For this reason it can be said that until now the outlook on the problem has been ambiguous. In Ref. [6] it was declared that our results on the Coulomb deexcitation rate [4] as well as on the isotope exchange [7] were ''*unreliable and must be carefully analyzed.*'' Despite such a strong statement, no clear physical motivations for such criticism are presented except for the comment that the number of partial waves involved in the process is too small ($l \sim M v \rho \leqslant 10$), for which reason the impact parameter approximation we used is not valid. Reference [6] stimulated us to reanalyze the approach we used in [4] and to scrutinize the assumptions we made. Here we present calculations of the Coulomb deexcitation rates for pionic hydrogen atoms with $n=4$, in order to compare them with the results of [6].

The effective potential of interaction of the excited mesic hydrogen atom with a hydrogen nucleus is asymptotically determined by

$$u(R) \simeq \tfrac{3}{2} n(n_1 - n_2)/R^2,$$

where R is the internuclear distance and (n,n_1,n_2) are parabolic quantum numbers. The validity condition for the WKB approximation $d\lambda/2\pi dR \ll 1$ is fulfilled here, since for $n_1 \neq n_2$ and $n \geqslant 2$

$$\frac{1}{2\pi}\frac{d\lambda}{dR} \sim (3Mn|n_1 - n_2|)^{-1/2} \ll 1.$$

M is the reduced mass of the colliding atoms.

As before [4], we use the asymptotic theory of the nonadiabatic transitions[1] developed in [8]. Coulomb deexcitation is considered as a nonadiabatic transition via the complex branch point of the T type [8], which connects the terms with parabolic quantum numbers (n,n_1,n_2,m) and $(n+1,n_1,n_2+1,m)$ and is determined by the promotion of the former term to the top of the barrier in the quasiangular equation of the problem of the two Coulomb centers. The position of the T point determines the region where the asymptotic expansion for the lower term is valid. This means that for the upper term the asymptotic expansion is not valid for $R \sim \mathrm{Re}\, R_T$. The branch point connects either two symmetric g states or, alternatively, two antisymmetric u states, and the real parts of these branch points are equal. However, only transitions between the g states are considered, because for the u states the imaginary parts of the branch points are twice as large as for g states, so the probability for such a transition is much smaller.

When solving the problem of mesic atom collisions with semiclassical methods one should choose the reduced mass of the system M and the unit of the mass m in order to use thereafter mesic atom units with $\hbar = m = e = 1$. Such a choice is simple and unambiguous in the physics of atomic collisions due to the smallness of the electron mass with respect to the nuclear ones. For mesic atom collisions several variants of the mass choice are possible; for example,

$$1/M = 1/(M_1 + \mu) + 1/M_2, \quad 1/m = 1/\mu + 1/M_1, \tag{3}$$

$$1/M = 1/M_1 + 1/M_2, \quad 1/m = 1/\mu + 1/M_1, \tag{4}$$

$$1/M = 1/M_1 + 1/M_2, \quad 1/m = 1/\mu + 1/(M_1 + M_2), \tag{5}$$

$$1/M = 1/M_1 + 1/M_2, \quad m = \mu, \tag{6}$$

where M_1 and M_2 are the masses of the hydrogen isotope nuclei in the initial and final mesic atoms, respectively, and μ is the mass of the light particle (muon or pion). The masses (3) correspond to the correct reduced mass of the system $\mathrm{H}\mu + \mathrm{H}'$ and correct asymptotic values of the momentum and energy in the input channel. Such a choice was

[1]This approach was called ''improved adiabatic approach'' (IAA) in [6] and ''adiabatic complex plane method'' (ACPM) in [9].

used in the improved two-level approximation [10] for a quantum-mechanical description of the system of three bodies, one of which is muon. The masses (4) and (5) are often used in the mesic atom physics. We used masses (4) in [4] when considering the Coulomb deexcitation, and masses (5) were used in [9] in the adiabatic hyperspherical approach in the study of low-energy scattering of a mesic atom in the ground state. The authors of [6] did not indicate what masses they used, so we have recalculated the reaction rates for all possible choices (3)–(6) of the masses [11] in order to compare them with the results of [6].

First of all we have realized that the approximate expression for the Massey parameter

$$\delta(\rho)=\frac{\pi\Delta u(\mathrm{Re}\ R_c)}{4v_c(\rho)}\ \mathrm{Im}\ R_c \tag{7}$$

that we used in [4] might be too rough. Here ρ is the impact parameter, $\Delta u(R)$ is the difference between the upper and lower terms, R_c is the complex branch point, v_c is the average radial velocity at the transition point $v_c(\rho)=(p_1+p_2)/2M$, $p_i=\sqrt{2M[\epsilon-u_i(\mathrm{Re}\ R_c)-\epsilon\rho^2/(\mathrm{Re}\ R_c)^2]}$, and $\epsilon=Mv^2/2$ is a relative energy of the colliding particles at $R\to\infty$. For all terms that we considered we recalculated the Massey parameter directly as a contour integral[2]

$$\delta(\rho)=\left|\mathrm{Im}\int_C p(R,\rho)dR\right|, \tag{8}$$

which depends on both the collision energy and the impact parameter, or, for fixed angular momentum l,

$$\delta(l)=\left|\mathrm{Im}\int_C p(R,l)dR\right|. \tag{9}$$

Here $p(R,\rho)=\sqrt{2M[\epsilon-u(R)-\epsilon\rho^2/R^2]}$ and $p(R,l)=\sqrt{2M[\epsilon-u(R)-l(l+1)/2MR^2]}$ are radial momenta, C is the contour that begins and ends on the real axis going around the complex branch point R_c. It turned out that the value of the $\delta(\rho)$ changed by only 10%, but it changed the cross section considerably because of the exponential dependence of the reaction probability on the Massey parameter:

$$w(\rho)=2\ \exp(-2\delta)[1-\exp(-2\delta)]. \tag{10}$$

The cross section is obtained then for each term as

$$\sigma_{n_1n_2}=\pi\int_0^{\rho^2_{\max}} w(\rho)d\rho^2 \tag{11}$$

or, for angular momentum l,

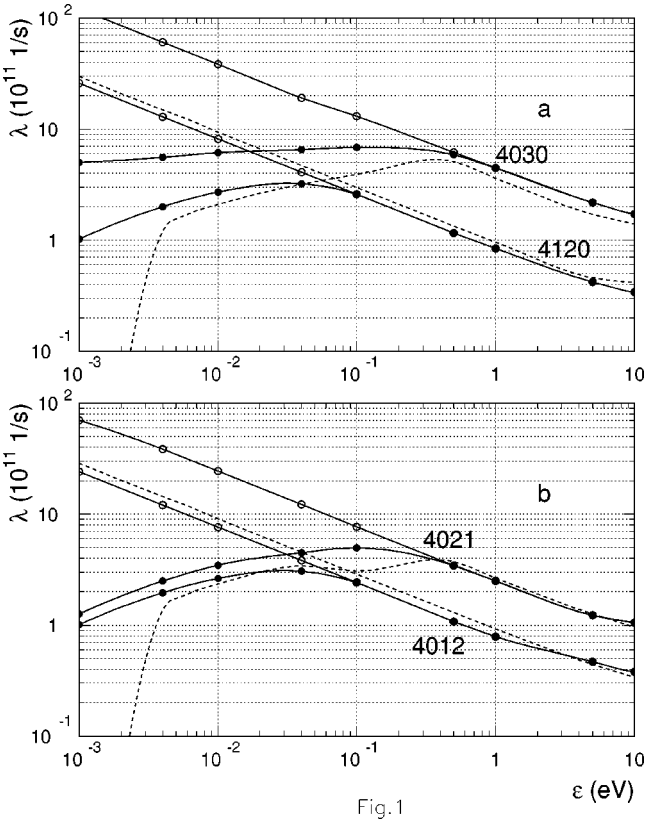

FIG. 1. Partial Coulomb deexcitation rates for $n=4$ [reaction (15)] calculated by summation over partial waves with masses (5). (a) Initial terms 4030 and 4120; (b) initial terms 4021 and 4012. Solid curves, the results of the present paper. Dashed curves, the results of paper [6]. Black circles, with the account of the screening correction; open circles, without screening correction.

$$\sigma_{n_1n_2}=\frac{\pi}{k^2}\sum_{l=0}^{l_{\max}}(2l+1)w(l), \tag{12}$$

where $l_{\max}$ is the maximum angular momentum for which the radial momentum is real on the trajectory, i.e., for $R\geqslant\mathrm{Re}\ R_c$. Since the transition region is determined by the position of the branch point R_c, we consider only trajectories with turning points $R_t\leqslant\mathrm{Re}\ R_c$. The reaction rate reduced to the liquid-hydrogen density $N_0=4.25\times10^{22}\ \mathrm{cm}^{-3}$ is

$$\lambda_{n_1n_2}=N_0\sigma_{n_1n_2}v. \tag{13}$$

The total rate for the given n is then obtained as [12]

$$\lambda=\frac{1}{2}\sum_{(n_1-n_2)<0}\frac{2-\delta_{0m}}{n^2}\lambda_{n_1n_2}, \tag{14}$$

where the summation is performed over all attracting terms and one-half means that only g terms are considered in the initial state.

The calculated rates for the Coulomb deexcitation reaction

$$(p\pi)^*_n\to(p\pi)^*_{n-1},\quad n=4 \tag{15}$$

are shown in Figs. 1(a) and 1(b) for masses (5). One can see that our partial rates reproduce quite well the results of Ref.

[2]It should be noted that we could do it only for terms with $n\leqslant5$, because for higher states the code that calculates the terms in the complex R plane does not work effectively for sufficiently high Re R. At the same time, for the fixed relative error in δ the relative error in the transition probability $w\sim\exp(-2\delta)$ is proportional to δ; i.e., it decreases with increasing n.

[6] for transitions 4012→3002 and 4120→3110, only if we neglect the screening correction. For transitions 4030 →3020 and 4021→3011 the agreement is quite good for energies $\epsilon > 0.5$ eV, where the screening correction is small.

In the absence of screening the effective potential has asymptotically the form $u(R) = -\beta/R^2$, $\beta > 0$ for attracting terms. Equating the radial momentum to zero, one can obtain the maximum impact parameter for the turning point $R_t = \mathrm{Re}\, R_c$ as $\rho_{\max}^2 = \beta/\epsilon + (\mathrm{Re}\, R_c)^2$, which gives for the cross section

$$\sigma \sim \beta/\epsilon + (\mathrm{Re}\, R_c)^2.$$

If $(\mathrm{Re}\, R_c)^2 \ll \beta/\epsilon$, one obtains for the reaction rate energy dependence for this case

$$\lambda = N_0 \sigma v \sim 1/\sqrt{\epsilon}.$$

Such a dependence is clearly seen in Fig. 1 for the rates calculated without the screening correction.

The effective potential with the screening correction [12] reads as

$$u_{\mathrm{eff}}(R) = -\beta(R^{-2} + 2R^{-1} + 2)e^{-2R} + \epsilon\rho^2/R^2.$$

A specific feature of such a potential is a barrier at large R. In order to find the maximum impact parameter, one has to find the maximum of the barrier and equate it to the energy, i.e., to solve the system

$$\frac{\partial u_{\mathrm{eff}}(R)}{\partial R} = 0,$$

$$u_{\mathrm{eff}}(R) = \epsilon. \tag{16}$$

The turning point can be found then from the equation

$$2R_t \exp(-2R_t) = \epsilon/\beta. \tag{17}$$

Obviously the left part of Eq. (17) cannot be higher than 1, so the system (16) has no solution for $\epsilon > \beta$. This means that for large energy $\epsilon > \beta$ the turning point is not determined by the top of the barrier. The maximum impact parameter is then determined by the value of the potential at $R = \mathrm{Re}\, R_c$ according to the requirement $p(\mathrm{Re}\, R_c, \rho_{\max}) = 0$.

The total rates [Fig. 2(a)] calculated with masses (5) for $\epsilon > 0.5$ eV coincide very well with those given in [6] if one corrects an obvious mistake made in [6]. It is easy to see that the total rates calculated by Eq. (9) of Ref. [6] should be two times smaller than those given in [6].

In contrast with paper [6] we did not consider the transition 4111→3101, but, as can be seen from [6], its contribution is very small. It should be expected because of the absence of the ''focusing'' for weakly attractive terms.

Figure 2(b) demonstrates the difference between the rates, calculated by integration over the impact parameter (11) and by summation over partial waves (12). The old results of Ref. [4] are shown as well. One can see that the difference in the total rates is quite small even for the lowest energy, despite the very small value of $l_{\max}$. The difference between the present results and those of Ref. [4] is explained mainly by the difference in the Massey parameters, roughly estimated in [4] by Eq. (7).

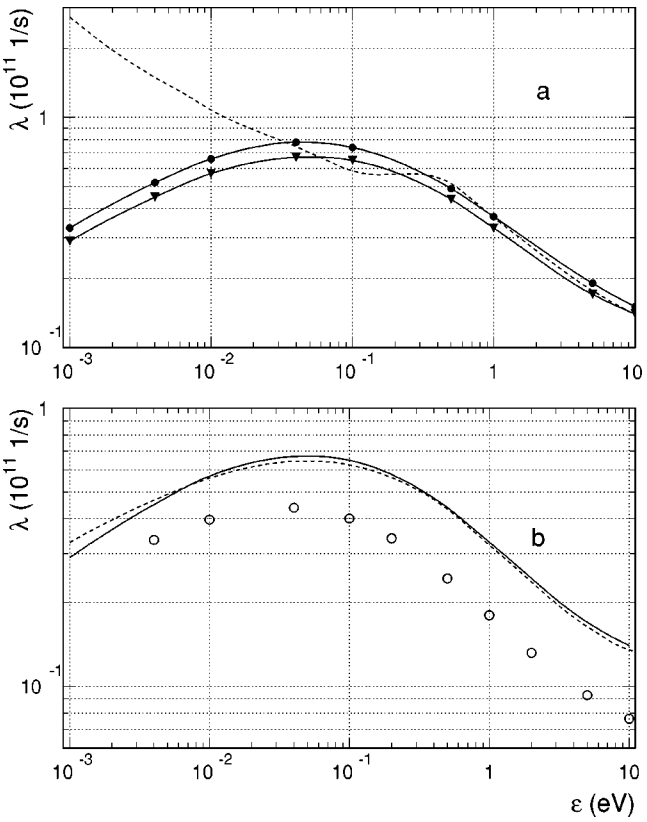

FIG. 2. Total rates of the Coulomb deexcitation (15) obtained by summation over angular momentum l. Triangles, calculation with masses (4). Circles, calculation with masses (5). The dashed line shows the results of [6] divided by 2. (b) Total Coulomb deexcitation rates (15) obtained with masses (4) by summation over angular momentum l (solid line) and by integration over the impact parameter ρ (dashed line). Circles show the results of [4].

Quasiresonant charge exchange (2) is characterized by the small splitting between the initial and final states of the reaction due to the small mass difference between nuclei H and H′. Solov'ev showed [13] that the difference in masses of isotopes H and H′ is equivalent to the difference in charges of nuclei, the heavier nucleus having the larger charge $1 + \Delta Z$ with

$$\Delta Z = \sqrt{M_2/(M_2 + m_\mu)} - \sqrt{M_1/(M_1 + m_\mu)},$$

where M_1 and M_2 are the masses of the light and heavy nuclei, respectively, and m_μ is the muon mass. The quasiresonant charge exchange reaction was considered in detail in the Rosen-Zener-Demkov model [14].

According to [8], transitions of this type are related with the branch points of the P series that connect the initial term (n, n_1, n_2, m) with the final one, which has the same quantum numbers but different muon localization. The transition is caused by the exchange interaction, which asymptotically reads as

$$u_{\mathrm{ex}}(R) = (-)^m \frac{2(2R/n)^{n-n_1+n_2} \exp[-n-(R/n)]}{n^3 n_2!(n_2+m)!}, \tag{18}$$

where m is the magnetic quantum number. The splitting value near the branch point can be expressed as

$$\Delta u(R)=\sqrt{d^2+u_{\rm ex}^2(R)}\,, \tag{19}$$

where d is the resonance defect. The branch point location is derived from the equation

$$d^2+u_{\rm ex}^2(R)=0,$$

which determines the infinite sequence of equidistant points, which have approximately equal Re R_P. Unlike the T-branch points, the branch points of the P series depend on the masses of the nuclei. For pd, pt, and dt, combinations the real parts of the P-type branch points are larger than those of the T points, so one may use the asymptotic expansion for the terms involved. The transition is characterized by the small value of the Massey parameter due to the small resonance defect $d\sim(0.008-0.03)/n^2$.

The reaction probability for the Rosen-Zener-Demkov case [14] was derived to be

$$w(\rho)=1/2\,\cosh^2(\delta), \tag{20}$$

where δ is determined by Eq. (8) for the branch point closest to the real axis. The difference between Eqs. (10) and (20) is caused by the presence of the infinite series of the branch points in the latter case. The total reaction rate should be calculated here as

$$\lambda=\sum_{(n_1-n_2)<0}\frac{2-\delta_{0m}}{n^2}\lambda_{n_1n_2}. \tag{21}$$

We chose the reduced masses according to Eq. (4), though the mass choice is less important here because of the small value of the Massey parameter. The cross section was calculated via integration over the impact parameter (11), which gives results very close to those obtained by summation over partial waves [15]. The results for $n=2$, 3, 4, and 5 are shown in Fig. 3. As seen from Fig. 3, our results do not differ much from those of Ref. [9] and the difference could beexplained by the asymptotic expansion we used for the terms instead of the accurate terms used in [9].

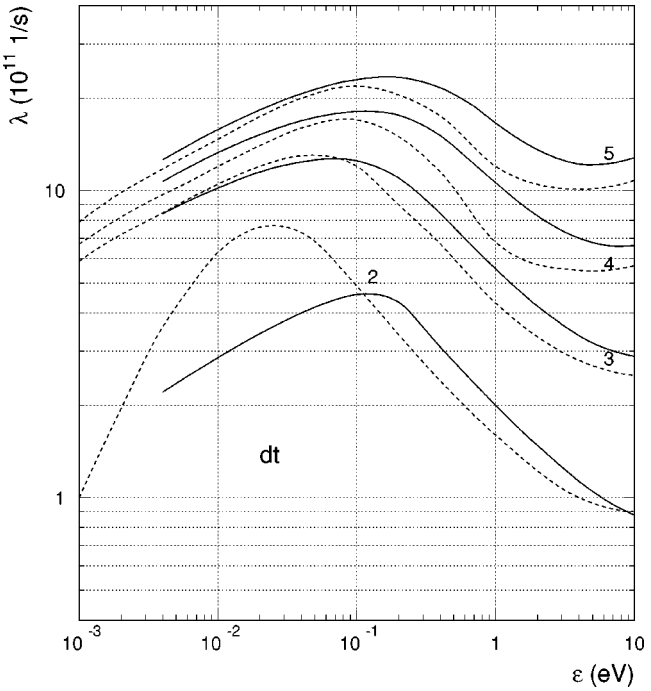

FIG. 3. Rates for the isotope exchange reaction (2) for H$=d$ and H$'=t$. Solid lines—the results of the present paper obtained by integration over the impact parameter, dashed lines—the results of Ref. [9]. Principal quantum numbers are shown at the curves.

Coulomb deexcitation and isotope exchange are considered here from the viewpoint of the asymptotic theory of nonadiabatic transitions. The rates, calculated by summation over partial waves and by integration over impact parameters, are close to each other, except for the lowest energies, where $l_{\rm max}\leqslant 1$. The results obtained for Coulomb deexcitation are close to those given in [6] for $\epsilon>0.5$ eV. The rates of the isotope exchange agree with the corresponding data of Ref. [9]. It is difficult to consider this coincidence to be accidental, which means that the approach we use is adequate for the problem in question, like that used in Refs. [6] and [9]. It is clear that the main difference between our results and those of [6] at low energy ($\epsilon<0.5$ eV) arises from the absence of the screening correction in the latter paper for transitions $4012\rightarrow 3002$ and $4120\rightarrow 3110$. This circumstance was not noted in [6]. It seems reasonable that one should explain why the screening correction does not change the Coulomb deexcitation rates in Ref. [6] for the transitions $4012\rightarrow 3002$ and $4120\rightarrow 3110$.

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