Resonant electron transfer in slow collisions of protons with Rydberg hydrogen atoms

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(Received 28 February 1983; revised manuscript received 8 November 1983)

The resonant charge-transfer reaction of protons on highly excited hydrogen atoms is considered by taking into account both the tunneling (under-barrier) and the over-barrier (classically allowed) electron transitions. It is demonstrated that in a wide range of variation of the reduced velocity $\tilde{v}=vn$, the classical transition mechanism is predominant. Cross-section calculations for principal quantum numbers n between 10 and 50 are presented. The results for $45\leq n\leq 50$ are compared with the available experimental data and with other theoretical calculations.

I. INTRODUCTION

Electron transfer collisions between ions and highly excited (Rydberg) atoms have attracted considerable attention in recent years.[1] In addition to contributing to our basic understanding of electron transfer reactions, these processes are important in the study of fusion plasmas,[2] in laser physics,[3] and in various astrophysical situations.[4] Of particular importance in this context is the simplest reaction of this class,

$$H^+ + H(n) \rightarrow H(n) + H^+, \quad n \gg 1 , \tag{1.1}$$

where n is the principal quantum number of the excited hydrogen atom. The resonant electron transfer reaction (1.1) has already been extensively studied theoretically, using various approximations. For high values of the reduced velocity (atomic units will be used throughout, unless otherwise explicitly stated) $\tilde{v}=v/v_n=nv$ (v is the relative collision velocity and $v_n=1/n$ is the classical velocity of the Rydberg electron), cross-section calculations for the reaction (1.1) have been performed by using the first Born and Brinkman-Kramers approximations,[5,6] as well as the classical-trajectory Monte Carlo (CTMC) method.[7–10] It is worthwhile noting that using a generalized correspondence principle,[7,8] the cross section of reaction (1.1) in this velocity region can be obtained by scaling the cross section of the corresponding ground state ($n=1$) reaction. In the low-velocity region ($\tilde{v}<1$), the reaction (1.1) has been studied for various values of n by employing two-state close-coupling models.[11–14] In this velocity region, classical mechanics can also be used to describe the electron transfer process.[15–17] The latter possibility is based on the fact that for internuclear distances R, smaller than the distance R_0 at which the electron binding energy becomes equal to the top of the potential barrier, the electronic motion takes place in a common potential well (over-barrier transitions). The critical distance R_0 can be shown to be given by[15]

$$R_0=6n^2[1+O(1/n)] \tag{1.2}$$

which yields an upper limit for the classical electron-capture cross section

$$\sigma_{\rm cl}=\tfrac{1}{2}\pi R_0^2=18\pi n^4 . \tag{1.3}$$

The only experimental information on the process (1.1) (for $n\gg 1$) is contained in the merged-beam-measured electron-loss (electron-capture *and* ionization) cross section of Koch and Bayfield,[18] performed for the band $44\leq n\leq 50$, and in the range $0.26\lesssim\tilde{v}\lesssim 3.3$. In the region $\tilde{v}<1$, the main contribution to the electron-loss process comes from the capture mechanism, and theoretical electron-capture cross sections can in this region be compared directly with the data. We note, however, that the experimental electron-loss data are uncertain to a factor of 2.[18] The two-state quantum calculations of Toshima[14] are a factor of 5 too low from the data (for a nominal value of $n=47$), while those based on the Rapp-Francis two-state model[11] are more than an order of magnitude too small.[18] The CTMC method also significantly underestimates the cross section (a factor of 3.65 at $\tilde{v}\approx 1$). The classical electron transfer model, based on the over-barrier electron transitions, when modified to account for the velocity dependence of the process,[17] predicts results that are consistent with the experimental data. This model, however, does not account for the under-barrier (tunneling) electron transitions, which at low velocities may also contribute to the electron capture.

In the present paper we shall study reaction (1.1) in the region $\tilde{v}\ll 1$, by taking into account both over- and under-barrier electron transitions. Attempts to account for the under-barrier ones have been made earlier by Bates and Reid[16] for $n\leq 5$. After formulating the electron

transfer problem in reaction (1.1) within the adiabatic approximation (Sec. II), we shall derive the classical (over-barrier) electron transition probability (Sec. III), and perform cross-section calculations for a number of typical values of n between $n=10$ and 50 (Sec. IV). The results of the calculations are compared with the low-velocity electron-loss data of Koch and Bayfield,[18] and with other theoretical calculations. In Sec. V we give some concluding remarks.

II. TRANSITION PROBABILITY AND CROSS SECTION IN THE ADIABATIC APPROXIMATION

In the low-velocity ($\tilde{v} \ll 1$) region the adiabatic electron states of the system $H^+ + H$ are determined from the Schrödinger equation

$$\left[-\frac{1}{2}\nabla^2_{\vec{r}} - \frac{1}{r_1} - \frac{1}{r_2}\right]\psi(\vec{r},\vec{R}) = E(R)\psi(\vec{r},\vec{R}) , \qquad (2.1)$$

where the internuclear distance R is held fixed, and the position vectors $\vec{r}_1$, $\vec{r}_2$, $\vec{r}$, and $\vec{R}$ are defined in Fig. 1. In the semiclassical description of the collision problem, the nuclear motion is described by the function $\vec{R}=\vec{R}(t)$, for which we shall adopt the straight-line trajectory approximation

$$\vec{R}(t) = \vec{b} + \vec{v}t, \quad \vec{b}\cdot\vec{v} = 0 , \qquad (2.2)$$

where b is the impact parameter. We assume that in the initial state ($t \to -\infty$) the electron is bound on the proton "2." If $P \equiv P(b,t)$ is the electron transfer probability at a given internuclear distance $R(t)$, the electron-capture cross section is

$$\sigma = 2\pi \int_0^\infty P(b, t=+\infty) b\, db . \qquad (2.3)$$

With respect to the critical internuclear distance $R_0 \simeq 6n^2$, defined in Sec. I, one can distinguish between two types of trajectories. For trajectories with $b > R_0$, the electron-capture process can occur only via tunneling (under-barrier) transitions. On the other hand, the trajectories with $b < R_0$ contain two essentially different parts (see Fig. 1): for $R > R_0$ [or $|t| > t_0$, with $t_0 > 0$ defined by $R_0 = R(t_0)$] again only under-barrier transitions determine the electron-capture process, while for $R < R_0$ ($|t| < t_0$) the process is dominated by over-barrier (classically allowed) transitions.

Let us first consider the region $R > R_0$. As is well known, due to the invariance of the electronic Hamiltonian with respect to interchange of the positions of protons "1" and "2," the electronic states are classified as gerade (even parity) or ungerade (odd parity). The energies of a gerade and an ungerade state, which at infinite internuclear separations are degenerate, in the asymptotic region of large R can be expressed in analytical form[19,20]

$$E_{g,u}(n,n_1,n_2,m;R) = E_{[n,n_1,n_2,m]}(R) \pm \tfrac{1}{2}\Delta E_{g\text{-}u}(n,n_1,n_2,m;R) , \qquad (2.4)$$

$$E_{[n,n_1,n_2,m]}(R) = -\frac{1}{2n^2} - \frac{1}{R} + \frac{3n\Delta}{2R^2} - \frac{n^2}{2R^3}(6\Delta^2 - n^2 + 1) + O(R^{-4}) , \qquad (2.5)$$

$$\Delta E_{g\text{-}u}(n,n_1,n_2,m;R) = \frac{1}{\pi n^3}\left[\frac{4}{n(n-\Delta)}\right]^{n-\Delta} R^{n-\Delta}\exp[-(R/n)-\Delta][1+O(R^{-1})+O(1/(n-\Delta))] , \qquad (2.6)$$

where $\Delta = n_1 - n_2$, $n = n_1 + n_2 + m + 1$, and n_1, n_2, and m are the parabolic quantum numbers of the electron bound to one of the protons.

It is important to note that in the region $R \gtrsim R_0$, the energies $E_{g,u}(R)$ do not intersect each other. Indeed, the closest levels $E_{[n,n_1,n_2,m]}(R)$ are those having the same values of n and Δ, but different values of m. The energy difference between these levels is given by[19] $\sim 9n^3(m^2 - m'^2)(n-\Delta)/16R^4$, where $m = n - |\Delta| - 1$, $n - |\Delta| - 3, \ldots, 0$ (or 1). For the nearest m sublevels, this difference becomes

$$\delta E = \frac{9n^3(n-\Delta)}{4R^4} \times \begin{cases} 1, & n - |\Delta| = 2k+1 \\ 2, & n - |\Delta| = 2k+2 \end{cases} \qquad (2.7)$$

where $k = 0, 1, 2, \ldots$. Hence the electronic energies (2.4) will not intersect each other provided $\Delta E_{g\text{-}u}/\delta E \lesssim 1$. This ratio depends on the value of Δ. For $\Delta = n-1$ (the maximum value of Δ), $\Delta E_{g\text{-}u}/\delta E$ is exponentially small for all $R \geq R_0$. For $\Delta = -(n-1)$ (the minimum value of Δ), $\Delta E_{g\text{-}u}/\delta E \lesssim 1$ for $R \gtrsim 1.02R_0$ ($n > 40$). Thus in nearly the entire region $R \gtrsim R_0$, one can use a two-state approximation in describing the electron transfer process, provided n is sufficiently large. The smallness of the ratio $\Delta E_{g\text{-}u}/\delta E$ in this region also justifies the use of the straight-line trajectory approximation for describing the nuclear motion.

In the two-state approximation, the total electron wave function may be represented as

$$\Psi(\vec{r},t) = C_-(b,t)\psi_-(\vec{r},t) + C_+(b,t)\psi_+(\vec{r},t) , \qquad (2.8)$$

where

$$\psi_\pm = 2^{-1/2}(\psi_g \pm \psi_u) \qquad (2.9)$$

and $\psi_{g,u}$ are the eigenfunctions of the gerade and ungerade

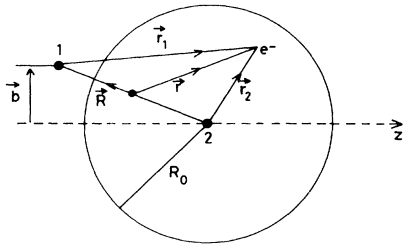

FIG. 1. Geometry of the collision problem.

states, corresponding to the electronic energies $E_{g,u}$. The functions $\psi_{g,u}$ and $\psi_{\pm}$ have the following asymptotic forms:

$$\psi_{g,u} \rightarrow 2^{-1/2}[\phi_1(\vec{r}_1) \pm \phi_2(\vec{r}_2)] \text{ as } R \rightarrow \infty \ , \tag{2.10}$$

$$\psi_{+,-} \rightarrow \phi_{1,2}(\vec{r}_{1,2}) \text{ as } R \rightarrow \infty \ , \tag{2.11}$$

where $\phi_1(\vec{r}_1)$ and $\phi_2(\vec{r}_2)$ are the atomic wave functions when the electron is bound on proton "1" and "2," respectively. Assuming that as $t \rightarrow -\infty$ the electron is bound on proton "2," the initial conditions for the expansion coefficients $C_{\pm}(b,t)$ in Eq. (2.8) are

$$C_-(b, t=-\infty)=1, \quad C_+(b, t=-\infty)=0 \ . \tag{2.12}$$

The electron transfer probability for a given impact parameter b and at time t is now given by[21]

$$P(b,t)=|C_+(b,t)|^2 = \sin^2\left[\tfrac{1}{2}\int_{-\infty}^{t} \Delta E_{g\text{-}u}(R(t'))dt'\right] . \tag{2.13}$$

For impact parameters $b > R_0$, we have $R > R_0$ along the entire trajectory and the electron capture probability (at $t \rightarrow +\infty$) is

$$P(b, t=+\infty)=\sin^2\left[\tfrac{1}{2}\int_{-\infty}^{\infty} \Delta E_{g\text{-}u}\, dt\right] . \tag{2.14}$$

Let us now examine a trajectory for which $b < R_0$. In the region $R \geq R_0$, $t \leq t_0$, the electron transfer probability is still expressed in the form (2.13), but for $R < R_0$ ($|t| < t_0$), the two-state approximation is no more valid. In the latter case, we shall use a classical description for the electron transfer process. Let $W(R)$ be the electron transition probability per unit time at a given distance R. The electron transfer probability for a given impact parameter satisfies the equation

$$\frac{dP(b,t)}{dt} = W(R)[1-P(b,t)] - W(R)P(b,t) \ , \tag{2.15}$$

for which the initial condition $P(b,-t_0)$ is given by Eq. (2.13) with $t=-t_0$. In Eq. (2.15) only the elastic and resonant electron transfer channels are taken into account. This can be justified only for sufficiently small values of reduced velocity $\tilde{v}$, when the resonant selectivity of the electron transfer process is well pronounced and other nonelastic transition processes are adiabatically improbable. The solution of Eq. (2.15) for $t < t_0$ is given by

$$P(b,t)=\frac{1}{2}\left[1-[1-2P(b,-t_0)] \times \exp\left[-2\int_{-t_0}^{t} W(R)dt'\right]\right] , \tag{2.16}$$

When the proton "1" enters the region $R \geq R_0$ ($t \geq t_0$), we do not know the quantum-mechanical state of the system, but only the electron transfer probability $P(b,t_0)$, given by Eq. (2.16) with $t=t_0$. We therefore represent the state of the system at $t=t_0$ as a weighted superposition

$$\Psi(\vec{r},t_0)=[1-P(b,t_0)]^{1/2}\psi_-(\vec{r},t_0) + [P(b,t_0)]^{1/2}\psi_+(\vec{r},t_0) \tag{2.17}$$

in which ψ_+ and ψ_- are taken to have the same phases. The electron capture probability for $t=+\infty$ is then

$$P(b, t=+\infty)=\lim_{t\rightarrow+\infty} |\langle \psi_+(\vec{r},t) | U(t,t_0)\Psi(\vec{r},t_0)\rangle|^2 , \tag{2.18}$$

where $U(t,t_0)$ is the adiabatic evolution operator, with

$$U(t,t_0)\psi_{g,u}(t_0)=\exp\left[-i\int_{t_0}^{t} E_{g,u}(R)dt'\right]\psi_{g,u}(t_0) \ . \tag{2.19}$$

The calculations in Eq. (2.18) give ($b \leq R_0$)

$$P(b, t=+\infty)=\tfrac{1}{2}\left[1-[1-2P(b,t_0)]\cos\left[\int_{t_0}^{\infty} \Delta E_{g\text{-}u}(R)dt\right]\right] + \{P(b,t_0)[1-P(b,t_0)]\}^{1/2}\sin\left[\int_{t_0}^{\infty} \Delta E_{g\text{-}u}(R)dt\right], \quad (b \leq R_0) \ . \tag{2.20}$$

Upon changing the variables from t to R, the electron-capture probabilities (2.20) and (2.14) for a given impact parameter b, respectively, become

$$P^{<}(b,v)=\tfrac{1}{2}(1-\cos^2\alpha^{<}\exp\beta) + \tfrac{1}{2}[1-\cos^2\alpha^{<}\exp(2\beta)]^{1/2}\sin\alpha^{<}, \quad b \leq R_0 \tag{2.21}$$

$$P^{>}(b,v)=\sin^2\alpha^{>}, \quad b \geq R_0 \tag{2.22}$$

where

$$\alpha^{<}=\frac{1}{v}\int_{R_0}^{\infty}\frac{\Delta E_{g\text{-}u}(R)R\,dR}{(R^2-b^2)^{1/2}} \ , \qquad \alpha^{>}=\frac{1}{v}\int_{b}^{\infty}\frac{\Delta E_{g\text{-}u}(R)R\,dR}{(R^2-b^2)^{1/2}} \ , \tag{2.23}$$

$$\beta=-\frac{4}{v}\int_{b}^{R_0}\frac{W(R)R\,dR}{(R^2-b^2)^{1/2}} \ . \tag{2.24}$$

For $b \rightarrow R_0$, the probabilities $P^{<}(b,v)$ and $P^{>}(b,v)$ become equal. By inserting (2.21) and (2.22) into Eq. (2.3), one obtains the electron-capture cross section in the form

$$\sigma=(\tilde{\sigma}^{<}+\tilde{\sigma}^{>})\sigma_0 \ , \tag{2.25}$$

where

$$\sigma_0=\tfrac{1}{2}\pi R_0^2 \ , \tag{2.26}$$

$$\tilde{\sigma}^{<}=1-\frac{2}{R_0^2}\int_0^{R_0}\{CD-[(1-C)(1-CD^2)]^{1/2}\}b\,db \ , \quad b \leq R_0 \tag{2.27}$$

$$\tilde{\sigma}^{>}=\frac{4}{R_0^2}\int_{R_0}^{\infty}\tilde{S}b\,db, \quad b \geq R_0 \tag{2.28}$$

and the quantities $\tilde{S}$, C, and D are given by

$$\tilde{S}=\sin^2\alpha^{>}, \quad C=\cos^2\alpha^{<}, \quad D=\exp(\beta) \ . \tag{2.29}$$

In order to perform cross-section calculations using the above formulas, one needs to determine first the transition probability per unit time, $W(R)$. This will be done in the next section.

III. OVER-BARRIER ELECTRON TRANSITION PROBABILITY PER UNIT TIME

Our method for determining the probability (per unit time) of the over-barrier electron transitions is similar to the one used by Grozdanov,[22] but includes also some quasiclassical arguments. The motion of the electron in the classically allowed region $R < R_0$ can be described in terms of the spatial probability density $f(\vec{r},t)$ which satisfies the continuity equation[23]

$$\frac{\partial f}{\partial t}+\vec{\nabla}\cdot(f\vec{\nabla}S)=0\ , \tag{3.1}$$

where $S(\vec{r},t)$ is the Hamilton principal function. This function is the solution of the Hamilton-Jacobi equation

$$\frac{\partial S}{\partial t}+H=0,\quad H=\frac{\vec{p}^{\,2}}{2}-\frac{1}{r_1}-\frac{1}{r_2}\ , \tag{3.2}$$

where H is the classical Hamiltonian of the electron whose momentum is $\vec{p}=\nabla S$. In the adiabatic approximation, H does not depend explicitly on time (R is treated as a parameter), and therefore the variables in Eq. (3.2) can be separated in the confocal elliptic coordinates

$$\xi=(r_1+r_2)/R,\quad \eta=(r_1-r_2)/R,\quad \phi=\arctan(y/x)\ ,$$
$$1\le\xi<\infty,\quad -1\le\eta\le 1,\quad 0\le\phi<2\pi\ . \tag{3.3}$$

The solution of Eq. (3.2) can then be obtained in the form[24]

$$S=-Et+\mu\phi\pm\int_1^{\xi}p_\xi(\xi')d\xi'\pm\int_{-1}^{\eta}p_\eta(\eta')d\eta'\ , \tag{3.4}$$

where

$$p_\xi(\xi)=\frac{\partial S}{\partial\xi}=\left[\frac{ER^2}{2}+\frac{2R\xi-\Lambda}{\xi^2-1}-\frac{\mu^2}{(\xi^2-1)^2}\right]^{1/2}, \tag{3.5a}$$

$$p_\eta(\eta)=\frac{\partial S}{\partial\eta}=\left[\frac{ER^2}{2}+\frac{\Lambda}{1-\eta^2}-\frac{\mu^2}{(1-\eta^2)^2}\right]^{1/2}, \tag{3.5b}$$

$$p_\varphi=\frac{\partial S}{\partial\phi}=\mu\ , \tag{3.5c}$$

and E and Λ are the electron energy and the separation constant, respectively. In the quasiclassical approximation the quantities E, Λ, and μ in Eqs. (3.4) and (3.5) have to be expressed by their quantum-mechanical values, so that $\mu=\pm m$ and[19]

$$E=-\frac{1}{2n^2}-\frac{1}{R}+O(R^{-2})\ , \tag{3.6a}$$

$$\Lambda=\frac{2n-1}{n}R+O(1)\ . \tag{3.6b}$$

The representation of E and Λ by the first terms of their asymptotic series is sufficient since, as will be seen later, the main contribution to the electron transition probability comes from the region of large R. We also note that, like in the quantum case, the flux of the transient particles with $\mu=m=0$ is predominant. Having this in mind, and the fact that in the over-barrier region the electronic motion is allowed in the entire range of η, the quasiclassical wave function $\tilde{\psi}\sim\exp(iS)$ can be written in the form

$$\tilde{\psi}=f^{1/2}\exp(-iEt)\sin\left[\int_1^{\xi}p_\xi d\xi'\right]\left[\exp\left[-i\int_{-1}^{\eta}p_\eta d\eta'\right]-\exp\left[+i\int_{-1}^{\eta}p_\eta d\eta'\right]\right]$$
$$\equiv\tilde{\psi}_1-\tilde{\psi}_2\ , \tag{3.7}$$

where the arguments of p_ξ and p_η have been omitted. For the case $m=0$, the particular solution of Eq. (3.1) is[22]

$$f=\frac{B}{p_\xi(\xi^2-1)p_\eta(1-\eta^2)} \tag{3.8}$$

with B being the normalization constant. From the condition $||\tilde{\psi}||=1$ one finds

$$B=\left[\pi R^3\int_1^{\xi_1}d\xi\int_{-1}^{1}\frac{d\eta(\xi^2-\eta^2)}{p_\xi(\xi^2-1)p_\eta(1-\eta^2)}\sin^2\left[\int_1^{\xi}p_\xi d\xi'\right]\sin^2\left[\int_{-1}^{\eta}p_\eta d\eta'\right]\right]^{-1}, \tag{3.9}$$

where ξ_1 is the turning point, $p_\xi(\xi_1)=0$, for the electron motion along the ξ direction, given by

$$\xi_1=-\frac{2}{RE}\left[1+\left[1+\frac{\Lambda E}{2}+\frac{R^2E^2}{4}\right]^{1/2}\right]. \tag{3.10}$$

In this expression, one can again use the asymptotic expansions (3.6) and (3.7) for E and Λ, respectively, since the region of small R is reached for small values of b, which do not contribute significantly to the cross section.

The probability per unit time for the over-barrier electron transitions from the field of proton "2" ($\eta=+1$) into the field of proton "1" ($\eta=-1$) is given by

$$W=\int_\Sigma\vec{j}\cdot d\vec{S},\quad \vec{j}=\mathrm{Re}\left[\tilde{\psi}_1^*\cdot\frac{1}{i}\vec{\nabla}\tilde{\psi}_1\right], \tag{3.11}$$

where $\tilde{\psi}_1$ is defined by Eq. (3.7), Σ is a plane defined by $\eta=0$, and $d\vec{S}$ is oriented along the negative η axis. The calculations give the following result

$$W=\pi BR\int_1^{\xi_1}\frac{d\xi}{p_\xi(\xi^2-1)}\sin^2\left[\int_1^{\xi}p_\xi d\xi'\right], \tag{3.12}$$

where B is given by Eq. (3.9). For the highly excited states considered here, the sine functions which appear in Eqs. (3.9) and (3.12) oscillate very rapidly and can be replaced by their mean values. The transition probability per unit time then becomes

$$W(R)=\frac{1}{R^2}\left[\int_1^{\xi_1}\frac{d\xi}{p_\xi(\xi^2-1)}\right]\times\left[\int_1^{\xi_1}d\xi\int_{-1}^{0}\frac{(\xi^2-\eta^2)d\eta}{p_\xi(\xi^2-1)p_\eta(1-\eta^2)}\right]^{-1}. \tag{3.13}$$

IV. CROSS-SECTION CALCULATIONS

Before presenting the results of cross-section calculations for the reaction (1.1), let us first examine the relative importance of the reduced cross sections $\tilde{\sigma}^<(b\le R_0)$ and $\tilde{\sigma}^>(b\ge R_0)$ at various collision energies and for various values of the principal quantum number n. Using the fact that for small values of the collision velocity, the function $\alpha^>(b,v)$ is large in the region of $b\sim R_0$ ($b>R_0$), and that $\Delta E_{g\text{-}u}(R)$ exponentially decreases with R, one can make an analytical evaluation of $\tilde{\sigma}^>$. For a given n, the main contribution to the reduced cross section $\tilde{\sigma}^>$ comes from the Stark state $n_1=0,n_2=n-1,m=0$, for which the electron exchange interaction $\Delta E_{g\text{-}u}(R)$ is maximum [see Eq. (2.6)]. In that case

$$\Delta E_{g\text{-}u}(R)=A(n)R^{2n-1}e^{-R/n},\qquad A(n)=\frac{1}{\pi n^3}\left[\frac{4}{(2n-1)n}\right]^{2n-1}e^{(2n-1)n} \tag{4.1}$$

and evaluating the integral (2.23) for $\alpha^>(b,v)$ asymptotically, one obtains

$$\alpha^>(b,v)=\frac{1}{v}\left[\frac{\pi nb}{2}\right]^{1/2}\Delta E_{g\text{-}u}(b). \tag{4.2}$$

Defining, further, an impact parameter $b^*=R_0+x$ such that for $b\le b^*$, $\alpha^>(b,v)$ is large, so that $\tilde{S}=\sin^2\alpha^>$ in Eq. (2.28) can be replaced by its mean value, and for $b>b^*$ $\tilde{S}\simeq(\alpha^>)^2$, the reduced cross section $\tilde{\sigma}^>$ can be obtained in the form

$$\tilde{\sigma}^>=\frac{1}{R_0^2}\left[(b^{*2}-R_0^2)+\pi\left[\frac{nb^*}{v}\Delta E_{g\text{-}u}(b^*)\right]^2\right]. \tag{4.3}$$

The critical impact parameter b^* can be evaluated from the condition $\alpha^>(b^*,v)=1/e\simeq0.3679$, which for the quantity $x=b^*-R_0$ gives

$$x=\begin{cases}0 & \text{for } \alpha^>(R_0,v)\lesssim 1/e\\ n[\ln\alpha^>(R_0,v)+1] & \text{for } \alpha^>(R_0,v)\ge 1/e\end{cases}. \tag{4.4}$$

An analytical evaluation of the reduced cross section $\tilde{\sigma}^<$ is not possible and it has to be calculated numerically. For collision energies (in the center-of-mass system) $E_{\text{c.m.}}=0.01$, 0.1, 1, and 10 eV, and for $n=10$, 20, 30, 40, and 50, the values of the reduced cross sections $\tilde{\sigma}^<$ and $\tilde{\sigma}^>$ are given in Table I. It can be seen from this table that in the considered range of $E_{\text{c.m.}}$ and n, the contribution of the under-barrier transitions from the region $b>R_0$ to the electron transfer cross section is negligibly small. However, it should be noted that the role of these transitions increases rapidly with decreasing collision energy and n.

In the region $b<R_0$ both tunneling ($R>R_0$) and over-barrier ($R<R_0$) transitions contribute to the electron transfer process. In order to examine the relative role of these two types of transitions, we shall analyze the probability $P^<(b,v)$ given by Eq. (2.21), [using the notation of (2.29)] by

$$P^<(b,v)=\tfrac{1}{2}(1-CD)+\tfrac{1}{2}[(1-C)(1-CD^2)]^{1/2} \tag{4.5}$$

as a function of the reduced variable

$$\tilde{b}=(1-b/R_0)^{1/2}. \tag{4.6}$$

The combinations $(1-C)$ and $(1-D)$ are connected with the tunneling and over-barrier transitions. For the value of $n=47$ and for energies $E_{\text{c.m.}}=0.01$, 0.1, 1, and 10 eV, the behavior of C and D as a function of $\tilde{b}$ is shown in Fig. 2. We see from this figure that for small values of $\tilde{b}$ ($b\sim R_0$), $D\sim1$ and, with decreasing the energy the elec-

TABLE I. Values of the reduced cross sections $\tilde{\sigma}^>$ and $\tilde{\sigma}^<$ for various energies and principal quantum numbers. (The numbers in parentheses indicate powers of ten.)

$E_{\text{c.m.}}$ (eV)		$n=10$	$n=20$	$n=30$	$n=40$	$n=50$
0.01	$\tilde{\sigma}^>$	2.61(−1)	7.22(−2)	5.13(−2)	1.51(−2)	6.92(−3)
	$\tilde{\sigma}^<$	1.00	1.00	1.00	9.97(−1)	9.94(−1)
0.1	$\tilde{\sigma}^>$	1.67(−1)	4.18(−2)	1.45(−2)	3.72(−3)	4.46(−4)
	$\tilde{\sigma}^<$	9.98(−1)	9.98(−1)	9.85(−1)	9.73(−1)	9.63(−1)
1	$\tilde{\sigma}^>$	9.65(−2)	1.70(−2)	1.15(−3)	1.99(−4)	4.46(−5)
	$\tilde{\sigma}^<$	9.96(−1)	9.53(−1)	9.18(−1)	8.87(−1)	8.57(−1)
10	$\tilde{\sigma}^>$	4.28(−2)	1.06(−3)	1.15(−4)	1.99(−5)	4.46(−6)
	$\tilde{\sigma}^<$	9.19(−1)	8.16(−1)	7.15(−1)	6.74(−1)	6.20(−1)

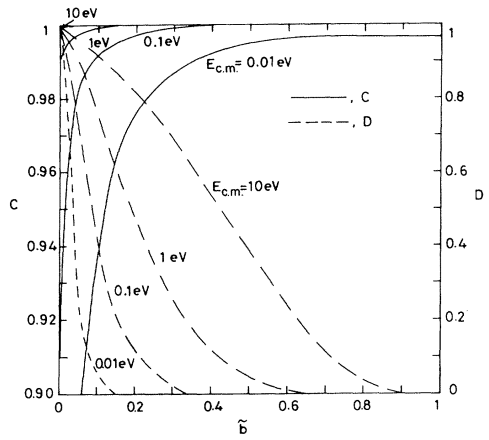

FIG. 2. Coefficients C (solid curves) and D (dashed curves) as functions of $\tilde{b}=(1-b/R_0)^{1/2}$, for $n=47$ and for center-of-mass energies $E_{\text{c.m.}}=0.01$, 0.1, 1, and 10 eV.

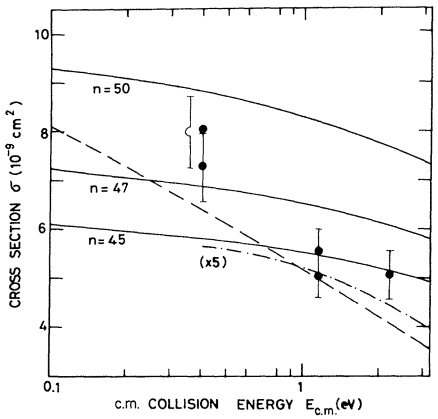

FIG. 4. Total electron transfer cross section σ_n as a function of the center-of-mass collision energy $E_{\text{c.m.}}$ for $n=45$, 47, and 50 (solid curves). The dots are the experimental points of Koch and Bayfield, Ref. 18. The dashed curve corresponds to the classical calculations of Smirnov for $n=47$ (Ref. 17). The dot-dashed curve refers to the PSS results of Toshima (Ref. 14), for $n=47$, multiplied by a factor of 5.

tron transfer probability is approximately given by its quantum-mechanical value, $P^{<}\sim 1-C$. However, in the prevailing part of the region $b<R_0$, in particular for energies above ~ 0.1 eV, the coefficient $C\sim 1$ and the electron transfer is dominated by the over-barrier transitions, $P^{<}\simeq(1-D)/2\simeq\frac{1}{2}$. Thus the main contribution to $\tilde{\sigma}^{<}$ comes from the over-barrier electron transitions.

Let us now turn to the question of the scaling of the electron transfer cross section. Within the framework of classical mechanics, the equations of the motion in a Coulomb field remain the same under the scale transformations $E\rightarrow n^2E$ and $L\rightarrow L/n^2$, where L denotes a length. Therefore, the cross sections scale like

$$\sigma_n(E)=(n/n_0)^4\sigma_{n_0}(n^2E/n_0^2)\ . \tag{4.7}$$

The n^4 scaling of σ_n also holds in the first Born approximation.[5] We have tested the scaling relationship (4.7) within our model by calculating the cross section σ_n for $n=10$, 20, 30, 40, and 50. The results are given in Fig. 3 as a function of the reduced velocity $\tilde{v}=nv$. We find that the n^4 scaling in our model holds approximately only for $n\gtrsim 30$.

In Fig. 4, we present the results of our cross-section calculations for $n=45$, 47, and 50 (the solid lines). They can be compared with the electron-loss data of Koch and Bayfield[18] (the solid circles) for the nominal band $45\leq n\leq 50$, which in the considered energy region can be attributed to the electron transfer process. Bearing in mind the claimed factor-of-2 uncertainty in the absolute value of the experimental data the agreement between our results and the experiment can be considered as satisfactory. In the same figure we have also plotted the results of the perturbed stationary state calculations of Toshima[14] (for $n=47$, the dot-dashed line), which in their low-energy part have the same energy dependence as our results, but are a factor of ~ 6 too low. The results of the classical model of Smirnov,[17] in which the velocity dependence of the cross section has been derived in a somewhat different way are shown in Fig. 4 (for $n=47$) by the dashed line.

Cross-section measurements of reaction (1.1) in a broader energy range would clearly be very useful in understanding in more detail the role of the tunneling and over-barrier transitions in the electron capture process.

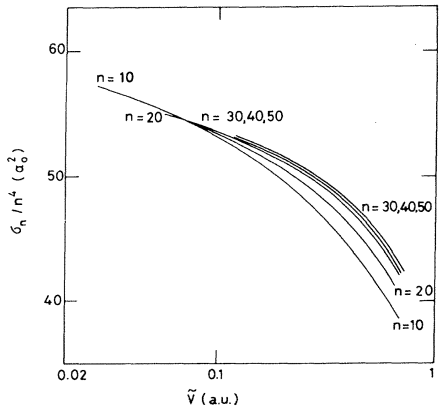

FIG. 3. Quantity σ_n/n^4 (in units of a_0^2) as a function of the reduced velocity $\tilde{v}=nv$, for $n=10$, 20, 30, 40, and 50.

V. CONCLUDING REMARKS

In the present paper, we have made an attempt to consider in a unified manner both the under-barrier and over-barrier transitions in the charge exchange problem of protons on highly excited hydrogen atoms. We have demonstrated that in the energy range in which both the adiabatic approximation and the impact parameter description of nuclear motion are applicable, the over-barrier transitions are the main mechanism governing the electron transfer process. Our treatment of the under-barrier transitions is largely simplified by using the two-state approximation, i.e., neglecting all the nonresonant transitions with a small energy defect. This approximation can only be justified at very low reduced velocities $\tilde{v}$.

However, in the considered range of n and $\tilde{v}$ the under-barrier transitions are expected to give a negligible contribution to the process, and this approximation can be used as a qualitative demonstration for that fact. For the low-lying excited states, the under-barrier transitions play a much more important role and they may "shield" the over-barrier transition mechanism. The probability (per unit time) of the over-barrier transitions has been determined by using the quasiclassical approximation. As a consequence of this is the fact that the n^4 scaling of the electron-capture cross section is observed only for states with $n \gtrsim 30$.

ACKNOWLEDGMENTS

One of us (N.N.N.) would like to thank the Université Libre de Bruxelles for the grant provided to her. The authors are indebted to Professor M. R. C. McDowell for several useful discussions. The partial support of the International Atomic Energy Agency, Vienna, Austria (Contract No. 2857/R2/RB) and by the U.S. National Bureau of Standards, Washington [Contract No. NBS(G)-279-Yu], as well as the Science and Engineering Research Council Research Fellowship (to R.K.J.), are gratefully acknowledged.

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