# Ionization of a hydrogen-like atom by slow ions

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(Submitted 3 June 1981)
Zh. Eksp. Teor. Fiz. **81**, 1681–1692 (November 1981)

The terms of the two-Coulomb-center problem are calculated in the complex plane of the internuclear distance $R$. The calculations reveal term intersection (branch) points of a new type: the adiabatic terms $E_{NLM}(R)$ and $E_{N+1LM}(R)$ successively intersect in pairs for all values of $N$ ($N$, $L$, and $M$ are the spherical quantum numbers of the united atom). At small values of $M$, the branch points are close to the real axis of $R$. This leads to the formation of infinite series of quasi-intersections than can be considered to be the result of the interaction of the diabatic term that goes over into the continuous spectrum with the Rydberg states of the quasimolecule. The cross section for ionization due to the evolution of the system along this diabatic term is obtained. The discovered branch points also play an important role in the united-atom approximation: the distance to them is the radius of convergence of the asymptotic expansions for $R \to 0$.

PACS numbers: 34.10. + x, 34.50.Hc

## 1. INTRODUCTION

The process of ionization of a hydrogen-like atom by slow ions does not at present have a validated mechanism within the framework of the adiabatic approximation. In the simpler case of negative-ion ionization the problem of the determination of the adiabatic term that goes over into the continuous spectrum as the nuclei approach each other; it is evolution of the system along this term that leads to the ionization. But such terms do not exist when the particles participating in the reaction are a neutral atom and a positively charged ion. The going-over of the term into the continuous spectrum prevents the Rydberg crowding of the levels below the boundary of the continuous spectrum. The ionization process could be explained by going over a diabatic term into the continuous spectrum, but such terms have thus far not been detected in real systems.

Among real systems, the term picture has been best studied for the two-Coulomb-center problem, which plays in the theory of collisions the same fundamental role played by the hydrogen-atom problem in the theory of the atom. There exists for this system a relatively simple algorithm allowing the exact computation of the adiabatic terms and the wave functions. The present paper is devoted to the computation of the terms of the two-Coulomb-center problem in the complex plane of the internuclear distance $R$. As far as we know, these computations have not been carried out before, although, as a rule, the characteristics of the terms in precisely the complex $R$ plane are required in applications involving the computation of inelastic processes (e.g., the transitions between the terms that undergo quasi-intersection).

The computations reveal term-intersection points of a new type: the adiabatic terms $E_{NLM}(R)$ and $E_{N+1LM}(R)$ successively intersect in pairs for all values of $N \geq L+1$ ($N$, $L$, and $M$ are the spherical quantum numbers of the united atom). When $M$ is small, the points of intersection are close to the real axis of $R$. As a result, there arise on this axis previously-unnoticed infinite series of quasi-intersections. These quasi-intersections can be considered to be the result of the interaction of the diabatic term that goes over into the continuous spectrum as the nuclei approach each other with the infinite series of Rydberg states. Such diabatic terms, which cause the ionization of the atom, have been successfully detected for the first time for real systems. Questions connected with the reason why the diabatic term goes over into the continuous spectrum are discussed in Sec. 4. In Sec. 5 we carry out quantitative estimates for the ionization cross section on the basis of the mechanism that attributes the ionization to the evolution of the system along this diabatic term. Another consequence of the going over of the diabatic term into the continuous spectrum is the possession of a minimum by the adiabatic terms with small values of $M$. The discovered intersection points play an important role in the united-atom approximation as well: the distance to these points is the radius of convergence of the asymptotic expansions for $R \to 0$ in the two-Coulomb-center problem. These questions are discussed in Sec. 3. In conclusion, we consider further possible applications of the results obtained in the present paper, and also discuss the applicability of these results to many-electron systems.

## 2. FORMULATION OF THE PROBLEM

The steady-state Schrödinger equation for the two-Coulomb-center problem admits, as is well known, the separation of the variables in the prolate spheroidal coordinates

$$\xi=(r_1+r_2)/R, \quad \eta=(r_1-r_2)/R, \quad \varphi=\operatorname{arctg}(x/y),$$
$$1\leqslant\xi<\infty, \quad -1\leqslant\eta\leqslant 1, \quad 0\leqslant\varphi<2\pi.$$

Here $R$ is the distance between the Coulomb centers and $r_1$ and $r_2$ are the distances from the electron to the first and second centers. If we represent the electron wave function in the form

$$\Psi(r)=F(\xi)\Phi(\eta)e^{im\varphi},$$

then we obtain the following equations[1] for the functions $F(\xi)$ and $\Phi(\eta)$ ($h=m=e=1$):

$$\left[\frac{d}{d\xi}(\xi^2-1)\frac{d}{d\xi}-p^2(\xi^2-1)+a\xi-\lambda-\frac{m^2}{\xi^2-1}\right]F(\xi)=0, \tag{1}$$

$$\left[\frac{d}{d\eta}(1-\eta^2)\frac{d}{d\eta}-p^2(1-\eta^2)+b\eta+\lambda-\frac{m^2}{1-\eta^2}\right]\Phi(\eta)=0, \tag{2}$$

$$p=(-2E)^{1/2}R/2, \quad a=(Z_2+Z_1)R, \quad b=(Z_2-Z_1)R,$$

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where $E$ is the electron energy in the field of two Coulomb centers with charges $Z_1$ and $Z_2$ and $\lambda$ is the separation constant. In the energy region $E<0$, the discrete energy levels (the adiabatic terms) $E(R)$ and the separation constant $\lambda(R)$ are determined from the boundary conditions

$$|\Phi(\pm1)|<\infty, \quad |F(1)|<\infty, \quad F(\xi)\underset{\xi\to\infty}{\longrightarrow}0. \tag{3}$$

The standard expansions of the functions $F(\xi)$ and $\Phi(\eta)$:

$$F(\xi)=(\xi^2-1)^{m/2}(\xi+1)^{\sigma}e^{-p(\xi-1)}\sum_{s=0}^{\infty}g_s\left(\frac{\xi-1}{\xi+1}\right)^s, \tag{4}$$

$$\Phi(\eta)=e^{-p(1+\eta)}\sum_{s=0}^{\infty}c_sP_{s+m}^{m}(\eta), \quad \sigma=\frac{a}{2p}-m-1, \tag{5}$$

allow us to obtain in place of the differential equations (1) and (2) the following relatively simple three-term recursion formulas[1] for the coefficients $g_s$ and $c_s$:

$$\alpha_sg_{s+1}+\beta_sg_s+\gamma_sg_{s-1}=0, \tag{6}$$

$$\rho_sc_{s+1}+\varkappa_sc_s+\delta_sc_{s-1}=0; \tag{7}$$

$$\alpha_s=(s+1)(s+m+1), \quad \beta_s=2s(s+2p-\sigma)-(m+\sigma)(m+1)-2p\sigma+\lambda,$$

$$\gamma_s=(s-1-\sigma)(s-1-m-\sigma), \quad \varkappa_s=(s+m)(s+m+1)-\lambda,$$

$$\rho_s=\frac{(s+2m+1)(b-2p(s+m+1))}{2(s+m)+3}, \quad \delta_s=\frac{s(b+2p(s+m))}{2(s+m)-1},$$

In order to get the expansions (4) and (5) to terminate on the side of negative $s$ values, we must set

$$g_{-1}=0, \quad c_{-1}=0. \tag{8}$$

At high $s$ values the solutions to the recursion formulas (6) and (7) have the asymptotic forms

$$g_s^-=(-1)^s\exp[-4(ps)^{1/2}], \quad g_s^+=(-1)^s\exp[4(ps)^{1/2}],$$

$$c_s^-=(-p)^s/s!, \quad c_s^+=s!/p^s.$$

The boundary conditions (3) are satisfied for the solutions with the asymptotic forms $c_s^-$ and $g_s^-$. The procedure for finding the eigenvalues $E(R)$ and $\lambda(R)$ is significantly simpler because of the relation between the three-term recursion formulas and infinite continued fractions. Let us, using the recursion formula (6), express the ratio $g_{-1}/g_0$ in terms of $g_{s+1}/g_s$ in the form of a finite continued fraction:

$$g_{-1}/g_0=D_\xi^s(E,\lambda,g_{s+1}/g_s)$$

$$=-\gamma_0^{-1}(\beta_0-\alpha_0\gamma_1/(\beta_1-\alpha_1\gamma_2/(\beta_2-\ldots(\beta_s-\alpha_s\gamma_{s+1}g_{s+1}/g_s)\ldots))). \tag{9}$$

If the solution satisfies the boundary conditions, then for $s\to\infty$ the ratio $g_{s+1}/g_s$ in the expression (9) can be neglected. This allows us to express $g_{-1}/g_0$ in terms of an infinite continued fraction:

$$g_{-1}/g_0=D_\xi(E,\lambda)=\lim_{s\to\infty}D_\xi^s(E,\lambda,g_{s+1}/g_s).$$

A similar expression is obtained for the ratio $c_{-1}/c_0$ connected with the angular Eq. (2). With allowance for (8), the problem of finding the eigenvalues $E(R)$ and $\lambda(R)$ now reduces to the problem of finding the common roots of the two infinite continued fractions:

$$D_\xi(E,\lambda)=0, \quad D_\eta(E,\lambda)=0. \tag{10}$$

For the coefficients, $g_s$ and $c_s$, having the asymptotic forms $g_s^+$ and $c_s^+$, the finite continued fractions $D_\xi^s$ and $D_\eta^s$ do not go over into the infinite continued fractions $D_\xi$ and $D_\eta$ as $s\to\infty$.

The solution to the spectral problem is described in such a detailed manner here because the connection of the infinite continued fractions with the boundary condition (3) through the asymptotic forms of the recursion formulas is sometimes overlooked, and this leads to errors. Thus, in Ref. 1 the use of the expansions of the wave functions (2.41) and (2.44) is proposed, but the continued fractions of these expansions are connected with spectral problems corresponding to other boundary conditions; for example, the expansion of (2.41) is connected with the spectral problem whose solutions are required to be regular in the interval $-1\leqslant\xi\leqslant1$, and not on the semiaxes $1\leqslant\xi<\infty$.

## 3. DISCUSSION OF THE RESULTS OF THE COMPUTATION OF THE TERMS IN THE COMPLEX PLANE OF THE INTERNUCLEAR DISTANCE

The $E(R)$ terms in the complex plane were numerically computed by solving the system of transcendental Eq. (10) with the aid of an algorithm similar to the one described in Truskova's[2] paper.[1)] Below, to classify the terms, we shall use either the spherical quantum numbers, $N$, $L$, and $M$, of the united atom, into whose energy levels the terms of the two-Coulomb-center problem go over as $R\to0$, or the numbers, $k$, $q$, and $m$, of zeros the wave function has in the variables $\xi$, $\eta$, and $\varphi$ respectively. These two sets of quantum numbers are connected with each other by the relations[1]

$$N=k+q+m+1, \quad L=q+m, \quad M=m. \tag{11}$$

Of greatest interest in the computation of the terms are the quasi-intersections. The quasi-intersection of two terms on the real axis of $R$ is, as is well known, due to the exact intersection of these terms at some complex value $R_0$, in whose neighborhood the difference between the terms has the form

$$\Delta E(R)=\text{const}\cdot(R-R_0)^{1/2}. \tag{12}$$

In going around the branch point $R_0$, we go over from one term to the other, since the two terms are different branches of the same analytic function. Thus far, in the two-Coulomb-center problem only those quasi-intersections of the pair of terms $E_{kqm}(R)$ and $E_{k'q'm'}(R)$ have been considered for which

$$k=k', \quad q=q'-1, \quad m=m'. \tag{13}$$

These quasi-intersections are due to the resonance subbarrier interaction between the states localized in the various potential wells in the angular Eq. (2).

In the present paper we find quasi-intersections of a new type, namely, quasi-intersections for which

$$k=k'-1, \quad q=q', \quad m=m'. \tag{14}$$

They occur for all values of the charges $Z_1$ and $Z_2$, including the case of the molecular hydrogen ion $H_2^+$, in which the quasi-intersections (13) do not occur. Formally, the quasi-intersections (14) can be considered to be quasi-intersections in the radial Eq. (1), since the states participating in them are those whose wave functions have different numbers of zeros in the variable $\xi$. But there is only one well in the radial equation, and therefore they cannot be as simply explained from the standpoint of a one-dimensional equation as the quasi-

TABLE I. The coordinates of points of intersection of the $Np\sigma$ terms for $H_2^+$.

| | N | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | 2 | 3 | 4 | 5 | 6 | 7 | 8 | ∞ |
| Re $R_{N10}$ | 0.786 | 0.768 | 0.759 | 0.755 | 0.752 | 0.751 | 0.749 | 0.746 |
| Im $R_{N10}$ | 1.099 | 1.050 | 1.034 | 1.027 | 1.023 | 1.021 | 1.020 | 1.015 |

intersections (13).

The points of intersection of the terms (14) in the complex $R$ plane were found directly in the computation. The terms $E_{NLM}(R)$ and $E_{N+1LM}(R)$ were found to intersect successively in pairs for all values of $N \geq L+1$ [the transition to the spherical quantum numbers $N$, $L$, and $M$ in (14) is accomplished in accordance with (11)]. The computed intersection points $R_{NLM}$,

$$E_{NLM}(R_{NLM}) = E_{N+1LM}(R_{NLM})$$

with different $N$ values and a fixed $LM$ set form an infinite series of branch points localized in a small region $\Omega$, and condensing toward some accumulation point

$$R_{LM} = \lim_{N\to\infty} R_{NLM}.$$

Table I illustrates this situation in the particular case of the $Np\sigma$-term series ($L=1, M=0$) for the $H_2^+$ system. All the terms of the $LM$ series in question are different branches of the same analytic function $E_{NLM}(R)$, and the points $R_{NLM}$ are the branch points of this function [see (12)]. In the vicinity of the region $\Omega$, the terms of the series in question are described with a high degree of accuracy by the formula ($Z = Z_1 + Z_2$)

$$E_{LM}(R) = -Z^2 \Big/ 2\Big[\frac{1}{2\pi i}\ln(R-R_{LM})\Big]^2, \qquad (15)$$

in which the expression in the square brackets play the role of the principal quantum number in the hydrogenic spectrum. As the computation shows, in going around the region $\Omega$ once, we go over from the given term $E_{NLM}(R)$ to the neighboring term $E_{N\pm1LM}(R)$ (the sign is determined by the circling direction). This agrees with the formula (15), in which the logarithm acquires an increment of $\pm 2\pi i$ when we go around the

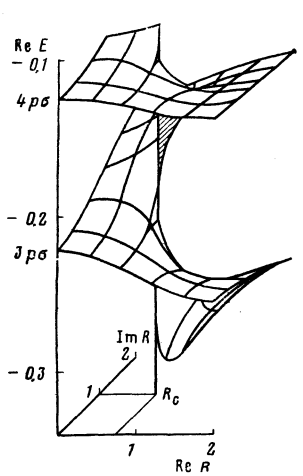


FIG. 1. Surface of the real part of the energy in the complex plane of the internuclear distance for $H_2^+$.

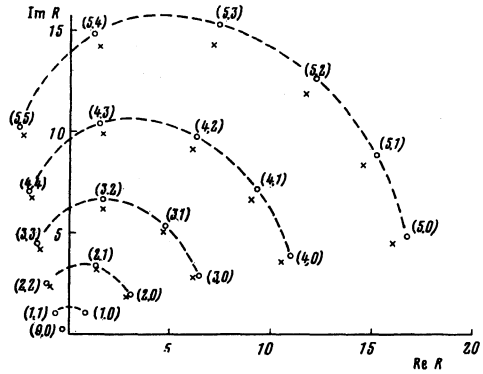


FIG. 2. Positions of the series of branch points in the complex $R$ plane for $H_2^+$: ○) the branch points $R_{L+1LM}$; ×) the branch points $R_{2L+LM}$.

point $R_{LM}$, which leads to the effective replacement of the principal quantum number $N$ by $N \pm 1$ in the Rydberg series. Figure 1 shows the results of the computation for the energy surface $\mathrm{Re}\,E_{LM}(R)$. On the chosen scale, all the branch points merge, and the surface has the form of a corkscrew (part of which is shown in the figure) with a pitch that decreases with increasing $N$ like the Rydberg-level spacing, i.e., like $N^{-3}$, which agrees with the formula (15). Figure 2 shows the disposition in the complex $R$ plane of series with different $L$ and $M$ values and the locations of the first two branch points $R_{L+1LM}$ and $R_{L+2LM}$ in each series. The following approximate relationships are evident from the figure. Inside a series, the points are located along a radius, and are crowded on the $R=0$ side; the series themselves form a regular structure: series with the same $L$ value and different $M$ values are evenly disposed on circles, and the greater $L$ is, the greater are the radii of the circles. The main effect of the charges $Z_1$ and $Z_2$ on the above-described picture is to change the characteristic scale in the $R$ plane. As the total charge $Z$ increases, all the distances decrease in proportion to $Z^{-1}$. The dependence on the charge ratio $Z_1/Z_2$ is a weak one. Figure 3 shows the locations of the points $R_{210}$ of intersection of the terms $2p\sigma$ and $3p\sigma$ for the charges $Z_1=1$, $Z_2 = 1-10, 20, 40$ in the $ZR$ plane. It is worth noting that, to within the accuracy with which the computations were carried out ($\Delta R \approx 10^{-3}$), all the points lie on one straight line in this plane.

The results allow us to take a new look at the struc-

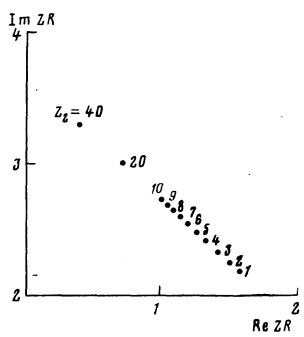


FIG. 3. Positions of the branch points $R_{L+LM}$ for different values of the charge $Z_2$ in the complex $ZR$ plane.

ture of the terms of the two-Coulomb-center problem. First, they clarify a number of questions connected with the expansion of the terms for small distances $R$ (the unified-atom approximation). These expansions are often used in applications, but it has thus far not been understood why in certain cases they describe well the actual behavior of the terms at fairly great distances, while in other cases the region of their applicability is extremely small. As is well known, the region of applicability of the expansions is determined by the distance to the nearest singular point. In the united-atom approximation, such singular points are precisely the discovered branch points $R_{NLM}$, the distance to which depends strongly on $L$ and weakly on $N$ and $M$ (the reasons why the dependence on the quantum numbers has such a character are discussed in Sec. 4). Thus, it turns out that the united-atom expansion is applicable, for example, in the case of $H_2^+$, to the $s$ state ($L=0$) up to $R=0.4$ a.u. and the $h$ state ($L=5$) up to $R=17$ a.u. (see Fig. 2).

Other singular points occur as a result of the possession of minima by the terms whose quantum numbers satisfy the condition[1]

$$L(L+1)>3M^2.$$

It has not become clear through the computation of the energy surface in the complex $R$ plane that these minima arise as a result of the presence near the real axis of an infinite series of singular points. Further, the larger $M$, the greater the distance of the series from the real axis (Fig. 2) and the less pronounced is the minimum of the term on the real axis of $R$, becoming more and more so as $M$ increases until it entirely disappears at $M>(L(L+1)/3)^{1/2}$. Figure 1 illustrates the formation of the minimum of the terms $3p\sigma$ and $4p\sigma$ under the influence of such a series, which imparts a helical character to the energy surface. It can also be seen from the figure that the position of the minimum should always be shifted to the right of the real coordinate of the series in question.

## 4. MECHANISM UNDERLYING THE FORMATION OF QUASI-INTERSECTIONS

Quasi-intersections are, from the standpoint of the application of these results in the theory of atomic collisions, the most interesting manifestation of singular points. At low $M$ values the branch points $R_{NLM}$ are close to the real axis of $R$, and there arise on the real axis infinite series of quasi-intersections that were not noticed before in the background of the minima. These quasi-intersections can be considered to be the result of the interaction of the diabatic term that goes over into the continuous spectrum as the nuclei approach each other with the infinite series of Rydberg states.

The diabatic terms are obtained from the adiabatic ones by replacing the quasi-intersections by exact intersections,[3] which we define as follows:

$$R^d_{NLM}=\mathrm{Re}\,R_{NLM},\quad E^d_{NLM}=\mathrm{Re}\,E_{NLM}(R_{NLM}), \tag{16}$$

where $R^d_{NLM}$ is the position of the point of intersection of the diabatic terms and $E^d_{NLM}$ is their value at this point. Joining successively the intersection points (16) in a given series, we obtain the diabatic term, which goes over into the continuous spectrum abruptly and, at $R>R^d_{L+1LM}$, into the lower adiabatic term of the given series. The remaining diabatic terms decrease monotonically with decreasing distance; the diabatic term coinciding at large distances with the adiabatic term $E_{NLM}(R)$ ($N\geq L+2$) goes over at $R=0$ into the adiabatic term $E_{N-1LM}(R)$. Figure 4 shows the adiabatic (continuous curves) and the diabatic (dashed curves) terms for $H_2^+$.

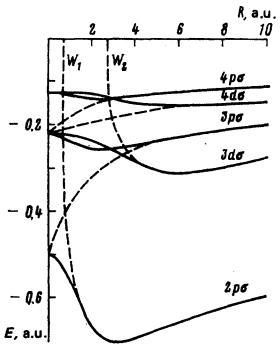


FIG. 4. Adiabatic (continuous curves) and diabatic (dashed curves) terms for $H_2^+$.

It is not entirely clear what makes a diabatic term go over into the continuous spectrum. To elucidate the mechanism underlying this phenomenon, we must separate in the Hamiltonian $H(R)$ of the system the Hamiltonian $H_0(R)$ for which the diabatic terms are exact eigenvalues and the interaction, $V(R)=H(R)-H_0(R)$, as a result of which the intersections are transformed into quasi-intersections. We cannot separate out $H_0(R)$ in a sufficiently simple and natural fashion. But we can adduce some qualitative arguments that show that these quasi-intersections are due to the reconstruction of the two-center geometry of the problem for $R\to\infty$ into a single-center geometry for $R=0$.

Let us first discuss the case in which $M=0$. The united atom's effective potential determining the state of the electron at small distances $R$ is the sum of the Coulomb interaction and a centrifugal core:

$$V_L(r)=-Z/r+L(L+1)/2r^2. \tag{17}$$

At large distances $R$ the potential consists of two potential wells, and, as the distance decreases, the total potential well at first deepens. The deepening of the potential well leads to the lowering of the energy levels, and this occurs until the centrifugal core of the united atom begins to form. For an electron with energy $E<0$ the width of the centrifugal core is determined from the condition

$$E=V_L(r_p) \tag{18}$$

and is equal to

$$D=2r_p=\{Z-[Z^2+2EL(L+1)]^{1/2}\}/(-E). \tag{19}$$

For $R<D$, the nuclei are screened off by the centrifugal core, and they act as a single Coulomb center. For $R>D$, however, both nuclei are in the region of classical-

ly allowed electron motion, and they manifest themselves individually. The changeover from a two-center electron wave function to a single-center one occurs at $R \approx D$, the changeover first occurring for the lowest energy level, since, according to (19), the lower the electron energy is, the wider is the centrifugal core. The appearance of the centrifugal core makes the effective potential well shallower; therefore, the adiabatic terms curve upward as $R$ decreases, and are then successively reflected from the higher-lying adiabatic term for all values of $N > L+1$, producing an infinite chain of quasi-intersections in the process. This chain of quasi-intersections was considered above to be the trace of the diabatic term $W_L(R)$ that goes over into the continuous spectrum. It follows from the mechanism proposed here for the formation of the quasi-intersections that the term $W_L(R)$ in the neighborhood of the point where it goes over into the continuous spectrum slides over the interior of the potential well (17), and should be approximately described in this region by the expression

$$W_L(R) = V_L(R/2)$$

$$= -2Z/R + 2L(L+1)/R^2, \tag{20}$$

which is connected with the condition (18), and is obtained with allowance for the relation $R = D = 2r_p$. Equating the energy $W_L$ in the expression (20) to zero, we find the distance $R_L$ at which the diabatic term goes over into the continuous spectrum:

$$R_L = L(L+1)/Z. \tag{21}$$

In Table II we present for comparison the $R_L$ values given by the formula (21) and the corresponding values extracted from the results of the numerical computation. There is good agreement in all the cases, which is surprising, considering the qualitative character of the above-performed investigation. Roughly the same agreement is obtained when the values for the slope of the diabatic term at the point where the term goes over into the continuous spectrum are compared. The centrifugal core does not arise in the $L = 0$ case. This explains why the terms of this series do not undergo quasi-intersections and do not possess minima.

In the $M \neq 0$ case there exists at all internuclear distances an axially symmetric centrifugal core, which weakens the effect of the formation of the spherical core of the united atom. As a result, the distance between the series of singular points and the real axis increases with increasing $M$ (see Fig. 2), and the quasi-intersections become less and less effective.

TABLE II. Approximate $R_L^a$, (21), and the exact $R_L^e$ values for the points at which the $M=0$ diabatic terms of $H_2^+$ go over into the continuous spectrum.

| | $L$ | | | | |
|---|---|---|---|---|---|
| | 1 | 2 | 3 | 4 | 5 |
| $R_L^a$ | 1 | 3 | 6 | 10 | 15 |
| $R_L^e$ | 0.75 | 2.6 | 5.6 | 9.9 | 15 |

## 5. IONIZATION

The obtained results allow us to consider within the framework of the adiabatic approximation the ionization process, to which the evolution of the system along the diabatic term that goes over into the continuous spectrum leads. The probability for ionization from the term $E_{N_0 LM}$ on account of the inelastic crossing of the quasi-intersections is equal to[4]

$$w_{N_0} = \prod_{N=N_0}^{\infty} \exp(-\Delta_N), \tag{22}$$

where

$$\Delta_N = 2 \left| \int_{\mathrm{Re}\, R_{NLM}}^{R_{NLM}} \{E_{N+1LM}(R) - E_{NLM}(R)\} \frac{dt}{dR} dR \right|$$

is the Massey parameter for the $N$-th quasi-intersection. As the computation shows, for $M=0$ the distance from the series of singular points to the real axis is given to within 10% by the expression

$$\mathrm{Im}\, R_{NLM} = 2L/Z, \tag{23}$$

and the splitting of the terms can be considered with the same degree of accuracy to be constant and equal to

$$E_{N+1LM}(R) - E_{NLM}(R) = Z^2/2N^2 - Z^2/2(N+1)^2 \tag{24}$$

right up to the point of intersection (the terms depend weakly on $R$ because of the existence of the points $R_{N+1\,LM}$ and $R_{N-1\,LM}$ close to the intersection point $R_{NLM}$, and sharply approach each other only in a small neighborhood of the point of intersection, i.e., in a neighborhood of dimension smaller than the distances to these points). With allowance for (21), (23), and (24), the Massey parameter in the straight-line-flight approximation ($R^2 = \rho^2 + v^2 t^2$) is equal to

$$\Delta_N = \frac{2ZL(2N+1)}{vN^2(N+1)^2} \left(1 + \frac{\rho^2}{2|R_{NLM}|^2}\right). \tag{25}$$

In deriving (25), we also used the inequality $\rho < |R_{LM}|$. Substituting (25) into (22), and then integrating over the impact parameter $\rho$, we obtain the ionization cross section

$$\sigma = \frac{\pi v N_0^2 |R_{NLM}|^2}{ZL} \exp\left(-\frac{2ZL}{vN_0^2}\right) \left\{1 - \exp\left[-\frac{L^3(L+1)^2}{vN_0^2 Z |R_{NLM}|^2}\right]\right\}. \tag{26}$$

Experimental data on the ionization of the hydrogen atom by protons at ionic energies higher than 5 keV are given in Ref. 5. The ionization cross sections obtained in that investigation exceed by a considerable factor the ionization cross section given by (26). This is due to the existence in the present case of another ionization channel. Resonance charge transfer occurs with a large cross section in slow hydrogen atom–proton collisions. Some of the electrons participating in the charge-transfer process break away in the course of the transition from one nucleus to the other, and get into the continuous spectrum. Although the fraction of such electrons in the charge-transfer process is not high, owing to the large magnitude of the charge-transfer cross section, the cross section for ionization through this channel turns out to be considerable. This two-stage ionization mechanism cannot be described within the framework of only the adiabatic approximation even

at very low collision energies. This approximation is applicable only to the first stage, i.e., to the charge transfer. To describe the second stage—the dynamical electron stripping—we must use an approximation similar to the approximation of instantaneous switching on of perturbation, in which the sudden switching on of the nuclear velocities is considered. Such an approximation has been used by Migdal[6] to compute the inelastic transitions induced in an atom by the neutron decay of the nucleus. Using the two-stage mechanism, we can obtain for the ionization cross section estimates that agree well with the experimental data given in Ref. 5. The comparison of the ionization cross section (26) with the experimental data should be carried out for those collisions in which resonance charge transfer does not occur, e.g., the collision of a hydrogen atom with an $\alpha$ particle. But there are no such data in the literature.

## 6. CONCLUSION

In the present paper we have far from exhausted the consequences of the existence of the adiabatic-term-related infinite series of branch points in the complex plane of the internuclear distance. Among further possible approximations, we can indicate, for example, the problem of the construction of approximate analytic expressions for the adiabatic terms of the two-Coulomb-center problem. There are at present asymptotic expansions for the terms for large and small internuclear distances.[1] The results obtained here pertain to the most complex transition region, in which an approximate analytical description that takes the fundamental features of the real terms into account is also possible (as an example, we can cite the expression (15)]. The joining of these results would allow us to obtain approximate expressions that are valid for all internuclear distances. All the terms of a given $LM$ series should then be described by a single analytic function $E_{LM}(R)$. A similar analytic energy-surface structure has been predicted on the basis of general arguments by Demkov.[7]

Another problem is connected with the fact that the going over of a diabatic term into the continuous spectrum should be accompanied by the appearance of a quasi-stationary state when $R < R_L$. We do not have at present a theory that would predict, even qualitatively, the dependence of the width of the quasi-stationary states on $R$ in the vicinity of the point where the diabatic term goes over into the continuous spectrum. In view of this, the computation of the poles of the $S$ matrix of the two-Coulomb-center problem in the complex energy ($E$) plane is of interest. Such a calculation will allow us to find the trajectory of the $S$-matrix poles corresponding to the quasi-stationary states and, thereby, the dependence of the width on $R$. This problem is apparently the simplest problem in which quasi-stationary states and the long-range Coulomb attraction occur at the same time. Knowledge of the width as a function of $R$ is necessary for the computation of the electron distribution in the continuous spectrum. Demkov and Komarov[4] have carried out such a computation of the energy distribution of the electrons for the Demkov–Osherov model, but it is as yet not clear to what extent this model is applicable to real systems, since it is virtually assumed in it that the diabatic term goes over into the continuous spectrum vertically, as a result of which the width of the quasi-stationary state is infinite.

The results obtained in the present paper pertain to the two-Coulomb-center problem, but they in fact have a more general character. The qualitative explanation, given in Sec. 4, of the mechanism underlying the formation of quasi-intersections can be applied on the same grounds to many-electron systems. These quasi-intersections were not discovered earlier apparently because of the fact that the splitting of the terms at a quasi-intersection point is large. But the probability for inelastic traversal of a quasi-intersection is determined not only by the splitting of the terms, but also by the strength of their interaction. The values obtained for the Massey parameter indicate that the interaction should be strong in the region of a quasi-intersection. The off-diagonal matrix elements for $H_2^+$ that describe the interaction between the terms of the $Np\sigma$ series in the adiabatic approximation are given in Ref. 8. Each of them has a sharp peak in the region of a quasi-intersection ($R \approx 1$ a.u.), in accordance with the results of the present paper.

The author is deeply grateful to Yu.N. Demkov, I.V. Komarov, and B.S. Pavlov for useful discussions of the results of the paper, as well as to M.N. Panov for his help in the analysis of the experimental ionization data.

[1] The formulas (10), (12), (29), and (32) in Ref. 2 contain typographical errors.

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Translated by A. K. Agyei