# Transition form factor of the hydrogen Rydberg atom

I. Bersons* and A. Kulsh
*Institute of Atomic Physics and Spectroscopy, University of Latvia, Raina boul. 19, Riga, LV-1586, Latvia*
(Received 24 May 1996; revised manuscript received 7 October 1996)

The form factor for the transition between the hydrogenic states with parabolic quantum numbers $n_1 n_2 m$ and $n_1' n_2' m'$ is obtained in a closed analytic form. The asymptotic limit of the transition form factor at large parabolic quantum numbers is derived, and a comparison with exact quantum calculations shows that the asymptotic limit is accurate in a wide region of parabolic quantum numbers and the momentum $p$ transferred to electrons. A simple quasiclassical formula for the transition probability is given, and the range of quantum numbers corresponding to quasiclassically forbidden transitions are defined. [S1050-2947(97)02803-5]

PACS number(s): 03.65.Db, 03.65.Sq, 32.80.Cy

## I. INTRODUCTION

The form factor for the $i \rightarrow f$ transition is defined by

$$T_{fi} = \langle \Psi_f | e^{i\mathbf{pr}} | \Psi_i \rangle, \tag{1.1}$$

where $|\Psi_i\rangle$ and $|\Psi_f\rangle$ are the electron wave functions for the initial and final atomic states, respectively, and $\mathbf{p}$ is the momentum transferred to electrons (atomic units are used throughout the paper).

The square of Eq. (1.1), $|T_{fi}|^2$, is the transition probability from the state $i$ to the state $f$, and it is the main factor in many theoretical treatments of the inelastic scattering of particles by atoms. Thus, in the Born and impulse approximations, $|T_{fi}|^2$ determines the cross sections of inelastic [1,2], $l$ mixing [3] and intercombination [4] transitions in atoms due to collisions with electrons, atoms, and ions. Recently it was shown [5,6] that the probability of excitation and ionization of a Rydberg atom by a short unipolar electromagnetic field pulse can be determined, in the sudden approximation, by the transition form factor. The vector $\mathbf{p} = \mathbf{F}_0 \tau$ is in this case the momentum transferred to the electron from the electric-field pulse of duration $\tau$ and the peak value $\mathbf{F}_0$. The matrix element for the electromagnetic transition between the atomic states can be reduced to Eq. (1.1) as well.

Direct calculation of the matrix element (1.1), even with hydrogenic wave functions, is laborious as the wave functions of highly excited states oscillate very rapidly and many matrix elements (1.1) have to be calculated for comparison with an experimentally measured cross section or a transition probability. The analytic expressions for the matrix element (1.1) have been obtained for transitions between two hydrogenic continuum states [7] and for the transition between the ground state and any parabolic discrete or continuum state [1]. Calculation of the form factor (1.1) in the spherical basis is more complicated than in the parabolic one. Therefore, to calculate the matrix elements $T_{fi}$ between the spherical states, Omidvar [8] at first calculated $T_{fi}$ between the parabolic states and then used the connection formula between the parabolic and spherical wave functions. Omidvar [8] has reduced the transition form factor $T_{fi}$ in parabolic coordinates to a fourfold sum. If the atom is placed in a constant electric field, the parabolic basis is preferable. Recent experimental studies [9,10] with unipolar half-cycle electromagnetic pulses focus on the excitation and ionization of parabolic atomic states. If the pulse duration is less than the Kepler period, the transition amplitude between the two parabolic states is determined directly by the form factor (1.1).

In the limit of small momentum $p$, the transition form factor (1.1) can be written as

$$T_{fi} = \delta_{fi} + ip T_{fi}^D, \tag{1.2}$$

where $T_{fi}^D$ is the dipole matrix element. The dipole matrix element with Coulomb wave functions is calculated analytically in a closed form in the spherical as well in the parabolic basis [11,12]. The approximate analytic formulas for $T_{fi}$ exist for close in energy states and for the case of transitions between remote bound states. Different approximations for the dipole matrix elements are discussed in the recent review article [13]. The transition form factor (1.1), as a function of its parameters, is a more complicated mathematical quantity than $T_{fi}^D$, and the approximate analytic formulas for $T_{fi}$ have been derived only in the case of small changes in principal and angular-momentum quantum numbers [2,4,14] when the Heisenberg correspondence principle can be used. For ionization and excitation processes involving large changes in the principal quantum number $n$, the methods based on the Heisenberg correspondence principle are not satisfactory. The purpose of this paper is to obtain an approximate analytic formula for the transition form factor $T_{fi}$ in the case of remote bound states.

In the present work, an analytic expression for the matrix element (1.1) between two parabolic quantum states of the hydrogen atom is obtained. A quantum-mechanical derivation of the main formula is given in Sec. II. In Sec. III we use the method of comparison equations and derive the uniform asymptotic limit of $T_{fi}$ at large parabolic quantum numbers. In Sec. IV the quasiclassical wave functions and the saddle-point method are used to estimate the matrix element (1.1). A comparison between the quantum-mechanical calculations and the different approaches are given and discussed in Sec. V. In conclusion we present a summary of the results.

*Electronic address: bersons@acad.latnet.lv

 

## II. FORM FACTOR FOR $n_1n_2m \to n_1'n_2'm'$ TRANSITION

The wave function of the hydrogen atom in the parabolic coordinates is given by [1,12]

$$\Psi_{n_1n_2m} = \frac{e^{im\varphi}}{\pi^{1/2}n^2} f_{n_1m}\left(\frac{\xi}{n}\right) f_{n_2m}\left(\frac{\eta}{n}\right), \tag{2.1}$$

$$f_{n_im}(x) = \frac{1}{m!}\left(\frac{(n_i+m)!}{n_i!}\right)^{1/2} x^{m/2} F(-n_i, m+1, x) e^{-(x/2)}, \tag{2.2}$$

$$n = n_1 + n_2 + m + 1, \quad m \geq 0, \tag{2.3}$$

where $F(-n_i, m+1, x)$ is the confluent hypergeometric function. If we choose the $z$ axis along the **p** direction, the integration over angular variable $\varphi$ is trivial and yields the conservation of the magnetic quantum number $m$. The transition form factor (1.1) can be presented as

$$T_{fi} = i\left[R(n_1, n_1')\frac{\partial R^*(n_2, n_2')}{\partial p} - R^*(n_2, n_2')\frac{\partial R(n_1, n_1')}{\partial p}\right], \tag{2.4}$$

where

$$R(n_1, n_1') = \frac{1}{(nn')^{(m/2)+1} m!^2}\left[\frac{(n_1+m)!(n_1'+m)!}{n_1!n_1'!}\right]^{1/2} \int_0^\infty d\xi\ \xi^m F\left(-n_1, m+1, \frac{\xi}{n}\right) F\left(-n_1', m+1, \frac{\xi}{n'}\right) \times \exp\left[-\frac{\xi}{2}\left(\frac{1}{n} + \frac{1}{n'} - ip\right)\right], \tag{2.5}$$

and $R^*(n_2, n_2')$ is the complex conjugate of $R(n_2, n_2')$.

The integral (2.5) is calculated analytically in a closed form [1], and can be written as

$$R(n_1, n_1') = \frac{2^{m+1}(nn')^{m/2}}{m!}\left[\frac{(n_1+m)!(n_1'+m)!}{n_1!n_1'!}\right]^{1/2} \frac{(n-n'-iy)^{n_1}(n'-n-iy)^{n_1'}}{(n+n'-iy)^{n_1+n_1'+m+1}} F(-n_1, -n_1', m+1; z), \tag{2.6}$$

$$y = pnn', \quad z = -\frac{4nn'}{(n-n')^2+y^2}, \tag{2.7}$$

where the hypergeometric function $F(-n_1, -n_1', m+1; z)$ is polynomial, symmetrical between $n_1$ and $n_1'$.

Differentiating of $R(n_1, n_1')$ and $R^*(n_2, n_2')$ with respect to $p$ according to Eq. (2.4) and using the recurrence relations for the hypergeometric functions [15] we obtain the final expression for the transition form factor (1.1)

$$T_{fi} = \frac{i2^{2m+1} yz (nn')^m}{m!^2}\left[\frac{(n_1+m)!(n_1'+m)!(n_2+m)!(n_2'+m)!}{n_1!n_1'!n_2!n_2'!}\right]^{(1/2)} \times \frac{(n-n'-iy)^{n_1}(n'-n-iy)^{n_1'}(n-n'+iy)^{n_2}(n'-n+iy)^{n_2'}}{(n+n'-iy)^{n_1+n_1'+m+1}(n'+n+iy)^{n_2+n_2'+m+1}} \left\{\frac{2nn'(n_1-n_2+iy)+(n_2'-n_1')(n^2+n'^2+y^2)}{(n+n')^2+y^2}\right. \times F(-n_1, -n_1', m+1; z) F(-n_2, -n_2', m+1; z) + n_1' F(-n_1, -n_1'+1, m+1; z) F(-n_2, -n_2', m+1; z) \left. - n_2' F(-n_1, -n_1', m+1; z) F(-n_2, -n_2'+1, m+1; z)\right\}. \tag{2.8}$$

In the limit of small $p$, the matrix element $T_{fi}$ is connected, according to Eq. (1.2), with the dipole matrix element in the parabolic basis [11,12]. Equation (2.8) is simplified, if $n_1 = n_2 = 0$, $m = n-1$ (the initial state is circular). The transition probability, in this case, is

$$|T_{fi}|^2 = \frac{(n_1'+n-1)!(n_2'+n-1)! y^2 z^{2n+2}[(n-n')^2+y^2]^{n+n'}[y^2+(n_1'-n_2')^2]}{[(n-1)!]^2 n_1'! n_2'! [(n+n')^2+y^2]^{n+n'+2}}, \tag{2.9}$$

$$n' = n_1' + n_2' + n \geq n.$$

For transitions from the ground state ($n=1$), Eq. (2.9) is identical with the one given by Landau and Lifshitz [1].

The transition form factor, in the spherical basis, can be calculated from Eq. (2.8), if the connection formula between the spherical and parabolic wave functions [16,17]

$$\Psi_{nlm}=\sum_k C\left(\frac{n-1}{2},\frac{m+k}{2},\frac{n-1}{2},\frac{m-k}{2},l,m\right)\psi_{nkm} \tag{2.10}$$

is used, where $C(\cdots)$ is the Clebsh-Gordon coefficient and $k=n_1-n_2$ is the electric quantum number.

At $n'=n$ and small $pn$, the argument of the hypergeometric function is large and from Eq. (2.8) we can obtain that the depletion of the initial state is equal to

$$|T_{ii}|^2=1-(n^2-m^2+3)\frac{(pn)^2}{4}. \tag{2.11}$$

This expression is independent of the parabolic quantum numbers $n_1$ and $n_2$ and it is true for the spherical quantum states too.

## III. ASYMPTOTIC LIMIT

In this section we shall obtain an asymptotic limit of the transition form factor at large quantum numbers. The problem is to find the asymptotic limit of the hypergeometric function $F(-n_1,-n_1',m+1;z)$. We shall further use the method of comparison equations for this purpose. This method [15] is successful to find the uniform asymptotic solution of a second-order differential equation presented in the form

$$\frac{d^2u_1}{dz^2}+[\lambda^2 p(z)+q(z)]u_1=0, \tag{3.1}$$

where $\lambda$ is a large parameter. Using the substitution

$$F=\frac{(1-z)^{(n_1+n_1'+m)/2}}{(-z)^{(m+1)/2}}u_1 \tag{3.2}$$

in the hypergeometric equation [15] we obtain an equation for the function $u_1$ in the form (3.1), where now

$$p(z)=-\frac{1}{(1-z)^2}-\frac{\alpha}{z(1-z)}-\frac{\beta}{z^2}, \tag{3.3}$$

$$q(z)=\frac{1}{4(1-z)^2}+\frac{1}{4z(1-z)}+\frac{1}{4z^2}, \tag{3.4}$$

$$\lambda=\frac{\nu_1+\nu_1'}{2}, \tag{3.5}$$

$$\alpha=\frac{4\nu_1\nu_1'+m^2}{(\nu_1+\nu_1')^2},\quad \beta=\frac{m^2}{(\nu_1+\nu_1')^2}, \tag{3.6}$$

$$\nu_1=n_1+\frac{m+1}{2},\quad \nu_1'=n_1'+\frac{m+1}{2}. \tag{3.7}$$

Thus, the method of comparison equations can be used, provided that the combination $\nu_1+\nu_1'$ of the parabolic quantum numbers is large.

The main term of the asymptotic solution of Eq. (3.1) is determined by the function $p(z)$. The zeros of the function $p(z)$ are called branching points. The method of the comparison equation is based on the idea that the function $p(z)$ can be replaced by a simpler function with the same branching points in some domain of $z$ and for which the analytic solution of the comparison equation is well known. However, in our case the situation is more complicated because the function $p(z)$ and, therefore, the branching points, depend on two additional parameters $\alpha$ and $\beta$. These parameters vary in the intervals: $0<\alpha<2$, $0<\beta<1$. Equation (3.1), for the function $u_1$, has two branching points (both negative)

$$z_1^-=\frac{-4\nu_1\nu_1'+m^2-b_1}{2(\nu_1-\nu_1')^2},\quad z_1^+=\frac{-4\nu_1\nu_1'+m^2+b_1}{2(\nu_1-\nu_1')^2}, \tag{3.8}$$

with

$$b_1^2=(4\nu_1\nu_1'-m^2)^2-4m^2(\nu_1-\nu_1')^2>0. \tag{3.9}$$

These branching points $z_1^-$ and $z_1^+$ depend only on parabolic quantum numbers $n_1,n_1'$ and $m$. In the case of the hypergeometric function $F(-n_2,-n_2',m+1,z)$, there are branching points $z_2^-$ and $z_2^+$ with $n_2$ and $n_2'$ instead of $n_1$ and $n_1'$, respectively. If $m=0$, both $z_1^+$ and $z_2^+$ are equal to zero. For $n_1=n_1'$ the branching point $z_1^-$ tends to infinity and $z_1^+$ is equal to $-m^2/(4\nu_1^2-m^2)$.

The asymptotic equation for $u_1$ can be presented now as

$$\frac{d^2u_1}{dz^2}-p_1(z)u_1=0, \tag{3.10}$$

where

$$p_1(z)=\frac{(\nu_1-\nu_1')^2(z_1^--z)(z_1^+-z)}{4z^2(1-z)^2}. \tag{3.11}$$

The argument $z$ is negative and according to Eq. (2.7) changes from $-4nn'/(n'-n)^2$ to zero. The function $u_1(z)$ oscillates in the region between the branching points, $z_1^-<z<z_1^+$, and exponentially decreases as $z$ tends to zero or to $-\infty$.

We are using the equation for the Airy function as a comparison equation [14] and are focusing our attention on a solution near the turning point $z_1^-$. For $z\leq z_1^-$, the asymptotic solution of Eq. (3.10) is given by

$$u_1=C\left(\frac{x_1}{p_1}\right)^{1/4}\mathrm{Ai}(x_1), \tag{3.12}$$

where

$$\gamma_1=\frac{2}{3}x_1^{3/2}=\int_z^{z_1^-}dz'[p_1(z')]^{1/2} \tag{3.13}$$

and $\mathrm{Ai}(x_1)$ is the Airy function. We will find in Sec. IV, that constant $C$ is

$$C=(-1)^{n_1}\frac{m!}{(n_1 n_1')^{m/2}}. \tag{3.14}$$

The integration in Eq. (3.13) yields

$$\frac{2}{3}x_1^{3/2}=(\nu_1+\nu_1')\ln\left|g_1^+\left(\frac{1-z_1^-}{1-z}\right)^{1/2}-g_1^-\left(\frac{1-z_1^+}{1-z}\right)^{1/2}\right|+|\nu_1-\nu_1'|\ln(g_1^++g_1^-)+m\ln\left[g_1^+\left(\frac{z_1^-}{z}\right)^{1/2}+g_1^-\left(\frac{z_1^+}{z}\right)^{1/2}\right], \tag{3.15}$$

with

$$g_1^{\pm}=\left(\frac{z_1^{\pm}-z}{z_1^+-z_1^-}\right)^{1/2}. \tag{3.16}$$

The argument of the Airy function is equal to zero at $z=z_1^-$.

For $z$ lying between the branching points, $z_1^-\leqslant z\leqslant z_1^+$, the function $p_1(z)$ is negative. The asymptotic solution of Eq. (3.10) is again given by Eq. (3.12) with a negative parameter $x_1$,

$$\gamma_1=\frac{2}{3}(-x_1)^{3/2}=\int_{z_1^-}^{z}dz'[-p_1(z')]^{1/2}. \tag{3.17}$$

After performing the integration, we obtain

$$\gamma_1=\frac{2}{3}(-x_1)^{3/2}=(\nu_1+\nu_1')\arctan\left[\tau_1\left(\frac{1-z_1^+}{1-z_1^-}\right)^{1/2}\right]-|\nu_1-\nu_1'|\arctan\tau_1-m\arctan\left[\tau_1\left(\frac{z_1^+}{z_1^-}\right)^{1/2}\right], \tag{3.18}$$

with

$$\tau_1=\left(\frac{z-z_1^-}{z_1^+-z}\right)^{1/2}. \tag{3.19}$$

As a result the asymptotic expression of the hypergeometric function $F(-n_1,-n_1',m+1;z)$ at large $\nu_1+\nu_1'$ and for $z\leqslant z_1^-$ and $z\geqslant z_1^-$ is given by Eqs. (3.2) and (3.12)–(3.19). The function $R(n_1,n_1')$ now becomes

$$R(n_1,n_1')=\left(\frac{4x_1}{d_1}\right)^{1/4}\mathrm{Ai}(x_1)e^{i\rho_1}, \tag{3.20}$$

with

$$d_1=4n^2n'^2(1-z)^2p_1(z)=\frac{n^2n'^2(\nu_1-\nu_1')^2(z_1^--z)(z_1^+-z)}{z^2}, \tag{3.21}$$

$$\rho_1=(\nu_1+\nu_1')\arctan\left(\frac{y}{n+n'}\right)-(\nu_1'-\nu_1)\arctan\left(\frac{y}{n'-n}\right). \tag{3.22}$$

The function $R^*(n_2,n_2')$ can be easily obtained from Eq. (3.20). Differentiation of $R(n_1,n_1')$ and $R^*(n_2,n_2')$ in Eq. (2.4) gives the following asymptotic estimate for the transition form factor:

$$T_{fi}=\frac{8nn'y}{Q}\left(\frac{x_1x_2}{d_1d_2}\right)^{1/4}\left\{nn'y\ \mathrm{Ai}(x_1)\mathrm{Ai}(x_2)+i\left[\left(\frac{d_1}{x_1}\right)^{1/2}\mathrm{Ai}'(x_1)\mathrm{Ai}(x_2)-\left(\frac{d_2}{x_2}\right)^{1/2}\mathrm{Ai}'(x_2)\mathrm{Ai}(x_1)\right]\right\}e^{i(\rho_1-\rho_2)}, \tag{3.23}$$

where

$$Q=(n'^2-n^2)^2+2y^2(n^2+n'^2)+y^4 \tag{3.24}$$

and $\mathrm{Ai}'(x)$ is the derivative of the Airy function. Here we ignore the derivatives of $(x_1/d_1)^{1/4}$ and $(x_2/d_2)^{1/4}$ which are much smaller than the derivative of the Airy function and the exponential factor.

The asymptotic limit of the transition form factor, Eq. (3.23), is valid for $z$ near the points $z_1^-$ and $z_2^-$. If $z$ approaches one of the branching points $z_1^+$ or $z_2^+$, Eq. (3.23) breaks down. However, Eq. (3.23) can also be used for $z$ near these points if we redefine the argument of the Airy functions. Thus, for $z>z_1^+$ the argument $x_1$ is defined again by Eq. (3.15) with

$$g_1^{\pm}=\left(\frac{z-z_1^{\pm}}{z_1^+-z_1^-}\right)^{1/2}. \tag{3.25}$$

At $z<z_1^+$ the argument $x_1$ is defined by Eqs. (3.18) and (3.19) if $z_1^-$ and $z_1^+$ are interchanged in both these equations.

When can we expect that the asymptotic limit of the form factor will not be correct? Firstly, when the parameter $\lambda$, Eq. (3.5), of the asymptotic expansion is small, i.e., $\nu_1+\nu_1'$ or $\nu_2+\nu_2'$ is small. In the second place, if the magnetic quantum number $m$ is very large and $n_1$ and $n_1'$ or $n_2$ and $n_2'$ are small. In this case $z_1^+$ or $z_2^+$ is close to $-m/2$, and $z_1^+$ approaches $z_1^-$ or $z_2^+$ approaches $z_2^-$. The asymptotic expansion in the vicinity of the isolated point is no longer correct. In the limiting case, if the initial or final state is circular one, the hypergeometric functions are equal to unity, and the transition probability is defined by Eq. (2.9) and has a bell-shaped form as a function of $pn$. At last, the asymptotic expansion breaks down, if the final state coincides with the initial one ($n_1'=n_1, n_2'=n_2, n'=n$), and we are looking at the matrix element $T_{ii}$ at small $pn$. When $n'=n$, the argument $z$ is equal to $-4/(pn)^2$ and is large at small $pn$. In this case, the dominant term in Eq. (3.1) proportional to $z^{-2}$ is absent in the main function $p(z)$, but the function $q(z)$, which we neglect to find the leading term of the asymptotic

expansion, contains such term. But this is just the case for developing an alternative method based on the Heisenberg correspondence principle.

For $z_1^- < z < z_1^+$, $z_2^- < z < z_2^+$ and large and negative $x_1$ and $x_2$, we can use the asymptotic expansion for the Airy function [15]. In this limit, the function $R(n_1, n_1')$ becomes

$$R(n_1, n_1') = \left(\frac{2}{\pi}\right)^{1/2} \frac{e^{i\rho_1}}{\kappa_1^{1/4}} \sin\left(\gamma_1 + \frac{\pi}{4}\right), \tag{3.26}$$

where

$$\kappa_1 = -d_1 \tag{3.27}$$

and $\gamma_1$ is defined by Eq. (3.18). The transition probability can be written as

$$|T_{fi}|^2 = \frac{16 n^2 n'^2 y^2}{\pi^2 Q^2 (\kappa_1 \kappa_2)^{1/2}} [V + \kappa_1 + \kappa_2 + L], \tag{3.28}$$

$$V = n^2 n'^2 y^2. \tag{3.29}$$

The rapidly oscillating term $L$ is given by

$$\begin{aligned} L = {} & (V - \kappa_1 + \kappa_2) \sin 2\gamma_1 + (V + \kappa_1 - \kappa_2) \sin 2\gamma_2 \\ & + \tfrac{1}{2}[V - \kappa_1 - \kappa_2 - 2(\kappa_1 \kappa_2)^{1/2}] \cos 2(\gamma_1 - \gamma_2) \\ & + \tfrac{1}{2}[-V + \kappa_1 + \kappa_2 - 2(\kappa_1 \kappa_2)^{1/2}] \cos 2(\gamma_1 + \gamma_2). \end{aligned} \tag{3.30}$$

Averaging Eq. (3.28) over these fast oscillations, we obtain a very simple estimate for the transition probability

$$\overline{|T_{fi}|^2} = \frac{16 n^2 n'^2 y^2}{\pi^2 Q^2 (\kappa_1 \kappa_2)^{1/2}} [V + \kappa_1 + \kappa_2], \tag{3.31}$$

where two parameters $\kappa_1$ and $\kappa_2$ are defined by Eqs. (3.21) and (3.27). Expression (3.28) for the transition probability will be found by the alternative, quasiclassical, method in Sec. IV, and we will call Eq. (3.28) the quasiclassical approximation and Eq. (3.31) the averaged quasiclassical approximation for the transition probability.

The quasiclassical formulas, Eqs. (3.28) and (3.31), diverge as $z$ tends to one of the branching point. Thus, we can use these formulas only in the $z$ domain

$$\max(z_1^-, z_2^-) < z < \min(z_1^+, z_2^+). \tag{3.32}$$

Transitions outside of this domain are quasiclassically forbidden. It means that in the quasiclassical approximation the transition probability between two parabolic states is zero at some $p$ values. Quantum mechanically, the transition probability at every finite $p$ differs from zero (at some $p$ values it can be very small). It is interesting to note that for some states the condition (3.32) never can be satisfied, i.e., transition between these states is quasiclassically forbidden. First, it happens if $z_1^+$ or $z_2^+$ is less than the minimal value of $z$:

$$z_1^+ < -\frac{4nn'}{(n-n')^2} \quad \text{or} \quad z_2^+ < -\frac{4nn'}{(n-n')^2}. \tag{3.33}$$

When $m = 0$, the branching points $z_1^+ = z_2^+ = 0$ and the condition (3.33) cannot be realized. But for $m > m_1$ or $m > m_2$, where

$$\begin{aligned} m_1 = {} & \frac{4nn'}{(n-n')^2} \left[ n_1 + n_1' + 1 + \frac{(n+n')}{(nn')^{1/2}} \right. \\ & \left. \times \left(n_1 + \frac{1}{2}\right)^{1/2} \left(n_1' + \frac{1}{2}\right)^{1/2} \right] \end{aligned} \tag{3.34}$$

and $m_2$ is defined similarly, the condition (3.33) is satisfied. In the second place, the transition between two states is quasiclassically forbidden, if the quasiclassical intervals $[z_1^-, z_1^+]$ and $[z_2^-, z_2^+]$ are not overlapping

$$z_2^- > z_1^+ \quad \text{or} \quad z_1^- > z_2^+. \tag{3.35}$$

In this case, there are no such $p$ values for which the condition (3.32) can be satisfied. A physical reason for these restrictions on the quasiclassical transitions probabilities will be given in Sec. IV.

Considering the limit of small $p$ in Eq. (3.23), we can find the asymptotic limit of the dipole matrix element in the parabolic basis for transition involving large changes in $n$

$$\begin{aligned} \langle n_1', n_2', m | z | n_1, n_2, m \rangle = {} & \frac{8 n^2 n'^2}{(n'^2 - n^2)^2} \\ & \times \left\{ \left(\frac{x_2 d_1}{x_1 d_2}\right)^{1/4} \mathrm{Ai}'(x_1) \mathrm{Ai}(x_2) \right. \\ & \left. - \left(\frac{x_1 d_2}{x_2 d_1}\right)^{1/4} \mathrm{Ai}'(x_2) \mathrm{Ai}(x_1) \right\}. \end{aligned} \tag{3.36}$$

The parameters $x_i$ and $d_i$ are defined above and

$$z = \frac{-4nn'}{(n-n')^2}. \tag{3.37}$$

An estimate of the dipole matrix element in the parabolic basis has been obtained recently in [13]. That presented in [13] formula contains the same combination of the Airy functions as Eq. (3.36), however the arguments of the Airy functions in two expressions are different. Note that at $p = 0$, when $z$ is given by Eq. (3.37), at least one of $z_1^-$ and $z_2^-$ exceeds $z$ and the condition (3.32) is not satisfied. Thus, in this limit we cannot employ the quasiclassical approximation for the function $R(n_1, n_2)$, given by Eq. (3.26). Therefore, we can never employ this approximation for Eq. (3.36).

## IV. QUASICLASSICAL APPROXIMATION

In this section an alternative method is proposed for estimating the transition form factor (1.1) at large quantum numbers. The quasiclassical wave functions and the saddle-point method are used. This method gives physical insight in the transition mechanism and allows us to find the constant $C$ undetermined in the preceding section.

The wave function (2.1) in the quasiclassical approximation is given by

$$\Psi_{n_1 n_2 m}=\frac{e^{im\varphi}\sin\left[S_{n_1}(\xi)+\frac{\pi}{4}\right]\sin\left[S_{n_2}(\eta)+\frac{\pi}{4}\right]}{n^2\pi^{3/2}[\xi\eta k_{n_1}(\xi)k_{n_2}(\eta)]^{1/2}}, \quad (4.1)$$

where

$$S_{n_1}(\xi)=\int_{\xi_{n_1}^-}^{\xi} d\xi' k_{n_1}(\xi'), \quad (4.2)$$

$$k_{n_1}^2(\xi)=-\frac{1}{4n^2}+\frac{\nu_1}{n\xi}-\frac{m^2}{4\xi^2}, \quad (4.3)$$

and the turning points $\xi_{n_1}^{\pm}$ are defined by

$$\xi_{n_1}^{\pm}=2n\nu_1(1\pm\varepsilon_{n_1}), \quad (4.4)$$

$$\varepsilon_{n_1}=\left(1-\frac{m^2}{4\nu_1^2}\right)^{1/2}. \quad (4.5)$$

For the coordinate $\eta$, there are equations, analogous to Eqs. (4.2)–(4.5).

The transition form factor can be presented again by Eq. (2.4), where the function $R(n_1,n_1')$ is now given by the integral

$$R(n_1,n_1')=\frac{1}{\pi nn'}\times\int\frac{d\xi\sin\left[S_{n_1}(\xi)+\frac{\pi}{4}\right]\sin\left[S_{n_1'}(\xi)+\frac{\pi}{4}\right]e^{(ip\xi)/2}}{\xi[k_{n_1}(\xi)k_{n_1'}(\xi)]^{1/2}}. \quad (4.6)$$

To calculate the quasiclassical integral like Eq. (4.6), the Heisenberg correspondence principle is usually used [2,4,6]. This method is based on the assumption that the difference between the actions $S_{n_1}$ and $S_{n_1'}$ is smaller than the actions themselves, but is larger than $p\xi/2$. This condition is fulfilled for small $p$. If $p\xi$ is comparable with $S_{n_1}$ and $S_{n_1'}$, the saddle-point method is more preferable [6]. The saddle-point method for evaluation of the quasiclassical integrals like (4.6) has been proposed in [18]. According to this method, the transitions arise only in the vicinity of stationary points.

A stationary point $\xi_0$ is defined by the equation

$$\frac{p}{2}=|k_{n_1'}(\xi_0)\pm k_{n_1}(\xi_0)|. \quad (4.7)$$

Equation (4.7) presents the momentum conservation: the sum (the difference) of the initial and final electron momentum (along the coordinate $\xi$) at the point $\xi_0$ is equal to half of the momentum transferred to electron. The sign ''+'' in Eq. (4.7) means that the electron changes the direction of motion along the classical orbit by changing the momentum. At $k_{n_1'}(\xi)=k_{n_1}(\xi)$, when Eq. (4.7) can be satisfied only for the sign ''+,'' the electron does not change the absolute value of its momentum, but changes the direction of motion. When $m=0$, the electron can approach the nucleus very closely and the momentum transferred to the electron can be large.

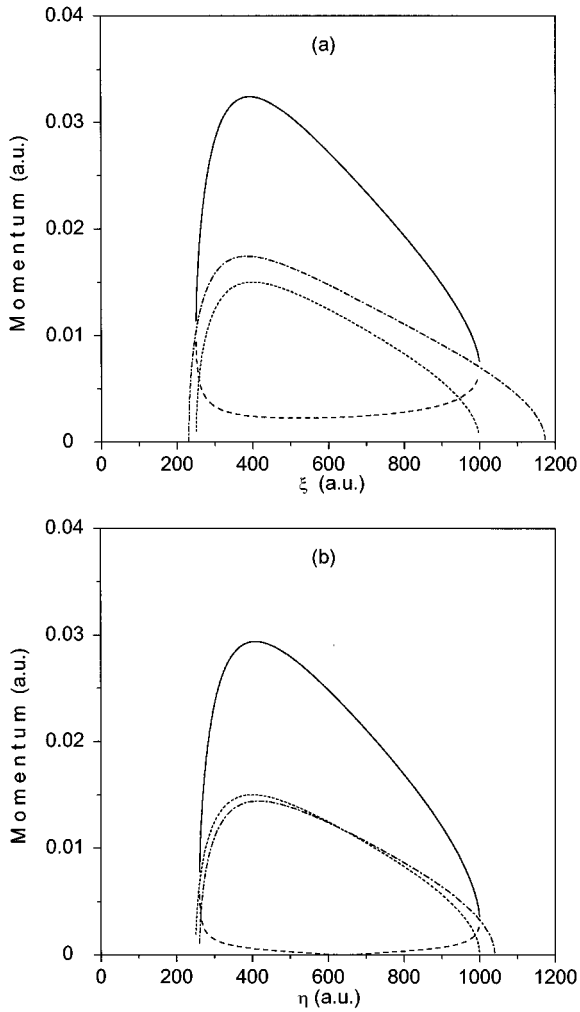


FIG. 1. (a) The electron momenta $k_{n_1}(\xi)$ (dotted line) and $k_{n_1'}(\xi)$ (dashed-dotted line), the sum $k_{n_1}(\xi)+k_{n_1'}(\xi)$ (solid line), and the absolute value of the difference $k_{n_1'}(\xi)-k_{n_1}(\xi)$ (dashed line) as a function of $\xi$; (b) the same for the coordinate $\eta$. Curves for the quantum numbers $n=25$, $n_1=2$, $n_2=2$, $m=20$, $n'=26$, $n_1'=3$, and $n_2'=2$ are shown.

In Fig. 1 we present the momenta $k_{n_1}(\xi), k_{n_1'}(\xi)$, the function $|k_{n_1'}(\xi)\pm k_{n_1}(\xi)|$, and the analogous momenta along the $\eta$ axis for the states with quantum numbers $n=25$, $m=20$, $n_1=2$, $n_2=2$, $n'=26$, $n_1'=3$, $n_2'=2$. For such quantum numbers, the momentum $k_{n_1'}(\xi)$ exceeds $k_{n_1}(\xi)$, and the transition is allowed for $\xi$ lying inside the classically allowed region, i.e., at $200<\xi<1000$. The momentum $k_{n_2}(\eta)$ exceeds $k_{n_2'}(\eta)$ at $\eta<633$, but at $\eta>633$, $k_{n_2}(\eta)<k_{n_2'}(\eta)$. Along the coordinate $\eta$ the transition is restricted by the range $260<\eta<1000$. We will call the right-hand side of Eq. (4.7), the two-valued function $|k_{n_1'}(\xi)\pm k_{n_1}(\xi)|$, the ovoid. For any $p/2$ inside of this ovoid, there are two roots of Eq. (4.7). The two roots are defined by

$$\xi_0^{\pm}=\frac{4nn'}{Q}[(n'^2-n^2)(\nu_1 n'-\nu_1' n) + (\nu_1' n+\nu_1 n')y^2 \pm 2y\kappa_1^{1/2}], \tag{4.8}$$

with

$$\kappa_1=nn'(n\nu_1-n'\nu_1')(\nu_1' n-\nu_1 n')+\nu_1\nu_1' nn' y^2-\frac{m^2}{16}Q = \frac{n^2 n'^2(\nu_1-\nu_1')^2(z-z_1^-)(z_1^+-z)}{z^2}. \tag{4.9}$$

On the top and the bottom of the ovoid, both stationary points $\xi_0^{\pm}$ coincide. As one can see from Eq. (4.9), the variable $z$ at these points is equal to $z_1^+$ and $z_1^-$ respectively. The standard saddle-point method is not correct in the vicinity of the top and the bottom of the ovoid, because the derivative of Eq. (4.7) at these points is equal to zero, and we should take into account the next term in the expansion of the exponential factor. This leads to the Airy function representation of the function $R(n_1,n_1')$. The standard saddle-point method gives the divergent form factor at the top and the bottom of ovoids. The quasiclassical approximation evaluates the transition form factor only in the range of $p$ values which are common for both ovoids. In Fig. 1 this range is $0.0022<p<0.029$. To make a transition from the initial to the final state, the momentum transferred to the electron cannot be less than 0.0022 and greater than 0.029. Outside this range the quasiclassical transition probability is equal to zero.

The transitions between some quantum states are quasiclassically forbidden for all $p$. It happens when both ovoids do not have a common interval of $p/2$. A fixed momentum can be transferred to the electron along one of the axes, but cannot be transferred along the other axis. As mentioned in the preceding section, this happens when $z_1^+<z_2^-$ or $z_2^+<z_1^-$. In the second place, the transition between the two states is quasiclassically forbidden, if the initial and final states do not have a common region in the electron classical motion, i.e., the areas under the curves $k_{n_1}(\xi)$ and $k_{n_1'}(\xi)$ or $k_{n_2}(\eta)$ and $k_{n_2'}(\eta)$ do not overlap. This occurs if the turning point $\xi_{n_1}^+<\xi_{n_1'}^-$ or $\xi_{n_1'}^+<\xi_{n_1}^-$ and similar for the motion along the axis $\eta$. It is easy to show that in this case $m>m_1$ or $m>m_2$, where $m_1$ is defined by Eq. (3.34). When $p$ is small, the momentum difference $|k_{n_1'}(\xi_0^{\pm})-k_{n_1}(\xi_0^{\pm})|$ is also small and using the saddle-point method is questionable. The Heisenberg correspondence method is preferable in this case.

In the saddle-point method, only the regions near four stationary points ($\xi_0^{\pm}$ for coordinate $\xi$ and $\eta_0^{\pm}$ for coordinate $\eta$) are important for transitions from the initial to the final electronic state. These stationary points are different for different final states. For the sign ''$-$'' in Eq. (4.7), the saddle-point method yields

$$R(n_1,n_1')=\frac{1}{(2\pi)^{1/2}\kappa_1^{1/4}}\left\{\exp\left[i\left(S_1(\xi_0^+)-\frac{\pi}{4}\right)\right] + \exp\left[i\left(S_1(\xi_0^-)+\frac{\pi}{4}\right)\right]\right\}, \tag{4.10}$$

where

$$S_1(\xi_0^{\pm})=S_{n_1}(\xi_0^{\pm})-S_{n_1'}(\xi_0^{\pm}), \tag{4.11}$$

$$S_{n_1}(\xi_0^{\pm})=2\nu_1\arctan\left[\frac{\xi_0^{\pm}-\xi_{n_1}^-}{\xi_{n_1}^+-\xi_0^{\pm}}\right]^{1/2} - m\arctan\left[\frac{(1+\varepsilon_{n_1})(\xi_0^{\pm}-\xi_{n_1}^-)}{(1-\varepsilon_{n_1})(\xi_{n_1}^+-\xi_0^{\pm})}\right]^{1/2}, \tag{4.12}$$

and $S_{n_1'}(\xi_0^{\pm})$ is defined for the final state in the same way as $S_{n_1}(\xi_0^{\pm})$ for the initial state. Comparing Eqs. (3.26) and (4.10) we see that they coincide if

$$\rho_1+\gamma_1=S_1(\xi_0^+), \quad \rho_1-\gamma_1=S_1(\xi_0^-). \tag{4.13}$$

These identities can be proved after some simple but lengthy algebra. The constant $C$ given by Eq. (3.14) is chosen on the basis of comparison of Eqs. (3.26) and (4.10). For the sign ''$+$'' in Eq. (4.7), the quasiclassical approximation again gives the function $R(n,n')$ identical with Eq. (3.26). According to Eq. (4.13), the argument of sin and cos in Eq. (3.30) is the difference between two actions. The transitions between two states take place in the vicinity of the stationary points, but the phase of the wave function of the initial and the final states is accumulating between these points. The phase is responsible for the oscillation of the transition probability by a variation of $p$.

## V. NUMERICAL RESULTS

In this section we compare various approximations for the transition probabilities with exact quantum-mechanical calculations. We present all results as a function of $pn$. In general, the transition probability increases with $pn$ increasing, has a maximum at some $pn$ and then decreases and oscillates with further increase of $pn$. The mathematical source of the oscillations of the transition probability is the oscillation of the hypergeometric functions in Eq. (2.8) at large $n_1,n_2,n_1'$ and $n_2'$.

In Fig. 2 the transition probability between two states of the $n=21$ manifold is presented. For the chosen quantum numbers the branching points $z_1^-=-35.0$, $z_2^-=-63.0$ and $z_1^+=z_2^+=0$. The parameters of the asymptotic expansion are large: $\lambda_1=9$ and $\lambda_2=12$. The asymptotic expansion developed in the vicinity of the points $z_1^-$ and $z_2^-$ and the quantum-mechanical calculations give practically the same results and cannot be distinguished in Fig. 2. The quasiclassical approximation also reproduces all oscillations, but it is not correct in the vicinity of $pn=0.338$ and below this point which corresponds to $z_1^-=-35$. In Fig. 3 we present the transition probability between two states of the neighboring $n$ manifolds with small $n_1,n_2,n_1',n_2'$, and large $m$. The corresponding picture of electron momenta is displayed in Fig. 1. The branching points $z_1^-=-273.5$, $z_2^-=-\infty$, $z_1^+=-1.46$ and $z_2^+=-1.78$. The asymptotic expansion near the points $z_1^-$ and $z_2^-$ reproduces the quantum calculations very

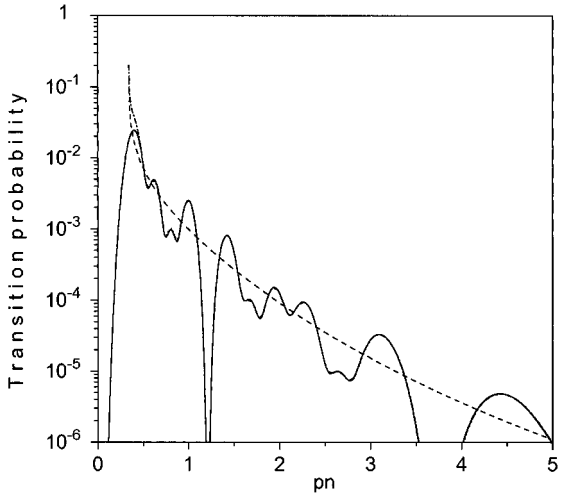


FIG. 2. Transition probability between the parabolic states with quantum numbers $n=n'=21$, $n_1=n_2=10$, $n_1'=7$, $n_2'=13$, and $m=0$ as a function of $pn$, in a.u. The solid line is the quantum-mechanical calculation; the dotted line is the asymptotic limit, Eq. (3.23); the dashed-dotted line is the quasiclassical approximation, Eq. (3.28); and the dash line is the averaged quasiclassical approximation, Eq. (3.31).

well but breaks down when $pn$ approaches value 1.47 which corresponds to the point $z_2^+$. On the other hand, the asymptotic expansion near the points $z_1^+$ and $z_2^+$ coincides well with the quantum calculations at large $pn$ but diverges when $pn$ tends to 0.11 which corresponds to the branching point $z_1^-$. There is a wide enough range of $pn$ values, where the asymptotic expansions near the points $z_1^-, z_2^-$ and $z_1^+, z_2^+$, as well as the quasiclassical approximation coincide. In Fig. 4 we present the transition between two states of very remote $n$ manifolds ($n=15$, $n'=180$), when the branching points $z_1^-=-0.837$, $z_2^-=-0.0686$ and $z_1^+=z_2^+=0$. Again, the asymptotic limit and quantum-mechanical results agree within a great accuracy. The quasiclassical approximation

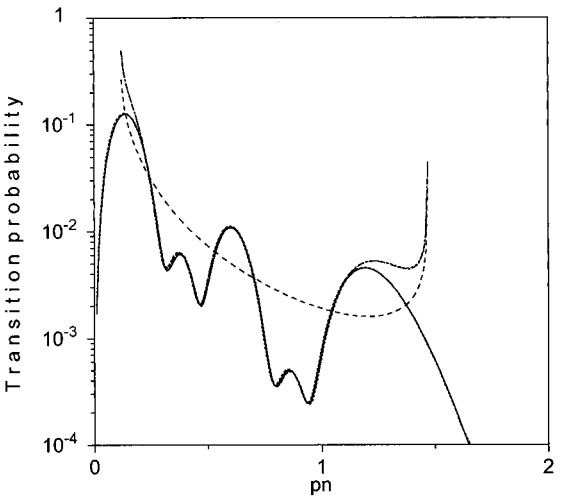


FIG. 3. The same as in Fig. 2 but for the states with $n=25$, $n_1=2$, $n_2=2$, $m=20$, $n'=26$, $n_1'=3$, and $n_2'=2$. The asymptotic expansion (dotted line) developed in the vicinity of the points $z_1^-$ and $z_2^-$ ($z_1^+$ and $z_2^+$) diverges at large (small) $pn$, in a.u.

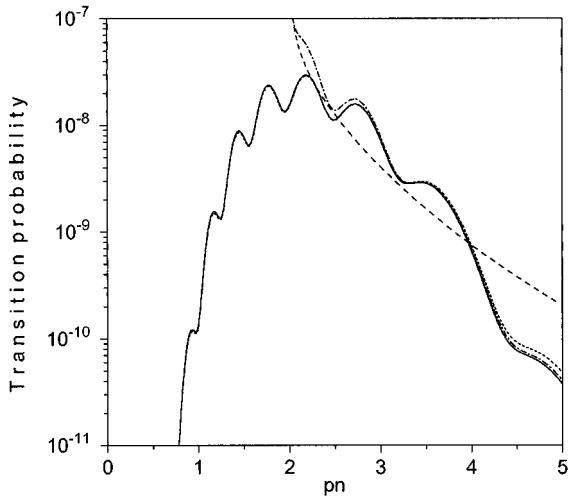


FIG. 4. The same as in Fig. 2 but for the states with $n=15$, $n_1=13$, $n_2=1$, $m=0$, $n'=180$, $n_1'=89$, and $n_2'=90$.

coincides with the quantum calculations at large $pn$ but diverges as $pn$ approaches 2.0 (the branching point $z_2^-$).

The two cases displayed in Fig. 5 and Fig. 6 are the worst of all for using the approximations developed in this paper. In Fig. 5 the initial state is the circular one and the hypergeometric functions in Eq. (2.8) are equal to unity. The branching points $z_1^+=-6.2$ and $z_2^+=-11.8$ are close to the points $z_1^-=-92.8$ and $z_2^-=-\infty$, respectively, and the asymptotic expansion near the isolated branching point is not justified. There is a very small range of $pn$ values for which the transitions are quasiclassically allowed. In Fig. 6 the depletion of the initial state (quantum numbers $n=21$, $n_1=20$, $n_2=m=0$) as a function of $pn$ is presented. In this case, the branching points $z_1^-=z_2^-=-\infty$, $z_1^+=z_2^+=0$ and the parameters of the asymptotic expansion $\lambda_1=20.5$ and $\lambda_2=0.5$. The parameter $\lambda_2$ is equal to the smallest possible value and using the method of comparison equation is not

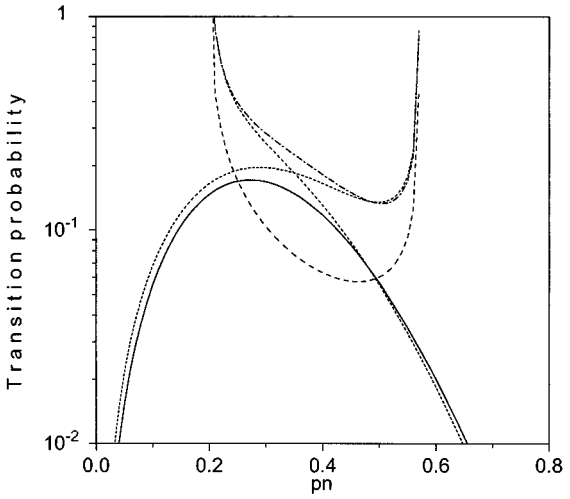


FIG. 5. The same as in Fig. 2 but for the states with $n=25$, $n_1=n_2=0$, $m=24$, $n'=26$, $n_1'=1$, and $n_2'=0$. The asymptotic expansion (dotted line) developed in the vicinity of the points $z_1^-$ and $z_2^-$ ($z_1^+$ and $z_2^+$) diverges at large (small) $pn$, in a.u.

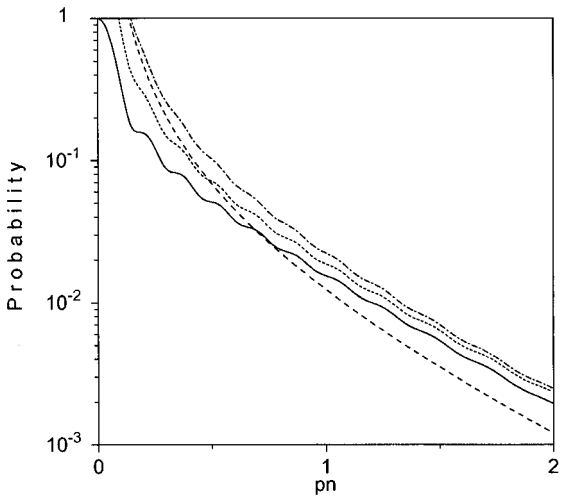


FIG. 6. The depletion of the initial state with quantum numbers $n=21$, $n_1=20$, $m=0$, as a function of $pn$, in a.u. The meaning of curves is the same as in Fig. 2.

correct. Nevertheless, the difference between the asymptotic limit and exact quantum calculations is only about 20–30% at large $pn$. As mentioned in Sec. III, the approximations developed in this paper diverge for the transition $i \rightarrow i$ as $pn$ tends to zero.

## VI. SUMMARY

The transition form factor (1.1) with parabolic Coulomb wave functions is calculated analytically in closed form. The final expression contains the hypergeometric functions and is similar to Gordon's formula for the dipole matrix element in the parabolic basis [11,12]. The numerical calculations show that the transition probability as a functions of $pn$ oscillates and has a maximum at some $pn$ value. In a general case, we have a superposition of two oscillations. Using the method of comparison equation, we approximate the hypergeometric function at large parameters by the Airy function. This asymptotic expansion is developed in the vicinity of one of the branching points of Eq. (3.10), and with a simple redefinition of the Airy function argument can be used in the vicinity of the other branching point. A comparison of the quantum-mechanical calculations with the asymptotic limit shows that the asymptotic limit is accurate in a wide region of $pn$ and parabolic quantum numbers. The asymptotic limit is not correct only for a description of the depletion of the initial state at small $pn$ and if the initial or the final state is close to the circular one.

The quasiclassical approximation and the saddle-point method are also used to estimate the transition form factor. In this approximation, the transitions between the initial and final states are located in the vicinity of four (two for the coordinate $\xi$ and two for the coordinate $\eta$) stationary points. These points lie in the classically allowed region of electron motion for the initial and final states. The transitions are quasiclassically allowed only if the momentum can be transferred to an electron along both coordinates. In Sec. IV, we have defined the conditions on the quantum numbers and $pn$, when the transition between two states is quasiclassically forbidden. There is a sufficiently broad region of $pn$ where the quasiclassical approximation gives fairly good results and reproduces all the oscillations in transition probabilities. Usually the experimentally measured value includes summation over many initial and final states. Such summation cancels out the fast oscillations in the individual transition probabilities and, therefore, for an evaluation of such sums, the simple averaged semiclassical approximation [Eq. (3.28)] should be good enough. This will be the subject of a separate work.

## ACKNOWLEDGMENTS

This work was supported by Latvian Sciences Council Grant No. 676 and European Community Contract No. ERB CIPD CT 940025.

[1] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Pergamon, Oxford, 1977).
[2] M. R. Flannery, in *Rydberg States of Atoms and Molecules*, edited by R. F. Stebbings and F. B. Dunning (Cambridge University Press, New York, 1983), p. 393.
[3] A. P. Hickman, R. E. Olson, and J. Pascall, in *Rydberg States of Atoms and Molecules*, edited by R. F. Stebbings and F. B. Dunning (Cambridge University Press, New York, 1983), p. 187.
[4] M. I. Syrkin, Phys. Rev. A **50**, 2284 (1994).
[5] P. Krstić and Y. Hahn, Phys. Rev. A **50**, 4629 (1994).
[6] I. Bersons, Latvian Journal of Physics and Technical Sciences, No. 5, 3 (1995).
[7] A. Nordsieck, Phys. Rev. **93**, 785 (1954).
[8] K. Omidvar, Phys. Rev. **188**, 140 (1969).
[9] R. R. Jones, N. E. Tielking, D. You, C. Raman, and P. H. Bucksbaum, Phys. Rev. A **51**, R2687 (1995).
[10] C. O. Reinhold, J. Burgdörfer, R. R. Jones, C. Raman, and P. H. Bucksbaum, J. Phys. B **28**, L457 (1995).
[11] W. Gordon, Ann. Phys. (Leipzig) **2**, 1031 (1929).
[12] H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms*, 2nd ed. (Plenum/Rosetta, New York, 1977).
[13] N. B. Delone, S. P. Goreslavsky, and V. P. Krainov, J. Phys. B **27**, 4403 (1994).
[14] E. Sobeslavsky, Ann. Phys. (Leipzig) **28**, 321 (1973).
[15] *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun (Dover, New York, 1972).
[16] D. Park. Z. Phys. **159**, 155 (1960).
[17] L. C. Biedenharn and J. D. Louck, *Angular Momentum in Quantum Physics* (Addison-Wesley, Massachusetts, 1981).
[18] B. D. Laihtman and J. V. Pogorelky, Zh. Éksp. Teor. Fiz. **75**, 2064 (1978).