

# Classical approximation for selective transitions in fast collisions of an atom with a charged particle

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(Submitted 25 May 1993)

Zh. Eksp. Teor. Fiz. **104**, 3928–3939 (December 1993)

Selective cross sections for  $(n, l) \rightarrow (n', l')$  transitions between subshells of a Rydberg atom and for ionization in a collision with a fast charged particle are derived in the binary approximation.

## 1. INTRODUCTION

Rydberg atomic states with a principal quantum number  $n \sim 10^2$  are currently the subject of active experimental and theoretical research (see, for example, Ref. 11). One specific feature of such states is their long lifetime with respect to radiative transitions,  $\tau \sim n^3$ . It is thus important to consider collisional transitions, whose cross section increases in proportion to  $n^4$  because the size of the Rydberg atom scales as  $d \sim n^2$ . A circumstance of importance from the standpoint of collision theory here is that the maximum of the cross section shifts toward lower energies with increasing principal quantum number. This tendency is clear from a comparison of the velocity of the Rydberg electron with the projectile velocity and also from the adiabatic approximation. According to the latter approximation, the cross section reaches a maximum at collision velocities  $v$  on the order of the Massey parameter, which varies in proportion to  $n^{-2}$  (Ref. 2). For collisions involving Rydberg atoms, it is thus legitimate to approximate by expanding in inverse powers of the collision velocity over a broad energy range  $E > n^{-4}$ . In addition, at large values of  $n$  it is legitimate to use the classical or semiclassical approximation. The classical approach has been taken in calculations on atomic collisions for a long time now, dating back to the paper by Thomas.<sup>3</sup> Using the binary approach, the semiclassical approximation was developed in Ref. 4 for calculations on transitions between shells,  $n \rightarrow n'$ . Below we derive the corresponding approximation for selective transitions between subshells,  $(n, l) \rightarrow (n', l')$ . Calculations on selective collisional transitions are required in order to fit these collisions into the overall scheme of kinetic equations, in which they compete with radiative transitions, which are closely related to the value of the orbital quantum number  $l$ .

From the mathematical standpoint, this approach amounts to a double asymptotic expansion in the limits  $v \rightarrow \infty$  and  $\hbar \rightarrow 0$ . Everywhere, we retain only the first order. The reason for this approach is not so much the desire to derive a result in the simplest possible form as it is the fact—well known in the theory of asymptotic expansions—that the range of agreement with the exact result narrows with increasing number of corrections, because the asymptotic

expansions diverge near the boundary of the range of applicability, and the corrections themselves are merely estimates of the accuracy of the given approximation.

## 2. ENERGY TRANSFER IN FAST COLLISIONS

We first consider the energy transfer in fast collisions in the classical approximation. Although this problem has already been solved by Percival and Richards,<sup>4</sup> our analysis has some substantial distinguishing features, concerning primarily the description of the Rydberg state, and the results are slightly different from those found previously.

The starting point in this approach is the solution of the dynamic problem in the form of the momentum transferred to an atomic electron by the projectile:

$$\Delta \mathbf{p} = \int_{-\infty}^{\infty} \mathbf{F}(t) dt, \quad (1)$$

where

$$\mathbf{F}(t) = \frac{Z\mathbf{R}(t)}{R(t)^3}$$

is the Coulomb force,  $Z$  is the charge of the projectile, and  $\mathbf{R}(t)$  is the radius vector of the projectile with respect to the electron. Here and below, unless otherwise stipulated, we are using the atomic system of units.

In the limit of high collision energies the motion of the projectile should be regarded as uniform and rectilinear in a first approximation. Furthermore, since the collision time tends toward zero in this limit, we can ignore the change in the positions of an atomic electron in the course of the collision. It then becomes possible to use for the projectile the coordinate system moving with the electron. We can then write  $\mathbf{R}(t) = \mathbf{b} + \mathbf{v}t$ , where  $\mathbf{v} = \text{const}$  is the projectile velocity, and  $\mathbf{b}$  is the vector impact parameter with respect to the electron ( $\mathbf{b} \perp \mathbf{v}$ ). In this approximation, the integral in (1) can be evaluated without difficulty; the result is

$$\Delta \mathbf{p}(t) = \frac{2Z\mathbf{b}}{vb^2}. \quad (2)$$

Using (2) we can write the energy transfer as

$$\Delta E(\mathbf{b}) = E' - E = \frac{(\mathbf{p} + \Delta \mathbf{p})^2}{2} - \frac{\mathbf{p}^2}{2} = \frac{2Zp_b}{vb} \cos(\chi) + \frac{2Z^2}{v^2 b^2}, \quad (3)$$

where  $E$  and  $E'$  are the energies of the electron respectively before and after the collision (everywhere below, the primes mean the parameters of the final state),  $p_b$  is the projection of the initial momentum  $\mathbf{p}$  onto the plane of the impact parameter, and  $\chi$  is the angle between  $\mathbf{p}_b$  and  $\mathbf{b}$ . The values of the potential energy before and after the collision in (3) cancel out, because the position of the electron is conserved during the collision. It can be seen from expression (3) that a decrease in the impact parameter corresponds to an increase in  $\Delta E$ . The boundary of the region of  $\mathbf{b}$  values which lead to an energy transfer greater than  $\varepsilon$  is specified by the equation  $\Delta E(\mathbf{b}) = \varepsilon$ , which, as can easily be verified, is the equation of a circle of radius

$$B = \left[ \frac{Z^2 p_b^2}{v^2 \varepsilon^2} + \frac{2Z^2}{v^2 \varepsilon} \right]^{1/2},$$

which is displaced along the  $\chi=0$  axis. As a result, the differential cross section with respect to  $\mathbf{r}$  for the transfer of an energy  $\Delta E \geq \varepsilon$ , which is given by the expression  $[\Theta(x) = 1$  for  $x \geq 0$  and  $\Theta(x) = 0$  for  $x < 0$ ]

$$\sigma(\varepsilon, \mathbf{r}) = \int \Theta(\Delta E(\mathbf{b}) - \varepsilon) d^2 \mathbf{b}, \quad (4)$$

is evidently

$$\sigma(\varepsilon, \mathbf{r}) = \pi B^2 = \frac{\pi Z^2}{v^2 \varepsilon^2} (p_b^2 + 2\varepsilon). \quad (5)$$

The total cross section is found by taking an average of (5) over the distribution of the electron in the atom:

$$\sigma(\varepsilon) = \int \sigma(\varepsilon, \mathbf{r}) q(\mathbf{r}) d^3 \mathbf{r}, \quad (6)$$

where  $q(\mathbf{r})$  is the probability density for finding an electron at the point  $\mathbf{r}$ .

To calculate  $p_b$  and  $q(\mathbf{r})$  below, we treat the atom in the one-electron approximation, and we specify the state of the atomic electron as a stationary ensemble of classical trajectories in a spherically symmetric effective potential  $U(r)$ . In this case, the oscillatory structure of  $q(\mathbf{r})$  due to the semiclassical phase shift  $\Phi = \int p dx$  drops out of the picture. The phase shift must be taken into account in order to analyze the local properties of the distribution  $q(\mathbf{r})$ , since the shift plays a leading role in this case. In integrals of the form (6), however, the shift appears in the form  $\sin^2(\Phi/\hbar) = [1 - \cos(2\Phi/\hbar)]/2$ , and the contribution from the rapidly oscillating cosine corresponds to corrections of higher order in  $\hbar$ . If the corrections are taken into account only partially, on the other hand, the effect is usually to degrade the result, since these corrections generally cancel out.

Various methods have been used in the literature to construct ensembles (see Ref. 5, for example). We will use that ensemble with fixed values of the energy  $E$ , of the

square of the angular momentum,  $L^2$ , and of its projection  $M$  which is the closest to the quantum description. These properties are related to the one-electron spherical quantum numbers  $(n, l, m)$  by  $E = E_{nl}$ ,  $L = \hbar(l + 1/2)$ , and  $M = \hbar m$ . The quantity  $p_b$  in (5) can then be expressed in terms of the integrals of motion through the use of the momentum components in the spherical coordinate system,  $r, \theta, \phi$ :

$$p_r = \sqrt{2 \left[ E_{nl} - U(r) - \frac{L^2}{2r^2} \right]},$$

$$p_\theta = \frac{1}{r} \sqrt{L^2 - \frac{M^2}{\sin^2 \theta}},$$

$$p_\phi = \frac{M}{r \sin \theta}.$$

This expression is

$$p_b^2 = p_\phi^2 + (p_\theta \cos \theta + p_r \sin \theta)^2. \quad (7)$$

In spherical coordinates, the probability density  $q(\mathbf{r})$  can be broken up into a product of 1D densities:

$$q(\mathbf{r}) = q(r)q(\theta)q(\phi).$$

In the general case of a 1D motion, the classical probability  $\Delta N$  for finding a particle in a given path interval  $\Delta x$  is proportional to the time spent in this interval or inversely proportional to the momentum  $p$ , and the probability density is

$$q = \frac{dN}{dx} = A \frac{1}{p}.$$

The proportionality factor  $A$  is determined by the normalization condition; it has the value  $A = 2/T$  in the case of libration and  $A = 1/T$  in the case of precession, where  $T$  is the period. The reason for the difference between libration and precession is that in the former case there are two states at each value of  $x$ , depending on the sign of the momentum, while in the latter case there is only one. In our case, motions in  $r$  and  $\theta$  are libration, while motion along  $\phi$  is precession, with periods

$$T_r = 2 \int_{r_1}^{r_2} \frac{dr}{p_r}, \quad T_\theta = 2 \int_{\theta_1}^{\theta_2} \frac{r d\theta}{p_\theta} = \frac{2\pi r^2}{L},$$

$$T_\phi = \int_0^{2\pi} \frac{r \sin \theta d\phi}{p_\phi} = \frac{2\pi r^2 \sin^2 \theta}{M},$$

where  $r_1, r_2, \theta_1$ , and  $\theta_2$  are the corresponding turning points. As a result the 1D distributions become

$$q(\phi) = \frac{1}{2\pi r \sin \theta}, \quad q(\theta) = \frac{L}{\pi r^2 p_\theta}, \quad q(r) = \frac{2}{T_r p_r}.$$

Alternatively, for the total distribution we find

$$q(n, l, m, \mathbf{r}) = q(r)q(\theta)q(\phi) = \frac{L}{\pi^2 r^3 \sin \theta p_\theta T_r p_r}. \quad (8)$$

After substituting (5), (7), and (8) into (6), we find that the 3D integral can be evaluated analytically. For the total cross section we find

$$\sigma(n, l, m, \varepsilon) = \frac{\pi Z^2}{v^2 \varepsilon^2} \left[ 2\varepsilon + \frac{M^2 + L^2}{L^2} (E_{nl} - \tilde{U}_{nl}) \right], \quad (9)$$

where

$$\tilde{U}_{nl} = \int U(r) q(n, l, m, \mathbf{r}) d^3 \mathbf{r}$$

is the average potential energy. If  $U(r)$  is a uniform function [i.e., if  $U(\alpha r) = \alpha^s U(r)$ ], then we have the following relation from the virial theorem (Ref. 6, for example):

$$\tilde{U}_{nl} = 2E_{nl}/(s+2). \quad (10)$$

It is a straightforward matter to work from the general expression (9) to find cross sections of certain other types. For comparison with experiment, one is usually interested in the cross section averaged over the orientation of the target, i.e., over the angular-momentum projection,

$$\sigma(n, l, \varepsilon) = \frac{1}{L} \int_0^L \sigma(n, l, m, \varepsilon) dM.$$

Substituting the cross section in the form (9) into the right side of this expression, we easily find

$$\sigma(n, l, \varepsilon) = \frac{\pi Z^2}{v^2 \varepsilon^2} \left[ 2\varepsilon + \frac{4}{3} (E_{nl} - \tilde{U}_{nl}) \right]. \quad (11)$$

Interestingly, for a Coulomb interaction this cross section does not depend on  $L$ , so it is the same as the total cross section for  $n \rightarrow n'$  transitions. The cross section for the loss of an electron,  $\sigma_{\text{loss}}$ , can be found by setting  $\varepsilon = -E_{nl} = I$  in (11):

$$\sigma_{\text{loss}}(n, l) = \frac{\pi Z^2}{v^2 I^2} \left[ 2I - \frac{4}{3} (I + \tilde{U}_{nl}) \right], \quad (12)$$

where  $I$  is the ionization potential.

To calculate the cross section for excitation to a state with a principal quantum number  $n'$ , we need to write  $\varepsilon$  in the form  $\varepsilon = E_{n'} - E_{nl}$  and then differentiate  $\sigma(\varepsilon)$  with respect to  $n'$ :

$$\sigma_{\text{ex}}(n') = \left| \frac{d\sigma(\varepsilon)}{d\varepsilon} \frac{dE_{n'}}{dn'} \right| = \left| \frac{2\pi}{T'_r} \frac{d\sigma(\varepsilon)}{d\varepsilon} \right|_{\varepsilon = E_{n'} - E_{nl}} \quad (13)$$

In expression (13) we have made use of the circumstance that in the semiclassical approximation the derivative of the energy with respect to the quantum number is equal to the classical frequency  $\Omega' = 2\pi/T'_r$  for a given energy. Substituting (9) and (11) into (13), we find

$$\sigma_{\text{ex}}(n, l, m \rightarrow n') = \frac{4\pi^2 Z^2}{T v^2 (E_{n'} - E_{nl})^3} \times \left[ E_{n'} - E_{nl} + \frac{M^2 + L^2}{L^2} (E_{nl} - \tilde{U}_{nl}) \right], \quad (14)$$

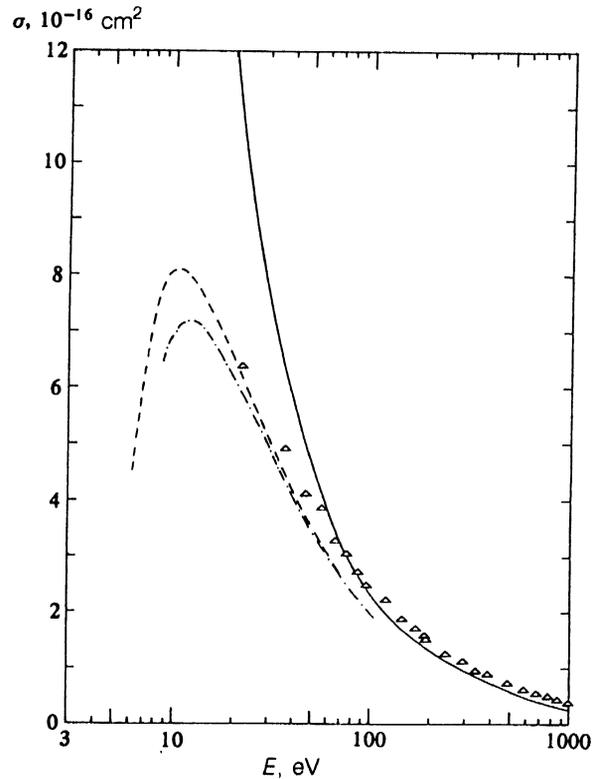


FIG. 1. Cross section for electron-impact ionization of helium in the metastable state,  $\text{He}(2^3S)$ . Solid curve—Calculated from expression (12); triangles—experimental results of Ref. 8; dashed curve—first Born approximation;<sup>9</sup> dot-dashed curve—binary approximation.<sup>9</sup>

$$\sigma_{\text{ex}}(n, l \rightarrow n') = \frac{4\pi^2 Z^2}{T v^2 (E_{n'} - E_{nl})^3} \times \left[ E_{n'} - E_{nl} + \frac{4}{3} (E_{nl} - \tilde{U}_{nl}) \right]. \quad (15)$$

For a hydrogen-like ion with an atomic number  $Z_a$ , these expressions take the following form, where we are using (10):

$$\sigma_{\text{ex}}(n, l, m \rightarrow n') = \frac{8\pi^2 Z^2 n^4 n'}{Z_a^2 v^2 (n'^2 - n^2)^2} \times \left[ 1 + \frac{[(l+1/2)^2 + m^2] n'^2}{(l+1/2)^2 (n'^2 - n^2)} \right], \quad (16)$$

$$\sigma_{\text{ex}}(n \rightarrow n') = \frac{8\pi^2 Z^2 n^4 n' (7n'^2 - 3n^2)}{3Z_a^2 v^2 (n'^2 - n^2)^3}. \quad (17)$$

In the limit  $n \gg |n' - n|$ , the cross section in (17) is given approximately by

$$\sigma_{\text{ex}}(n \rightarrow n') = \frac{4\pi^2 Z^2 n^4}{3Z_a^2 v^2 (n' - n)^3},$$

and it agrees with that found in Ref. 4 for this case.

Figures 1 and 2 show results calculated for a helium atom, in comparison with some results found previously. For helium we use the effective one-electron potential from Ref. 7:

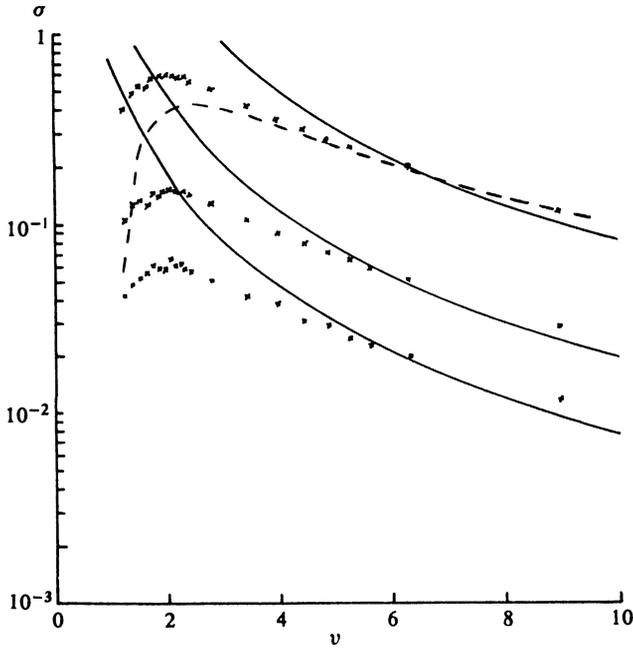


FIG. 2. Cross section for excitation of helium from the ground state, He( $1^1S$ ), to states with main quantum numbers  $n'=2, 3, 4$ . Solid curves—Calculated from (15); points—recommended experimental data for excitation of helium by protons;<sup>10</sup> dashed curve—recommended data for excitation of helium by electron impact.<sup>11</sup>

$$U(r) = -\frac{1}{r} - \frac{1}{r} (1 + 1.665r) \exp(-3.36r).$$

Figure 1 illustrates a calculation on the electron-impact ionization of helium in the metastable state, He( $2^3S$ ), from expression (12). Shown for comparison are some other results, both experimental<sup>8</sup> and theoretical.<sup>9</sup> In this case the binding energy is  $E_{n'} = -0.175$  a.u., and the average potential is  $\tilde{U} = -0.374$  a.u. Figure 2 shows cross sections for the excitation of helium from the ground state, He( $1^1S$ ) ( $E_{n'} = -0.903$  a.u.,  $\tilde{U} = -2.15$  a.u.), to states with  $n'=2, 3, 4$ , as calculated from expression (15). [In this case, the cross section in (15) should be doubled to allow for the two equivalent electrons.] Also shown in Fig. 2 are recommended data for excitation of He( $1^1S$ ) by protons<sup>10</sup> and by electron impact.<sup>11</sup> It can be seen from these figures that simple classical expressions give good agreement with both experimental and theoretical results, even for low-lying states of a two-electron atom. The discrepancy at very high energy is common to all classical approaches. It results from quantum-mechanical corrections logarithmic in  $E$ .

In the case of the one-electron atom, the ionization cross section in (12) agrees with the result of Ref. 12 at high energies.

### 3. CROSS SECTION FOR SELECTIVE TRANSITIONS

To calculate the cross section for selective excitation,  $\sigma(n, l \rightarrow n', l')$ , we need, in addition to the energy transfer in (3), the magnitude of the angular-momentum transfer.

For this purpose we resolve  $\mathbf{p}$  and  $\Delta\mathbf{p}$  into two components, one directly along the radius vector  $\mathbf{r}$  of the electron and one lying in the plane  $\pi$  perpendicular to  $r$ :

$$\mathbf{p} = \mathbf{p}_r + \mathbf{p}_\pi, \quad \Delta\mathbf{p} = \Delta\mathbf{p}_r + \Delta\mathbf{p}_\pi. \quad (18)$$

The square of the angular momentum in the final state can then be written

$$\begin{aligned} L'^2 &= |\mathbf{r}(\mathbf{p} + \Delta\mathbf{p})|^2 \\ &= r^2(\mathbf{p}_\pi + \Delta\mathbf{p}_\pi)^2 \\ &= L^2 + r^2(2p_\pi\Delta p_\pi \cos \alpha + \Delta p_\pi^2), \end{aligned} \quad (19)$$

where  $\alpha$  ( $0 \leq \alpha \leq 2\pi$ ) is the angle between  $\mathbf{p}_\pi$  and  $\Delta\mathbf{p}_\pi$ .

Transitions from the  $(n, l)$  subshell imply an average of the initial distribution (8) over  $M$ :

$$q(n, l, \mathbf{r}) = \frac{1}{L} \int_0^L q(n, l, m, \mathbf{r}) dm = \frac{1}{2\pi r^2 T p_r}. \quad (20)$$

As in the quantum-mechanical case, this distribution turns out to be isotropic. On the other hand, this averaging step is equivalent to choosing an ensemble of initial states which are distributed uniformly with respect to the angle  $\alpha$ . Taking that fact into account, we can write the normalized distribution with respect to  $L'$  for fixed values of  $\mathbf{r}$  and  $\mathbf{b}$  as follows:

$$\lambda(\mathbf{r}, \mathbf{b}, L') = \frac{1}{2\pi} \left| \frac{d\alpha}{dL'} \right|.$$

Evaluating the derivative of  $\alpha$  with respect to  $L'$  with the help of (19), we can put this expression in the form

$$\lambda(\mathbf{r}, \mathbf{b}, L') = \frac{2L'}{\pi r^2} \frac{1}{\sqrt{(\Delta p^2 - \Delta p_r^2 - \mu^2)(\nu^2 + \Delta p_r^2 - \Delta p^2)}}, \quad (21)$$

where  $\mu = (L' - L)/r$  and  $\nu = (L' + L)/r$ .

By analogy with (4), the differential cross section with respect to  $n', L'$ , and  $\mathbf{r}$  is given by

$$\sigma(n', L', \mathbf{r}) = \frac{dE_{n'}}{dn'} \int \delta(\Delta E(\mathbf{b}) - \varepsilon) \lambda(\mathbf{r}, \mathbf{b}, L') b db d\chi, \quad (22)$$

where  $\delta(x)$  is the Dirac  $\delta$ -function. This  $\delta$ -function arises from the differentiation of the  $\Theta$  function of the energy in (4) in accordance with rule (13). The expression for the selective cross section becomes

$$\sigma(n, l \rightarrow n', l') = \int \sigma(n', L', \mathbf{r}) q(n, l, \mathbf{r}) r^2 \sin \theta dr d\theta d\phi. \quad (23)$$

When  $\Delta E$ ,  $q$ , and  $\lambda$  from (3), (20), and (21), respectively, are substituted into these expressions, four of the five integrations in (22) and (23) can be carried out analytically (see the Appendix). The final result is found as a single radial integral over the classically allowed region which is common to the initial and final states ( $\rho_1 \leq r \leq \rho_2$ ):

$$\sigma(n, l \rightarrow n', l') = \frac{32\pi Z^2 L'}{3T_r T_r' v^2} \sum_{i=1}^2 \int_{\rho_1}^{\rho_2} \frac{dr}{r^2 p_r p_r' A_i^3 B_i^4}$$

$$\times [2(A_i^2 + B_i^2)E(g_i) - B_i^2 K(g_i)]. \quad (24)$$

Here  $g_1 = (A_i^2 - B_i^2)/B_i^2$ ; the quantities  $A_i^2$  and  $B_i^2$  are defined in the Appendix;  $T_r$  and  $T'_r$  are the periods of the radial oscillations in the initial and final states; and  $K(x)$  and  $E(x)$  are the complete elliptic integrals of the first and second kinds as defined in Ref. 13. The summation over  $i$  in (24) corresponds to two directions of the radial momentum, parallel and antiparallel to the radius vector  $r$ . It can be seen from expression (24) that, in addition to the known scaling properties in  $Z$  and  $v$ , the nontrivial part of the cross section,

$$Q(n, l; n' l') = \frac{v^2 \sigma(n, l \rightarrow n' l')}{Z^2 L'}, \quad (25)$$

is symmetric under interchange of the initial and final states.

The derivation of a distribution with respect to  $L'$  for the ionization process differs from that for the excitation process only in that the differentiation with respect to  $n'$  in (22) is replaced by differentiation with respect to  $E'$ . The final result is

$$\begin{aligned} \sigma(n, l \rightarrow E' l') &= \frac{16Z^2 L'}{3T_r v^2} \sum_{i=1}^2 \int_{\rho_1}^{\rho_2} \frac{dr}{r^2 p_i p'_i A_i^3 B_i^4} \\ &\times [2(A_i^2 + B_i^2)E(g_i) - B_i^2 K(g_i)]. \end{aligned} \quad (26)$$

The literature reveals no data on selective transitions between Rydberg states. For the data available for small values of  $l$  and  $l'$ , expression (24) does not give a satisfactory description, in contrast with the case of  $n \rightarrow n'$  transitions. This is the standard situation. It occurs because there is a qualitative change in the structure of the caustics in the case  $l=0$ . As a result, at small values of  $l$  the semiclassical approximation in terms of angular variables is far poorer than for the radial variables.

Figure 3 shows the results of a numerical calculation of the reduced cross section for the case of a Coulomb interaction  $U(r)$  for selective transitions (25) from the  $n=50$  shell. It can be seen from this figure that the cross section has a maximum at  $l \approx l'$ . For  $n \neq n'$  we find a second maximum, which occurs because, with increasing  $l'$ , the inner turning point in the effective potential of the final state approaches the outer turning point in the effective potential of the initial state. As a result, there is an increase in the overlap integral of the initial and final states. Figure 4 shows the reduced distribution with respect to  $L'$  in the continuous spectrum,

$$Q_{\text{ion}}(n, l; E' l') = v^2 \sigma(n, l \rightarrow E' l') / Z^2 L', \quad (27)$$

for values of  $E'$  which are multiples of half the ionization potential:  $E' = I/2, I, 3I/2, 2I, 5I/2$ . We see the following in this figure:

a) With increasing initial value of  $L$ , there is a decrease in the maximum value  $L'_{\text{max}}$ .

b) With increasing final energy  $E'$ , the maximum in the distribution shifts toward larger values of  $L'$ .

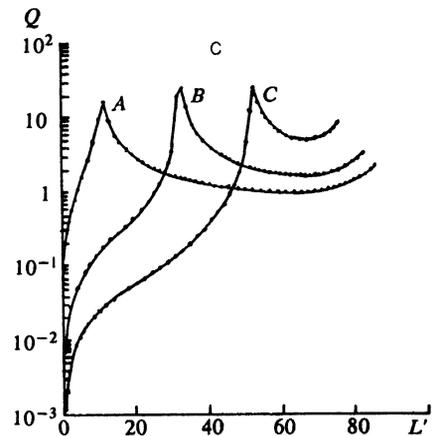
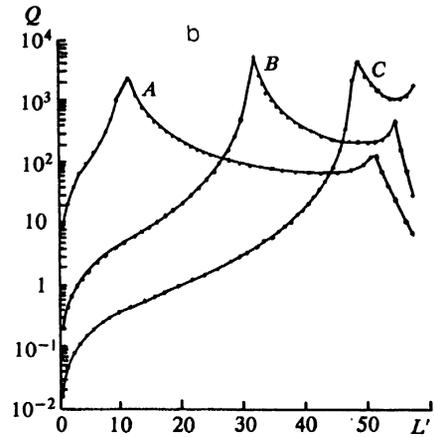
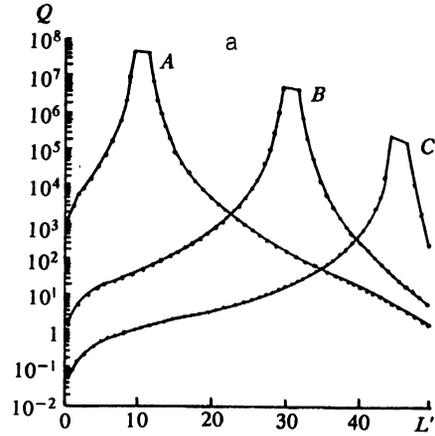


FIG. 3. Reduced cross section for selective transitions, (25), for the case of a Coulomb interaction from the  $n=50$  shell to the following shells: a)  $n'=50$ ; b)  $n'=58$ ; c)  $n'=100$ . Curves  $A$ ,  $B$ , and  $C$  corresponding to initial values  $l=10, 30$ , and  $45$  of the orbital quantum number.

c) Toward  $L'_{\text{max}}$ , there is an increase in the cross section, because of the decrease in the distance between the turning points in the initial and final states as outlined above.

We wish to thank R. K. Yanev for useful discussions and critical comments. This work was supported by the

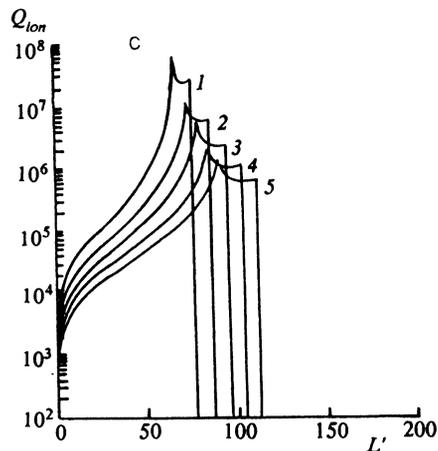
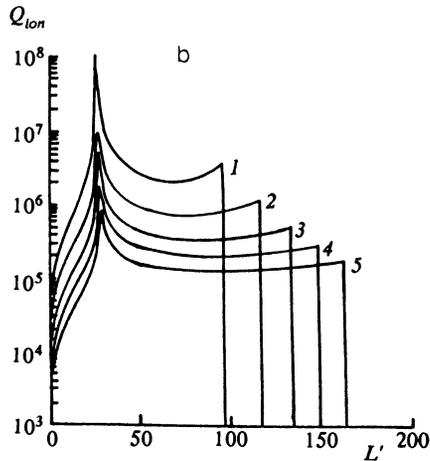
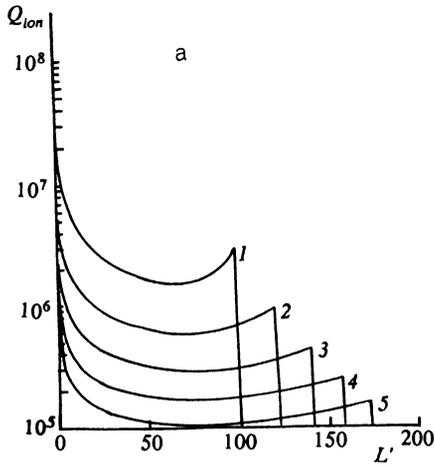


FIG. 4. Reduced distribution with respect to  $L'$  in the continuous spectrum [expression (27)] for ionization from the  $n=50$  shell. a: The initial orbital quantum number is  $l=0$ . b:  $l=25$ . c:  $l=49$ . 1) The final energy is  $E'=I/2$ ; 2)  $I$ ; 3)  $3I/2$ ; 4)  $2I$ ; 5)  $5I/2$ , where  $I$  is the ionization potential.

Ministry of Science of the Republic of Macedonia through Grant 08-0565/5.

## APPENDIX

To calculate the selective cross sections in (24) and (26), we write the energy transfer in (3) in terms of the momentum components in (18):

$$\Delta E(\mathbf{b}) = p_r \Delta p_r + p_\pi \Delta p_\pi \cos(\alpha) + \frac{1}{2} \Delta p^2.$$

We then substitute  $\alpha$  from (19):

$$\Delta E(\mathbf{b}) = \frac{L'^2}{2r^2} - \frac{L^2}{2r^2} + p_r \Delta p_r + \frac{1}{2} \Delta p_r^2.$$

Now solving the equation  $\Delta E(\mathbf{b}) = E_{n'l'} - E_{nl}$ , we easily find that the  $\delta$ -function in (22) is nonzero for  $\Delta p_r = \kappa_1 = -p_r - p'_r$  and  $\Delta p_r = \kappa_2 = -p_r + p'_r$ . Expressing  $\Delta p_r$  in terms of  $\mathbf{b}$  in spherical coordinates in accordance with (2),

$$\Delta p_r = \frac{2Z}{vb} \sin(\theta) \cos(\chi),$$

where the angle  $\chi$  is measured from the projection of  $\mathbf{r}$  onto the plane of the impact parameter, and integrating over  $\chi$  in (22), we find

$$\sigma(n', L', \mathbf{r})$$

$$= \frac{4L'}{T'_r p'_r r^2} \sum_{i=2}^2 \int \frac{bdb}{\sqrt{(\Delta p^2 - A_i^2)(B_i^2 - \Delta p^2)(\Delta p^2 \sin^2(\theta) - \kappa_i^2)}}, \quad (\text{A1})$$

where  $A_i^2 = \kappa_i^2 + \mu^2$ ,  $B_i^2 = \kappa_i^2 + \nu^2$ . After substituting (A1) into (23), we first evaluate the integrals over  $\phi$  and  $\theta$ . The integral over  $\phi$  is trivial, since the integrand is independent of this variable. The integral over  $\theta$  reduces to an Abel integral and can also be handled analytically. The resulting expression,

$$\sigma(n', L', \mathbf{r})$$

$$= \frac{8\pi L'}{T'_r T_r} \sum_{i=1}^2 \int \frac{drbdb}{r^2 p'_r \cdot p_r \sqrt{(\Delta p^2 - A_i^2)(B_i^2 - \Delta p^2) \Delta p}},$$

takes the form (24) after we integrate over  $b$  and use (2).

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Translated by D. Parsons