

## ATOMIC SPECTROSCOPY

# Generalized Correspondence Rules for Quasi-Classical Dipole Matrix Elements

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**Abstract**—Based on the requirement of the orthogonality of quasi-classical wave functions, generalized correspondence rules are formulated for calculations of radial dipole matrix elements in the semi-classical approximation. The rules are used for the derivation of quite simple analytic representations of the oscillator strengths for electronic transitions accompanied by large variations in principal quantum numbers in the discrete and continuous spectra. Comparison with exact quantum-mechanical calculations of photoionization cross sections for alkali atoms shows the possibility of the analytic description with the help of formulas for the Cooper minimum. Conditions of the rearrangement of the hydrogen-like photorecombination spectrum are formulated for the example of the model Sommerfeld potential, and the tendency to the appearance of the inverse population of the lowest excited states is demonstrated.

### INTRODUCTION

Information on dipole matrix elements  $R_{j,j'}$  =  $\langle \Psi_{j'} | r | \Psi_j \rangle$  is required for the solution of many problems. The oscillator strengths determine the efficiency of various radiative processes involved in bound-bound, bound-free, and free-free electronic transitions and also appear in many expressions for calculations of cross sections for different collision reactions. The exact analytic representations of  $R_{j,j'}$  are known only for the hydrogen atom and hydrogen-like ions [1]. The corresponding Gordon formula contains hypergeometric functions with a set of indices which depend in a complicated way on the principal ( $n$ ) and orbital ( $l$ ) quantum numbers of the states under study. For this reason, this formula is inconvenient and can be reasonably simplified only under restricted conditions [2–4]. In this connection, a number of authors, beginning with papers [5, 6], suggest to use the quasi-classical approximation for calculations of dipole matrix elements. The leading term of quasi-classical formulas for  $R_{j,j'}$  is determined by a Fourier series of the radial coordinate of an electron moving along the average Kepler orbit  $j_a$  with the energy  $\epsilon_a$  and the orbital moment  $L_a$ . For transitions between the states with close quantum numbers  $j = \{n^*, l\}$ ,  $j' = \{n'^*, l'\}$ , parameters of the orbit  $j_a = \{\epsilon_a, L_a\}$  can be easily found assuming that  $\{j\} \approx \{j'\}$ :

$$\begin{aligned} \epsilon_a &= -z^2 / (2n_a^{*2}) \approx (\epsilon + \epsilon') / 2, \\ L_a &= (L + L') / 2 = (l + l' + l) / 2, \end{aligned} \quad (1)$$

where  $z$  is the effective charge of the ion atomic core and  $n^*$  is the effective principal quantum number.

Below, we will use the atomic system of units. The quasi-classical orbital moment  $L$  of an electron differs from its corresponding quantum value by the Langer

correction  $L = l + 0.5$  [7]. For this reason,  $L_a$ , for the average orbit  $j_a$ , is taken as the arithmetic mean of  $L$  and  $L'$ . The main obstacle to the applicability of the quasi-classical transition in the case of widely separated levels  $s \equiv |n'^* - n^*| \gg 1$  is a great uncertainty in the choice of the energy  $\epsilon_a$  (or the corresponding effective quantum number  $n_a^*$ ) for the orbit  $j_a$ , which should reflect parameters of each of the initial states  $j$  and  $j'$ . This uncertainty in  $n_a^*$  gave rise to numerous recipes (correspondence rules) for determining  $n_a^*$ , which were not physically substantiated. Note here that because  $l$  and  $l'$  differ from each other only by unity, the choice of  $L_a$  (1) mentioned above is optimum [8, 9].

In this paper, we start from two fundamental principles, the orthogonality of the wave functions and Bohr's correspondence principle, to determine the value of  $n_a^*$  from  $n^*$  and  $n'^*$  in a physically meaningful way. The formulated correspondence rules are used for substantial simplification of quasi-classical formulas for  $R_{j,j'}$  in the limit of "long" transitions ( $s \gg 1$ ), which allows us to analytically describe effects of the type of the appearance of Cooper's minimum in radiative processes [10]. Such a simplification is not coincidental, but is due to the fact [11] that the energy  $\epsilon_a$  of the average orbit is absent in the parametric representation of the trajectory of its movement near the continuum boundary.

### QUASI-CLASSICAL MATRIX ELEMENTS

Let us formulate briefly the quasi-classical scheme for determining radial matrix elements of the form

$$R_{j,j'}^{(m)} = \int_0^\infty dr r^m \Psi_j(r) \Psi_{j'}(r). \tag{2}$$

Here, the normalized radial wave functions  $\Psi_j$  in the quasi-classical approximation have the form [7]

$$\Psi_j(r) = 2/[\sqrt{T p_c(r)}] \cos[S_c(r) + \pi\mu_1], \tag{3}$$

$$p_c(r) = \sqrt{2\varepsilon + 2z/r - L^2/r^2},$$

$$S_c(r) = \int_{r_1}^r dr p_c(r) - \pi/4, \tag{4}$$

$$\varepsilon = -z^2/(2n^{*2}), \quad T = 2\pi n^{*3}/z^2,$$

where  $p_c(r)$  is the momentum of an electron with the energy  $\varepsilon$  and orbital moment  $L = l + 0.5$  moving in the Coulomb field with the charge  $z$ . The phase  $S_c$  of the wave function (3) is determined by the Coulomb truncated action  $S_c(r)$  (4), which also includes the phase jump  $\pi/4$  appearing after the passage by an electron of the left turning point  $r_1$ . The quantum defect  $\mu_1$  takes into account the phase incursion of the wave function due to the deviation of the real one-electron potential from the Coulomb potential near the atomic core ( $r \approx 0$ ). The quantity  $\mu_1$  changes the value of the principal quantum number ( $n \rightarrow n^* = n - \mu_1$ ), resulting in the shift of energy levels and an increase in the period  $T$  of radial motion of the Rydberg electron. Note that if we take  $m = 0$  and  $l = l'$  in (2), then matrix elements  $R_{j,j'}^{(0)} = 0$  ( $n \neq n'$ ) because of the orthogonality of radial wave functions.

Substitution of functions  $\Psi_j(r)$  (3) in the radial integral (2) yields

$$R_{j,j'}^{(m)} = \frac{z^2}{\pi \sqrt{n^{*3} n'^{*3}}} \tag{5}$$

$$\times \int_{r_1}^{r_r} dr r^m / \left[ \sqrt{p_c(r) p'_c(r)} \right] \cos[\Delta S_c(r) + \pi\Delta\mu],$$

$$\begin{aligned} \Delta S_c(r) &= (\partial S(r)/\partial \varepsilon)\Delta\varepsilon + (\partial S(r)/\partial L)\Delta L \\ &= t(r)\Delta\varepsilon - \theta(r)\Delta l \end{aligned} \tag{6}$$

by omitting rapidly oscillating terms of the type  $\cos(S_c(r) + S'_c(r))$ . If the orbits are close, i.e., the parameters  $j = \{\varepsilon, l\}$  and  $j' = \{\varepsilon', l'\}$  are close, then the difference  $\Delta S_c(r)$  of truncated actions for the orbits is reduced to a linear combination (6) of differences in the parameters  $\Delta\varepsilon$  and  $\Delta l$ . The position of the left ( $r_1$ ) and right ( $r_r$ ) turning points is determined from the requirement that the electron velocity vanishes:  $p_c(r_1; r_r) \approx p'_c(r_1; r_r) = 0$ . The partial derivatives  $\partial S_c(r)/\partial \varepsilon$  and

$-\partial S_c(r)/\partial L$  of the truncated action are equal to the time  $t(r)$  and the turning angle  $\theta(r)$  of an electron in polar coordinates  $\{r, \theta\}$  with the Coulomb charge  $r = 0$  [12]. Under these assumptions, the radial integral (5) is reduced to the time-averaged product  $r^m \cos(\dots)$  over some average weighted Kepler orbit  $j_a = \{\varepsilon_a, L_a\}$ :

$$R_{j,j'}^{(m)} = \frac{z^2}{\pi \sqrt{n^{*3} n'^{*3}}} \int_0^{T_a/2} dt r^m \cos[t\Delta\varepsilon - \theta(r)\Delta l + \pi\Delta\mu], \tag{7}$$

where an electron passes the left  $r_l$  and right  $r_r$  turning points at instants  $t = 0$  and  $t = T_a/2$ , which correspond to the perigee and apogee of the orbit  $j_a$ .

### GENERALIZED CORRESPONDENCE RULES

Expression (7) can be also used for the calculation of  $R_{j,j'}^{(m)}$  in the general case for widely separated energy levels, provided the concept of the average trajectory is retained. The problem to be solved with the help of the correspondence rules is the determination of parameters  $j_a = \{\varepsilon_a, L_a\}$ .

To determine the effective quantum number  $n_a^*$  (or the energy  $\varepsilon_a$ ) of the average orbit, we will use the fundamental property of the orthogonality of radial wave functions with  $l = l'$ . This means that, by setting  $\Delta l = 0$  and  $m = 0$  in (7), we arrive at the relation

$$\begin{aligned} &\Delta\varepsilon \int_0^{T_a/2} dt \cos(t\Delta\varepsilon + \pi\Delta\mu) \\ &= \sin(\Delta\varepsilon T/2 + \pi\Delta\mu) - \sin(\pi\Delta\mu) = 0. \end{aligned} \tag{8}$$

In other words, the argument of sine takes a discrete series of allowed values

$$\begin{aligned} \Delta\varepsilon T_a/2 + \pi\Delta\mu &= \pi(\Delta n_r + k), \\ \Delta\varepsilon &= (2\pi/T_a)(\Delta n^* + k). \end{aligned} \tag{9}$$

Here,  $\Delta n_r + k$  is an integer. It can be conveniently written as a sum of  $\Delta n_r$  (the difference of radial quantum numbers) with some integer addition not yet determined. In the case of close energy levels within one series,  $\Delta\mu = 0$ , so that  $\Delta n^* = \Delta n$ . The quantity  $k$  should vanish according to Bohr's correspondence principle [7], which is expressed by the second equality in (9) for  $k = 0$ . It is obvious that as the hydrogen-like level  $\{j'\}$  is moving away from  $\{j\}$ , there is no reason for the jump-like change of  $k$  by unity, therefore,  $k \equiv 0$ . Moreover, even in the case of the interaction between channels, the difference of quantum defects  $\Delta\mu$  changes by  $\pi$  after the term of series  $\{j'\}$  passes the perturbing energy level. Thereby,  $\Delta\mu$  contains the possible unit jump of  $k$ .

The generalized correspondence rule (9) for  $k \equiv 0$  defines the effective quantum number  $n_a^*$  of the average orbit as

$$n_a^{*3} = 2n^{*2}n'^{*2}/(n^* + n'^*) \quad (10)$$

and allows us to calculate matrix elements  $R_{j,j}^{(m)}$  of transitions in the quasi-classical approximation (7) by using the Coulomb parametrization [12]

$$r = a_a(1 - e_a \cos \xi), \quad t = T_a/(2\pi)(\xi - e_a \cos \xi),$$

$$\cos \theta = (\cos \xi - e_a)/(1 - e_a \cos \xi), \quad (11)$$

$$\sin \theta = \sin \xi (\sqrt{1 - e_a^2})/(1 - e_a \cos \xi),$$

$$e_a = \sqrt{1 - L_a^2/n_a^{*2}}, \quad (12)$$

$$a_a = n_a^{*2}/z, \quad T_a = 2\pi n_a^{*3}/z^2$$

for the average Kepler orbit  $j_a = \{\varepsilon_a, L_a\}$ . A change of  $t$  within the half-period  $T_a/2$  corresponds to the region  $0 \leq \xi \leq \pi$  of values of the parameter  $\xi$ . One can see that the only undetermined parameter is the eccentricity  $e_a$  (12), which can be found by comparing quasi-classical and quantum results [9, 13] for dipole matrix elements. By setting  $\Delta\varepsilon = 0$  ( $\varepsilon = \varepsilon'$ ) and  $\Delta l = \pm 1$ , it is easy to show that after substitution of parametrization (11, 12) the right-hand side of (7) is reduced to the form

$$R_{j,j}^{(1)} = -1.5e_a a_a \cos(\pi\Delta\mu) + 2a_a \Delta l \sqrt{1 - e_a^2} \sin(\pi\Delta\mu)/\pi. \quad (13)$$

Meanwhile, the exact result for the hydrogen atom [4, 13] is  $R_{j,j}^{(1)} = -1.5e_a a_a$ , with the eccentricity containing the orbital moment  $L_a$  (1), which can be rewritten in the form  $L_a = \max\{l, l'\}$ . This fact determines the correspondence rule (1) for orbital moments. Another approach for the substantiation of the choice of  $L_a$  (1) in the case of large quantum numbers and widely separated energy levels was suggested in [9].

### DIPOLE MATRIX ELEMENT FOR LONG TRANSITIONS

The Coulomb parametrization (11) also allows one to express the quasi-classical dipole matrix element in terms of the Anger function  $\mathfrak{S}_s(x)$  and its derivative  $\mathfrak{S}'_s(x)$  [4, 6]

$$R_{j,j}^{(1)} = (-1)^{\Delta n} n_a^{*2} \frac{z}{\Delta\varepsilon \sqrt{n^{*3} n'^{*3}}} \times \left\{ \sin(\pi s)/(\pi s) [s(1 - e_c) - \Delta l \sqrt{1/e_a^2 - 1}] \right. \quad (14)$$

$$\left. - \mathfrak{S}'_s(-se_a) + \Delta l \sqrt{1/e_a^2 - 1} \mathfrak{S}_s(-se_a) \right\}, \quad s = n^* - n'^*,$$

$$\mathfrak{S}_s(x) = \frac{1}{\pi} \int_0^\pi d\xi \cos(s\xi - x \sin \xi). \quad (15)$$

Note that the phase factor  $(-1)^{\Delta n}$  in (14) is absent in [6], because the authors [6] chose the opposite sign for quasi-classical wave functions (3). Expression (15) is a starting relation in most papers in this field, their results being different in methods of specifying  $n_a^*$  and approximation of the Anger function. The problem of the determination of  $R_{j,j}^{(1)}$  for not widely separated levels can be considered solved [11], because several auxiliary functions for calculations of  $\mathfrak{S}_s(x)$  with high accuracy were tabulated in [6, 13]. However, for long transitions ( $s \gg 1$ ), the differences in the choice of  $n_a^*$  become noticeable. In addition, expression (14) cannot be used for the analytic continuation of the dipole matrix element to the region of bound-free transitions [3, 14], when the formally effective quantum number of the final state becomes purely imaginary ( $n'^* \rightarrow iz/p$ ), so that the energy of a photoelectron with the momentum  $p$  would become positive:  $\varepsilon' = -z^2/2n'^{*2} \rightarrow p^2/2$ . The photoionization cross section  $\sigma(n^*l \rightarrow pl')$  can be obtained from the expression [14]

$$\sigma(n^*l \rightarrow pl') = (2\pi^2 \omega) / (3cz^2 p^3) |R_{j,j}^{(1)}|^2; \quad (16)$$

$$n'^* = iz/p; \quad \omega = \varepsilon' - \varepsilon = p^2/2 + z^2/2n^{*2}.$$

The advantage of the definition of  $n_a^*$  (10), along with the fundamental principle of orthogonality inherent in it, is the possibility of the natural continuation of  $R_{j,j}^{(1)}$  (14) to the region of energy continuum. For large values of  $s$  and  $e_a \approx 1$ , the method of stationary phase can be applied to the integral representation (14, 15) of Anger functions  $\mathfrak{S}_s(se_a)$  and  $\mathfrak{S}'_s(se_a)$ , which reduces these functions to a linear combination of Airy functions [15]. By omitting intermediate calculations, we present the final result

$$R_{j,j}^{(1)} = \frac{L_c^2 z}{\omega \pi \sqrt{n^{*3} n'^{*3}}} \times [-0.5 \sin(\pi\Delta\mu) - (\sqrt{\pi/x})\Phi'(x) + \Delta l_q \sqrt{\pi/x}\Phi(x)], \quad (17)$$

$$x = (s/2)^{2/3} L_c^2/n_c^{*3} = (0.5\omega L_c^3/z^2)^{2/3},$$

$$\Delta l_q = \Delta l + (\varepsilon' + \varepsilon)/(5\omega L_a), \quad \omega = \varepsilon' - \varepsilon > 0,$$

$$\Phi(x) = \int_0^{\pi} d\xi \cos(x\xi + \xi^3/3 + \Delta\mu), \quad (18)$$

$$\Phi'(x) = \frac{d\Phi(x)}{dx}.$$

Expression (17) assumes a certain rule for the ordering of levels: the difference of energies  $\Delta\varepsilon$  (17) corresponding to the transition frequency  $\omega$  should be positive. In other words, the lower level is assumed to be the initial state  $j = \{n^*, l\}$ , while the quantum numbers of the level close to continuum are assigned to the final state  $j' = \{n'^*, l'\}$  ( $n'^* > n^*$ ). Signs of  $\Delta l = l' - l$  and  $\Delta\mu = \mu_1' - \mu_1$  are chosen in accordance with the adopted ordering. The important feature of our approach is the appearance of the dimensionless parameter  $x$  in (17), which does not contain quantum numbers  $n^*$  and  $n'^*$ . The latter circumstance is caused by the choice of  $n_a^*$  according to (10). We introduced into expression (10) the modification of the difference of orbital quantum numbers  $\Delta l \rightarrow \Delta l_q$ , which takes into account quantum corrections for quasi-classical formulas obtained in [2, 4] and substantially improves their accuracy. Finally, the important advantage of representation (17) is the possibility of the direct continuation of  $R_{j,j'}^{(1)}$  to the region of energy continuum of the states involved in the optical transition [see (16)].

In the case of the hydrogen atom ( $\Delta\mu = 0$ ), expression (17) coincides with the results obtained in papers [3, 14] where the region of applicability of representations of the type (17) was carefully analyzed:

$$n^*, n'^* \gg 1, \quad \Delta s \gg 1, \quad n'^* \gg L', \quad p \ll z/L'. \quad (19)$$

Further simplifications of  $R_{j,j'}^{(1)}$  (17) are connected with the existence of the following asymptotic expressions for functions  $\Phi(x)$  and  $\Phi'(x)$ :

$$\begin{aligned} \Phi(x) &= -\sin(\pi\Delta\mu)/(\sqrt{\pi}x) \\ &+ \sqrt{x}/(3\pi)\cos(\pi\Delta\mu)K_{1/3}(2/3x^{2/3}), \quad x \rightarrow \infty, \end{aligned} \quad (20)$$

$$\begin{aligned} \Phi'(x) &= -\sin(\pi\Delta\mu)/(\sqrt{\pi}x^2) \\ &+ x/\sqrt{3\pi}\cos(\pi\Delta\mu)K_{2/3}(2/3x^{2/3}), \quad x \rightarrow \infty, \end{aligned} \quad (21)$$

$$\begin{aligned} \Phi(x) &= \sin(\pi/3 - \pi\Delta\mu)\Gamma(1/3)/(\sqrt{\pi}3^{2/3}), \\ &x \rightarrow 0, \end{aligned} \quad (22)$$

$$\begin{aligned} \Phi'(x) &= \sin(\pi/3 + \pi\Delta\mu)\Gamma(2/3)/(\sqrt{\pi}3^{1/3}), \\ &x \rightarrow 0. \end{aligned} \quad (23)$$

Here,  $K_{1/3}$  and  $K_{2/3}$  are cylinder functions of the imaginary argument, and  $\Gamma$  is the Euler gamma function [15].

One can see from the above expressions that the dipole matrix element consists of a sum of three terms, which differently depend on  $x$  in (17). The relative weight and signs of these terms are controlled by the difference of quantum defects of series, so that  $R_{j,j'}^{(1)}$  can vanish for some relations between them. In physics of atomic spectra, this leads to the appearance of a deep minimum (the so-called Cooper minimum) of experimental and theoretical dependences of the oscillator strengths on the energy of the final state of the optical transition [16]. It is obvious that the maximum error of quasi-classical formulas should be manifested when the efficiency of optical processes is reduced and small deviations in the values of mutually compensating terms can result in a substantial deviation of their sum from the true value.

### PHOTOIONIZATION CROSS SECTIONS IN THE REGION OF THE COOPER MINIMUM

Consider the use of expression (17) for calculations of photoionization cross sections in the most unfavorable for the quasi-classical approximation case of the presence of the Cooper minimum. Figure 1 shows the results of quantum-mechanical calculations [17] of photoionization cross sections  $\sigma(nS \rightarrow \varepsilon'P)$  for different terms of the  $S$  series of the sodium atom (solid curves). Figure 1a corresponds to the wavelength range adjacent to the photoionization threshold. Figure 1b demonstrates the behavior of  $\sigma$  in the vicinity of the Cooper minimum. The dashed curves describe the dependence of the cross section  $\sigma$  on  $\lambda$  calculated from our quasi-classical formula (16, 17). Note that specific features of the dependence  $\sigma(\lambda)$  are sensitive to variations even in the third sign of  $\Delta\mu$  (which is beyond the accuracy limit of the data on  $\Delta\mu$  reported in the literature and this fact was mentioned above). Moreover, the Cooper minimum  $\varepsilon'_c$  is far removed from the photoionization threshold ( $\varepsilon'_c \cong 1-2$  eV), so that, in principle, the tendency of the phase difference  $\Delta\mu_a(n) = \mu_p(\varepsilon'_c) - \mu_s(n)$  to shift from its asymptotic value  $\Delta\mu_r(n) = \mu_p(\varepsilon' = 0) - \mu_s(n)$  should be taken into account. The table presents the  $\Delta\mu(n)$  values taken from [18] and changed, by us, in the second or third sign to obtain the better agreement between the solid and dashed curves in Fig. 1. Note that shifts of  $\Delta\mu(n)$  relative to data [18] obtained by us agree with the behavior of  $\mu_p(\varepsilon)$  for  $\varepsilon \rightarrow \varepsilon'_c$ .

Figure 2 shows dependences of threshold values of photoionization cross sections  $\sigma(nS \rightarrow \varepsilon' = 0, P)$  on the principal number of the  $S$  state of the strontium ion. Unlike the case in Fig. 1, all values of  $\mu_1$  required for the quasi-classical approach can be found in the literature. Asymptotic values of  $\mu_1(\varepsilon' \rightarrow 0)$  are taken from [19], and the relative dependence  $\mu_s(n)$  for the  $S$  series of  $\text{Sr}^+$  is plotted according to data [20].

PHOTORECOMBINATION SPECTRUM FOR THE MODEL SOMMERFELD POTENTIAL

Consider also radiative processes (which are inverse to photoionization) upon movement of a Rydberg electron in the model Sommerfeld potential  $U_s$  [21]

$$U_s(r) = -1/r + \alpha/2r^2, \tag{24}$$

$$U_{\text{eff}}(r) = -1/r + L_{\text{eff}}/2r^2, \quad L_{\text{eff}} = \sqrt{L^2 + \alpha}.$$

For a given  $l$  series, the radial movement of the electron occurs in the effective potential  $U_{\text{eff}}(r)$  with the effective angular momentum  $L_{\text{eff}}$ . Positions of the energy levels of the Sommerfeld atom can be obtained from those in the Coulomb field by the replacement  $L = l + 0.5 \rightarrow L_{\text{eff}}$ , so that

$$n^* = n_r + L_{\text{eff}} + 0.5, \quad \mu_l = l + 0.5 - L_{\text{eff}}. \tag{25}$$

In studies of emission spectra of the Rydberg electron, we will restrict ourselves to the case of the zero energy  $\epsilon \rightarrow 0$  ( $n_r \rightarrow \infty$ ), which allows us to consider the shapes of spectra of spontaneous and photorecombination emission coincident. Figure 3 shows the dependence  $W(n_r)$  of the probability of the radiative transition of the  $P$  electron with  $\epsilon = 0$  (the normalization of the wave function corresponds to the bound state) to the  $n_r$ th level of the  $S$  series.  $W(n_r)$  is related to the dipole matrix element by the expression [22]

$$W = (2\omega^3 L_a) / [3c(l + 0.5)] |R_{j,j}^{(1)}|^2. \tag{26}$$

The solid curves were obtained quantum-mechanically, and the dashed curves correspond to the quasi-classical approximation (17). The curves are normalized to unity for the most intense transition. One can see that quasi-classical expression (17) is in good agreement with quantum-mechanical calculations, even beyond the region of its applicability [see (19)] for small values of  $n_r$ . The accuracy of calculations was improved due to the introduction of the quantum correction to (17).

The curves in Fig. 3 demonstrate the interesting effect of the reconstruction of the hydrogen photorecombination spectrum (curves with  $\alpha = 0$ ) in the Sommerfeld atom. As the repulsive centrifugal term in (24) increases (due to increasing  $\alpha$ ), the initially most intense transition  $W(n_r = 0)$  is suppressed, and, beginning with the value of the parameter  $\alpha > 2$ , the third and fourth levels of the  $S$  series become the dominating lower states. In other words, the data in Fig. 3 show that there is the tendency to formation of the inverse population upon photorecombination of the  $P$  electron to the  $S$  state. It is interesting that this tendency correlates with the phenomenon of "glory" upon scattering of an electron from an ion core [23]. Indeed, consider the relation between the parameter  $\alpha$  of the Sommerfeld potential and the angle of rotation  $\theta$  of a subthermal

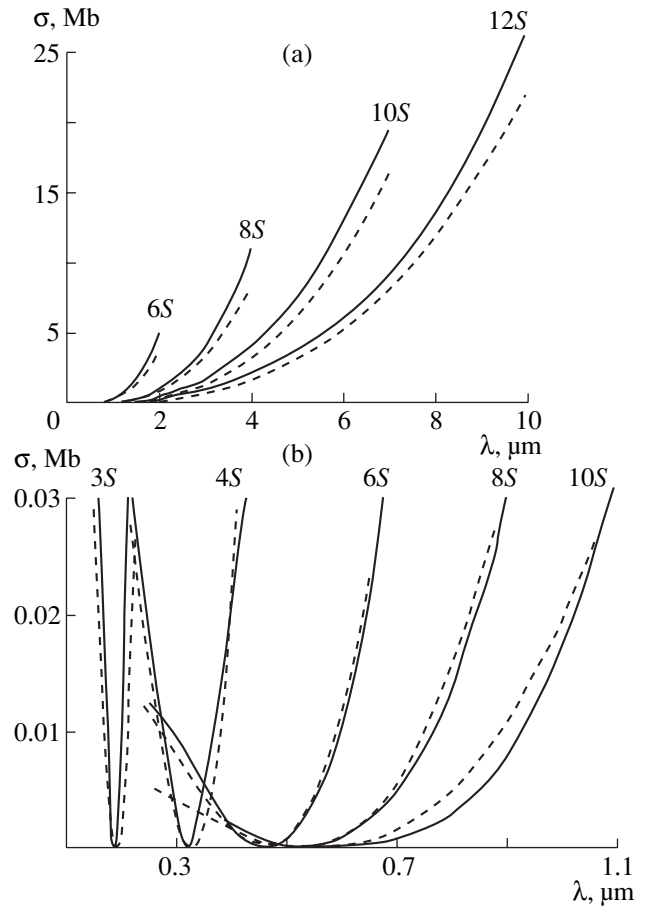


Fig. 1. Dependence of the photoionization cross section  $\sigma$  on the emission wavelength  $\lambda$  for the  $S$  state of a sodium atom. The principal quantum numbers  $n$  are indicated near the curves. The solid and dashed curves correspond to quantum-mechanical calculations [17] and quasi-classical approximation (16, 17), respectively.

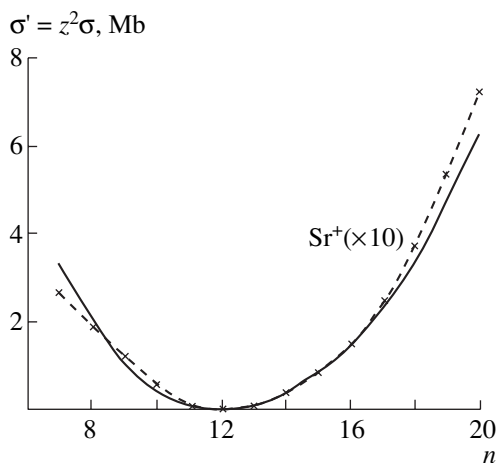
electron ( $\epsilon \rightarrow 0 \sim n_r \rightarrow \infty$ ) around the core during its scattering [23]:

$$\theta = -\partial S_R / \partial L, \quad S_R = 2\pi(n_r - \mu), \quad \theta = 2\pi L / L_{\text{eff}}. \tag{27}$$

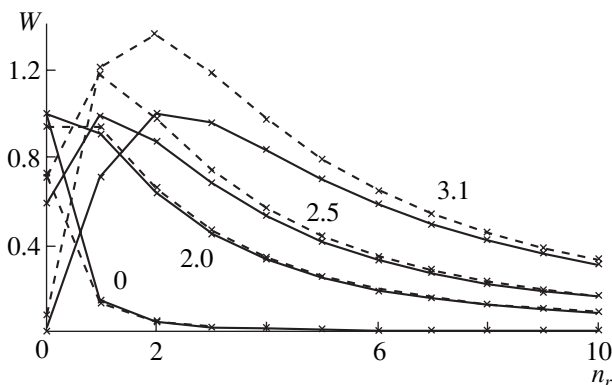
Expression (27) also determines the classical scattering angle  $\varphi = \theta - \pi = 2\pi(L/L_{\text{eff}} - 0.5)$  of the electron. The parameter  $\alpha = 1$  (Fig. 1), at which the transition to the ground state proves to be completely suppressed [because  $R_{j,j}^{(1)}$  vanishes (17)], corresponds to a quite small scattering angle  $\varphi = 2\pi \times 0.14$ . For this reason, the propagation direction of the electron weakly changes after the passage of the region of interaction with the

Values of the difference  $\Delta\mu(n)$  of quantum defects for optical  $nS \rightarrow \epsilon'P$  transitions in a sodium atom

$n$	3	4	6	8	10	12
$-\Delta\mu(n)$	0.550	0.517	0.503	0.498	0.496	0.496



**Fig. 2.** Dependence of the reduced threshold photoionization cross section  $\sigma' = z^2\sigma$  on the principal quantum number of the S series for the strontium ion. The solid and dashed curves correspond to quantum-mechanical calculations [10] and quasi-classical approximation (16, 17), respectively.



**Fig. 3.** Profile of the emission spectrum upon photorecombination of a subthermal electron. The numbers near the curves indicate values of the parameter  $\alpha$  of the Sommerfeld atom.

atomic core. Other aspects of the relation between the phenomenon of glory and special features of the spontaneous emission spectra are discussed in papers [23, 24].

### CONCLUSIONS

Note first that various correspondence rules for calculations of quasi-classical matrix elements have been formulated in many papers (see [9] and references therein and review [11]). Unlike other authors, we suggested the principle of obtaining these rules, which is, in our opinion, physically more substantiated. The principal effective quantum number  $n_a^*$  (10) obtained by us for the average trajectory coincides with the corresponding number found in [9] from heuristic considerations. Further, the authors [9] complicated the rules for

determining  $n_a^*$ , which resulted in rather cumbersome expressions for dipole matrix elements. We showed that our correspondence rules (10) could be used for continuation of the matrix elements (17) for "long" transitions to the continuum. After minor modification that takes into account the corresponding quantum corrections [2, 4], expression (17) yields cross sections for radiative processes with an accuracy not worse than in [9].

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