Excitation and ionization of multicharged ions by electron collisions

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Investigations of the processes of excitation and ionization of multicharged ions by electron collisions are reviewed. It is shown that the Coulomb-Born method with exchange, for calculating cross sections of these processes, is identified here with the perturbation theory in a small parameter—the reciprocal of the ion charge. Resonant scattering substantially alters excitation cross section in a small region of collision energies; however, its contribution to excitation constant is small. Relativistic effects are also considered.

PACS numbers: 34.80.Dp

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INTRODUCTION

Lately, for a variety of reasons, attention has turned to intensive studies of a plasma at very high temperatures, of the order of several or even tens of keV. At such temperatures, light-element atoms in a plasma are completely stripped, and heavy-element atoms are partially stripped. Multicharged ions, which contain electrons, may be excited by the plasma particles, thus giving rise to a time spectrum that may be used to decide on the plasma parameters.

The general spectral properties of multicharged ions and the spectroscopy of a high-temperature plasma were considered by Presnyakov.¹ This review contains the results of investigations of the electron inelastic scattering by multicharged ions. Specifically, the excitation and ionization processes are discussed.

The physics of the electron inelastic scattering by multicharged ions contains a number of interesting properties. In addition to the direct Coulomb excitation of multicharged ions, and the direct ionization of the same, inelastic electron scattering is characterized by the possibility of formation (in the course of a collision process) of long-lived, so-called self-ionized states which break up in a time interval much longer than required for the orbital motion of the electrons. In nuclear physics such states are called compoundnuclei. When electrons are scattered by multicharged ions the formation of self-ionized states occurs by means of excitation of one of the ion-bound electrons

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0038-5670/81/040276-19\$01.10

and the transition of an incident electron from the continuous spectrum into a discrete spectrum state: the Auger-decay of such a state leads to the resonance excitation of a multicharged ion; or by means of exciting an electron from the inner ion shells: the Auger-decay of such a state leads to ionization of multicharged ions.

The relativistic effects begin to appear in the process of electron scattering by multicharged ions essentially at temperatures already attainable in a laboratory plasma. In view of this the very general questions, concerning the role of magnetic interactions and the delay effects in the process of excitation and ionization of multicharged ions when the ion multiplicity increases, require elucidation.

The interaction between electrons, which is the cause of inelastic processes, is considerably weaker than the energy of interaction between electrons and a multicharged ion. This fundamental fact permits us to consider from a unique viewpoint the entire broad range of questions associated with the processes of electron inelastic scattering by multicharged ions.

The data concerning the results of calculations of the electron excitation cross sections of multicharged ions by means of the Coulomb-Born method are presented in the Vainshtein, Sobel'man, Yukov book,² which contains original results by the authors. Today, a large number of calculations of the electron excitation of multicharged ions obtained by other methods is available. In the vicinity of the excitation threshold all available methods may be used only numerically; moreover, especially important is the clearly expressed viewpoint concerning the methodology of the process: what is the accuracy of the method used? In which case and what advantages does this method offer over others, etc.

1. GENERAL CHARACTERISTICS OF INELASTIC COLLISIONS BETWEEN ELECTRONS AND MULTICHARGED IONS

a. Applicability of perturbation theory in the case of near-threshold excitation

The binding energies of the ground and nearest excited states of multicharged ions of one isoelectron series may be considered proportional to Z_2^2 (ion charge $Z_2 \gg 1$).¹⁾ Ion excitation requires, therefore, an energy $\sim Z_2^2$, excluding the transitions with the principal quantum number unchanged, $\Delta n = 0$. In order to verify the applicability of the perturbation theory in the interaction between electrons, it becomes necessary to explain which interelectron distances are significant for excitation or ionization.

In quantum mechanics, relatively large interelectron distances contribute to the cross section, such that perturbation theory appears to be applicable.³ This

follows from qualitative considerations such as in the case of the long-range nature of the Coulomb interelectron coupling the intrinsic region is defined by electron wavelengths (for a bound electron, simply the dimension of its wave function). The size of the intrinsic region should be of the order of or greater than the sum of wavelengths of both electrons. In other words, this dimension cannot be smaller than the size of the wave function of the bound electron which is ${}^{-1/2}_{2}$.

Thus, in quantum mechanics

(a) The effective interelectron distances are large or of the order of Z_2^{-1} ;

(b) the perturbation theory of interaction between electrons is applicable.

The same conclusion holds also for transitions between degenerated states, a result that may be obtained from estimates by means of the perturbation theory of degenerated states.⁴

In this problem the following typical situation takes place: Although, according to the classical mechanics, electrons separated by distances $\sim Z_2^{-1}$ may not interchange energies $\Delta E \sim Z_2^2$, such exchange occurs in quantum mechanics although with a low probability, which is proportional to $(V/\Delta E)^2 \sim Z_2^2$. By multiplying this probability by the geometric transverse cross section of a bound state we obtain the effective cross section $\sim Z_2^4$.

Thus, the well-known and frequently used Coulomb-Born (C-B) approximation for calculating the electron excitation cross section of multicharged ions constitutes a strict perturbation theory with respect to the small parameter $Z_2^{-1} \ll 1$ up to the reaction threshold. Inasmuch as the required symmetrization of the wave functions with respect to electron transposition tends to change them even in the zero approximation, the Coulomb-Born approximation with exchange (CBE) is the absolutely strict perturbation theory. We note that unlike the case of the Born-Oppenheimer approximation, the wave functions of the initial and terminal states in this case are orthogonal with respect to each other, as are wave functions of one and the same Hamiltonian.

Among other methods widely used in the literature for calculating the excitation cross sections of multicharged ions, the method of perturbed waves with polarized orbitals and the strong interaction method are the most interesting. We shall focus briefly on these.

In the case of the method of perturbed waves with polarized orbitals (see Refs. 25 and 26), the wave function of an incident electron is determined not only by including the ion field, but also the bound electron field and the correlation among electrons. However, at Z_2 $\gg 1$ these effects are small, contribute to only higher orders of the parameter Z_2^{-1} and, therefore, taking them into the consideration without allowing for the secondorder perturbation theory with respect to interelectron coupling actually exaggerates the accuracy (but does not lead, as seen below, to appreciable numerical errors).

The strong coupling method indicates the following:

¹Further, all values are measured in atomic units for which the energy unit is 27.21 eV; the mass unit is the electron mass; the length is Bohr's radius $a_0 = 5.29 \times 10^{-9}$; the cross section is measured in units $a_0^2 = 0.28 \times 10^{-16}$ cm².

The total wave function of the ion-incident electron system decomposes with respect to ion wave functions. The coefficients of this expansion are functions of the coordinates of the incident electron and their set describes the state of this electron, i.e., it represents its wave functions. The resultant sum is symmetrized with respect to electron transpositions. Subsequently, only several terms remain in this infinite sum which are states pertaining to the physics of the subject transition. As a result of this, a system of several integradifferential equations must be solved to calculate the cross section. A detailed description of the strong coupling method may be found in Refs. 88 and 89.

The method of strong coupling involving more than two states means taking into account transitions through several intermediate states (for example, $1s \rightarrow 2p \rightarrow 2s$, $1s \rightarrow 2s \rightarrow 2p$). When the perturbation theory applies, i.e., when the small parameter exists ($\mathbb{Z}_2^{-1} \ll 1$), the above allowance may mean that accuracy has been exaggerated—incomplete allowance for the second approximation of perturbation theory. To calculate the second approximation fully requires the summation of the contribution of transitions through all intermediate states. However, allowance for only certain of these may impair the final result.

Thus, when the perturbation theory applies, the strong coupling method, generally speaking, fails to guarantee improved results as compared to the CBE approximation with properly picked wave functions. However, this method also yields correct results for multicharged ion scattering.

From experience with calculations of the excitation cross sections of neutral atoms by electrons, we know that when the Born approximation is used, the contribution of individual moments may exceed a theoretical limit. For this reason a majority of the Bornian calculations with neutral atoms tend to overestimate cross sections near the threshold. To eliminate this disadvantage, an artificial procedure is used: the Born approximation is normalized. The purpose of this operation is to constrain the contribution of above mentioned methods to a theoretical limit. According to Seaton,⁵ this goal is attained if the reaction matrix is calculated which automatically ensures unitarity of the scattering matrix. According to Vainshtein and coworkers,² the calculated cross section may be renormalized. Both methods are equivalent and are meaningful only when the Born approximation substantially (several fold) exceeds the result.

In the case when the multicharged ions are excited by electrons, i.e., under the conditions of strong perturbation theory, contributions of arbitrary moments may not exceed the theoretical limit. For this reason there is no need for normalization. Accuracy is exceeded when the latter is used, a fact that has little effect or the numerical results.

b. Dipole approximation

The specific calculations of the excitation cross sections fail to yield analytical results for even hydrogen-

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like ions. This is occasioned by the fact that continuous spectrum Coulomb functions must be used for an incident electron, which are expressed in terms of a degenerate hypergeometric function. Thus, in order to obtain qualitative results, numerical methods are used, and for the estimating use is frequently made of Bethe's dipole approximation.⁶ In the context of the latter, in the expansion of the interelectron coupling in terms of the Legendre polynomials

$$r_{12}^{-1} = \sum_{l=0}^{\infty} \frac{1}{r_{>}} \left(\frac{r_{<}}{r_{>}}\right)^{l} P_{l}(\cos\theta)$$
(1)

[where $r_{z} = \min(r_{1}, r_{2}, r_{z} = \max(r_{1}, r_{2}); \theta$ is an angle between radius vectors \overline{r}_{1}, r_{2} of the bound and incident electrons], contains only the dipole (l=1) term. The zero term (l=0) contributes nothing due to the orthogonality of the wave functions.

We shall transform the dipole term in Eq. (1) by means of relationships of the classical mechanics which hold for matrix elements in the quantum mechanics:

$$r_{12}^{-1} \approx \frac{r_1 r_2}{r_2^3} = -\frac{\Delta E^3}{Z_2} (r_1 r_2).$$
 (2)

If the exchange is neglected in the CB method the use of Eq. (2) to calculate dipole transition cross sections permits one to adopt Sommerfeld's results, derived from bremsstrahlung theory,⁷ namely to adopt a dipole matrix element between continuous spectrum functions. The ion dipole transition cross sections were derived in this manner and tabulated by Galilitis.⁸

Inasmuch as the CB method in this case represents the strong perturbation theory, there is a need to explain the conditions under which simplification of this method—use of the dipole approximation [Eq. (2)]—may also be completely justified. In other words, it is necessary to identify instances in which the excitation cross section is determined by large distances of the incident electron, which are greater than the dimension of a bound electron state where, while using dipolarity, it is possible simultaneously to neglect exchange.

It will be shown further that among the unknowns are cases of small energy transfer $\Delta E \ll Z_2^2$; more precisely, ΔE is much smaller than the ionization potential of the excited ion, i.e., cases of dipole transitions between components of the fine structure and between states without a change in the principal quantum number (Δn =0). For example, the $2s \neq 2p$ transitions in lithiumlike ions; $2s^2 \rightarrow 2s2p$, $2p^2$, in beryllium-like ions; etc. These states are split as a state electrons, such that These states are split as a result of different exchange and other couplings with ground state electrons, such that $\Delta E \sim Z_2 \ll Z_2^2$.

We shall calculate cross sections of these transitions, assuming that the incident electron travels along a classical Coulomb trajectory, a hyperbola. We shall consider the bound electron to be quantized. A justification of all approximations will be given after the derivation of results.

With this approach the excitation cross section is

$$Q_{0n} = 2\pi \int_{0}^{\infty} \omega(\rho) \rho \, \mathrm{d}\rho, \qquad (3)$$

where the excitation probability $\omega(\rho)$ in the case of dipole coupling [Eq. (2)] and a given impact parameter ρ is

$$\omega(\rho) = \frac{\Delta E^4}{Z_2^2} |(\mathbf{r}_1)_{0n} (\mathbf{r}_2 (\Delta E, \rho))|^2;$$
(4)

where $\bar{r}_2(\Delta E, \rho)$ is the Fourier component of a radius vector of an incident electron. This quantity was calculated in Sec. 70 in Ref. 9. We get

$$\omega(\rho) = \frac{\Delta E^4}{Z_2^2} |(x_1)_{0n} (x_2 (\Delta E, \rho)) + (y_1)_{0n} (y_2 (\Delta E, \rho))|^2,$$
(5)
$$x_2 (\Delta E, \rho) = \frac{\pi Z_2}{2\pi \Delta E} H_{iv}^{(1)'}(iv\varepsilon), \quad y_2 = -\frac{\pi Z_2 \sqrt{\varepsilon^2 - 1}}{2\pi \Delta E} H_{iv}^{(1)}(iv\varepsilon),$$
(6)

$$(\Delta E, \rho) = \frac{2E_2}{2E\Delta E} H_{iv}^{(1)}(iv\varepsilon), \quad y_2 = -\frac{2E_2}{2E\Delta E} H_{iv}^{(1)}(iv\varepsilon), \quad (6)$$
$$\varepsilon = \sqrt{1 + \left(\frac{2E\rho}{Z_*}\right)^2}, \quad v = \frac{Z_2\Delta E}{(2E)^{3/2}}, \quad (7)$$

where $x_{1,2}$ and $y_{1,2}$ are the coordinates of a bound electron and incident particle in the trajectory plane; $H_{i\nu}^{(1)}$ is the Hankel function. We are interested in a probability which has been averaged with respect to the initial and summed over the final substates. The latter pertain to different projections of the moments. In this case $(x_1)_{0n}^2 = (y_1)_{0n}^2 = |d_{0n}|^2$. Then, in the same manner as is used in calculating bremsstrahlung,⁹ we obtain the excitation cross section

$$Q_{0n} = \frac{\alpha^3 f_{0n}}{(2l_0 - \tau) \Delta E} \frac{F(v)}{v_e^2},$$
(8)

$$F(\mathbf{x}) = \mathbf{v} \| H_{i\mathbf{x}}^{(1)}(i\mathbf{x}) \| H_{i\mathbf{x}}^{(1)'}(i\mathbf{x})$$
(9)

 $(l_0$ is the orbital momentum of initial state), where $f_{0n} = 2\Delta E |d_{0n}|^2$ is the oscillator strength of the investigated transition. The cross section is expressed as a function of a single universal quantity ν .

We shall now find conditions under which Eq. (8) holds; these are determined when the classical approximation is used for the incident electron and by means of coupling dipolarity.

The distance of least approach of an electron to a positive ion is^{10}

$$r_{\min} = \frac{Z_2}{2E} \left(\sqrt{1 + \left(\frac{2E\rho}{Z_2}\right)^2} - 1 \right).$$
 (10)

In order to obtain criteria for the correctness of theory, the function $\omega(\rho)$ or, according to Eq. (5) and (6), the dependence of the Hankel function $H_{i\nu}^{(1)}(i\nu \varepsilon)$ on ε must be analyzed. By neglecting the trivial details of such analysis we arrive at the final conclusions. The incident electron trajectories are characterized by different degrees of curvature depending on ν . At $\nu \gg 1$, i.e., in a near-threshold energy region, dipolarity $r_{\min} \gg Z_2^{-1}$ and the classical character (contributions to cross section made by large moments of the incident electron) are achieved when

$$\Delta E \ll Z_2^2. \tag{11}$$

We have assumed that the energy transfer ΔE to a bound electron has no effect on the trajectory of an incident electron. This is valid if energy of the latter in the reaction zone, i.e., at $r_2 \sim r_{\min}$, is much greater than ΔE . At $\nu \gg 1$

$$r_{\min} \approx \frac{Z_2^{1/3}}{6^{1/3} (\Delta E)^{2/3}}.$$
 (12)

It is clear from the foregoing that the condition $Z_2 | r_{min} \gg \Delta E$ is automatically fulfilled when Eq. (11) is

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satisfied, at $\nu \gg 1$ the trajectories are pronouncedly bent.

At $\nu \sim 1$, $\nu < 1$ and $\nu \ll 1$ contributions to cross section are made by $\varepsilon - 1 \sim \nu^{-1}$. Moreover,

$$r_{\min} \sim \rho \sim \frac{Z_2}{2E} \frac{1}{\gamma},\tag{13}$$

i.e., trajectories are slightly bent. Dipolarity is achieved again under a condition in Eq. (11) and $E \le Z_2^2$ (the latter because of the smallness of electron diffraction effect).

The function in Eq. (9) approaches analytical form in the range of small ($\nu \ll 1$) and large ($\nu \gg 1$) "frequencies." ⁹ Accordingly, there are two limits for the cross section:

$$(E/\Delta E)^{3/2} \gg \frac{Z_2}{2\sqrt{2\Delta E}}$$
 (v < 1), (14)

$$Q_{0n} \approx \frac{4\pi f_{0n}}{(2l_0+1)\,\Delta E} \frac{1}{v_e^2} \ln\left(\frac{4E}{\Delta E} \frac{\sqrt{2E}}{\gamma Z_2}\right),\tag{15}$$

where $\gamma = e^{C} = 1.781$ (C is Euler constant),

$$\left(\frac{E}{\Delta E}\right)^{3/2} \ll \frac{Z_2}{2\sqrt{2\Delta E}} \quad (\nu \gg 1),$$
(16)

$$Q_{0n} \approx \frac{4\pi^2 f_{0n}}{\sqrt{3} (2l_0 + 1) \Delta E} - \frac{1}{v_e^2}.$$
 (17)

We note that Eq. (8) may be obtained from the quantum result⁸ in a quasi-classical limit for a hypergeometric function; moreover, Eq. (17) corresponds to a quasi-classical Kramers limit in bremsstrahlung.¹¹ The asymptotic behavior of one cross section at high energies [Eq. (15)] does not go over to the known result yielded by the Bethe-Born approximation, and the logarithmic term fails to coincide. The reason for that, as was said earlier, is diffraction—the quantum nature of electron scattering at very small angles. The resultant formula [Eq. (8)] in the Born interval of collision energies $E \gg Z_2^2$ is inapplicable. The cross sections of transitions with a low excitation energy in the Born limit were calculated in other works.^{12,90}

c. Resonance excitation

The effective cross sections of interaction between electrons and positive ions under investigation are characterized by a wealth of resonances. The values of cross sections in very narrow energy regions of the incident electron exhibit sharp jumps which occur due to the presence of autoionization states in a system incident electron ion. The incident electron may excite any ion level and cross over to a bound orbit of the same ion. In this manner a system containing two excited electrons is formed which is unstable and subjected to autoionization, i.e., capable of reverting to the initial state as a result of a backward energy exchange between electrons (Fig. 1a). The formation of an intermediate autoionization complex is indeed the cause of resonances in the elastic scattering of electrons by positive ions.¹³ An ion's electron which is in the ground state prior to collision may be excited when an autoionization complex is formed, not to the first level but to a higher excited level (Fig. 1b). In the course of reverse decay of such a state, this electron may move to a lower-lying excited state. This results in an ion excitation. In fact, such is the mechanism of



resonance formation in the case of inelastic scattering.^{3,14} Inasmuch as an incident electron may "sit" on a highly-excited ion level, the resonances under consideration are grouped in the cross sections in the form of Coulomb bunching in an energy region before the opening of the next inelastic channel. The abundance of these resonances may in fact lead to their making a notable contribution to the mean cross section, while the width of each individual resonance is small.

In the case of electron scattering on neutral atoms similar resonances are also possible, although the number of these is limited since the number of autoionization states which correspond to a negative ion configuration is limited.

The resonant structure of cross sections, as well as the potential part, may be examined, generally speaking, by means of perturbation theory (in second order, allowing for the widths and shifts of states occurring as a result of the summing up the entire series of perturbation theories over $1/Z_2$), as is done in the theory of resonance fluorescence.¹⁵

We shall analyze the role of resonance excitation using as an example a single autoionization state whose width is considerably smaller than the energy gap between adjacent autoionization states. In this case, perturbation theory leads to the same expression for the resonance scattering cross section $Q_{\rm res}$ as in the Breit-Wigner theory⁴:

$$Q_{\rm res} = \frac{2l+1}{2} \frac{\pi}{E} \frac{\Gamma_1 \Gamma_2}{(E-E_0)^2 + (\Gamma^2/4)}; \qquad (18)$$

where l is the resonant moment of an incident electron; E_0 is energy of an autoionization state; E is energy of an incident electron; Γ is the total width of an autoionization state; Γ_1 and Γ_2 are widths at the input and output channels, respectively. Equation (18) represents the resonance cross section for an ion transition from state 1 to state 2.

Inasmuch as the incident electron energy $E \sim Z_2^2$, Eq. (18) clearly shows that the resonance cross section decreases with increasing Z_2 less than the potential: the resonance cross section $\sim Z_2^{-2}$; at resonance, the cross section increases from $\sim Z_2^{-4}$ to $\sim Z_2^{-2}$. The area under the resonance peak $Q_{\rm res}(E-E_0)$ is also $\sim Z_2^{-2}$. Nevertheless, the resonance scattering contribution to

the total excitation rate $K = \langle vQ \rangle$ is of the same order in Z_2 as the potential scattering contribution. The parentheses $\langle \cdots \rangle$ denote averaging with respect to the velocity distribution function of the plasma electrons

$$K = \int Qv \,\frac{\mathrm{d}f}{\mathrm{d}E} \,\mathrm{d}E \tag{19}$$

(v is the electron speed).

The integration in Eq. (19) with the Maxwellian distribution function leads to the following contribution of the resonance cross section [Eq. (18)] to excitation rate:

$$K_{\rm res} = \pi \sqrt{2\pi} \left(2l + 1 \right) \frac{\Gamma_1 \Gamma_2}{\Gamma^{TS/2}} e^{-E_0/T},$$
(20)

where T is electron temperature. At $T \sim Z_2^2$, we get

$$K_{\rm res} \sim \frac{1}{Z_{\star}^2} \frac{\Gamma_1 \Gamma_2}{\Gamma} e^{-E_0/T}.$$
(21)

The above expression contains, in addition to Z_2^{-3} , small widths (at $\Gamma_1 \sim \Gamma_2 \sim \Gamma \ll 1$). For this reason $K_{\rm res}$ is $\Gamma \ll 1$ times smaller than $K_{\rm pot}$. It follows from calculations of the autoionization widths that $\Gamma_{1,2} \sim 0.01$ for the lowest excited state and that it is practically independent of Z_2 . Nevertheless, on the whole, the ratio $K_{\rm res}/K_{\rm pot}$ may attain values ~0.1 due to a large number of autoionization levels.

The resonance denominator of Eq. (18) contains the total width for the decay of a given state in all possible channels. This includes, as a component of T, the radiation width, which corresponds to emission of a photon during transition of one of the electrons into the ground or a much lower excited state of the ion. In the case of such a radiative decay of the newly-formed autoionization state, coupling occurs between an incident electron and ion (after such an electron also completes radiative transition to ground state). This process is known as dielectric recombination. Its cross section may be obtained if Γ_2 in Eq. (18) is considered to be the radiation width. Thus dielectric recombination and resonance excitation of ions are competing processes. Inasmuch as the autoionization and radiative widths are different functions of Z_2 , each of these processes is predominant in different regions of Z_2 values.

The autoionization width, as stated earlier, is almost independent of Z_2 and it may be estimated for a lower excited level as $\Gamma_{aut} \sim 0.01$ a.u. The radiation width highly increases with increasing Z_2 :

$$\Gamma_{\rm rad} \approx \frac{4}{3} \frac{\omega^3}{(137)^3} |d|^2;$$
 (22)

where ω is the transition frequency; *d* is the dipole matrix element of transition. Clearly, $\Gamma_{\rm rad} \sim Z_2^4/137^3$. This value should be compared with the constant auto-ionization width ~0.01. These are comparable when

.

$$Z_0 \sim (0.01 \cdot 137^3)^{1/4} \approx 13.$$
 (23)

At $Z_2 < 13$, resonance excitation predominates, and at $Z_2 > 13$, $\Gamma \sim \Gamma_{rat}$ and the contribution of resonance excitation cross section to K is proportional to the product of three small quantities:

$$K_{\rm res} \sim Z_a^{-3} \frac{\Gamma_{\rm lout} \Gamma_{\rm sout}}{\Gamma_{\rm rad}}$$
 (24)

Thus, if at $Z_2 \le 13$ the contribution of resonances to excitation is ~10-20%, at $Z_2 > 13$ it sharply decreases.

d. Relativistic formulation of the problem

As the nuclear charge Z increases, the role of relativistic effects also grows requiring, as a result, that their contribution to the excitation cross section of multicharged ions by electron impact must be known.

Both the relativistic and non-relativistic theories make use of a perturbation theory of interelectron coupling. The total Hamiltonian in the relativistic case is

$$H = \sum_{i=1}^{2} H_{i}^{(0)} + H_{\gamma}^{(0)} + V_{ee} + \sum_{i=1}^{2} V_{\gamma e_{i}},$$
(25)

where $H_i^{(0)} = mc^2 P_i + cp_i \alpha_i + e^2/r_i$ is the Dirac Hamiltonian of an electron in the field of a point charge Z_2 with infinite mass; H_{ν} is the Hamiltonian of a free electromagnetic field; $V_{ee} = r_{12}^{-2}$; $V_{vei} = e \alpha_i A$ is a coupling operator between the electron and the transverse electromagnetic field which is defined by a vector potential A; α is the Dirac matrix triplet.

Inasmuch as photons in the initial and terminal states are nonexistent, ion excitation due to coupling via a virtual transverse electromagnetic field is described in second order perturbation theory in terms of V_{ue} . The amplitude of the excitation probability, moreover, is proportional to

$$A_{if} \sim \int dk \, \frac{\langle 1', \, 2' | \alpha_1 e^{ikr_1} | v \rangle \langle v | e^{-ikr_2} | \mathbf{1}, \, 2 \rangle}{E_1 - E_f - k} \,, \tag{26}$$

where E_i and E_f are initial and final energies of an incident electron; $|1,2\rangle$; $|V\rangle$; and $|1',2'\rangle$ are the eigenfunctions of the Dirac Hamiltonian of two non-interacting electrons (at $r_{12} \rightarrow \infty$, states $|1,2\rangle$ and $|1',2'\rangle$ become initial and final states of a system, respectively); k is the wave vector of an intermediate photon. The identical character of the electron is reached by antisymmetrization of the Hamiltonian eigenfunctions $H_1^{(0)}$ $+H_2^{(0)}$. The transition amplitude, in addition to "direct" term also contains an "exchange" term.

Inasmuch as

$$(E_1 - E_t - k)^{-1} = i\pi\delta (E_1 - E_t - k) + P \frac{1}{E_1 - E_t - k},$$

the main portion of the integral in Eq. (26) may be combined with the excitation probability amplitude in first order perturbation theory with respect to the Coulomb interaction r_{12}^{-1} and, after a series of identical transformations, it may be reduced to

$$A_{if} = \langle 1', 2' | r_{12}^{-1} \cdot e^{i(E_1 - E_f)r_{12}} \cdot (1 - \alpha_1 \alpha_2) | 1, 2 \rangle.$$
(27)

In fact, Walter used this expression initially.¹⁶ This clearly shows what Walker actually neglected: a polar term in the transition probability amplitude [Eq. (16)] describes a process of excitation via an intermediate resonant stage of bremsstrahlung photon emission by an incident electron, and the subsequent absorption of the same by an ion. In this case, the law of conservation of energy may be fulfilled in the intermediate state at resonance and, subsequently, the virtual state becomes

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real. This process, which is forbidden to free electrons, scattering from each other and causing energy to be transferred, becomes possible in the external Coulomb field of a nucleus.

Regardless of a substantially different dependence of the cross section of such a process on Z_2 (increase $\sim Z_2^2$) than the dependence of direct excitation cross section ($\sim Z_2^4$), its neglect is justified for real values of Z_2 . This conclusion permits a precise analysis to be made in the second order perturbation theory.

We shall note a possibility of using a more elegant, relativistically invariant form of perturbation theory [see, for example, Eq. (17)] which leads, in the end, to the same results. In this theory, a covariant Lorentz gauge is used in which the electromagnetic field is equally quantized into longitudinal and transverse photons, and interaction between the electron and photon fields is characterized by a single universal constant $e^2/\hbar c$.

The relativistic effects are very distinctly manifested when non-dipole transitions between the fine structure components of complex multicharged ions are excited. For example, the $3D_{5/2} \rightarrow 3D_{3/2}$ radiative transition of a potassium-like ion Mo²³⁺ is the M1 transition-magnetic dipole transition. But, when this transition is excited by charged-particle impact, the electric quadrupole excitation (E2) may also be dominant. The magnetic dipole excitation cross section has the order of smallness $(Ze^2/\hbar c)^2 (v/c)^2$ with respect to the electric dipole, since the amplitude of a magnetic field which travels with a speed of charge v is v/c-fold smaller than the amplitude of an electric field. However, the quadrupole electric excitation cross section is of the order of $(E/Z)^2$ with respect to the electric dipole. Therefore, when $E \gg Z^6/M(137)^4$ (where M is the mass of an incident particle), the magnetic excitation is smaller than the electric quadrupole. For protons, this condition is more than satisfied under the conditions of a high-temperature plasma ($T \sim 10$ keV). Either E2 or M1 may be dominant for electron-shock excitation in accordance with the condition above.

2. EXCITATION AND IONIZATION OF HYDROGEN-LIKE IONS BY ELECTRONS

Hydrogen-like ions are the simplest of all cases under consideration. The wave functions of the continuous spectrum, which at large distances from an ion become plane waves with a given direction of propagation, i.e., a given vector k,⁴ are:

$$\psi_{k} = e^{\pi Z_{2}/2k} \Gamma\left(1 - \frac{iZ_{2}}{2k}\right) e^{ikr} F\left(\frac{iZ_{2}}{k}; 1; i\left(kr - \mathbf{kr}\right)\right).$$
(28)

Total and differential scattering cross sections are:

$$Q_{0n} = 2\pi \int Q_{0n} (\theta) \sin \theta \, \mathrm{d}\theta, \qquad (29)$$

$$Q_{0n}(\theta) = \frac{k_n}{k_0} \left[\frac{1}{4} |f(\theta) + g(\theta)|^2 + \frac{3}{4} |f(\theta) - g(\theta)|^2 \right];$$
(30)

where k_0 and k_n are initial and final momenta of an incident electron. The direct $f(\theta)$ and exchange $g(\theta)$ scattering amplitudes are

- 1

$$f(\theta) = \frac{1}{2\pi} \int \psi_n^{\bullet}(\mathbf{r}_2) \psi_0(\mathbf{r}_2) \psi_{h_0}(\mathbf{r}_1) \psi_{h_n}^{\bullet}(\mathbf{r}_1) \frac{d\mathbf{r}_1 d\mathbf{r}_2}{r_{12}}, \qquad (31)$$

$$g(\theta) = \frac{1}{2\pi} \int \kappa_N(\mathbf{r}_1) \psi_0(\mathbf{r}_2) \psi_{k_0}(\mathbf{r}_1) \psi_{k_n}^*(\mathbf{r}_2) \frac{d\mathbf{r}_1 d\mathbf{r}_2}{r_{19}}.$$
 (32)

It follows from Eqs. (28) and (30) that at the threshold when $k_n = 0$ the excitation reaction cross section $0 \rightarrow n$ is finite. It is also evident that the cross section of the reverse process of de-excitation by very slow electrons with a momentum $k_n \rightarrow 0$ proceeds in proportion k_n^{-2} . This conclusion also follows from the detailed balance principle:

$$k_{n}^{2}Q_{0n} = k_{n}^{2}Q_{n0}.$$
(33)

The divergence of de-excitation cross section by slow electrons can be explained in terms of attraction by the ion Coulomb field which effectively increases the electron flow in the reaction region.

The aforementioned properties of the finiteness of excitation cross sections and the divergence of the de-excitation cross section can be explained only in terms of the Coulomb field attraction and, therefore, take place when electrons are scattered by positive ions, with any number of bound electrons.

It follows from the properties of wave functions and scattering amplitudes that the excitation cross section Q_{0n} of the $0 \rightarrow n$ transition may be represented as follows

$$Q_{0n} = Z_{-1}^{-4} \varphi_{0n}(x); \quad x = \frac{E}{AE},$$
(34)

where φ_{0n} is independent of Z_2 and is determined only by a given transition for a given number of isoelectronic ions. The proportionality $Q_{0n} \sim Z_2^4$ holds only for transitions with the excitation energy $\sim Z_2^2$.

a. Excitation of hydrogen-like ions

The CBE method for the excitation of hydrogen-like ions was used in several works^{2,18-20}; elsewhere,²¹⁻²⁴ the CB method was used and, in Refs. 20 and 21, expansion in terms of moments for the $S \rightarrow S$ transitions was avoided. A method of perturbed waves with polarized orbitals was used,^{25,28} while a complex combined method, tested on experimentally studied cases of excitation of H and He atoms, was also introduced.²⁸ All these calculation methods should yield identical results in view of correctness of the perturbation theory.

Figures 2 and 3 show normalized (or scanned) cross sections Z^4Q for the excitation from ground to *p*-states: $1s \rightarrow n, l=1$. According to Eq. (34), such a product should be a universal function for the isoelectronic series under consideration, which depends on the normalized energy *x* of an incident electron and on a specific transition $0 \rightarrow n$. Evidently, the function Z^4Q_{0n} is actually independent of Z_2 at high values of Z_2 .

Figures 2 and 3 clearly show that taking into consideration exchange between incident and bound electrons has a weak effect on the results for the excitation of hydrogen-like ions. This can be explained by the proximity of values of direct and exchange amplitudes.

We shall examine the behavior of cross sections as $n \rightarrow \infty$, i.e., when the principal quantum number of an excited state increases. For this purpose it is con-

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FIG. 2. Normalized excitation cross section $Z^{4}Q$ $(1s \rightarrow 2p)$ (nonrelativistic) of the $1s \rightarrow 2p$ transition of hydrogen-like ions by electron shock as a function of ratio of kinetic electron energy and transmitted energy $x = E/\Delta E$. Calculations wihout allowing for exchange: $1-CB^{18,23}2-Ref. 2$. Calculations allowing for exchange: $3-CBE^{18}$; method of perturbed waves with polarized orbitals; $4-Z=26^{25}$; 5-Z=10; $6-Z=6^{26}$; 7-Ref.27; 8-method of strong coupling 1s, 2s, 2p, Z=6 and 10^{29} .

venient to express cross section in terms of so-called impact force Ω^{18} :

$$Z^{4}Q(1s \rightarrow n) = \frac{\pi}{n^{3} - n} \frac{\widetilde{\Omega}(x)}{x}, \qquad (35)$$

where the normalized impact force $\tilde{\Omega}$ is related to Ω as follows

$$\hat{\Omega} = n^3 Z^2 \Omega. \tag{36}$$

When $Z_2 \rightarrow \infty$ and $n \rightarrow \infty$, $\tilde{\Omega}$ tends to a constant limit which is a certain universal function of x. Table I shows a limit of function $\tilde{\Omega}$ at $n, Z \rightarrow \infty$ calculated by Tully using the CB approximation without exchange.²³ The table, when supported by Eq. (35), may be used to calculate cross sections for any values of $Z_2 \ge 4$ and $n \ge 4$. If we compare the results of this calculation with the excitation cross sections of level n=4—shown in Fig. 3—we see that the error due to the use of the critical impact force $\tilde{\Omega}(x)|_{n,r=\infty}$ is 15% for n=4. This error decreases



FIG. 3. Normalized excitation cross section $Z^{4}Q$ (1s $\rightarrow np$) (nonrelativistic) of the 1s $\rightarrow np$ transition of hydrogen-like ions by electron shock. Calculations without allowing for exchange (CB method): 1—Ref. 2; 2—Ref. 23; 3—Ref. 24. Calculations allowing for exchange: 4—method of perturbed waves with polarized orbitals, $Z = 26^{25}$; 5—CBE.¹⁹

TABLE I. Limit at $n, Z \to \infty$ of normalized collision force $\tilde{\Omega}_{1s+nl}$ (see Ref. 55), which depends on the incident electron energy, in threshold units $x = E/\Delta E$.²³

ł	x = 1	x = 2	x = 3	x = 4
0	1.843	1.883	1,878	1.869
1	6.94	10.14	12.27	13.8
2	0.835	1.342	1,59	1,74

as n increases.

Hayes and Seaton²⁹ calculated the normalized impact forces $Z_2^2\Omega$ for the excitation of the 2s and 2p levels of He^{*}, Li^{2*}, C^{5*}, and Ne^{9*} ions. Calculations were made using the perturbing wave and strong interaction (1s, 2s, 2p) methods with exchange. It was found that results for C^{5*}, calculated by both methods, are already similar. This coincidence is due to the applicability of the perturbation theory: both methods in different ways take into consideration only a portion of the next approximation. For this reason neither one of these methods should be given preference. However, it may be stated with confidence that the perturbation theory the CBE method—yields reliable results already for C^{5*} ions.

We note that the absolute values $Z_2^2\Omega$ obtained in Ref. 29, are 5-10% lower than the same values obtained elsewhere.^{18,25}

Equations (8), (15) and (17) may be used to calculate excitation cross sections of transitions between fine structure components. Fine splitting of the $2P_{3/2} \rightarrow 2S_{1/2}$, $2P_{1/2}$ levels strongly increases with increasing Z,³⁰ giving rise to a strong increase in the electric fields which leads to the $2s \neq 2p$ mixing. The $2s \rightarrow 3p$, 7p, $Z \rightarrow \infty$ transition cross sections were calculated by the CB method.³¹

Hayes and Seaton³² investigated contributions of resonances to excitation of the 2s, 2p levels of C^{5*} and Ne^{9*} ions from the ground state using the strong coupling method, allowing for the 1s, 2s and 2p ion states and the autoionization states $3s^2$, $3p^2$ and $3d^2$. Figure 4 shows transition strengths $Z^2\Omega$ calculated by these authors. Clearly, good separation exists between resonances. This figure may be used to estimate roughly the average resonance width for C^{5+} (0.2 eV) which is comparable to values normally obtained in calculations of autoionization state widths. The same authors³² have estimated the contribution of resonances to excitation rate K as ~20% for the $1s \rightarrow 2s$ transitions, and ~10% for the 1s $\rightarrow 2p$ transition. Higher autoionization states nl, n'l'with n, n' > 3 contribute even less since Γ_{aut} decreases strongly with increasing n.

Figure 5 shows results of calculations of the $1_{S} \rightarrow 2s_{1/2}$, $2P_{1/2}$ and $2P_{3/2}$ transitions¹⁶ by means of the CBE method in the relativistic approximation, using Eq. (27). The figure clearly shows that the most changeable as Z increases—due to the relativistic effects—is the cross section at lower incident electron energies, in particular, near the threshold, i.e., at x = 1. (In the nonrelativistic approximation each curve in Fig. 5 should become a straight line parallel to the abscissa.) As



 $Z^2 \Omega (1s - 2s)$ Z2 Q (15-25) 36 3.0 62+ 2.0 2.0 1,0 1.0 107 104 100 107 104 108 ti 102 x ь) a) Z2 9 (15-2p) $Z^2 \Omega(1s - 2\rho)$ 8.0 8.0 C2+ 6.0 6,0 4.0 4.0 2.0 2.0 102 102 104 100 100 æ c) d)

FIG. 4. Resonance structure in the normalized collision force $Z^{2} \dot{\Omega}$ of au electron with $C^{5^{*}}$ and $Ne^{3^{*}}$ ions for the $1s \rightarrow 2s$ and $1s \rightarrow 2p$ transitions. Calculations by means of a strong coupling method of the 1s, 2s, 2p states with autoionization states $3s^{2}$, $3p^{2}$, $2d^{2}$.³²

this energy increases, the effect of relativistic effects decreases. It can be also seen that allowing for the relativistic effect changes cross sections at Z = 100 more than twofold. The electron binding energy in the 1s state at Z = 50 is ~37 keV. Therefore, a conclusion may be made on the basis of Walker's results¹⁶ that relativistic effects become noticeable during excitation of electrons with binding energies \geq 40 keV.

b. Ionization of hydrogen-like ions

In order to calculate ionization cross sections by means of perturbation theory it is necessary to replace in Eqs. (29)-(32) the terminal state function of a bound electron by a wave function of the continuous spectrum with a diverging wave at infinity. As was the case for excitation, the first approximation of pertur-



FIG. 5. Normalized electron excitation cross sections Z^4Q of the $1s \rightarrow 2s_{1/2}$ and $1s \rightarrow 2p_{1/2,3/2}$ transitions of hydrogenlike ions as a function of Z (allowing for exchange), calculated by Walker¹⁶ in the relativistic pproximation by Eq. (37) for three values of relative energy $x = E/\Delta E$: 1.07(-.-), 1.33(--), and 5.33(-).

×. .

bation theory leads to an expression for the ionization cross section that is similar to Eq. (34), i.e., ionization cross section decreases with increasing nuclear charge $\sim Z^{-4}$ and can be characterized by an energy dependence in threshold units x = E/I (*I* is ion ionization potential) which is universal for the entire isoelectronic series. A distinctive feature of this function is the conversion of the ionization cross section to zero at threshold. This can be explained by a tendency toward zero of the energy interval when $E \rightarrow I$, in which the knock-on electron spectrum is different from zero.

The nonrelativistic CBE method was used to calculate the ionization cross section of hydrogen-like ions (H, He, and Z = 128)³³ and $(Z = \infty)$.³⁴ Salop³⁵ calculated the ionization cross sections of many multicharged ions, including hydrogen-like ions C⁵⁺, N⁶⁺, O⁷⁺, and Ne⁹⁺, using a method of pair collisions between electrons, i.e., a modified Grizinskiy method which utilizes classical mechanics concepts.

Experimentally, ionization was also investigated for many multicharged ions,³⁸⁻³⁸ including hydrogen-like N^{6^+} , O^{7^+} and Ar^{17^+} ions.³⁸ The measuring technique, similar to the one used in these works, has been used elsewhere.^{39,40}

Figure 6 shows a comparison of theoretical and experimental values of normalized cross section Z^4Q for a number of elements. Clearly, there is a good general agreement between experiment and theory, except at two data points. Certain experimental points near the threshold are ~50% above theoretical. It should be noted that derivation of experimental cross sections from observed values requires solving a system of a large number of coupled algebraic equations. The results of calculations based on classical mechanics³⁵ are closer to experimental points. However, accuracy of such calculations is indefinite. Practice with calculations of ionization cross sections of neutral atoms shows their accuracy is of the order of 2 (i.e., ~200%).

c. Excitation and ionization rates of hydrogen-like ions

Calculations of radiation intensities from a plasma require that ion excitation rates must be known, i.e., K = vQ (v is electron speed), which are averaged with respect to electron velocity distribution function (see Ref. 19). We shall use Maxwell's distribution function with temperature T.



FIG. 6. Normalized ionization cross section $Z^4Q_{ton}(1s \rightarrow k)$ of hydrogen-like ions by electrons.

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Using cross sections obtained elsewhere $^{18-28,31}$ and calculating the integral [Eq. (19)], we get excitation rates of hydrogen-like ions:

$$K (1s \rightarrow 2p) = \frac{3.5}{Z^3} \alpha^{1/2} e^{-\alpha} [-0.12 + (2.74 + 1.84\alpha) e^{\alpha} I(\alpha)], \quad (37)$$

$$K(1s \to 2s) = \frac{1.5}{7^3} \alpha^{1/2} e^{-\alpha} [1 + 0.058 e^{\alpha} I(\alpha)],$$
(38)

$$K(1s \rightarrow 3s) = \frac{0.32}{7^s} \alpha^{1/2} e^{-\alpha},$$
 (39)

$$K(1s \to 3p) = \frac{\alpha^{1/4}}{Z^3} e^{-\alpha} [-0.52 + (1.83 + 1.70\alpha) e^{\alpha} I(\alpha)], \qquad (40)$$

$$K (1s \to ns) = \frac{6.54}{Z^3 n^3} \alpha^{1/2} e^{-\alpha},$$

$$K (1s \to np) = \frac{\alpha^{1/2} e^{-\alpha}}{Z^3 n^3} [24.6 + 17.2 e^{\alpha} I(\alpha)],$$

$$K (1s \to n d) = \frac{\alpha^{1/2} e^{-\alpha}}{Z^3 n^3} [2.98 + 2.41 e^{\alpha} I(\alpha)],$$

$$\alpha = \frac{\Delta E}{Z^3}, \quad 0.05 \leqslant \alpha < \infty.$$
(41)

The $I(\alpha)$ function is related to the integral exponential function⁴¹ and it can be calculated using the following approximation:

$$I(\alpha) = \int_{0}^{\infty} \frac{e^{-\alpha x}}{x} dx = \begin{cases} \ln\left(\frac{0.562}{\alpha}\right) + \alpha - \frac{\alpha^2}{4} + \frac{\alpha^3}{18} - \frac{\alpha^4}{96}, & \alpha \leqslant 1, \\ \frac{e^{-\alpha}}{\alpha} - 1.29e^{-2j i 6\alpha}, & \alpha \geqslant 1. \end{cases}$$
(42)

The rate of ionization of a hydrogen-like ion from a state with the principal quantum number n was approximated as follows³³

$$K_{\rm ton}(n, z) = 10^{-8} \ {\rm cm}^3/{\rm s} \left(\frac{2n^3}{Z^2}\right)^{3/2} e^{-\alpha} \sum_{m=0}^5 \varkappa_m \alpha^m, \quad \alpha = \frac{I_n}{T}, \tag{43}$$

where I_n is the ionization potential of the *n*th state and the matching coefficients \varkappa_m are

The rate of excitation (or de-excitation) in those cases where the cross section is determined as a dipole approximation by means of Eqs. (8), (15) and (17), is

$$K_{dip} (\alpha) = \frac{V^2 \pi i_{on}}{(2l_o+1) \Delta E^{3/2}} \sqrt{\alpha} \left[\frac{2}{3} \alpha^{-\alpha} \ln \left(\frac{4 \sqrt{2\Delta E}}{\gamma Z} \right) + I(\alpha) \right],$$

$$\alpha^{-3/2} \gg Z/2 \sqrt{2\Delta E}, \qquad \gamma = 1.781 \dots, \qquad (44)$$

$$K_{dip} (\alpha) = \frac{3 \sqrt{6\pi} i_{on}}{(2l_o+1) \Delta E^{3/2}} \sqrt{\alpha} e^{-\alpha},$$

$$\alpha^{-3/2} \ll Z/2 \sqrt{2\Delta E}. \qquad (45)$$

We should point out that the atomic unit of the reaction rate is $K_0 = a_0^2 v_0 = 6.12 \times 10^{-9} \text{ cm}^3/\text{s}$, where a_0 is Bohr's radius and $v_0 = 2.188 \times 10^8 \text{ cm/s}$ is the atomic rate unit.

3. BOUND STATE ENERGIES OF COMPLEX MULTICHARGED IONS

One of the difficulties facing theory when addressing helium-like and more complex ions is the calculation of the excited and ground state energies. There are no strict analytical formulas for these energies for ions with two or more electrons; instead, they are obtained by a variational method or, using the perturbation theory, by expansion in terms of the small parameter $1/Z_2$.

Ivanova and Safronova⁴² have calculated energies of ground and certain excited states of ions with the electron configurations $1s^22s^{n_1}2p^{n_2}$ $(n_1=0-2, n_2=0-6)$ as a nonrelativistic approximation by means of a field

form of perturbation theory. These energies can be written out as a series in 1/Z: $E = E_0 Z^2 + E_1 Z + E_2 + \cdots$.

Excited state energies of a {He} series have been calculated.^{43,44} Blanchard has processed a large number of variational calculations (based on Ref. 45) and other calculations based on the perturbation theory.⁴³ He presented the total energy of two electrons as a power series in $Z^{-1} [E_0 = -0.5(1 + n^{-2})]$ and determined 5-8 first coefficients E_k by comparing these series with the results of original calculations. His work⁴³ provides nonrelativistic energy values of the n^1 , ³S and n^1 , ³P (n=2-5) states. The $1s^2$, 2^1 , ³P and 2^1 , ³S state energies were calculated by means of the perturbation theory allowing for relativistic effects.⁴⁴ Numerical results for $Z = 10, 20, 30, \ldots$, 100 are given.

A comparison of theoretical^{43,45} and experimental⁴⁶ values of ionization potentials and excitation energies for certain states of helium-like ions demonstrates an excellent agreement of calculated and experimental data. As Z increases, theory and experiment diverge (in the fourth, fifth signs) due to relativistic effects neglected in theory.

In addition to conducting relativistic calculations, available experimental values of energy at $Z \le 10$ may be extrapolated to a higher Z region. This operation was carried out for ions of several isoelectron series $(1 \le Z \le 30)$ by comparing the expansion of unknown energies in powers of Z^{-1} with their experimental values.⁴⁷ Lotz's results⁴⁷ very accurately reproduce the experimental value of ionization potential for Fe²⁴⁺.⁴⁸

The results of calculations of selected levels of lithium- 49,50 and beryllium-like⁵¹ ions are in a good agreement with the results of Ivanova and Safronova.⁴²

The foregoing may be used to conclude that very many levels of a large number of multicharged ions may be determined in some manner, either on the basis of theoretical calculations or extrapolation of spectroscopic data⁴⁶ with an accuracy that is sufficient for the calculation of cross sections of various processes.

4. EXCITATION OF DIPOLE TRANSITION OF MULTICHARGED IONS WITH SMALL EXCITATION ENERGY

We shall compare values of cross sections given by Eq. (8) with those calculated by more complex computer methods.

The function $F(\nu)$ has been adequately studied in the theory of electromagnetic excitation of nuclei by positive ions⁵² and in the theory of bremsstrahlung of a classical particle in a Coulomb field. This function was tabulated in the $0.1 \le \nu \le 4$ region⁵² and was the subject of a dissertation over the broader region $0.01 \le \nu \le 20$.⁵³

The function F(v) may be approximated by the following relationship:

$$F(\mathbf{v}) \approx \begin{cases} \frac{4}{\pi^8} \ln \frac{1.123}{\mathbf{v}} + 1.46 \mathbf{v}^{0.7}, & \mathbf{v} \leq 0.2, \\ \frac{4}{\pi \sqrt{3}} + \frac{0.163}{\sqrt{\mathbf{v}}}, & \mathbf{v} \geq 0.2. \end{cases}$$
(46)

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a. Lithium-like ions (Li), $2s \rightarrow 2p$ transition

The cross section of this transition was calculated for several ions in a number of works: by means of the Coulomb-Born (CB) method for Be^{*}, N^{4*} and Ne^{7*} ions,⁵⁴ and N^{4*} ions⁵⁵; by means of the CB and strong coupling methods for Be^{* 56}; by the strong coupling method, allowing for five states nearest to the ground state for N^{4* 57} and C^{3*} and Ar^{15* 58} ions. Resonances were studied by use of the strong coupling method when this transition was excited by electrons with energies 1.4 $Ry \le E \le 2.6 \text{ Ry}$.⁵⁹ A large number of narrow resonances were identified (Fig. 7); however, their contribution to the averaged out cross section was small (~5%).

The experimental cross section of the aforementioned transition was measured only for C^{3*} ions⁶⁰ (in an energy region 8-500 eV), and N^{4*} ions⁶¹ (130-305 eV).

Figure 8 shows comparisons of excitation cross section of this transition for various ions, determined by means of Eq. (8), with those obtained by numerical methods. To calculate cross sections by means of Eq. (8), we used the oscillator strengths of the 2s - 2ptransition of lithium-like ions, assembled in Ref. 62. These data may be approximated by the following relationship:

$$f_{2s-2p}\{\mathrm{Li}\} = \frac{1.35}{Z} + \frac{2.20}{Z^3}, \qquad (47)$$

which is well confirmed by more recent measurements for lithium-like sulfur ions.⁶³

The energy differences were taken from Ref. 42:

$$\Delta E_{28-2p} \{ \text{Li} \} = 0.0707Z - 0.120; \tag{48}$$

where Z is nuclear charge, as opposed to Z_2 , ion charge.

Figure 8 shows that the results from all sources are in a good agreement with each other at sufficiently high Z's. An exception to this is the C^{3^*} ion for which Eq. (8) exceeds results by 1.5-2-fold (which may be explained by insufficient smallness of Z_2^{-1} for this ion), while results obtained by means of the strong coupling method coincide with experimental results.

In the case of large ion charges Z_2 differences between the fine components $2P_{1/2}$ and $2P_{3/2}$ become substantial, such that two dipole transitions $2S_{1/2} - 2P_{1/2}$ and $2S_{1/2} - 2P_{3/2}$ must be distinguished. Table II shows

FIG. 7. Electron excitation cross section of the $2s \rightarrow 2p$ transition of C^{3^*} ion (threshold 8eV = 0.59 Ry), calculated by strong coupling method⁵⁹ with autoionization states C^{2^*} . Dash line—cross section averaged with respect to resonance.





FIG. 8. Electron excitation cross sections of lithium-like ions as a function of energy in threshold units $x = E/\Delta E$. $-\times$ ---Eq. (8); ----its limit Eq. (17); a: 1--experiment; ⁶⁰ 2-strong coupling method (2s, 2p, 3s, 3p); ⁵³ b: 1--CB method, ⁵⁵ 2--strong coupling; ⁵⁷ c: 1--CB method; ⁶⁴ d: 1--strong coupling. ⁵⁸

the parameters of these transitions for iron Fe^{23+} and molybdenum Mo^{39+62} ions, as also the cross sections of these when excited by electrons and protons (see Ref. 52) at energies of 0.5, 1 and 2 keV.²⁾ Clearly, the proton cross sections are small due to repulsion in this energy region, but they sharply increase with increasing E.

b. Beryllium-like ions {Be}, $1s^22s^2|^1S \rightarrow 1s^22s2p|^1P$ transition

The collisional and cross section values for this transition were calculated by Osterbrock for B^{*}, C²⁺, N³⁺, O^{4+} and Ne⁶⁺ ions using the strong coupling method.⁶⁵ Parks and Sampson calculated cross sections of the same transition by means of hydrogen-like functions

TABLE II. Parameters f and ΔE^{62} and excitation cross section of lithium-like ions of iron and molybdenum, calculated from Eq. (8) for electrons (Q_g) and from a formula in Ref. 52 for protons (Q_g) .

	Fe ³³⁺		
Δ <i>E</i>	$1s^{2}2s S \rightarrow 1s^{2}2p P_{3/2}$ 2.371 a.u. = 64.51 eV	$\begin{array}{c} 1s^{3}2s \mid S - 1s^{3}2p \mid P_{1/2} \\ 1,785 \ a.u. = 48.57 \ eV \end{array}$	
- t	0.048	0,018	
E, keV Qe Qp	$\begin{array}{c} 0.5 & 1 & 2 \\ 5.0 \cdot 10^{-19} \mathrm{cm}^2 \ 3.1 \cdot 10^{-19} \mathrm{cm}^3 \ 1.9 \cdot 10^{-19} \mathrm{cm}^3 \\ 10^{-43} \mathrm{cm}^2 & 3 \cdot 10^{-86} \mathrm{cm}^3 & 5 \cdot 10^{-20} \mathrm{cm}^3 \end{array}$	$\begin{array}{c} 0,5 & 1 & 2 \\ 2.6.40^{-19} \mathrm{cm}^3 & 1.6.40^{-19} \mathrm{cm}^3 & 1.0.40^{-19} \mathrm{cm}^3 \\ 10^{-38} \mathrm{cm}^3 & 4.10^{-36} \mathrm{cm}^3 & 2.8.40^{-19} \mathrm{cm}^3 \end{array}$	
	M	038+	
Δ <i>E</i>	$\begin{array}{c} 1s^{2}2s \mid S \rightarrow 1s^{2}2p \mid P_{3/2} \\ 7.881 a.u. = 214.44 eV \end{array}$	$\begin{array}{c} 1s^{2}2s \mid S \rightarrow 1s^{2}2p \mid P_{1/2} \\ 3.276 a.u. = 89.14 \text{ eV} \end{array}$	
	0,056	0,011	
E, keV Qe Qp	$ \begin{smallmatrix} 0.5 & 1 & 2 \\ 1.4 \cdot 10^{-19} \text{ cm}^3 8.1 \cdot 10^{-39} \text{ cm}^3 4.7 \cdot 10^{-39} \text{ cm}^3 \\ 0 & 0 & 10^{-36} \text{ cm}^3 \end{smallmatrix} $	$ \begin{array}{c} 0,5 & 1 & 2 \\ 10,5 \cdot 10^{-20} \text{ cm}^3 & 4.4 \cdot 10^{-50} \text{ cm}^3 & 2.7 \cdot 10^{-20} \text{ cm}^3 \\ 0 & 0 & 1.2 \cdot 10^{-85} \text{ cm}^3 \end{array} $	

 2Recently measured values of Fe $^{23+}$ oscillator strengths coincide with those shown in Table II. 64

and the CB method for an interval $Z = \infty$.⁶⁶ Berrington and coworkers studied resonances in the collision forces for C²⁺ and O⁴⁺ ions.⁶⁷ Nakazaki and Hashino analyzed the roles of various approximations for the wave functions of ions' bound electrons within the framework of the CB method.

Some difficulty for the numerical calculations of cross sections of transitions under consideration is presented by the fact that the many moments of an incident electron contribute in this case. Osterbrock's work⁶⁵ shows the principal cross sections for excitation of the $2s2p|^{1,3}P$ states of the C^{2*} and O^{4*} ions in the near-threshold energy region. In the excitation of an inter-combined transition to the ${}^{3}P$ state, only 3-4 moments are substantial, while the excitation of a dipole-allowed transition to ${}^{1}P$ involves 10 moments.

Cross sections calculated by means of Eq. (8) are compared in Fig. 9 with the parameters f and ΔE taken from spectroscopic data,⁴⁶ and those calculated by the strong coupling method for C²⁺, N³⁺, O⁴⁺ and Ne⁶⁺ by Osterbeck⁸⁵ and Nakazaki and Hashino.⁶⁸

The spectroscopic data^{46,63} may be approximated by the following relationships:

$$f_{2s^{2} \to 2s^{2}p|'P} (Be) = \frac{3.30}{Z} + \frac{5.60}{Z^{2}}, \qquad (49)$$

$$\Delta E_{2s^2 \to 2s2pl'P} \text{(Be)} = 0.132Z - 0.350.$$
(50)

c. Sodium-like ions $\{Na\}$, $3s \rightarrow 3p$ transition

The approximation relationships of tabulated data⁴⁶ for the oscillator strengths and transition energies are

$$f_{3s-3p}(Ns) = \frac{8.44}{Z} - \frac{28.8}{Z^3},$$
 (51)

$$\Delta E_{38 \to 3p} \{ Na \} = 0.076Z - 0.732.$$
 (52)

Blaha and Davis⁶⁹ used the method of perturbed waves without exchange to calculate collision strengths of the 3s - 3p, 3d, 4s, 4p, 4d, and 4f transitions for the CaX, FeXVI, KrXXVI, and MoXXXII ions. The same authors give excitation energies and oscillator strengths of the



FIG. 9. Electron excitation cross sections of beryllium-like ions as a function $x = E/\Delta E$. C—calculation by strong coupling method; ⁶⁵ \square —CB method; ⁶⁸ \times —Eq. (8) with parameters fand ΔE equal to:⁴⁶ (a) f = 0.81, $\Delta E = 0.466$; (b) $f = 0.64 \Delta E$ = 0.595; (c) f = 0.53, $\Delta E = 0.723$; (d) f = 0.57, $\Delta E = 0.979$.

foregoing transitions of these ions. We shall compare the excitation cross sections of the $3S \rightarrow 3P_{1/2}$, $3P_{3/2}$ transitions of the MoXXXII ion $(3S \rightarrow 3P_{1/2}: \Delta E = 2.57)$ a.u., f = 0.073; $3S \rightarrow 3P_{3/2}$: $\Delta E = 3.53$ a.u., f = 0.201), given by Eq. (8), with those obtained by Blaha and Davis.⁶⁹ Using Eq. (8) we get the following: x = 1:Q $(3S \rightarrow 3P_{1/2}) = 3.5 \times 10^{-16} \text{ cm}^2$, $Q(3S \rightarrow 3P_{3/2}) = 5.0 \times 10^{-18}$ cm²; $X = 16: Q(3S \rightarrow 3P_{1/2}) = 3.9 \times 10^{-19} \text{ cm}^2; Q(3S \rightarrow 3P_{3/2})$ $=5.8 \times 10^{-19}$ cm². The corresponding cross sections are⁶⁹: x = 1: $Q_{1/2} = 3.5 \times 10^{-18} \text{ cm}^2$; $Q_{3/2} = 4.5 \times 10^{-18} \text{ cm}^2$; x = 16: $Q_{1/2} = 2.9 \times 10^{-19} \text{ cm}^2$, $Q_{3/2} = 4.1 \times 10^{-19} \text{ cm}^2$.

Evidently, machine-calculated cross sections are also somewhat smaller here (clearly, for the same reason as also for the $\{Li\}$ ions) than those calculated from Eq. (8).

d. Helium-like (He) ions, $2'S \rightarrow 2'P$, $2^3S \rightarrow 2^3P$ transitions

The tabulated values of oscillator strengths and energy differences⁴⁶ are approximated by the following relationships:

2'S
$$\rightarrow$$
 2'P:
$$\begin{cases} f = \frac{0.50}{Z} + \frac{0.33}{Z^2} \\ \Delta E = 0.028Z - 0.040, \end{cases}$$
 (53)

$$2 \,{}^{3}S \rightarrow 2 \,{}^{3}P: \begin{cases} f = \frac{0.67}{Z} + \frac{0.69}{Z^{2}}, \\ \Delta E = 0.036Z - 0.009, \end{cases}$$
(54)

which may be used to calculate cross sections for Eq. (8).

In addition to dipole transitions there exists a large number of non-dipole transitions with $\Delta n = 0$ for which $\Delta E \ll Z_2^2$. The electron excitation cross sections of these, as shown in the analysis, can be calculated by neither multipole expansion of interelectron interaction

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nor classical description of the incident electron. In this case, quantum calculations by means of the Coulomb-Born method with exchange are required.

-a - **b**

The excitation reaction rates $K = \langle vQ \rangle$, which are determined by the cross section [Eq. (8)] can be obtained by averaging the product vQ with respect to Maxwell's electron energy distribution function. Since $F(\nu)$ is a slowly varying electron energy function E, K may be calculated by means of a method proposed earlier.⁷⁰ We then get

$$K_{e} = \frac{\sqrt{2} \pi^{5/2} f_{on}}{(2l_{o}+1) \Delta E \sqrt{T}} e^{-\Delta E/T} F(\tilde{\mathbf{v}}), \qquad (55)$$
$$\tilde{\mathbf{v}} = \frac{Z_{p} \Delta E}{(2L_{o}+1) (2L_{o}+1) (2$$

$$f = \frac{Z_{9}\Delta E}{[2(\Delta E + 1.78T)]^{3/4}}.$$
 (56)

Representation of the reaction rate in this form is convenient because to calculate it and also the cross section one can use the function $F(\nu)$ which is shown as an approximation formula [Eq. (46)].

We shall compare excitation rates of the $2s \rightarrow 2p$ transition of a lithium-like argon ion Ar^{15+} ($\Delta E = 1.15$ a.u.; f=0.082), given by Eq. (55), with those obtained by Vainshtein and coworkers.² At three temperatures: $T = \Delta E/2 = 0.575$; $T = \Delta E = 1.15$; $T = 3\Delta E = 3.45$, Eq. (55) yields K=1.6, 3.3 and 4.2×10^{-9} cm³/s, respectively. The corresponding values obtained by Vainshtein² are 1.5, 2.5 and $3.2 \times 10^{-19} \text{ cm}^3/\text{s}$.

5. EXCITATION OF TRANSITIONS WITH $\Delta n \neq 0$

a. Helium-like ions

We shall now direct our attention to transition cross sections with a variable principal quantum number, which require an excitation energy $\sim Z_2^2$.

The excitation cross sections of the 2^1 , 3S and 2^1 , 3P states of helium-like Li^{*}, Be^{2*}, B^{3*}, C^{4*}, N^{5*}, O^{6*}, Fe^{7*}, Ne^{8*}, Si^{12*}, Ca^{18*} and Fe^{24*} ions from the ground state 'S were calculated as a nonrelativistic approximation by a method of distorted waves with exchange,⁷¹ and also by the CB method. The excitation cross sections of the 2'S ind 2'P states of ions with $3 \le Z \le 10$ and Si¹²⁺, Ca¹⁸⁺ d Fe²⁴⁺ were calculated by a method of perturbed waves with polarized orbitals, taking exchange into account also as a nonrelativistic approximation.²⁶ The excitation cross sections of the n'S and n'P states (n=2-6) were calculated by the CB method without exchange by Tully.⁷² The CBE method was used also to calculate excitation cross sections of heliumlike ions.73,74

In view of the correctness of the perturbation theory the most consistent method for calculating cross sections is the CBE method with hydrogen-like functions. Such calculations were made by Burgess and cowork ers^{75} ($1S \rightarrow 2^{3}P$, $1'S \rightarrow 2^{3}S$, $Z = \infty$) and Sampson and coworkers⁷⁶ (1'S $\rightarrow n'$, 3S, P, D; 2', ${}^{3}S \rightarrow n^{1}$, ${}^{3}S$, P, D, n = 2 - 5).

Figure 10 shows normalized cross sections Z^4Q of the 2^1 , 3S and 2^1 , 3P states excited from the ground 1'S state by electron shock and calculated by different methods. Clearly, results obtained by different meth-

1



FIG. 10. Normalized electron excitation cross sections Z^4Q of helium-like ion states. Calculation by distorted wave method with exchange⁷¹: $a - Li^*$; $2 - Be^{2^*}$; $3 - B^{2^*}$; $4 - C^{4^*}$; $5 - N^{5^*}$; $6 - 0^{6^*}$; $7 - F^{7^*}$; $8 - Ne^{8^*}$; $9 - Si^{12^*}$; $10 - Ca^{18^*}$; $11 - Fe^{24^*}$. Calculation by CBE method with hydrogen-like functions: -9 - -Ref. 75; -9 - -Ref. 76; -9 - - approximating relations: (a) $1.7/x^2$ +5.35 ln x/x) 10⁻¹⁶ cm²; (b) (5+2.55 ln x) $x^{-1} \cdot 10^{17}$ cm²; (c) 1.8 $x^{-1} \cdot 10^{-16}$ cm²; (d) (8.2/x³) - (5.2/x⁴) 10⁻¹⁷ cm².

ods are in satisfactory agreement with each other. An exception to this is the excitation cross section of the $2^{3}P$ state obtained by Sampson and coworkers⁷⁶ which clearly constitutes a numerical error. The coherence of results obtained by different methods is attributed to the applicability of perturbation theory. It is evident from Fig. 10 that as the ion charge increases the results obtained by Bhatia and Temkin⁷¹ tend to converge on the curves obtained with hydrogen-like functions. 75,76

Figure 11 shows twice-normalized excitation cross sections $n^{3}Z^{4}Q$ of higher levels (n=3, 4, 5) from the ground state 1'S, calculated by the CBE method with hydrogen-like functions.⁷⁶ A relatively good convergence is seen between these cross sections with increasing n and the universal functions of x which we approximate by the following relationships (Z is element number):

{He}

$$n^{3}Z^{4}Q(1's \rightarrow n'S) = \left(\frac{3.38}{x} - \frac{1.53}{x^{3}}\right) \cdot 10^{-16} \,\mathrm{cm}^{2},$$
 (57)

$$n^{3}Z^{4}Q(1s \rightarrow n^{3}S) = \left(\frac{2.82}{x^{4}} - \frac{1.32}{x^{4}}\right) \cdot 10^{-i8} \,\mathrm{cm}^{2} \,, \qquad (58)$$

$$n^{3}Z^{4}Q(1's \rightarrow n'P) = \left(\frac{13.7 \ln x}{x} + \frac{5.0}{x^{4}}\right) \cdot 10^{-16} \text{ cm}^{2}, \quad (59)$$

$$n^{3}Z^{4}Q(1's \rightarrow n^{3}P) = \frac{3.40 + 2.16 \ln x}{x} \cdot 10^{-16} \text{ cm}^{2},$$
 (60)

$$n^{3}Z^{4}Q(1'S \rightarrow n'D) = \frac{-6.30 + 5.6 \ln x}{x} \cdot 10^{-17} \text{ cm}^{2},$$
 (61)

$$n^{3}Z^{4}Q(1's \rightarrow n^{3}D) = \left(\frac{6.6}{x} + \frac{0.4}{x^{3}}\right) \cdot 10^{-17} \text{ cm}^{2}.$$
 (62)

The above expressions may be used to calculate excitation cross sections of levels with any $n \ge 3$ for any ion $Z_2 \ge 4$; they hold in the region $1 \le x \le 10$.

Figure 12 also shows twice-normalized excitation

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FIG. 11. Twice normalized excitation cross sections $n^{3}Z^{4}Q$ of states n^1 , ${}^{3}S$, n^1 , ${}^{3}P$, n^1 , ${}^{3}D$ (n = 3, 4, 5), from ground state of helium-like ions by electron shock, calculated by CBE method with hydrogen-like functions.⁷⁶ $\bigcirc -n = 2; \bullet -n = 3; \times -n = 4;$ +-n = 5; — approximating relations, Eqs. (57)-69).



FIG. 12. Twice normalized excitation cross sections n^3Z^4Q of states n^1 , 3S , P, D (n = 3, 4, 5) from 2^3S metastable state of helium-like ions by electron shock, calculated by CBE method.⁶⁷ $\bullet -n = 3$; $\times -n = 4$; + -n = 5; - -approximating relations, Eqs. (63)-(68).

cross sections $n^3 Z^4 Q$ (n=3, 4, 5) of states from the metastable state $2^3 S$, calculated by the same authors and method.⁷⁶ The approximating relationships of these cross sections are as follows:

{He}

$$n^{3}Z^{4}Q(2^{3}s \rightarrow n^{4}S) = \frac{10^{-15} \text{ cm}^{2}}{2},$$
 (63)

$$n^{3}Z^{4}Q(2^{3}s \rightarrow n^{3}S) = \frac{1.7 \cdot 10^{-14} \,\mathrm{cm}^{2}}{7},$$
 (64)

$$n^{3}Z^{4}Q(2^{3}s \rightarrow n'P) = \frac{3.6 \cdot 10^{-15} \text{ cm}^{2}}{x},$$
 (65)

$$n^{3}Z^{4}Q(2^{3}s \rightarrow n^{3}P) = \frac{5.5 + 6.7 \ln z}{\tau} \cdot 10^{-15} \text{ cm}^{2},$$
 (66)

$$n^{3}Z^{4}Q (2^{3}s \rightarrow n'D) = \left(\frac{9.0}{x^{2}} - \frac{2.0}{x^{3}}\right) \cdot 10^{-15} \text{ cm}^{2},$$
 (67)

$$n^{3}Z^{4}Q (2^{3}s \rightarrow n^{3}D) = \left(\frac{16.5}{x^{3}} - \frac{9.0}{x^{3}}\right) \cdot 10^{-15} \text{ cm}^{2}.$$
 (68)

The analysis of excitation of hydrogen-like ions has shown that the effect of exchange on cross section values was weak. The position is different for heliumlike ions: excitation of intercombinational transitions with a change in the spin—is impossible without exchange of an incident electron with a bound electron. However, exchange shows up substantially exerted in the values of excitation cross sections of transitions without spin changes. Excitation cross sections of helium-like C^{4+} , N^{5+} , O^{6+} and Ne^{8+} ions from the ground state to 2'P and 3'P, calculated by Nakazaki by means of the CB method without exchange,⁷⁷ are ~2 times greater near the threshold than same values calculated with allowance for the exchange.

We shall now give the excitation rates for helium-like ions scattered by electrons K, which are averaged with respect to Maxwell's electron velocity distribution function with temperature T. If we integrate the approximating cross sections of the function (see, Fig. 10), we get

{He}

$$K(1's \to 2'P) = 2 \sqrt{\frac{2\Delta E}{\pi Z^3}} \frac{\sqrt{\alpha}}{Z^3} (6.07\alpha + 19.1) I(\alpha),$$
(69)

$$K(\mathbf{1's} \rightarrow \mathbf{2'S}) = 2 \sqrt{\frac{2\Delta E}{\pi Z^3}} \frac{\sqrt{\alpha}}{Z^3} (0.91\alpha + 1.80) l(\alpha), \qquad (70)$$

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$$K (1'S \rightarrow 2^{3}P) = 12.9 \sqrt{\frac{2\Delta E}{\pi Z^{4}}} \frac{\alpha^{3/2}}{Z^{3}} (e^{-\alpha} - \alpha I (\alpha)),$$
(71)

$$K (1'S \rightarrow 2^{3}S) = 2 \sqrt{\frac{2\Delta E}{\pi Z^{4}}} \frac{\alpha^{3/2}}{Z^{3}} [(2 + 0.93\alpha) e^{-\alpha} - \alpha (2.93 + 0.93\alpha) I (\alpha)],$$

$$=\frac{\Delta E}{T}$$

The integral exponential function $I(\alpha)$ was determined in Eq. (42).

α

The excitation rates of high states, whose cross sections are given by Eqs. (57)-(62), are:

{He}

$$K (1'S \rightarrow n'S) = 2 \sqrt{\frac{2\Delta E}{\pi Z^4}} \frac{\sqrt{\alpha}}{n^3 Z^3} (12.1e^{-\alpha} - 5.46\alpha I(\alpha)),$$
(73)

$$K(1'S \rightarrow n^{3}S) = 2 \sqrt{\frac{2\Delta E}{\pi Z^{2}}} \frac{\alpha^{3/2}}{n^{3}Z^{3}} [(7.75 + 2.35\alpha) e^{-\alpha} - \alpha (10.1 + 2.35\alpha) I(\alpha)]$$
(74)

$$K (\mathbf{1'S} \rightarrow n'\mathbf{P}) = 2 \sqrt{\frac{\overline{2\Delta E}}{\pi Z^2}} \frac{\sqrt{\alpha}}{n^3 Z^3} (17.9\alpha + 48.9) I(\alpha), \tag{75}$$

$$K\left(\mathbf{1'S} \rightarrow n^{\mathbf{3}}\mathbf{P}\right) = 2\sqrt{\frac{2\Delta E}{\pi Z^{\mathbf{2}}}} \frac{\sqrt{\alpha}}{n^{3}Z^{\mathbf{3}}}\left(\mathbf{12.1}e^{-\alpha} + 7.71I\left(\alpha\right)\right),\tag{76}$$

$$K(\mathbf{1}'\mathbf{S} \rightarrow \mathbf{n}'\mathbf{D}) = 2 \sqrt{\frac{2\Delta E}{\pi Z^2}} \frac{\gamma \alpha}{n^3 Z^3} (2.25e^{-\alpha} + 2I(\alpha)), \tag{77}$$

$$K\left(\mathbf{1}^{\prime}\mathbf{S} \rightarrow n^{3}\mathbf{D}\right) = 2\sqrt{\frac{2\Delta E}{\pi Z^{3}}}\frac{\sqrt{\alpha}}{n^{3}Z^{3}}\left(2.36e^{-\alpha} + 0.14\alpha I\left(\alpha\right)\right).$$
(78)

The rates of transitions from the excited 2^3 S state, whose cross sections are given by Eqs. (63)-(68), are: (He)

$$K(2^{3}S \rightarrow n'S) = 2 \sqrt{\frac{2\Delta E}{\pi Z^{3}}} \sqrt{\frac{2}{n^{3}Z^{3}}} 35.7e^{-\alpha},$$
(79)

$$K(2^{3}S \rightarrow n^{3}S) = 2 \sqrt{\frac{2\Delta E}{\pi Z^{2}}} \frac{\sqrt{\alpha}}{n^{3}Z^{3}} 607e^{-\alpha}, \qquad (80)$$

$$K (2^{3}S \rightarrow n'P) = 2 \sqrt{\frac{2\Delta E}{\pi Z^{2}}} \frac{\sqrt{\alpha}}{n^{3}Z^{3}} 129 e^{-\alpha}, \qquad (81)$$

$$K(2^{3}S \to n^{3}P) = 2 \sqrt{\frac{2\Delta E}{\pi Z^{3}}} \frac{\sqrt{\alpha}}{n^{3}Z^{3}} (196 \ e^{-\alpha} + 239I(\alpha)), \tag{82}$$

$$K(2^{3}S \rightarrow n'D) = 2 \bigvee \frac{2\Delta E}{\sqrt{\pi^{2}}} \frac{\sqrt{\alpha}}{n^{3}Z^{3}} [-71\alpha e^{-\alpha} + (321\alpha + 71\alpha^{2})I(\alpha)], \quad (83)$$

$$K\left(2^{3}S \rightarrow n^{3}D\right) = 2 \sqrt{\frac{2\Delta L}{\pi Z^{3}}} \frac{\nu^{\alpha}}{n^{3}Z^{3}} \left[-321\alpha e^{-\alpha} + (321\alpha + 589\alpha^{2}) I(\alpha)\right].$$
(84)

We now compare the existing results of the experimental measurements of aggregate rates of excitation of the $1'S \rightarrow (2'P + 2'S)$, $1'S \rightarrow (2^3P \rightarrow 2^3S)$ transitions of the O^{6+} ion.⁷⁸ These were carried out at an electron temperature of 250 eV and speed given by Eqs. (69)-(72), and using Vainshtein's calculations.² The experimental values are $K_{2'S+2'P} = 3.1 \times 10^{-11} \text{ cm}^3/\text{s}$, $K_{2\ S+2\ P}^{3}$ = $1.5 \times 10^{-11} \text{ cm}^3/\text{s}$. The experimental error, according to the authors,⁷⁸ was 100%. Equations (69)–(72) yield the following values (T = 250 eV): $K_{2'S+2'P} = 2.1$ $\times 10^{-11} \text{ cm}^3/\text{s}, K_2^{3}_{s+2}^{3}_{P} = 0.67 \times 10^{-11} \text{ cm}^3/\text{s}.$ Data tabulated in Vainshtein's work are²: $K_{2'S+2'P} = 3.8 \times 10^{-11}$ cm³/s, $K_{2^3S+2^3P} = 2.2 \times 10^{-11}$ cm³/s. The results of theoretical sources, while at variance with each other, generally agree with the experiment within experimental error. At T = 250 eV, which is 2.2 times ($\alpha = 2.2$) smaller than transferred energy ΔE , the basic contribution to K comes from near-threshold values of cross sections. The latter, shown in Fig. 10 and when calculated,² are sufficiently close to each other.

b. Lithium-like ions

The cross sections of the 2s - np (n = 2-7) transitions

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of the Be⁺, N⁴⁺ and Ne⁷⁺ ions were calculated by Bely using the CB method without exchange.⁵⁴ Gan and Henrv used the strong coupling method with exchange of the $1s^22s$, $1s^22p$, $1s^23s$, $1s^23p$, $1s^23d$ states for calculating excitation cross sections of the $2s \rightarrow 2p$, 3s, 3p, 3d, $2p \rightarrow 3s$, 3d, 3p transitions of the C³⁺ and Ar¹⁵⁺ ions.⁵⁸ In both calculations use was made of the Hartree-Fock wave functions. The $1s^2$ core electrons were considered to be "frozen," i.e., their wave functions remained unchanged in the course of transitions of the 2s orbital electron. Figure 13 shows normalized excitation cross sections Z^4Q of the $2s \rightarrow 3p$ transitions of certain ions. Clearly, although exchange varies the nature of the energy dependence of cross sections near the threshold, such a change is numerically small. An exception to this is the C^{3+} ion for which the perturbation theory remains unfeasible. It can be seen from Fig. 13 that the cross section Z^4Q of this transition is well represented by the approximating function. The spectroscopic values of excitation energy ΔE of the $2s \rightarrow 3p$ transition may be approximated by the following expression

{Li},
$$\Delta E (2s \rightarrow 3p) = 0.069Z^2$$

-0.175Z + 0.024. (85)

The rate constant of this transition is:

$$K_{2s \rightarrow 3p}^{\text{(Li)}} = 2 \sqrt{\frac{2\Delta E}{\pi Z^3}} \frac{\sqrt{\alpha}}{Z^s} (185 + 98\alpha) I(\alpha).$$
(86)

The twice-normalized excitation cross sections in n^3Z^4Q of the $2s \rightarrow np$ transitions, calculated by Bely using the CB method without exchange,⁵⁴ for the N⁴⁺ and Ne⁷⁺ ions are well approximated by the function $(4.0/x^2 + 6.6 \ln x/x) \times 10^{-15} \text{ cm}^2$; this yields the following rate constant for these processes:

$$K_{2s-np}^{\text{[L1]}} = 2 \sqrt{\frac{2\Delta E}{\pi Z^3}} \frac{\sqrt{\alpha}}{\pi^3 Z^3} (2.4 \cdot 10^3 + 1.4 \cdot 10^3 \alpha) I(\alpha).$$
(87)

Using the results of calculations by means of the strong coupling method with exchange⁵⁸ for the Ar^{15+} ion, we get the following approximating functions for rate constants:

{Li}

$$2s \rightarrow 3s: \quad K = \sqrt{\frac{2\pi}{\Delta E}} \frac{\sqrt{\alpha}}{2Z^4} e^{-\alpha} \left(9.6 + \frac{0.7}{\alpha}\right), \quad (88)$$

$$2s \rightarrow 3 d: \quad K = \sqrt{\frac{2\pi}{\Delta E}} \frac{\sqrt{\alpha}}{2Z^2} e^{-\alpha} \left(19.0 + \frac{3.5}{\alpha}\right), \quad (89)$$

$$2\mathbf{p} \to 3\mathbf{s}; \quad K = \sqrt{\frac{2\pi}{\Delta E} \frac{V \,\alpha}{6Z^4} (2.2e^{-\alpha} + \alpha I(\alpha))}, \quad (90)$$



FIG. 13. Normalized excitation cross sections Z^4Q (2s \rightarrow 3p) of the 2s \rightarrow 3p transition of lithium-like ions by electron shock. CB method without exchange⁵⁴: $1-\text{Ne}^{7*}$; $2-\text{N}^{4*}$. Strong coupling method. 2s, 2p, 3s, 3p states with exchange⁵⁸: $3-\text{Ar}^{15*}$; $4-\text{C}^{3*}$; 5-approximating relation (2.7 $x^{-1}\ln x$) 10^{-15} cm².

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$$\mathbf{p} \to 3\mathbf{p}$$
: $K = \sqrt{\frac{2\pi}{\Delta E}} \frac{\sqrt{\alpha}}{6Z^3} (22e^{-\alpha} + 2.5 \alpha I(\alpha)),$ (91)

$$2p \rightarrow 3d$$
: $K = \sqrt{\frac{2\pi}{\Delta E}} \frac{\sqrt{\alpha}}{6Z^3} (91e^{-\alpha} + 68\alpha I(\alpha)).$ (92)

These functions hold in the $1 \le x \le 5-10$ and $0.2 \le \alpha \le \infty$ regions.

The strong coupling method was used to calculate the contribution of the resonance excitation processes to the cross section for the $2s \rightarrow 3s$, $2p \rightarrow 3s$ transitions of lithium-like oxygen $O^{5^*,3}$ The resonance scattering in a narrow energy region tends to increase the cross section substantially, although its contribution to the constant K is small.

c. Beryllium-like ions

2

The $2s^{2} {}^{1}S' \rightarrow 2s2p^{3}P$ intercombination transition cross section with a small excitation energy

$$\Delta E = 0.068Z - 0.170 \tag{93}$$

was calculated by Osterbrock for the B^{*}, C^{2*}, N^{3*}, O^{4*} and Ne^{6*} ions using the strong coupling method.⁶⁵ Contribution of the $2s2p^{1}P$, *nl* resonance configurations was taken into consideration when averaging with respect to *nl* by means of the Gailitis formula.⁷⁹ The collision forces for the excitation of this transition of the C²⁺ and O⁴⁺ ions also are shown graphically elsewhere.⁶⁷

The rate constant for the cross section of this transition was obtained by the authors by means of the following approximating function of cross section Z^4Q :

$$K (2s^{2/4}S' \to 2s^{2}p/^{3}P) = 2 \sqrt{\frac{2\Delta E}{\pi Z^{4}}} \frac{\sqrt{\alpha}}{Z^{3}} [2.7 \cdot 10^{3}e^{-\alpha} + 1.25 \cdot 10^{3}\alpha I (\alpha)].$$
(94)

The oscillator strength of the $2s2p|^{3}P \rightarrow 2s^{2}|^{1}S'$ radiative transition increases with increasing Z and, in the case of the P^{11*} ion, is 1.1×10^{-4} .

The collision forces for transitions with a change in the principal quantum number of beryllium-like ions from the ground $2s^2$ state and $2s2p^1$, 3p states were calculated by Parks and Sampson⁸⁰ who used the CBE method and hydrogen-like single-electron functions. The $Z = \infty$ interval was considered. Displacement of the initial and final state configurations was taken into consideration, which was due to relativistic effects. The results are shown for two values of energy in threshold units: x = 1 and 1.5.

6. IONIZATION OF MULTICHARGED IONS

Ionization of multicharged ions has been studied more thoroughly than excitation. Donets and coworkers, using ion-trap method have observed ionization of atoms to very high multiples; in fact, they observed Xe^{37*} ions.³⁶⁻³⁶ Data from observation of ion spectrum evolution in a trap, obtained by means of solving a system of ionization balance equations, have yielded ionization cross sections of ions of all multiples for nitrogen, oxygen and argon atoms. These cross sections are shown in Fig. 14 alongside results of calculations



FIG. 14. Ionization cross sections of nitrogen (a) oxgyen (b), and argon (c) ions. Φ -experiment; ³⁸ - - -Salpo's calculations by binary classical method; ⁸¹ Coulomb-Born approximation: ⁸² \blacktriangle -N³⁺; \blacksquare -N⁴⁺.

by means of pair collision method involving an incident and bound electrons in a classical treatment (a modified Grizinskiy method).⁸¹ In Salop's work,⁸¹ calculations were made for all ions of C, N, O. Ne and Ar atoms. Figure 13a also shows the ionization cross sections of N³⁺ and N⁴⁺ ions calculated by Moores as a Coulomb-Born approximation without exchange. The results of this calculation are in a satisfactory agreement with Salop's results.⁸¹

The latter's calculations take also into account ionization from the $2p^6$ shell in the course of ionization of argon ions with a small number of electrons in a shell with the principal quantum number n=3. This noticeable increased the cross section. Vainshtein's book provides numerical values of ionization rates all the way to neon-like ions.²

A comparison of data given in Fig. 14 shows that the theoretical cross section follows the power law Z^{-4} well, while the experimental does not follow it so well. The ionization coefficients $K_{1,\infty}$ of certain nitrogen, oxygen and neon ions in a theta-pinch plasma were measured.^{83,84} Luminescence of these ions was measured which yielded information concerning their concentration. Ionization coefficient of lithium-like oxygen was the same: $K_{1,\infty}$ (T = 128 eV) = 2.2×10⁻⁹ cm³/s; K_i (T = 119 eV) = 2.6×10⁻⁹ cm³/s. Estimating the ionization cross section by means of a relation Q = K/v we get—using these rates—the following values: $Q_{1,\infty}$ (128 eV) = 3.2×10⁻¹⁸ cm². These values are 2–3-fold higher than Salop's cross sections

(see Fig. 14b).⁸¹ Extrapolation of the measured cross sections³⁸ in a small energy region (120 eV) (see Fig. 14b) yields good qualitative agreement with aforementioned experimental values.

Rudge and Schwartz calculated ionization cross sections of Fe XV and Fe XVI ions using the CB and CBE methods.⁸⁵

Their calculations (see Ref. 49) were repeated by Golden and coworkers using hydrogen-like functions by means of the CBO method.⁸⁶ The results were found to be in a good agreement.

The resultant cross sections^{85,86} are well described by Lotz's empirical formula⁸⁷

$$Q_{10n}^{nl} = \frac{4.5 \cdot 10^{-14} \text{cm}^2}{(I_{nl})^2} N_{nl} \frac{\ln X_{nl}}{X_{nl}}, \qquad (95)$$

where I_{nl} is the ionization potential (in eV) of the nl shell, from which an electron is removed, N_{nl} is the number of equivalent electrons in the *n* shell, $X_{nl} = E/I_{nl}$.

A comparison of Lotz's formula [Eq. (95)] with the Donets-Ovsyannikov experiments results (see Fig. 14c)³⁶ goes as follows. At 2-keV energies of the Ar⁸⁺(I = 423eV), Ar⁹⁺(I = 479 eV), Ar¹⁰⁺(I = 539 eV) and Ar¹¹⁺(I = 618eV) ions, experimental cross sections are 7.0; 5.3; 4.0; 2.7; ×10⁻¹⁹ cm², respectively. However, Eq. (95) for ionization from only the outer shell yields the following values: 4.9; 3.3; 2.2; 1.3×10^{-19} cm². The increasing divergence as the number of ionized electrons decreases may be reduced if ionization of the $2s^2$ electrons is taken into consideration [also from Eq. (95)].

In the case of ionization (see Fig. 14b) of the $O^{6+}(I = 739 \text{ eV})$ and $O^{7+}(I = 871 \text{ eV})$ ions, experimental cross sections at E = 2 keV are 7.4 and $3.1 \times 10^{-20} \text{ cm}^2$, respectively. Equation (95), however, yields 5.9 and $2.1 \times 10^{-20} \text{ cm}^2$. Thus, in all aforementioned cases, Lotz's empirical formula yields ~30% divergence.

To calculate the contributions of the inner electrons of complex ions to the total cross section of direct ionization, results of Moores' work⁹¹ may be used, whereby the CBE method is used to calculate ionization cross sections of the 1s, 2s, 2p, 3s, 3p and 3d shells. These calculations were carried out with hydrogen-like wave functions in the energy region 1.125 $\leq x_{nl} \leq 6.0$ in threshold units.

When calculating ionization cross sections of positive ions, contribution of excitation of autoionization states of the same ion must be taken into account. The autoionization states of a system ion + incident electron, discussed in Sec. 1c, cannot contribute to ionization. In this case, different autoionization states are involved, which form when an incident electron excites orbital electrons to free discrete excited levels. These states are states of the initial ion without an incident electron present. The autoionization decay of these leads to formation of the next higher multiple ion, i.e., to ionization. The significant difference between this process and the process of excitation via the autoionization state stage is the fact that the cross section for the formation of an intermediate state is not resonant in nature

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but, instead, is comparable to the excitation cross section of an inner electron. Consequently, the contribution of this excitation to ionization may be greater than that of direct ionization of all ion shells.

A particularly important role, for ions with a small number of outer electrons, is played by excitation of inner electrons. Bely's estimates for sodium-like $Fe^{15+}(1s^2, 2s^22p^33s)$, Ca^{9^+} , P^{4^+} , Al^{2^+} and Mg^+ ions show that the cross section of ionization via the formation of autoionization states $1s^2 2s^2 2p^5 3s 3(s, p, d)$ and $1s^2 2s 2p^6 3s 3(s, p, d)$ of an iron atom ion is approximately 10 fold greater than direct ionization cross section of the 3s electron.⁹² In this work, however, radiative stabilization of autoionization states, which competes with autoionization decay, was not taken into consideration. In Hahn's calculations,⁹³ radiative stabilization was included in the form of an approximation formula for emission probability, although its accuracy has not been validated. A more detailed analysis of the process of ionization via excitation of inner electrons for the Fe¹⁵⁺ and Mo¹³⁺ ions was carried out by Cowan and Mann.⁹⁴ However, rates of direct ionization and excitation of inner electrons were calculated from empirical formulas whose accuracy is unknown.

In the experimental work by Crandall and coworkers a method of crossed ion and electron beams was used to measure the ionization cross sections of lithiumlike ions C^{3+} , N^{4+} , and O^{5+} in the energy region from threshold to 15 keV.95 In addition to the principal maximum, a second maximum was observed at large energies in the function which relates ionization cross section and ionizing electron speed. Its value increased from C^{3+} to O^{5+} ions. The occurrence of a second maximum was explained by excitation of autoionization states $1s2s^2/2S$, 1s2s2p/4P, and 2P . Henry⁹⁶ used the method of strong coupling of six states to calculate excitation cross section of autoionization states observed in the experiment. The calculated and measured cross sections are in a good agreement with each other. Moores' calculations, which allow for only the direct ionization from the $1s^2$ and 2s shells, failed to reveal the second peak of ionization cross section of the C³⁺ and N⁴⁺ ions.

These first works unquestionably underscore the importance of the effect of excitation of inner electrons, although its quantitative contribution to ionization has not been established with sufficient reliability.

CONCLUSIONS

The foregoing comparison of calculations of excitation and ionization cross sections of multicharged ions by electrons, carried out by different methods, shows good agreement with results at $Z_2 \ge 5$. This pertains also to excitation of degenerate levels. Thus, evidence of the applicability of the perturbation theory considered in this review has been specifically confirmed numerically.

Although the CBE method may be used only numerically, it is much simpler than other numerical methods. We note that electron scattering by multicharged ions represents the second case in the physics of electron-atom collisions (despite the Born approximation), for which a theoretically well-founded method of calculating cross sections may be given.

An incident electron was shown to be a possible source for the excitation of dipole transitions with small transition energy ($\Delta E < Z_2^2$), considered as a classical particle, and to assume its interaction with a bound electron same as with a dipole. As a result of such consideration, a very simple analytical formula was obtained for the cross section, which holds in the interval from the threshold to the Born region, and whose accuracy is also determined by the reciprocal of the ion charge.

Investigation of the relativistic formulation of the problem of electron scattering by a positive ion shows that a matrix element of the Breit operator is sufficient for calculating the inelastic scattering amplitude. The numerical calculations of the excitation of hydrogenlike ions show that the relativistic effects for the excitation of transitions with a change in the principal quantum number become noticeable for ions with a charge $Z_2 \ge 50$. A different situation takes place for transitions without a change in the principal quantum number. Relativistic effects occurring during direct interaction between incident and bound electrons also play a small part. However, variation in the bound electron parameters (transition energy, oscillator strength), caused by relativistic effects becomes substantial for $Z \ge 20$. This, as is evident from Eqs. (8), (15), and (17), has a substantial effect on the value of cross section both near threshold and at large energies.

Electron scattering by positive ions differs by the rich resonant structure which is inherent in the dependence of cross sections on collision energy. These resonances depend on the formation of autoionization states of an ion-incident electron system. The value of cross section in a resonance is approximately Z_2^2 -fold greater than normal cross section.

Radiative losses of a plasma at G thermonuclear temperature consist not only of the emission of excited valence electrons. So-called satellite emission lines are also observed. They occur in the course of radiative transition from an autoionization state. Excitation cross sections of satellite transitions must be known to study the plasma. Evidence concerning such cross sections is only beginning to be seen at this time.

Upon collision with an ion, incident electron may excite inner electrons. In this case autoionization states are formed which leads to ionization of an ion. For ions with a small number of outer electrons, the cross section of such Auger-ionization may substantially exceed direct ionization cross section.

In this review we have examined relatively simple ions containing a small number of bound electrons. In the case of more complex ions the CBE approximation will experience an additional difficulty: the determination of the zero approximation wave functions. These functions must take into consideration interaction of the ion core with electrons.

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Translated by Y. Ksander

Edited by R. T. Beyer