

NATIONAL INSTITUTE FOR FUSION SCIENCE**LS-Averaged $1/Z$ Method as a Tool of Studying
the Interactions of Highly Charged Ions with
a Metal Surface**

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**LS-AVERAGED $1/Z$ METHOD AS A TOOL
OF STUDYING THE INTERACTIONS OF HIGHLY
CHARGED IONS WITH A METAL SURFACE**

Inga Yu. Tolstikhina

[Keywords: ion-surface interaction, $1/Z$ perturbation theory, LS-averaged transition energy, radiative probability, autoionizing width]

Abstract

In the present paper, a new theoretical approach is described for the calculation of the atomic characteristics of the multiply charged ions (MCI) in various electronic configurations. This theoretical approach is based on the perturbation theory using the nuclear charge of the ion as a parameter and the inter electron interaction and relativistic corrections as a perturbation. In order to reduce a large number of the calculations of atomic data for many different electron configurations which may be formed in MCI colliding with a surface, the transition energies, radiative transition probabilities and autoionizing rates are averaged over the orbital and spin quantum numbers. It turned out that these atomic characteristics can be expressed in analytical forms as a function of the number of electrons in different shells of the ions and the suggested method can be applied for the calculation of the atomic characteristics of practically any atomic system with arbitrary number of electrons.

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I. Introduction

At present much attention is being paid to experimental and theoretical studies of interactions of slow, highly charged ions with a surface. This attention is caused by the formation of a new physical object - so-called "hollow atom". The main feature of such a state of atom is a great number of vacancies in inner shells while the ionization degree of atom is low - almost neutral. With today's availability of powerful multicharged ion sources such as electron cyclotron resonance (ECR) sources, the electron-beam ion trap source (EBIS), and the electron-beam ion trap (EBIT), investigations on mechanisms of productions and decays of such "hollow atoms" near solid surfaces have become a subject of considerable interest. These investigations are mainly aimed at understanding the neutralization dynamics of highly charged ions as they approach the surface and penetrate into the solid. Such highly charged projectile ions carry very large potential energy up to several hundred keV and X-ray emission studies are particularly suited to illuminate different deexcitation and interaction processes which lead to the transfer of this energy to the surface. Furthermore, such new experiments allow the observation of surface modifications induced by a medium-to-heavy ion impact.

1. Formation of "hollow atom": Reviews of neutralization processes

The scenario so far developed for the interaction of a slow multicharged ion (MCI) with a metal surface has evolved from numerous experimental investigations of total electron yields, electron emission statistics and fast Auger electron energy distributions, together with the analysis of scattered projectiles and soft X-ray emission [1]. Up to now, it is best described in terms of so-called "classical over-barrier model", which has recently been developed by Burgdoerfer *et al.* [2,3]. The approach of a slow MCI (charge state q ; its velocity is much smaller than the Fermi velocity of electrons inside the metal target) towards the metal surface (characterized by a conduction band with the work function W_ϕ , and the Fermi energy E_F , see Fig.I.1.1) causes a collective response of the metal electrons which at a large distance from surface R can be described by the classical image potential (the atomic units are used through the present paper, unless otherwise noted)

$$V_{im}(R) = \frac{q^2}{4R}, \tag{I.1.1}$$

where q is the charge of projectile.

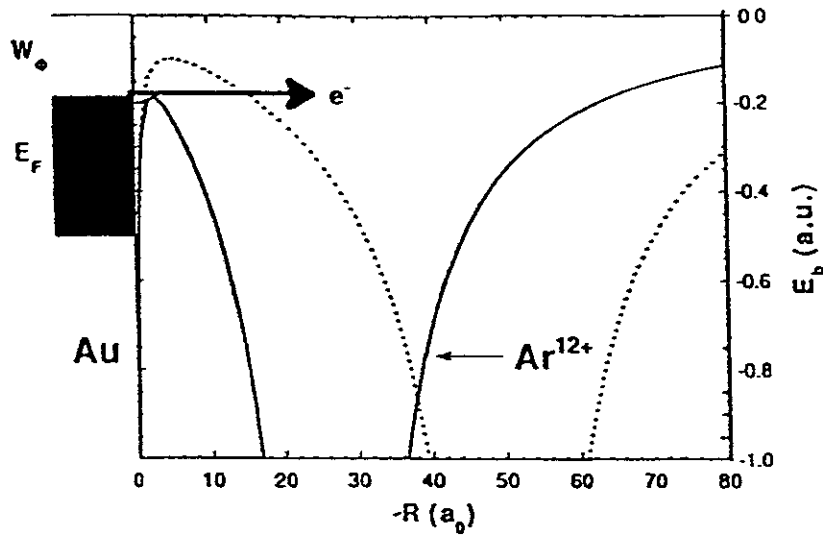


Fig.I.1.1. Electronic potential barrier between the MCI and the metal surface, exemplified for the cases of Ar^{12+} projectile ion at about 50 a.u. (dotted curve) and 26 a.u. (full curve), respectively, above an Au surface. In the second case, the potential barrier has decreased below the Fermi level of Au, and then the electron capture becomes classically permitted [1].

This image potential accelerates MCI towards the metal surface and therefore imposes the lower limit to the projectile impact velocity, corresponding to an upper limit for the available MCI-surface interaction time. In addition, the image interaction causes a shift of the projectile electronic states and decreases the height of electronic potential barrier between the ion and surface, which is formed by the projectile's potential, its image potential, and the image potential of the particular electron to be captured. At a critical distance

$$R_c(q) = \frac{1}{2W_\phi} \sqrt{8q+2} , \quad (\text{I.1.2})$$

(W_ϕ is the work function of metal), this potential barrier decreases below the Fermi level of the metal and the ion starts to capture electrons resonantly from the conduction band into highly excited states of projectiles (resonant neutralization - RN, see Fig.I.1.2). The electron capture can in principle occur at larger distances than RN via tunneling processes through the potential barrier but this has been found to be of minor importance.

The classical over-barrier model also predicts the principal quantum number of the highly excited states of projectiles in which the RN takes place:

$$n_c \leq \frac{q}{\sqrt{2W_\phi}} \left(1 + \frac{q-0.5}{\sqrt{8q}} \right)^{-\frac{1}{2}}.$$

(I.1.3)

The RN stops as soon as the captured electrons have screened the ion charge and, as a consequence, the potential barrier has moved up again above the Fermi level. With further approach of the projectile towards the surface, the over-the-barrier condition will be restored as the image interaction mentioned above and the screening of the projectile charge by the electrons already captured will shift the energy levels of the projectile upwards ("image shift", IS, and "screening shift", SS, see Fig.I.1.2), and again RN can go on. Thus, n_c in Eq.I.1.3 designates the highest n-shell of the projectile which can be reached during the whole neutralization sequence.

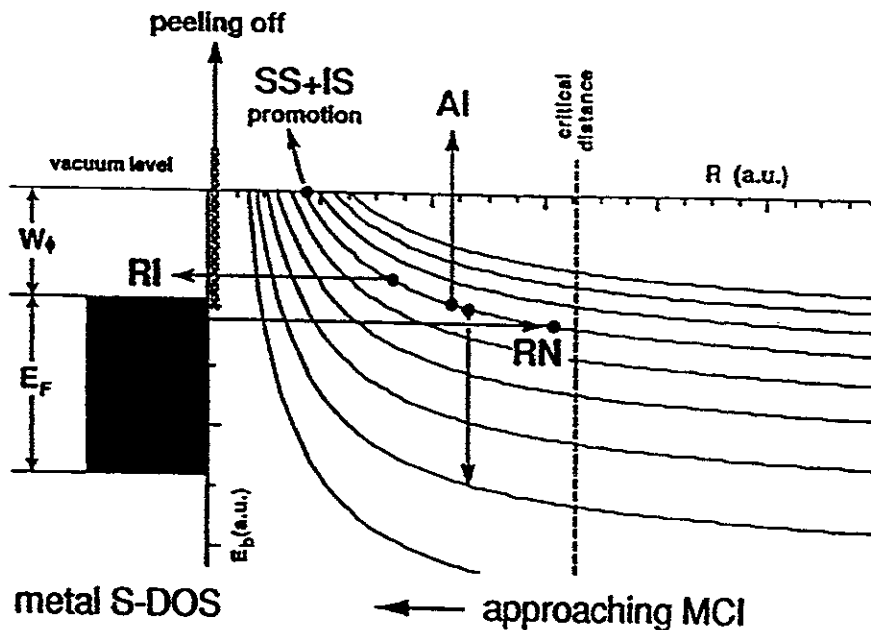


Fig.I.1.2. States of a neutralizing MCI approaching a metal surface.

Electrons captured via RN can be emitted via autoionization (AI), promotion into vacuum due to screening and image shift (SS/IS), and "peeling off" of all electrons which can not stay bound to the projectile inside the solid. Furthermore, electrons can be recaptured into the solid via resonant ionization (RI) [1].

Further evolution of such a multiply excited projectile depends on

competition between resonant neutralization and other classes of electronic transitions such as intra-atomic Auger transitions, Auger deexcitation and interatomic Auger transitions (see Fig.I.1.3). However, all electrons lost from the projectile are rapidly replaced by RN and finally a fully neutralized "hollow atom" is formed.

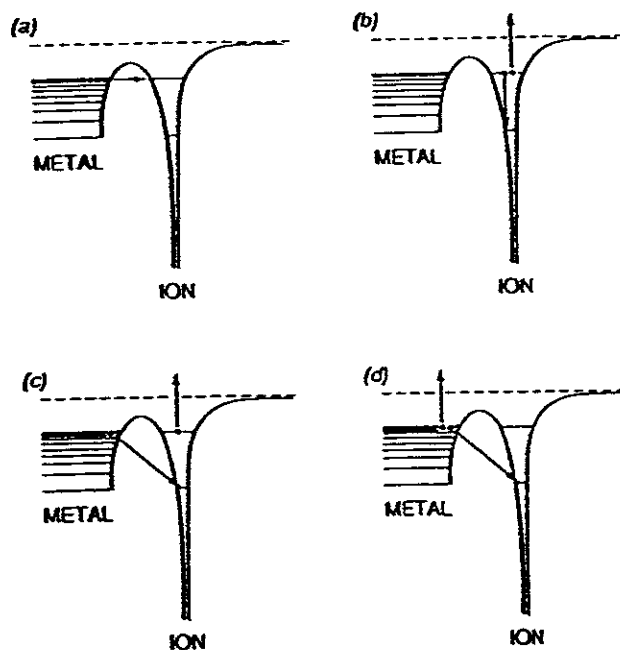


Fig.I.1.3. Energy diagrams describing (a) resonant neutralization, (b) intra-atomic Auger transition, (c) Auger deexcitation, and (d) and interatomic Auger transition [4,5].

The complete deexcitation of this highly excited species to its neutral ground state, via the above mentioned manifold of electronic interactions, would require a time not available because of the upper limit set by image charge attraction. When such a highly excited "hollow atom" approach the surface, electrons of the projectile with Rydberg radius $r_R = n^2/q$ larger than the screening length within the solid, $\lambda_s = v_F/w_p$ (v_F is the Fermi velocity of electrons inside the metal and w_p is the surface plasmon frequency) can be removed (ionized) from projectile ("peeling off" effect). However, such electrons removed are rapidly refilled by electrons from the conduction band of the solid and a "hollow atom" in

less excited states is formed.

Further relaxation of the projectile within the solid will be finished with the filling of inner shell vacancies not yet recombined through a series of cascade processes and electron transfer between inner shells of projectile and metal. These transitions result in the majority of the observed fast (projectile) Auger electrons, in competition with X-ray emission.

2. Brief reviews of studies on deexcitation processes in a "hollow atom"

Deexcitation of this short-lived complex can take place via various electronic transitions between intra-atomic states in the particle or between the particle and metal. Besides their fundamental interest, this process is also of practical relevance for plasma - wall interactions in gas discharges including thermonuclear fusion experiments or ion beam-activated material modification.

Various neutralization-deexcitation processes in interactions of MCI with surface are the subject of numerous papers. Hagstrum [4,5] and Arifov *et al.* [6] first treated such cases both experimentally and theoretically. They assumed multiple-resonant transitions to take place between MCI and surface thus rapidly forming a multiply excited neutral particle which then starts to decay via sequential autoionization processes. The shake-off process and Auger decay in the production and the decay of "hollow atoms", and the final charge state distributions of projectile have been studied in work of Omar and Hahn [7,8]. Donets [9,10] was the first to observe the $np-1s$ radiative decay in the interaction of Ar^{17+} ions with Be target. The X-ray spectra produced by MCI such as Ar^{17+} , Xe^{44-48+} , U^{62-73+} interacting with solid surface have been theoretically and experimentally studied by Briand *et al.* [11,12], Clark *et al.* [13], Andra [14], and Schuch *et al.* [15]. The review of some recent theoretical investigations of autoionization rates for highly ionized atoms has been written by Desclaux [16] in which the dependence of the Auger rates as a function of the level of the capture (i.e., the principal and orbital quantum numbers), the total angular momentum of the initial state and the number of electrons (either in the same shell or in different ones) has been considered. Competition between Auger and radiative processes has also been studied.

A number of papers devoted to investigations of the "hollow atom" show that the transfer of many electrons in low velocity collisions between MCI and neutral atomic, molecular, and solid state targets have now been the subject of extensive investigations.

3. Purpose of the present work

To calculate the atomic characteristics of neutralization-deexcitation processes such as electron transition energy, radiative transition probability and autoionization rate, a series of methods have been developed. The most accurate methods are based on the perturbation theory [17-22], Hartree-Fock-Pauli approximation (HFP) [23,24], multiconfiguration Dirac-Fock method (MCDF) [25-27], and model potential methods [28]. All the methods mentioned above take a lot of time to calculate atomic characteristics of complex many-electron systems. Although there exist very powerful numerical calculation techniques such as super computers, there still remains strong need for efficient analytical approaches. Indeed, in cases (for example, in interpretation of the observed spectra including a large number of unresolved line groups) the high accuracies of the calculations may not be necessary.

In this work an attempt is made to find a compromise between precision and general applicability of theoretical approach. Thus, the purpose of the present work is to obtain explicit formulas for calculating the atomic characteristics averaged over the orbital and spin quantum numbers and to create numerical codes which need a considerably less time in comparison with the well known methods in order to calculate these atomic characteristics with the accuracies sufficient for various applications. The author introduces in the present theoretical approach the combination of the $1/Z$ -expansion method based on the perturbation theory over $1/Z$ (Z being the nuclear charge), the screening parameter for the each subshell of the electronic configuration, and the averaging over the orbital and spin quantum numbers LS . Such a combination allows us to reduce the vast number of possible states for a complex, many-electron system, to take into account the screening effect for each atomic subshell and to calculate the atomic characteristics of the atomic system as a function of the number of electrons in different subshells of the system. Therefore, the present theoretical method can be applied to calculate atomic characteristics of practically any atomic system with arbitrary number of electrons.

This approach has been applied to study the deexcitation process of "hollow atom" during the interactions of multicharged Xe^{q+} ($q=44-48$) and Ar^{q+} ($q=17$) ion with a metal surface [13,32,38,37]. The deexcitation process involves different mechanisms which result in a large number of intermediate states of the atom before it decays to the ground state. That is why the X-ray or electron spectra observed in the interactions includes a large number of unresolved line groups and it takes a lot of time to identify or simulate these spectra using the accurate methods mentioned above. The present approach considerably facilitates this problem reducing the number of possible states and, as the $1/Z$ -expansion method, which the

present theoretical approach is based on, is especially useful for multicharged ions with a number of electrons N much smaller than the nuclear charge of ions, has been found to give the generally good results for the identification of the experimental spectra and for the simulation of the deexcitation process of the "hollow atom".

It has been also shown by comparison with other theoretical data that this method gives good results even for almost neutral atomic system which is usually difficult to treat theoretically [38].

All results obtained by the present theoretical method allow us to conclude that the method is very useful for study the atomic processes involved the large number of atomic and ionic states in a wide region of nuclear charge Z .

4.Theoretical approach

As mentioned above, the "hollow atom" decays finally to the ground state via various electronic transitions (including satellite transitions) between states in the particle and the surface. Calculation of atomic characteristics of the satellite radiative transitions is one of the subjects of the present work. The detailed description of the theoretical method is given in Chapter II. Here we shall describe briefly the main idea of the theoretical approach.

In view of applications of this theoretical method to multicharged ions we shall proceed with the perturbation theory using the nuclear charge Z of projectile as a parameter. The electronic interactions between electrons and relativistic effects which are taken into account in the frame of Breit operator are included as perturbations. To describe atomic orbitals, the H-like wave functions are used. Therefore, all atomic characteristics can be given by a series of $1/Z$ powers. For the energy we have a series of powers of Z and αZ :

$$E = \sum_{i=0}^{\infty} \sum_{k/2=0}^{\infty} E_{ik} (\alpha Z)^k Z^{2-i}, \quad (\text{I.4.1})$$

where α is the fine structure constant and E_{ik} are the expansion coefficients of the i -th order of the non-relativistic ($k=0$) and relativistic ($k/2 \geq 1$) energy. Here we shall confine ourselves to the first order of perturbation theory by $1/Z$.

In order to improve accuracies of calculation, the screening parameter σ which depends on the electronic states of ions is introduced both for relativistic and non-relativistic parts of energy. The effective charge for projectile with an electron in the (n) state is represented as

$$Z(nl) = Z - \sigma(nl), \quad (\text{I.4.2})$$

where $\sigma(nl)$ is determined from the variational principle.

To reduce a vast number of possible states for complex, many-electron system Q ($Q = 1s^{k_1} 2s^{k_2} 2p^{k_3} 3s^{k_4} \dots$, where k_i is the electron occupation number), all the atomic characteristics have to be averaged over the orbital and spin quantum numbers.

This method allows us to express the desired atomic properties in analytical forms as a function of the electron numbers in various shells of the ion. It can be applied practically to any atomic system with arbitrary number of electrons.

II. Theoretical method

1. Z-expansion method

The non-relativistic Schrodinger equation for the atom with the nuclear charge Z can be written in the form (atomic units are used):

$$\left[\sum_i \left(-\frac{1}{2} \Delta_i - \frac{Z}{r_i} \right) + \frac{1}{2} \sum'_{ij} \frac{1}{r_{ij}} \right] \psi = E^N \psi. \quad (\text{II.1.1})$$

The first term of this equation describes the kinetic and potential energy of each electron (Δ_i is the operator of kinetic energy of the i -th electron) and the second term describes the inter-electron interaction. The summation is performed over the total number of electrons in the atom. The wave function ψ being the solution of the Eq.(II.1.1) describes the stationary state with the definite value of non-relativistic energy E^N [29]. To illustrate the designation used in the Eq.(II.1.1) we present the following picture (Fig. II.1.1) :

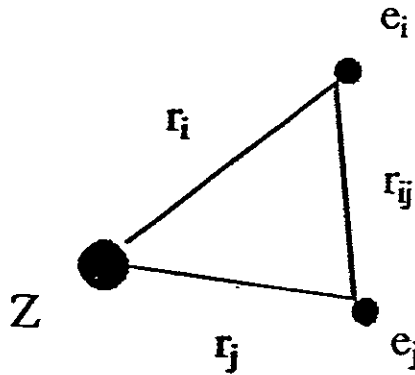


Fig. II.1.1

The perturbation theory with using a hydrogenic basis set [30], known to be the most systematic and straightforward theory for highly charged ions, is used. The inter-electron interaction $1/r_{ij}$ and the relativistic energy are treated as a perturbation. To extract $1/Z$ -dependence the variables r_i and r_{ij} are replaced by r_i'/Z and r_{ij}'/Z respectively. After such a replacement (and division by Z^2), Eq.(II.1.1) results in the following :

$$\left[\sum_i \left(-\frac{1}{2} \Delta_i - \frac{1}{r_i'} \right) + \frac{1}{2} \frac{1}{Z} \sum'_{ij} \frac{1}{r_{ij}'} \right] \psi = \frac{E^N}{Z^2} \psi. \quad (\text{II.1.2})$$

Based on the perturbation theory with $1/Z$ we can express the eigen-function and eigen-energy in the form of series of expansion in $1/Z$:

$$\Psi = \Psi_0 + \frac{1}{Z} \Psi_1 + \frac{1}{Z^2} \Psi_2 + \dots, \quad (\text{II.1.3})$$

$$E^N = Z^2 \left(E_0^N + \frac{1}{Z} E_1^N + \frac{1}{Z^2} E_2^N + \dots \right), \quad (\text{II.1.4})$$

where Ψ_0 and E_0^N are the hydrogenic wave function and non-relativistic hydrogenic energy, and E_i^N ($i \geq 1$) represents the non-relativistic energy of the i -th order in Z -expansion. Ψ_i ($i \geq 1$) is the i -th order of wave function.

The relativistic energy is taken into account in the frame of Breit operator [31] and, as it was already mentioned, plays a part of the perturbation. The Breit operator allows us to calculate the corrections to the non-relativistic energy up to relative order $(\alpha Z)^2$. The $(\alpha Z)^2$ corrections give the energy to the same order of accuracy as the Pauli approximation for hydrogenic atoms. The Breit operator includes the following terms:

1. one-particle operators

$$H_1(\mathbf{r}) = -\frac{\alpha^2}{8} \mathbf{p}^4,$$

$$H_4(\mathbf{r}) = \frac{\alpha^2}{2} \pi Z \delta^3(\mathbf{r}),$$

$$H_3(\mathbf{r}) = \frac{\alpha^2}{2} Z \frac{\mathbf{L} \cdot \mathbf{S}}{r^3},$$

2. two-particle operators

$$H_2(\mathbf{r}_{12}) = -\frac{\alpha^2}{2} \frac{1}{r_{12}} \left(\mathbf{p}_1 \mathbf{p}_2 + \frac{\mathbf{r}_{12} (\mathbf{r}_{12} \cdot \mathbf{p}_1) \mathbf{p}_2}{r_{12}^2} \right),$$

$$H_3'' = -\frac{\alpha^2}{r_{12}^3} (\mathbf{r}_{12} \times \mathbf{p}_1) \cdot (\mathbf{s}_1 + 2\mathbf{s}_2),$$

$$H_4^r(\mathbf{r}_{12}) = -\alpha^2 \pi \delta^3(\mathbf{r}_{12}),$$

$$H_5^r(\mathbf{r}_{12}) = -\frac{8}{3} \alpha^2 \pi \mathbf{s}_1 \mathbf{s}_2 \delta^3(\mathbf{r}_{12}),$$

$$H_5^s = \frac{\alpha^2}{r_{12}^3} \left[\mathbf{s}_1 \mathbf{s}_2 - \frac{3}{r_{12}^2} (\mathbf{s}_1 \mathbf{r}_{12})(\mathbf{s}_2 \mathbf{r}_{12}) \right],$$

(II.1.5)

where α is the fine structure constant, \mathbf{r}_{12} is the radii-vector, \mathbf{p} is the momentum operator, \mathbf{s} is the spin operator, $\delta^3(\mathbf{r})$ is the three dimensional Dirac delta-function, and L and S are the orbital and spin momenta, respectively. The physical significance of the various terms in Eq.(II.1.5) is as follows :

H_1 is the relativistic correction due to the "variation of mass with velocity" (which does not depend on electron spin).

H_2 corresponds to the classical relativistic correction to the interaction between electrons. This correction is due to the retardation of the electromagnetic field produced by an electron.

H_3^r is the interaction between the spin magnetic moment and the orbital magnetic moment of the electrons (spin-orbit coupling).

H_5^r and H_5^s represent the interaction between the spin magnetic dipole moments of the two electrons.

H_4^r , H_4^s and H_3^s are the contact terms.

The relativistic part of energy can be presented also in terms of $1/Z$ expansion:

$$E^R = \alpha^2 Z^4 \left(E_0^R + \frac{1}{Z} E_1^R + \frac{1}{Z^2} E_2^R + \dots \right).$$

(II.1.6)

Here E_i^R ($i > 0$) represents the relativistic energy of the i -th order and E_0^R equals to

$$E_0^R = -\frac{2}{n^3} \left(\frac{2}{2l+1} - \frac{3}{4n} - \delta(l,0) \right),$$

(II.1.7)

where $\delta(l,0)$ is the delta function, l is the orbital momentum of the electron, and n is the principal quantum number.

Then the total energy of atom is given as the sum of non-relativistic and relativistic energies:

$$E = E^N + E^R. \quad (\text{II.1.8})$$

2. Screening parameter

In the zeroth approximation all electrons move in the Coulomb field of the nucleus, with the interelectron interaction being absent. We note that the nuclear charge Z is a good approximation for the innermost shell, i.e., the K-shell electrons, independent of the number of electrons in the other shells. On the other hand if one approximates the effective field by the Coulomb field in which the outer electron moves, the corresponding effective charge must be close to that in the spectroscopic notation $Z_s = (Z - N_e - 1)$, where N_e is the total number of electrons, but is not necessarily close to the nuclear charge. For understanding the optimal charge and correspondingly the non-relativistic screening parameter (σ^N) we rewrite Eq. (II.1.4) in the form

$$E^N = E_0^N (Z - \sigma^N)^2. \quad (\text{II.2.1})$$

By comparing Eqs.(II.1.4) and (II.2.1) we can determine the screening parameter σ^N :

$$E_0^N Z^2 + E_1^N Z + E_2^N + \dots = E_0^N Z^2 - 2E_0^N Z \sigma^N + E_0^N (\sigma^N)^2,$$

$$\sigma^N = - \frac{E_1^N}{2E_0^N}, \quad (\text{II.2.2})$$

if we neglect the third, fourth and higher order contributions in Eq.(II.1.4) and assume $Z \gg \sigma^N$. Now we can rewrite Eq.(II.1.4) in the form:

$$E^N = E_0^N (Z - \sigma^N)^2 + \varepsilon(\sigma^N), \quad (\text{II.2.3})$$

where

$$\varepsilon(\sigma^N) = E_2^N - E_0^N (\sigma^N)^2. \quad (\text{II.2.4})$$

In the actual computation of E_2^N for all states, numerical difficulties are encountered [20]. If $\varepsilon(\sigma^N)$ is a small part of E_2^N , a large amount of the second order is already accounted for by the lower orders of perturbation theory. In other

words, the introduction of the screening parameter actually enables us to reach appreciable accuracy without computation of more elaborate terms of the second order of the perturbation theory. The comparison of E_2^N and $\varepsilon(\sigma^N)$ for different states given in [32] shows that $\varepsilon(\sigma^N)$ reaches 40-50% of E_2^N .

The screening parameter can be introduced also for the relativistic energy and is expressed as follows:

$$\sigma^R = - \frac{E_1^R}{3E_0^R} \quad (\text{II.2.5})$$

3. Non-relativistic part of energy: Averaging over LS

Generally we can represent each configuration of any atomic system in the following form :

$$1s^{k_1} 2s^{k_2} 2p^{k_3} 3s^{k_4} 3p^{k_5} 3d^{k_6} \dots \quad (\text{II.3.1})$$

Averaging over the total angular momentum of the atomic system (LS) is equivalent to averaging all the sets of one-electron quantum numbers (n, j, m, m_s) , where n and j are the principal and orbital quantum numbers, and m and m_s are the projections of the orbital and spin momenta [33].

For simplicity we shall first consider the two-electron systems. For this case the energy in the first-order perturbation theory is

$$E_1^N(njn'j', LS) = N_0(2j+1)(2j'+1) \sum_k \left[R_k(njn'j'; nj'nj) \begin{pmatrix} j & j & k \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} j' & j' & k \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} j & j' & L \\ j' & j & k \end{pmatrix} (-1)^{L+s} \right. \\ \left. R_k(njn'j'; nj'nj) \begin{pmatrix} j & j' & k \\ 0 & 0 & 0 \end{pmatrix}^2 \begin{pmatrix} j & j' & L \\ j & j' & k \end{pmatrix} (-1)^s \right], \quad (\text{II.3.2})$$

where we use the common designation for $3j$ and $6j$ Wigner's coefficients. The first term of the sum in Eq.(II.3.2) describes the Coulomb energy of two electron interaction. The second term defines the so-called exchange part of the interaction energy and has not any clear physical interpretation because there is no analog of

the exchange energy in the classical electrodynamics. The presence of the two terms in the expression for the energy of the two electron interaction is caused by the fact that the Schroedinger equation does not contain the spins. The spins are taken into account by requirement for the wave function to be antisymmetric. The exchange part of the electrostatic interaction has the purely quantum character. The radial integral $R_k(n_1j_1n_2j_2; n_4j_4n_3j_3)$ can be expressed as [29]

$$R_k(n_1j_1n_2j_2;n_4j_4n_3j_3)=$$

$$\int_0^\infty r_1^2 dr_1 \int_0^\infty r_2^2 dr_2 R_{n_1j_1}(r_1)R_{n_2j_2}(r_2) \frac{r_1^k}{r_1^{k+1}} R_{n_4j_4}(r_2)R_{n_3j_3}(r_1), \quad (\text{II.3.3})$$

where $R_{nj}(r)$ is the hydrogenic radial function, and r_1^k and r_1^{k+1} are the smaller and the larger values of the absolute values of r_1 and r_2 . The normalization constant N_0 in Eq.(II.3.2) is equal to 1 for nonequivalent electrons ($nj \neq n'j'$) and $2(2j+1)/4j+1$ for equivalent electrons ($nj = n'j'$). For equivalent electrons we can rewrite Eq.(II.3.2) in the form

$$E_1^N(njn_j, LS) = N_0 (2j+1)^2 \sum_k R_k(njn_j; njnj) \begin{pmatrix} j & j & k \\ 0 & 0 & 0 \end{pmatrix}^2 \begin{Bmatrix} j & j & L \\ j & j & k \end{Bmatrix} [(-1)^L + (-1)^S]. \quad (\text{II.3.4})$$

Averaging over LS is equivalent to calculating

$$E_1^N(njn'j') = \frac{\sum_L \sum_S (2L+1)(2S+1) E_1^N(njn'j', LS)}{\sum_L \sum_S (2L+1)(2S+1)}. \quad (\text{II.3.5})$$

After averaging over LS we obtain for $E_1^N(njn'j')$ and $E_1^N(njn_j)$ the following expressions :

$$E_1^N(njn'j') = F_0(nj, n'j') - \frac{1}{2} \sum_k \begin{pmatrix} j & j' & k \\ 0 & 0 & 0 \end{pmatrix}^2 G_k(nj, n'j'), \quad (\text{II.3.6})$$

$$E_1^N(njn_j) = F_0(nj,n_j) - \sum_k \frac{(2j+1)}{(4j+1)} \begin{pmatrix} j & j & k \\ 0 & 0 & 0 \end{pmatrix}^2 F_k(nj,n_j), \quad (\text{II.3.7})$$

where we use the usual designation [29]

$$\begin{aligned} F_k(nj,n'_j) &= R_k(njn'_j;n'_jn_j), \\ G_k(nj,n'_j) &= R_k(njn'_j;njn'_j). \end{aligned} \quad (\text{II.3.8})$$

In averaging over LS for a many-electron system it is sufficient to consider states associated with electrons in two configurations, i.e., $(nj)^k(n'_j)^{k'}$. The energy in the first order perturbation theory after averaging over LS can be expressed in terms of $E_1^N(njn_j)$, $E_1^N(n'_jn'_j)$ and $E_1^N(njn'_j)$ as follows :

$$E_1^N[(nj)^k(n'_j)^{k'}] = \frac{k(k-1)}{2} E_1^N(njn_j) + \frac{k'(k'-1)}{2} E_1^N(n'_jn'_j) + kk' E_1^N(njn'_j). \quad (\text{II.3.9})$$

The first two terms in Eq.(II.3.9) describe the interaction of the electrons belonging to the same subshell and the third term the interaction between the electrons of different subshells.

We can represent each configuration Q of a multi-electron atomic system with N subshells in the form

$$Q = 1s^{k_1} 2s^{k_2} 2p^{k_3} 3s^{k_4} 3p^{k_5} 3d^{k_6} 4s^{k_7} 4p^{k_8} \dots n_j i^{k_i} \dots n_N j_N^{k_N}, \quad (\text{II.3.10})$$

where k_i is the number of electrons in the i-th subshell $n_j i$. Using Eq.(II.3.9) we obtain the energy of the configuration Q :

$$E_1^N(Q) = \frac{1}{2} \sum_{i=1}^N k_i(k_i-1) E_1^N(n_j i n_j i) + \sum_{m=2}^N \sum_{i < m} k_i k_m E_1^N(n_j i n_m j_m). \quad (\text{II.3.11})$$

The energy of such a system in the zero-th order of perturbation theory is given as the sum of the hydrogenic energies of all electrons of the system :

$$E_0^N(Q) = - \frac{1}{2} \sum_{i=1}^N \frac{k_i}{n_i^2}. \quad (\text{II.3.12})$$

Introducing the screening parameter σ^N in accordance with Eq.(II.2.1) we can express the total non-relativistic energy of the system with the configuration Q in the form

$$E^N(Q) = E_0^N(Q)(Z - \sigma^N)^2, \quad (\text{II.3.13})$$

where

$$\sigma^N = - \frac{E_1^N(Q)}{2E_0^N(Q)}.$$

The same type of the screening procedure can be applied for the calculation of n_1j_1 - n_2j_2 transition energies, namely,

$$\begin{aligned} E^N[Q] - E^N[(n_1j_1)^{-1}n_2j_2Q] &\cong Z^2 [E_0^N(n_1j_1) - E_0^N(n_2j_2)] + Z \{E_1^N[Q] - E_1^N[(n_1j_1)^{-1}n_2j_2Q]\} \\ &= [E_0^N(n_1j_1) - E_0^N(n_2j_2)](Z - \sigma^N)^2, \end{aligned} \quad (\text{II.3.14})$$

where

$$\sigma^N = - \frac{E_1^N[Q] - E_1^N[(n_1j_1)^{-1}n_2j_2Q]}{2 [E_0^N(n_1j_1) - E_0^N(n_2j_2)]}, \quad E_0^N(nj) = -\frac{1}{2n^2}.$$

4. Relativistic part of energy: Averaging over LS

For intermediate Z atomic system, the relativistic effects can be accounted for by adding additional terms resulting from the reduction of the Dirac equation and the Breit interaction [32] to the non-relativistic Hamiltonian. Since we are interested in the LS averaged energies, only those terms of the Breit operator which cause the energy shifts are incorporated here. These operators can be written as

$$H_1(\mathbf{r}) = - \frac{\alpha^2}{8} \mathbf{p}^4,$$

$$H_4(\mathbf{r}) = \frac{\alpha^2}{2} \pi Z \delta^3(\mathbf{r}),$$

$$H_{4''}(\mathbf{r}_{12}) = -\alpha^2 \pi \delta^3(\mathbf{r}_{12}),$$

$$H_2(\mathbf{r}_{12}) = -\frac{\alpha^2}{2} \frac{1}{r_{12}} \left(\mathbf{p}_1 \mathbf{p}_2 + \frac{\mathbf{r}_{12}(\mathbf{r}_{12} \mathbf{p}_1) \mathbf{p}_2}{r_{12}^2} \right),$$

$$H_{5'}(\mathbf{r}_{12}) = -\frac{8}{3} \alpha^2 \pi \mathbf{s}_1 \mathbf{s}_2 \delta^3(\mathbf{r}_{12}).$$

(II.4.1)

By using these operators we can calculate the relativistic correction.

The calculation of the relativistic part of the energy is more difficult than that of the non-relativistic part. This is connected with the absence of the equation analogous to Schroedinger equation. However, it is possible to write the expression for the relativistic energy using the S-matrix [34] and obtain a perturbation theory expansion in the same way as for the non-relativistic part of the energy. Therefore, we can represent the relativistic part of energy in the form

$$E^R = \alpha^2 (E_0^R Z^4 + E_1^R Z^3 + E_2^R Z^2 + E_3^R Z + \dots).$$

(II.4.2)

Similar to the non-relativistic part of energy we consider here only the first two terms: E_0^R and E_1^R . The zero-th order of one-particle operators will contribute to the zero-th order of the relativistic energy, and the first order of one-particle operators and the zero-th order of two-particle operators to the first order of the relativistic energy.

First we will consider the one-particle Breit operators.

1. One-particle Breit operators :

$$H_1(\mathbf{r}) = -\frac{\alpha^2}{8} p^4, \quad H_{4'}(\mathbf{r}) = \frac{\alpha^2}{2} \pi Z \delta(\mathbf{r}).$$

It is possible to separate the angular and radial parts of the $V_{njn'j'}^i$ matrix element with $i=1$ and $4'$.

$$V_{njn'j'}^1 = \delta(m, m') \delta(m_s, m'_s) M^1(nj, n'j'),$$

(II.4.3)

$$V_{njn'j'}^{4'} = \delta(m, m') \delta(m_s, m'_s) \delta(m, 0) M^{4'}(nj, n'j'),$$

(II.4.4)

where

$$M^1(nj,n'j')= - \alpha^2 Z^4 \frac{1}{8} \delta(j,j') \int_0^\infty r^2 dr \left(\frac{2}{r} - \frac{1}{n^2} \right) \left(\frac{2}{r} - \frac{1}{n'^2} \right) R_{nj}(r) R_{n'j'}(r), \quad (\text{II.4.5})$$

$$M^4(nj,n'j')= \alpha^2 Z^4 \frac{1}{2} \delta(j,0) \delta(j',0) R_{nj}(0) R_{n'j'}(0) \quad (\text{II.4.6})$$

and $R_{nj}(r)$ is the radial hydrogenic function.

We can describe the matrix element for many-electron system by taking into account the inter-electron interaction potential [35] :

$$V_{n_1 j_1 n_2 j_2; n_4 j_4 n_3 j_3} = \int d\mathbf{r}_1 \int d\mathbf{r}_2 \sum_{v_1} \sum_{v_2} \frac{1}{r_{12}} \phi_{n_1 j_1}^*(\mathbf{r}_1, v_1) \phi_{n_2 j_2}^*(\mathbf{r}_2, v_2) \phi_{n_4 j_4}(\mathbf{r}_2, v_2) \phi_{n_3 j_3}(\mathbf{r}_1, v_1), \quad (\text{II.4.7})$$

where $\phi_{nj}(\mathbf{r}, v)$ is the wave function and v is the spin variable.

The zero-th order relativistic energy for the the n-electron system can be written as

$$E_0^R(H_i) = \sum_{\beta_1 \dots \beta_n} \sum_{\beta_1'} V_{\beta_1 \beta_1'}^i C_{\beta_1 \dots \beta_n}^{LS} C_{\beta_1' \beta_2 \dots \beta_n}^{LS}, \quad (\text{II.4.8})$$

where $\beta_i = n_i j_i m_i m_s$ and i in the case under consideration is equal to 1 and 4'. The angular part of the $C_{\beta_1 \dots \beta_n}^{LS}$ -coefficients consists of products of 3j Wigner coefficients which couple states with two angular (j, m) and spin ($1/2, m_s$) momenta of electrons in total angular ($L_{12} M_{12}$) and spin ($S_{12} M_{12}^S$) momenta of the two-electron system. In the second step we add momenta of the third electron to the intermediate states LM, SM^S . We obtain $C_{\beta_1 \dots \beta_n}^{LS}$ for the n-electron system:

$$C_{\beta_1 \dots \beta_n}^{LS} = \sum_{K_{12}} \dots \sum_{K_{1n-1}} A(\beta_1 \beta_2 K_{12}) A(K_{12} \beta_3 K_{13}) \dots A(K_{1n-1} \beta_n K) C_{j_1 n_1 j_1 \dots j_n n_n} (L_{12} S_{12}, L_{12}^S S_{12}^S, \dots, LS), \quad (\text{II.4.9})$$

where $K = LMSM^S$ and $A(K_1 K_2 K_3)$ is equal to the product of 3j Wigner coefficients:

$$A(K_1 K_2 K_3) = (-1)^{L_1 - L_2 + M_3} \sqrt{(2L_3 + 1)} \begin{pmatrix} L_1 & L_2 & L_3 \\ M_1 & M_2 & M_3 \end{pmatrix} \times$$

$$(-1)^{S_1-S_2+M_3^S} \sqrt{(2S_3+1)} \begin{pmatrix} S_1 & S_2 & S_3 \\ M_1^S & M_2^S & M_3^S \end{pmatrix} \quad (\text{II.4.10})$$

The coefficients $C_{j_1 n_1 j_1 \dots j_n n_n j_n} (L_{12} S_{12}, L''_{12} S''_{12}, \dots, LS)$ provide the antisymmetry of the coefficients $C_{\beta_1 \dots \beta_n}^{LS}$. For a specific case of equivalent electrons, i.e., at $n_1 j_1 = n_2 j_2 = \dots = n_n j_n$ the coefficients $C_{j_1 n_1 j_1 \dots j_n n_n j_n} (L_{12} S_{12}, L''_{12} S''_{12}, \dots, LS)$ are the parentage coefficients.

Eq. (II.4.8) represents the contribution of the zero-th order relativistic energy. Then, the first order correction is given as [35]:

$$E_1^R(H^i) = - \frac{1}{(n-2)!} \sum_{\beta_1 \dots \beta_n} \sum_{\beta_1 \beta_2} C_{\beta_1 \dots \beta_n}^{LS} C_{\beta_1 \beta_2 \beta_3 \dots \beta_n}^{LS} \times \\ \sum_k \left(\frac{1}{E_k + E_{\beta_2} - E_{\beta_1} - E_{\beta_2}} V_{k\beta_1} V_{\beta_1 \beta_2; \beta_2 k} + \frac{1}{E_k + E_{\beta_2} - E_{\beta_1} - E_{\beta_2}} V_{\beta_1 k} V_{k\beta_2; \beta_2 \beta_1} \right) \quad (\text{II.4.11})$$

with the summation over the index k which involves all the quantum number $n_j m_{j_s}$.

After evaluation of the summation over angular and spin states we can express the zero-th (Eq.(II.4.8)) and the first (Eq.(II.4.11)) order contribution in radial form. The zero-th order contribution is equal to the sum of the one-electron contributions, where $q(n_j)$ is the number of electrons in each shell belonging to sets of f shells:

$$E_0^R(H_i) = \sum_{n_j \in f} q(n_j) [M^1(n_j, n_j) + M^{4'}(n_j, n_j)]. \quad (\text{II.4.12})$$

The first order contribution depends on the quantum numbers for each electron and also on the intermediate quantum numbers: $n_1 j_1 n_2 j_2 (L_{12} S_{12}) n_3 j_3 \dots LS$. In this basic set we obtain the diagonal elements of the H_1 and H_4 operators:

$$E_1^R(H_i) = \frac{1}{2(n-2)!} \sum_{j_1} \sum_{j_2} \sum_{j_1'} \sum_{j_2'} \sum_l \sum_{L_{12}} \sum_{S_{12}} (-1)^{L_{12}+j_1+j_2} \begin{Bmatrix} j_1 & j_2 & L_{12} \\ j_1' & j_2' & l \end{Bmatrix} \times \\ \sqrt{(2j_1+1)(2j_2+1)(2j_1'+1)(2j_2'+1)} E_l^i(n_1 j_1 n_2 j_2; n_2 j_2 n_1 j_1) \times$$

$$\sum_{j_3} \dots \sum_{j_n} \sum_{L_{13}} \sum_{S_{13}} \dots \sum_{L_{1n-1}} \sum_{S_{1n-1}} C_{j_1 n_1 j_1 \dots j_n n_n j_n} (L_{12} S_{12}, L_{12}'' S_{12}'', \dots, LS) \times$$

$$C_{j_1 n_1 j_1 j_2 n_2 j_2 j_3 n_3 j_3 \dots j_n n_n j_n} (L_{12} S_{12}, L_{12}'' S_{12}'', \dots, LS),$$
(II.4.13)

where

$$E_l^i(n_1 j_1 n_2 j_2; n_4 j_4 n_3 j_3) = \sum_n \frac{1}{E_n + E_{n_2} - E_{n_4} - E_{n_3}} \begin{pmatrix} l & j_1 & j_3 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l & j_2 & j_4 \\ 0 & 0 & 0 \end{pmatrix} \times$$

$$M^i(n_{j_1}, n_{1j_1}) R_l(n_{j_2}, n_{2j_2}; n_{4j_4}, n_{3j_3}).$$
(II.4.14)

The sum over n includes the summation over discrete states and the integration over continuous states :

$$\sum_n = \sum_{n=1}^{\infty} + \int_0^{\infty} dk.$$
(II.4.15)

2. Two-particle Breit operators.

We consider now the contributions of the two-particle operators. These operators can be written as follows, as already given before :

$$H_4^n(\mathbf{r}_{12}) = -\alpha^2 \pi \delta(\mathbf{r}_{12}),$$

$$H_2(\mathbf{r}_{12}) = \frac{-\alpha^2}{2} \frac{1}{r_{12}} \left(\mathbf{p}_1 \mathbf{p}_2 + \frac{\mathbf{r}_{12} (\mathbf{r}_{12} \mathbf{p}_1) \mathbf{p}_2}{r_{12}^2} \right),$$

$$H_5(\mathbf{r}_{12}) = -\frac{8}{3} \alpha^2 \pi \mathbf{s}_1 \mathbf{s}_2 \delta(\mathbf{r}_{12}).$$

For these operators we can use the formula obtained before for $1/r_{12}$ operator [35]:

$$V_{n_1 j_1 n_2 j_2; n_4 j_4 n_3 j_3} =$$

$$\int d\mathbf{r}_1 \int d\mathbf{r}_2 \sum_{v_1} \sum_{v_2} \phi_{n_1 j_1}^*(\mathbf{r}_1, \mathbf{v}_1) \phi_{n_2 j_2}^*(\mathbf{r}_2, \mathbf{v}_2) H_i(\mathbf{r}_1 \mathbf{v}_1; \mathbf{r}_2 \mathbf{v}_2) \phi_{n_4 j_4}(\mathbf{r}_2, \mathbf{v}_2) \phi_{n_3 j_3}(\mathbf{r}_1, \mathbf{v}_1).$$

In the zero-th approximation the contribution of each of the three operators is equal to

$$E_0^R(H^i) = -\frac{1}{2(n-2)!} \sum_{\beta_1 \dots \beta_n} \sum_{\beta_1 \beta_2} V_{n_1 j_1 n_2 j_2; n_4 j_4 n_3 j_3} C_{\beta_1 \dots \beta_n}^{LS} C_{\beta_1 \beta_2 \beta_3 \dots \beta_n}^{LS} \quad (\text{II.4.17})$$

After summation over all the quantum numbers we obtain the same expression as for the first order contribution of the one-particle Breit operators (Eq.(II.4.13)) by only changing the expression for $E_l^i(n_1 j_1 n_2 j_2; n_2 j_2 n_1 j_1)$. Here we give expressions for the $E_l^i(n_1 j_1 n_2 j_2; n_2 j_2 n_1 j_1)$ with $i=4, 5, 2$:

$$E_l^{4''}(n_1 j_1 n_2 j_2; n_4 j_4 n_3 j_3) = - (2l+1) \begin{pmatrix} l & j_1 & j_3 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l & j_2 & j_4 \\ 0 & 0 & 0 \end{pmatrix} T(n_1 j_1 n_2 j_2; n_4 j_4 n_3 j_3), \quad (\text{II.4.18})$$

$$E_l^{5'}(n_1 j_1 n_2 j_2; n_4 j_4 n_3 j_3) = 2(2l+1) \begin{pmatrix} l & j_1 & j_3 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l & j_2 & j_4 \\ 0 & 0 & 0 \end{pmatrix} \times$$

$$T(n_1 j_1 n_2 j_2; n_4 j_4 n_3 j_3) (-1)^{1+S_{12}''} \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 1 \\ \frac{1}{2} & \frac{1}{2} & S_{12}'' \end{pmatrix}, \quad (\text{II.4.19})$$

where

$$T(n_1 j_1 n_2 j_2; n_4 j_4 n_3 j_3) = \int_0^\infty r_1^2 dr_1 \int_0^\infty r_2^2 dr_2 R_{n_1 j_1}(r_1) R_{n_2 j_2}(r_2) R_{n_4 j_4}(r_2) R_{n_3 j_3}(r_1). \quad (\text{II.4.20})$$

As the expression for $E_l^2(n_1 j_1 n_2 j_2; n_4 j_4 n_3 j_3)$ is very cumbersome to write [20], we give here only the radial integral to illustrate the contribution of orbit-orbit operator:

$$K_l(n_1 j_1 n_2 j_2; n_4 j_4 n_3 j_3) = \int_0^\infty r_1^2 dr_1 \int_0^\infty r_2^2 dr_2 \theta(r_1 - r_2) \frac{r_2^l}{r_1^{l+1}} R_{n_1 j_1}(r_1) R_{n_2 j_2}(r_2) \frac{d^2}{dr_1 dr_2} R_{n_4 j_4}(r_2) R_{n_3 j_3}(r_1). \quad (\text{II.4.21})$$

To obtain the first order of relativistic energy E^R_1 (Eq.(II.4.2)) we combine the first order for one-particle operators and the zero-th order for two-particle operators. For a common case we can rewrite Eq.(II.4.13) in the form :

$$\begin{aligned}
E^R_1(H^i) = & \frac{1}{2(n-2)!} \sum_{j_1} \sum_{j_2} \sum_{j_1'} \sum_{j_2'} \sum_l \sum_{L_{12}} \sum_{S_{12}} (-1)^{L_{12}+j_1+j_2} \left\{ \begin{matrix} j_1 & j_2 & L_{12}'' \\ j_1' & j_2' & l \end{matrix} \right\} \times \\
& \sqrt{(2j_1+1)(2j_2+1)(2j_1'+1)(2j_2'+1)} E_l^R(n_1j_1n_2j_2;n_2j_2n_1j_1') \times \\
& \sum_{j_3} \dots \sum_{j_n} \sum_{L_{13}} \sum_{S_{13}} \dots \sum_{L_{1n-1}} \sum_{S_{1n-1}} C_{j_1n_1j_1' \dots j_n n_n j_n'}(L_{12}S_{12}, L_{12}''S_{12}'', \dots, LS) \times \\
& C_{j_1n_1j_1' j_2n_2j_2' j_3n_3j_3' \dots j_n n_n j_n'}(L_{12}S_{12}, L_{12}''S_{12}'', \dots, LS),
\end{aligned} \tag{II.4.22}$$

where

$$\begin{aligned}
E_l^R(n_1j_1n_2j_2;n_2j_2n_1j_1') = & E_l^1(n_1j_1n_2j_2;n_2j_2n_1j_1') + E_l^{4'}(n_1j_1n_2j_2;n_2j_2n_1j_1') \\
+ E_l^{4''}(n_1j_1n_2j_2;n_2j_2n_1j_1') + & E_l^5(n_1j_1n_2j_2;n_2j_2n_1j_1') + E_l^2(n_1j_1n_2j_2;n_2j_2n_1j_1').
\end{aligned} \tag{II.4.23}$$

To average the relativistic energy over LS we have to consider its zero-th and first order terms (Eqs. (II.4.12) and (II.4.22)). The zero-th order of relativistic energy which is the zero-th order for the one-particle operators H_1 and H_4 , is independent of LS . After substitution of Eqs.(II.4.5) and (II.4.6) to Eq.(II.4.12) we obtain the zero-th order of relativistic part of energy for the configuration Q (Eq.II.3.10) :

$$E_0^R(Q) = \sum_{i=1}^N k_i E_0^R(n_i j_i), \tag{II.4.24}$$

where

$$E_0^R(n_i j_i) = - \frac{2}{n_i^3} \left(\frac{2}{2j_i+1} - \frac{3}{4n_i} - \delta(j_i, 0) \right). \tag{II.4.25}$$

The angular part of E_l^R is the same as that for the non-relativistic first order

energy. In this case we can use all formulas obtained for the $1/r_{12}$ operator by changing only the radial part.

$$E_1^R(Q) = \frac{1}{2} \sum_{i=1}^N k_i(k_i-1) E_1^R(n_{ij}; n_{ij}) + \sum_{m=2}^N \sum_{i < m} k_i k_m E_1^R(n_{ij}; n_{mj}), \quad (\text{II.4.26})$$

where

$$E_1^R(n_{ji}; n_{jj}) = E_0^R(n_{ji}; n_{jj}; n_{jj}; n_{ji}) (-1)^{j_i+j_j} \sqrt{(2j_i+1)(2j_j+1)} - \frac{1}{2} \sum_l E_l^R(n_{ji}; n_{jj}; n_{jj}; n_{ji}), \quad (\text{II.4.27})$$

$$E_1^R(n_{ji}; n_{ji}) = (2l+1) E_0^R(n_{ji}; n_{ji}; n_{ji}; n_{ji}) - \frac{2l+1}{4l+1} \sum_{l>0} E_l^R(n_{ji}; n_{ji}; n_{ji}; n_{ji}), \quad (\text{II.4.28})$$

$E_l^R(n_{ji}; n_{jj}; n_{ji}; n_{jj})$ is determined from Eq.(II.4.23).

The zero-th and the first order relativistic energies for the configuration Q can be represented in the form of screening formula :

$$E^R(Q) = \alpha^2 Z E_0^R(Q) \left[Z + \frac{E_1^R(Q)}{3E_0^R(Q)} \right]^3. \quad (\text{II.4.29})$$

Then, the relativistic part of $Q-(n_{1j_1})^{-1}n_{2j_2}Q$ transition energy is :

$$E^R[Q] - E^R[(n_{1j_1})^{-1}n_{2j_2}Q] = \alpha^2 Z [E_0^R(n_{1j_1}) - E_0^R(n_{2j_2})] (Z - \sigma^R)^3, \quad (\text{II.4.30})$$

where

$$\sigma^R = - \frac{E_1^R[Q] - E_1^R[(n_{1j_1})^{-1}n_{2j_2}Q]}{3 [E_0^R(n_{1j_1}) - E_0^R(n_{2j_2})]}. \quad (\text{II.4.31})$$

5. X-ray transition energy averaged over LS

The total X-ray transition energy can be expressed as a sum of non-relativistic and relativistic transition energies. Combining Eqs.(II.3.14) and (II.4.30) we obtain the Q-

$$E[Q-(n_1j_1)^{-1}n_2j_2Q] = [E_0^N(n_1j_1)-E_0^N(n_2j_2)](Z - \sigma^N)^2 + \alpha^2 Z[E_0^R(n_1j_1)-E_0^R(n_2j_2)](Z - \sigma^R)^3, \quad \text{tr} \quad (\text{II.5.1})$$

where

$$\sigma^N = - \frac{E_1^N[Q]-E_1^N[(n_1j_1)^{-1}n_2j_2Q]}{2 [E_0^N(n_1j_1)-E_0^N(n_2j_2)]},$$

$$\sigma^R = - \frac{E_1^R[Q]-E_1^R[(n_1j_1)^{-1}n_2j_2Q]}{3 [E_0^R(n_1j_1)-E_0^R(n_2j_2)]},$$

$$E_0^N(n_ji) = - \frac{1}{2n_i^2},$$

$$E_0^R(n_ji) = - \frac{2}{n_i^3} \left(\frac{2}{2j_i+1} - \frac{3}{4n_i} - \delta(j_i,0) \right),$$

and the configuration Q is given by Eq.(II.3.10).

It is important to note that these formulas can be used for calculation of the transition energies for any atomic system.

6. Autoionization widths of levels averaged over L and S

In the present section we will obtain the expression for the autoionization widths of levels averaged over the total momentum L and S. To derive the formula for the autoionization width for the multielectron system we will proceed first with the two-electron $(n_1j_1n_2j_2;LS)$ system. The autoionization level width for the two-electron system where one of the electrons goes to continuum k and the other to n_1j_1 , is given by [34]

$$\Gamma(n_1j_1n_2j_2;LS) = \frac{2\pi}{k} \sum_{n_1j_1j_2'} \left| \left\langle n_1j_1n_2j_2LS \left| \frac{1}{r_{12}} \right| n_1j_1'kj_2'LS \right\rangle \right|^2, \quad (\text{II.6.1})$$

where n_i and j_i are the principal and orbital quantum numbers of an electron and k

is the wave vector of an electron in continuum. The Coulomb matrix element in Eq.(II.6.1) can be expressed as

$$\begin{aligned} & \left\langle n_1 j_1 n_2 j_2 LS \left| \frac{1}{r_{12}} \right| n_1 j_1' k j_2' LS \right\rangle = \sqrt{(2j_1+1)(2j_2+1)(2j_1'+1)(2j_2'+1)} \times \\ & \sum_l (-1)^{L+l+\frac{1}{2}(j_1+j_1'-j_2-j_2')} \left[\begin{matrix} j_1 & j_2 & L \\ j_2' & j_1' & l \end{matrix} \right] P_l(n_1 j_1 n_2 j_2; k j_2' n_1 j_1') + (-1)^{L+S} \left[\begin{matrix} j_1 & j_2 & L \\ j_1' & j_2' & l \end{matrix} \right] P_l(n_1 j_1 n_2 j_2; n_1 j_1' k j_2') \end{aligned} \quad (\text{II.6.2})$$

where

$$P_l(n_1 j_1 n_2 j_2; k j_2' n_1 j_1') = (l j_1 j_1) (l j_2 j_2) R_l(n_1 j_1 n_2 j_2; k j_2' n_1 j_1'). \quad (\text{II.6.3})$$

$(l j_1 j_1)$ and $(l j_2 j_2)$ in Eq.(II.6.3) are the $3j$ symbols and $R_l(n_1 j_1 n_2 j_2; k j_2' n_1 j_1')$ is the Coulomb radial integral with one continuous parameter given by

$$R_l(n_1 j_1 n_2 j_2; k j_2' n_1 j_1') = \int_0^\infty dr_1 r_1^2 \int_0^\infty dr_2 r_2^2 U_l(r_1, r_2) R_{n_1 j_1}(r_1) R_{n_2 j_2}(r_2) R_{k j_2'}(r_2) R_{n_1 j_1'}(r_1),$$

$$U_l(r_1, r_2) = \Theta(r_1 - r_2) \frac{r_2^l}{r_1^{l+1}} + \Theta(r_2 - r_1) \frac{r_1^l}{r_2^{l+1}},$$

where $U_l(r_1, r_2)$ is the operator of the electrostatic interaction, $\Theta(r_1 - r_2)$ is the theta function. To get the averaged autoionization width $\Gamma(n_1 j_1 n_2 j_2; LS)$ we consider the function $A(n_1 j_1 n_2 j_2; k j_2' n_1 j_1')$ determined as follows :

$$A(n_1 j_1 n_2 j_2; k j_2' n_1 j_1') = \frac{2\pi}{k} \frac{\sum_{LS} (2L+1)(2S+1) \left| \left\langle n_1 j_1 n_2 j_2 LS \left| \frac{1}{r_{12}} \right| n_1 j_1' k j_2' LS \right\rangle \right|^2}{\sum_{LS} (2L+1)(2S+1)}. \quad (\text{II.6.4})$$

Then, evidently, the averaged width for the configuration $n_1 j_1 n_2 j_2$ is :

$$\Gamma(n_1 j_1 n_2 j_2; LS) = \sum_{n_1 j_1' j_2'} A(n_1 j_1 n_2 j_2; k j_2' n_1 j_1'). \quad (\text{II.6.5})$$

Using the expression for the matrix element (Eq.(II.6.2)) and the sum rules for the 6j-symbols [29]

$$\sum_L (2L+1) \begin{Bmatrix} j_1 & j_2 & L \\ j_2' & j_1' & l \end{Bmatrix} \begin{Bmatrix} j_1 & j_2 & L \\ j_2' & j_1' & l \end{Bmatrix} = \frac{1}{(2l+1)}$$

and

$$\sum_L (-1)^{L+l+l'} (2L+1) \begin{Bmatrix} j_1 & j_2 & L \\ j_2' & j_1' & l \end{Bmatrix} \begin{Bmatrix} j_1 & j_2 & L \\ j_1' & j_2' & l' \end{Bmatrix} = \begin{Bmatrix} j_1 & j_1' & l' \\ j_2 & j_2' & l \end{Bmatrix},$$

we obtain the following expressions for the autoionization width of two-electron system averaged over the orbital and spin quantum numbers :

Two typical cases are considered here :

1. $n_1 j_1 \neq n_2 j_2$ (nonequivalent electrons)

$$A(n_1 j_1 n_2 j_2; k j_2 n_1 j_1) = \frac{2\pi}{k} (2j_1+1)(2j_2+1) \times \sum_{l'l'} \left[\frac{\delta(l,l')}{2l+1} P_{l'}^2(n_1 j_1 n_2 j_2; k j_2 n_1 j_1) + \frac{\delta(l,l')}{2l+1} P_{l'}^2(n_1 j_1 n_2 j_2; n_1 j_1 k j_2) - (-1)^{l+l'} \begin{Bmatrix} j_1 & j_2' & l' \\ j_2 & j_1' & l \end{Bmatrix} P_l(n_1 j_1 n_2 j_2; k j_2 n_1 j_1) P_l(n_1 j_1 n_2 j_2; n_1 j_1 k j_2) \right], \quad (\text{II.6.6})$$

2. $n_1 j_1 = n_2 j_2$ (equivalent electrons)

$$A(n_1 j_1 n_1 j_1; k j_2 n_1 j_1) = \frac{4\pi}{k} \frac{(2j_1+1)}{(4j_1+1)} (2j_1+1)(2j_2+1) \times \sum_{l'l'} 2 \left[\frac{\delta(l,l')}{2l+1} P_{l'}^2(n_1 j_1 n_1 j_1; k j_2 n_1 j_1) - (-1)^{l+l'} \begin{Bmatrix} j_1 & j_2' & l' \\ j_1 & j_1' & l \end{Bmatrix} P_l(n_1 j_1 n_1 j_1; k j_2 n_1 j_1) P_l(n_1 j_1 n_1 j_1; k j_2 n_1 j_1) \right]. \quad (\text{II.6.7})$$

Here we take into account that the statistical weight of configuration $n_1 j_1 n_2 j_2 LS$ is $2(2j_1+1)2(2j_2+1)$ for nonequivalent electrons and $(2j_1+1)(4j_1+1)$ for equivalent electrons. The numerical values of $A(n_1 j_1 n_2 j_2; k j_2 n_1 j_1)$ and $A(n_1 j_1 n_1 j_1; k j_2 n_1 j_1)$ for two-electron system with configuration up to 4d4d are given in Table II.6.1.

Formulae (II.6.6) and (II.6.7) can be considerably simplified in some important cases when the final state contains a 1s-electron :

$n_1j_1 \neq n_2j_2$:

$$A(n_1j_1n_2j_2;kj_2'1s) = \frac{2\pi}{k} (2j_2'+1)(j_1j_2j_2')^2 \times \left[\frac{1}{(2j_1+1)^2} R_{j_1}^2(n_1j_1n_2j_2;kj_2'1s) + \frac{1}{(2j_2+1)} R_{j_2}^2(n_1j_1n_2j_2;1skj_2') - \frac{(-1)^{(j_1+j_2)}}{(2j_1+1)(2j_2+1)} R_{j_1}(n_1j_1n_2j_2;kj_2'1s) R_{j_2}(n_1j_1n_2j_2;1skj_2') \right], \quad (\text{II.6.8})$$

$n_1j_1 = n_2j_2$:

$$A(n_1j_1n_1j_1;kj_2'1s) = \frac{4\pi}{k} \frac{(2j_2'+1)}{(4j_1+1)(2j_1+1)} (j_1j_2j_2')^2 \times R_{j_1}^2(n_1j_1n_1j_1;kj_2'1s). \quad (\text{II.6.9})$$

The expressions (II.6.6-9) give the autoionization rates of the two-electron system averaged over the orbital and spin quantum numbers. To generalize this problem to multi-electron system we have to consider two cases : two electrons which change their states in autoionization process belong to one group or to two different groups of equivalent electrons. One of these electrons goes to continuum and the other changes its state in the atom. Therefore, to calculate the autoionization width in general multi-electron systems we have to consider variations of states of the following configurations :

$$(n_1j_1)^{p_1}(n_2j_2)^{p_2}(n_3j_3)^{p_3} \quad (\text{II.6.10})$$

and

$$(n_1j_1)^{p_1}(n_2j_2)^{p_2}.$$

In the first case we consider the transition of the type

$$(n_1j_1)^{p_1}(n_2j_2)^{p_2}(n_3j_3)^{p_3} \rightarrow (n_1j_1)^{p_1-1}(n_2j_2)^{p_2-1}(n_3j_3)^{p_3+1}kl \quad (\text{II.6.11})$$

and in the second case of the type

$$(n_1j_1)^{p_1}(n_3j_3)^{p_2} \rightarrow (n_1j_1)^{p_1-2}(n_3j_3)^{p_2+1}kl.$$

The probabilities of the autoionization decay are given as follows :

1. case where three subshells are involved in autoionization decay:

$$A[(n_1j_1)^{p_1}(n_2j_2)^{p_2}(n_3j_3)^{p_3}-(n_1j_1)^{p_1-1}(n_2j_2)^{p_2-1}(n_3j_3)^{p_3+1}kl]=$$

$$p_1p_2\left(1-\frac{p_3}{2(2j_3+1)}\right)A(n_1j_1n_2j_2;k/n_3j_3),$$
(II.6.13)

2. case where two subshells are involved in autoionization decay:

$$A[(n_1j_1)^{p_1}(n_2j_2)^{p_2}-(n_1j_1)^{p_1-2}(n_2j_2)^{p_2+1}kl]=\frac{1}{2}p_1(p_1-1)\left(1-\frac{p_2}{2(2j_2+1)}\right)A(n_1j_1n_1j_1;k/n_2j_2),$$
(II.6.14)

where $A(n_1j_1n_2j_2;k/n_3j_3)$ and $A(n_1j_1n_1j_1;k/n_2j_2)$ are determined by Eqs.(II.6.6) and (II.6.7).

Formulae (II.6.13) and (II.6.14) should not be changed if we would add new groups of equivalent electrons to the configurations (II.6.10) because the operator $1/r_{12}$ changes the state of no more than two electrons. To determine the widths of autoionization states it is necessary to sum up A over all the finite states, i.e., over all rearrangements of the indices (i,g,m) as well as over indices of the emitted electron l and to combine both formulae (II.6.13) and (II.6.14). Finally we find the following autoionization width:

$$\Gamma((n_1j_1)^{p_1}(n_2j_2)^{p_2}\dots(n_Nj_N)^{p_N}) =$$

$$\sum_{i,g,m}^N A[(n_1j_1)^{p_1}(n_2j_2)^{p_2}\dots(n_mj_m)^{p_m}-(n_1j_1)^{p_1-1}(n_2j_2)^{p_2-1}\dots(n_mj_m)^{p_m+1}kl]\times\delta(E_k+E_{n_m}-E_{n_1}-E_{n_g})+$$

$$\sum_{i,m}^N A[(n_1j_1)^{p_1}(n_mj_m)^{p_m}-(n_1j_1)^{p_1-2}(n_mj_m)^{p_m+1}kl]\times\delta(E_k+E_{n_m}-2E_{n_1}),$$
(II.6.15)

where $E_k = k^2/2$ is the kinetic energy of the emitted electron and E_{n_i} , E_{n_g} and E_{n_m} are the one-particle non-relativistic energies of the bound electrons all of which are equal to $-1/2n^2$. In Eq.(II.6.15) we have written out in an explicit form the Kronecker's symbol for energies of the initial and final states. This restricts the summation over m . From the energy conservation

$$\frac{1}{2}k^2 + E_{n_m} = E_{n_i} + E_{n_g},$$

$E_{n_i} + E_{n_g} - E_{n_m}$ must be positive, i.e., the quantum number n_m must be smaller than the quantum numbers n_i and n_g .

For the illustration of the above formulae we present the autoionization width Γ for typical configurations in $1s2s^{p_1}2p^{p_2}n_j$ system :

$$\Gamma(1s2s^{p_1}2p^{p_2}n_j) =$$

$$\frac{1}{4}p_1(p_1-1)A(2s2s;ks1s) + \frac{1}{2}p_1p_2A(2s2p;kp1s) +$$

$$\frac{1}{2}p_1A(2sn_j;kj1s) + \frac{1}{4}p_2(p_2-1)\{A(2p2p;ks1s) + A(2p2p;kd1s)\} +$$

$$\frac{1}{2}p_2\{A(2pn_j;k(j-1)1s) + A(2pn_j;k(j+1)1s)\}.$$

(II.6.16)

Table II.6.1. Mean values of square of the matrix element, eV*.

Electronic configuration $n_1j_1n_2j_2n_1j_1k_{j_2}$	$A(n_1j_1n_2j_2;n_1j_1k_{j_2})$	Electronic configuration $n_1j_1n_2j_2n_1j_1k_{j_2}$	$A(n_1j_1n_2j_2;n_1j_1k_{j_2})$
202010k0	0.1353742E+00	313110k0	0.4334630E-03
202110k1	0.4007047E-01	313110k2	0.4349244E-02
203010k0	0.1713699E-01	313120k0	0.2123355E-04
203110k1	0.1142916E-01	313120k2	0.5108035E-02
203210k2	0.1137283E-02	313121k1	0.1846140E+00
204010k0	0.6909104E-02	313210k1	0.1086592E-04
204110k1	0.4757865E-02	313210k3	0.5422759E-03
204210k2	0.5989454E-03	313220k1	0.1143075E-02
204310k3	0.1194274E-04	313220k3	0.1131785E-01
212110k0	0.6836230E-02	313221k0	0.1210498E-01
212110k2	0.8197643E-01	313221k2	0.1037155E+00
213010k1	0.8239322E-02	314010k1	0.8885289E-03
213110k0	0.1486025E-02	314020k1	0.1428472E-01
213110k2	0.1567209E-01	314021k0	0.2188851E-01
213210k1	0.7047191E-04	314110k0	0.1443133E-03
213210k3	0.3228880E-02	314110k2	0.1416621E-02
214010k1	0.3103617E-02	314120k0	0.6745998E-05
214110k0	0.6061064E-03	314120k2	0.1432632E-02
214110k2	0.6114865E-02	314121k1	0.4736068E-01
214210k1	0.3767503E-04	314210k1	0.5814587E-05
214210k3	0.1652319E-02	314210k3	0.2829510E-03
214310k2	0.5225128E-06	314220k1	0.4781162E-03
214310k4	0.1174001E-03	314220k3	0.2744082E-02
303010k0	0.8452666E-02	314221k0	0.2888935E-02
303020k0	0.1298267E+00	314221k2	0.3639755E-01
303110k1	0.2358414E-02	314310k2	0.1252982E-06
303120k1	0.6606562E-01	314310k4	0.1626205E-04
303121k0	0.5445527E-01	314320k2	0.6460321E-03
303210k2	0.2050333E-03	314320k4	0.3973397E-02
303220k2	0.6868159E-01	314321k1	0.3657072E-04
303221k1	0.4613040E-03	314321k3	0.5279547E-02
304010k0	0.1690209E-02	323210k0	0.1240500E-06
304020k0	0.2077584E-01	323210k2	0.7386578E-06
304110k1	0.9830592E-03	323210k4	0.6972003E-04
304120k1	0.2628151E-01	323220k0	0.1620228E-02
304121k0	0.1181018E-01	323220k2	0.1755390E-02
304210k2	0.1078268E-03	323220k4	0.3823095E-01
304220k2	0.2571912E-01	323221k1	0.2194059E-01
304221k1	0.1997177E-03	323221k3	0.2729374E+00
304310k3	0.1828313E-05	324010k2	0.7440466E-04
304320k3	0.6673792E-02	324020k2	0.1540260E-01
304321k2	0.2190811E-02	324021k1	0.6974708E-04

* 0.4007047E-01 means 0.4007047*10⁻¹

Table II.6.1. Continuation.

Electronic configuration $n_1j_1n_2j_2n_1j_1'k_j_2'$	$A(n_1j_1n_2j_2;n_1j_1'k_j_2')$	Electronic configuration $n_1j_1n_2j_2n_1j_1'k_j_2'$	$A(n_1j_1n_2j_2;n_1j_1'k_j_2')$
324110k1	0.3754825E-05	414220k3	0.8050460E-03
324110k3	0.1905760E-03	414221k0	0.1307118E-02
324120k1	0.5813416E-03	414221k2	0.8895547E-02
324120k3	0.3637278E-02	414310k2	0.5166560E-07
324121k0	0.5698759E-02	414310k4	0.5378402E-05
324121k2	0.2648852E-01	414320k2	0.1680534E-03
324210k0	0.4822074E-07	414320k4	0.8878215E-03
324210k2	0.3536460E-06	414321k1	0.7659674E-05
324210k4	0.2978746E-04	414321k3	0.8463108E-03
324220k0	0.4238389E-03	424210k0	0.2275004E-07
324220k2	0.6644706E-03	424210k2	0.2074035E-06
324220k4	0.5917673E-02	424210k4	0.1586524E-04
324221k1	0.6858957E-02	424220k0	0.9707705E-04
324221k3	0.6470531E-01	424220k2	0.2333356E-03
324310k1	0.9251373E-08	424220k4	0.1628462E-02
324310k3	0.5794120E-07	424221k1	0.2120880E-02
324310k5	0.1907893E-05	424221k3	0.1892440E-01
324320k1	0.3653635E-04	424310k1	0.4922826E-08
324320k3	0.6792153E-03	424310k3	0.2857428E-07
324320k5	0.6621568E-02	424310k5	0.8355666E-06
324321k0	0.7684954E-04	424320k1	0.2494282E-04
324321k2	0.6576700E-03	424320k3	0.1856463E-03
324321k4	0.2744000E-01	424320k5	0.7730885E-03
404010k0	0.1348413E-02	424321k0	0.3888767E-04
404020k0	0.1157387E-01	424321k2	0.8244574E-04
404110k1	0.3704147E-03	424321k4	0.4126228E-02
404120k1	0.5707020E-02	434310k0	0.5620801E-10
404121k0	0.4734870E-02	434310k2	0.2670124E-09
404210k2	0.3906301E-04	434310k4	0.2919349E-08
404220k2	0.5396224E-02	434310k6	0.3461214E-07
404221k1	0.5404846E-04	434320k0	0.1471619E-07
404310k3	0.6386833E-06	434320k2	0.1425021E-04
404320k3	0.1035849E-02	434320k4	0.1344863E-03
404321k2	0.8229092E-03	434320k6	0.5235595E-03
414110k0	0.6874160E-04	434321k1	0.4720087E-05
414110k2	0.6646596E-03	434321k3	0.8137828E-05
414120k0	0.9266958E-05	434321k5	0.1500449E-02
414120k2	0.5859216E-03		
414121k1	0.1606276E-01		
414210k1	0.2006968E-05		
414210k3	0.1000068E-03		
414220k1	0.1777911E-03		

7. LS-averaging of radiative transition probability:

First order of Z-expansion method for dipole matrix element

In the present section we derive the analytical formulae for the radiative transition probability averaged over the L and S quantum numbers with regard to the first order of the perturbation theory by 1/Z-parameter for the dipole matrix element and present the results of calculation. The dipole matrix element is considered in the non-relativistic approach.

We shall start with the general formulae for the radiative transition probability, W, of the two-electron system in the LS-coupling scheme :

$$W(n_1j_1n_2j_2LS-n_1j_1n_2j_2L'S)=$$

$$\frac{2}{(2L+1)(2S+1)}[E(n_1j_1n_2j_2LS)-E(n_1j_1n_2j_2L'S)]^3[P(n_1j_1n_2j_2LS-n_1j_1n_2j_2L'S)]^2,$$

(II.7.1)

where n_ij_i is the electronic configuration of the i-th electron, L and S are the total angular and spin momenta, $E(n_1j_1n_2j_2LS)$ is the energy of the LS state and P is the dipole matrix element. Averaging of (II.7.1) over LS and L' can be done through the following procedure :

$$W(n_1j_1n_2j_2-n_1j_1n_2j_2')=\frac{\sum_{L'} \sum_{LS} (2L+1)(2S+1)W(n_1j_1n_2j_2LS-n_1j_1n_2j_2'L'S)}{\sum_{LS} (2L+1)(2S+1)},$$

(II.7.2)

and performed separately for the transition energy and the dipole matrix element. As averaging of the energy has been already done in the previous sections, here we will treat only the dipole matrix element. After averaging the energy we have the following radiative transition probability :

$$W(n_1j_1n_2j_2-n_1j_1n_2j_2')= \frac{2}{g} (E(n_1j_1n_2j_2)-E(n_1j_1n_2j_2'))^3 \sum_{L'} \sum_{LS} [P(n_1j_1n_2j_2LS-n_1j_1n_2j_2'L'S)]^2, \quad (\text{II.7.3})$$

where $g=4(2j_1+1)(2j_2+1)$ is the statistical weight.

We can represent the dipole matrix element as a series of $1/Z$ powers and, taking into account the $1/Z$ -dependence of its zero-th order, we can write:

$$ZP(n_1j_1n_2j_2LS-n_1j_1n_2j_2'L'S)= P^{(0)}(n_1j_1n_2j_2LS-n_1j_1n_2j_2'L'S)+\frac{1}{Z}P^{(1)}(n_1j_1n_2j_2LS-n_1j_1n_2j_2'L'S), \quad (\text{II.7.4})$$

where $P^{(i)}$ is the i -th order of dipole matrix element.

To average the square of dipole matrix element with regard to the first order we have to consider the expression:

$$Z^2 \sum_{L'} \sum_{LS} P(n_1j_1n_2j_2LS-n_1j_1n_2j_2'L'S)^2= \sum_{L'} \sum_{LS} [\{P^{(0)}(n_1j_1n_2j_2LS-n_1j_1n_2j_2'L'S)\}^2+ \frac{2}{Z}P^{(0)}(n_1j_1n_2j_2LS-n_1j_1n_2j_2'L'S)P^{(1)}(n_1j_1n_2j_2LS-n_1j_1n_2j_2'L'S)], \quad (\text{II.7.5})$$

where

$$P^{(0)}(n_1j_1n_2j_2LS-n_1j_1n_2j_2'L'S)=Q(n_2j_2,n_2j_2')(-1)^{j_1} \begin{Bmatrix} L & L' & 1 \\ j_2' & j_2 & j_1 \end{Bmatrix} \sqrt{(2L+1)(2L'+1)(2S+1)/3} \quad (\text{II.7.6})$$

and

$$P^{(1)}(n_1j_1n_2j_2LS-n_1j_1n_2j_2'L'S)= T(n_1j_1n_2j_2L;n_2j_2'n_1j_1L')+T(n_1j_1n_2j_2L';n_2j_2'n_1j_1L)+ (-1)^{j_1+j_2+L+S} [T(n_2j_2n_1j_1L;n_2j_2'n_1j_1L')+T(n_1j_1n_2j_2L';n_1j_1n_2j_2L)]+$$

$$(-1)^{j_1+j_2+L'+S} [T(n_1j_1n_2j_2L;n_1j_1n_2j_2L')+T(n_2j_2n_1j_1L';n_2j_2n_1j_1L)] +$$

$$(-1)^{j_2+j_2'+L+L'} [T(n_2j_2n_1j_1L;n_1j_1n_2j_2L')+T(n_2j_2n_1j_1L';n_1j_1n_2j_2L)]$$

(II.7.7)

with the following notations:

$$Q(nj,n'j') = \sqrt{(2j+1)(2j'+1)} \begin{pmatrix} j & j' & 1 \\ 0 & 0 & 0 \end{pmatrix} R(nj,n'j'),$$

(II.7.8)

$$T(n_1j_1n_2j_2L;n_2j_2n_1j_1L') =$$

$$-\sum_l \sum_{l'} t_{ll'}(n_1j_1n_2j_2;n_2j_2n_1j_1') (-1)^{l+L'+(j_2+j_1-j_1'-j_2+1)/2} \times$$

$$\sqrt{(2L+1)(2L'+1)(2S+1)/3} \begin{pmatrix} l & j_2 & L' \\ j_2' & j_1' & l' \end{pmatrix} \begin{pmatrix} L & L' & 1 \\ l & j_1 & j_2 \end{pmatrix},$$

(II.7.9)

where

$$t_{ll'}(n_1j_1n_2j_2;n_2j_2n_1j_1') =$$

$$-\sum_n \frac{2l+1}{E_n + E_{n_2} - E_{n_2'} - E_{n_1'}} R(nl,n_1j_1) R_{l'}(nln_2j_2;n_2j_2n_1j_1') \times$$

$$\sqrt{(2j_1+1)(2j_2+1)(2j_1'+1)(2j_2'+1)} \begin{pmatrix} l & j_1 & 1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l & j_1' & l' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} j_2 & j_2' & l' \\ 0 & 0 & 0 \end{pmatrix},$$

(II.7.10)

$R(n_1j_1,n_2j_2)$ and $R_l(n_1j_1n_2j_2;n_2j_2n_1j_1')$ are the dipole and Coulomb radial integrals, respectively, and the last multiplier in Eq.(II.7.10) is the product of the Wigner's 3-j symbols. The summation over n in Eq.(II.7.10) means the summation over discrete states and the integration over continuum; E_n and E_{n_i} are the non-

relativistic one-particle energies equal to $-1/2n^2$.

The summation over LS in Eq.(II.7.5) can be made for both $(P^{(0)})^2$ and $P^{(0)}P^{(1)}$ terms. The final results for two terms in Eq.(II.7.5) are as follows :

$$\sum_{L'} \sum_{LS} [(P^{(0)}(n_1j_1n_2j_2LS-n_1j_1n_2j_2L'S))]^2 =$$

$$\sum_{L'} \sum_{LS} [Q(n_2j_2, n_2j_2')]^2 \begin{Bmatrix} L & L' & 1 \\ j_2 & j_2' & j_1 \end{Bmatrix}^2 (2L+1)(2L'+1)(2S+1)/3 = \frac{g}{3(2j_2+1)} [Q(n_2j_2, n_2j_2')]^2,$$

(II.7.11)

and

$$\sum_{L'} \sum_{LS} P^{(0)}(n_1j_1n_2j_2LS-n_1j_1n_2j_2L'S)P^{(1)}(n_1j_1n_2j_2LS-n_1j_1n_2j_2L'S) = \frac{2}{3} Q(n_2j_2, n_2j_2')^2 (-1)^{j_2+j_2'+1} \times$$

$$\left\{ 2\sqrt{(2j_1+1)} \left(t_{j_2 0}(j_2j_1; j_1j_2')/\sqrt{(2j_2+1)} + t_{j_2 0}(j_2j_1; j_1j_2)/\sqrt{(2j_2+1)} \right) + \right.$$

$$\left. \frac{2}{3} \sum_l (-1)^{l+j_1+1} (t_{l1}(j_1j_2; j_2j_1) + t_{l1}(j_1j_2'; j_2j_1)) - \right.$$

$$\left. \sum_l \left(t_{j_2 l}(j_2j_1; j_2j_1)/(2j_2+1) + t_{j_2 l}(j_2j_1'; j_2j_1)/(2j_2+1) \right) - \right.$$

$$\left. \sum_l \sum_{l'} (-1)^{l+j_1+1} \left[\begin{Bmatrix} j_2' & l & l' \\ j_1 & j_2 & 1 \end{Bmatrix} t_{ll'}(j_1j_2; j_1j_2') + \begin{Bmatrix} j_2 & l & l' \\ j_1 & j_2' & 1 \end{Bmatrix} t_{ll'}(j_1j_2'; j_1j_2) \right] \right\}.$$

(II.7.12)

Combining Eqs. (II.7.3), (II.7.5), (II.7.11) and (II.7.12) we can write the final expression of the radiative transition probability averaged over LS for two-electron system in the form :

$$W(n_1j_1n_2j_2-n_1j_1n_2j_2') =$$

$$\frac{2}{3(2j_2+1)} \frac{1}{Z^2} [E(n_1j_1n_2j_2) - E(n_1j_1n_2j_2')]^3 [Q(n_2j_2, n_2j_2')]^2 \left[1 + \frac{2}{Z} S(n_1j_1n_2j_2-n_1j_1n_2j_2') \right],$$

(II.7.13)

where $S(n_1j_1n_2j_2-n_1j_1n_2j_2')$ is given by

$$\begin{aligned}
 S(n_1j_1n_2j_2-n_1j_1n_2j_2') = & \frac{1}{2(2j_1+1)Q(n_2j_2, n_2j_2')} \times \\
 & \left\{ 2\sqrt{(2j_1+1)} \left((t_{j_20}(j_2j_1; j_1j_2) / \sqrt{(2j_2+1)} + (t_{j_20}(j_2j_1; j_1j_2) / \sqrt{(2j_2+1)}) \right) + \right. \\
 & \quad \left. \frac{2}{3} \sum_l (-1)^{l+j_1+1} (t_{l1}(j_1j_2; j_2j_1) + t_{l1}(j_1j_2'; j_2j_1)) - \right. \\
 & \quad \left. \sum_l \left(\{l_{1j_2'}\} t_{j_2l}(j_2j_1; j_2j_1) / (2j_2+1) + \{l_{1j_2}\} t_{j_2l}(j_2j_1; j_2j_1) / (2j_2+1) \right) - \right. \\
 & \quad \left. \sum_l \sum_{l'} (-1)^{l+j_1+1} \left[\begin{matrix} j_2' & l & l' \\ j_1 & j_2 & 1 \end{matrix} \right] t_{ll'}(j_1j_2; j_1j_2') + \left[\begin{matrix} j_2 & l & l' \\ j_1 & j_2' & 1 \end{matrix} \right] t_{ll'}(j_1j_2'; j_1j_2) \right] \left. \right\}.
 \end{aligned}
 \tag{II.7.14}$$

In two equivalent electron system the denominator in the first multiplier in Eq.(II.7.14) should be replaced to $2(2j_1+1/2)Q(n_2j_2, n_2j_2')$.

To generalize this result for many-electron system we will consider the following transition $(nj)^{k+1}(n'j')^{k'-1}\Phi - (nj)^k(n'j')^{k'}\Phi$, where Φ is the electronic configuration (for convenience we change the designation Q which has been used in the previous sections) and in the present case is : $\Phi = 1s^{k_1}2s^{k_2}2p^{k_3}3s^{k_4}3p^{k_5}3d^{k_6}4s^{k_7}4p^{k_8}4d^{k_9}4f^{k_{10}}$ and nj and $n'j'$ belonging to any subshell of this configuration. The generalization gives the following result :

$$\begin{aligned}
 W((nj)^{k+1}(n'j')^{k'-1}\Phi - (nj)^k(n'j')^{k'}\Phi) = & \\
 & \frac{1}{Z^2} \frac{4}{3} [E((nj)^{k+1}(n'j')^{k'-1}\Phi) - E((nj)^k(n'j')^{k'}\Phi)]^3 [Q(nj, n'j')]^2 \times \\
 & \frac{k'}{2(2j'+1)} \left(1 - \frac{k}{2(2j+1)} \right) \left[1 + \frac{2}{Z} \sum_{i=1}^N (k_i - \delta(n_j, n'j')) S(n_j, n_j - n_j, n'j') \right],
 \end{aligned}
 \tag{II.7.15}$$

where the summation is performed over all the subshells, i.e., over all the groups of electrons with different quantum numbers n and j .

The analytical expressions obtained can be used for the calculation of X-ray

emission rates for different atoms .

The main part of the calculation is to calculate the value of $S(n_1j_1n_2j_2-n_1j_1n_2j_2)$ which is given by Eq.(II.7.14). Here we present some details of this calculation. As mentioned above, the sum in Eq.(II.7.10) means the sum over both the discrete spectrum and the integration over the continuous spectrum. The following Coulomb and dipole radial integrals in Eq.(II.7.10) with all discrete parameters and with one continuous parameter have been treated analytically :

$$R_l(n_1j_1n_2j_2;n_2j_2n_1j_1) = \int_0^\infty dr_1 r_1^2 \int_0^\infty dr_2 r_2^2 U_l(r_1, r_2) R_{n_1j_1}(r_1) R_{n_2j_2}(r_2) R_{n_2j_2}(r_2) R_{n_1j_1}(r_1),$$

$$R_l(kj_1n_2j_2;n_2j_2n_1j_1) = \int_0^\infty dr_1 r_1^2 \int_0^\infty dr_2 r_2^2 U_l(r_1, r_2) R_{kj_1}(r_1) R_{n_2j_2}(r_2) R_{n_2j_2}(r_2) R_{n_1j_1}(r_1),$$

where

$$U_l(r_1, r_2) = \Theta(r_1 - r_2) \frac{r_2^l}{r_1^{l+1}} + \Theta(r_2 - r_1) \frac{r_1^l}{r_2^{l+1}},$$

$$R(n_1j_1, n_2j_2) = \int_0^\infty dr r^2 R_{n_1j_1}(r) r R_{n_2j_2}(r),$$

$$R(kj_1, n_2j_2) = \int_0^\infty dr r^2 R_{kj_1}(r) r R_{n_2j_2}(r).$$

The radial functions of the discrete and continuous states are [31] :

$$R_{nj}(r) = \frac{1}{(2j+1)!} \left\{ \frac{(n+j)!}{(n-j-1)!} \right\}^{1/2} \frac{2}{n^2} e^{-r/n} \left(\frac{2}{r} \right)^j F(-n+j+1, 2j+2, \frac{2r}{n})$$

and

$$R_{kj}(r) = \sqrt{\frac{2}{\pi}} k e^{\pi/2} \frac{|\Gamma(j+1+1/ik)|}{(2j+1)!} (2kr)^j e^{-ikr} F(-1/ik, 2j+2, 2ikr),$$

where Θ is the theta-function, F is the confluence hypergeometric function and Γ is the gamma-function. The radial function of continuous spectrum is normalized in the k -scale.

The sum over the discrete spectrum in Eq.(II.7.10) has been calculated for the quantum numbers $n=1-50$ and asymptotical evaluation of the Coulomb integrals proportional to $1/n^3$ has been used to take into account the contribution of the rest part of the spectrum. The integral over continuum has been calculated numerically by the extended Simpson's rule with the step $h=0.05$ and $k=0.01-5$. The relative uncertainties of the present calculation of the sum in Eq.(II.7.10) are estimated to be of the order of 10^{-4} .

The numerical values of $S(n_1j_1n_2j_2-n_1j_1n_2j_2')$ given by Eq.(II.7.14) for different transitions are presented in Table II.7.1.

Table II.7.1. Numerical values of $S(n_1j_1n_2j_2-n_1j_1n_2j_2')$

Electronic configuration $n_1j_1n_2j_2, n_1j_1n_2j_2'$	$S(n_1j_1n_2j_2-n_1j_1n_2j_2')$	Electronic configuration $n_1j_1n_2j_2, n_1j_1n_2j_2'$	$S(n_1j_1n_2j_2-n_1j_1n_2j_2')$
10211010	-0.154775	10311020	-0.044860
20212010	-0.161135	20312020	-0.087249
21212110	-0.151501	21312120	-0.157203
30213010	-0.029340	30313020	-0.123708
31213110	-0.056669	31313120	-0.051133
32213210	-0.051318	32313220	-0.008191
40214010	-0.011483	40314020	-0.045120
41214110	-0.016213	41314120	-0.055522
42214210	-0.015795	42314220	-0.011704
43214310	-0.005128	43314320	-0.034314
10211020	0.823184	10311030	0.899480
20212020	0.265608	20312030	0.558128
21212120	0.076032	21312130	0.571122
30213020	0.201151	30313030	0.247069
31213120	-0.099027	31313130	0.172067
32213220	-0.830387	32313230	-0.041756
40214020	0.465830	40314030	0.200510
41214120	0.073440	41314130	0.117172
42214220	-0.724366	42314230	-0.226866
43214320	-1.058331	43314330	-0.792079
10301021	2.456648	10321021	-0.762947
20302021	0.959442	20322021	-0.004509
21302121	1.571283	21322121	-0.047090
30303021	0.222180	30323021	0.111903
31303121	0.249491	31323121	0.043286
32303221	0.008348	32323221	-0.109460
40304021	-0.043408	40324021	0.035411
41304121	0.039322	41324121	0.000447
42304221	-0.055137	42324221	-0.037954
43304321	0.006379	43324321	0.029505
10311010	0.365955	10321031	-1.023694
20312010	-0.241941	20322031	-0.795314
21312110	-0.048184	21322131	-0.833575
30313010	-0.218407	30323031	-0.301699
31313110	-0.186980	31323131	-0.250255
32313210	-0.233723	32323231	-0.055310
40314010	-0.049825	40324031	-0.279541
41314110	-0.141400	41324131	-0.144495
42314210	-0.101365	42324231	0.191111
43314310	-0.131533	43324331	0.809640
10311020	-0.044860	10401021	2.216724
20312020	-0.087249	20402021	0.708640

Table II.7.1. Continuation

Electronic configuration $n_1j_1n_2j_2, n_1j_1n_2j_2$	$S(n_1j_1n_2j_2-n_1j_1n_2j_2)$	Electronic configuration $n_1j_1n_2j_2, n_1j_1n_2j_2$	$S(n_1j_1n_2j_2-n_1j_1n_2j_2)$
21402121	0.920852	40414030	-0.079185
30403021	0.540886	41414130	0.034799
31403121	0.231688	42414230	0.006766
32403221	0.430041	43414330	0.095338
40404021	-0.024957	10411032	-1.777307
41404121	0.061388	20412032	-2.549926
42404221	-0.031404	21412132	-2.888766
43404321	-0.068051	30413032	-1.082949
10401031	2.339532	31413132	-1.300756
20402031	1.531662	32413232	-2.268968
21402131	1.705634	40414032	-0.406483
30403031	0.677181	41414132	-0.545066
31403131	0.695820	42414232	-0.366843
32403231	0.963797	43414332	0.082881
40404031	0.293417	10411040	0.926948
41404131	0.321338	20412040	0.698754
42404231	0.188459	21412140	0.727444
43404331	-0.132277	30413040	0.442760
10411010	0.508325	31413140	0.435212
20412010	-0.231610	32413240	0.423642
21412110	-0.074805	40414040	0.233068
30413010	-0.382246	41414140	0.191593
31413110	-0.153852	42414240	0.101066
32413210	-0.404749	43414340	-0.105374
40414010	-0.264919	10421021	-0.932565
41414110	-0.220250	20422021	-0.611744
42414210	-0.202157	21422121	-0.889690
43414310	-0.352215	30423021	-0.068872
10411020	0.309046	31423121	-0.134451
20412020	0.255476	32423221	-0.245648
21412120	0.098552	40424021	0.111572
30413020	-0.106088	41424121	0.083019
31413120	0.098903	42424221	0.001069
32413220	0.065481	43424321	0.062469
40414020	-0.148267	10421031	-0.696506
41414120	-0.094902	20422031	-0.077912
42414220	-0.040375	21422131	-0.102992
43414320	-0.122624	30423031	0.077158
10411030	-0.047119	31423131	0.063497
20412030	-0.062888	32423231	0.143341
21412130	0.061419	40424031	0.097656
30413030	-0.044126	41424131	0.102670
31413130	-0.074366	42424231	-0.025404
32413230	0.018507	43424331	-0.195047

Table II.7.1. Continuation.

Electronic configuration $n_1j_1n_2j_2n_1j_1n_2j_2$	$S(n_1j_1n_2j_2-n_1j_1n_2j_2')$	Electronic configuration $n_1j_1n_2j_2n_1j_1n_2j_2$	$S(n_1j_1n_2j_2-n_1j_1n_2j_2')$
10421041	-1.015977	32433232	0.104547
20422041	-0.886908	40434032	-0.104312
21422141	-0.919824	41434132	-0.020097
30423041	-0.552912	42434232	0.110587
31423141	-0.563651	43434332	0.411925
32423241	-0.566942	10431042	1.002636
40424041	-0.258772	20432042	1.067460
41424141	-0.236651	21432142	1.055556
42424241	-0.151023	30433042	0.747195
43424341	0.057177	31433142	0.765509
10431032	0.988523	32433242	0.814757
20432032	0.578020	40434042	0.333849
21432132	0.642961	41434142	0.306280
30433032	0.076139	42434242	0.234213
31433132	0.064929	43434342	0.043724

III. Summaries

The purpose of the present work was to develop and suggest the theoretical method and create numerical codes for the calculation of the atomic characteristics (such as radiative transition energy, radiative transition probabilities and autoionizing rates) of the highly ionized atoms with an arbitrary number of electrons and in any electronic configuration (including highly excited Rydberg states). These requirements have arisen in order to apply the theoretical method to study the formation-deexcitation processes in "hollow atoms" which are formed via neutralization under the interactions of highly charged ions with a metallic surface. The mechanisms of formation and deexcitation of such a highly excited state of atom have been described in Chapter I.

The satellite transitions and Auger cascades play an important role in the deexcitation of such a "hollow atom" and the calculation of the atomic characteristics of these processes was one of the main subjects of the present work. In view of applications to highly charged ions the theoretical method has been based on the perturbation theory using the nuclear charge Z of the ion as a parameter and the inter electron interaction and relativistic correction as perturbations (the so-called Z -expansion method). The perturbation theory gives all atomic characteristics expressed as a series of expansion in $1/Z$. The screening parameter has been introduced in order to improve the accuracy of the calculation. To facilitate the calculation and reduce a vast number of possible states for many-electron systems all the atomic characteristics have been averaged over the total orbital and spin quantum numbers and found to be expressed in analytical forms as a function of the electron numbers in various shells of the ion. The derivation of the analytical formulae and the description of the theoretical approach are given in the Chapter II.

The present method has the following advantages :

1. An important advantage of this method is that expansion coefficients for energy including relativistic corrections are the same for all ions belonging to a given isoelectronic sequence. Moreover, all radial integrals in perturbation theory formulas are the same for all atoms and ions. This feature of the theoretical method is very important in calculation of the energies and radiative probabilities of the satellite transitions.
2. The introduction of the screening parameter described in Chapter II allows us to take into account a part of the second order correction of the non-relativistic as well as relativistic energy and to obtain appreciable accuracy without the necessity to compute more elaborate terms of the second and higher orders perturbation

theory.

3. The expansion coefficients for the energy E can be extrapolated on the principal quantum number n , i.e., if we have the coefficient for $n=n_0$ then the following formula is used for $n>n_0$:

$$E(n) = E(n_0) \left(\frac{n_0}{n}\right)^3.$$

This extrapolation allows us to calculate the atomic characteristics of the ions in highly excited states.

4. The averaging over LS reduces the vast number of possible states of many-electron system and allows us to express the atomic characteristics as a function of number of electrons in different shells of the ion. Therefore, this theoretical method can be applied practically to any atomic system with arbitrary number of electrons.

5. The numerical codes for the calculation of the atomic characteristics which have been created on the base of the present theoretical approach need considerably less time in comparison with other methods well known.

The theoretical method suggested has been applied for the study of deexcitation processes and identification of the observed X-ray spectrum resulted from the interaction of highly charged Xe^{q+} ($q=44-48$) [13,32] and Ar^{q+} ($q=17$) ions [36,37] with metallic surfaces (Cu and Ag, respectively). It was found that the present method of calculation gives generally good results (a comparison was made with results obtained by other methods) and allows to describe the main features of the X-ray spectrum and determine the possible states of ions which contribute to the observed spectrum lines. The accuracy of the calculations can be improved by increasing the number of the screening parameters, i.e., by introducing the screening parameter for each subshell of the ion (the states with the same principal and orbital quantum numbers n and j). This method has been also applied to calculate the K_{α} X-ray emission rates for atoms with $Z=10-36$ [38] in order to study the contribution of the first order of the dipole matrix elements to the radiative transition probability. The comparison with other theoretical data shows that the present method can be also applied for the calculation of the atomic characteristics of nearly neutral atoms.

The results of various applications of the suggested theoretical approach allow us to conclude that this method can be very useful for calculation of the atomic characteristics of the multi-electron highly charged ions including ions in highly excited states. The present approach can be also useful for study and simulation of the neutralization-deexcitation processes which take place during the interaction of the highly charged ions with a surface.

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