ADIABATIC ASYMPTOTIC THEORY OF THE TWO-ELECTRON EXCHANGE AT RELATIVISTIC BINDING ENERGIES

V.Yu. Lazur, O.K. Reity, S.I. Myhalyna

Department of Theoretical Physics, Uzhhorod National University, Voloshin Str. 54, Uzhhorod 88000, Ukraine

An asymptotic (over a large internuclear distance) theory of two-electron exchange in collision of a multielectron atom and multiply charged ion is constructed. In the framework of the quasirelativistic Dirac-Breit approximation the matrix element of two-electron exchange interaction is analytically calculated. This approach allows to take into account the relativistic effects connected with the magnetic and retardation interelectron interactions. In the nonrelativistic limit the matrix element obtained proceeds to the result of paper [6].

Introduction

Processes of heavy particle collisions with forming of vacancies in inner shells of atoms form the basis of many widely applicable practical methods of quantitative and qualitative analysis of matters, such as a Auger-spectroscopy, photo- and x-ray electron spectroscopy, electron and proton x-ray spectroscopy etc. The set of these processes is one of the main information sources about the structure and properties of inner shells of atoms. Therefore, detailed experimental and theoretical study of various collision processes of forming and decay of vacancies in inner shells of atoms is of the great applied and fundamental importance.

The collisions of the multiply charged ions $B^{Z_b+}(Z_b >> 1)$ with neutral atoms A with large performance can lead to forming of two and more vacancies in inner shells of A. Under favourable conditions the mechanisms of nonadiabatic bound cause multielectronic transitions with effective cross-sections $10^{-16} - 10^{-18} cm^2$. In symmetrical systems $A + A^{Z+}$ with a completely stripped ("bare") ion A^{Z+} forming of two vacancies in the K-shell can occur at the expense of processes of two-electronic recharge

$$A + A^{Z+} \to A^{++} + A^{(Z-2)+}(1s^2) \qquad (1)$$

at distances that are larger than sizes of a united atom. Also, other more complicated mechanisms of forming of two vacancies in K-shell and higher shells are possible. If the two-electron vacancies are forming due to nonadiabatic two-electron transitions, the correlation effects play an essential role and the consideration of the problem is hardly possible in the framework of approximation of one-electron molecular orbitals. Furthermore, if the collision energy is not too large, the connection of processes with inner-shell electrons and of similar processes where the transitions execute by outer electrons is observed. Unfortunately, all these phenomena are little studied, and for processes including highly charged ions and bare nuclei are not investigated at all. This situation is a surprising example of inertia in a theoretical field in the face of deficiency of experimental data that is not of the principal character and very likely connected with the difficulties in construction of sources of multiply charged ions and formation of beams of rather slow particles. In last decade in this range of studies the targeted work is carried out (see, for example, [1, 2]), and the creation of the theory of multielectronic processes in ion-atomic and ion-ionic collisions is one of the most important problems.

In this paper the process of exchange of two electrons at collision of the multielectronic atom A with the multiply charged ion B^{Z_b+} we shall study on the elementary exam-

ple of collision of He-like ion $A^{(Z_a-2)+}(e_1,e_2)$ with the stripped nucleus; for the helium atom and α-particle $Z_a = Z_b = 2$:

$$A^{(Z_a-2)+}(e_1,e_2) + B^{Z_b+} \rightarrow \\ \rightarrow A^{Z_a+} + B^{(Z_b-2)+}(e_1,e_2). \qquad (2)$$

Nevertheless, developed below theoretical ideas about physical features of two-electron exchange are of the general character. The formal construction of the theory will be given in the form, suitable for the description of collisions of arbitrary atomic particles.

Since the binding energy of inner-shell electrons rapidly increases with increasing nuclear charge Z_i $(i = a,b)$, at tight collisions of heavy nuclei with own atoms the inner-shell electrons fall in the two-centre potential

$$V_{ab}(\vec{r}) = -\frac{Z_a e^2}{r_1} - \frac{Z_b e^2}{r_2}, \quad r_{1,2} = \left|\vec{r} \pm \vec{R}/2\right|,$$

of the united system $A^{Z_a+} + B^{Z_b+}$ with forming of a heavy quasimolecule.

The traditional description of processes with rearrangement of electrons at slow ion-atomic collisions is based on the introduction of the matrix element of the two-electron exchange interaction.

General structure of the matrix element of two-electron exchange interaction in the Dirac-Breit approximation

The process of the electron capture at collision of He-like ion $A^{(Z_a-2)+}$ and bare nucleus B^{Z_b+} can be realized either as a result of two successive one-electron transitions in one collision event including of intermediate state $A^{(Z_a-1)+} + B^{(Z_b-1)+}$:

$$A^{(Z_a-2)+} + B^{Z_b+} \rightarrow A^{(Z_a-1)+} + B^{(Z_b-1)+} \rightarrow \\ \rightarrow A^{Z_a+} + B^{(Z_b-2)+}(e_1,e_2), \qquad (3)$$

or as a result of the straight two-electron transition in points of quasi-crossing of adiabatic potential curves of original and final states of reaction (2) in one collision.

The first mechanism (3) is simpler and studied much more than the simultaneous transition of two-electrons from one nucleus to the other one (reaction (2)). The studies of resonant two-electron capture (in collision of atom A and two-charged ion A^{++} of the same chemical element), carried out in [3, 4], have shown that the process of exchange of two electrons in a direct way (2) comprises a number of interesting features that are not inherent in the mechanism of serial drift of electrons from atom A to ion A^{++}. In this sense the nonresonance exchange of two electrons (in collision of different atom and ion) is not an exception (see [5, 7] and review [8]).

In adiabatic range of collision velocities the capability of a qualitative analysis of the transitions dynamics in reaction (2) yields the approach based on separation of the so-called ranges of non-adiabaticity [9]. Adiabatic evolution of the electronic subsystem on quasimolecular potential curves leads to the fact that the probabilities of transitions between levels separated by considerable energy interval are exponentially small. The nonadiabatic transitions are localized in small vicinity of crossing point R_c of diabatic quasimolecular potential curves of original and final states of process (2). In each of such vicinities the adiabatic potential curves form the quasi-crossing, and spacing interval between potential curves $\Delta E(R)$ at R_c is equal to the matrix element of the exchange interaction $\Delta(R)$ of two-electron diabatic states $A^{(Z_a-2)+} + B^{Z_b+}$ and $A^{Z_a+} + B^{(Z_b-2)+}$.

The large values of total cross-sections of two-electron capture allow to assume that the process (2) is determined by transitions at large enough internuclear distances R. It enables to carry out the analytical investigation in asymptotic approximation, as was done in all of the above mentioned articles [3]-[8].

For asymptotic interatomic distances the main purpose of analytical investigation of process (2) is the determination of the matrix element of the two-electron exchange interaction $\Delta E(R)$. In the general nonresonance case $(Z_a \neq Z_b)$ the value $\Delta E(R)$ is determined as the doubled matrix element $H_{ab}(R) = \langle \Psi_a | \hat{H} | \Psi_b \rangle = \Delta E(R)/2$ of the electron Hamiltonian $\hat{H}$ between the electron wave functions Ψ_a, Ψ_b of original $A^{(Z_a-2)+} + B^{Z_b+}$ and final $A^{Z_a+} + B^{(Z_b-2)+}$ dia-

batic states of quasimolecule.

At the same time, in all of the papers quoted above [3]-[7] when determining the parameters of particle interaction in two-electron exchange it was supposed that the electrons and nuclei interact instantaneously. The retardation connected with the finiteness of the velocity of light c was not taken into account. However on large internuclear separations R, at which the propagation time of interaction R/c becomes of the same order with a mean time of electron transitions, besides the "instantaneous" Coulomb interaction e^2/r_{12} it is necessary to take into account the effects of retardation leading to arise of the additional terms in the operator of interelectron interaction. If in reactions (1), (2) the nuclear charges of both colliding particles are large, so that $Z_m \le 1$ (where $\alpha = e^2/\hbar c$ is the fine structure constant, Z_m is the greater of nuclear charges Z_a, Z_b), and the electron capture takes place from internal (not optical) shells, alongside of retardation effects it is necessary to take into account the essential deviations of the angular and spin moments from LS-coupling scheme, and also relativistic character of motion of rapid inner-shell electrons in heavy quasi-molecule $(AB)^{Z_a+Z_b-2}$.

There are some ways of taking into account the relativistic effects in a problem of calculation of the matrix element $\Delta E(R)$. In a case of not too heavy He-like ions $A^{(Z_a-2)+}$ and bare nuclei B^{Z_b+} in the nonrelativistic Hamiltonian of the two-centre system $A^{(Z_a-2)+} + B^{Z_b+}$ it is possible to introduce the additional members from the Breit-Pauli Hamiltonian [11]. When they are small enough, they can be taken into account in the perturbation theory.

The alternate approach apparently reasonable for heavy quasi-molecules $(AB)^{Z_a+Z_b-2}$ with the total charge of nuclei $Z_a + Z_b \ge 137$ consists in constructing the asymptotic (on large internuclear distances) theory of process of two-electron exchange (2) on the basis of the Dirac-Breit equation [11]. Such approach allows to take into account the orbital and spin degrees of freedom of active electrons, most natural for heavy atoms jj-coupling scheme of the angular and spin moments, and also effects of retardation of interelectronic interaction at large R.

For stationary states the quasirelativistic wave Dirac-Breit equation describing motion of two interacting one another electrons in the field of two fixed Coulomb centres with charges Z_a and Z_b is of the form ($\hbar = e = m_e = 1$):

$$\hat{H}\Psi = (\hat{H}_1 + \hat{H}_2 + V)\Psi = E\Psi,$$
$$\hat{H}_i(\vec{r}_i) = c\hat{\vec{\alpha}}_i\hat{\vec{p}}_i + c^2\beta_i - \frac{Z_a}{r_{ia}} - \frac{Z_b}{r_{ib}}. \quad (4)$$

Here $\Psi = \Psi(\vec{r}_1, \vec{r}_2; R)$ is the 16-component wave function, E is the total energy of two electrons, including their rest energy; the indexes a, b number the nuclei A^{Z_a+}, B^{Z_b+} with charges Z_a and Z_b, respectively; the index $i = 1,2$ distinguishes quantities, relating to the first and second electrons; $\vec{R}$ is the vector between nuclei; $\vec{r}_i$ is the vector joining the centre of segment R with the i-th electron; r_{ia} and r_{ib} are the distances from the i-th electron to nuclei A^{Z_a+} and B^{Z_b+}, respectively; $\{\vec{\alpha}_1, \beta_1\}$ and $\{\vec{\alpha}_2, \beta_2\}$ are two commuting sets of the Dirac matrices of the first and second particles; $\hat{H}_i$ is the Dirac Hamiltonian of the two-centre problem $Z_a e Z_b$, describing motion of the i-th electron in the field of two fixed nuclei with charges Z_a and Z_b separated by distance R. The symbol $V = V(\vec{r}_1, \vec{r}_2)$ in (4) indicates the potential of the interelectron interaction:

$$V = \frac{1}{r_{12}} + V_B,$$
$$V_B = -\frac{1}{2r_{12}}\left[\vec{\alpha}_1\vec{\alpha}_2 + \frac{(\vec{\alpha}_1\vec{r}_{12})(\vec{\alpha}_2\vec{r}_{12})}{r_{12}^2}\right]. \quad (5)$$

The first term r_{12}^{-1} describes the instantaneous Coulomb interaction of electrons, and the Breit operator V_B is sometimes represented in the form of the sum of magnetic V_m and retardation V_r interactions:

$$V_B = V_m + V_r, \qquad (6)$$

$$V_m = -(\vec{\alpha}_1\vec{\alpha}_2)/r_{12},$$

$$V_r = -\frac{1}{2}(\vec{\alpha}_1\vec{\nabla}_1)(\vec{\alpha}_2\vec{\nabla}_2)\vec{r}_{12} =$$

$$= -\frac{1}{2r_{12}}\left[\vec{\alpha}_1\vec{\alpha}_2 - \frac{(\vec{\alpha}_1\vec{r}_{12})(\vec{\alpha}_2\vec{r}_{12})}{r_{12}^2}\right]. \qquad (7)$$

where r_{12} is the distance between electrons.

Calculation of the matrix element of two-electron exchange interaction

As it was already mentioned in the previous section, the matrix element of the two-electron exchange interaction is given by

$$\Delta E(R) = 2\left\langle \Psi_a \left| \hat{H} \right| \Psi_b \right\rangle. \qquad (8)$$

As well as in a nonrelativistic case [4] it is possible to represent the two-electron atomic wave functions $\Psi_{a,b}(\vec{r}_1,\vec{r}_2)$ in the form of linear combination of products of one-electron functions (orbitals) $\psi(\vec{r})$:

$$\Psi_a = \psi_{1a}(\vec{r}_1)\psi_{2a}(\vec{r}_2) + \psi_{1a}(\vec{r}_2)\psi_{2a}(\vec{r}_1), \qquad (9)$$

where ψ_{1a}, ψ_{2a} are the wave functions of ions $A^{Z_a+}(1s)$ and $A^{(Z_a-1)+}(1s)$ in ground states, respectively.

For splitting (8), by using the function (9), we obtain the following expression in terms of one-electron orbitals:

$$\Delta E(R) = \Delta E_1 + \Delta E_2,$$

$$\Delta E_1 = 2\int [\psi_{1a}(\vec{r}_1)\psi_{2a}(\vec{r}_2)\hat{H}\psi_{2b}(\vec{r}_1)\psi_{1b}(\vec{r}_2)]\, d\vec{r}_1 d\vec{r}_2; \qquad (10)$$

$$\Delta E_2 = 2\int [\psi_{1a}(\vec{r}_{1b})\psi_{2a}(\vec{r}_{2a})\hat{H}\psi_{1b}(\vec{r}_1)\psi_{2b}(\vec{r}_2)]\, d\vec{r}_1 d\vec{r}_2. \qquad (11)$$

As it is seen from (10), the first contribution in splitting ΔE_1 gives the crossover transitions: the electron 1 of the outer orbit of atom $A^{(Z_a-1)+}\psi_{1a}$ passes into the internal orbit of atom $B^{Z_b+}\psi_{2b}$, and the electron 2 of the internal orbit of atom $A^{Z_a+}\psi_{2a}$ passes into the outer orbit of atom $B^{(Z_b-1)+}\psi_{1b}$. The second contribution ΔE_2 is determined by "parallel" transitions of electrons: $\psi_{1a} \to \psi_{1b}, \psi_{2a} \to \psi_{2b}$.

In [12] the wave function ψ_{1a} of the outer electron of atom in the vicinity of another nucleus B^{Z_b+} was constructed by the means of the Green function method and is of the form:

$$\psi_{1a}(\vec{r}_{1b}) = x^{-3/2}\sum_{j=|m_{1a}|} C_j(R) \sum_{l=j\pm 1/2} \begin{pmatrix} f^+_{j,l}(x)\Omega_{jl|m_{1a}|}(\vec{n}_{1b}) \\ i\, f^-_{j,l}(x)\Omega_{jl'|m_{1a}|}(\vec{n}_{1b}) \end{pmatrix}, \quad l' = 2j - l, \quad x = 2\lambda_{1a}r_{1b}, \qquad (12)$$

where

$$C_j(R) = D_j R^{\varepsilon_{1a}(Z_a+Z_b-2)/\lambda_{1a} - (|m_{1a}|+1/2)} e^{-\lambda_{1a}R - \varepsilon_{1a}Z_b/\lambda_{1a}}, \qquad (13)$$

$$D_j = 2A_{1a}(1+\varepsilon_{1a})^{-1/2}(2\lambda_{1a})^{\varepsilon_{1a}Z_b/\lambda_{1a}}(|m_{1a}|-1/2)!(2/\lambda_{1a})^{|m_{1a}|-1/2} L_{j_{1a}m_{1a}}$$

$$\times(-1)^{j+|m_{1a}|-1} L_{jm_{1a}} \frac{\Gamma(\gamma_j - \varepsilon_{1a}Z_b/\lambda_{1a})}{\Gamma(2\gamma_j+1)}, \quad L_{jm} = \frac{1}{2^{|m|}(|m|-1/2)!}\left(\frac{(j+|m|)!}{(j-|m|)!}\right)^{1/2}. \qquad (14)$$

Here $\gamma_j = \sqrt{\aleph_j^2 - Z_b^2\alpha^2}$, $\aleph_j = (-1)^{j-l+1/2}(j+1/2)$, $\lambda_{1a} = c\sqrt{1-\varepsilon_{1a}^2}$, $\varepsilon_{1a} = E_{1a}/c^2$, and E_{1a} is the energy of the bound state $(n_{1a}, j_{1a}, l_{1a}, m_{1a})$ of an electron in the field of nucleus with charge $Z_a - 1$, c is the velocity of light, $\alpha = 1/c \approx 1/137$ is the fine structure constant, $\Gamma(z)$ is the Euler gamma-function. The asymptotic coefficient A_{1a} of the relativistic Coulomb wave function is given by

$$A_{1a}=\lambda_{1a}(2\lambda_{1a})^{\frac{\varepsilon_{1a}(Z_a-1)}{\lambda_{1a}}}\left(\frac{(1+\varepsilon_{1a})\left(\frac{(Z_a-1)}{\lambda_{1a}}-\aleph_{1a}\right)}{2Z_a\Gamma\left(\frac{\varepsilon_{1a}(Z_a-1)}{\lambda_{1a}}-\gamma_{1a}+1\right)\Gamma\left(\frac{\varepsilon_{1a}(Z_a-1)}{\lambda_{1a}}+\gamma_{1a}+1\right)}\right)^{1/2}, \qquad (15)$$

where $\gamma_{1a}=\sqrt{\aleph_{1a}^2-(Z_a-1)^2\alpha^2}$, $\aleph_{1a}=(-1)^{j_{1a}-l_{1a}+1/2}(j_{1a}+1/2)$.

The radial wave functions $f_{j,l}^{\pm}(x)$ are expressed as linear combinations of the Whittaker functions $M_{\mu,\nu}(x)$:

$$f_{j,l}^{\pm}(x)=\sqrt{1\pm\varepsilon_{1a}}\left[\left(\gamma_j-\frac{\varepsilon_{1a}Z_b}{\lambda_{1a}}\right)M_{\mu_-,\gamma_j}(x)\pm\left(\frac{Z_b}{\lambda_{1a}}-\aleph_j\right)M_{\mu_+,\gamma_j}(x)\right],\ \mu_{\pm}=\frac{\varepsilon_{1a}Z_b}{\lambda_{1a}}\pm\frac{1}{2}. \qquad (16)$$

For the wave function ψ_{2b} of ground state hydrogen-like ion B^{Z_b+} we use the known expression [11]:

$$\psi_{2b}(\vec{r}_{1b})=A_{2b}r_{1b}^{\gamma_{2b}-1}e^{-Z_b r_{1b}}\begin{pmatrix}\Omega_{\frac{1}{2},0,\frac{1}{2}}(\vec{n}_{1b})\\ -i\sqrt{\frac{1-\gamma_{2b}}{1+\gamma_{2b}}}\Omega_{\frac{1}{2},1,\frac{1}{2}}(\vec{n}_{1b})\end{pmatrix}, \qquad (17)$$

$$A_{2b}=(2Z_b)^{\gamma_{2b}+\frac{1}{2}}\sqrt{\frac{1+\gamma_{2b}}{2\Gamma(2\gamma_{2b}+1)}},\quad \gamma_{2b}=\sqrt{1-Z_b^2\alpha^2}.$$

The wave functions ψ_{1b} and ψ_{2a} are obtained from expressions (12) and (17), respectively, by simultaneous replacement of indices $a\leftrightarrow b$ in all quantities.

Since ψ_{1a} is orthogonal to ψ_{2b} and ψ_{1b} is orthogonal to ψ_{2a}, the contribution to the integral (10) gives only the correlation part of interelectronic interaction V (see (6), (7)). As this operator consists of three summands, it is convenient to divide the matrix element (10) into three parts as well:

$$\Delta E_1=\Delta E_{in}+\Delta E_m+\Delta E_r, \qquad (18)$$

$$\Delta E_{in}=4\langle\psi_{1a}(\vec{r}_{1b})\psi_{2a}(\vec{r}_{2a})|\frac{1}{r_{12}}|\psi_{2b}(\vec{r}_{1b})\psi_{1b}(\vec{r}_{2a})\rangle, \qquad (19)$$

$$\Delta E_m=4\langle\psi_{1a}(\vec{r}_{1b})\psi_{2a}(\vec{r}_{2a})|-\frac{\vec{\alpha}_1\vec{\alpha}_2}{r_{12}}|\psi_{2b}(\vec{r}_{1b})\psi_{1b}(\vec{r}_{2a})\rangle, \qquad (20)$$

$$\Delta E_r=4\langle\psi_{1a}(\vec{r}_{1b})\psi_{2a}(\vec{r}_{2a})|-\frac{1}{2}(\vec{\alpha}_1\vec{\nabla}_1)(\vec{\alpha}_2\vec{\nabla}_2)r_{12}|\psi_{2b}(\vec{r}_{1b})\psi_{1b}(\vec{r}_{2a})\rangle. \qquad (21)$$

Let us calculate the matrix elements (19)-(21) separately, beginning from the first of them.

For electrons belonging to different atoms the instantaneous interaction

$$r_{12}^{-1}=[R^2+2R(r_{1b}\cos\theta_{1b}-r_{2a}\cos\theta_{2a})+r_{1b}^2+$$
$$+r_{2a}^2-2r_{1b}r_{2a}(\cos\theta_{1b}\cos\theta_{2a}+$$
$$+\sin\theta_{1b}\sin\theta_{2a}\cos(\varphi_{1b}-\varphi_{2a}))]^{-1/2}$$

can be expanded in inverse powers of R:

$$r_{12}^{-1}=R^{-1}-(r_{1b}\cos\theta_{1b}-r_{2a}\cos\theta_{2a})R^{-2}+$$
$$+[r_{1b}^2(3\cos^2\theta_{1b}-1)+r_{2a}^2(3\cos^2\theta_{2a}-1)-$$
$$-2r_{1b}r_{2a}(2\cos\theta_{1b}\cos\theta_{2a}-\sin\theta_{1b}\sin\theta_{2a}\times$$
$$\times\cos(\varphi_{1b}-\varphi_{2a}))]/2R^{-3}+O(R^{-4}). \qquad (22)$$

Note that both spherical angles θ_{1b} and θ_{2a} are measured from the z-axis, connecting centers of charges Z_a and Z_b.

After substituting only the first three terms of the expansion (22) into the matrix element

(19) and evaluating integrals in a spherical system of coordinates it can be seen that due to orthogonality of the function ψ_{1a} to ψ_{2b} and ψ_{1b} to ψ_{2a} and also selection rules for spherical harmonics the nonzero contribution to this matrix element gives only one term of (22) containing the product $r_{1b}r_{2a}\cos\theta_{1b}\cos\theta_{2a}$, i.e.

$$\Delta E_{in} = \frac{8}{R^3}\langle\psi_{1a}(\vec{r}_{1b})\,|r_{1b}\cos\theta_{1b}|\psi_{2b}(\vec{r}_{1b})\rangle\times$$
$$\times\langle\psi_{2a}(\vec{r}_{2a})\,|r_{2a}\cos\theta_{2a}|\psi_{1b}(\vec{r}_{2a})\rangle. \quad (23)$$

At first, consider the first of the two matrix elements which are included in (23). The integration over angular variables θ_{1b}, φ_{1b} leads to

$$\langle\psi_{1a}(\vec{r}_{1b})\,|r_{1b}\cos\theta_{1b}|\psi_{2b}(\vec{r}_{1b})\rangle =$$
$$-\frac{A_{2b}}{3(2\lambda_{1a})^{3/2}}\left[C_{1/2}(R)\left(I^{+}_{1,\frac{1}{2},1}-\sqrt{\frac{1-\gamma_{2b}}{1+\gamma_{2b}}}I^{-}_{1,\frac{1}{2},1}\right)-\right.$$
$$\left.-\sqrt{2}C_{3/2}(R)\left(I^{+}_{1,\frac{3}{2},1}-\sqrt{\frac{1-\gamma_{2b}}{1+\gamma_{2b}}}I^{-}_{1,\frac{3}{2},1}\right)\right], \quad (24)$$

where $I^{\pm}_{n,j,l}$ is the integral with the radial functions:

$$I^{\pm}_{n,j,l} = \int_0^{\infty} r_{1b}^{n+\gamma_{2b}-1/2}e^{-Z_b r_{1b}}\,f^{\pm}_{j,l}(2\lambda_{1a}r_{1b})\,dr_{1b}. \quad (25)$$

By using the table integral [13]

$$\int_0^{\infty} e^{-st}t^{\alpha}M_{\mu,\nu}(t)\,dt = \frac{\Gamma(\alpha+\nu+3/2)}{(s+1/2)^{\alpha+\nu+3/2}}\times$$
$$F(\alpha+\nu+3/2,-\mu+\nu+1/2;2\nu+1;2/(2s+1)),$$

where $F(a,b;c;z)$ is the hypergeometric function, we obtain the expression for the radial integrals:

$$I^{\pm}_{n,j,l} = \sqrt{1\pm\varepsilon_{1a}}\,\frac{(2\lambda_{1a})^{\gamma_j+1/2}\Gamma(g_{nj})}{(Z_b+\lambda_{1a})^{g_{nj}}}\times$$
$$\times\left[\left(\gamma_j-\frac{\varepsilon_{1a}Z_b}{\lambda_{1a}}\right)F_1\pm\left(\frac{Z_b}{\lambda_{1a}}-\aleph_j\right)F_0\right], \quad (26)$$

$$F_k = F\left(g_{nj},\gamma_j-\frac{\varepsilon_{1a}Z_b}{\lambda_{1a}}+k;2\gamma_j+1;\frac{2\lambda_{1a}}{Z_b+\lambda_{1a}}\right),$$
$$k=0,1,\quad g_{nj}=\gamma_j+\gamma_{2b}+n+1.$$

Having selected the explicit dependence on internuclear distance R by (13) one can write the final result for the matrix element (24) in the form

$$\langle\psi_{1a}(\vec{r}_{1b})\,|r_{1b}\cos\theta_{1b}|\psi_{2b}(\vec{r}_{1b})\rangle =$$
$$=\Delta_{ab}R^{\varepsilon_{1a}(Z_a+Z_b-1)/\lambda_{1a}-(|m_{1a}|+1/2)}e^{-\lambda_{1a}R-\varepsilon_{1a}Z_b/\lambda_{1a}}, \quad (27)$$

where

$$\Delta_{ab} = -\frac{A_{2b}}{3(2\lambda_{1a})^{3/2}}\left[D_{1/2}\left(I^{+}_{1,\frac{1}{2},1}-\sqrt{\frac{1-\gamma_{2b}}{1+\gamma_{2b}}}I^{-}_{1,\frac{1}{2},1}\right)\right.$$
$$\left.-\sqrt{2}D_{3/2}\left(I^{+}_{1,\frac{3}{2},1}-\sqrt{\frac{1-\gamma_{2b}}{1+\gamma_{2b}}}I^{-}_{1,\frac{3}{2},1}\right)\right]. \quad (28)$$

The second matrix element is calculated in the similar way

$$\langle\psi_{2a}(\vec{r}_{2a})\,|r_{2a}\cos\theta_{2a}|\psi_{1b}(\vec{r}_{2a})\rangle =$$
$$=\Delta_{ba}R^{\varepsilon_{1b}(Z_a+Z_b-1)/\lambda_{1b}-(|m_{1b}|+1/2)}e^{-\lambda_{1b}R-\varepsilon_{1b}Z_a/\lambda_{1b}}, \quad (29)$$

where the quantity Δ_{ba} can be obtained from the formula (28) for Δ_{ab} by making the simultaneous replacement of indices $a\leftrightarrow b$.

Thus, by substituting (27) and (29) into (23) we arrive at the expression for the matrix element of instantaneous interelectronic interaction:

$$\Delta E_{in} = \frac{8}{R^3}\Delta_{ab}\Delta_{ba}\times$$
$$\times R^{\frac{\varepsilon_{1a}}{\lambda_{1a}}+\frac{\varepsilon_{1b}}{\lambda_{1b}}(Z_a+Z_b-1)-(|m_{1a}|+|m_{1b}|+1)}\times$$
$$\times e^{-(\lambda_{1a}+\lambda_{1b})R-\frac{\varepsilon_{1a}Z_b}{\lambda_{1a}}-\frac{\varepsilon_{1b}Z_a}{\lambda_{1b}}}. \quad (30)$$

Let us proceed to the calculation of the second term ΔE_m of the sum (18). Here, in contrast to the matrix element ΔE_{in} besides the term that is proportional to R^{-3} the terms $\sim R^{-1}$ and $\sim R^{-2}$ exist as well:

$$\Delta E_m = -4\{Z^{00}_{ab}Z^{00}_{ba}R^{-1}-(Z^{11}_{ab}Z^{00}_{ba}+Z^{00}_{ab}Z^{11}_{ba})R^{-2}$$
$$+[Z^{00}_{ab}(3Z^{22}_{ba}-Z^{20}_{ba})+(3Z^{22}_{ab}-Z^{20}_{ab})Z^{00}_{ba}$$
$$4Z^{11}_{ab}Z^{11}_{ba}-4X_{ab}X_{ba}-4Y_{ab}Y_{ba}]R^{-3}/2\}$$

$$\times R^{\frac{\varepsilon_{1a}}{\lambda_{1a}}+\frac{\varepsilon_{1b}}{\lambda_{1b}}(Z_a+Z_b-1)-(|m_{1a}|+|m_{1b}|+1)} \times$$

$$\times e^{-(\lambda_{1a}+\lambda_{1b})R-\frac{\varepsilon_{1a}Z_b}{\lambda_{1a}}-\frac{\varepsilon_{1b}Z_a}{\lambda_{1b}}}, \quad (31)$$

$$X_{ab}=\langle\psi_{1a}|\alpha_x r_{1b}\sin\theta_{1b}\cos\varphi_{1b}|\psi_{2b}\rangle$$
$$=\langle\psi_{1a}|\alpha_y r_{1b}\sin\theta_{1b}\sin\varphi_{1b}|\psi_{2b}\rangle,$$
$$Y_{ab}=\langle\psi_{1a}|\alpha_y r_{1b}\sin\theta_{1b}\cos\varphi_{1b}|\psi_{2b}\rangle$$
$$=-\langle\psi_{1a}|\alpha_x r_{1b}\sin\theta_{1b}\sin\varphi_{1b}|\psi_{2b}\rangle,$$
$$X_{ba}=\langle\psi_{2a}|\alpha_x r_{2a}\sin\theta_{2a}\cos\varphi_{2a}|\psi_{1b}\rangle$$
$$=\langle\psi_{2a}|\alpha_y r_{2a}\sin\theta_{2a}\sin\varphi_{2a}|\psi_{1b}\rangle,$$
$$Y_{ba}=\langle\psi_{2a}|\alpha_y r_{2a}\sin\theta_{2a}\cos\varphi_{2a}|\psi_{1b}\rangle$$
$$=-\langle\psi_{2a}|\alpha_x r_{2a}\sin\theta_{2a}\sin\varphi_{2a}|\psi_{1b}\rangle,$$
$$Z_{ab}^{nn'}=\langle\psi_{1a}|\alpha_z r_{1b}^n\cos^{n'}\theta_{1b}|\psi_{2b}\rangle,$$
$$Z_{ba}^{nn'}=-\langle\psi_{2a}|\alpha_z r_{2a}^n\cos^{n'}\theta_{2a}|\psi_{1b}\rangle, n,n'=0,1,2. \quad (32)$$

After integration over the angular variables θ_{1b}, θ_{2a}, φ_{1b}, φ_{2a} in the matrix elements (32), belonging to the formula (31), we obtain the following expressions:

$$X_{ab}=\frac{iA_{2b}}{15(2\lambda_{1a})^{3/2}}\Bigg[5D_{1/2}\Bigg(I^{-}_{1,\frac12,0}+\sqrt{\frac{1-\gamma_{2b}}{1+\gamma_{2b}}}I^{+}_{1,\frac12,0}\Bigg)+\frac{D_{3/2}}{\sqrt2}\Bigg(5I^{-}_{1,\frac32,2}-\sqrt{\frac{1-\gamma_{2b}}{1+\gamma_{2b}}}I^{+}_{1,\frac32,2}\Bigg)-2\sqrt3 D_{5/2}\sqrt{\frac{1-\gamma_{2b}}{1+\gamma_{2b}}}I^{+}_{1,\frac52,2}\Bigg], \quad (33)$$

$$Y_{ab}=-\frac{A_{2b}}{3(2\lambda_{1a})^{3/2}}\Bigg[D_{1/2}\Bigg(I^{-}_{1,\frac12,0}-\sqrt{\frac{1-\gamma_{2b}}{1+\gamma_{2b}}}I^{+}_{1,\frac12,0}\Bigg)+\frac{D_{3/2}}{\sqrt2}\Bigg(I^{-}_{1,\frac32,2}-\sqrt{\frac{1-\gamma_{2b}}{1+\gamma_{2b}}}I^{+}_{1,\frac32,2}\Bigg)\Bigg], \quad (34)$$

$$Z_{ab}^{n0}=-\frac{iA_{2b}}{3(2\lambda_{1a})^{3/2}}\Bigg[D_{1/2}\Bigg(3I^{-}_{n,\frac12,1}-\sqrt{\frac{1-\gamma_{2b}}{1+\gamma_{2b}}}I^{+}_{n,\frac12,1}\Bigg)-2\sqrt2\,D_{3/2}\sqrt{\frac{1-\gamma_{2b}}{1+\gamma_{2b}}}I^{+}_{1,\frac32,2}\Bigg], \ n\in Z, \quad (35)$$

$$Z_{ab}^{11}=\frac{iA_{2b}}{15(2\lambda_{1a})^{3/2}}\Bigg[5D_{1/2}\Bigg(I^{-}_{1,\frac12,0}+\sqrt{\frac{1-\gamma_{2b}}{1+\gamma_{2b}}}I^{+}_{1,\frac12,0}\Bigg)-\sqrt2 D_{3/2}\Bigg(5I^{-}_{1,\frac32,2}-\sqrt{\frac{1-\gamma_{2b}}{1+\gamma_{2b}}}I^{+}_{1,\frac32,2}\Bigg)+4\sqrt3 D_{5/2}\sqrt{\frac{1-\gamma_{2b}}{1+\gamma_{2b}}}I^{+}_{1,\frac52,2}\Bigg], \quad (36)$$

$$Z_{ab}^{22}=\frac{iA_{2b}}{105(2\lambda_{1a})^{3/2}}\Bigg[-7D_{1/2}\Bigg(5I^{-}_{2,\frac12,1}+\sqrt{\frac{1-\gamma_{2b}}{1+\gamma_{2b}}}I^{+}_{2,\frac12,1}\Bigg)+14\sqrt2 D_{3/2}\Bigg(I^{-}_{2,\frac32,1}+2\sqrt{\frac{1-\gamma_{2b}}{1+\gamma_{2b}}}I^{+}_{2,\frac32,1}\Bigg)-2\sqrt3 D_{5/2}\Bigg(7I^{-}_{2,\frac52,3}-\sqrt{\frac{1-\gamma_{2b}}{1+\gamma_{2b}}}I^{+}_{2,\frac52,3}\Bigg)+24D_{7/2}\sqrt{\frac{1-\gamma_{2b}}{1+\gamma_{2b}}}I^{+}_{2,\frac72,3}\Bigg], \quad (37)$$

where the quantities $I^{\pm}_{n,j,l}$ are given by the previous formulae (26), and the matrix elements X_{ba}, Y_{ba}, $Z_{ba}^{nn'}$ are obtained from (33)–(37) by making the simultaneous replacements of indexes $a\leftrightarrow b$.

For calculation of the matrix element ΔE_r of retardation interaction V_r (see (7)) besides the expansion (22) it is also necessary to use the expansion of r_{12}^{-3} in inverse powers of large internuclear distance R. Without going into details we give the final result for ΔE_r:

$$\Delta E_r=-4\{(X_{ab}Z_{ba}^{00}+Z_{ab}^{00}X_{ba})R^{-2}+[Z_{ab}^{00}(Z_{ba}^{22}-Z_{ba}^{20})+(Z_{ab}^{22}-Z_{ab}^{20})Z_{ba}^{00}-4X_{ab}Z_{ba}^{11}-4Z_{ab}^{11}X_{ba}+8X_{ab}X_{ba}-4\delta_{ab}Z_{ba}^{00}-4Z_{ab}^{00}\delta_{ba}]R^{-3}/2\}$$
$$\times R^{\frac{\varepsilon_{1a}}{\lambda_{1a}}+\frac{\varepsilon_{1b}}{\lambda_{1b}}(Z_a+Z_b-1)-(|m_{1a}|+|m_{1b}|+1)} \times$$
$$\times e^{-(\lambda_{1a}+\lambda_{1b})R-\frac{\varepsilon_{1a}Z_b}{\lambda_{1a}}-\frac{\varepsilon_{1b}Z_a}{\lambda_{1b}}}, \quad (38)$$

where the quantities $X_{ab,ba}$, $Y_{ab,ba}$, $Z_{ab,ba}^{nn'}$ are determined in (33)-(37),

$$\delta_{ab} = = \langle \psi_{1a} \ | \alpha_x r_{1b}^2 \sin\theta_{1b} \cos\theta_{1b} \cos\varphi_{1b} | \psi_{2b} \rangle$$

$$= \frac{iA_{2b}}{105(2\lambda_{1a})^{3/2}} \Bigg[-14 D_{1/2} \sqrt{\frac{1-\gamma_{2b}}{1+\gamma_{2b}}} I^{+}_{2,\frac{1}{2},1}$$

$$+ \frac{7}{\sqrt{2}} D_{3/2} \left(3 I^{-}_{2,\frac{3}{2},1} + \sqrt{\frac{1-\gamma_{2b}}{1+\gamma_{2b}}} I^{+}_{2,\frac{3}{2},1} \right)$$

$$+ \sqrt{3} D_{5/2} \left(7 I^{-}_{2,\frac{5}{2},3} - \sqrt{\frac{1-\gamma_{2b}}{1+\gamma_{2b}}} I^{+}_{2,\frac{5}{2},3} \right)$$

$$- 12 D_{7/2} \sqrt{\frac{1-\gamma_{2b}}{1+\gamma_{2b}}} I^{+}_{2,\frac{7}{2},3} \Bigg], \qquad (39)$$

and δ_{ab} one can obtain from (39) by making the simultaneous replacement of indices $a \leftrightarrow b$.

In the nonrelativistic limit the quantities $\gamma_{2b} \to 1$, $\varepsilon_{1a} \to 1$, and, therefore, all the matrix elements $X_{ab,ba}$, $Y_{ab,ba}$, $Z^{nn'}_{ab,ba}$, $\delta_{ab,ba}$ tend to zero. Thus, when $c \to \infty$ the contribution ΔE_m, ΔE_r to the exchange splitting of Breit interactions disappear, and the exchange matrix element ΔE_1, corresponding to crossbar transitions, in the resonant case $Z_a = Z_b = Z$ proceeds into the result of paper [6]:

$$\Delta E_1 = 2^8 A^2 \Gamma^2 (1 - nZ) \left(\frac{n\sqrt{Z}}{nZ+1} \right)^{10} \left(\frac{2}{ne} \right)^{2nZ}$$

$$\times \left(\frac{nZ-1}{nZ+1} \right)^{2nZ-4} R^{2n(2Z-1)-5} e^{-2R/n}, \qquad (40)$$

where $n = 1/\lambda$, λ is the ionization potential, and *A* is the nonrelativistic asymptotic coefficient.

References

1. A. Belkacem, H. Could, B. Feinberg, R. Bossngham, W.E. Meyerhof, Phys. Rev. A56, 2806 (1997).
2. A. Belkacem, N. Claytor, T. Dinneen, B. Feinberg, H. Could, Phys. Rev. A58, 1253 (1998).
3. I.V. Komarov, R.K. Janev, Zh. Eksp. Teor. Fiz., 1712 (1966).
4. M.I. Chibisov, Zh. Eksp. Teor. Fiz., 1687 (1976).
5. T.P. Grozdanov, R.K. Janev, J. Phys. B13, 3341 (1980).
6. M.I. Karbovanets, V.Yu. Lazur, M.I. Chibisov, Zh. Eksp. Teor. Fiz., 84 (1984).
7. T.P. Grozdanov, R.K. Janev, V.Yu. Lazur, Phys. Scripta, 64 (1985).
8. M.I. Chibisov, R.K. Janev, Phys. Rep., 1 (1988).
9. E.E. Nikitin, S.Ya. Umanskii, Nonadiabatic Transitions at Slow Atomic Collisions [in Russian], Moscow, Atomizdat, 1979.
10. I.K. Fetisov, O.B. Firsov, Zh. Eksp. Teor. Fiz., 95 (1959).
11. A.I. Akhiezer and V. B. Berestetskii, Quantum Electrodynamics [in Russian] (2nd ed.), Nauka, Moscow, 1981; English transl. prev. ed., Elements of Quantum Electrodynamics, Oldbourne, London, 1962.
12. P.P. Gorvat, V.Yu. Lazur, S.I. Migalina, I.M. Shuba, R.K. Yanev, Theor. Math. Phys., 1423 (1996).
13. I.S. Gradshtein, I.M. Ryzhik, Tables of Integrals, Series, and Products, Academic Press, New York, 1969.
14. H. Bateman and A. Erdelyi, eds., Higher Transcendental Functions (based on notes left by H. Bateman), Vol. 1, 2, McGraw-Hill, New York, 1953.
15. V.S. Popov, Zh. Eksp. Teor. Fiz., 35 (1973).
16. H.A. Bethe, E.E. Salpeter, Quantum Mechanics of One- and Two-Electron Atoms, Springer, Berlin, 1957.

АДІАБАТИЧНА АСИМПТОТИЧНА ТЕОРІЯ ДВОЕЛЕКТРОННОЇ ПЕРЕЗАРЯДКИ ПРИ РЕЛЯТИВІСТСЬКИХ ЕНЕРГІЯХ ЗВ'ЯЗКУ

В.Ю. Лазур, О.К. Рейтій, С.І. Мигалина

Ужгородський національний університет, вул. Волошина, 54, Ужгород, 88000, Україна

Побудовано асимптотичну (за великими між'ядерними відстанями) теорію двоелектронної перезарядки при зіткненні багато електронного атома з багатозарядним іоном. В рамках квазірелятивістського наближення Дірака-Брейта розраховано матричний елемент двоелектронної обмінної взаємодії. Даний підхід дозволяє врахувати релятивістські ефекти пов'язані з магнітною та запізнюючою міжелектронними взаємодіями. В нерелятивістській границі отриманий матричний елемент переходить в результат роботи [6].