

EXPERIMENTAL PHYSICS

**INSTITUTE OF EXPERIMENTAL PHYSICS
SLOVAK ACADEMY OF SCIENCES**



**THE 11th SMALL TRIANGLE MEETING
on theoretical physics**

ACADEMY OF SCIENCES

September 20. – 23. 2009
Kysak



Relativistic Operator of Interaction of Two Quasimolecular Electrons with Emission (Absorption) of Real Photon

V.Yu. Lazur, O.K. Reity, S.I. Myhalyna, and O.F. Pavlyk

*Department of Theoretical Physics, Uzhgorod National University,
Voloshyna Street 54, Uzhgorod 88000, Ukraine*

Abstract

The problem of interaction of two quasimolecular electrons located at an arbitrary distance from each other and near different atoms (nuclei) is solved. Effects of the third order of quantum electrodynamics, which include the exchange of a virtual photon between the electrons, and emission (absorption) of a real photon, are considered. The general expression for the matrix elements of the operator of the effective interaction energy of the two quasi-molecular electrons with the external radiation field, which allows to calculate the probabilities of inelastic processes with rearrangement in slow collisions of multiply charged ions with relativistic atoms, is obtained. Carrying out consistently the procedure of symmetrization of the retardation factor with respect to both the electrons results in the appearance of additional terms in the relativistic operator of the interaction of two quasi-molecular electrons in comparison with Breit operators known previously.

Introduction

Inelastic collisions of atomic particles, especially multielectron ones, are accompanied by many processes of modification of their charge and electronic states. The simplest examples, which are studied quite well, are one-electron ion-atom processes with rearrangement (for example, the resonance and quasi-resonance charge exchange), in which only one electron changes the state and the other one can be considered frozen. Such processes have high efficiency and play an important role in formation of the inverse population of ionic levels in solar coronal plasma and new thermonuclear facilities [1, 2]. However, the two-electron processes with rearrangement have either the same or larger probabilities when compared with the one-electron processes [3, 4, 5, 6, 7] at thermal energies of collisions. Various Auger processes studied by Kishinevsky and Parilis [7], the two-electron capture [3, 4, 5, 6], and the two-electron capture with simultaneous excitation of an ion [4] occupy an important place among the two-electron processes. Large values of total cross-sections and velocity constants allow us to assume that the specified processes with rearrangement are determined by electron transitions when the distance R between colliding particles is rather large. The presence of a small parameter $1/R$ gives a chance to elaborate a consistent asymptotic theory of such processes.

Additionally, during last decades the considerable attention was given to study the influence of intensive electromagnetic radiation on characteristics of the inelastic processes accompanying collisions of highly charged ions with heavy atoms. Interest in this range of problems is caused by the possibility of inducing (by means of laser radiation) various processes occurring in ion-atom collisions, which involve electrons of outer and inner shells. In the majority of theoretical and experimental papers, the two-electron processes with rearrangement (see, e.g., [2, 6, 8, 9, 10, 11, 12] and references therein), which happen at large internuclear distances and are accompanied by absorption (emission) of photons, has been considered. Clarification of the basic features and basic mechanisms of radiative collisional processes with rearrangement is crucial for this field.

Since the future interest in similar investigations will doubtlessly increase, it is worthwhile to consider in detail the course of quantum processes corresponding to the Feynman diagrams presented

in figure 1. To do that, it is necessary to take into account the fact that the followed exchange mechanism is typical for all two-electron processes with rearrangement: one of the active electrons of atom (ion) $A^{(Z_a-2)+}$ tunnels to a "foreign" ion B^{Z_b+} with the following dipole-multipole simultaneous transition of two electrons located near different nuclei. Therefore, we assume in the present paper that the exchange matrix element corresponding to the course of two-electron processes with rearrangement is determined by the configuration when the active electrons are far apart – near different atoms (nuclei). In the case when under favourable conditions, the mechanisms of nonadiabatic coupling cause multielectronic transitions by involving the electrons of inner shells, the realistic calculations of parameters of the interaction of heavy (relativistic) atomic particles in the course of the collision should be based on the completely relativistic theory. However, even the formulation of the two-particle problem in the relativistic quantum theory encounters principal mathematical and logical obstacles. As early as 1929, Breit demonstrated [13] that accounting for the first (non-zero) term of such an expansion is a good approximation for the relativistic interaction between the two electrons under the condition of smallness of the retardation effects in the spectrum of He-like atoms. The expression for the relativistic operator of the interaction of two electrons obtained by Breit is of the form [13]

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

where $\vec{\alpha}_1$ and $\vec{\alpha}_2$ are the two commuting sets of the Dirac matrices, $\vec{r}_{12} = \vec{r}_1 - \vec{r}_2$, and the lower indices 1 and 2 distinguish the quantities relating to the first and second electron, respectively.

However, the applicability of the Breit operator (1) is restricted by the requirement of smallness of the time $T_{int} = r_{12}/c$ of interaction transmission when compared with the average time $T_0 = 2\pi/\omega_0$ of electronic transitions, where ω_0 is the characteristic frequency of a spectrum of interacting electrons. It is obvious that this requirement is certainly satisfied when the distances between electrons are not too large, e.g., the interatomic distances of He-like atoms.

In view of this, in our previous paper [9], we have given the arguments that cast doubt on the possibility of using the Breit operator (1) for determination of the asymptotics of the exchange interaction, corresponding to simultaneous capture of two electrons in slow collisions of multiply charged ions with atoms [3, 4]. In essence, these arguments pertain equally to other two-electron processes with rearrangement, including radiative collisional ones, if the basic contribution to the transition probability comes from the configuration when the electrons are located near different nuclei and the approximation of independent electrons is valid as a zero approximation. In fact, we meet here a new quantum electrodynamic problem of interaction of two quasimolecular electrons with emission (absorption) of a real photon that has no satisfactory solution until now. As far back as in the early seventies of the last century, the interest in the given problem arose in the connection with the intensive study of multiatomic systems placed into a field of radiation. The credit for the realization and development of new ideas in this direction goes to the authors of papers [15, 16, 17], where the problem of interaction of two bound electrons belonging to two hydrogen-like atoms was considered by using methods of quantum electrodynamics without any restrictions on interatomic distances. However, the generalized Breit operator constructed in the above quoted papers does not manifest the symmetry with respect to the interacting particles, and therefore, cannot be utilized in the consistent relativistic quantum theory. It is precisely this circumstance that motivated us to return to the problem of two quasimolecular electrons anew.

The matrix of effective energy of the interaction of two quasimolecular electrons at an arbitrary distance from each other

Describing a quasimolecule $(AB)^{(Z_a+Z_b-2)+}$ by methods of quantum electrodynamics, we consider it as a system of two electrons that interact via quantized electromagnetic field and move in an external (electric) field of two fixed nuclei A^{Z_a+} and B^{Z_b+} with charges Z_a and Z_b located at distance R from each other. Hereinafter, the nuclei are assumed to be infinitely heavy, pointlike, and structureless.

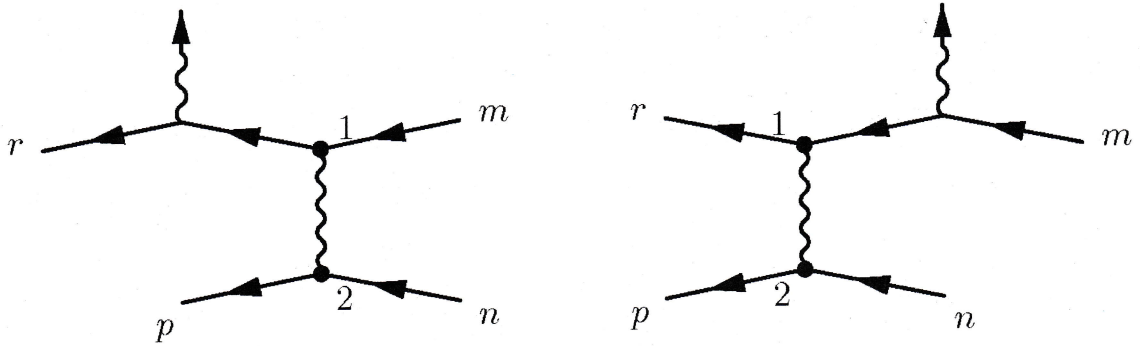


Figure 1: The Feynman diagrams of the third order effects of QED for the interaction of the two quasimolecular electrons with emission or absorption of the real photon.

In standard quantum mechanical form (see, e.g., [3, 4, 18]), the matrix element of the two-electron exchange interaction of the atom $A^{(Z_a-2)+}$ with the ion B^{Z_b+} is determined as a non-diagonal matrix element of the operator of interelectron interaction calculated between (adiabatic) electron wave functions of the quasimolecule $(AB)^{(Z_a+Z_b-2)+}$, which correspond to the cases of various localizations of active electrons in the initial and final states. In the quantum electrodynamic approach used below, this matrix element is a constituent of a more general matrix element of the operator of effective energy of interaction of the system of two quasimolecular electrons with an external field of radiation. In this case, the third order effects of quantum electrodynamics, which include the exchange of virtual photons between the electrons and emission (absorption) of a real photon, are considered. The Feynman diagrams of these effects are presented in figure 1; two parts of the interaction, each of which takes into account the intermediate states in the quasimolecular spectrum with either positive or negative frequency, are separated.

Let the coefficients m and n (p and r) denote sets of quantum numbers of the initial (final) states of the electrons. Integrating in the S-matrix with respect to time, frequencies, and wave vectors of the virtual photons, we arrive at an expression for the matrix of the effective interaction energy of two atomic electrons (here $\hbar = c = 1$) [19]:

$$\begin{aligned}
 U_{mn,pr}^{(3)} = e^3 \int d\vec{r}' d\vec{r}'' d\vec{r}''' \left\{ -\frac{1}{|\vec{r}''' - \vec{r}''|} \sum_{l_{\pm}} \frac{\exp\{i|\omega_p - \omega_n||\vec{r}'' - \vec{r}'''\}}{\omega_l(1-i0) - \omega - \omega_r} \bar{\Psi}_r(\vec{r}') \hat{A}(\vec{r}') \right. \\
 \times \Psi_l(\vec{r}') \bar{\Psi}_l(\vec{r}'') \gamma_{\mu}'' \Psi_m(\vec{r}'') \bar{\Psi}_p(\vec{r}''') \gamma_{\mu}''' \Psi_n(\vec{r}''') - \frac{1}{|\vec{r}' - \vec{r}''|} \sum_{l_{\pm}} \frac{\exp\{i|\omega_p - \omega_n||\vec{r}' - \vec{r}'''\}}{\omega_l(1-i0) + \omega - \omega_m} \\
 \left. \times \bar{\Psi}_r(\vec{r}') \gamma_{\mu}' \Psi_l(\vec{r}') \bar{\Psi}_l(\vec{r}'') \hat{A}(\vec{r}'') \Psi_m(\vec{r}'') \bar{\Psi}_p(\vec{r}''') \gamma_{\mu}''' \Psi_n(\vec{r}''') \right\}, \quad (2)
 \end{aligned}$$

where $\Psi_{m(n)}$, $\Psi_{r(p)}$, and Ψ_l are the coordinate wave functions of the electrons (without the time factors), and \vec{r}' , \vec{r}'' , \vec{r}''' are the position vectors of the first and second electrons, respectively. The matrix element (11) corresponds to two of the eight processes that occur due to the interaction of the active electrons via the field of virtual photons and are accompanied by emission (absorption) of a real photon. Other processes can be taken into account by the corresponding change of notation of the wave functions.

The generalized Breit operator

Following the previous section, one can represent the general expression for the matrix of the effective energy of interaction of the two bound quasimolecular electrons with the external field of radiation in

the form

$$U_{i \rightarrow f}^{(3)} = U_{mn,pr}^{(3)} - U_{nm,pr}^{(3)}. \quad (3)$$

According to (11), the matrix element $U_{mn,pr}^{(3)}$ reads

$$\begin{aligned} U_{mn,pr}^{(3)} = & e^3 \int \Psi_r^+(\vec{r}') \Psi_p^+(\vec{r}''') \sum_{l\pm} \left\{ \gamma'_4 \gamma'_\delta A'_\delta \frac{\Psi_l(\vec{r}') \Psi_l^+(\vec{r}'')}{\omega_l(1-i0) - \omega - \omega_r} \right. \\ & \times \frac{1 - \vec{\alpha}'' \vec{\alpha}'''}{|\vec{r}'' - \vec{r}'''} \exp\{i|\omega_p - \omega_n||\vec{r}'' - \vec{r}'''\} \} + \frac{1 - \vec{\alpha}' \vec{\alpha}'''}{|\vec{r}' - \vec{r}'''} \exp\{i|\omega_p - \omega_n||\vec{r}' - \vec{r}'''\} \\ & \left. \times \frac{\Psi_l(\vec{r}') \Psi_l^+(\vec{r}'')}{\omega_l(1-i0) + \omega - \omega_m} \gamma''_4 \gamma''_\delta A''_\delta \right\} \Psi_m(\vec{r}'') \Psi_n(\vec{r}''') d\vec{r}' d\vec{r}'' d\vec{r}'''. \end{aligned} \quad (4)$$

Here $\vec{\alpha}'$, $\vec{\alpha}''$, $\vec{\alpha}'''$ are the Dirac matrices, the operator $\vec{\alpha}''(\vec{\alpha}')$ acts on the function $\Psi_m(\vec{r}'')$ ($\Psi_l(\vec{r}'')$), and the operator $\vec{\alpha}'''$ acts on the function $\Psi_n(\vec{r}''')$; A_δ are the components of the vector potential without the time factors, the index δ covers the values of 1, 2, 3, and the summation over the twice repeated index δ is carried out from $\delta = 1$ to $\delta = 3$.

Let us consider the first term in (13), and inside it, we separate the factor

$$K(\vec{r}'', \vec{r}'''; \omega_{pn}) = \frac{1 - \vec{\alpha}'' \vec{\alpha}'''}{|\vec{r}'' - \vec{r}'''} \exp \left\{ \frac{i}{c} |\omega_{pn}| |\vec{r}'' - \vec{r}'''| \right\}, \quad (5)$$

corresponding to the exchange of virtual photons between the two electrons. Here, $\omega_{pn} = \omega_p - \omega_n$, and we use the system of units where $c \neq 1$. Because the retardation factor $\exp\{\frac{i}{c} |\omega_{pn}| |\vec{r}'' - \vec{r}'''\}$, which depends explicitly on the initial and final energies of the system, appears in this expression, in the general case we cannot introduce the operator of the interaction between the two electrons $B_{1l}(\vec{r}'', \vec{r}''')$, whose matrix element would be equal to $U_{mn,pr}^{(3)}$. However, we can construct such an operator within the approximation of small velocities ($v/c \ll 1$, where v is the velocity of the electron in the atom and c is the velocity of light in the vacuum) as well as when obtaining the Breit expression (1). However, in the case of interaction of the two quasimolecular electrons located at an arbitrary distance from each other near different nuclei, the situation becomes complicated because the absolute value of the exponents in $U_{mn,pr}^{(3)}$ -matrix (13) becomes larger than a unit and the exponential factors become rapidly oscillating functions in the (asymptotic) domain of interelectron distances of interest. The specified circumstance renders the impossibility of direct usage of the several first terms of the c^{-1} -expansion of the retardation factor to construct the relativistic operator of interaction of the two bound electrons at arbitrary distances between them (including arbitrarily large ones). At the same time, this far domain of interelectron distances determines the probabilities of processes with rearrangement in the asymptotic limit ($R \rightarrow \infty$) in many two-electron problems of the theory of slow atomic collisions. In this domain, which we shall call *the domain of far electron correlations*, the effects of retardation of interaction of charged particles are amplified essentially.

If the domains of spatial localization of the electrons near the different nuclei (of the first electron near the nucleus B^{Z_b+} , and of the second one near A^{Z_a+}) are rather small (of the order of atomic sizes) and rather far apart, then the relative distance between the electrons can be expanded in powers of the ratio $\Delta r/R$ under the condition $\Delta r < R < \infty$,

$$|\vec{r}'' - \vec{r}'''| = R \left(1 + \frac{\vec{R} \Delta \vec{r}}{R^2} + \frac{M}{R} \right). \quad (6)$$

Here, $\Delta \vec{r} = \vec{r}_{1b} - \vec{r}_{2a}$, $\Delta r = |\Delta \vec{r}|$, \vec{r}_{1b} (\vec{r}_{2a}) is the position vector of the first (second) electron with respect to the nucleus B^{Z_b+} (A^{Z_a+}), $M = M(\Delta \vec{r}, \vec{R})$ are small corrections containing higher powers of $\Delta r/R$. Therewith, the smallness of the parameter $\Delta r/R$ means that the electrons are located close to the different atoms (nuclei).

To assign the exact meaning to the K -factor (14), we transform it as follows:

$$K(\vec{r}''', \vec{r}''''; \omega_{pn}) = \frac{1 - \vec{\alpha}'' \vec{\alpha}''''}{|\vec{r}'' - \vec{r}''''|} e^{\frac{i}{c} |\omega_{pn}| R} e^{\frac{i}{c} |\omega_{pn}| (|\vec{r}'' - \vec{r}''''| - R)}. \quad (7)$$

For the quasimolecular electrons located near the different nuclei, the performed transformation is convenient due to the factorization of the R -dependent relativistic factor $\exp\{\frac{i}{c} |\omega_{pn}| R\}$ of the amplification of the effects of dynamic retardation of the interaction.

Henceforth, we shall assume that the requirement

$$\frac{1}{c} |\omega_{pn}| \frac{\vec{R} \Delta \vec{r}}{R} \ll 1 \quad (8)$$

is satisfied. The distance R between the nuclei can vary in the range $\Delta r \leq R < \infty$ and has a dynamical meaning in our problem, i.e., it appears in the expression for the energy spectrum. The exponential factor $\exp\{\frac{i}{c} |\omega_{pn}| (|\vec{r}'' - \vec{r}''''| - R)\}$ in the right hand side of (12) is small, compared to an unity. This fact allows to formally expand the K -factor (12) in powers of $1/c$. We have the expansion up to the terms of the order of c^{-2} inclusively:

$$K(\vec{r}''', \vec{r}''''; \omega_{pn}) = (1 - \vec{\alpha}'' \vec{\alpha}'''') \exp\left\{\frac{i}{c} |\omega_{pn}| R\right\} \times \left\{ f_0(\vec{r}''', \vec{r}'''') + \frac{i}{c} |\omega_{pn}| f_1(\vec{r}''', \vec{r}'''') - \frac{1}{2c^2} \omega_{pn}^2 f_2(\vec{r}''', \vec{r}'''') \right\}. \quad (9)$$

We provide the explicit form of the coefficient functions f_0 , f_1 , and f_2 , finally determining the dependence of the required relativistic operator $B_{1l}(\vec{r}'', \vec{r}''')$ on the spatial positions of the electrons:

$$\begin{aligned} f_0(\vec{r}'', \vec{r}''') &= \frac{1}{g_0(\vec{r}'', \vec{r}''')} = \frac{1}{|\vec{r}'' - \vec{r}'''|}, \\ f_1(\vec{r}'', \vec{r}''') &= \frac{g_1(\vec{r}'', \vec{r}''')}{g_0(\vec{r}'', \vec{r}''')} = \frac{|\vec{r}'' - \vec{r}'''| - R}{|\vec{r}'' - \vec{r}'''|}, \\ f_2(\vec{r}'', \vec{r}''') &= \frac{g_2(\vec{r}'', \vec{r}''')}{g_0(\vec{r}'', \vec{r}''')} = \frac{(|\vec{r}'' - \vec{r}'''| - R)^2}{|\vec{r}'' - \vec{r}'''|}. \end{aligned} \quad (10)$$

We eliminate the frequencies in expression (17) by using the Dirac equations:

$$\hat{H}'' \Psi_m(\vec{r}'') = \omega_m \Psi_m(\vec{r}''), \quad \hat{H}''' \Psi_n(\vec{r}''') = \omega_n \Psi_n(\vec{r}'''). \quad (11)$$

Evidently, in order to take into account completely the retardation effects of interaction of the electrons, we should transform the expansion of the K -factor (17) such that it takes the form that is symmetric with respect to both the electrons. We shall carry out such symmetrization below and simultaneously represent the required relativistic operator $B_{1l}(\vec{r}'', \vec{r}''')$ in the form that is convenient for perturbative calculations.

In order to move from frequencies to operators, we shall first transform the second term (in the right hand side of (17)) into a slightly different equivalent form. Namely, by means of the easily checkable relation $\omega_n - \omega_p = R_{1l}(\omega_l - \omega_m)$, we divide this term into two groups of terms:

$$|\omega_{pn}| f_1(\vec{r}'', \vec{r}''') \equiv \pm \frac{1}{2} [R_{1l}(\omega_l - \omega_m) + (\omega_n - \omega_p)] f_1(\vec{r}'', \vec{r}'''). \quad (12)$$

Here, $R_{1l} = (\omega_n - \omega_p)/(\omega_l - \omega_m)$, the plus sign in (20) corresponds to the case $\omega_p < \omega_n$, and the minus sign corresponds to the case $\omega_p > \omega_n$. Because in the calculations of the matrix elements (13), the quantity $K(\vec{r}'', \vec{r}''''; \omega_{pn})$ is always multiplied by $\Psi_l^+(\vec{r}'') \Psi_p^+(\vec{r}''')$ from the left and by $\Psi_m(\vec{r}'') \Psi_n(\vec{r}''')$ from the right and subsequently integrated over \vec{r}'' and \vec{r}'''' , one can replace the frequencies ω_m and ω_n in the last expression by the operators \hat{H}'' and \hat{H}''' to the right of the factor $f_1(\vec{r}'', \vec{r}''')$ and replace

the frequencies ω_l and ω_p with the operators \hat{H}'' and \hat{H}''' to the left of the factor $f_1(\vec{r}'', \vec{r}''')$. After such transformations, the expression in the right hand side of (20) takes the following form:

$$|\omega_{pn}|f_1(\vec{r}'', \vec{r}''') \rightarrow \pm \frac{1}{2} \left\{ R_{1l} \left[\hat{H}'' f_1(\vec{r}'', \vec{r}''') - f_1(\vec{r}'', \vec{r}''') \hat{H}'' \right] + f_1(\vec{r}'', \vec{r}''') \hat{H}''' - \hat{H}''' f_1(\vec{r}'', \vec{r}''') \right\} = \pm \frac{1}{2} \left\{ R_{1l} [\hat{H}'', f_1(\vec{r}'', \vec{r}''')] + [f_1(\vec{r}'', \vec{r}'''), \hat{H}'''] \right\}. \quad (13)$$

Hereinafter, the square brackets denote the commutators of corresponding quantities.

Taking into account the relation $\omega_n - \omega_p = R_{1l}(\omega_l - \omega_m)$ and transforming the third term in the expansion (17) to the symmetric form, we arrive at the following transformation of the K -factor:

$$K(\vec{r}'', \vec{r}'''; \omega_{pn}) \rightarrow (1 - \vec{\alpha}'' \vec{\alpha}''') e^{\frac{i}{c} |\omega_{pn}| R} \left\{ f_0(\vec{r}'', \vec{r}''') \pm \frac{i}{2c} \left(R_{1l} [\hat{H}'', f_1(\vec{r}'', \vec{r}''')] + [f_1(\vec{r}'', \vec{r}'''), \hat{H}'''] \right) + \frac{R_{1l}}{2c^2} \left[\hat{H}'', [\hat{H}''', f_2(\vec{r}'', \vec{r}''')] \right] \right\}. \quad (14)$$

The motion of the separate electrons in the two-centre system $A^{(Z_a-2)+} + B^{Z_b+}$ is described by the Dirac one-electron Hamiltonian for the problem of two fixed Coulomb centres at the distance R from each other:

$$\begin{aligned} \hat{H}'' &= c \vec{\alpha}'' \hat{p}'' + \beta'' mc^2 - \frac{Z_a e^2}{|\vec{r}'' - \vec{R}_a|} - \frac{Z_b e^2}{|\vec{r}'' - \vec{R}_b|}, \\ \hat{H}''' &= c \vec{\alpha}''' \hat{p}''' + \beta''' mc^2 - \frac{Z_a e^2}{|\vec{r}''' - \vec{R}_a|} - \frac{Z_b e^2}{|\vec{r}''' - \vec{R}_b|}. \end{aligned} \quad (15)$$

Here, we keep $\hbar \neq 1$ explicitly, $Z_a e$ and $Z_b e$ are the charges of the point nuclei, $\hat{p}'' = -i\hbar \vec{\nabla}''$ and $\hat{p}''' = -i\hbar \vec{\nabla}'''$ denote the operators of momentum of the electrons. All the position vectors in (18) are measured from the origin of the laboratory system of coordinates, \vec{R}_a and \vec{R}_b are the position vectors of nuclei A^{Z_a+} and B^{Z_b+} , respectively; the internuclear distance can be expressed as $R = |\vec{R}_b - \vec{R}_a|$.

Having calculated the commutators appearing in the right hand side of (21) we obtain the operator, which describes (in the $U_{mn,pr}^{(3)}$ -matrix (13)) the interaction of the two electrons via the field of virtual photons, is of the form

$$\begin{aligned} B_{1l}(\vec{r}'', \vec{r}''') &= e^2 \exp \left\{ \frac{i}{c} |\omega_{pn}| R \right\} \left\{ \frac{1 - \vec{\alpha}'' \vec{\alpha}'''}{|\vec{r}'' - \vec{r}'''|} \pm R \frac{R_{1l} \vec{\alpha}'' \vec{n} + \vec{\alpha}''' \vec{n}}{2|\vec{r}'' - \vec{r}'''|^2} \right. \\ &\quad \left. + \frac{R_{1l}}{2} \left(\frac{\vec{\alpha}'' \vec{\alpha}''' - (\vec{\alpha}'' \vec{n})(\vec{\alpha}''' \vec{n})}{|\vec{r}'' - \vec{r}'''|} - R^2 \frac{\vec{\alpha}'' \vec{\alpha}''' - 3(\vec{\alpha}'' \vec{n})(\vec{\alpha}''' \vec{n})}{|\vec{r}'' - \vec{r}'''|^3} \right) \right\}. \end{aligned} \quad (16)$$

The first term in (24) represents the energy of the instantaneous (Coulomb) interaction of the electrons, and other ones take into account the corrections due to the retardation of relativistic interaction and the presence of the electron spins.

Similarly, we consider the exchange of virtual photons in the second term of the matrix (13) (see the second diagram in figure 1). After necessary transformations of the corresponding retardation factor, we arrive at the operator $B_{2l}(\vec{r}', \vec{r}''')$, which can be obtain from (24) after replacing the coefficient R_{1l} by $R_{2l} = (\omega_n - \omega_p)/(\omega_r - \omega_l)$.

In the special case of the resonance exchange of photons, we have $R_{1l} = 1$, and the operator (24) is transformed into the generalized Breit operator [9] for the interaction of the two quasimolecular electrons without emission or absorption of real photons. The condition $R_{1l} = 1$ implies that the transition of the system of the two particles into the intermediate state should be carried out according to the law of conservation of energy: $E_n - E_p = E_l - E_m$. As it is expected, the operator (24) is transformed into the known Breit operator (1) for the interaction of the two atomic electrons in He-like atoms at $R_{1l} = 1$ and $R \rightarrow 0$ (the united-atom limit). Thereby, one can consider the operator (24)

as a natural generalization of the Breit operator [13, 19] to the case of arbitrarily large interelectron distances where influence of the effect of dynamic retardation on the spin interactions of the electrons is amplified. The nontrivial moment of such a generalization is the presence of additional (compared to the Breit expression (1)) retardation terms depending on both the dimensional parameter R and the spin operators of the electrons in expression (24) for $B_{1l}(\vec{r}'', \vec{r}''')$.

According to the improvement of the Breit operator made in the present paper, it is justifiable to call the expression (24) *the generalized radiative Breit operator of the long-range type* (to stress the possibility of using it to solve a wide range of two-electron problems in physics of radiative atom-molecule collisions [2, 6, 8, 9, 10, 11, 12], in the theory of quasimolecular Auger spectroscopy [7], and in several important problems of nonlinear and quantum optics [9, 15, 16, 17, 20]).

Note that the obtained expression (24) for the operator $B_{1l}(\vec{r}'', \vec{r}''')$ is symmetrical with respect to both the electrons. This is the result of the appropriate symmetrization of all the terms in expansion (17) of the K -factor with respect to both the electrons.

In the series of papers [15, 16, 17] that actually led to the present stage of the investigations of the problem of two electrons, the following expression has been obtained for the relativistic operator of interaction of the two atomic electrons at an arbitrary distance from each other within the of the third order effects of quantum electrodynamics:

$$\begin{aligned} \tilde{B}_{1l}(\vec{r}'', \vec{r}''') = e^2 \exp \left\{ \frac{i}{c} |\omega_{pn}| R \right\} & \left\{ \frac{1 - \vec{\alpha}'' \vec{\alpha}'''}{|\vec{r}'' - \vec{r}'''|} + R \frac{\vec{\alpha}'' \vec{n}}{|\vec{r}'' - \vec{r}'''|^2} \right. \\ & \left. + \frac{R_{1l}}{2} \left(\frac{\vec{\alpha}'' \vec{\alpha}''' - (\vec{\alpha}'' \vec{n})(\vec{\alpha}''' \vec{n})}{|\vec{r}'' - \vec{r}'''|} - R^2 \frac{\vec{\alpha}'' \vec{\alpha}''' - 3(\vec{\alpha}'' \vec{n})(\vec{\alpha}''' \vec{n})}{|\vec{r}'' - \vec{r}'''|^3} \right) \right\}. \end{aligned} \quad (17)$$

As can be readily seen from the structure of the second term of (25), which is proportional to R , the principal drawback of this operator is the absence of the symmetry in the description of the pair of interacting particles.

Conclusion

The problem of interaction of two quasimolecular electrons via a field of virtual photons that is accompanied by emission or absorption of a real photon is solved in the current paper. Such an interaction is considered as a third order effect of quantum electrodynamics described by the Feynman diagrams in figure 1. We now shall list main properties of this interaction.

We have two domains of the configuration space where the generalized Breit operator of the long-range interaction type (24) behaves differently if the relative distance $r_{12} = |\vec{r}'' - \vec{r}'''|$ between the two electrons changes. For instance, in the united-atom limit ($R \rightarrow 0$), formula (24) for the operator $B_{1l}(\vec{r}'', \vec{r}''')$ becomes the limiting (Breit) expression (1), which correctly describes the retardation effects of the relativistic interaction only at a small interparticle distance r_{12} . More precisely, we can conclude that the domain of applicability of the Breit formula (1) is given by

$$\omega_0 r_{12} / c \ll 1, \quad (18)$$

where ω_0 is a characteristic frequency of the spectrum of the interacting electrons. Let Ω_{cl} denote such a domain of the configuration space, which we call the domain of close electron correlations. However, in the domain Ω_f , where the electrons belong to the different nuclei and inequality (16) is satisfied for all $\Delta r \leq R < \infty$, the Breit operator (1) fails to describe even qualitatively the relativistic interaction of the two electrons. At the same time, the relativistic operator B_{1l} (24) constructed herein describes the retarded interaction of the two quasimolecular electrons in the domain Ω_{cl} of close electron correlations as well as in the domain Ω_f of far electron correlations. Therefore, this operator can be used to solve many two-electron problems in atomic and molecular spectroscopy, astrophysics, theory of slow atomic collisions, etc. Moreover, it is necessary to employ the relativistic operator of interaction of the two electrons (24) in mathematical modelling of atomic clusters [21], investigation of optical properties

of various nanostructural systems in intense optical fields [22], and solving some important problems of recording, reading, and transmission of quantum information from one two-level atom (qubit) to another [23, 24].

References

- [1] J.D. Gillaspay, *J. Phys. B* **34** (2001) R93.
- [2] P. Verma, P.H. Mokler et al., *Nucl. Inst. Meth. Phys. Res. B* **235** (2005) 309.
- [3] M.I. Karbovanets, V.Yu. Lazur, and M.I. Chibisov, *Sov. Phys.—JETP* **59** (1984) 47.
- [4] M.I. Chibisov and R.K. Janev, *Phys. Rep.* **166** (1988) 1.
- [5] T.P. Grozdanov, R.K. Janev, and V.Yu. Lazur, *Phys. Scr.* **32** (1985) 64.
- [6] M. Barat and P. Roncin, *J. Phys. B* **25** (1992) 2205.
- [7] E.S. Parilis, L.M. Kishinevskii, V.I. Matveev, and B.G. Krakov, *Auger Processes at Atomic Collisions*, PhAN, Tashkent, 1989 (in Russian).
- [8] J. Eichler and W.E. Meyerhof, *Relativistic Atomic Collisions*, Academic Press, New-York, 1995.
- [9] M.Ya. Agre and L.P. Rapoport, *Sov. Phys.—JETP* **50** (1979) 37.
- [10] P. Beiersdorfer, L. Schweikhard, R. Olson et al., *Phys. Scr.* **T80A** (1999) 121;
- [11] K. Tökesi, Y. Awaya, T. Kambara et al., *Phys. Scr.* **T80B** (1999) 408.
- [12] A.V. Lankin, I.V. Morozov, G.E. Norman, and I.Yu. Skobelev, *JETP* **106** (2008) 608.
- [13] G. Breit, *Phys. Rev.* **34** (1929) 553.
- [14] V.Yu. Lazur, S.I. Migalina, and A.K. Reiti, *Theor. Math. Phys.* **158** (2009) 333.
- [15] O.N. Gadomskii, V.R. Nagibarov, and N.K. Solovarov, *Sov. Phys.—JETP* **36** (1973) 390; **43** (1976) 225.
- [16] O.N. Gadomsky and K.K. Altunin, *JETP* **87** (1998) 842.
- [17] O.N. Gadomskii, *Phys. Usp.* **43** (2000) 1071.
- [18] E.E. Nikitin and B.M. Smirnov, *Slow Atomic Collisions*, Energoatomizdat, Moscow, 1990 (in Russian); B.M. Smirnov, *Phys. Usp.* **44** (2001) 221.
- [19] A.I. Akhiezer and V.B. Berestetskiy, *Quantum Electrodynamics*, Nauka, Moscow, 1969 (in Russian); Wiley, New-York, 1965 (Engl. transl. pr. ed.).
- [20] G.W.F. Drake, *Phys. Rev. A* **5** (1972) 1979.
- [21] Y. Yamamoto, T. Miura et al., *Phys. Rev. Lett.* **93** (2004) 011801.
- [22] O.N. Gadomsky and A.G. Glukhov, *JETP* **103** (2006) 23.
- [23] O.N. Gadomsky and Yu.Yu. Voronov, *JETP* **94** (2002) 882.
- [24] O.N. Gadomskii and Yu.Ya. Kharitonov, *Quantum electronics* **34** (2004) 249.