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On the Quantum Electrodynamic Problem of Two Interacting Electrons

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Abstract

The problem of interaction of two quasi-molecular electrons, being at an arbitrary distance from one another – near different atoms (nuclei), is solved. Interaction is considered as the second-order effect of the quantum electrodynamic perturbation theory in the coordinate representation. The successive account of a natural requirement of symmetry of the retardation factor, electronic spins and retardation effects of the relativistic interaction of two quasi-molecular electrons localised near various nuclei, leads to the occurrence of additional terms in the expression for the electron-electron interaction operator, in comparison with the standard Breit operator [6,7].

Introduction

Almost all two-electron processes with rearrangement (two-electron capture, capture followed by excitation or ionisation etc.) accompanying inelastic collisions of the multicharged ions with atoms are inevitably related to the correlated transitions of electrons from a field of one ionic core (or the bare nucleus) to the field of another. The main contribution to probability of such transitions comes from the region of two-electron configuration space, in which two active electrons of parent ion are localised around different nuclei, and the approximation of independent electrons is valid as a zero one (see, for example, the review [1] and the literature quoted therein). At low energies of collision quasi-resonance processes with rearrangement are characterised by large cross sections when compared with an atomic diameter, and are defined substantially by transitions at large internuclear distances R , which allows to construct the asymptotic theory of such processes (see [2]; as examples of later development of this direction the reviews [1, 3, 4] can be recommended). Expanding the asymptotic theory of processes with rearrangement to the field of the relativistic binding energies leads to the necessity of the consecutive accounting of correlations of two electrons pulled apart to different nuclei, which are located at large distances from one another when compared with the characteristic wavelengths λ_0 in a spectrum of interacting atoms. Namely this far region of interelectron distances $r_{12} = |\vec{r}_1 - \vec{r}_2|$ defines the probabilities of two-electron processes with rearrangement in an asymptotic limit $r_{12} \sim R \rightarrow \infty$; we will term it further as a region of far electron correlations ($r_{12} \sim R > \lambda_0$).

The analysis of autoionisation states of the heavy multicharged quasi-molecules with two excited electrons shows [4, 5] that the main correlation effect corresponds to the configurations in which electrons are far apart – near different atoms. For the study of spectroscopy of autoionisation states of such quasi-molecules the completely relativistic consideration is necessary. In comparison with the autoionisation states of nuclear systems, in this case other physical aspects that demand detailed study of rather general questions about the role of magnetic interactions and retardation effects in processes of Auger ionisation of atoms by slow highly charged ions appear on the foreground.

However, even the formulation of a two-particle problem within the relativistic quantum theory encounters principal difficulties of mathematical and logical character. With known reservations one can say that to this day there is no satisfactory relativistic theory of two-particle systems. Immediate generalisation of the Dirac equation to the case of two-electron system is impossible due to the absence of the local Lorentz-invariant operator that takes into account the relativistic character of interelectronic interaction (retardation effects).

Without discussing weakly studied problems of the relativistic two-particle interactions in more details, we note only that the complete relativistic Hamiltonian of the system could be represented in the form of a series in powers of α^2 (where α is the fine structure constant). As long ago as 1929 Gregory Breit has shown [6] that taking into account the first term of this expansion turns out to be good approximation of the relativistic interaction between two electrons under the condition of smallness of retardation effects in a spectrum of He-like atom. The relativistic operator of interelectronic interaction obtained by Breit is of the following form [6, 7]:

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

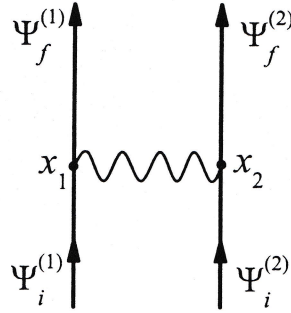
Here $\vec{\alpha}_1$ and $\vec{\alpha}_2$ – two commuting sets of the Dirac matrices, $\vec{r}_{12} = \vec{r}_1 - \vec{r}_2$, and the subindices 1 and 2 distinguish the quantities corresponding to the first and second electron respectively. The first term in (1) describes the electrostatic interaction of electrons, and remaining the Breit part $V_B(\vec{r}_{12})$ takes into account the magnetic spin-spin interactions and retardation corrections connected with the finiteness of velocity of the interaction expansion. Using the terminology accepted in the quantum electrodynamics one can say that the retardation interaction is caused by the exchange of transversal virtual photons between electrons, while the Coulomb interaction is caused by the exchange of "longitudinal" and "scalar" photons [7].

However, it is necessary to remember that the Breit expression (1) is a good approximation for description of the retardation interaction only while the distance r_{12} between electrons remains small when compared to $\lambda_0 = 2\pi c/\omega_0$, where ω_0 is the characteristic frequency in a spectrum of interacting electrons. It cannot be used in the two-electron problems related to slow atomic collisions because in this case, on the contrary, large interelectron distances r_{12} are essential. Therefore, the problem of two electrons belonging to two neutral atoms, being at an arbitrary distance from one another, has attracted a new wave of interest in the early seventies in connection with intensive study of multiatomic systems in the radiation field. The key step in this direction has been made in papers [8, 9, 10] where by methods of quantum electrodynamics the problem of interaction of two electrons belonging to two hydrogen-like atoms was considered in the general definition, not related to any restrictions to interatomic distances. The generalized Breit operator of interaction of two electrons through the field of the virtual photons as the effect of the second order of quantum electrodynamic perturbation theory has been obtained in [9, 10]. However, in the quoted works the account of relativistic effects has not been carried out consequentially. Particularly it is manifested in the absence of symmetry in the description of pair of interacting particles in the operator constructed in [10]. For the complete account of retardation effects in electron interaction it is necessary to satisfy the natural requirement of symmetry of the "retardation factor" with respect to the interacting particles that leads to the rise of the new ("retarded") term in the relativistic operator of interaction of two electrons (21) when compared to the corresponding operator in paper [10].

Our investigations are based on papers of Gadomsky with collaborators [10, 11] who within the last three decades have carried out extensive studies of the problem of two interacting electrons in the framework of effects of the 3rd order of the quantum electrodynamics, including process of radiation (or absorption) of a real photon. Importance of this approach for the general statement and solution of some basic problems of classical, non-linear and quantum optics increases rapidly. In particular, it gives an way of description of polarising fields in a system of two hydrogen-like atoms in whose terms one succeeded in constructing the nonlocal equations of extending of photons and electromagnetic waves in various mediums depending on types of quantum transitions and the intermediate states in the spectrum of interacting atoms. The certain completion of this range of problems can be found in the review [12].

Matrix of effective energy of interaction of two quasi-molecular electrons being at an arbitrary distance from one another

Interaction of two electrons in an external electrostatic field we shall consider as an effect of the second order of the quantum electrodynamics with the Feynman diagram shown below.



After integration over time, frequencies and wave vectors of the virtual photons in S -matrix we obtain the known expression for the matrix element [7]

$$S_{i \rightarrow f}^{(2)} = -2\pi i U_{i \rightarrow f}^{(2)} \delta(\omega_{fi}^{(1)} + \omega_{fi}^{(2)}), \quad (2)$$

where $U_{i \rightarrow f}^{(2)}$ denotes the matrix of the effective electrostatic energy of the two electrons, determined by the equation (see, for example, [13, 14])

$$U_{i \rightarrow f}^{(2)} = e^2 \int d\vec{r}_1 \int d\vec{r}_2 \Psi_f^{(2)+}(\vec{r}_2) \Psi_f^{(1)+}(\vec{r}_1) \frac{1 - \vec{\alpha}_1 \vec{\alpha}_2}{|\vec{r}_1 - \vec{r}_2|} \cos(|\omega_{fi}^{(2)}| |\vec{r}_1 - \vec{r}_2| / c) \Psi_i^{(2)}(\vec{r}_2) \Psi_i^{(1)}(\vec{r}_1). \quad (3)$$

Here $\Psi_i^{(n)}$ and $\Psi_f^{(n)}$ are wave functions of initial and final states of the n th electron ($n = 1, 2$), and $\omega_{fi}^{(n)} = E_f^{(n)} - E_i^{(n)}$ is the transition frequency. The quantities $E_i^{(1)}$ ($E_f^{(1)}$) and $E_i^{(2)}$ ($E_f^{(2)}$) are initial (final) energies of the 1st and 2nd electrons respectively. The indices i and f in (2), (3) characterise initial and final states of two electrons. Appearance of one-dimensional δ -functions from a difference between the total energies of two electrons in initial and final states as a factor in (2) is due to the energy conservation law:

$$E_f^{(1)} + E_f^{(2)} = E_i^{(1)} + E_i^{(2)}, \quad (4)$$

which represents demonstration of symmetry with respect to the continuous operation of time shift. According to this conservation law we shall further write $|\omega_{fi}^{(1)}|$ and $|\omega_{fi}^{(2)}|$ in the simplified form $|\omega_{fi}|$ (implying satisfaction of equalities $|\omega_{fi}| = |\omega_{fi}^{(1)}| = |\omega_{fi}^{(2)}|$).

All formulae given in this section concern the matrix element (2). To obtain the complete expression for $S_{i \rightarrow f}^{(2)}$ it is enough to add to the matrix element (3) the corresponding exchange matrix element representing an indistinguishability of two electrons.

Expression (3) explicitly depends on initial and final energies of the system, therefore here it is impossible to write (in the general case) the Hamiltonian of interaction of two electrons, i.e. the operator \hat{V} for which the following relation is satisfied

$$U_{i \rightarrow f}^{(2)} = \langle f | V | i \rangle = \int d\vec{r}_1 \int d\vec{r}_2 \Psi_f^{(2)+}(\vec{r}_2) \Psi_f^{(1)+}(\vec{r}_1) \hat{V} \Psi_i^{(2)}(\vec{r}_2) \Psi_i^{(1)}(\vec{r}_1). \quad (5)$$

However, at small velocities ($v_e/c \ll 1$ where v_e is the velocity of electrons in atom) such an operator can be constructed. For this purpose consider the situation, when one of electrons of atom

$A^{(Z_a-2)+}$, say the electron 1 moves into the immediate vicinity of other nucleus B^{Z_b+} , and the second electron remains near its own nucleus A^{Z_a+} . If the regions of space localisation of electrons on different nuclei (1st – close to B^{Z_b+} , and 2nd – close to A^{Z_a+}) are sufficiently small (do not exceed atomic sizes) and are far enough from one another then when the condition $\Delta r < R < \infty$ is satisfied, the relative distance r_{12} of pair of electrons pulled apart to different nuclei can be expanded in powers of $\Delta r/R$:

$$|\vec{r}_1 - \vec{r}_2| = R \left(1 + \frac{\vec{R}\Delta\vec{r}}{R^2} + \frac{M_1}{R} \right). \quad (6)$$

Here $\Delta\vec{r} = \vec{r}_{1b} - \vec{r}_{2a}$, $\Delta r = |\Delta\vec{r}|$, \vec{r}_{1b} and \vec{r}_{2a} – position vectors of 1st and 2nd electron with respect to the corresponding nuclei, and $M_1 = M_1(\Delta\vec{r}, \vec{R})$ – the small corrections including high powers of the ratio $\Delta r/R$. Corresponding (to the described picture of electrons localisation) region of two-particle configuration space we shall denote Ω_f and term it as a region of far electronic correlations.

In the matrix of the effective energy of interaction (3) let us separate the factor

$$K(\vec{r}_1, \vec{r}_2; \omega_{fi}) = \frac{\cos(|\omega_{fi}||\vec{r}_1 - \vec{r}_2|/c)}{|\vec{r}_1 - \vec{r}_2|}, \quad (7)$$

being responsible for exchanging of the virtual photons between two electrons. In the previous works [6, 7] at constructing the expansion of the retardation factor (7) the quantity $\omega_0 r_{12}/c \ll 1$ (or, equivalently, $1/c$; ω_0 – the characteristic frequency in a spectrum of interacting electrons) was supposed to be the unique small parameter. The expansion of the K -factor (7) below is constructed for a case when $1/c$ and $\Delta r/R$ are small parameters simultaneously. Such a choice of small parameters corresponds to a region of far electronic correlations and is realised within the used two-center model $A^{(Z_a-2)+} + B^{Z_b+}$, for example, when electrons are far apart – near different atoms (nuclei).

By the means of the elementary transformations the K -factor (7) is reduced to the form

$$K(\vec{r}_1, \vec{r}_2; \omega_{fi}) = \frac{\cos[|\omega_{fi}|(r_{12} - R)/c] \cos(|\omega_{fi}|R/c) - \sin[|\omega_{fi}|(r_{12} - R)/c] \sin(|\omega_{fi}|R/c)}{r_{12}}. \quad (8)$$

For the electrons which are at an arbitrary distance from one another, the transformation carried out above is convenient because it separates the additional retardation defined by the real $\cos(|\omega_{fi}|R/c)$ and imaginary $\sin(|\omega_{fi}|R/c)$ parts of the retardation factor $\exp\{i|\omega_{fi}|R/c\}$. Presence of the difference $r_{12} - R$ of the relative distances of electrons r_{12} and of nuclei R in arguments of the trigonometrical functions included in (8) specifies that the expansion of the K -factor should be carried out not only in powers of $1/c$ but in powers of small parameter $\Delta r/R$, too.

Henceforth, according to this we shall suppose that

$$\frac{|\omega_{fi}| \Delta r}{c R} \ll 1. \quad (9)$$

When condition (9) is satisfied the argument $|\omega_{fi}|(r_{12} - R)/c$ of trigonometrical functions in r.h.s. of (8) is small, so it is possible to expand the K -factor in powers of small parameter (9) and to restrict ourselves, as usual, only to the lowest terms of cosine and sine expansions:

$$K(\vec{r}_1, \vec{r}_2; \omega_{fi}) = \cos\left(\frac{|\omega_{fi}|R}{c}\right) \left\{ f_0(r_{12}) - \frac{\omega_{fi}^2}{2c^2} f_2(r_{12}) \right\} - \sin\left(\frac{|\omega_{fi}|R}{c}\right) \frac{|\omega_{fi}|}{c} f_1(r_{12}). \quad (10)$$

In turn, the coefficients

$$\begin{aligned} f_0(r_{12}) &= \frac{1}{g_0(r_{12})} = \frac{1}{|\vec{r}_1 - \vec{r}_2|}, \\ f_1(r_{12}) &= \frac{g_1(r_{12})}{g_0(r_{12})} = \frac{|\vec{r}_1 - \vec{r}_2| - R}{|\vec{r}_1 - \vec{r}_2|}, \\ f_2(r_{12}) &= \frac{g_2(r_{12})}{g_0(r_{12})} = \frac{(|\vec{r}_1 - \vec{r}_2| - R)^2}{|\vec{r}_1 - \vec{r}_2|} \end{aligned} \quad (11)$$

of the expansion (10) are series in powers of $\Delta r/R$ which can be written by means of asymptotic representations of functions g_0, g_1, g_2 at small values of parameter $\Delta r/R$:

$$g_0(\Delta\vec{r}, \vec{R}) = R \left[1 + (\vec{R}\vec{\Delta}r)/R^2 + M_1/R \right],$$

$$g_1(\Delta\vec{r}, \vec{R}) = \left[(\vec{R}\vec{\Delta}r)/R + M_1 \right], \quad g_2(\Delta\vec{r}, \vec{R}) = \left[(\vec{R}\vec{\Delta}r)/R + M_1 \right]^2.$$

The obtained expansion (10) is valid in a wide range of parameter R : $\Delta r \leq R < \infty$.

Let us eliminate the frequency in the matrix element by using the Dirac equations

$$\hat{H}_n^{(0)}(\vec{r}_n)\Psi_i^{(n)}(\vec{r}_n) = E_i^{(n)}\Psi_i^{(n)}(\vec{r}_n), \quad \hat{H}_n^{(0)}(\vec{r}_n)\Psi_f^{(n)}(\vec{r}_n) = E_f^{(n)}\Psi_f^{(n)}(\vec{r}_n), \quad (12)$$

$$\hat{H}_n^{(0)}(\vec{r}_n) = c\vec{\alpha}_n\hat{p}_n + \beta_n mc^2 - \frac{Z_a e^2}{r_{na}} - \frac{Z_b e^2}{r_{nb}}. \quad (13)$$

Hereinafter $\{\beta_1, \vec{\alpha}_1\}$ and $\{\beta_2, \vec{\alpha}_2\}$ are two sets of the Dirac matrices commuting among themselves and acting on various one-electron wave functions; $\hat{p}_n = -i\hbar\vec{\nabla}_n$ is the momentum operator of the n th electron; \vec{r}_{na} and \vec{r}_{nb} are position vectors of the n th electron with respect to the nuclei A^{Z_a+} and B^{Z_b+} respectively. The index n specifies that the one-electron relativistic Hamiltonian $\hat{H}_n^{(0)}(\vec{r}_n)$ (13) acts in space of the Dirac wave functions $\Psi_{i,f}^{(n)}(\vec{r}_n)$ of electron with the number n .

In a given form (10) the expansion of the K -factor does not reveal the symmetry with respect to interacting particles in any way. To write this expansion in symmetrical form we shall use the relation $\omega_{fi}^{(1)} = -\omega_{fi}^{(2)}$ which represents the energy conservation law (4). Moreover, according to the two possibilities $E_f^{(1)} > E_i^{(1)}$ and $E_f^{(1)} < E_i^{(1)}$ it is necessary to consider two cases $\omega_{fi}^{(1)} > 0$ and $\omega_{fi}^{(1)} < 0$ separately. If $E_f^{(1)} > E_i^{(1)}$ ($E_f^{(1)} < E_i^{(1)}$), then $\omega_{fi}^{(1)} = -\omega_{fi}^{(2)} > 0$ ($\omega_{fi}^{(1)} = -\omega_{fi}^{(2)} < 0$) and $|\omega_{fi}^{(1)}| = \omega_{fi}^{(1)}$ ($|\omega_{fi}^{(1)}| = -\omega_{fi}^{(1)}$). Using these relations, we transform the last term in r.h.s. of (10) to the symmetrical form:

$$|\omega_{fi}|f_1(r_{12}) = |\omega_{fi}^{(1)}|f_1(r_{12}) = \pm\omega_{fi}^{(1)}f_1(r_{12}) = \pm\frac{1}{2} \left[E_f^{(1)} - E_i^{(1)} + E_i^{(2)} - E_f^{(2)} \right] f_1(r_{12}). \quad (14)$$

In (14) '+' corresponds to $E_f^{(1)} > E_i^{(1)}$ ($\omega_{fi}^{(1)} > 0$), and '-' corresponds to $E_f^{(1)} < E_i^{(1)}$ ($\omega_{fi}^{(1)} < 0$). Meaning that expression (10) is multiplied by $\Psi_i^{(2)}(\vec{r}_2)\Psi_i^{(1)}(\vec{r}_1)$ from the right and by $\Psi_f^{(2)+}(\vec{r}_2)\Psi_f^{(1)+}(\vec{r}_1)$ from the left and is integrated over \vec{r}_1 and \vec{r}_2 , we can replace energies $E_i^{(1)}$ and $E_i^{(2)}$ in (14) by the operators $\hat{H}_1^{(0)}$ and $\hat{H}_2^{(0)}$, arranged to the right of the factor $f_1(r_{12})$. The energies $E_f^{(1)}$ and $E_f^{(2)}$ can be similarly replaced by the operators $\hat{H}_1^{(0)}$ and $\hat{H}_2^{(0)}$, arranged to the left of $f_1(r_{12})$:

$$\begin{aligned} |\omega_{fi}|f_1(r_{12}) &\rightarrow \pm\frac{1}{2} \left\{ \hat{H}_1^{(0)}f_1(r_{12}) - f_1(r_{12})\hat{H}_1^{(0)} + f_1(r_{12})\hat{H}_2^{(0)} - \hat{H}_2^{(0)}f_1(r_{12}) \right\} \\ &= \pm\frac{1}{2} \left\{ [\hat{H}_1^{(0)}, f_1(r_{12})] + [f_1(r_{12}), \hat{H}_2^{(0)}] \right\}. \end{aligned} \quad (15)$$

Hereinafter the square brackets denote commutators of corresponding quantities.

In a similar way (having used again the equations (12) and relations $\omega_{fi}^{(1)} = -\omega_{fi}^{(2)}$) we shall eliminate the frequencies in the second term of (10) that is proportional to c^{-2} :

$$\begin{aligned} -\omega_{fi}^2 f_2(r_{12}) &= (E_f^{(1)} - E_i^{(1)})(E_f^{(2)} - E_i^{(2)})f_2(r_{12}) \rightarrow f_2(r_{12})\hat{H}_1^{(0)}\hat{H}_2^{(0)} - \hat{H}_1^{(0)}f_2(r_{12})\hat{H}_2^{(0)} \\ &\quad - \hat{H}_2^{(0)}f_2(r_{12})\hat{H}_1^{(0)} + \hat{H}_1^{(0)}\hat{H}_2^{(0)}f_2(r_{12}) = \left[\hat{H}_1^{(0)}, [\hat{H}_2^{(0)}, f_2(r_{12})] \right]. \end{aligned} \quad (16)$$

Having substituted the operator expressions (15) and (16) into r.h.s. of (10) we arrive at the following transformation of the K -factor:

$$K(\vec{r}_1, \vec{r}_2; \omega_{fi}) \rightarrow \cos\left(\frac{\omega_{fi}R}{c}\right) \left\{ f_0(r_{12}) + \frac{1}{2c^2} [\hat{H}_1^{(0)}, [\hat{H}_2^{(0)}, f_2(r_{12})]] \right\} - \frac{1}{2c} \sin\left(\frac{\omega_{fi}R}{c}\right) \left([\hat{H}_1^{(0)}, f_1(r_{12})] + [f_1(r_{12}), \hat{H}_2^{(0)}] \right). \quad (17)$$

To symmetrize the further formulae with respect to both electrons, we shall replace the exchange energy of electrons $\omega_{fi} = E_f^{(1)} - E_i^{(1)} = E_i^{(2)} - E_f^{(2)}$ by the average difference of energies of the one-particle states $\bar{\omega}_{fi} = (E_f^{(1)} - E_i^{(1)} + E_f^{(2)} - E_i^{(2)})/2$. It is obvious that $\bar{\omega}_{fi}$ is nonzero only for exchange transitions.

So the K -factor (7) is presented by double expansion (10) in powers of $1/c$ and $\Delta r/R$. Herewith in the expansion in powers of $1/c$ we have restricted ourselves to the terms $1/c^2$, and there are no restrictions in the expansion in powers of small parameter $\Delta r/R$ because the function M_1 contains all higher correction terms. For this reason all subsequent consideration takes into account the interaction of two quasi-molecular electrons of the arbitrary multipolarity.

In approximation of noninteracting electrons the motion of each electron in the two-centre system $A^{(Z_a-2)+} + B^{Z_b+}$ is described by one-electron Dirac Hamiltonian (13) of the two-Coulomb-centre problem (Z_a, e, Z_b). For higher precision other terms, which take into account, for example, unpointness and spin of nucleus, screening the nuclear field by electron shell of atomic core etc., should be considered in the Hamiltonian (13). However, within the present consideration these can be neglected. Except for limit cases (of large ($R \gg 1$) and small ($R \ll 1$) internuclear distances) the problem of eigenvalues for such a Hamiltonian cannot be solved in an explicit form.

Using formulae (13) let us previously calculate commutators in r.h.s. of (17). It is easy to see that only one term in $\hat{H}_n^{(0)}$ is not commuting with $f_1(r_{12})$ and $f_2(r_{12})$, namely $c\vec{\alpha}_n\hat{p}_n$. For this reason substituting the operators $\hat{H}_1^{(0)}, \hat{H}_2^{(0)}$ into commutators (17), in expressions (13) at once we can omit the terms noncontaining the matrices $\vec{\alpha}_n$:

$$[\hat{H}_1^{(0)}, f_1] = c[\vec{\alpha}_1\hat{p}_1, f_1], \quad [f_1, \hat{H}_2^{(0)}] = c[f_1, \vec{\alpha}_2\hat{p}_2], \quad [\hat{H}_1^{(0)}, [\hat{H}_2^{(0)}, f_2]] = c^2[\vec{\alpha}_1\hat{p}_1, [\vec{\alpha}_2\hat{p}_2, f_2]]. \quad (18)$$

With the help of (18) and the obvious auxiliary formula $[\vec{\alpha}_n\hat{p}_n, f_{1,2}] = -i\hbar(\vec{\alpha}_n\vec{\nabla}_n)f_{1,2}$, it is easy to be convinced that the contributions of linear and quadratic in $1/c$ terms in expansion (17) are determined by the following operator expressions:

$$-\frac{1}{2c} \left([\hat{H}_1^{(0)}, f_1(r_{12})] + [f_1(r_{12}), \hat{H}_2^{(0)}] \right) = i\hbar R \frac{\vec{\alpha}_1\vec{n} + \vec{\alpha}_2\vec{n}}{2|\vec{r}_1 - \vec{r}_2|^2}, \quad (19)$$

$$\frac{1}{2c^2} [\hat{H}_1^{(0)}, [\hat{H}_2^{(0)}, f_2(r_{12})]] = -\frac{\hbar^2}{2} (\vec{\alpha}_1\vec{\nabla}_1)(\vec{\alpha}_2\vec{\nabla}_2)|\vec{r}_1 - \vec{r}_2| - \frac{\hbar^2 R^2}{2} (\vec{\alpha}_1\vec{\nabla}_1)(\vec{\alpha}_2\vec{\nabla}_2) \frac{1}{|\vec{r}_1 - \vec{r}_2|}, \quad (20)$$

where $\vec{n} = (\vec{r}_1 - \vec{r}_2)/|\vec{r}_1 - \vec{r}_2|$. Thus, quantity $\langle f|V|i \rangle$ indeed can be represented in the form (5) where the operator \hat{V} describing exchange of virtual photons in the matrix (3), is determined by the formula ($\hbar = 1$)

$$V(\vec{r}_1, \vec{r}_2; R) = e^2 \cos\left(\frac{\bar{\omega}_{fi}R}{c}\right) \left\{ \frac{1}{|\vec{r}_1 - \vec{r}_2|} - \frac{\vec{\alpha}_1\vec{\alpha}_2 + (\vec{\alpha}_1\vec{n})(\vec{\alpha}_2\vec{n})}{2|\vec{r}_1 - \vec{r}_2|} - R^2 \frac{\vec{\alpha}_1\vec{\alpha}_2 - 3(\vec{\alpha}_1\vec{n})(\vec{\alpha}_2\vec{n})}{2|\vec{r}_1 - \vec{r}_2|^3} \right\} + ie^2 R \sin\left(\frac{\bar{\omega}_{fi}R}{c}\right) \frac{\vec{\alpha}_1\vec{n} + \vec{\alpha}_2\vec{n}}{2|\vec{r}_1 - \vec{r}_2|^2}. \quad (21)$$

The first term $e^2 \cos(\bar{\omega}_{fi}R/c)r_{12}^{-1}$ in (21) represents the relativistic generalisation of the Coulomb interaction of electrons which are at the arbitrary distance from one another. Other terms in (21)

take into account the corrections caused by retardation of the relativistic interaction and presence of electron spins.

The obtained formula (21) for the operator of interelectron interaction corresponds to Feynman gauge of electromagnetic potentials [15]. Having changed the gauge, we can obtain various alternative forms of representation for this operator. In some cases the selection of either representation for the operator of electron-electron interaction takes on essential significance. The expression (21) is convenient for the analysis of effects of retardation of interelectron interaction since it allows to proceed immediately to the limit $c \rightarrow \infty$ (corresponding to "switching off" of the retardation effects).

In the united-atom limit ($R \rightarrow 0$) the operator (21) proceeds to the relativistic Breit operator (1) for interaction of two atomic electrons in He-like atoms. Thereby the operator (21) can be considered as an immediate generalisation of the Breit operator (1) to the range of arbitrarily large interelectron distances where the relativistic character of interaction of moving charges shows itself most striking. The nontrivial moment of such generalisation is the presence in expression (21) of the additional (in comparison with (1)) retardation terms which are proportional to the first and second power of R . This additional contribution in (21) is purely of relativistic character and appears at the expense of additional retardation of the relativistic interaction of the electrons being at arbitrarily large distances from one another when compared to $\lambda_0 = 2\pi c/\omega_0$.

According to specification of the Breit operator, represented in this paper, it is appropriate to call the expression (21) as the generalized Breit operator of the long-range type (in order to emphasize a possibility of its use in solving multielectronic problems of physics of slow atomic collisions [1, 3, 16, 17, 18, 19, 20, 21, 22], problems of theory of the quasimolecular Auger spectroscopy [5, 22], and some important problems of non-linear and quantum optics [8, 9, 10, 11, 12]).

Let us also pay attention to the fact that the discovered representation of the operator (21) in an explicit form reveals the symmetry with respect to the interacting particles and remains invariable under their permutation. Thus, the constructed relativistic operator of interaction of two electrons (21) opens a possibility for mathematically correct calculations of parameters of interaction of atomic particles at large distances, which are responsible for transitions between two-electron states in slow collisions. Note that in this connection the formula (21) not only considerably increases the limits of applicability of the Breit approximation when compared to (1), but also gives the chance to trace the structure and contribution to the matrix elements of the operator (21) of various relativistic effects within the terms $\sim \alpha^2$.

References

- [1] M.I. Chibisov, R.K. Janev, Phys. Rep. **166** (1988) 1.
- [2] V.M. Galitskii, E.E. Nikitin, B.M. Smirnov, Theory of Collisions of Atomic Particles [in Russian], Nauka, Moscow, 1981.
- [3] B.M. Smirnov, Uspekhi Fiz. Nauk, **171** (2001) 233.
- [4] B.G. Krakov, E.S. Parilis, Uspekhi Fiz. Nauk, **157** (1989) 477.
- [5] E.S. Parilis, L.M. Kishinevskii, V.I. Matveev, B.G. Krakov, Auger Processes in Atomic Collisions [in Russian], Fan, Tashkent, 1989.
- [6] G. Breit, Phys. Rev. **34** (1929) 553; **39** (1932) 616.
- [7] 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.

- [8] C.S. Chang, P. Stehle, *Phys. Rev. A.* **4** (1971) 630.
- [9] O.N. Gadoskii, V.R. Nagibarov, N.K. Solovarov, *Zh. Eksp. Teor. Fiz.* **63** (1972) 813.
- [10] O.N. Gadoskii, V.R. Nagibarov, N.K. Solovarov, *Zh. Eksp. Teor. Fiz.* **70** (1976) 435.
- [11] O.N. Gadoskii, K.K. Altunin, *Zh. Eksp. Teor. Fiz.* **114** (1998) 1555.
- [12] O.N. Gadoskii, *Uspekhi Fiz. Nauk* **170** (2000) 1145.
- [13] J. Sucher, *J. Phys. B* **21** (1988) L585.
- [14] L.N. Labzovskii, *Theory of Atom. Quantum Electrodynamics of Electronic Shells and Radiation Processes*, Fizmatgiz, Moscow, 1996.
- [15] V.B. Berestetskii, E.M. Lifshitz, L.P. Pitaevskii, *Quantum Electrodynamics*, Pergamon Press, Oxford, 1982.
- [16] I.V. Komarov, R.K. Janev, *Zh. Eksp. Teor. Fiz.* **51** (1966) 1712.
- [17] M.I. Chibisov, *Zh. Eksp. Teor. Fiz.* **70** (1976) 1687.
- [18] T.P. Grozdanov, R.K. Janev, *J. Phys.* **B13** (1980) 3341.
- [19] M.I. Karbovanets, V.Yu. Lazur, M.I. Chibisov, *Zh. Eksp. Teor. Fiz.* **86** (1984) 84.
- [20] T.P. Grozdanov, R.K. Janev, V.Yu. Lazur, *Phys. Scripta* **32** (1985) 64.
- [21] E.E. Nikitin, S.Ya. Umanskii, *Nonadiabatic Transitions at Slow Atomic Collisions* [in Russian], Moscow, Atomizdat, 1979.
- [22] E.E. Nikitin, B.M. Smirnov, *Slow Atomic Collisions* [in Russian], Energoatomizdat, Moscow, 1990.