

## THE RELATIVISTIC OPERATOR OF INTERACTION OF TWO QUASIMOLECULAR ELECTRONS AS A THIRD-ORDER EFFECT OF QUANTUM ELECTRODYNAMICS

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*We solve the problem of interaction two quasimolecular electrons located at an arbitrary separation near different atoms (nuclei). We consider third-order effects in quantum electrodynamics, which include the virtual photon exchange between electrons with emission (absorption) of a real photon. We obtain the general expression for matrix elements of the operator of the effective interaction energy of two quasimolecular electrons with the external radiation field, which allows calculating probabilities of inelastic processes with rearrangement at slow collisions of multicharge ions with relativistic atoms. We demonstrate that consistently taking the natural condition of the interaction symmetry with respect to the two electrons into account results in the appearance of additional terms in the operators of spin–orbit, spin–spin, and retarded interactions compared with the previously obtained expressions for these operators. We construct the operator of the dipole–dipole interaction of two neutral atoms located at an arbitrary separation.*

**Keywords:** interelectron interaction, retardation effect, Breit operator, quantum electrodynamics, quasimolecular electron

### 1. Introduction

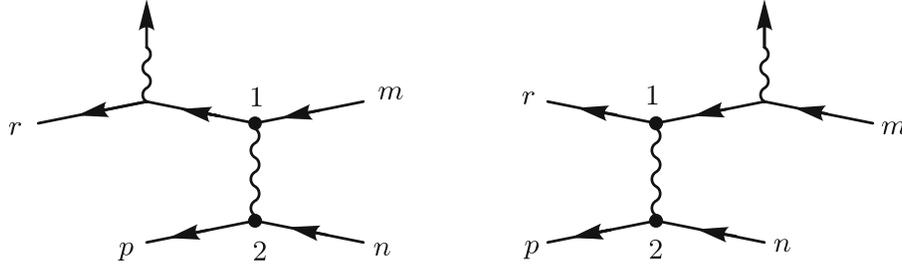
Inelastic collisions of atomic particles, especially multielectron ones, are accompanied by multiple processes of changing their charge and electron states. The simplest well-studied examples are one-electron ion–atom processes with rearrangement (for instance, resonance or quairesonance charge exchange) in which only one electron changes its state while the other electrons can be considered frozen. Such processes are highly effective and play an important role in creating the inverse population of ion levels in the solar corona plasma and in newly developed installations for controlled thermonuclear fusion [1], [2]. But at heat-scale collision energies, two-electron processes with rearrangement [3]–[7] become equally probable or even sometimes prevail over one-electron processes. These two-electron processes include various Auger processes [7], the two-electron charge exchange processes [3]–[6], and the charge exchange with simultaneous ion excitation [4]. Because the total cross sections and rate constants of these processes are large, we can assume that these processes with rearrangement are governed by electron transitions at relatively large distances  $R$  between colliding particles. The presence of the small parameter  $1/R$  allows developing a consistent asymptotic theory of the process under investigation. This is why several “memorable” results in the theory of multielectron atom–ion processes with rearrangement were obtained in the framework of the asymptotic approach [3], [4], [6].

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**Fig. 1.** Feynman diagrams for the third-order QED effects for interaction of two quasimolecular electrons accompanied by emission or absorption of a real photon.

At the same time, studying the influence of intensive electromagnetic radiation on characteristics of inelastic processes accompanying collisions of highly charged ions with heavy atoms attracted much attention in recent decades. The interest in these problems is due to the possibility of laser radiation stimulation of various processes occurring in ion–atom collisions and involving electrons of both the outer and the inner electron shells. Most theoretical and experimental papers dealt with two-electron processes with rearrangement (see, e.g., [2], [6], [8]–[12] and the references therein), which occurs at large internuclear distances and are accompanied by absorption (emission) of photons. These processes include strongly correlated electronic transitions recently intensively studied both experimentally [2], [10] and theoretically [8], [11]. Clarifying the principal features and basic mechanisms of radiation–collision processes with rearrangement affects all the recent activity in this field.

Because the interest in investigations of this sort will definitely increase in the future, it is important to consider quantum processes corresponding to the Feynman diagrams in Fig. 1 in detail. We must then take into account that the exchange mechanism is intrinsic for all the two-electron processes with rearrangement: one of the active, i.e., participating in transitions, electrons of the atom (ion)  $A^{(Z_a-2)+}$  tunnels to the “foreign” ion  $B^{Z_b+}$  with the subsequent dipole–multipole simultaneous transition of two electrons belonging to different nuclei. We therefore begin here with the assumption that the exchange matrix element governing two-electron processes with rearrangement is determined by a configuration in which active electrons are situated far from each other near different atoms (nuclei). In the case where, under favorable conditions, the mechanisms of nonadiabatic interaction result in multielectron transitions involving electrons of inner electron shells, realistic calculations of the interaction parameters for collision processes involving heavy (relativistic) atomic particles must be based on a totally relativistic theory. In fact, the very formulation of the two-particle problem in relativistic quantum theory encounters principal mathematical and logical difficulties. This is mainly because a local Lorentz-invariant operator taking the relativistic character of interelectron interaction (“retardation effects”) into account is lacking. The contemporary quantum field theory of electromagnetic interaction, quantum electrodynamics (QED), based on the  $S$ -matrix formalism and the Feynman diagram technique provides only the recipe for constructing such operators in the form of an expansion in powers of  $\alpha^2$  (where  $\alpha \approx 1/137$  is the fine structure constant). As early as 1929, Breit demonstrated [13] that such an expansion up to the first (nonzero) correction term provides a good approximation for the relativistic interaction of two electrons under the assumption that retardation effects in the spectrum of the helium-like atom are small. Breit obtained the relativistic operator of the interelectron interaction [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 two commuting sets of Dirac matrices,  $\vec{r}_{12} = \vec{r}_1 - \vec{r}_2$ , and the subscripts 1 and 2 distinguish quantities related to the first and second electrons.

Expression (1) for the interelectron interaction operator is currently fundamental for most Dirac–Breit quasirelativistic equation applications to multielectron problems in atomic physics and astrophysics. In particular, QED corrections of the Breit type  $V_B$  are often taken into account when calculating atomic structures perturbatively [14], but they are still being omitted when calculating electron structures of heavy multicharged quasimolecules. The applicability of Breit operator (1) is restricted by the condition that the interaction transfer time  $T_B = r_{12}/c$  is small compared with the mean electron transition time  $T_0 = 2\pi/\omega_0$ , where  $\omega_0$  is the characteristic frequency in the spectrum of interacting electrons. This condition is obviously satisfied for relatively small interelectron distances, for example, for intra-atomic distances in helium-like atoms.

The foregoing is why we advanced arguments in our preceding paper [15] that cast doubt on the possibility of using Breit operator (1) to find asymptotic expressions for the exchange interaction responsible for the simultaneous capture of two electrons during slow collisions of multicharge ions with atoms [3], [4]. These arguments are equally applicable to other two-electron processes (including radiation–collision) with rearrangement as soon as the leading contribution to the transition probability comes from the configuration in which these electrons are captured by different nuclei and the zeroth-order approximation is the independent-electron approximation. In fact, we here encounter the new QED problem of interaction two quasimolecular electrons with emission (absorption) of a real photon, which has no satisfactory solution as yet. The interest in this problem appeared in the early 1970s in relation to the intensive study of multiatom systems in a radiation field. The authors of [16]–[19] can be credited with creating and developing new ideas in this direction; in those papers, the problem of interaction two electrons belonging to two different hydrogen-like atoms was studied by QED methods in the general setting without imposing any restriction on the interatom distances. But the generalized Breit operator constructed there is not symmetric with respect to the pair of interacting particles and therefore cannot be applied in a consistent relativistic quantum theory. We therefore return to the problem of two quasimolecular electrons.

In Sec. 2, we present the general expression for matrix elements of the operator of the effective interaction energy of the system of two quasimolecular electrons and an external radiation field. In Sec. 3, we construct the relativistic interaction operator for two quasimolecular electrons coupled via a virtual photon field with simultaneous emission (absorption) of a real photon. This operator is a generalization of Breit operator (1). In Sec. 4, passing from relativistic Dirac spinors to nonrelativistic Pauli spinors in the matrix of the effective interaction energy allows finding the explicit form of the generalized Breit operator for the interaction of two quasimolecular electrons located at an arbitrary separation. In Sec. 5, we discuss the final results and compare them with the corresponding results in previous papers devoted to the problem of two electrons.

## 2. Effective interaction energy matrix for two quasimolecular electrons at an arbitrary separation

Describing the quasimolecule  $(AB)^{(Z_a+Z_b-2)+}$  by QED methods, we treat it as a system of two electrons interacting with each other via the quantized electromagnetic field and propagating in the external (electric) field of two stable  $A^{Z_a+}$  and  $B^{Z_b+}$  nuclei with the respective charges  $Z_a$  and  $Z_b$  separated by the distance  $R$ . We consider the nuclei here to be infinitely heavy, pointlike, and structureless.

The simplest examples of such systems are two-electron heteronuclear quasimolecules  $\text{HeH}^+$ ,  $\text{HeBe}^{4+}$ ,  $\text{HeC}^{6+}$ , etc. Such quasimolecules are created in stellar atmospheres and in experiments with thermonuclear plasma and with atomic (ionic) beams. As objects of theoretical interest, they can be compared to the helium atom in the theory of multielectron atoms. The laws and theoretical methods developed for these

systems can be used in the future to study more complex quasimolecular objects.

The QED perturbation theory based on the  $S$ -matrix formalism and the Feynman diagram technique provides a natural base for the field treatment of quantum mechanical problems. It allows expressing all the relevant physical quantities through the  $S$ -matrix including potentials of (exchange and long-range) particle interactions during the collision of the two-electron atom  $A^{(Z_a-2)+}$  with the slow multicharge ion  $B^{Z_b+}$ , while the  $S$ -matrix itself can be calculated using the standard QED Feynman rules. In the standard quantum mechanical form (see, e.g., [3], [4], [20]), the matrix element of the two-electron exchange interaction between the atom  $A^{(Z_a-2)+}$  and ion  $B^{Z_b+}$  is defined as a nondiagonal element of the interelectron interaction operator calculated on (adiabatic) electron wave functions of the quasimolecule  $(AB)^{(Z_a+Z_b-2)+}$  corresponding to cases of different localizations of electrons in the initial and final states. In the QED approach below, this matrix element is a component of a more general matrix element of the energy operator for the effective interaction of the system of two quasimolecular electrons with the external radiation field. Moreover, we then take third-order QED effects into account, including the virtual photon exchange between the electrons with emission (absorption) of a real photon. We present Feynman diagrams for this process in Fig. 1. In these effects, we separate two parts of the interaction, each of which takes intermediate states in the quasimolecular spectrum with either positive or negative frequencies into account.

To solve the stated problem, we consider processes of the interaction of two quasimolecular electrons located near different nuclei accompanied by emission or absorption of real photons. We do not assume the interelectron distances to be small compared with the characteristic wave lengths  $\lambda_0 = 2\pi c/\omega_0$  in the spectrum of interacting electrons, as was assumed in previous papers [13], [21], [22]; all the formulas below hold for all, including arbitrarily large, interelectron distances. This situation occurs (see [4]) when seeking the asymptotic behavior as  $R \rightarrow \infty$  for the exchange interaction responsible for the dynamics of various multielectron processes with rearrangement at slow collisions of atoms with multicharge ions. A typical example of a process with rearrangement caused by the direct interaction of two electrons belonging to different atoms is the quasisonance two-electron charge exchange of  $A^{(Z_a-2)+}$  atoms (for example, of helium He) on multicharge ions  $B^{Z_b+}$  (nitrogen  $N^{5+}$  [23], argon  $A^{6+}$  [24], or carbon  $C^{4+}$  [3]–[5]). At collision velocities smaller than orbital velocities of bound electrons, the two-electron capture occurs at large distances between the colliding atomic particles:  $R \sim |\vec{r}'' - \vec{r}'''| \gg 1$ , where  $\vec{r}''$  and  $\vec{r}'''$  are the radius vectors of the respective first and second electrons. In the active (i.e., asymptotic) domain of internuclear distances, the process essentially decomposes into a superposition of two inelastic transitions for each of the electrons: an electron from an outer or inner shell of the  $A^{(Z_a-2)+}$  atom travels to a respective inner or outer shell of the  $B^{(Z_b-2)+}$  atom. Inelastic transitions are possible only because of the electron interaction with each other via the virtual photon field. These electron “cross transitions” [3], [4] result in populating intermediate excited states of the incident multicharge ion with subsequent emission of a photon belonging to the short-wave ultraviolet or long-wave X-ray spectrum range.

Optical spectroscopy methods were recently used (see, e.g., [25]) to determine cross sections of radiation emission for separate level transitions in excited multicharge ions created by capturing electrons of helium (argon) atoms or of hydrogen molecules by ions with charges  $Z_b = 3, \dots, 8$  ( $Z_b = 10, 18, 36$ ). In particular, the existence of radiational two-electron charge exchange was confirmed experimentally [23] in collisions of ions  $N^{5+}$  with helium atoms at energies 0.357–4.28 KeV per unit charge in which the emission of the line 76.5 nm (the transition  $2s^2\ ^1S - 2s2p\ ^1P$  in  $N^{3+}$ ) was observed.

We now introduce the  $S$ -matrix of the QED third-order effects under consideration with the Feynman diagrams depicted in Fig. 1. We let the subscripts  $m$  and  $n$  denote the sets of quantum numbers of initial electron states and the subscripts  $p$  and  $r$  denote those of final states. Following the general rules formulated, for example, in [21], we obtain the expression for the matrix element

$$S_{i \rightarrow f}^{(3)} = S_{mn,pr}^{(3)} - S_{nm,pr}^{(3)}, \quad (2)$$

where

$$S_{mn,pr}^{(3)} = -ie^3 \int \bar{\Psi}_r(x'_1) \bar{\Psi}_p(x''_2) \mathcal{K}_{12}^{(3)}(1, 2; 3) \Psi_m(x'_1) \Psi_n(x''_2) d^4x'_1 d^4x''_1 d^4x''_2 \quad (3)$$

and  $S_{nm,pr}^{(3)}$  differs from  $S_{mn,pr}^{(3)}$  by interchanging the subscripts  $m$  and  $n$ . In expression (3) and hereafter, we use the system of units where  $\hbar = c = 1$ ,  $e = -|e|$  is the electron charge,  $\Psi_{m(n)}$  are solutions of the Dirac equation with the potential of two Coulomb centers for given electron initial states  $m(n)$ ,  $\bar{\Psi}_{r(p)} \equiv \Psi^+ \gamma_4$ , where  $\Psi^+$  are Hermitian conjugate two-center wave functions of final electron states  $r(p)$ ,  $x \equiv (\vec{r}, it)$  is the four-vector, and  $\vec{r}$  is the electron three-dimensional radius vector with respect to either nucleus  $A^{Z_a+}$  or nucleus  $B^{Z_b+}$ . We use the subscripts 1 and 2 to distinguish between quantities pertaining to electrons with the corresponding numbers.

Using the standard correspondence rules [21], we find that the operator  $\mathcal{K}_{12}^{(3)}(1, 2; 3)$  in (3) has the analytic structure

$$\mathcal{K}_{12}^{(3)}(1, 2; 3) = \hat{A}(x'_1) S(x'_1, x''_1) \gamma'_{\mu_1} D(x''_1 - x''_2) \gamma'''_{\mu_2} + \gamma'_{\mu_1} S(x'_1, x''_1) \hat{A}(x''_1) \gamma'''_{\mu_2} D(x'_1 - x''_2). \quad (4)$$

Here,  $\gamma_\mu \equiv (\vec{\gamma}, \gamma_4)$  is the covariant form of the Dirac matrices,  $\vec{\gamma} = -i\beta\vec{\alpha}$ ,  $\gamma_4 = \beta$ ,

$$\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix},$$

$\vec{\sigma}$  are the Pauli matrices, and 0 and  $I$  are the zero and unit  $2 \times 2$  matrices. We use the symbol  $\hat{A}$  to denote the contraction of the four-vector components  $A_\mu$  ( $\mu = 1, 2, 3, 4$ ) with the Dirac matrices  $\gamma_\mu$ :  $\hat{A} = \sum_\mu \gamma_\mu A_\mu$ . In the secondary quantization representation, the operator of the four-dimensional electromagnetic field potential is

$$A_\mu(x) = \sum_{\vec{k}, \lambda} g_{\vec{k}} e_{\mu\vec{k}}^\lambda (\hat{C}_{\vec{k}\lambda}^- e^{ikx} + \hat{C}_{\vec{k}\lambda}^+ e^{-ikx}), \quad (5)$$

where  $kx = \vec{k}\vec{r} - \omega_{\vec{k}}t$  is the scalar product of the four-vector  $x = (\vec{r}, it)$  and four-vector wave vector  $k = (\vec{k}, i\omega_{\vec{k}})$  satisfying the condition  $k^2 = \vec{k}^2 - \omega_{\vec{k}}^2 = 0$ ,  $\omega_{\vec{k}} \equiv \omega$  is the real photon frequency,  $e_{\mu\vec{k}}^\lambda$  are the unit vectors of the real photon polarizations (the values  $\lambda = 1, 2$  correspond to the transverse polarizations), and  $\hat{C}_{\vec{k}\lambda}^+$  and  $\hat{C}_{\vec{k}\lambda}^-$  are the operators of creation and annihilation of real photons in states with the polarization  $\lambda = 1, 2$ , momentum  $\vec{k}$ , and energy  $\omega$ . The coupling constants  $g_{\vec{k}} = (2\pi/\omega\Omega)^{1/2}$  contain the normalizing volume  $\Omega$ ; because they do not enter the final expression, we hereafter set  $\Omega = 1$ .

We set the electron propagator in the Furry picture [21]

$$S(x'_1, x''_1) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} d\omega'' e^{i\omega''(t'_1 - t''_1)} \sum_{l_\pm} \frac{\Psi_l(\vec{r}'_1) \bar{\Psi}_l(\vec{r}''_1)}{\omega_l(1 - i0) + \omega''} \quad (6)$$

into correspondence with the inner electron lines in the figure diagrams. In formula (6), we sum over all intermediate electron states with both positive ( $l = l_+$ ) and negative ( $l = l_-$ ) frequencies. We set the propagators

$$D(x''_1 - x''_2) = \frac{4\pi}{i(2\pi)^4} \int \frac{e^{i[k'(\vec{r}''_1 - \vec{r}''_2) - \omega'(t''_1 - t''_2)]}}{\vec{k}'^2 - \omega'^2 - i0} d\vec{k}' d\omega' \quad (7)$$

into correspondence with the internal photon lines in the Feynman gauge, where  $\vec{k}'$  denotes wave vectors of virtual photons with the frequency  $\omega'$ .

Primes on the four-vectors  $x = (\vec{r}, it)$  and  $\gamma$ -matrices in operator (4) and in the wave functions determine the integration domains with respect to space-time coordinates of interacting particles in  $S$ -matrix (3). The Dirac matrices  $\gamma_\mu$  with different primes then mutually commute.

We can represent the matrix element  $S_{mn,pr}^{(3)}$  in a form convenient for applications and admitting a simple physical interpretation. For this, we segregate the time factors in the wave functions in expression (3),

$$\Psi_m(x_1'') = \Psi_m(\vec{r}_1'')e^{-i\omega_m t_1''} \quad (8)$$

(and analogously for  $\Psi_n$ ,  $\Psi_r$ , and  $\Psi_p$ ). We now pass from the  $S$ -matrix to the matrix  $U_{mn,pr}^{(3)}$  of the effective interaction energy for the system of two bound electrons determined by the expression

$$S_{mn,pr}^{(3)} = -2\pi i U_{mn,pr}^{(3)} \delta(\omega + \omega_p - \omega_m + \omega_r - \omega_n), \quad (9)$$

where  $\omega_m = E_m/\hbar$  and  $\omega_n = E_n/\hbar$  are the frequencies of initial electron states and  $\omega_r = E_r/\hbar$  and  $\omega_p = E_p/\hbar$  are those of their final states. We here explicitly reconstruct the dependence on the Planck constant  $\hbar$ ; the sign of the optical photon frequency  $\omega$  in relation (9) indicates that in vector potential operator (5), we select the positive-frequency part proportional to the creation operator for the photon in the corresponding mode  $\vec{k}\lambda$ . Segregating the factor in the form of the one-dimensional  $\delta$ -function as usual expresses the energy conservation law common for all third-order effects under consideration (electron interaction via the virtual photon field accompanied by emission or absorption of a real photon),

$$E_p - E_m + E_r - E_n + \hbar\omega = 0. \quad (10)$$

For absorption of a real photon, we must change the sign of the frequency  $\omega$  in formulas (9) and (10).

Substituting explicit expressions (6)–(8) for propagators and wave functions in matrix element (3) and integrating in the matrix  $S_{mn,pr}^{(3)}$  over the times  $t_1'$ ,  $t_1''$ , and  $t_2'''$  and the wave vectors, we obtain the effective interaction energy matrix ( $\hbar = c = 1$ )

$$\begin{aligned} U_{mn,pr}^{(3)} = e^3 \int d\vec{r}' d\vec{r}'' d\vec{r}''' \left\{ -\frac{1}{|\vec{r}'' - \vec{r}'''}| \sum_{l\pm} \frac{e^{i|\omega_p - \omega_n| |\vec{r}'' - \vec{r}'''}|}}{\omega_l(1 - i0) - \omega - \omega_r} \overline{\Psi}_r(\vec{r}') \hat{A}(\vec{r}') \times \right. \\ \times \Psi_l(\vec{r}') \overline{\Psi}_l(\vec{r}'') \gamma'_\mu \Psi_m(\vec{r}'') \overline{\Psi}_p(\vec{r}''') \gamma''_\mu \Psi_n(\vec{r}''') - \\ \left. - \frac{1}{|\vec{r}' - \vec{r}'''}| \sum_{l\pm} \frac{e^{i|\omega_p - \omega_n| |\vec{r}' - \vec{r}'''}|}}{\omega_l(1 - i0) + \omega - \omega_m} \times \right. \\ \left. \times \overline{\Psi}_r(\vec{r}') \gamma'_\mu \Psi_l(\vec{r}') \overline{\Psi}_l(\vec{r}'') \hat{A}(\vec{r}'') \Psi_m(\vec{r}'') \overline{\Psi}_p(\vec{r}''') \gamma''_\mu \Psi_n(\vec{r}''') \right\}, \quad (11) \end{aligned}$$

where  $\Psi_{m(n)}$ ,  $\Psi_{r(p)}$ , and  $\Psi_l$  are the coordinate wave functions of electrons (without the time factors), the radius vectors  $\vec{r}'$  and  $\vec{r}''$  pertain to the first electron, and the radius vector  $\vec{r}'''$  pertains to the second electron. Matrix (2) describes one of eight processes that occur because of active electron interactions via the virtual photon field and are accompanied by emission (absorption) of a real photon. Other processes can be taken into account by changing the notation in the wave function accordingly.

### 3. The generalized Breit operator

The general expression for the matrix of the effective interaction energy of the system of two bound quasimolecular electrons with the external radiation field is [21]

$$U_{i \rightarrow f}^{(3)} = U_{mn,pr}^{(3)} - U_{nm,pr}^{(3)}. \quad (12)$$

According to (11), we can represent the matrix element  $U_{mn,pr}^{(3)}$  in the form

$$\begin{aligned}
U_{mn,pr}^{(3)} = & e^3 \int \Psi_r^+(\vec{r}') \Psi_p^+(\vec{r}''') \sum_{l\pm} \left\{ \gamma'_4 \gamma'_\delta A'_\delta \frac{\Psi_l(\vec{r}') \Psi_l^+(\vec{r}'')}{\omega_l(1-i0) - \omega - \omega_r} \times \right. \\
& \times \frac{1 - \bar{\alpha}'' \bar{\alpha}'''}{|\vec{r}'' - \vec{r}'''} e^{i|\omega_p - \omega_n| |\vec{r}'' - \vec{r}'''} + \frac{1 - \bar{\alpha}' \bar{\alpha}'''}{|\vec{r}' - \vec{r}'''} e^{i|\omega_p - \omega_n| |\vec{r}' - \vec{r}'''} \times \\
& \left. \times \frac{\Psi_l(\vec{r}') \Psi_l^+(\vec{r}'')}{\omega_l(1-i0) + \omega - \omega_m} \gamma''_4 \gamma''_\delta A''_\delta \right\} \Psi_m(\vec{r}'') \Psi_n(\vec{r}''') d\vec{r}' d\vec{r}'' d\vec{r}'''. \quad (13)
\end{aligned}$$

Here,  $\bar{\alpha}'$ ,  $\bar{\alpha}''$ , and  $\bar{\alpha}'''$  are Dirac matrices with the operators  $\bar{\alpha}''$ ,  $\bar{\alpha}'$ , and  $\bar{\alpha}'''$  acting on the respective functions  $\Psi_m(\vec{r}'')$ ,  $\Psi_l(\vec{r}')$ , and  $\Psi_n(\vec{r}''')$ ,  $A_\delta$  are the vector potential components without the time factors, the subscript  $\delta$  takes the values 1, 2, and 3, and we assume summation from 1 to 3 over the repeated index  $\delta$ . We stress that the one-electron quasimolecular wave functions in expression (13) depend parametrically on  $R$  (see formula (27) below).

We consider the first term in (13) and segregate the factor

$$K(\vec{r}'', \vec{r}'''; \omega_{pn}) = \frac{1 - \bar{\alpha}'' \bar{\alpha}'''}{|\vec{r}'' - \vec{r}'''} e^{i|\omega_{pn}| |\vec{r}'' - \vec{r}'''|/c}, \quad (14)$$

which is responsible for the virtual photon exchange between two electrons belonging to two different nuclei,  $|\vec{r}'' - \vec{r}'''| \sim R$ . Here,  $\omega_{pn} = \omega_p - \omega_n$ , and we use the system of units where  $c \neq 1$ . Because this expression contains the ‘‘retardation factor’’  $e^{i|\omega_{pn}| |\vec{r}'' - \vec{r}'''|/c}$  explicitly depending on the initial and final energies of the system, in the general case, we cannot introduce an operator of the interaction of two electrons  $B_{1l}^{(\pm)}(\vec{r}'', \vec{r}''')$  whose matrix element would be  $U_{mn,pr}^{(3)}$ . But we can construct such an operator in the small velocity approximation ( $v/c \ll 1$ , where  $v$  is the orbital speed of electrons in the atom and  $c$  is the vacuum speed of light).

Because expression (13) holds in the limit of the united atom ( $R \rightarrow 0$ ,  $Z = Z_a + Z_b$ ), it is instructive to perform the procedure of replacing retardation factor (14) with the corresponding operator in the simple example of two interacting electrons in a helium-like atom. For the characteristic value of  $\omega_{pn}$ , we then have the estimate  $|\omega_{pn}| \sim m(\alpha Z)^2$ , where  $Z = Z_a + Z_b$  is the total charge of the  $A^{Z_a+}$  and  $B^{Z_b+}$  nuclei. We further take into account that the characteristic value of the interelectron distance is of the order of the atomic distances,  $|\vec{r}'' - \vec{r}'''| \sim (m\alpha Z)^{-1}$ . For  $\alpha Z \ll 1$ , the exponent in expression (14) is then a small quantity of the order  $\alpha Z$ , and we can expand the exponential in a power series in  $1/c$  up to the order  $c^{-2}$  inclusively. We then pass from this expansion to its operator form in the  $c^{-2}$  approximation by properly symmetrizing all the retained terms of the  $c^{-1}$  expansion for retardation factor (14) and subsequently (using the Dirac equation) replacing frequencies with the corresponding Hamiltonian operators for the separated electrons. As a result, we obtain known expression (1) for the Breit operator [13], [21], [22], which depends not only on the displacement of the electron pair but also directly on the electron spin variables.

The situation becomes principally different for the interaction of two quasimolecular electrons belonging to two different nuclei and located at an arbitrary separation. The situation is then complicated by the absolute value of the exponent in the  $U_{mn,pr}^{(3)}$  matrix (13) exceeding unity in the (asymptotic) domain of interelectron distances under investigation, and the exponentials themselves become rapidly oscillating functions. This circumstance makes it impossible to construct a relativistic interaction operator for two bound electrons at arbitrarily large interelectron distances based on the first few terms of the  $c^{-1}$  expansion. At the same time, just this domain of large interelectron distances determines the probabilities of processes with rearrangement in the asymptotic limit ( $R \rightarrow \infty$ ) in many two-electron problems in the theory of slow

atomic collisions (for instance, in the problem of the quasisonance two-electron charge exchange of the type  $\text{He} + \text{N}^{5+} \rightarrow \text{He}^{2+} + \text{N}^{3+}$ ). In this domain of long-range electron correlations, as we call it, the effects of the retardation of the charged particle interaction are significantly enhanced.

As mentioned in the introduction, the possibility in principle of generalizing the Breit operator to the case of quasimolecular electrons was established in [17], [18] in the example of the problem of the interaction of two bound electrons belonging to two hydrogen-like atoms located at an arbitrary separation. But we found [15] in examining these papers that the generalized Breit operator obtained there is not symmetric with respect to the interacting particles and therefore cannot be applied in a consistent relativistic quantum theory. As mentioned in [15], the essential drawback of the procedure for passing from the retardation factor to the corresponding operator accepted in [17], [18] is that the interacting particles from the pair are treated unequally. The problem of two quasimolecular electrons with emission (absorption) of a real photon therefore needs further detailed study.

The method we use to solve this important QED problem is a further development of the method used in [15], [17] to solve the problem of the interaction of two atomic electrons in the framework of second-order QED effects. As shown below, symmetrizing the retardation factor consistently with respect to the two particles results in the appearance of additional terms in the relativistic operator of the two-electron interaction compared with both original Breit operator (1) and the generalized Breit operator in [18].

It is known [3], [4], [26] that the exponential coordinate dependence of the one-electron two-center wave functions results in the integration over  $\vec{r}''$  or  $\vec{r}'$  in expression (13) becoming localized primarily near the nucleus  $\text{B}^{Z_b+}$  in the regime of large internuclear distances  $R$ . Integration over  $\vec{r}'''$  in expression (13) is then localized near the nucleus  $\text{A}^{Z_a+}$ , and the leading contributions to the corresponding integrals of matrix (13) at large  $R$  are from the two spherical coordinate domains  $|\vec{r}' - \vec{R}| (|\vec{r}'' - \vec{R}|) \lesssim (m\alpha Z_b)^{-1}$  and  $|\vec{r}'''| \lesssim (m\alpha Z_a)^{-1}$ , which physically correspond to localizing electrons near different centers. Those are the domains of the electron coordinates for which we must construct the operator  $B_{1l}^{(\pm)}(\vec{r}'', \vec{r}''')$  describing the virtual photon exchange in the corresponding terms of matrix (13).

After these preliminary notes, we pass to directly deriving the relativistic interaction operator for two quasimolecular electrons located at an arbitrary separation. We begin with the two-electron atom  $\text{A}^{(Z_a-2)+}$  and the bare nucleus  $\text{B}^{Z_b+}$  separated by an arbitrary distance  $R$ . We now consider the typical situation (for processes with rearrangement) in which one of the active electrons of the  $\text{A}^{(Z_a-2)+}$  atom, for example, the first electron, tunnels in the vicinity of the “foreign”  $\text{B}^{Z_b+}$  nucleus while the second electron remains located near the “host”  $\text{A}^{Z_a+}$  nucleus. If the domains of spatial localization of electrons near different nuclei (near the  $\text{B}^{Z_b+}$  nucleus for the first electron and near the  $\text{A}^{Z_a+}$  nucleus for the second) are sufficiently small (of the order of atomic sizes) and sufficiently separated and if the condition  $\Delta r < R < \infty$  is satisfied, then we can expand the relative distance between the electrons in a power series in the ratio  $\Delta r/R$ ,

$$|\vec{r}'' - \vec{r}'''| = R \left( 1 + \frac{\vec{R} \Delta \vec{r}}{R^2} + \frac{M}{R} \right). \quad (15)$$

Here,  $\Delta \vec{r} = \vec{r}_{1b} - \vec{r}_{2a}$ ,  $\Delta r = |\Delta \vec{r}|$ ,  $\vec{r}_{1b}$  and  $\vec{r}_{2a}$  are the radius vectors of the respective first and second electrons relative to the respective  $\text{B}^{Z_b+}$  and  $\text{A}^{Z_a+}$  nuclei, and  $M = M(\Delta \vec{r}, \vec{R})$  are small corrections in higher powers of the ratio  $\Delta r/R$ . The small parameter  $\Delta r/R$  then selects the situation that physically corresponds to the electrons localized near different atoms (nuclei).

It was assumed in expanding the retardation factor in previous papers [13], [21], [22] that the only small parameter was the quantity  $\omega_0 r/c \ll 1$  (or formally  $1/c$ ), where  $r$  is the interelectron distance. This condition is obviously satisfied for not too large interelectron distances, for instance, for intra-atomic distances in helium-like atoms. Below, we construct the asymptotic expansion for  $K$ -factor (14) in the case where both  $1/c$  and  $\Delta r/R$  are natural small parameters simultaneously. Such a choice of small parameters

differs from the limit case of a single (united) helium-like atom ( $R = 0$ ) studied by Drake [22], and our case is realized in the adopted quasimolecule model, for example, when electrons are located far from each other near different centers.

To make the meaning of  $K$ -factor (14) precise, we transform it as

$$K(\vec{r}'' , \vec{r}''' ; \omega_{pn}) = \frac{1 - \vec{\alpha}'' \vec{\alpha}'''}{|\vec{r}'' - \vec{r}'''} e^{i|\omega_{pn}|R/c} e^{i|\omega_{pn}|(|\vec{r}'' - \vec{r}'''| - R)/c}. \quad (16)$$

For the quasimolecular electrons belonging to different nuclei, this transformation is convenient because the ( $R$ -dependent) relativistic factor  $e^{i|\omega_{pn}|R/c}$  of the amplification of the effects of dynamical interaction retardation, which are encoded in the dependence of this factor on the initial and final system energies,  $\omega_{pn} = E_p - E_n$ , is segregated. But the principal argument in favor of this transformation is that by applying it, we can reduce the problem of expanding retardation factor (14) to that of expanding the special exponential factor  $e^{i|\omega_{pn}|(|\vec{r}'' - \vec{r}'''| - R)/c}$  (for the quasimolecular model under consideration with electrons located near different centers). The presence of the difference  $|\vec{r}'' - \vec{r}'''| - R$  in the exponent of the last exponential factor implies that we must expand not only in powers of  $1/c$  but also in powers of the small parameter  $\Delta r/R$ .

In what follows, we assume that the condition

$$\frac{1}{c} |\omega_{pn}| \frac{\vec{R} \Delta \vec{r}}{R} \ll 1 \quad (17)$$

is satisfied. The internuclear distance  $R$  can then vary in the range  $\Delta r \leq R < \infty$  and has a dynamical meaning in our problem, i.e., it enters the expression for the energy spectrum.

The above analysis demonstrates that the exponent in  $e^{i|\omega_{pn}|(|\vec{r}'' - \vec{r}'''| - R)/c}$  in the right-hand side of (16) is small compared with unity if condition (17) is satisfied. This allows formally expanding  $K$ -factor (16) in powers of  $1/c$ . Through the terms of the order  $c^{-2}$ , we obtain the expansion

$$K(\vec{r}'' , \vec{r}''' ; \omega_{pn}) = (1 - \vec{\alpha}'' \vec{\alpha}''') e^{i|\omega_{pn}|R/c} \times \left\{ f_0(\vec{r}'' , \vec{r}''') + \frac{i}{c} |\omega_{pn}| f_1(\vec{r}'' , \vec{r}''') - \frac{1}{2c^2} \omega_{pn}^2 f_2(\vec{r}'' , \vec{r}''') \right\}. \quad (18)$$

We also write the coefficient functions  $f_0$ ,  $f_1$ , and  $f_2$  determining the dependence of the sought relativistic operator  $B_{1l}^{(\pm)}(\vec{r}'' , \vec{r}''')$  on the spatial arrangement of electrons explicitly,

$$\begin{aligned} f_0(\vec{r}'' , \vec{r}''') &= \frac{1}{g_0(\vec{r}'' , \vec{r}''')} = \frac{1}{|\vec{r}'' - \vec{r}'''} , \\ f_1(\vec{r}'' , \vec{r}''') &= \frac{g_1(\vec{r}'' , \vec{r}''')}{g_0(\vec{r}'' , \vec{r}''')} = \frac{|\vec{r}'' - \vec{r}'''} - R}{|\vec{r}'' - \vec{r}'''} , \\ f_2(\vec{r}'' , \vec{r}''') &= \frac{g_2(\vec{r}'' , \vec{r}''')}{g_0(\vec{r}'' , \vec{r}''')} = \frac{(|\vec{r}'' - \vec{r}'''} - R)^2}{|\vec{r}'' - \vec{r}'''} . \end{aligned} \quad (19)$$

Using the fact that the problem under study contains the small parameter  $\Delta r/R$  (in addition to  $1/c$ ), we expand the functions  $g_0$ ,  $g_1$ , and  $g_2$  in the right-hand sides of equalities (19) in power series in  $\Delta r/R$ ,

$$\begin{aligned} g_0(\Delta \vec{r}, \vec{R}) &= R \left[ 1 + \frac{\vec{r} \Delta \vec{r}}{R^2} + \frac{M}{R} \right], \\ g_1(\Delta \vec{r}, \vec{R}) &= \frac{\vec{R} \Delta \vec{r}}{R} + M, \quad g_2(\Delta \vec{r}, \vec{R}) = \left[ \frac{\vec{R} \Delta \vec{r}}{R} + M \right]^2. \end{aligned} \quad (20)$$

We note that formulas (15) and (20) are heuristic here because we write explicitly only the leading terms of the asymptotic expansions in them.

The form of expressions (15) and (20) formally implies that the expansion parameter in (18) is actually small dimensionless quantity (17), not  $1/c$ . In turn, the coefficients of expansion (18) are then obviously power series in  $\Delta r/R$ . This actually means that in the case where the interelectron distance is comparable to the internuclear distance, we can use formulas (20) to expand the functions  $f_0$ ,  $f_1$ , and  $f_2$  in expression (18) in power series in  $\Delta r/R$ . If we do not perform such an expansion, then we can take quasielectron interactions of all multiplicities into account in the closed form (in the  $c^{-2}$  approximation under investigation).

We use the Dirac equations to eliminate frequencies from (18),

$$\hat{H}''\Psi_m(\vec{r}'') = \omega_m\Psi_m(\vec{r}''), \quad \hat{H}'''\Psi_n(\vec{r}''') = \omega_n\Psi_n(\vec{r}'''). \quad (21)$$

For taking the retardation effects in the interelectron interactions fully into account, we must obviously bring  $K$ -factor expansion (18) to a form symmetric with respect to both electrons. We perform such a symmetrization below, simultaneously representing the sought relativistic operator  $B_{1l}^{(\pm)}(\vec{r}'', \vec{r}''')$  in a form convenient for perturbation theory calculations.

To pass from frequencies to operators, we first transform the second term in the right-hand side of (18) into a somewhat different equivalent form. Namely, using the easily verified relation  $\omega_n - \omega_p = R_{1l}(\omega_l - \omega_m)$ , we split it into two groups of terms,

$$|\omega_{pn}|f_1(\vec{r}'', \vec{r}''') \equiv \pm \frac{1}{2}[R_{1l}(\omega_l - \omega_m) + (\omega_n - \omega_p)]f_1(\vec{r}'', \vec{r}'''). \quad (22)$$

Here,  $R_{1l} = (\omega_n - \omega_p)/(\omega_l - \omega_m)$ , the plus sign corresponds to the case  $\omega_p < \omega_n$ , and the minus sign corresponds to the case  $\omega_p > \omega_n$ . Because 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 is integrated over  $\vec{r}''$  and  $\vec{r}'''$  when calculating matrix elements (13), we can replace the frequencies  $\omega_m$  and  $\omega_n$  in the expression for the  $K$ -factor with the respective operators  $\hat{H}''$  and  $\hat{H}'''$  on the right of  $f_1(\vec{r}'', \vec{r}''')$  and replace the frequencies  $\omega_l$  and  $\omega_p$  with the respective operators  $\hat{H}''$  and  $\hat{H}'''$  on the left of  $f_1(\vec{r}'', \vec{r}''')$ . After these transformations, the expression in the right-hand side of formula (22) becomes

$$\begin{aligned} |\omega_{pn}|f_1(\vec{r}'', \vec{r}''') &\rightarrow \pm \frac{1}{2}\{R_{1l}[\hat{H}''f_1(\vec{r}'', \vec{r}''') - f_1(\vec{r}'', \vec{r}''')\hat{H}''] + \\ &\quad + f_1(\vec{r}'', \vec{r}''')\hat{H}''' - \hat{H}'''f_1(\vec{r}'', \vec{r}''')\} = \\ &= \pm \frac{1}{2}\{R_{1l}[\hat{H}'', f_1(\vec{r}'', \vec{r}''')] + [f_1(\vec{r}'', \vec{r}'''), \hat{H}''']\}. \end{aligned} \quad (23)$$

Here and hereafter, the square brackets denote the commutators of the corresponding quantities.

Taking the relation  $\omega_n - \omega_p = R_{1l}(\omega_l - \omega_m)$  into account, we transform the third term in expansion (18) into the symmetric form

$$-\omega_{pn}^2 f_2(\vec{r}'', \vec{r}''') = R_{1l}(\omega_l - \omega_m)(\omega_p - \omega_n)f_2(\vec{r}'', \vec{r}'''). \quad (24)$$

Replacing frequencies with operators in (24) analogously to what was done in formula (23), we obtain the transformation

$$\begin{aligned} -\omega_{pn}^2 f_2(\vec{r}'', \vec{r}''') &\rightarrow R_{1l}\{f_2(\vec{r}'', \vec{r}''')\hat{H}''\hat{H}''' - \hat{H}''f_2(\vec{r}'', \vec{r}''')\hat{H}''' - \\ &\quad - \hat{H}'''f_2(\vec{r}'', \vec{r}''')\hat{H}'' + \hat{H}''\hat{H}'''f_2(\vec{r}'', \vec{r}''')\} = \end{aligned}$$

$$= R_{1l}[\hat{H}'', [\hat{H}''', f_2(\vec{r}'', \vec{r}''')]]. \quad (25)$$

Introducing operator expressions (23) and (25) into the right-hand side of expansion (18), we obtain the transformation of the  $K$ -factor

$$K(\vec{r}'', \vec{r}'''; \omega_{pn}) \rightarrow (1 - \bar{\alpha}'' \bar{\alpha}''') e^{i|\omega_{pn}|R/c} \left\{ f_0(\vec{r}'', \vec{r}''') \pm \frac{i}{2c} (R_{1l}[\hat{H}'', f_1(\vec{r}'', \vec{r}''')]) + [f_1(\vec{r}'', \vec{r}'''), \hat{H}'''] + \frac{R_{1l}}{2c^2} [\hat{H}'', [\hat{H}''', f_2(\vec{r}'', \vec{r}''')]] \right\}. \quad (26)$$

The functions  $f_0$ ,  $f_1$ , and  $f_2$  in this expression are still given by equalities (19). We note that the obtained  $K$ -factor representation (26) ensures describing the pair of interacting particles on an equal footing.

In our approach,  $K$ -factor (14) is therefore described by double expansion (18), (20) in powers of  $1/c$  and  $\Delta r/R$ . In the  $1/c$  expansion, we restrict ourself to the first three terms while no restrictions are imposed on the expansion in the small parameter  $\Delta r/R$  because the function  $M$  contains all the correction terms. We thus take interactions of the two quasimolecular electrons of all multiplicities into account in what follows.

The motion of separate electrons in the two-center system  $A^{(Z_a-2)+} + B^{Z_b+}$  is described by the Dirac one-electron Hamiltonian for the problem of two stable Coulomb centers separated by the distance  $R$ ,

$$\begin{aligned} \hat{H}'' &= c\bar{\alpha}'' \hat{p}'' + \beta'' mc^2 - \frac{Z_a e^2}{|\vec{r}'' - \vec{R}_a|} - \frac{Z_b e^2}{|\vec{r}'' - \vec{R}_b|}, \\ \hat{H}''' &= c\bar{\alpha}''' \hat{p}''' + \beta''' mc^2 - \frac{Z_a e^2}{|\vec{r}''' - \vec{R}_a|} - \frac{Z_b e^2}{|\vec{r}''' - \vec{R}_b|}. \end{aligned} \quad (27)$$

Here, we explicitly introduce  $\hbar \neq 1$ ,  $Z_a e$  and  $Z_b e$  are charges of the pointlike nuclei, and  $\hat{p}'' = -i\hbar \vec{\nabla}''$  and  $\hat{p}''' = -i\hbar \vec{\nabla}'''$  are the electron momentum operators. All the radius vectors in expressions (27) are drawn from the origin of the laboratory reference frame,  $\vec{R}_a$  and  $\vec{R}_b$  are the radius vectors of the respective  $A^{Z_a+}$  and  $B^{Z_b+}$  nuclei, and the internuclear distance is  $R = |\vec{R}_b - \vec{R}_a|$ .

The above calculations imply that result (26) can be obviously generalized to the case where additional terms, for example, taking the effects of the finite size of the nucleus and its spin, the screening of the nucleus field by electron shells of the atomic core, etc., into account, are added to Hamiltonian (27). But we must remember that except in limit cases (e.g., large internuclear distance [26]), the problem of calculating eigenvalues (21) for such a Hamiltonian cannot be solved explicitly.

We now calculate the commutators in the right-hand side of (26). We first note that only one of the terms in  $\hat{H}''$  and in  $\hat{H}'''$ , namely, the respective terms  $c\bar{\alpha}'' \hat{p}''$  and  $c\bar{\alpha}''' \hat{p}'''$ , do not commute with  $f_1(\vec{r}'', \vec{r}''')$  and  $f_2(\vec{r}'', \vec{r}''')$ . In expressions (27) for the operators  $\hat{H}''$  and  $\hat{H}'''$ , we can then omit all the terms not containing  $\bar{\alpha}''$  and  $\bar{\alpha}'''$  when substituting these expressions in the commutators in expansion (26):

$$\begin{aligned} [\hat{H}'', f_1] &= c[\bar{\alpha}'' \hat{p}'', f_1], & [f_1, \hat{H}'''] &= c[f_1, \bar{\alpha}''' \hat{p}'''], \\ [\hat{H}'', [\hat{H}''', f_2]] &= c^2[\bar{\alpha}'' \hat{p}'', [\bar{\alpha}''' \hat{p}''', f_2]]. \end{aligned} \quad (28)$$

Calculating commutators (28) using the easily verified formulas  $[\bar{\alpha}'' \hat{p}'', f_{1,2}] = \bar{\alpha}'' \hat{p}'' f_{1,2}$  and  $[\bar{\alpha}''' \hat{p}''', f_{1,2}] = \bar{\alpha}''' \hat{p}''' f_{1,2}$ , we obtain the contributions from the second and the third terms in expansion (26) given by the

operator expressions

$$\pm \frac{i}{2c}(R_{1l}[\widehat{H}'', f_1] + [f_1, \widehat{H}''']) = \pm \hbar R \frac{R_{1l}\vec{\alpha}''\vec{n} + \vec{\alpha}'''\vec{n}}{2|\vec{r}'' - \vec{r}'''|^2}, \quad (29)$$

$$\begin{aligned} \frac{1}{2c^2} R_{1l}[\widehat{H}'', [\widehat{H}''', f_2]] = & -\frac{\hbar^2}{2} R_{1l} \left[ (\vec{\alpha}''\vec{\nabla}'')(\vec{\alpha}'''\vec{\nabla}''')|\vec{r}'' - \vec{r}'''| + \right. \\ & \left. + R^2(\vec{\alpha}''\vec{\nabla}'')(\vec{\alpha}'''\vec{\nabla}''')\frac{1}{|\vec{r}'' - \vec{r}'''|} \right], \end{aligned} \quad (30)$$

where  $\vec{n} = (\vec{r}'' - \vec{r}''')/|\vec{r}'' - \vec{r}'''|$ . The operator describing the two-electron interaction via the virtual photon field in the matrix  $U_{mn,pr}^{(3)}$  given by (13) therefore becomes

$$\begin{aligned} B_{1l}^{(\pm)}(\vec{r}'', \vec{r}''') = e^2 e^{i|\omega_{pn}|R/c} & \left\{ \frac{1 - \vec{\alpha}''\vec{\alpha}'''}{|\vec{r}'' - \vec{r}'''|} \pm R \frac{R_{1l}\vec{\alpha}''\vec{n} + \vec{\alpha}'''\vec{n}}{2|\vec{r}'' - \vec{r}'''|^2} + \right. \\ & \left. + \frac{R_{1l}}{2} \left( \frac{\vec{\alpha}''\vec{\alpha}'''}{|\vec{r}'' - \vec{r}'''|} - \frac{(\vec{\alpha}''\vec{n})(\vec{\alpha}'''\vec{n})}{|\vec{r}'' - \vec{r}'''|} - R^2 \frac{\vec{\alpha}''\vec{\alpha}'''}{|\vec{r}'' - \vec{r}'''|^3} - 3\frac{(\vec{\alpha}''\vec{n})(\vec{\alpha}'''\vec{n})}{|\vec{r}'' - \vec{r}'''|^3} \right) \right\}. \end{aligned} \quad (31)$$

The plus sign of the term containing  $R$  corresponds to the case  $\omega_p < \omega_n$ , and the minus sign corresponds to the case  $\omega_p > \omega_n$ . The first term in formula (31) is the energy of the instant (Coulomb) electron interaction, and the other terms take corrections due to the relativistic interaction retardation and the electron spins into account.

We can analogously take the virtual photon exchange into account in the second term of matrix (13) (the second diagram in Fig. 1). After the necessary transformations of the corresponding retardation factor, we obtain the operator  $B_{2l}(\vec{r}', \vec{r}''')$  in a form analogous to expression (31) but with the coefficient  $R_{1l}$  replaced with  $R_{2l} = (\omega_n - \omega_p)/(\omega_r - \omega_l)$ .

In the particular case of the resonant photon exchange, we have  $R_{1l} = 1$ , and operator (31) becomes the generalized Breit operator [15] of the interaction of two quasimolecular electrons without emission or absorption of real photons. The condition  $R_{1l} = 1$  implies that the transition of the two-particle system into an intermediate state obeys the energy conservation law:  $E_n - E_p = E_l - E_m$ . At  $R_{1l} = 1$  and as  $R \rightarrow 0$  (the united atom limit), operator (31), as it should, becomes the known Breit operator (1) for the interaction of two atomic electrons in helium-like atoms. Operator (31) can therefore be considered the natural generalization of the Breit operator [13], [21] to the domain of arbitrarily large interelectron distances where the influence of the dynamical retardation effect on the electron spin interactions increases. A nontrivial point of this generalization is that additional retardation terms (compared with expression (1)) depending on the dimensional parameter  $R$  and the electron spin operators appear in expression (31) for  $B_{1l}^{(\pm)}(\vec{r}'', \vec{r}''')$ . We also note that this additional contribution to  $B_{1l}^{(\pm)}(\vec{r}'', \vec{r}''')$  is principally relativistic and appears because of the additional retardation of the relativistic interaction of two quasimolecular electrons located at large separation compared with  $\lambda_0 = 2\pi c/\omega_0$ .

In accordance with our refinement of the Breit operator here, expression (31) can be reasonably called the generalized radiational Breit operator of the long-range interaction type (to emphasize the possibility of using it to solve a broad class of two-electron problems in the physics of atom–molecule collisions with photon emission [2], [6], [8]–[12] and in the theory of quasimolecular Auger spectroscopy [7] and also to solve numerous important problems of nonlinear and quantum optics [15]–[19], [22]).

We also mention that expression (31) obtained for the operator  $B_{1l}^{(\pm)}(\vec{r}'', \vec{r}''')$  is symmetric with respect to both electrons. This is a result of properly symmetrizing all the retained terms in  $K$ -factor expansion (18) with respect to the two electrons. We note in passing that a symmetric representation for the relativistic

operator of the interaction of two quasimolecular electrons was first obtained in [15] from the consistent treatment of all second-order QED effects including exchange by virtual photons of all polarizations.

The following result for the relativistic operator of interaction of two atomic electrons located at an arbitrary separation was obtained in the series of papers [16]–[19], which actually initiated the contemporary investigations of the two-electron problem:

$$\begin{aligned} \tilde{B}_{1l}(\vec{r}'', \vec{r}''') = e^2 e^{i|\omega_{pn}|R/c} & \left\{ \frac{1 - \vec{\alpha}'' \vec{\alpha}'''}{|\vec{r}'' - \vec{r}'''}|} + R \frac{\vec{\alpha}'' \vec{n}}{|\vec{r}'' - \vec{r}'''}|^2} + \right. \\ & \left. + \frac{R_{1l}}{2} \left( \frac{\vec{\alpha}'' \vec{\alpha}'''}{|\vec{r}'' - \vec{r}'''}|} - \frac{(\vec{\alpha}'' \vec{n})(\vec{\alpha}''' \vec{n})}{|\vec{r}'' - \vec{r}'''}|} - R^2 \frac{\vec{\alpha}'' \vec{\alpha}'''}{|\vec{r}'' - \vec{r}'''}|^3} - 3 \frac{(\vec{\alpha}'' \vec{n})(\vec{\alpha}''' \vec{n})}{|\vec{r}'' - \vec{r}'''}|^3} \right) \right\}. \end{aligned} \quad (32)$$

An essential drawback of this operator is the absence of symmetry in the description of the pair of interacting particles. This follows from the structure of the second term proportional to  $R$  in expression (32).

An important remark, which follows from comparing formulas (31) and (32), is that as a result of consistently symmetrizing the two last terms in retardation factor expansion (18), final expression (31) for the operator  $B_{1l}^{(\pm)}(\vec{r}'', \vec{r}''')$  also contains the new term  $\pm R_{1l} R \vec{\alpha}'' \vec{n} / (2|\vec{r}'' - \vec{r}'''}|^2)$ , which was missed in (32) and is due to the additional retardation in the interaction of electrons separated by arbitrarily large distances. Calculations based on using operator (32) of [16]–[19] may therefore yield incorrect results.

## 4. Passing to two-component Pauli spinors

**4.1. The generalized two-particle Breit–Pauli operator.** In the  $U_{mn,pr}^{(3)}$  matrix in (13), we pass to the approximate two-component wave functions  $\Phi_m(\vec{r}'')$ ,  $\Phi_l(\vec{r}'')$ , and  $\Phi_n(\vec{r}''')$ ,  $\Phi_p(\vec{r}''')$  using the transformations [21]

$$\begin{aligned} \Psi_{m,l}(\vec{r}'') &= \begin{pmatrix} \varphi_{m,l}(\vec{r}'') \\ \frac{\vec{\sigma}'' \hat{p}''}{2mc} \varphi_{m,l}(\vec{r}'') \end{pmatrix}, & \varphi_{m,l}(\vec{r}'') &= \left( 1 - \frac{\hat{p}''^2}{8m^2 c^2} \right) \Phi_{m,l}(\vec{r}''), \\ \Psi_{n,p}(\vec{r}''') &= \begin{pmatrix} \varphi_{n,p}(\vec{r}''') \\ \frac{\vec{\sigma}''' \hat{p}'''}{2mc} \varphi_{n,p}(\vec{r}''') \end{pmatrix}, & \varphi_{n,p}(\vec{r}''') &= \left( 1 - \frac{\hat{p}'''^2}{8m^2 c^2} \right) \Phi_{n,p}(\vec{r}'''). \end{aligned} \quad (33)$$

Here, the  $2 \times 2$  Pauli matrices  $\vec{\sigma}''$  and  $\vec{\sigma}'''$  and the operators  $\hat{p}''$  and  $\hat{p}'''$  act respectively on those variables on which the wave functions  $\Phi_{m,l}(\vec{r}'')$  and  $\Phi_{n,p}(\vec{r}''')$  depend. Formulas (33) demonstrate the convenience of the Pauli approximation when considering a nonrelativistic limit for the four-component spinors  $\Psi_{m,l}$  and  $\Psi_{n,p}$ . In this limit, we have  $c \rightarrow \infty$ , and spinors (33) effectively become two-component ones.

Using functions (33), we transform the matrix element

$$\langle lp | B_{1l}^{(\pm)} | mn \rangle = \langle \Psi_l^*(\vec{r}'') \Psi_p^*(\vec{r}''') | B_{1l}^{(\pm)}(\vec{r}'', \vec{r}''') | \Psi_m(\vec{r}'') \Psi_n(\vec{r}''') \rangle \quad (34)$$

such that it becomes

$$\langle \Phi_{lp}^* | V_{BP}^{(\pm)} | \Phi_{mn} \rangle = \langle \Phi_l^*(\vec{r}'') \Phi_p^*(\vec{r}''') | V_{BP}^{(\pm)}(\vec{r}'', \vec{r}''') | \Phi_m(\vec{r}'') \Phi_n(\vec{r}''') \rangle, \quad (35)$$

where we can treat  $V_{BP}^{(\pm)}(\vec{r}'', \vec{r}''')$  as the interaction energy operator for two quasimolecular electrons located at an arbitrary separation. The wave functions  $\Phi_{mn} = \Phi_m(\vec{r}'') \Phi_n(\vec{r}''')$  and  $\Phi_{lp} = \Phi_l(\vec{r}'') \Phi_p(\vec{r}''')$  in formula (35) are nonsymmetrized products of two-component normalized wave functions (33) of the separate

electrons in the respective initial and final states. The electron coordinates in the functions  $\Psi_{n,p}(\vec{r}''')$  and  $\Psi_{m,l}(\vec{r}'')$  are taken with respect to the respective  $A^{Z_a+}$  and  $B^{Z_b+}$  nuclei.

We first consider the problem of reducing matrix element (34) of the Coulomb interaction operator  $e^2/|\vec{r}'' - \vec{r}'''|$  to form (35). Substituting functions (33) in (34) and performing the necessary transformations, we obtain the expression up to terms of the order  $O(1/c^2)$

$$\begin{aligned}
& e^2 e^{i|\omega_{pn}|R/c} \left\langle \Phi_{lp}^* \left| \frac{1}{|\vec{r}'' - \vec{r}'''} \right| \Phi_{mn} \right\rangle = \\
& = e^2 e^{i|\omega_{pn}|R/c} \int \left\{ \Phi_l^*(\vec{r}'') \Phi_p^*(\vec{r}''') \Phi_m(\vec{r}'') \Phi_n(\vec{r}''') - \right. \\
& \quad - \frac{1}{8m^2 c^2} \Phi_l^*(\vec{r}'') \Phi_p^*(\vec{r}''') \Phi_m(\vec{r}'') [\hat{p}''^2 \Phi_n(\vec{r}''')] - \\
& \quad - \frac{1}{8m^2 c^2} \Phi_l^*(\vec{r}'') \Phi_p^*(\vec{r}''') [\hat{p}''^2 \Phi_m(\vec{r}'')] \Phi_n(\vec{r}''') - \\
& \quad - \frac{1}{8m^2 c^2} \Phi_l^*(\vec{r}'') [\hat{p}''^2 \Phi_p(\vec{r}''')]^* \Phi_m(\vec{r}'') \Phi_n(\vec{r}''') - \\
& \quad - \frac{1}{8m^2 c^2} [\hat{p}''^2 \Phi_l(\vec{r}'')]^* \Phi_p^*(\vec{r}''') \Phi_m(\vec{r}'') \Phi_n(\vec{r}''') + \\
& \quad + \frac{1}{4m^2 c^2} [\vec{\sigma}'' \hat{p}'' \Phi_l(\vec{r}'')]^* [\vec{\sigma}'' \hat{p}'' \Phi_m(\vec{r}'')] \Phi_p^*(\vec{r}''') \Phi_n(\vec{r}''') + \\
& \quad \left. + \frac{1}{4m^2 c^2} \Phi_l^*(\vec{r}'') \Phi_m(\vec{r}'') [\vec{\sigma}''' \hat{p}''' \Phi_p(\vec{r}''')]^* [\vec{\sigma}''' \hat{p}''' \Phi_n(\vec{r}''')] \right\} \frac{d\vec{r}'' d\vec{r}'''}{|\vec{r}'' - \vec{r}'''} . \quad (36)
\end{aligned}$$

We can bring expression (36) to the form

$$\langle \Phi_{lp}^* | V_1 | \Phi_{mn} \rangle = \int \Phi_l^*(\vec{r}'') \Phi_p^*(\vec{r}''') V_1 \Phi_m(\vec{r}'') \Phi_n(\vec{r}''') d\vec{r}'' d\vec{r}''' . \quad (37)$$

For this, we must first integrate by parts. We take into account that for the quasimolecular model under consideration with two electrons located near different centers, the higher powers of  $1/|\vec{r}'' - \vec{r}'''|$  do not become infinite when varying the internuclear distance  $R$  in the range  $\Delta r < R < \infty$ . But higher powers of  $1/|\vec{r}'' - \vec{r}'''|$  may obviously result in nontrivial  $\delta$ -function-like contributions to the operator of the two-electron interaction energy in the limit of the united atom in which  $R \rightarrow 0$ . Indeed, as  $R$  decreases, the field in which electrons propagate becomes closer and closer to the field of the united helium-like atom with the total nucleus charge  $Z = Z_a + Z_b$ . This in fact means that in the range  $0 \leq R < \Delta r$ , where the wave functions localized near different centers essentially overlap, electrons perceive the two nuclei as a united Coulomb center. In this range, it is physically justified to replace the exact quasimolecular wave functions with the simpler wave functions of the united atom. In this case, all the electron coordinates are taken with respect to the united center, where we conveniently place the origin. Because the integrand in (36) contains higher powers of  $1/|\vec{r}'' - \vec{r}'''|$ , we preliminarily segregate the above point ( $\vec{r}'' = \vec{r}'''$ ), i.e., the origin. The integral over the sphere with the center at the origin is finite as  $\vec{r}'' \rightarrow \vec{r}'''$ . Because the result depends only on the value of the integrand at  $\vec{r}'' = \vec{r}'''$ , it can also be imitated by the volume integral of an expression containing the three-dimensional Dirac delta function  $\delta(\vec{r}'' - \vec{r}''')$ .

In a more formal language,  $\delta$ -function-like terms arising here customarily appear when integrating by parts or, more precisely, when we "transfer" the action of the operators  $\hat{p}'' = -i\vec{\nabla}''$  and  $\hat{p}''' = -i\vec{\nabla}'''$  from the functions  $\Phi_l(\vec{r}'')$  and  $\Phi_p(\vec{r}''')$  to the quantity  $1/|\vec{r}'' - \vec{r}'''|$ . The singular expressions thus appearing

have the operator form

$$\hat{p}''2 \frac{1}{|\vec{r}'' - \vec{r}'''}| = \hat{p}'''2 \frac{1}{|\vec{r}'' - \vec{r}'''}| = -\hat{p}'' \hat{p}''' \frac{1}{|\vec{r}'' - \vec{r}'''}| = 4\pi\delta(\vec{r}'' - \vec{r}'''). \quad (38)$$

In what follows, we rewrite the products of Pauli  $\vec{\sigma}$ -matrices arising in the above transformations using the known matrix relations [21]

$$(\vec{\sigma}\vec{a})(\vec{\sigma}\vec{b}) = \vec{a}\vec{b} + i\vec{\sigma}[\vec{a} \times \vec{b}], \quad (39)$$

$$(\vec{\sigma}\vec{a})\vec{\sigma} = \vec{a} + i[\vec{\sigma} \times \vec{a}], \quad \vec{\sigma}(\vec{\sigma}\vec{a}) = \vec{a} + i[\vec{a} \times \vec{\sigma}], \quad (40)$$

where  $\vec{a}$  and  $\vec{b}$  are arbitrary vectors.

Using these transformations, we can write expression (36) in form (37), where the sought operator  $V_1$  is

$$V_1 = e^2 e^{i|\omega_{pn}|R/c} \left\{ \frac{1}{|\vec{r}'' - \vec{r}'''}| + \frac{1}{4m^2 c^2} \frac{\vec{\sigma}'''[\vec{n} \times \hat{p}'''] - \vec{\sigma}''[\vec{n} \times \hat{p}'']}{|\vec{r}'' - \vec{r}'''}|^2} - \frac{\pi}{m^2 c^2} \delta(\vec{r}'' - \vec{r}''') \right\}. \quad (41)$$

In the united atom limit ( $R \rightarrow 0$ ), the first term

$$V_{1C} = e^2 e^{i|\omega_{pn}|R/c} \frac{1}{|\vec{r}'' - \vec{r}'''}| \quad (42)$$

in the right-hand side of (41) becomes the standard Coulomb electron interaction  $V_C(|\vec{r}'' - \vec{r}'''|) = e^2/|\vec{r}'' - \vec{r}'''|$ . The operator  $V_{1C}$  in (42) is then naturally the analogue of the Coulomb interaction of electrons located at an arbitrary separation, but this new operator differs from the standard operator  $V_C(|\vec{r}'' - \vec{r}'''|)$  because the former depends explicitly on the initial and final energies of the system:  $|\omega_{pn}| = |E_p - E_n|$ . This reflects the primarily purely relativistic effects of retardation for the interaction of charged particles separated by arbitrarily large distances.

Below, we return to discussing the other terms of the operator  $V_1$  in (41) in detail. Here, we only note the key property of the operator  $V_{1C}$  in (42): it is a periodic function of the internuclear distance  $R$ .

Using wave functions (33), we transform matrix element (34) for other terms of the operator  $B_{1l}$  in (31). We here stress that transforming the retarded terms (containing  $\vec{\alpha}$ -matrices) in expression (31) pertains to merely replacing  $\varphi_{m,l}(\vec{r}'')$  and  $\varphi_{n,p}(\vec{r}''')$  with  $\Phi_{m,l}(\vec{r}'')$  and  $\Phi_{n,p}(\vec{r}''')$  because these functions already contain the factor  $1/c^2$ .

We perform transformations analogous to those performed in obtaining explicit expression (41) for the operator  $V_1$ . Then, because the integrand develops a strong singularity at the origin as  $R \rightarrow 0$ , calculations for the atomic ( $0 \leq R < \Delta r$ ) and the quasimolecular ( $\Delta r < R < \infty$ ) domains differ somewhat.

At large internuclear distances ( $\Delta r < R < \infty$ ), the domains of the configuration space corresponding to electrons localized near different centers can be considered nonoverlapping. This in fact means that in contrast to the case of a single helium-like atom ( $R \rightarrow 0$ ) considered in [21], the higher powers of the quantities

$$(\vec{a}\vec{n})(\vec{b}\vec{n}) \frac{1}{|\vec{r}'' - \vec{r}'''}|, \quad R(\vec{a}\vec{n}) \frac{1}{|\vec{r}'' - \vec{r}'''}|^2, \quad R^2(\vec{a}\vec{n})(\vec{b}\vec{n}) \frac{1}{|\vec{r}'' - \vec{r}'''}|^3, \quad (43)$$

where  $\vec{a}$  and  $\vec{b}$  are arbitrary vectors, do not become infinite when  $R$  varies in the quasimolecular range  $\Delta r < R < \infty$ . The roughest approximation in this range must already take the difference in the nucleus

locations into account (in contrast to calculations in the interval  $0 \leq R < \Delta r$ ), and the simultaneous interactions between the electrons and the stable nuclei must be taken into account.

In the above transformations, we often encounter operator expressions of the form

$$(\hat{p}''\vec{a})(\hat{p}'''\vec{b})\frac{1}{|\vec{r}''-\vec{r}'''} = -\frac{1}{|\vec{r}''-\vec{r}'''}^3\left\{\vec{a}\vec{b}-\frac{3\vec{a}(\vec{r}''-\vec{r}''')\vec{b}(\vec{r}''-\vec{r}''')}{|\vec{r}''-\vec{r}'''}^2}\right\}, \quad (44)$$

which contain constant vectors  $\vec{a}$  and  $\vec{b}$ . But the last formula holds only if the wave functions sandwiched by matrix elements (34) and (35) are not spherically symmetric. For spherically symmetric functions, the matrix element of the operator in the right-hand side of (44) vanishes. This follows from the elementary integration over angle variables.

We now pass to studying singularities of higher powers of quantities (43) and (44) as  $R$  tends to zero. The limit expressions thus obtained are improper functions and may contain  $\delta$ -function-like singularities at the origin. A consistent mathematically rigorous description of these singularities requires the apparatus of generalized function theory [27]. We can nevertheless establish the structure of leading singularities using considerations based on systematically exploiting the symmetry properties of the system under consideration. For example, in the spherically symmetric case, which can be realized only in the united atom limit ( $R \rightarrow 0$ ), we can change the variables in the integrand ( $x = x'' - x'''$ ,  $y = y'' - y'''$ ,  $z = z'' - z'''$ ),

$$(\vec{\nabla}''\vec{a})(\vec{\nabla}'''\vec{b})\frac{1}{|\vec{r}''-\vec{r}'''} = \left(a_x b_x \frac{\partial^2}{\partial x^2} + a_y b_y \frac{\partial^2}{\partial y^2} + a_z b_z \frac{\partial^2}{\partial z^2}\right)\frac{1}{|\vec{r}''-\vec{r}'''} . \quad (45)$$

Indeed, the symmetry considerations imply that terms with the mixed derivatives  $\partial^2/\partial x\partial y$  vanish when integrating over angle variables. Again, because of the spherical symmetry, all the three terms in the right-hand side of (45) contribute the same. Therefore,

$$(\vec{\nabla}''\vec{a})(\vec{\nabla}'''\vec{b})\frac{1}{|\vec{r}''-\vec{r}'''} = \frac{1}{3}\vec{a}\vec{b}\Delta\frac{1}{|\vec{r}''-\vec{r}'''} = -\frac{4\pi}{3}\vec{a}\vec{b}\delta(\vec{r}''-\vec{r}'''). \quad (46)$$

Obtained expressions (44) and (46) can be unified into the single formula

$$(\hat{p}''\vec{a})(\hat{p}'''\vec{b})\frac{1}{|\vec{r}''-\vec{r}'''} = -\frac{1}{|\vec{r}''-\vec{r}'''}^3\left\{\vec{a}\vec{b}-\frac{3\vec{a}(\vec{r}''-\vec{r}''')\vec{b}(\vec{r}''-\vec{r}''')}{|\vec{r}''-\vec{r}'''}^2}\right\} + \frac{4\pi}{3}\vec{a}\vec{b}\delta(\vec{r}''-\vec{r}'''), \quad (47)$$

which holds in an arbitrary case.

We can find the structure of other singularities appearing in course of the above transformations by repeating the arguments that resulted in representation (47) and subsequently reducing the similar terms. We note that all the higher powers of quantities (43) that contain  $R$  (or  $R^2$ ) contribute zero in the limit as  $R \rightarrow 0$  because of the presence of the factor  $R$  (or  $R^2$ ). Of course, nontrivial  $\delta$ -function-like singularities arise in the limit  $R \rightarrow 0$  only from those higher powers of quantities (43) that do not contain a factor  $R$  or  $R^2$ .

Collecting all the expressions coming from both Coulomb and retarded terms in formula (31), we write the final result for the interaction energy operator for two quasimolecular electrons up to terms of the order  $\sim 1/c^2$  inclusively:

$$V_{\text{BP}}^{(\pm)} = V_{\text{IC}} + \tilde{V}_{\text{BP}}^{(\pm)} = V_{\text{IC}} + V_{\text{D}} + V_{\text{LL}}^{(\pm)} + V_{\text{SS}} + V_{\text{SL}}. \quad (48)$$

Here, we set

$$V_D = -\pi \left( \frac{e\hbar}{mc} \right)^2 e^{i|\omega_{pn}|R/c} \delta(\vec{r}'' - \vec{r}'''), \quad (49)$$

$$\begin{aligned} V_{LL}^{(\pm)} = & -\frac{e^2}{2m^2c^2} e^{i|\omega_{pn}|R/c} \left\{ \left( 1 - \frac{1}{2} R_{1l} \right) \frac{\hat{p}'' \hat{p}'''}{|\vec{r}'' - \vec{r}'''}|} + \frac{1}{2} R_{1l} \frac{\vec{n}(\vec{n} \hat{p}'') \hat{p}'''}{|\vec{r}'' - \vec{r}'''}|} \right. \\ & \left. + \frac{1}{2} R_{1l} \frac{R^2}{|\vec{r}'' - \vec{r}'''}|^3} [\hat{p}'' \hat{p}'' - 3\vec{n}(\vec{n} \hat{p}'') \hat{p}'''] \right\} \pm \\ & \pm \frac{e^2}{2mc} e^{i|\omega_{pn}|R/c} \frac{R}{|\vec{r}'' - \vec{r}'''}|^2} [R_{1l} \vec{n} \hat{p}'' + \vec{n} \hat{p}'''], \end{aligned} \quad (50)$$

$$\begin{aligned} V_{SS} = & \left( \frac{e\hbar}{2mc} \right)^2 e^{i|\omega_{pn}|R/c} \left\{ \frac{1}{|\vec{r}'' - \vec{r}'''}|^3} [\vec{\sigma}'' \vec{\sigma}''' - 3(\vec{\sigma}'' \vec{n})(\vec{\sigma}''' \vec{n})] + \right. \\ & \left. + \frac{R_{1l} R^2}{|\vec{r}'' - \vec{r}'''}|^5} [15(\vec{\sigma}'' \vec{n})(\vec{\sigma}''' \vec{n}) - 9\vec{\sigma}'' \vec{\sigma}'''] - \frac{8\pi}{3} \vec{\sigma}'' \vec{\sigma}''' \delta(\vec{r}'' - \vec{r}''') \right\}, \end{aligned} \quad (51)$$

$$\begin{aligned} V_{SL} = & \frac{e^2 \hbar}{4m^2 c^2} e^{i|\omega_{pn}|R/c} \left\{ \frac{1}{|\vec{r}'' - \vec{r}'''}|^2} [-(\vec{\sigma}'' + 2\vec{\sigma}''') [\vec{n} \times \hat{p}'']] + \right. \\ & \left. + (\vec{\sigma}''' + 2\vec{\sigma}'') [\vec{n} \times \hat{p}'''] \right\} + \frac{3R_{1l} R^2}{|\vec{r}'' - \vec{r}'''}|^4} [\vec{\sigma}'' [\vec{n} \times \hat{p}'''] - \vec{\sigma}''' [\vec{n} \times \hat{p}'']] \}. \end{aligned} \quad (52)$$

All the terms of the operator  $V_{BP}^{(\pm)}$  in (48) admit a clear physical interpretation and describe well-known physical effects appearing in the system of two interacting quasimolecular electrons. For example, the operators  $V_D$  in (49) and  $V_{LL}^{(\pm)}$  in (50) are purely orbital, and the  $\delta$ -function-like structure of the operator  $V_D$  in (49) admits a clear physical interpretation: in the limit  $R \rightarrow 0$ , this operator becomes the two-particle singular part  $-\pi(e\hbar/mc)^2 \delta(\vec{r}'' - \vec{r}''')$  of the known Darwin (contact) interaction of electrons with nuclei and with each other [13], [21]. The  $\delta$ -function-like structure in (49) of the operator  $V_D$  also implies that taking this operator into account makes sense only in the range of atomic distances  $0 \leq R < \Delta r$ .

We now discuss the physical meaning of the operator  $V_{LL}^{(\pm)}$  in (50). As  $R \rightarrow 0$  with  $R_{1l} = 1$ , it becomes the standard operator of the retarded interaction of two electrons in the united helium-like atom [21]. The operator  $V_{LL}^{(\pm)}$  in (50) can then be naturally considered the operator of the retarded interaction of two quasimolecular electrons located at an arbitrary separation.

At  $R_{1l} = 1$  (the case of the resonance electron interaction), an absolutely equivalent result for the operator  $V_{LL}^{(\pm)}$  follows from the classical Hamilton function of the system of interacting charges propagating in an external electromagnetic field [28] if we substitute quantum mechanical momentum operators for the corresponding classical particle momenta [16]. This correspondence between classical and quantum theories might be a foundation for constructing a more complete relativistic quantum mechanical theory of ion-atom interactions.

We also present the expression for the operator of retarded interaction of two quasimolecular electrons obtained in [16]–[19]. In our notation, it is

$$\begin{aligned} V_{LL} = & -\frac{e^2}{2m^2c^2} e^{i|\omega_{pn}|R/c} \left\{ \left( 1 - \frac{1}{2} R_{1l} \right) \frac{\hat{p}'' \hat{p}'''}{|\vec{r}'' - \vec{r}'''}|} + \frac{1}{2} R_{1l} \frac{\vec{n}(\vec{n} \hat{p}'') \hat{p}'''}{|\vec{r}'' - \vec{r}'''}|} \right. \\ & \left. + \frac{1}{2} R_{1l} \frac{R^2}{|\vec{r}'' - \vec{r}'''}|^3} [\hat{p}'' \hat{p}'' - 3\vec{n}(\vec{n} \hat{p}'') \hat{p}'''] \right\} + \frac{e^2}{mc} e^{i|\omega_{pn}|R/c} \frac{R}{|\vec{r}'' - \vec{r}'''}|^2} \vec{n} \hat{p}'''. \end{aligned} \quad (53)$$

But this expression is not symmetric with respect to the interacting particles and therefore cannot be applied in a consistent relativistic quantum theory. As mentioned, the operator  $V_{LL}^{(\pm)}$  in (50) constructed here is universal and symmetric with respect to the two particles; this follows directly from its structure.

Comparing formulas (50) and (53), we find that the operator  $V_{LL}^{(\pm)}$  differs from the operator  $V_{LL}$  not only by the additional factor  $\pm R_{1l}/2$  in the last term in expression (50) but also by the additional retarded term

$$\pm \frac{e^2}{2mc} e^{i|\omega_{pn}|R/c} \frac{R}{|\vec{r}'' - \vec{r}'''|^2} \vec{n} \hat{p}''''$$

proportional to  $R$ . Expression (50) therefore provides a more complete description of retardation effects in the electron interaction than expression (53) from [16]–[19].

We now discuss the physical meaning of the operator  $V_{SS}$  in (51). We first note that in the limit  $R \rightarrow 0$ , it becomes the standard operator of spin–spin electron interaction in the helium-like atom [21]. The operator  $V_{SS}$  in (51) then naturally generalizes the spin–spin interaction operator to the case of two quasimolecular electrons separated by an arbitrary distance.

We mention that expression (51) agrees with the corresponding result in [16]–[19] only in the quasimolecular range  $\Delta r < R < \infty$ . But we note that singularities of the integrand in (34) in the atomic range  $0 \leq R < \Delta r$  were not considered in those papers. As is known [21], [29], the singular part of the operator  $V_{SS}$  in (51) arises from the so-called spin–contact interelectron interaction (the Fermi interaction) and is related to the  $\delta$ -function-like singularity in (47) at the origin. Similarly to the case of the operator  $V_D$  in (49), the  $\delta$ -function term ( $\sim \vec{\sigma}'' \vec{\sigma}''' \delta(\vec{r}'' - \vec{r}''')$ ) in formula (51) contributes nontrivially to matrix element (35) only as  $R \rightarrow 0$ , and we can neglect this term in all other cases  $\Delta r \leq R < \infty$  where the overlap between wave functions located near different centers is negligibly small.

We now find the physical meaning of the operator  $V_{SL}$  in (52). In the limit as  $R \rightarrow 0$ , it becomes the corresponding spin–orbit term in the Breit–Pauli operator [21], [29] describing the interaction between spin and orbital magnetic moments of the electrons in the helium-like atom. The last term  $V_{SL}$  in expression (48) is therefore just the operator of the spin–orbit interaction of electrons located at an arbitrary separation.

We also note that the second term  $-3R^2 \vec{\sigma}''' [\vec{n} \times \hat{p}'''] / |\vec{r}'' - \vec{r}'''|^4$  in the last square brackets in expression (52) was missed in [17], [18] (it was also missed in [19]; see formula (3.8)). As is clear from expression (52), the operator  $V_{SL}$  is symmetric with respect to both electrons and therefore takes the spin–orbit retardation of the interaction of two quasimolecular electrons into account compared with the corresponding operator in [18], [19].

We also comment concerning the obtained expression for the generalized Breit–Pauli operator  $V_{BP}^{(\pm)}$ . Although we are mostly interested in the quasimolecular range ( $\Delta r < R < \infty$ ), formulas (48)–(52) are written in a form valid in the whole range of  $R$  ( $0 \leq R < \infty$ ). As  $R$  tends to zero, the operator  $V_{BP}^{(\pm)}$  in (48) becomes the corresponding two-particle term of the Breit–Pauli operator in the coordinate space [21], [29]. It then turns out that independently of the smallness of the coupling constant, the  $\delta$ -function-like terms become relevant in the limit expression. These  $\delta$ -function-like terms in generalized Breit–Pauli operator (48)–(52) therefore ensure the mathematical consistency of the limit transition to the case of a single helium-like atom ( $R \rightarrow 0$ ) investigated in [21].

In conclusion, we stress that a special meaning (for instance, the presence of an especially strong interaction) should not be given to the singular parts of the operators  $V_D$  in (49) and  $V_{SS}^{(\pm)}$  in (51) becoming infinite (at  $R = 0$  and  $\vec{r}'' = \vec{r}'''$ ). The integral quantity of all correction terms  $\tilde{V}_{BP}^{(\pm)}$  in the particle interaction operator  $V_{BP}^{(\pm)}$  is the same, and by the expansion assumption, all these terms are small compared with the first term  $V_{1C}$  in (42), which is an analogue of the Coulomb interaction.

**4.2. Electric dipole–dipole interaction of two quasimolecular electrons.** The role of different terms in interaction operator (48) is determined by the type of quantum transition in the spectrum of

the quasimolecule  $(AB)^{(Z_a+Z_b-2)+}$ . Here, we consider the interaction between two electrons belonging to different nuclei taking only orbital degrees of freedom into account. The operator  $V_{1C} + V_{LL}^{(\pm)}$  with a purely orbital origin is responsible for this component of the interelectron interaction. Below, we consider the case  $\omega_0 R/c \sim 1$  in detail, i.e., we assume that the internuclear distance is comparable to the characteristic wavelength in the spectrum of interacting electrons. At large  $R$ , we can expand the functions  $1/|\vec{r}'' - \vec{r}'''|$ ,  $1/|\vec{r}'' - \vec{r}'''|^2$ , and  $1/|\vec{r}'' - \vec{r}'''|^3$  in the operator  $V_{1C} + V_{LL}^{(\pm)}$  with respect to multipoles and restrict ourself to the first few terms of this expansion. A convenient form of the multipole expansion for the operator  $1/|\vec{r}'' - \vec{r}'''|$  was obtained in [30] (also see [31]). In the case under consideration, where the radius vectors  $\vec{r}_{1b}$  and  $\vec{r}_{2a}$  of electrons 1 and 2 are calculated with respect to the corresponding  $B^{Z_b+}$  and  $A^{Z_a+}$  nuclei and the axes  $z_A$  and  $z_B$  of the corresponding coordinate systems are parallel to  $\vec{R}$ , the bipole expansion of the operator  $1/|\vec{r}'' - \vec{r}'''|$  is

$$\begin{aligned} \frac{1}{|\vec{r}'' - \vec{r}'''|} &= \frac{1}{R} + \frac{\vec{n}_R \vec{r}_{2a} - \vec{n}_R \vec{r}_{1b}}{R^2} + \frac{3(\vec{n}_R \vec{r}_{2a})^2 - r_{2a}^2 + 3(\vec{n}_R \vec{r}_{1b})^2 - r_{1b}^2}{2R^3} + \\ &+ W(\vec{r}_{1b}, \vec{r}_{2a}) + O(R^{-4}). \end{aligned} \quad (54)$$

Here,  $\vec{r}''$  and  $\vec{r}'''$  are the radius vectors of the first and second electrons in an arbitrary coordinate system, and  $\vec{n}_R$  is the unit vector in the direction of  $\vec{R}$ . The correlation term  $W(\vec{r}_{1b}, \vec{r}_{2a})$  depends on the product of the coordinates of both electrons,

$$W(\vec{r}_{1b}, \vec{r}_{2a}) = \frac{\vec{r}_{1b} \vec{r}_{2a} - 3(\vec{n}_R \vec{r}_{1b})(\vec{n}_R \vec{r}_{2a})}{R^3}, \quad (55)$$

and each remaining term in (54) depends on the coordinates of only one of the electrons. Replacing the initial operator with multipole series (54) for  $|\vec{r}'' - \vec{r}'''|^{-1}$  is meaningful if the condition  $R \gg r_{1b} + r_{2a}$  is satisfied. Bipolar expansions for  $|\vec{r}'' - \vec{r}'''|^{-2}$  and  $|\vec{r}'' - \vec{r}'''|^{-3}$  have analogous structures and can be easily obtained from multipole expansion (54), (55) for  $|\vec{r}'' - \vec{r}'''|^{-1}$ .

In actual calculations, we customarily deal with dipole–dipole and quadrupole–quadrupole interactions. Here, we restrict ourself to considering only electric dipole transitions for which the corresponding operator is

$$\begin{aligned} V_{1C, \text{dip}} + V_{LL, \text{dip}}^{(\pm)} &= e^{i|\omega_{pn}|R/c} \left\{ \frac{\vec{d}_{1b} \vec{d}_{2a} - 3(\vec{n}_R \vec{d}_{1b})(\vec{n}_R \vec{d}_{2a})}{R^3} \pm \right. \\ &\pm \frac{e}{2mc} \left[ \frac{\vec{d}_{1b} \hat{p}_2 - 3(\vec{n}_R \vec{d}_{1b})(\vec{n}_R \hat{p}_2)}{R^2} - R_{1l} \frac{\vec{d}_{2a} \hat{p}_1 - 3(\vec{n}_R \vec{d}_{2a})(\vec{n}_R \hat{p}_1)}{R^2} \right] - \\ &- \frac{e^2}{m^2 c^2} \left[ \left(1 - \frac{1}{2} R_{1l}\right) \frac{\hat{p}_1 \hat{p}_2}{R} + \frac{1}{2} R_{1l} \frac{(\vec{n}_R \hat{p}_1)(\vec{n}_R \hat{p}_2)}{R} + \right. \\ &\left. + \frac{1}{2} R_{1l} \frac{\hat{p}_1 \hat{p}_2 - 3(\vec{n}_R \hat{p}_1)(\vec{n}_R \hat{p}_2)}{R} \right] \left. \right\}, \end{aligned} \quad (56)$$

where  $\vec{d}_{1b} = e\vec{r}_{1b}$  and  $\vec{d}_{2a} = e\vec{r}_{2a}$  are the electric dipole moment operators of separate electrons and  $\hat{p}_1$  and  $\hat{p}_2$  are the momentum operators for the first and second electrons. Obtained operator (56) is the operator of the electric dipole–dipole interaction of two electrons belonging to different nuclei and located at an arbitrarily large separation. It turns out that correctly taking the retardation effects in the electron interaction into account leads to the appearance of the additional term

$$\mp \frac{e}{2mc} R_{1l} \frac{\vec{d}_{2a} \hat{p}_1 - 3(\vec{n}_R \vec{d}_{2a})(\vec{n}_R \hat{p}_1)}{R^2}$$

in dipole–dipole interaction operator (56) compared with the corresponding operator in [18] (see formula (3.9)).

The dipole–dipole interaction contributes to the first perturbative correction only when pairs of states of isolated atoms having opposite parities enter the initial functions of the leading approximation. Such a situation occurs, for example, in the resonant and almost-resonant excitation transmission in collisions of atoms of alkali metals [32], [33].

## 5. Conclusion

We have solved the problem of the interaction of two quasimolecular electrons via the virtual photon field accompanied by emission or absorption of a real photon. Such an interaction is the third-order QED effect described by the Feynman diagrams in Fig. 1. We now list the main properties of this interaction.

There are two domains of the configuration space in which the generalized Breit operator of a long-range interaction of type (31) behaves differently depending on the variation of the relative interelectron distance  $|\vec{r}'' - \vec{r}'''|$ . For example, in the united atom limit ( $R \rightarrow 0$ ), formula (31) for the operator  $B_{1l}^{(\pm)}(\vec{r}'', \vec{r}''')$  becomes limit expression (1), which correctly describes the retardation effects of the relativistic interaction only at relatively small interparticle distances  $|\vec{r}'' - \vec{r}'''|$ . More precisely, the applicability domain of Breit expression (1) is bounded by the condition on the relative coordinates of the interacting particles

$$\frac{\omega_0 |\vec{r}'' - \vec{r}'''}{c} \ll 1, \quad (57)$$

where  $\omega_0$  is the characteristic frequency in the spectrum of the interacting electrons. We let  $\Omega_c$  denote the corresponding configuration space domain, and we call it the domain of close electron correlations. In contrast, in the domain  $\Omega_d$ , where the electrons belong to different nuclei and inequality (17) holds for all  $\Delta r \leq R < \infty$ , Breit operator (1) ceases to describe the relativistic interaction between two electrons properly, even on the qualitative level. At the same time, relativistic operator  $B_{1l}^{(\pm)}$  given by (31) constructed here describes the retarded interaction of two quasimolecular electrons uniformly and equally in both the domains  $\Omega_c$  and  $\Omega_d$  of close and distant electron correlations and can therefore be used to solve many two-electron problems in atomic and molecular spectroscopy, astrophysics, the theory of slow atomic collisions, etc. Moreover, the relativistic operator of two-electron interaction (31) can be used for mathematical modeling of atomic clusters [34], for investigating the optical properties of various nanostructure systems in intense optical fields [35], [36], and also for solving several important problems of recording, reading, and transferring quantum information from one two-level atom (qubit) to another [37], [38].

Each of the domains  $\Omega_c$  and  $\Omega_d$  of interelectron distances  $|\vec{r}'' - \vec{r}'''|$  has its own time scale of interaction transfer and correspondingly its own computational approximation that allows segregating small parameters and taking different types of intermediate states in the interacting electron spectrum and also different interaction types into account. We therefore have additional justification for using the generalized Breit operator  $B_{1l}^{(\pm)}(\vec{r}'', \vec{r}''')$  to solve multielectron two-center problems together with a clear view of the incompleteness of the QED interaction picture of two atomic electrons described by standard Breit operator (1).

As shown in Sec. 3, it was assumed in [21] in deriving Breit operator (1) that quantity (57) is the only small parameter for expanding the retardation factor. This means that in addition to the characteristic (mean) time of electron transitions  $T_e = 2\pi/\omega_0$ , the uniform time scale  $T_t = |\vec{r}'' - \vec{r}'''|/c$  (corresponding to the domain  $\Omega_c$ ) is also used. This time can be interpreted as the time necessary for transmitting the interaction. The condition  $2\pi T_t \ll T_e$  must be satisfied, i.e., substantial changes of electronic density occur in the system of two interacting electrons during the the interaction transfer time.

At sufficiently large interelectron distances (in the domain  $\Omega_d$ ), where the interaction transfer time  $T_t = R/c$  is large compared with the mean time  $T_e$  of electron transitions, the natural small parameter

is dimensionless quantity (17). Exchange by virtual photons at these distances results in the interelectron interaction of form (31), where other relativistic terms depending on the spin electron operators and on the interelectron distance  $R$  are involved in addition to the Breit and Coulomb interaction terms (1). These terms appear because of the additional retardation in the interaction of two quasimolecular electrons located at an arbitrary, including arbitrarily large, separation. Expression (31) obtained for the relativistic operator  $B_{1l}^{(\pm)}(\vec{r}'', \vec{r}''')$  then differs from the analogous result (32) from [16]–[19] not only by the additional factor  $\pm 1/2$  in the second term in (31) but also by the additional term  $\pm RR_{1l}\vec{\alpha}''\vec{n}/2|\vec{r}'' - \vec{r}'''|^2$  taking the additional retardation in the interaction of two quasimolecular electrons into account.

We derived the explicit representation for the generalized two-particle Breit–Pauli operator  $V_{BP}^{(\pm)}$  given by (48) by passing in the matrix  $U_{mn,pr}^{(3)}$  in (13) for the effective interaction energy  $B_{1l}^{(\pm)}$  in (31) from relativistic four-component Dirac spinors to the nonrelativistic two-component Pauli spinors. We demonstrated that consistently taking the natural condition of the interaction symmetry with respect to both electrons into account results in the appearance of new terms in the operators of spin–orbit (52), spin–spin (51), and retarded (50) interactions; these terms were missed in the corresponding operator expressions in [16]–[19]. Generalized Breit–Pauli operator (48)–(52) constructed here therefore takes the orbital and spin degrees of freedom rigorously into account and also takes the interaction retardation effects for two quasimolecular electrons located at an arbitrary separation into account. This opens possibilities for mathematically rigorous calculations of both molecular structures and atomic clusters and of the parameters of the exchange–correlation interaction of atomic particles in collision processes.

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