Sum rules for the polarization correlations in photoionization and bremsstrahlung

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The polarization correlations in doubly differential cross sections are investigated for photoionization and ordinary bremsstrahlung. These correlations describe the polarization transfer between incident light and ejected photoelectrons as well as between an incoming electron beam and bremsstrahlung light, respectively. They are characterized by a set of seven real parameters C_{ij}. We show that the squares of these parameters are connected by simple "sum rules." These sum rules can be applied for both one-electron systems and also for atoms, if the latter are described within the independent particle approximation. In particular, they are exact in their simplest form (i) for the photoionization of K-, $L_{I,II}$-, and $M_{I,II}$-atomic shells, as well as (ii) for bremsstrahlung in which the electron is scattered into $s_{1/2}$ or $p_{1/2}$ states, as in the tip (bremsstrahlung) region. Detailed calculations are performed to verify the derived identities and to discuss their possible applications for the analysis of modern photoionization and bremsstrahlung experiments. In particular, we argue that the sum rules may help to determine the entire set of (significant) polarization correlations in the case when not all C_{ij} are available for experimental observation.

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I. INTRODUCTION

With the recent experimental advances in polarized electron and coherent-light sources, more possibilities arise to study the polarization phenomena in electronic, ionic, and photonic collisions. Of special interest in these studies are the correlations between the polarization of incident and outgoing particles. During the last decade, for example, a number of experiments have been performed to investigate the *polarization correlations* in atomic bremsstrahlung [1–4], (time-reversed) photoionization [5], and elastic photon scattering by heavy neutral atoms [6]. When compared with the theoretical predictions, based on the relativistic Dirac theory [7–10], results of these measurements have provided valuable information about atomic (and ionic) structure and details of electron-photon interaction in the presence of strong electromagnetic fields.

Polarization transfer in atomic collision processes may be characterized in terms of the so-called correlation parameters C_{ij}, with indices associated with the particles being observed. Two important questions can be addressed for each particular process: (i) How many parameters are needed to describe *all* the possible polarization correlations for various experimental setups, and (ii) whether these parameters are independent of each other. In the past these issues were investigated for elastic Rayleigh scattering of photons [11] and for Coulomb scattering of electrons [12]. In both cases the general matrix element is characterized by two complex amplitudes (F and G in electron scattering), and the corresponding cross sections are characterized by the unpolarized cross section and three other real functions, associated with polarization correlations. In electron scattering it was noted that the *three* correlation parameters S, L, and R, that enter the differential cross section Eq. (6.01) of Ref. [13], are related to each other as

$$S^2 + L^2 + R^2 = 1. \qquad (1)$$

This simple "sum rule" is exact and can be used to predict the magnitude of one of the correlations if the other two are known. A similar identity was derived for the elastic scattering of photons by an atom [11].

While the sum rules for the (squares of) polarization correlation coefficients have been derived and discussed for elastic photon and elastic electron scattering, corresponding relationships have not yet been established for such basic processes as photoionization and ordinary bremsstrahlung, even just for doubly differential cross sections, which involve at least seven such distinct correlations. A possible approach has been recently proposed by Jakubassa-Amundsen, who conjectured a relation, similar to Eq. (1), for the polarization correlations in atomic bremsstrahlung [14]. Her conjectured identity is based on the relationship between elastic electron scattering and bremsstrahlung [15]. It was proposed only for the (inelastic) scattering of highly relativistic electrons by high-Z targets, in the case when the electron gives away all its energy to the emitted photon. The validity of this conjecture is not yet clear. In any event, for the analysis of the present-day experimental data one would like a sum rule (or other relationship connecting the coefficients) for bremsstrahlung as well as for photoionization that is valid for a wider range of energies and nuclear charges of a target.

Motivated by the proposal of Jakubassa-Amundsen [14], here we obtain exact sum rules for (doubly differential) polarization correlations in atomic photoionization and bremsstrahlung. This requires further specification of the states being observed. First, we define the polarization correlations in Sec. II. We show that one needs *seven* parameters C_{ij} in order to characterize the doubly differential polarization transfer both in photoionization and bremsstrahlung. The relationships among the squares of the coefficients C_{ij}, i.e., the sum rules, are presented in Secs. II A and II B. A brief discussion of the derivation of these rules and of their numerical verification is given in Sec. III. In particular, we display two tables with the results of our calculations of the parameters C_{ij} for both processes. As will be seen from these calculations, performed for low-Z one-electron systems, the derived relations are exact (under certain conditions) and can be applied for any collision energy. In Sec. IV we consider how the obtained sum rules can be used to analyze experimental data and to extract from it unknown correlations C_{ij}. In order to support our discussion, we present (in six figures) the results of the relativistic calculations for the K-shell photoionization of hydrogenlike Be^{3+}, Ar^{17+}, and Xe^{53+} ions as well as for the bremsstrahlung produced by the electron scattering by bare Be^{4+}, Ar^{18+}, and Xe^{54+} ions. Although the examples of computations in the present paper are shown for the single-electron case, we argue that the sum rules (as well as their applications) are also exact for many-electron ions and atoms, if those can be described within the independent particle approximation (IPA). A summary of our results is given in Sec. V.

II. POLARIZATION CORRELATIONS AND THEIR SUM RULES

A. Atomic photoeffect

The polarization correlations in the atomic photoeffect are defined by seven nontrivial coefficients C_{02}, C_{10}, C_{12}, C_{21}, C_{23}, C_{31}, and C_{33}. These allowed correlations follow from symmetry arguments [7], and enter the doubly differential cross section as [16,17]

$$\frac{d\sigma}{d\Omega} = \left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{unpol}} \left[\frac{1}{2}\sum_{i,j=0}^{3} C_{ij}\,\xi_i\,\zeta_j\right], \tag{2}$$

which is obtained upon averaging over the projections μ_b of the total angular momentum j_b of a bound electron [18]. Here, $(d\sigma/d\Omega)_{\mathrm{unpol}}$ is the cross section for the absorption of unpolarized light when the polarization state of emitted electrons remains unobserved. In Eq. (2), moreover, the Stokes parameters ξ_i $(i = 0,\ldots 3)$ describe the polarization of incident light. These parameters,

$$\begin{aligned} \xi_1 &= \epsilon_1^*\epsilon_1 - \epsilon_2^*\epsilon_2\,, \quad \xi_2 = \epsilon_1\epsilon_2^* + \epsilon_2\epsilon_1^*, \\ \xi_3 &= i(\epsilon_1\epsilon_2^* - \epsilon_2\epsilon_1^*), \quad \xi_0 = 1, \end{aligned} \tag{3}$$

are expressed in terms of the components ϵ_1 and ϵ_2 of the photon polarization vector, taken parallel and perpendicular to the reaction plane, respectively. As usual, the reaction plane is defined by the momenta of incoming photon $\boldsymbol{k}$ and outgoing electron $\boldsymbol{p}$. In experiment, the Stokes parameters ξ_1 and ξ_2 are determined by the intensities I_χ of light, *linearly* polarized at different angles χ with respect to the reaction plane: $\xi_1 = (I_0 - I_{90})/(I_0 + I_{90})$ and $\xi_2 = (I_{45} - I_{135})/(I_{45} + I_{135})$. The third parameter ξ_3 reflects the degree of *circular* polarization of photons.

The polarization state of the outgoing electron is described by its spin vector $\boldsymbol{\zeta}$. This vector is defined in the electron's rest frame. Its components ζ_1 and ζ_2 are perpendicular to the electron momentum $\boldsymbol{p}$ and are chosen *in* and *perpendicular* (along $\boldsymbol{k}\times\boldsymbol{p}$) to the reaction plane, respectively. The component ζ_3 characterizes the longitudinal—along its momentum $\boldsymbol{p}$—electron polarization, and, finally, ζ_0 is unity.

Having discussed the polarization correlations C_{ij} we are ready now to introduce their sum rule. Namely, the linear combination of squares of the correlation coefficients,

$$R_{\mathrm{ph}} = C_{10}^2 + C_{21}^2 + C_{31}^2 + C_{02}^2 + C_{23}^2 + C_{33}^2 - C_{12}^2, \tag{4}$$

is a constant, *exactly* unity, for the photoionization cross section (2) obtained from the summation (or averaging) over the *two* bound single-electron substates $|j_b\mu_b\rangle$ with the same modulus of the magnetic quantum number μ_b:

$$R_{\mathrm{ph}} = 1, \quad \text{if } \mu_b = \pm|\mu_0|. \tag{5}$$

Note there is a separate sum rule Eq. (4) for the cross section associated with each magnitude of the electron magnetic substate, i.e., with each $|\mu_0|$. Since the inner-shell radiative processes in many-electron systems can be understood fairly well within the independent particle approximation [17], Eqs. (4) and (5) are directly valid for the full K, $L_{I,II}$ and $M_{I,II}$ ionization of atoms, since only one value of magnitude of magnetic substate, $\mu_b = \pm 1/2$, is involved.

B. Atomic-field bremsstrahlung

Similar to the photoeffect, the polarization correlations in atomic-field bremsstrahlung are also parametrized in terms of the coefficients C_{ij}. Again, *seven* such coefficients are needed to describe the polarization transfer between an incident electron with the momentum $\boldsymbol{p}$, energy E_{el}, and spin $\boldsymbol{\zeta}$, and emitted photon with wave vector $\boldsymbol{k}$ and energy $E_\gamma = \hbar ck$. Here we assume, moreover, that the (final) outgoing electron with the energy $E_f = E_i - E_\gamma$ remains unobserved. For such a scenario, the doubly differential bremsstrahlung cross section reads as [8,18]

$$\frac{d\sigma}{d\Omega} = \left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{unpol}} \left[\frac{1}{2}\sum_{i,j=0}^{3} C_{ij}\,\zeta_i\,\xi_j\right], \tag{6}$$

where $(d\sigma/d\Omega)_{\mathrm{unpol}}$ is averaged over the initial electron spins and summed over the final photon polarizations, and the Stokes parameters ξ_i $(i = 0,\ldots 3)$ characterize the polarization of bremsstrahlung radiation.

As seen from Eq. (6), the first index of the correlation C_{ij} refers now to the incident electron spin projection while the second to the emitted photon polarization, conversely to the photoionization case [cf. Eq. (2)]. Moreover, by following the convention introduced by Tseng and Pratt [8] we redefine the indices of the (photon) Stokes parameters in such a way that ξ_3 and ξ_1 describe the linear polarization and ξ_2 the circular polarization of bremsstrahlung radiation, i.e., we made a substitution $(1,2,3) \to (3,1,2)$ in C_{ij}.

One can again define the linear combination of (squares of) polarization correlations C_{ij} for the atomic-field bremsstrahlung:

$$R_{\mathrm{br}} = C_{03}^2 + C_{11}^2 + C_{12}^2 + C_{20}^2 + C_{31}^2 + C_{32}^2 - C_{23}^2. \tag{7}$$

If an electron after bremsstrahlung is in a state with well-defined total angular momentum j_f and if summation over the magnetic quantum number μ_f is restricted to only the two values $\pm|\mu_0|$ with $|\mu_0| \leqslant j_f$, the equality holds:

$$R_{\mathrm{br}} = 1, \quad \text{if } \mu_f = \pm|\mu_0|. \tag{8}$$

In reality, this sum rule would be valid if an electron is scattered into the $s_{1/2}$ or $p_{1/2}$ states, or in the separate partitions of states

TABLE I. Polarization correlation coefficients C_{ij} for the K-shell photoionization of hydrogenlike beryllium ($Z = 4$). Results are presented for two energies E_γ of the incident light and for various electron emission angles. In the last column, moreover, we present the coefficient R_{ph} defined by Eq. (4).

				$E_\gamma = 100$ keV				
θ(deg)	C_{02}	C_{10}	C_{12}	C_{21}	C_{23}	C_{31}	C_{33}	R_{ph}
0	0.000	0.000	0.000	0.000	0.000	0.000	1.000	1.000
30	0.000	0.987	0.000	0.002	−0.001	−0.104	0.120	1.000
60	0.001	0.982	0.001	0.003	−0.001	−0.184	0.047	1.000
90	0.004	0.974	0.004	0.006	−0.002	−0.220	−0.058	1.000
120	0.009	0.965	0.011	0.013	−0.003	−0.200	−0.169	1.000
150	0.023	0.958	0.031	0.032	−0.004	−0.128	−0.255	1.000
180	0.000	0.000	0.000	0.000	0.000	0.000	−1.000	1.000
				$E_\gamma = 1$ MeV				
θ(deg)	C_{02}	C_{10}	C_{12}	C_{21}	C_{23}	C_{31}	C_{33}	R_{ph}
0	0.000	0.000	0.000	0.000	0.000	0.000	1.000	1.000
30	0.008	0.312	0.016	−0.013	−0.008	−0.652	0.691	1.000
60	0.000	−0.221	0.015	−0.003	−0.019	−0.690	0.690	1.000
90	−0.018	−0.511	0.018	0.008	−0.028	−0.512	0.690	1.000
120	−0.051	−0.651	0.028	0.023	−0.033	−0.313	0.689	1.000
150	−0.130	−0.711	0.058	0.056	−0.035	−0.108	0.682	1.000
180	0.000	0.000	0.000	0.000	0.000	0.000	−1.000	1.000

with $j_f > 1/2$. Since the final (as well as initial) electron state in bremsstrahlung is a superposition of partial waves with different total angular momenta j_f, in most observations Eq. (8) holds only approximately at best. It is most useful in the tip region of low-Z elements at not too low energy, where the final $s_{1/2}$ cross section dominates.

III. DERIVATION AND NUMERICAL VERIFICATION OF SUM RULES

Not much has to be said about the derivation of the sum rules (4)–(5) and (7)–(8). These rules follow immediately from the explicit form of the polarization correlation coefficients C_{ij} as obtained from the relativistic independent particle approximation (IPA). Within the IPA, the evaluation of the cross sections (2) and (6) both for many-electron atoms and hydrogenlike ions can be traced back to the *single-electron* transition amplitude. For the photoionization, for example, this amplitude reads as [16,17,19]

$$M_{\text{if}} = -\sqrt{\frac{2\pi}{k}} \int \psi_f^\dagger(\boldsymbol{r})\, \boldsymbol{\alpha} \cdot \boldsymbol{\epsilon}\, e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\, \psi_i(\boldsymbol{r})\, d\boldsymbol{r}, \tag{9}$$

where $\boldsymbol{\alpha}$ is the vector of Dirac α matrices, $\boldsymbol{k}$ and $\boldsymbol{\epsilon}$ are the photon wave and polarization vectors, and $\psi_i(\boldsymbol{r})$ and $\psi_f(\boldsymbol{r})$ are the wave functions for the initial (bound) and final (continuum) electron, respectively. These wave functions are solutions of the Dirac equation for either the pure Coulomb or some effective "screened" potential. The latter potential is used to account for the (spherical part of the) electron-electron interaction in the ionization of neutral atoms or many electron ions.

The computation of the photoionization matrix element (9) is based on the partial-wave expansion of both electron-photon interaction operator $R = \boldsymbol{\alpha} \cdot \boldsymbol{\epsilon}\, e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$ and the continuum-electron wave function $\psi_f(\boldsymbol{r})$. These expansions have been discussed in detail previously (see, e.g., Refs. [16,20–22]), and will not be repeated here. We just recall that the multipole decomposition of the continuum electron wave and the interaction operator allow one to represent the amplitude M_{if} and, hence, the photoionization cross section in terms of integrals over the radial components of electronic wave functions [16,19]. By making use of these—rather lengthy—expressions, we have derived the sum rule (5).

The relations (7)–(8) between the squares of the polarization correlations C_{ij} for atomic bremsstrahlung can be easily obtained from the photoionization formulas (4)–(5). This can be expected since the analysis of both photoionization and bremsstrahlung processes is traced back to the matrix elements of the *same* operator $R = \boldsymbol{\alpha} \cdot \boldsymbol{\epsilon}\, e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$. The polarization correlations for photoionization and bremsstrahlung obey the same symmetry relations and sum rules. Therefore, one can obtain the bremsstrahlung sum rules from Eqs. (4)–(5) just by interchanging the photon and electron indices, $C_{ij}(\text{ph}) = C_{ji}(\text{br})$ and by making the substitution $j = (1,2,3) \to j = (3,1,2)$. The latter is due to the different conventions for the components of the photon's polarization vector ϵ_j as used for the description of the photoionization [16] and bremsstrahlung [8].

In order to verify the sum rules $R_{\text{ph}} = 1$ and $R_{\text{br}} = 1$ numerically we have carried out a series of calculations for different targets and for a wide range of photon (electron) energies. These calculations were performed within the rigorous relativistic approach based on the partial-wave representation of the Dirac wave functions for the purely Coulombic field case. Since the details of the numerical procedure have been presented in our previous works [8,9,16,23], we will not discuss them here and proceed immediately to the results. For both photoionization and bremsstrahlung, Eqs. (5) and (8) have been confirmed within the accuracy of our analysis. In Table I, for example, we display the polarization correlation coefficients for the K-shell ionization of hydrogenlike beryllium by x rays with energy $E_\gamma = 100$ keV and 1 MeV. Results were

TABLE II. Polarization correlation coefficients C_{ij} for bremsstrahlung produced by the scattering of 100 keV and 1 MeV electrons on the bare Be^{4+} ion. The coefficients were calculated for the scattered electron in the $s_{1/2}$ state with kinetic energy 1 eV. In the last two columns we display the linear combination of squares of polarization correlations (7) as obtained after summation over all allowed partial waves of the final electron, R_{br}(all), and if this summation is restricted to the $s_{1/2}$ state, $R_{br}(s_{1/2})$.

$E_i = 100\,\text{keV}, E_f = 1\,\text{eV}$									
θ(deg)	C_{03}	C_{11}	C_{12}	C_{23}	C_{31}	C_{32}	C_{20}	$R_{br}(s_{1/2})$	R_{br}(all)
0	0.000	0.000	0.000	0.000	0.000	1.000	0.000	1.000	0.051
30	0.987	−0.002	−0.104	0.000	0.001	0.120	0.000	1.000	0.994
60	0.982	−0.003	−0.184	−0.000	0.001	0.047	−0.001	1.000	0.996
90	0.974	−0.006	−0.220	−0.001	0.002	−0.058	−0.003	1.000	0.995
120	0.965	−0.013	−0.200	−0.003	0.003	−0.169	−0.009	1.000	0.989
150	0.958	−0.032	−0.129	−0.009	0.004	−0.256	−0.023	1.000	0.955
180	0.000	0.000	0.000	0.000	0.000	−1.000	0.000	1.000	0.023
$E_i = 1\,\text{MeV}, E_f = 1\,\text{eV}$									
θ(deg)	C_{03}	C_{11}	C_{12}	C_{23}	C_{31}	C_{32}	C_{20}	$R_{br}(s_{1/2})$	R_{br}(all)
0	0.000	0.000	0.000	0.000	0.000	1.000	0.000	1.000	0.845
30	0.312	0.013	−0.652	−0.014	0.008	0.691	−0.008	1.000	0.999
60	−0.221	0.003	−0.690	−0.015	0.019	0.689	−0.000	1.000	0.999
90	−0.509	−0.007	−0.512	−0.009	0.027	0.691	0.019	1.000	1.000
120	−0.651	−0.023	−0.313	0.006	0.032	0.689	0.051	1.000	0.998
150	−0.711	−0.056	−0.108	0.040	0.035	0.682	0.130	1.000	0.990
180	0.000	0.000	0.000	0.000	0.000	−1.000	0.000	1.000	0.585

obtained for different electron emission angles θ as defined with respect to the propagation direction of the incident light. We note that the C_{ij} coefficients have not been presented on a fine enough mesh to display their rapid variation at very small and large angles, related to the vanishing of nonrelativistic, but not relativistic, cross sections at such angles. In the last column of Table I, moreover, the coefficient R_{ph} is also displayed. As expected, this parameter is unity for both energies and for all emission angles. In sample calculations we have also obtained similar results in screened potentials.

The polarization correlation coefficients obtained for the bremsstrahlung of 100 keV and 1 MeV electrons, colliding with bare beryllium ions Be^{4+}, are displayed in Table II. Here, the computations have been performed for the so-called tip region where the electron transfers all its kinetic energy to the photon. For this region we have restricted the partial-wave expansion of the final electron wave function to the single $s_{1/2}$ state. As seen from the ninth column of the table, where the linear combination $R_{br}(s_{1/2})$ of squares of C_{ij} is presented, the sum rule (8) holds true in this case. Of course,

TABLE III. Polarization correlation coefficients C_{ij} for bremsstrahlung produced by the scattering of 100 keV and 1 MeV electrons on the bare Be^{4+} ion. The coefficients were calculated for the scattered electron in the $s_{1/2}$ state with half the initial kinetic energy. In the last two columns we display the linear combination of squares of polarization correlations (7) as obtained after summation over all allowed partial waves of the final electron, R_{br}(all), and if this summation is restricted to the $s_{1/2}$ state, $R_{br}(s_{1/2})$.

$E_i = 100\,\text{keV}, E_f = 50\,\text{keV}$									
θ(deg)	C_{03}	C_{11}	C_{12}	C_{23}	C_{31}	C_{32}	C_{20}	$R_{br}(s_{1/2})$	R_{br}(all)
0	0.000	0.000	0.000	0.000	0.000	1.000	0.000	1.000	0.009
30	0.995	−0.003	−0.079	0.000	0.000	0.060	0.002	1.000	0.143
60	0.993	−0.004	−0.118	0.000	0.000	0.023	0.000	1.000	0.231
90	0.989	−0.006	−0.148	0.000	0.001	−0.028	−0.002	1.000	0.152
120	0.983	−0.011	−0.164	−0.001	0.001	−0.083	−0.007	1.000	0.054
150	0.969	−0.023	−0.206	−0.003	0.001	−0.133	−0.020	1.000	0.010
180	0.000	0.000	0.000	0.000	0.000	−1.000	0.000	1.000	0.005
$E_i = 1\,\text{MeV}, E_f = 500\,\text{keV}$									
θ(deg)	C_{03}	C_{11}	C_{12}	C_{23}	C_{31}	C_{32}	C_{20}	$R_{br}(s_{1/2})$	R_{br}(all)
0	0.000	0.000	0.000	0.000	0.000	1.000	0.000	1.000	0.167
30	0.862	0.000	−0.437	−0.001	0.002	0.258	−0.005	1.000	0.124
60	0.384	−0.010	−0.918	−0.007	0.009	0.099	−0.008	1.000	0.119
90	−0.415	−0.029	−0.898	−0.024	0.022	−0.146	−0.003	1.000	0.081
120	−0.838	−0.044	−0.200	−0.028	0.026	−0.507	0.012	1.000	0.038
150	−0.398	−0.034	0.320	−0.026	0.011	−0.860	0.017	1.000	0.044
180	0.000	0.000	0.000	0.000	0.000	−1.000	0.000	1.000	0.061

in bremsstrahlung experiments it is very difficult to select out final electron states of particular parity and symmetry, as, e.g., $s_{1/2}$. However, for the tip region and low-Z targets the s-wave generally gives the dominant contribution to the partial wave expansion of the final electron state and, hence, the equality $R_{\rm br} = 1$ may be (approximately) valid in this case. In order to prove this, in the last column of the table we display the linear combination $R_{\rm br}$(all) obtained from Eq. (7) after summation over all allowed multipoles of the final-electron wave. As expected, $R_{\rm br}$(all) does not deviate from unity by more than 0.5% for almost the entire angular range, except for $\theta \approx 0$ deg and $\theta \approx 180$ deg. For these very forward and very backward directions there is only one nonvanishing parameter C_{32} that describes the circular polarization of emitted light if an incident electron is longitudinally polarized. For the case when the summation over the final-electron partial waves is restricted to the $s_{1/2}$ state, $C_{32}(\theta = 0) = 1$ and $C_{32}(\theta = 180) = -1$ as it can be expected from the conservation of the projection of the total angular momentum. However, if one takes into account the higher electron multipoles, $p_{1/2}$ and $p_{3/2}$, the parameter C_{32} and, hence, the $R_{\rm br}$(all) significantly deviate from unity even for the low-Z regime.

Assuming that the electron after the bremsstrahlng is in the $s_{1/2}$ state, the sum rule (8) holds also throughout the entire spectrum. In Table III, for example, we display the C_{ij} polarization correlations and their linear combination $R_{\rm br}(s_{1/2})$ for the case when only *half* of the incident electron energy E_i is carried away by the photon. As seen from the table, the $R_{\rm br}(s_{1/2})$ is, of course, unity for all photon emission angles. In contrast to the tip region, however, the approximation of the scattered electron by a single $s_{1/2}$ wave is very inaccurate for the middle of the spectrum. For this energy range the higher multipoles in the expansion of the (final-state) electron wave function are of paramount importance. Each magnitude of magnetic substate, i.e., each $|\mu_0|$ for a particular multipole, has its own sum rule, with its own set of C_{ij}'s. When summed together, however, the higher-order partial waves result in the significant difference between the $R_{\rm br}(s_{1/2})$ and the rigorous estimate of the linear combination $R_{\rm br}$(all), presented in the last column of Table III.

IV. APPLICATION OF SUM RULES

We have discussed above the sum rules that establish the connection between the squares of *seven* polarization correlations C_{ij} for photoionization and for bremsstrahlung. By using these rules one can determine the (absolute value of) one of the coefficients C_{ij} if the other six are known and if the applicability conditions of Eqs. (5) and (8) are fulfilled. The determination of an unknown C_{ij} in this way is especially feasible if only a *few* of the correlation coefficients are significantly nonzero, while the others are very small. In order to illustrate such a study of polarization correlations and discuss its (possible) application for the analysis of experimental data let us discuss first the K-shell photoionization of low- and medium-Z ions. In Fig. 1 we display, for example, the results of our relativistic partial-wave calculations for hydrogenlike beryllium and photon energies $E_\gamma = 100$ keV (upper panel), 500 keV (middle panel), and 1 MeV (lower panel). As seen from the figure, only three coefficients, C_{10}, C_{31}, and C_{33},

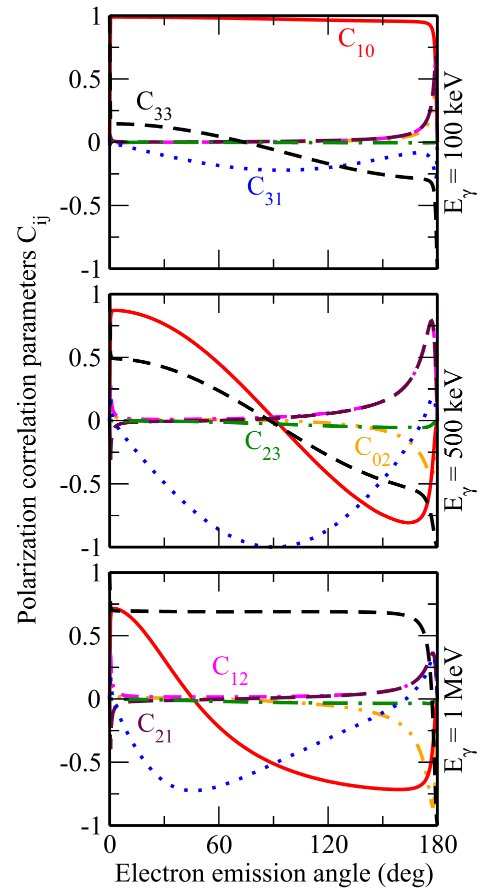

FIG. 1. The polarization correlation parameters C_{ij} for K-shell ionization of hydrogenlike beryllium ($Z = 4$) by 100 keV (upper panel), 500 keV (middle panel), and 1 MeV (lower panel) photons. Different curves are used to represent the correlations: C_{10} (red solid line), C_{33} (black short-dashed line), C_{31} (blue dotted line), C_{23} (green long-dash-dotted line), C_{02} (orange short-dash-double-dotted line), C_{21} (maroon long-dashed line), and C_{12} (pink short-dash-dotted line). Moreover, we have additionally labeled various among the curves in different panels.

are dominant for this low-Z target at most emission angles. This result is expected from the predictions of the Born approximation discussed in Ref. [7]. In particular, it was shown that C_{10}, C_{31}, and $C_{33} \sim O(1)$ while the other correlations are $\sim O(\alpha Z)$, where α is the fine-structure constant. Such a behavior of C_{ij} coefficients leads to the simplified sum rule:

$$C_{10}^2 + C_{31}^2 + C_{33}^2 \simeq 1, \tag{10}$$

which is, again, valid for low-Z targets. With the help of Eq. (10) one can determine, for example, the (module of) coefficient C_{33} that describes the production of longitudinally polarized electrons from circularly polarized photons, if the other two correlations, C_{10} and C_{31}, are known. The latter correlations reflect the sensitivity of the photoelectron angular distribution on the linear polarization of incident light C_{10}, and describe how the transversely polarized (in the x direction) electrons are produced by circularly polarized light C_{31}. For x rays with the energy $E_\gamma = 500$ keV and electron emission angle $\theta = 30$ deg, these coefficients are $C_{10} = 0.761$ and

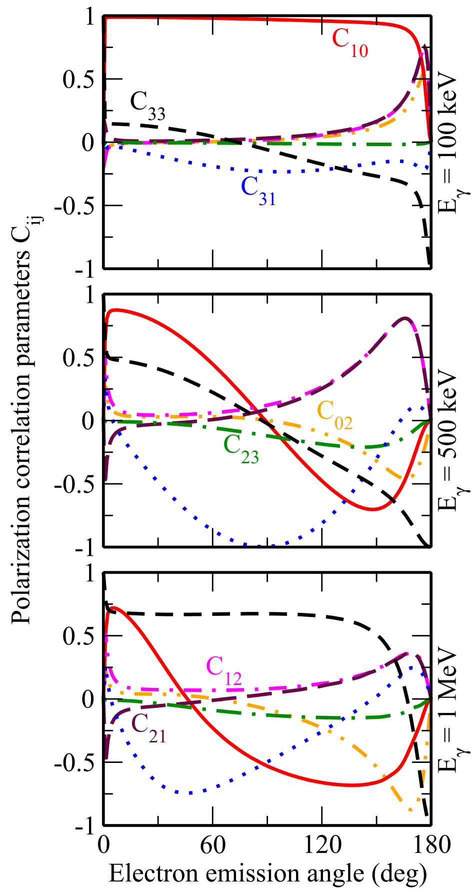

FIG. 2. The same as Fig. 1 but for K-shell ionization of hydrogenlike argon ($Z = 18$).

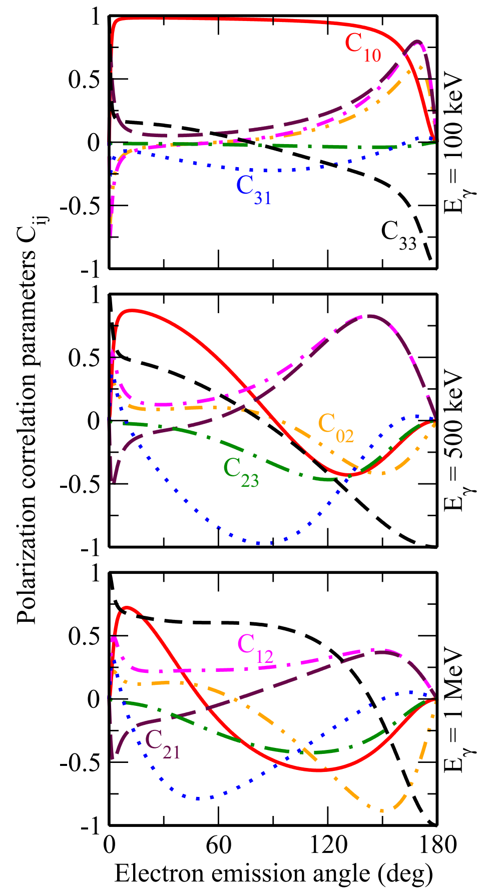

FIG. 3. The same as Fig. 1 but for K-shell ionization of hydrogenlike xenon ($Z = 54$).

$C_{31} = -0.495$. By making use of Eq. (10), we can deduce from these data $|C_{33}| = 0.420$ which is in perfect agreement with the results of our relativistic calculations.

As seen from Figs. 2 and 3, the simplified sum rule (10) fails with increase of the nuclear charge Z. In this case, the coefficients of the order of $O(\alpha Z)$ become comparable in magnitude with C_{10}, C_{31}, and C_{33}. Of course, the general rule (5) will be still valid in this case, although its practical application can be hampered by the need to determine up to six other correlations C_{ij}.

Apart from the low-Z, Born approximation case, for which Eq. (10) is approximately true, one can also simplify the sum rule in the ultrarelativistic regime. As was shown by one of us in Ref. [7], there are three nonvanishing correlations, C_{33} and $C_{12} = -C_{21}$, that appear in this regime. The additional C_{ij} terms that appear in the cross sections of Eq. (9) of that reference cancel when cross sections with the opposite sign of magnetic substate are summed. Equation (5) converges then to the trivial result:

$$C_{33}^2 \simeq 1. \tag{11}$$

The numerical verification of this relation with the help of the partial-wave-expansion approach is at present a rather difficult task. It requires the summation over a very large number of electron multipoles and, hence, it is very computationally demanding. In our present work, therefore, we do not attempt to perform ultrarelativistic photoionization calculations. We note Ref. [24], in which Eq. (11) was proved within the framework of the Sommerfeld-Maue approximation.

Until now we have discussed the applications of the sum rule (4)–(5) for the photoionization coefficients C_{ij}. Similar relations (7)–(8) have been derived also for atomic bremsstrahlung. As we mentioned already above, the bremsstrahlung result was obtained assuming that summation in cross sections over the projection of a specified total angular momentum magnitude for the final electron is restricted to two values $\pm|\mu_0|$. The sum rule $R_{\rm br} = 1$ can be applied, therefore, only if the final electron (spin–) state $|j_f\, \mu_f = \pm|\mu_0|\rangle$ is "fixed" and results for a relevant two magnetic substates are summed or averaged. This is most easily achieved if the final electron is scattered as an $s_{1/2}$ or $p_{1/2}$ wave. Based on our relativistic calculations, we argue that an initial electron of not very low energy, which lost (almost) all its kinetic energy during the scattering by a low-Z ion or atom, is predominantly in the $s_{1/2}$ state and, hence, the bremsstrahlung sum rule (7)–(8) is valid. In Fig. 4 we display, for example, the polarization correlations C_{ij} and the linear combination $R_{\rm br}$ of squares of these coefficients (gray solid line) for collision of 100-keV (upper panel), 500-keV (middle panel), and 1-MeV (lower panel) electrons by a bare beryllium ion. Calculations have been performed for the bremsstrahlung tip region, where the final electron energy is 1 eV, and for the entire range of

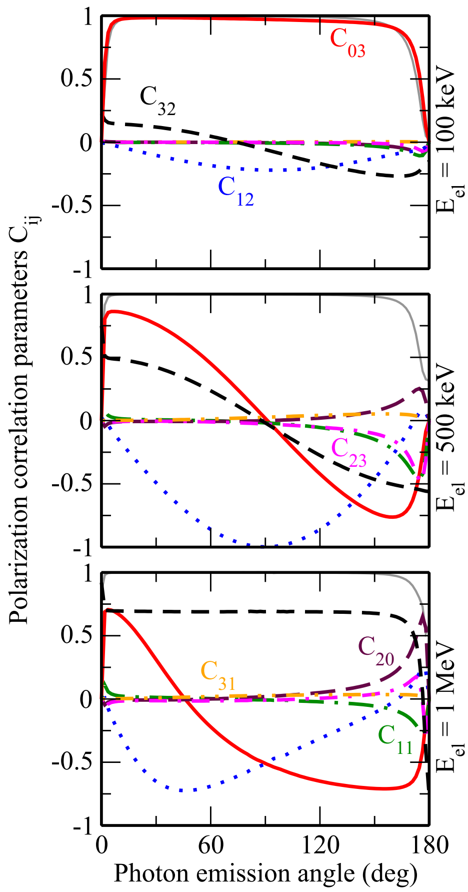

FIG. 4. The polarization correlation parameters C_{ij} for bremsstrahlung produced by 100 keV (upper panel), 500 keV (middle panel), and 1 MeV (lower panel) electrons scattered by a bare beryllium ion ($Z = 4$). Different curves are used to represent the correlations: C_{03} (red solid line), C_{32} (black short-dashed line), C_{12} (blue dotted line), C_{11} (green long-dash-dotted line), C_{31} (orange short-dash-double-dotted line), C_{20} (maroon long-dashed line), and C_{23} (pink short-dash-dotted line). Moreover, the linear combination of squares of correlations R_{br} is shown on an absolute scale by the thin gray solid curve.

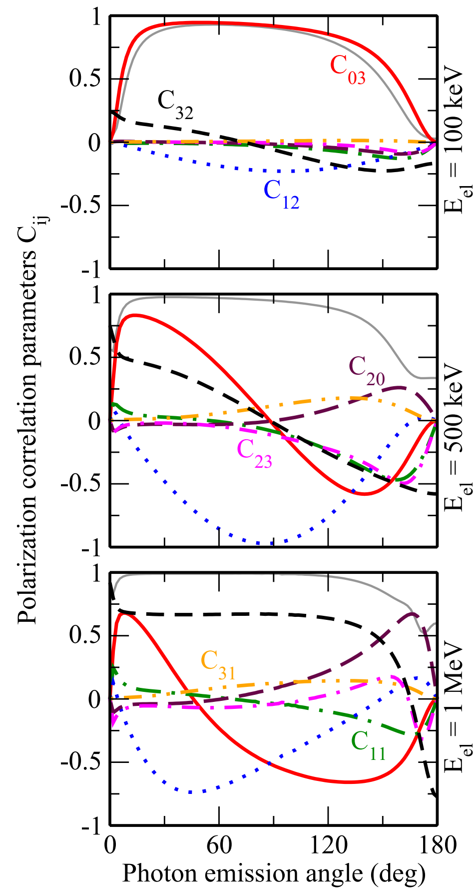

FIG. 5. The same as Fig. 4 but for electron scattering by the bare argon ion ($Z = 18$).

photon emission angles θ. As seen from this figure, the R_{br} is almost identical to unity for $5 \leqslant \theta \leqslant 130$ deg. For these angles, moreover, as in photoeffect, only the three polarization correlations, C_{03}, C_{12}, and C_{32}, are manifestly nonzero, thus leading to the simplified sum rule:

$$C_{03}^2 + C_{12}^2 + C_{32}^2 \simeq 1. \tag{12}$$

Again, this result is expected from the Born-approximation analysis, which predicts that C_{03}, C_{12}, and C_{32} are the leading-order coefficients, proportional to $O(1)$, while the other four C_{ij}'s are $\sim O(\alpha Z)$.

One can use Eq. (12) to analyze the bremsstrahlung polarization correlations in the low-Z, Born-approximation regime. For example, from the measurements of the parameters C_{03} and C_{12}, which characterize the production of linearly (within the reaction plane) and circularly polarized light by the scattering of unpolarized and transversely (in the x direction) electrons, respectively, we can extract the information about the C_{32}. The latter correlation describes the circular polarization of bremsstrahlung radiation for the case when the electron beam is longitudinally polarized. For the energy $E_{\mathrm{el}} = 500\,\mathrm{keV}$ and photon emission angle $\theta = 30\,\mathrm{deg}$, our partial-wave calculations predict that $C_{03} = 0.755$ and $C_{12} = 0.505$. Based on these data, one finds $|C_{32}| = \sqrt{1 - C_{03}^2 - C_{12}^2} = 0.417$ which is, again, in a perfect agreement with the results of calculations. The simplified sum rule (12) of course becomes invalid with the increase of the nuclear charge Z of a target, owing to the growth of the other C_{ij}'s, see Figs. 5 and 6.

The bremsstrahlung sum rules remain valid in the ultrarelativistic regime, in which the only nonvanishing correlations are C_{32} and $C_{23} = -C_{11}$ [7]. Similar to the photoionization case, this leads to the trivial result:

$$R_{\mathrm{br}} \simeq C_{32}^2 \simeq 1. \tag{13}$$

Again, due to the computation difficulties we did not attempt to verify this relation in computations with our Dirac partial-wave approach. Instead, we refer to recent Dirac-Sommerfeld-Maue calculations, which confirm Eq. (13) for heavy targets and incident electron energy higher than 10 MeV [14].

As noted earlier, another possible form of a sum rule for the ultrarelativistic bremmstrahlung regime and high-Z targets was conjectured recently by Jakubassa-Amundsen in Ref. [14]:

$$C_{32}^2 + C_{12}^2 + C_{20}^2 \simeq 1. \tag{14}$$

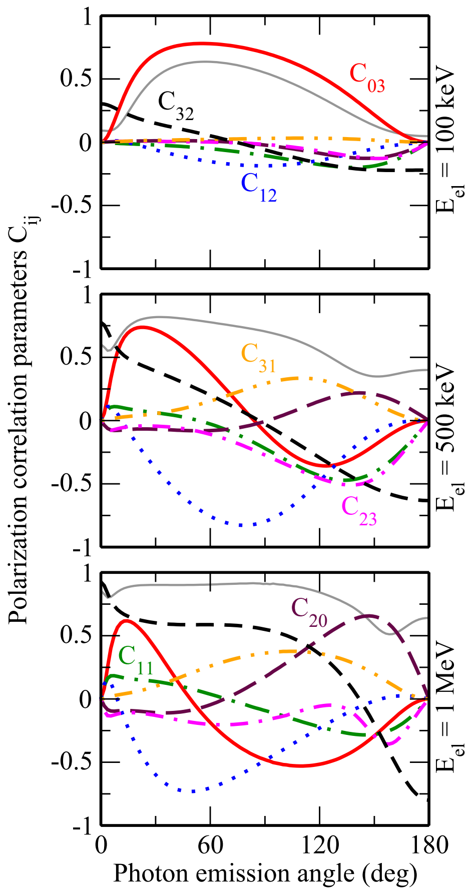

FIG. 6. The same as Fig. 4 but for electron scattering by the bare xenon ion ($Z = 54$).

This proposed identity was based on the earlier discussion by Johnson and Rozics [15] of the relationship between elastic electron scattering and bremsstrahlung for $E_{\rm el} \to \infty$. Some argument for the conjecture (14) was presented in Table I of Ref. [14]. In that table, however, only the sum of the squares of C_{32}, C_{12}, and C_{20}, but not these coefficients separately, was presented for incident energies 5–20 MeV in Xe, with good agreement for the sum at least above 10 MeV. In this asymptotic region Eq. (14) trivially agrees with our (asymptotic) sum rule (13) since $C_{32} \to 1$ while C_{12} and C_{20} vanish in the ultrarelativistic regime.

The above discussions of the sum rules for both photoionization and bremsstrahlung were based on our relativistic partial-wave calculations. These calculations provide estimates of the correlation parameters C_{ij} which are *exact* within the framework of the independent-particle approximation. In experimental studies, however, the coefficients C_{ij} are always measured with some error. Such uncertainties in the determination of polarization correlations may hamper the application of Eqs. (5) and (8). For example, a 10% inaccuracy in the sum rule leads to a 20%–30% error in one of the C_{ij}. Despite this drawback, the sum rules and, especially their simplified forms (10) and (12), can be useful for the analysis of experimental data. This reflects the recent developments in solid-state Compton polarimeters and, hence, increasing accuracy of photoionization and bremsstrahlung experiments.

V. SUMMARY

In summary, we have reconsidered the polarization correlations between (i) incident photon and emitted electron in photoionization, and (ii) incident electron and emitted photon in atomic-field bremsstrahlung. In both cases the correlations are characterized by *seven* coefficients C_{ij} that enter the differential photoionization (2) and bremsstrahlung (6) cross sections, respectively. We have found simple relations (4)–(5) and (7)–(8) connecting the squares of the correlation coefficients C_{ij}. These relations can be applied both for one-electron systems and—within the independent particle approach—for many-electron atoms and ions. In particular, the derived sum rules are exact (i) for the ionization of an electron from the K, $L_{I,II}$, $M_{I,II}$ atomic shells, as well as (ii) for the tip bremsstrahlung process, in which an outgoing low energy electron is primarily in a $s_{1/2}$ state. The structure of the relations between the coefficients C_{ij} in photoeffect and bremsstrahlung is similar to that found in elastic electron and elastic photon scattering. This suggests a common origin for the behavior of polarization correlations observed in such processes. No explanation for this common behavior has yet been found.

While no practical use has been proposed for a relationship involving all seven polarization correlations, there are scenarios in which only few C_{ij} coefficients contribute to the cross sections. In particular, for low-Z ionic (or atomic) targets three correlation parameters are manifestly nonvanishing for both photoionization and bremsstrahlung, thus giving rise to simplified sum rules (10) and (12). For such a Born-approximation scenario, the knowledge of two of the C_{ij}'s predicts the magnitude of the third one. The simplified sum rules can be employed, therefore, to determine a complete set of (nonvanishing) polarization correlations in modern photoionization and bremsstrahlung experiments.

[1] S. Tashenov, T. Back, R. Barday, B. Cederwall, J. Enders, A. Khaplanov, Y. Poltoratska, K. U. Schassburger, and A. Surzhykov, Phys. Rev. Lett. **107**, 173201 (2011).

[2] R. Märtin, G. Weber, R. Barday, Y. Fritzsche, U. Spillmann, W. Chen, R. D. DuBois, J. Enders, M. Hegewald, S. Hess, A. Surzhykov, D. B. Thorn, S. Trotsenko, M. Wagner, D. F. A. Winters, V. A. Yerokhin, and Th. Stöhlker, Phys. Rev. Lett. **108**, 264801 (2012).

[3] S. Tashenov, T. Back, R. Barday, B. Cederwall, J. Enders, A. Khaplanov, Y. Fritzsche, K. U. Schassburger, A. Surzhykov, V. A. Yerokhin, and D. Jakubassa-Amundsen, Phys. Rev. A **87**, 022707 (2013).

[4] O. Kovtun, V. Tioukine, A. Surzhykov, V. A. Yerokhin, B. Cederwall, and S. Tashenov, Phys. Rev. A **92**, 062707 (2015).

[5] S. Tashenov, Th. Stöhlker, D. Banas, K. Beckert, P. Beller, H. F. Beyer, F. Bosch, S. Fritzsche, A. Gumberidze, S. Hagmann,

C. Kozhuharov, T. Krings, D. Liesen, F. Nolden, D. Protic, D. Sierpowski, U. Spillmann, M. Steck, and A. Surzhykov, Phys. Rev. Lett. **97**, 223202 (2006).

[6] K. H. Blumenhagen *et al.* (unpublished).

[7] R. H. Pratt, R. D. Levee, R. L. Pexton, and W. Aron, Phys. Rev. **134**, A916 (1965).

[8] H. K. Tseng and R. H. Pratt, Phys. Rev. A **7**, 1502 (1973). Note that the analysis beginning with Eq. (2.12) and yielding (2.18) of this reference is incorrect. However the remainder of the paper did not utilize this. The numerical results have been confirmed subsequently, and the expressions (2.19)–(2.22) do lead to the sum rule stated in the present work. Note that the coefficients of Eq. (2.18) of this reference, although incorrect, do in fact satisfy the same sum rule as Eq. (7) of the present paper.

[9] V. A. Yerokhin and A. Surzhykov, Phys. Rev. A **82**, 062702 (2010).

[10] A. Surzhykov, V. A. Yerokhin, Th. Stöhlker, and S. Fritzsche, J. Phys. B **48**, 144015 (2015).

[11] S. C. Roy, B. Sarkar, L. D. Kissel, and R. H. Pratt, Phys. Rev. A **34**, 1178 (1986).

[12] F. Gursey, Phys. Rev. **107**, 1734 (1957).

[13] J. W. Motz, H. Olsen, and H. W. Koch, Rev. Mod. Phys. **36**, 881 (1964).

[14] D. H. Jakubassa-Amundsen, Phys. Rev. A **85**, 042714 (2012).

[15] W. R. Johnson and J. D. Rozics, Phys. Rev. **128**, 192 (1962).

[16] R. H. Pratt, R. D. Levee, R. L. Pexton, and W. Aron, Phys. Rev. **134**, A898 (1965).

[17] R. D. Schmickley and R. H. Pratt, Phys. Rev. **164**, 104 (1967).

[18] The doubly differential cross section $d\sigma/d\Omega$, if corresponding to (i) a specific initial photoeffect bound state $|j_b\mu_b\rangle$ or (ii) a specific final bremsstrahlung continuum state $|j_f\mu_f\rangle$, involve 16 parameters C_{ij}. Rather, if summed or averaged over $\pm|\mu_b|$ (or $\pm|\mu_f|$), it is those quantities that are connected by the seven C_{ij} as stated.

[19] R. D. Schmickley, Ph.D thesis, Stanford University, Stanford, CA, 1966.

[20] R. H. Pratt, A. Ron, and H. K. Tseng, Rev. Mod. Phys. **45**, 273 (1973).

[21] A. Surzhykov, S. Fritzsche, and Th. Stöhlker, J. Phys. B **35**, 3713 (2002).

[22] J. Eichler and Th. Stöhlker, Phys. Rep. **439**, 1 (2007).

[23] R. A. Müller, V. A. Yerokhin, and A. Surzhykov, Phys. Rev. A **90**, 032707 (2014).

[24] R. H. Pratt, Phys. Rev. **123**, 1508 (1961).