

Interaction of relativistic elementary atoms with matter. I. General formulas

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The problem of the interaction of relativistic elementary atoms (Coulomb bound states of elementary particles such as positronium, pionium, etc.) with matter is studied in the reference frame where the atom is initially at rest. An atom of matter is treated as a spinless structureless fast particle. The amplitudes of elementary-atom interaction are derived in the Born approximation under the assumption that a momentum transfer to the atom does not significantly exceed an inverse Bohr radius of the atom. The elementary-atom excitation and ionization processes are considered. The transitions where the spin projection of the atom component is reversed are also studied. In particular the matrix elements for para-ortho and ortho-para transitions are given. The spin structure of the amplitudes is discussed in detail. The sum rules, which allow the calculation of the cross sections summed over atom final states are found. Finally the formulas of the atom interaction cross sections are presented.

I. INTRODUCTION

Elementary atoms are the Coulomb bound states of two elementary particles. One can enumerate here positronium, pionium, or the recently discovered¹ atom of a pion and a muon. In our previous paper² we have studied the interaction of elementary atoms with atoms of matter in the nonrelativistic approximation. This paper is devoted to a relativistic generalization of those calculations. The general formulas are given here while the results of numerical calculations are presented in the following paper.³ To omit repetitions we invite the reader to read as an introduction the first section of Ref. 2, where the history of elementary atoms and existing literature are discussed. Let us consider here only some "relativistic" aspects of the problem. We first mention that the relativistic calculations are of practical, not only academic, interest. The motion of some elementary atoms, e.g., $A_{\mu\pi}$,¹ in laboratory experiments is really relativistic. (A_{ab} denotes the elementary atom of a positively charged particle a and a negatively charged particle b ; A_{2c} denotes the atom composed of a particle c and an antiparticle \bar{c} .) Recently ultrarelativistic positronia with the Lorentz γ factor of 10^3 – 10^4 have been registered⁴ and the experiment to study the interaction of such positronia with matter is just in progress.

The relativistic treatment of bound states is faced with well-known difficulties which can be partly overcome for weakly bound states by means of the Bethe-Salpeter approach. In our description of the elementary-atom interaction we use the less refined formalism where the atom is treated in a nonrelativistic manner. It is justified because of two circumstances: (1) In the atom rest frame the atom component motion is quite nonrelativistic; (2) the characteristic momentum transfer to the elementary atom in the interaction process is of order of the inverse Bohr radius of the atom and consequently it is small when compared to the atom component masses.

Both circumstances, which follow from the smallness of the electrodynamic coupling constant, allow the nonrelativistic description of the atom in the reference frame where the atom is initially at rest. On the basis of such an approach collisions with high momentum transfer cannot be studied. However, as long as we are interested in the bulk characteristics of elementary-atom interactions, in particular, in the integrated cross sections, such collisions are of no importance. Therefore in this paper we consider the interaction of an elementary atom with matter in the reference frame, where the atom is initially at rest while the atom of matter is represented by a fast spinless particle. The effect of electron screening of the electromagnetic field is taken into account by modification of a photon propagator.

The analogous problem of the relativistic particle interaction with a hydrogen atom was studied more than 50 years ago by Møller⁵ and Bethe.⁶ In the case of the hydrogen atom the proton can be treated as infinitely heavy (when compared to an electron) and consequently only the electron plays an active role in the interaction. Møller and Bethe, of course, used this approximation and it makes their calculations inapplicable to elementary atoms with components of comparable masses. This fact has not been noticed by Prasad,⁷ who used the Møller and Bethe formulas to study the interaction of $A_{\mu\pi}$. Although the electron mass has been replaced by the reduced mass of a pion and a muon, the results of Ref. 7 have nothing to do with the $A_{\mu\pi}$ interaction.

The calculations of relativistic positronium collisions with atoms of matter have been performed by Kotzinian and Dulian.⁸ However the general formulas have not been derived since it has been (correctly) argued that if the electric transition is allowed the role of the magnetic part of the interaction is negligible. The magnetic transitions have been considered only for processes where the atom spin is changed. For other critical comments on Ref. 8 see Ref. 2.

II. ATOMIC WAVE FUNCTIONS

Our first task is to write down the atomic wave functions in the form appropriate for relativistic calculations. As explained above, in the reference frame where the atom is initially at rest or its motion is nonrelativistic, the final-state motion also can be described nonrelativistically. In such a description the center-of-mass motion and the relative motion of the atom can be separated from one another; i.e., the wave functions factorize into the functions describing the center-of-mass motion and relative motion, respectively. We introduce two sets of variables: positions and momenta of the atom components in the laboratory frame $(\mathbf{r}_1, \mathbf{p}_1)$ and $(\mathbf{r}_2, \mathbf{p}_2)$; the position and momentum of the center of mass of the atom (\mathbf{R}, \mathbf{P}) and the position and momentum of the atom component in the center-of-mass frame (\mathbf{r}, \mathbf{p}) . Both sets of variables are connected by the simple relations

$$\mathbf{R} = \zeta \mathbf{r}_1 - \eta \mathbf{r}_2, \quad \mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2, \quad (1)$$

$$\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2, \quad \mathbf{p} = -\eta \mathbf{p}_1 - \zeta \mathbf{p}_2,$$

where, as in Ref. 2, $\zeta = m_1/M$, $\eta = -m_2/M$ with m_1 , m_2 , and M the masses of the atom components and of the atom. Because of the small value of the atomic binding energy $\zeta - \eta = 1$.

Let us also introduce for convenience the four-vector positions and four-momenta:

$$X = (t, \mathbf{R}), \quad \mathcal{P} = (E, \mathbf{P}),$$

$$x_i = (t, \mathbf{r}_i), \quad p_i = (E_i, \mathbf{p}_i),$$

$$\psi_{s_1 s_2}(x_1, x_2) = \frac{1}{\sqrt{V}} e^{-i\mathcal{P}X} \int \frac{d^3 \mathbf{p}}{(2\pi)^3} \left[\frac{m_1 m_2}{E_1 E_2} \right]^{1/2} e^{i\mathbf{p} \cdot \mathbf{r}} \tilde{\phi}(\mathbf{p}) u(s_1, \mathbf{p}_1) v(s_2, \mathbf{p}_2), \quad (4)$$

where V is the normalization volume and $\phi(\mathbf{r})$ is the nonrelativistic, spin-independent wave function of relative motion. ϕ is normalized in the standard way and

$$\tilde{\phi}(\mathbf{p}) = \int d^3 \mathbf{r} e^{-i\mathbf{p} \cdot \mathbf{r}} \phi(\mathbf{r}).$$

$u(s, \mathbf{p})$, $v(s, \mathbf{p})$ are the Dirac spinors⁹ normalized by the condition

$$\bar{u}(s, \mathbf{p}) u(s', \mathbf{p}) = \bar{v}(s, \mathbf{p}) v(s', \mathbf{p}) = \delta_s^{s'}. \quad (5)$$

s_1, s_2 are the atom component spin projections on the quantization axis. The normalization coefficients of the wave functions (2)–(4) are chosen to satisfy the equation

$$\int d^3 \mathbf{r}_1 d^3 \mathbf{r}_2 \psi^\dagger(x_1, x_2) \psi(x_1, x_2) = 1, \quad (6)$$

where a dagger denotes Hermitian conjugation and it is understood that the spin indices of ψ^\dagger and ψ (if any) coincide.

In the case of the spin- $\frac{1}{2}$ - $\frac{1}{2}$ atoms it is more adequate to use other spin variables which describe the total atomic spin σ and the atomic spin projection σ_3 . New functions are expressed as

where $i=1,2$ and $E=(M^2+\mathbf{P}^2)^{1/2}$, $E_i=(m_i^2+\mathbf{p}_i^2)^{1/2}$. We use the units where $c=\hbar=1$. The metric is $(+, -, -, -)$. The time components of all these four-vector positions are the same, which is characteristic of nonrelativistic approach.

The elementary-atom components are spin- $\frac{1}{2}$ or spinless particles. Therefore one has to consider three types of atoms: (1) atoms of two spinless components, e.g., $A_{2\pi}$, $A_{\pi K}$; (2) atoms of spin-0 and spin- $\frac{1}{2}$ particles, e.g., $A_{e\pi}$, $A_{\mu\pi}$; (3) the atoms of two spin- $\frac{1}{2}$ components, e.g., A_{2e} , $A_{e\mu}$. Three kinds of elementary atoms are, later on, called the spin-0-0 atoms, the spin-0- $\frac{1}{2}$ atoms, and the spin- $\frac{1}{2}$ - $\frac{1}{2}$ atoms, respectively.

The atomic wave functions are chosen in the following form.

(1) For the spin-0-0 atoms

$$\psi(x_1, x_2) = \frac{1}{\sqrt{V}} e^{-i\mathcal{P}X} \phi(\mathbf{r}), \quad (2)$$

(2) for the spin-0- $\frac{1}{2}$ atoms

$$\psi_{s_2}(x_1, x_2) = \frac{1}{\sqrt{V}} e^{-i\mathcal{P}X} \times \int \frac{d^3 \mathbf{p}}{(2\pi)^3} \left[\frac{m_2}{E_2} \right]^{1/2} e^{i\mathbf{p} \cdot \mathbf{r}} \tilde{\phi}(\mathbf{p}) v(s_2, \mathbf{p}_2), \quad (3)$$

(3) for the spin- $\frac{1}{2}$ - $\frac{1}{2}$ atoms

$$\psi_{\sigma, \sigma_3}(x_1, x_2) = C_{s_1 s_2}^{\sigma \sigma_3} \psi_{s_1 s_2}(x_1, x_2),$$

where the spin matrices are easily found by means of the Clebsch-Gordan coefficients

$$\begin{aligned} C_{s_1 s_2}^{00} &= \frac{1}{\sqrt{2}} (\delta_{s_1}^{1/2} \delta_{s_2}^{-1/2} - \delta_{s_1}^{-1/2} \delta_{s_2}^{1/2}), \\ C_{s_1 s_2}^{10} &= \frac{1}{\sqrt{2}} (\delta_{s_1}^{1/2} \delta_{s_2}^{-1/2} + \delta_{s_1}^{-1/2} \delta_{s_2}^{1/2}), \\ C_{s_1 s_2}^{1\pm 1} &= \delta_{s_1}^{\pm 1/2} \delta_{s_2}^{\pm 1/2}. \end{aligned} \quad (7)$$

III. TRANSITION MATRIX ELEMENTS

The transition matrix element in the Born approximation reads

$$S_{if} = -i \int d^4 x_1 j_\mu^{if}(x_1) A_{if}^\mu(x_1) + i \int d^4 x_2 j_\mu^{if}(x_2) A_{if}^\mu(x_2), \quad (8)$$

where j_μ^{if} is the transition four-current related to the

atom component motion and A_{if}^μ is the transition electromagnetic four-potential of the projectile.

If the projectile is a spinless particle of Ze charge, one finds in the Lorentz gauge the potential⁹

$$A_{if}^\mu(x) = Ze \frac{k_i^\mu + k_f^\mu}{2(\epsilon_i \epsilon_f)^{1/2} V} e^{-iqx} \Delta(q), \quad (9)$$

where $q = k_f - k_i$ and $k_i, (k_f)$ is the initial (final) four-momentum of the projectile, $k_{i,f} = (\epsilon_{i,f}, \mathbf{k}_{i,f})$; $\Delta(q)$ is the photon propagator in the Lorentz gauge, which should be modified to take into account the screening effect.

The transition currents are

$$j_\mu^{if}(x_1) = \int d^3 \mathbf{r}_2 \psi_f^\dagger(x_1, x_2) \hat{J}_\mu^1 \psi_i(x_1, x_2), \quad (10)$$

$$j_\mu^{if}(x_2) = \int d^3 \mathbf{r}_1 \psi_f^\dagger(x_1, x_2) \hat{J}_\mu^2 \psi_i(x_1, x_2), \quad (11)$$

where the current operator equals

$$\hat{J}_\mu^{1,2} = \left[e, \frac{ie}{2m_{1,2}} \nabla_{1,2} \right]$$

for spin-0 atom components and

$$\hat{J}_\mu^{1,2} = e \gamma^0 \gamma_\mu$$

for spin- $\frac{1}{2}$ atom components.

Substituting the wave functions (2)–(4) in Eqs. (10) and (11) one finds the explicit expressions for the currents. Then, substituting them and the four-potential (9) in Eq. (8) we get after simple manipulations the formulas for S -matrix transition elements for three kinds of elementary atoms.

(1) The spin-0-0 atoms

$$S_{if} = \frac{-iZe^2}{V^2(\epsilon_i \epsilon_f)^{1/2}} (2\pi)^4 \delta^{(4)}(\mathcal{P}_f + k_f - \mathcal{P}_i - k_i) \Delta(q) \left[\left[\epsilon_i + \frac{\mathbf{k}_i \cdot (\mathbf{P}_i + \mathbf{P}_f)}{2M} \right] [F_{if}(\eta q) - F_{if}(\zeta q)] + \frac{\mathbf{k}_i}{2} \cdot \left[\frac{1}{m_1} \mathbf{G}_{if}(\eta q) + \frac{1}{m_2} \mathbf{G}_{if}(\zeta q) \right] \right], \quad (12)$$

(2) the spin-0- $\frac{1}{2}$ atoms

$$S_{if} = \frac{-iZe^2}{V^2(\epsilon_i \epsilon_f)^{1/2}} (2\pi)^4 \delta^{(4)}(\mathcal{P}_f + k_f - \mathcal{P}_i - k_i) \times \Delta(q) \left\{ \delta_{s_2'}^{s_2} \left[\left[\epsilon_i + \frac{\mathbf{k}_i \cdot (\mathbf{P}_f + \mathbf{P}_i)}{2M} \right] F_{if}(\eta \mathbf{q}) + \frac{\mathbf{k}_i}{2m_1} \cdot \mathbf{G}_{if}(\eta \mathbf{q}) \right] - \int \frac{d^3 \mathbf{p}}{(2\pi)^3} \frac{m_2}{(E_2 E_2')^{1/2}} \bar{v}(s_2', \mathbf{p}_2 + \mathbf{q}) \gamma_\mu k_i^\mu v(s_2, \mathbf{p}_2) \bar{\phi}_f^*(\mathbf{p} - \zeta \mathbf{q}) \bar{\phi}_i(\mathbf{p}) \right\}, \quad (13)$$

(3) the spin- $\frac{1}{2}$ - $\frac{1}{2}$ atoms

$$S_{if} = \frac{-iZe^2}{V^2(\epsilon_i \epsilon_f)^{1/2}} (2\pi)^4 \delta^{(4)}(\mathcal{P}_f + k_f - \mathcal{P}_i - k_i) \Delta(q) C_{s_1 s_2}^{\sigma \sigma_3} C_{s_1' s_2'}^{\sigma' \sigma_3'} \times \left[\delta_{s_2'}^{s_2} \int \frac{d^3 \mathbf{p}}{(2\pi)^3} \frac{m_1}{(E_1 E_1')^{1/2}} \bar{u}(s_1', \mathbf{p}_1 + \mathbf{q}) \gamma_\mu k_i^\mu u(s_1, \mathbf{p}_1) \bar{\phi}_f^*(\mathbf{p} - \eta \mathbf{q}) \bar{\phi}_i(\mathbf{p}) - \delta_{s_1'}^{s_1} \int \frac{d^3 \mathbf{p}}{(2\pi)^3} \frac{m_2}{(E_2 E_2')^{1/2}} \bar{v}(s_2', \mathbf{p}_2 + \mathbf{q}) \gamma_\mu k_i^\mu v(s_2, \mathbf{p}_2) \bar{\phi}_f^*(\mathbf{p} - \zeta \mathbf{q}) \bar{\phi}_i(\mathbf{p}) \right], \quad (14)$$

where

$$E_{1,2}' \equiv [m_{1,2}^2 + (\mathbf{p}_{1,2} + \mathbf{q})^2]^{1/2},$$

$$F_{if}(\mathbf{q}) = \int d^3 \mathbf{r} e^{i\mathbf{q} \cdot \mathbf{r}} \phi_f^*(\mathbf{r}) \phi_i(\mathbf{r}),$$

$$\mathbf{G}_{if}(\mathbf{q}) = i \int d^3 \mathbf{r} e^{i\mathbf{q} \cdot \mathbf{r}} \phi_f^*(\mathbf{r}) \nabla \phi_i(\mathbf{r}).$$

The final-state variables are denoted by the index f or by prime, and the initial-state variables are denoted by the index i .

Because the currents (10) and (11) depend on $x_{1,2}$ as $e^{iqx_{1,2}}$ the conservation current condition $\partial^\mu j_\mu(x) = 0$ can

be written in the form

$$q^\mu j_\mu^{if}(x_{1,2}) = 0. \quad (15)$$

The condition (15) has been used in the derivation of formulas (12)–(14), i.e., the expression $(k_i^\mu + k_f^\mu)$ from Eq. (9) has been replaced by $2k_i^\mu$.

Let us now discuss the spin structure of the amplitude (14), which can be written down as

$$S_{if} = C_{s_1 s_2}^{\sigma \sigma_3} C_{s_1' s_2'}^{\sigma' \sigma_3'} [\delta_{s_2'}^{s_2} A(s_1', s_1) + \delta_{s_1'}^{s_1} B(s_2, s_2')].$$

The amplitudes A and B are related to the interaction of

TABLE I. The spin structure of the interaction amplitude.

$\sigma, \sigma_3 \backslash \sigma', \sigma'_3$	0,0	1,-1	1,0	1,1
0,0	$A_n + B_n$	$\frac{1}{\sqrt{2}}(A_f - B_f)$	0	$\frac{1}{\sqrt{2}}(A_f - B_f)$
1,-1	$\frac{1}{\sqrt{2}}(A_f - B_f)$	$A_n + B_n$	$\frac{1}{\sqrt{2}}(A_f + B_f)$	0
1,0	0	$\frac{1}{\sqrt{2}}(A_f + B_f)$	$A_n + B_n$	$\frac{1}{\sqrt{2}}(A_f + B_f)$
1,1	$\frac{1}{\sqrt{2}}(A_f - B_f)$	0	$\frac{1}{\sqrt{2}}(A_f + B_f)$	$A_n + B_n$

the first and the second atom component, respectively. The following relations are assumed:

$$\begin{aligned} A(s_1, s_1) &= A(-s_1, -s_1) \\ &\equiv A_n \text{ (spin nonflip) ,} \\ A(-s_1, s_1) &= A(s_1, -s_1) \\ &\equiv A_f \text{ (spin flip) ,} \end{aligned}$$

and analogous relations for the B amplitude which follow from the invariance of the electrodynamics under P and T transformations. Sixteen amplitudes describing all possible transitions $\sigma\sigma_3 \rightarrow \sigma'\sigma'_3$ collected in Table I have been found using the explicit form of the spin matrices (7). It is seen that the transition is forbidden (in Born approximation) if (1) $\sigma \neq \sigma'$ and $\sigma_3 = \sigma'_3$, (2) $|\sigma'_3 - \sigma_3| > 1$. One also sees that the amplitudes A_f and B_f contribute to the complete amplitude with the same sign for the processes with $\sigma = \sigma'$ and with opposite sign for $\sigma \neq \sigma'$.

When the atom is composed of a particle and antiparticle there occurs the selection rule for transitions in the Born approximation. The transition is allowed if the charge parity of the atom changes in the course of interaction, i.e., when

$$(-1)^{l+\sigma} = -(-1)^{l'+\sigma'} . \quad (16)$$

Otherwise the transition is forbidden. The selection rule (16) can be found in two ways.

(1) The atom of particles and antiparticles is an eigenstate of the charge-parity operator C with the eigenvalue $(-1)^{l+\sigma}$ the photon is also an eigenstate of C and the eigenvalue is -1 . Keeping in mind that charge parity is conserved in electrodynamic interactions one finds the selection rule (16) since the Born approximation relates to the one-photon-exchange process.

(2) The selection rule (16) directly follows from the amplitudes (12) and (14). In the case of the atom of spinless particles it is enough to observe that

$$F_{if}(-\mathbf{q}) = (-1)^{l-l'} F_{if}(\mathbf{q})$$

and

$$\mathbf{G}_{if}(-\mathbf{q}) = (-1)^{l-l'-1} \mathbf{G}_{if}(\mathbf{q}) .$$

The above relations follow from the well-known parity properties of nonrelativistic Coulomb wave functions.

For the spin- $\frac{1}{2}$ - $\frac{1}{2}$ atoms, let us write down the amplitude (14) in the form

$$\begin{aligned} S_{if} &= \frac{-iZe^2}{V^2(\epsilon_i \epsilon_f)^{1/2}} (2\pi)^4 \delta^{(4)}(\mathcal{P}_f + k_f - \mathcal{P}_i - k_i) \\ &\times \Delta(\mathbf{q}) C_{s'_1 s'_2}^{\sigma' \sigma'_3} C_{s_1 s_2}^{\sigma \sigma_3} \int \frac{d^3 \mathbf{p}}{(2\pi)^3} \frac{m_1}{\sqrt{E_1 E'_1}} \bar{\phi}_f^*(\mathbf{p} + \frac{1}{2}\mathbf{q}) \phi_i(\mathbf{p}) \\ &\times [\delta_{s'_2}^{s'_1} \bar{u}(s'_1, \mathbf{p}_1 + \mathbf{q}) \gamma_\mu k_i^\mu u(s_1, \mathbf{p}_1) - (-1)^{l-l'} \delta_{s_1}^{s'_1} \bar{v}(s'_1, \mathbf{p}_2 + \mathbf{q}) \gamma_\mu k_i^\mu v(s_2, \mathbf{p}_2)] . \end{aligned}$$

To obtain the above formula we have changed \mathbf{p} into $-\mathbf{p}$ in the second term of (14) and we have taken into account the parity properties of the Coulomb wave functions. Then, keeping in mind that

$$\bar{u}(s', \mathbf{p}') \gamma_\mu k^\mu u(s, \mathbf{p}) = \bar{v}(s', \mathbf{p}') \gamma_\mu k^\mu v(s, \mathbf{p})$$

and using the results from Table I one finds the selection rule (16).

If one considers the hypothetical atom of the equal-

mass particles with spin- $\frac{1}{2}$ and spin-0, respectively, the selection rule (16) does not hold, because such an atom is not an eigenstate of the charge-conjugation operator.

The changes of the atomic spin are due to the magnetic transitions which are much less effective than the electric one.³ Therefore the simpler selection rule is realized in practice. Namely, the transitions for atoms of equal-mass components are strongly damped if

$$l' - l = 0, \pm 2, \pm 4, \dots . \quad (17)$$

For the atoms of the components of close but not equal mass, as $A_{\mu\pi}$, the transitions (17) are also significantly damped.²

IV. THE AMPLITUDES IN THE ATOMIC REST FRAME

In this section we consider the amplitudes (12)–(14) in the rest frame of the initial atom, where important simplifications of the formulas (12)–(14) occur.

The transition matrix element of the spin-0-0 atoms in the atomic rest frame reads

$$S_{if} = -i \frac{Ze^2}{V^2} (2\pi)^4 \delta^{(4)}(\mathcal{P}_f + k_f - \mathcal{P}_i - k_i) \Delta(q) \times \left[\left[1 + \frac{\mathbf{q} \cdot \mathbf{v}}{2M} \right] [F_{if}(\eta\mathbf{q}) - F_{if}(\zeta\mathbf{q})] + \frac{\mathbf{v}}{2M} \cdot [\zeta^{-1} \mathbf{G}_{if}(\eta\mathbf{q}) - \eta^{-1} \mathbf{G}_{if}(\zeta\mathbf{q})] \right], \quad (18)$$

where $\mathbf{v} \equiv \mathbf{k}_i / \epsilon_i$ is the projectile initial velocity. To derive Eq. (18) we have assumed that

$$|\epsilon_i - \epsilon_f| \ll \epsilon_i \quad (19)$$

which means that the projectile is heavy when compared to the atomic mass (projectile can be treated as an external field) or/and the projectile is initially sufficiently fast. In fact, condition (19) coincides with that of applicability of the Born approximation.

If $m_1 \gg m_2$ as for a hydrogen atom one finds, for inelastic transitions,

$$\Xi(\mathbf{p}', \mathbf{k}, \mathbf{p}) = \frac{1}{2m} \{ [(E+m)(E'+m)]^{1/2} + [(E-m)(E'-m)]^{1/2} [1 + i\boldsymbol{\sigma} \cdot (\mathbf{n}' \times \mathbf{n})] \} \epsilon - [(E'-m)(E+m)]^{1/2} [\mathbf{n} \cdot \mathbf{k} + i\boldsymbol{\sigma} \cdot (\mathbf{n}' \times \mathbf{k})] - [(E'+m)(E-m)]^{1/2} [\mathbf{n} \cdot \mathbf{k} - i\boldsymbol{\sigma} \cdot (\mathbf{n} \times \mathbf{k})],$$

where $k^\mu = (\epsilon, \mathbf{k})$, $E = (m^2 + \mathbf{p}^2)^{1/2}$, $E' = (m^2 + \mathbf{p}'^2)^{1/2}$,

$$\mathbf{n} \equiv \mathbf{p} / |\mathbf{p}|, \quad \mathbf{n}' \equiv \mathbf{p}' / |\mathbf{p}'|,$$

and $\boldsymbol{\sigma}$ denotes the vector of Pauli matrices. For the nonrelativistic momenta \mathbf{p} and \mathbf{p}' the above formula essentially simplifies to

$$\Xi(\mathbf{p}', \mathbf{k}, \mathbf{p}) \simeq \epsilon - \frac{\mathbf{k} \cdot (\mathbf{p} + \mathbf{p}')}{2m} - i \frac{\boldsymbol{\sigma} \cdot (\mathbf{q} \times \mathbf{k})}{2m}, \quad (23)$$

where $\mathbf{q} \equiv \mathbf{p}' - \mathbf{p}$. If the spin projections s and s' are equal, the first and the second terms of (23) contribute while for $s \neq s'$ there is the contribution of the third term only. So one can write

$$W^\dagger(\pm s) \Xi(\mathbf{p}', \mathbf{k}, \mathbf{p}) W(\pm s) = \epsilon - \frac{\mathbf{k} \cdot (\mathbf{p} + \mathbf{p}')}{2m}, \quad (24)$$

$$W^\dagger(\pm s) \Xi(\mathbf{p}', \mathbf{k}, \mathbf{p}) W(\mp s) = i \frac{Q |\mathbf{k}| \sin \alpha}{2m} (\sin \beta \mp i \cos \beta),$$

where $Q \equiv |\mathbf{q}|$, α and β are the polar and azimuthal angles of the vector \mathbf{k} in the coordinate system where the z

$$S_{if} = i \frac{Ze^2}{V^2} (2\pi)^4 \delta^{(4)}(\mathcal{P}_f + k_f - \mathcal{P}_i - k_i) \times \Delta(q) \left[F_{if}(\mathbf{q}) - \frac{\mathbf{v}}{2m_2} \cdot \mathbf{G}_{if}(\mathbf{q}) \right], \quad (20)$$

where the term from Eq. (18) which is proportional to $\mathbf{q} \cdot \mathbf{v} / 2M$ has been omitted because the characteristic momentum transfer (of an order of the inverse Bohr radius of the atom) is much smaller than M for $m_1 \gg m_2$.

In the nonrelativistic limit ($v^2 \ll 1$) the formula (18) gives the result known from Ref. 2:

$$S_{if} = -i \frac{Ze^2}{V^2} (2\pi)^4 \delta^{(4)}(\mathcal{P}_f + k_f - \mathcal{P}_i - k_i) \times \Delta(q) [F_{if}(\eta\mathbf{q}) - F_{if}(\zeta\mathbf{q})]. \quad (21)$$

The structure of the amplitudes (13) and (14) is much more complicated than that of (12) and for further study of these amplitudes one has to calculate the spinor products present in Eqs. (13) and (14). Using the standard representation of Dirac matrices⁹ one finds

$$\bar{u}(s', \mathbf{p}') \gamma_\mu k^\mu u(s, \mathbf{p}) = W^\dagger(s') \Xi(\mathbf{p}', \mathbf{k}, \mathbf{p}) W(s), \quad (22)$$

where $W(s)$ is the two-dimensional spinor normalized as

$$W^\dagger(s) W(s') = \delta_s^{s'};$$

$W(s)$ describes the particle spin projection on a quantization axis in the particle rest frame; the operator Ξ reads

axis, which is the spin quantization axis, coincides with the vector \mathbf{q} .

As seen in Table I the atomic interaction process is described by two spin-flip (A_f and B_f) or by two non-spin-flip amplitudes (A_n and B_n). There is no mixture of the spin-flip and non-spin-flip amplitudes. Therefore the processes where the atomic spin is conserved, or the atomic spin or spin projection is changed, can be considered separately. Let us now consider the spin-flip processes for the spin-0- $\frac{1}{2}$ and spin- $\frac{1}{2}$ - $\frac{1}{2}$ atoms. It is seen from Eqs. (24) that the spinor product depends on \mathbf{p} and \mathbf{p}' only through \mathbf{q} in the case of the spin-flip process. Then the spinor products can be placed in front of the integrals (13) and (14). The normalization coefficients are replaced by unity in the atomic rest frame since

$$\sqrt{M/E} = 1 + O(\mathbf{p}^2/m^2).$$

As it easily can be shown our calculations are valid up to the linear terms of the dimensionless parameter $(ma)^{-1}$ where a is the Bohr atom radius. Therefore the

quantities $O(\mathbf{p}^2/m^2)$ can be neglected.

Finally the spin-flip amplitude for the spin-0- $\frac{1}{2}$ atom in the atomic rest frame reads

$$S_{if} = -\frac{Ze^2}{2V^2}(2\pi)^4\delta^{(4)}(\mathcal{P}_f+k_f-\mathcal{P}_i-k_i)\Delta(q) \times \frac{Q|\mathbf{v}|\sin\alpha}{m_2}(\sin\beta \mp i\cos\beta)F_{if}(\xi\mathbf{q}). \quad (25)$$

In this case the amplitude of the spinless particle interaction does not contribute to the transition matrix element. The double sign in Eq. (25) is of no physical meaning because the β dependence disappears in the respective cross section ($|\sin\beta \mp i\cos\beta|^2=1$).

The spin-change amplitude for the spin- $\frac{1}{2}$ - $\frac{1}{2}$ atom is

$$S_{if} = \frac{Ze^2}{2\sqrt{2}V^2}(2\pi)^4\delta^{(4)}(\mathcal{P}_f+k_f-\mathcal{P}_i-k_i)\Delta(q) \times Q|\mathbf{v}|\sin\alpha \left[\frac{\sin\beta+i\chi_1\cos\beta}{m_1}F_{if}(\eta\mathbf{q}) - (-1)^{\sigma-\sigma'}\frac{\sin\beta+i\chi_2\cos\beta}{m_2}F_{if}(\xi\mathbf{q}) \right]$$

$$S_{if}=0 \text{ for } \sigma_3=\sigma'_3 \text{ or } |\sigma'_3-\sigma_3|>1,$$

where $\chi_{1,2}=\pm 1$ and the sign depends on the initial value of the spin projection of the atomic components. Keeping in mind that the spin projection of only one atomic component can be changed in the course of the interaction (because of the one-photon-exchange approximation) one finds that $\chi_1=\chi_2$. Therefore one can write

$$S_{if} = \frac{Ze^2}{2\sqrt{2}V^2}(2\pi)^4\delta^{(4)}(\mathcal{P}_f+k_f-\mathcal{P}_i-k_i)\Delta(q) \times Q|\mathbf{v}|\sin\alpha(\sin\beta \pm i\cos\beta) \times \left[\frac{1}{m_1}F_{if}(\eta\mathbf{q}) - (-1)^{\sigma-\sigma'}\frac{1}{m_2}F_{if}(\xi\mathbf{q}) \right]. \quad (26)$$

The respective cross section is β independent.

Let us now consider the process where the atomic spin and the atomic spin projection are conserved. Observing that

$$\int \frac{d^3\mathbf{p}}{(2\pi)^3}\bar{\phi}_f^*(\mathbf{p}-\mathbf{q})\bar{\phi}_i(\mathbf{p})=F_{if}(\mathbf{q})$$

$$\begin{aligned} & \sum_f |F_{if}(\eta\mathbf{q})-F_{if}(\xi\mathbf{q})+\mathbf{x}\cdot[\xi^{-1}\mathbf{G}_{if}(\eta\mathbf{q})-\eta^{-1}\mathbf{G}_{if}(\xi\mathbf{q})]|^2 \\ &= (1-\xi^{-1}\mathbf{q}\cdot\mathbf{x})^2+(1+\eta^{-1}\mathbf{q}\cdot\mathbf{x})^2+4(\xi^{-2}+\eta^{-2})K_i(\mathbf{x},\mathbf{q}=0)+2[(1-\xi^{-1}\mathbf{q}\cdot\mathbf{x})\xi^{-1}+(1+\eta^{-1}\mathbf{q}\cdot\mathbf{x})\eta^{-1}]\mathbf{x}\cdot\mathbf{G}_{ii}(\mathbf{q}=0) \\ & \quad -2(1-\xi^{-1}\mathbf{q}\cdot\mathbf{x})(1+\eta^{-1}\mathbf{q}\cdot\mathbf{x})F_{ii}(\mathbf{q})-4(1-\xi^{-1}\mathbf{q}\cdot\mathbf{x})\eta^{-1}\mathbf{x}\cdot\text{Re}\mathbf{D}_{ii}(\mathbf{q})-4(1+\eta^{-1}\mathbf{q}\cdot\mathbf{x})\xi^{-1}\mathbf{x}\cdot\text{Re}\mathbf{D}_{ii}(-\mathbf{q}) \\ & \quad -8\xi^{-1}\eta^{-1}K_i(\mathbf{x},\mathbf{q})\equiv\Sigma_i(\mathbf{x},\mathbf{q}), \end{aligned} \quad (29)$$

where \mathbf{x} is a real vector. We have introduced two form factors:

$$\mathbf{D}_{if}(\mathbf{q})=i\int d^3\mathbf{r}e^{i\mathbf{q}\cdot\mathbf{r}}\phi_f^*(\mathbf{r})\nabla\phi_i(\mathbf{r}) \quad (30)$$

and

$$\int \frac{d^3\mathbf{p}}{(2\pi)^3}\mathbf{p}\bar{\phi}_f^*(\mathbf{p}-\mathbf{q})\bar{\phi}_i(\mathbf{p})=\frac{1}{2}[\mathbf{G}_{if}(\mathbf{q})+i\mathbf{q}F_{if}(\mathbf{q})]$$

one easily finds the amplitudes for the spin-conserved processes of the spin-0- $\frac{1}{2}$ and of the spin- $\frac{1}{2}$ - $\frac{1}{2}$ atoms which are equal to the amplitude of the spin-0-0 atom (18). One may wonder whether this result is correct since it is well known that the cross sections of spin-0 and spin- $\frac{1}{2}$ particle scattering differ from one another.⁹ However the difference is significant for the high-momentum-transfer interactions which have been neglected in our calculations.

V. THE SUM RULES

It is well known that

$$\sum_f |F_{if}(\mathbf{q})|^2=1,$$

where the summation is performed over the complete set of (nonrelativistic) wave functions describing final states. In Ref. 2 we have found that

$$\sum_f |F_{if}(\eta\mathbf{q})-F_{if}(\xi\mathbf{q})|^2=2-2\text{Re}F_{ii}(\mathbf{q}). \quad (27)$$

Because the parity of the Coulomb wave functions is well defined, i.e.,

$$\phi(-\mathbf{r})=\pm\phi(\mathbf{r}),$$

the form factor F_{ii} is real. The sum rule (27) has been used in Ref. 2 to obtain the total cross section of the elementary-atom interaction.

In the relativistic calculations considered here, there are three kinds of amplitudes (18), (25), and (26). To get the respective cross sections summarized over final states new sum rules have to be derived. With no difficulties one finds

$$\begin{aligned} & \sum_f |\xi^{-1}F_{if}(\eta\mathbf{q})\pm\eta^{-1}F_{if}(\xi\mathbf{q})|^2 \\ &= \xi^{-2}+\eta^{-2}\pm 2(\xi\eta)^{-1}F_{ii}(\mathbf{q})\equiv\Omega_i^\pm(\mathbf{q}). \end{aligned} \quad (28)$$

Simple but lengthy calculations provide the sum rule

and

$$K_i(\mathbf{x},\mathbf{q})=\int d^3\mathbf{r}e^{i\mathbf{q}\cdot\mathbf{r}}|\mathbf{x}\nabla\phi_i(\mathbf{r})|^2. \quad (31)$$

Because the Coulomb wave functions vanish at space infinities one finds the relation connecting the form factors \mathbf{G} , \mathbf{D} , and F :

$$\mathbf{G}_{if}(\mathbf{q}) = 2\mathbf{D}_{if}(\mathbf{q}) - \mathbf{q}F_{if}(\mathbf{q}). \quad (32)$$

VI. THE CROSS SECTIONS

In this section we give the cross sections of the elementary-atom interactions with atoms of matter which have been derived from the amplitudes (18), (25), and (26).

The initial elementary-atom state is defined by the quantum numbers $(n, l, m, \sigma, \sigma_3)$ while the final one is defined by $(n', l', m', \sigma', \sigma'_3)$. Since we consider the transitions with definite values of the projections of the

atomic orbital momentum and/or of the atomic spin projections on the quantization axis, the cross sections $d\sigma_{nlm\sigma\sigma_3}^{n'l'm'\sigma'\sigma'_3}$ depend on the azimuthal angle ϕ . In the case of initially unpolarized atoms the cross sections of physical meaning have to be independent of the choice of the quantization axis and ϕ independent. One finds these cross sections from $d\sigma_{nlm\sigma\sigma_3}^{n'l'm'\sigma'\sigma'_3}$ by averaging them over m and σ_3 and by summation over m' and σ'_3 . Namely,

$$d\sigma_{nl\sigma}^{n'l'\sigma'} = \frac{1}{(2l+1)(2\sigma+1)} \sum_{\sigma_3, \sigma'_3} \sum_{m, m'} d\sigma_{nlm\sigma\sigma_3}^{n'l'm'\sigma'\sigma'_3}.$$

It is explicitly demonstrated in Ref. 3 that the cross sections $d\sigma_{nl\sigma}^{n'l'\sigma'}$ are indeed ϕ independent.

The cross section of the elementary spin-0-0 atom excitation is

$$d\sigma_{nlm}^{n'l'm'} = \frac{Z^2 e^4}{(2\pi)^2 v^2} |\Delta(q)|^2 \left| \left[1 + \frac{\mathbf{q} \cdot \mathbf{v}}{2M} \right] \left[F_{nlm}^{n'l'm'}(\eta\mathbf{q}) - F_{nlm}^{n'l'm'}(\xi\mathbf{q}) \right] - \frac{\mathbf{v}}{2M} \cdot \left[\xi^{-1} \mathbf{G}_{nlm}^{n'l'm'}(\eta\mathbf{q}) - \eta^{-1} \mathbf{G}_{nlm}^{n'l'm'}(\xi\mathbf{q}) \right] \right|^2 Q dQ d\phi. \quad (33)$$

Keeping in mind condition (19) one finds the minimal momentum transfer

$$Q_{\min} = \frac{\epsilon_{n'} - \epsilon_n}{v}, \quad (34)$$

where ϵ_n and $\epsilon_{n'}$ are the atomic binding energies of initial and final states. The maximal value of the momentum transfer which follows from energy-momentum conservation is of no importance here because, as explained in Sec. I, the processes of high momentum transfer give negligible contribution to the integrated (over momentum transfer) cross sections. On the other hand, these processes cannot be studied on the basis of the formalism presented in this paper.

The angle α between \mathbf{q} and \mathbf{k}_i vectors is determined due to energy-momentum conservation and this angle can be expressed through $|\mathbf{k}_i|$, $|\mathbf{k}_f|$, and the scattering angle Θ . Let us remember that

$$q^2 = \mathbf{k}_f^2 + \mathbf{k}_i^2 - 2|\mathbf{k}_i||\mathbf{k}_f| \cos\Theta.$$

If $\mathbf{k}_i^2 \approx \mathbf{k}_f^2$ that is the case because of condition (19)

$$Q \approx 2|\mathbf{k}_i| \sin\frac{1}{2}\Theta.$$

Then one easily finds that

$$\cos\alpha \approx \sin\frac{1}{2}\Theta \approx \frac{Q}{2|\mathbf{k}_i|}.$$

In practical calculations one can assume that \mathbf{q} is perpendicular to \mathbf{v} because the characteristic momentum transfer is much less than the initial momentum for the relativistic elementary atoms studied here.

The photon propagator $\Delta(q)$ depends on the four-momentum squared

$$q^2 = q_0^2 - \mathbf{q}^2,$$

where

$$q_0 = \mathbf{q}^2/2M - \epsilon_n + \epsilon_{n'}.$$

Keeping in mind that the characteristic momentum transfer is of order of the inverse Bohr radius of the atom one finds that

$$q_0^2/q^2 \sim e^4 \ll 1.$$

Therefore $q^2 \approx -\mathbf{q}^2$ and, as in the nonrelativistic case, the interaction can be treated as instantaneous.

For the atom of equal-mass components the cross section (33) reads

$$d\sigma_{nlm}^{n'l'm'} = [1 - (-1)^{l'-l}] \frac{Z^2 e^4}{2\pi^2 v^2} |\Delta(q)|^2 \times \left| \left[1 + \frac{\mathbf{q} \cdot \mathbf{v}}{2M} \right] F_{nlm}^{n'l'm'}(\frac{1}{2}\mathbf{q}) - \frac{\mathbf{v}}{M} \cdot \mathbf{G}_{nlm}^{n'l'm'}(\frac{1}{2}\mathbf{q}) \right|^2 Q dQ d\phi.$$

Formula (33) holds for the spin-0- $\frac{1}{2}$ and spin- $\frac{1}{2}$ - $\frac{1}{2}$ atoms when the interaction process does not lead to the change of the atomic spin or spin projection.

The cross section of the spin-flip transition of the spin-0- $\frac{1}{2}$ atom is

$$d\sigma_{nlms}^{n'l'm'-s} = \frac{Z^2 e^4}{8\pi} |\Delta(q)|^2 \times \frac{Q^3 \sin^2 \alpha}{m_2^2} |F_{nlm}^{n'l'm'}(\xi \mathbf{q})|^2 dQ, \quad (35)$$

where the trivial integration over azimuthal angle ϕ has been performed.

The cross section of the spin- $\frac{1}{2}$ - $\frac{1}{2}$ atomic interaction with change of the atomic spin and/or atomic spin projection reads

$$d\sigma_{nlm\sigma\sigma_3}^{n'l'm'\sigma'\sigma'_3} = \frac{Z^2 e^4}{16\pi} |\Delta(q)|^2 \frac{Q^3 \sin^2 \alpha}{M^2} |\xi^{-1} F_{nlm}^{n'l'm'}(\eta \mathbf{q}) + (-1)^{\sigma'-\sigma} \eta^{-1} F_{nlm}^{n'l'm'}(\xi \mathbf{q})|^2 dQ, \quad (36)$$

$$d\sigma_{nlm\sigma\sigma_3}^{n'l'm'\sigma'\sigma'_3} = 0 \text{ for (1) } \sigma \neq \sigma' \text{ and } \sigma_3 = \sigma'_3, \text{ (2) } |\sigma'_3 - \sigma_3| > 1.$$

The integration over ϕ has been performed. For the atom of the particle and antiparticle, e.g., positronium, the cross section (36) changes to the form

$$d\sigma_{nlm\sigma\sigma_3}^{n'l'm'\sigma'\sigma'_3} = \frac{Z^2 e^4}{32\pi} [1 - (-1)^{l'+\sigma'-l-\sigma}] |\Delta(q)|^2 \frac{Q^3 \sin^2 \alpha}{M^2} |F_{nlm}^{n'l'm'}(\frac{1}{2}\mathbf{q})|^2 dQ, \quad (37)$$

$$d\sigma_{nlm\sigma\sigma_3}^{n'l'm'\sigma'\sigma'_3} = 0 \text{ for (1) } \sigma \neq \sigma' \text{ and } \sigma_3 = \sigma'_3, \text{ (2) } |\sigma'_3 - \sigma_3| > 1, \text{ (3) } l' + \sigma' - l - \sigma = 0, 2, 4, \dots$$

The cross sections of elementary-atom ionization are quite analogous to those of (33)–(37); however the right-hand side of Eqs. (33)–(37) should be multiplied by the phase-space element $d^3\mathbf{p}/(2\pi)^3$, the form factors $F_{nlm}^{n'l'm'}$, $\mathbf{G}_{nlm}^{n'l'm'}$ should be replaced by F_{nlm}^p , \mathbf{G}_{nlm}^p , and the kinematics should be, respectively, modified. Let us remember that \mathbf{p} denotes the atomic component momentum in the atomic center-of-mass frame.

If the values of Q_{\min} and Q_{\max} are shifted to zero and infinity, respectively, the initial energy dependence of the cross sections is the same ($1/v^2$) for all final states. Then we can use the sum rules discussed in the previous section to calculate the cross sections summarized over the complete set of “nonrelativistic” atomic final states. The word nonrelativistic means that we consider the set of states which is complete in the Hilbert space spanned by the solutions of the nonrelativistic Schrödinger equation. In other words, we consider the final states where the spin quantum numbers are fixed, and the radiation and particle creation processes are not taken into account. The cross sections (33), (35), and (36) summarized over the final states are

$$d\sigma_{nlm} = \frac{Z^2 e^4}{(2\pi)^2 v^2} |\Delta(q)|^2 \left[1 + \frac{\mathbf{q} \cdot \mathbf{v}}{2M} \right]^2 \times \Sigma_{nlm}(\mathbf{x}, \mathbf{q}) Q dQ d\phi, \quad (38)$$

$$d\sigma_{nlms}^{-s} = \frac{Z^2 e^4}{8\pi v^2} |\Delta(q)|^2 \frac{Q^3 \sin^2 \alpha}{m_2^2} dQ, \quad (39)$$

$$d\sigma_{nlm\sigma\sigma_3}^{\sigma'\sigma'_3} = \frac{Z^2 e^4}{16\pi v^2} |\Delta(q)|^2 \Omega_{nlm}^{\pm}(\mathbf{q}) \frac{Q^3 \sin^2 \alpha}{M^2} dQ, \quad (40)$$

where Σ_{nlm} and Ω_{nlm}^{\pm} are determined by Eqs. (28), (29), and

$$\mathbf{x} = \frac{\mathbf{v}}{2M + \mathbf{q} \cdot \mathbf{v}}.$$

As stressed several times the cross sections given in this paper are correct for the processes with $\mathbf{q}^2 \ll m_{1,2}^2$. Therefore, $\sin^2 \alpha$ can be replaced by unity in Eqs. (38) and (39). Then, the cross sections [(38) and (39)] integrated over momentum transfer are, in contrast with all other integrated cross sections, divergent at high momentum transfer. It is not surprising since the spin-flip processes are usually effective at high momentum transfer; however, it shows the limitations of our approach. Anyway formulas (38) and (39) integrated over the momentum-transfer interval where the formulas are correct provide the reasonable estimation of the respective cross sections due to the logarithmic character of the divergence.

VII. SUMMARY AND CONCLUSIONS

The problem of the interaction of relativistic elementary atoms with atoms of matter has been studied in the reference frame where the initial and final atomic motion is nonrelativistic. The most proper would be the Breit system, i.e., the system where the atomic momentum is reversed in the course of the interaction ($\mathbf{p}_i = -\mathbf{p}_f$). The value of the atomic momentum is minimal in this frame and the nonrelativistic description of the atom is better justified here than in any other frame. Because of the smallness of the characteristic momentum transfer to the atom we have used the reference frame where the atom is initially at rest. In this frame the interaction process description is simpler than in the Breit system.

An atom of matter has been treated as a structureless spinless relativistic particle of the electric charge Ze . The effect of electron screening of the nucleus field has been taken into account by modification of the photon propagator. Since the atom of matter is treated as structureless it is implicitly assumed that the initial and final states of the atom of matter coincide. Therefore we take into account the coherent interactions only. For the atoms of matter with $Z \gg 1$ the incoherent interactions,

i.e., the processes of the atom of matter excitations, are much less effective because the coherent interaction cross sections are roughly proportional to Z^2 while the incoherent ones are proportional to Z . The incoherent interactions have been discussed in the context of elementary atoms in Ref. 10.

Because the elementary-atom components are spin-0 or spin- $\frac{1}{2}$ particles we have considered three kinds of atoms: the spin-0-0 atoms, the spin-0- $\frac{1}{2}$ atoms, and the spin- $\frac{1}{2}$ - $\frac{1}{2}$ atoms. For these three kinds of elementary atoms we have derived the transition amplitudes in the Born approximation. The atomic excitation and ionization processes have been considered. Particular attention has been paid to the spin structure of the amplitude of spin- $\frac{1}{2}$ - $\frac{1}{2}$ atom interactions. It has been shown that

the atom composed of a particle and antiparticle can interact if the charge parity of the atom changes in the course of the interaction.

We have derived the sum rules which allow the calculation of the cross sections summed over elementary-atom final states. Finally we have given formulas of elementary-atom interaction cross sections. In the following paper³ we present the results of numerical calculations of the cross sections of some elementary atoms interacting with typical targets.

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