arXiv:hep-ph/0109208 22 Sep 2001

Contribution of α^2-terms to the total interaction cross sections of relativistic elementary atoms with atoms of matter

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(Dated: January 29, 2002)

It is shown that the corrections of α^2 order for the total interaction cross sections of elementary hydrogen-like atoms with target atoms, found in the previous paper [S.Mrówczyński, Phys.Rev. **D36**, 1520], does not include some terms of the same order of magnitude. This results to significant contribution of these corrections in particular cases. It is shown that the full α^2-correction is really small and could be omitted for most practical applications.

PACS numbers: 11.80.Fv, 34.50.-s, 36.10.-k

The experiment DIRAC [1], which now under way at PS CERN, aims to measure the lifetime of hydrogen-like elementary atoms (EA) consisting of π^+ and π^- mesons ($A_{2\pi}$) with accuracy of 10%. The interaction of $\pi^+\pi^-$-atoms with matter is of great importance for the experiment as $A_{2\pi}$ dissociation (ionization) in such interactions is exploited to observe $A_{2\pi}$ and to measure its lifetime. In the experiment the ratio between the number of $\pi^+\pi^-$-pairs from $A_{2\pi}$ dissociation inside a target and the number of produced atoms will be measured. The lifetime measurement is based on the comparison of this experimental value with its calculated dependence on the lifetime. Accuracy of the interaction cross sections of relativistic EA with ordinary atoms, which are behind all these calculations [2], is essential for the extraction of the lifetime.

Study of interactions of fast hydrogen-like atoms with atoms has a long history starting from Bethe. One of the resent calculations for hydrogen and one-electron ions was published in [3]. Interactions of various relativistic EA consisting of $e^\pm$, $\pi^\pm$, $\mu^\pm$, $K^\pm$ were considered in different approaches [4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16]. In this paper we reconsider corrections of α^2 order to the EA total interaction cross sections obtained in [7]. (Through this paper α is the fine-structure constant.)

As shown in [7] analysis of the relativistic EA interaction with the Coulomb field of target atoms can be performed conveniently in the rest frame of the projectile EA (anti-lab frame). As the characteristic transfer momentum is of order of the EA Bohr momentum, in this frame after the interaction EA has a non-relativistic velocity and thus initial and final states of EA can be treated in terms of the non-relativistic quantum mechanics. In this manner the well-known difficulties of the relativistic treatment of bound states can be get round.

As in the EA rest frame a target atom moves with the relativistic velocity its electromagnetic field is no longer pure Coulomb. It is described by the 4-vector potential $A_\mu = (A_0, \boldsymbol{A})$ with components related to its rest Coulomb potential $U(r)$:

$$A_0 = \gamma U \qquad \boldsymbol{A} = \gamma \boldsymbol{\beta} U \ . \tag{1}$$

Here $\boldsymbol{\beta} = \boldsymbol{v}/c$, $\boldsymbol{v}$ is the target atom velocity in the EA rest frame and γ is its Lorentz-factor. The time-like component A_0 of the 4-potential interacts with the charges of particles forming EA and the space component with their currents.

In this paper we consider only EA consisting of spinless particles (π, K-mesons etc.) which are of interest for the DIRAC experiment. In the Born approximation the amplitudes of transition from the initial state i to the final f due to the interaction with A_μ can be written as:

$$A_{fi} = U(Q) a_{fi}(\boldsymbol{q}) \ , \tag{2}$$

$$U(Q) = 2\int_0^\infty U(r) \frac{\sin Qr}{Q} r dr \ , \tag{3}$$

$$a_{fi}(\boldsymbol{q}) = \rho_{fi}(\boldsymbol{q}) - \boldsymbol{\beta} \boldsymbol{j}_{fi}(\boldsymbol{q}) \ . \tag{4}$$

The transition densities $\rho_{fi}(\boldsymbol{q})$ and transition currents $\boldsymbol{j}_{fi}(\boldsymbol{q})$ are expressed via the the EA wave functions ψ_i and ψ_f for the the initial and final states:

$$\rho_{fi}(\boldsymbol{q}) = \int \rho_{fi}(\boldsymbol{r}) \left(e^{i\boldsymbol{q}_1\boldsymbol{r}} - e^{-i\boldsymbol{q}_2\boldsymbol{r}}\right) d^3r \ , \tag{5}$$

$$\boldsymbol{j}_{fi}(\boldsymbol{q}) = \int \boldsymbol{j}_{fi}(\boldsymbol{r}) \left(\frac{\mu}{m_1} e^{i\boldsymbol{q}_1\boldsymbol{r}} + \frac{\mu}{m_2} e^{-i\boldsymbol{q}_2\boldsymbol{r}}\right) d^3r \ , \tag{6}$$

$$\rho_{fi}(\boldsymbol{r}) = \psi_f^*(\boldsymbol{r}) \psi_i(\boldsymbol{r}) \tag{7}$$

$$\boldsymbol{j}_{fi}(\boldsymbol{r}) = \frac{i}{2\mu} \left[\psi_i(\boldsymbol{r}) \boldsymbol{\nabla} \psi_f^*(\boldsymbol{r}) - \psi_f^*(\boldsymbol{r}) \boldsymbol{\nabla} \psi_i(\boldsymbol{r})\right] \ . \tag{8}$$

The EA wave functions $\psi_{i,f}$ and the binding energies $\varepsilon_{i,f}$ obey the Schrödinger equation

$$H\psi_{i,f} = \varepsilon_{i,f} \psi_{i,f} \tag{9}$$

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$$H = -\frac{\Delta}{2\mu} + V(r)$$

with the Hamiltonian H. It is worth noting that the explicit form of the potential $V(r)$ of the interaction between the EA components have no influence on the final result of this paper.

In the above equations $m_{1,2}$ are masses of EA components, $q = (q_0, \boldsymbol{q})$ is the transfer 4-momentum, and all other kinematic variables are related by the following equations:

$$\begin{gathered}
\boldsymbol{q}_1 = \frac{\mu}{m_1}\boldsymbol{q}\,, \quad \boldsymbol{q}_2 = \frac{\mu}{m_2}\boldsymbol{q}\,, \quad \mu = \frac{m_1 m_2}{M}\,, \quad M = m_1 + m_2\,, \\
q = (q_0, \boldsymbol{q})\,, \qquad \boldsymbol{q} = (q_L, \boldsymbol{q}_T)\,, \\
q_0 = \omega_{fi} + \frac{Q^2}{2M} = \boldsymbol{\beta q} = \beta q_L\,, \quad \omega_{fi} = \varepsilon_f - \varepsilon_i\,, \qquad (10) \\
Q = \sqrt{Q^2}\,, \qquad Q^2 = \boldsymbol{q}^2 - q_0^2 = \boldsymbol{q}_T^2 + q_L^2(1-\beta^2)\,.
\end{gathered}$$

The differential and integral cross sections of the EA transition from the initial state i to the final f due to interaction with the electromagnetic field of the target atom are related to the amplitudes (2):

$$\begin{aligned}
\frac{d\sigma_{fi}}{d\boldsymbol{q}_T} &= \frac{1}{\beta^2}|A_{fi}(q)|^2 \\
\sigma_{fi} &= \frac{1}{\beta^2}\int |A_{fi}(q)|^2 d^2\boldsymbol{q}_T\,. \qquad (11)
\end{aligned}$$

Formulae (2–11) allow to calculate the transition (partial) cross sections in the Born approximation. But for applications (for example see [2]) the total cross sections of the EA interaction with target atoms are required also. Because the Born amplitudes of the EA elastic scattering are pure real values the optical theorem can not be used to calculate the total cross sections. Thus they should be calculated as the sum of all partial cross sections:

$$\sigma_i^{\text{tot}} = \sum_f \sigma_{fi}\,. \qquad (12)$$

Usually to get a closed expression for the sum of this infinite series (the so-called "sum rule") the transition amplitudes (2) are rewrite as:

$$A_{fi}(q) = \langle f|\widehat{A}(q)|i\rangle\,, \qquad (13)$$

where the operator $\widehat{A}(q)$ does not contain an explicit dependence on the EA final state variables (for example its energy ε_f , see bellow). Then using of the completeness relation

$$\sum_f |f\rangle\langle f| = 1\,, \qquad (14)$$

the sum (12) can be written in the form:

$$\sigma_i^{\text{tot}} = \frac{1}{\beta^2}\int \langle i|\widehat{A}^*(q)\widehat{A}(q)|i\rangle d^2\boldsymbol{q}_T\,. \qquad (15)$$

However one should to take some caution while going from the exact expressions (2–10) for the transition amplitudes, with explicitly dependence on the ε_f (through the time-like q_0 and longitudinal q_L components of 4-vector q), to the approximate one without such dependence. Otherwise, it is possible to obtain a physically improper result as it has happened to the authors of the the paper [7] at deriving of the sum rules for the total cross section of interaction of ultrarelativistic EA ($\beta = 1$) with target atoms. Below we discuss this problem in detail.

The most essential simplification, that arises in the case of $\beta = 1$ is that $Q^2 = \boldsymbol{q}_T^2$. Thus $U(Q) = U(\boldsymbol{q}_T)$ [see (10)] and only A_{fi} in (2) depends on ε_f through the exponential factors $\exp(i\boldsymbol{q_1 r})$ and $\exp(-i\boldsymbol{q_2 r})$ in (5) and (6)

$$\boldsymbol{q}_{1,2}\boldsymbol{r} = \frac{\mu}{m_{1,2}}\boldsymbol{qr} = \frac{\mu}{m_{1,2}}(q_L z + \boldsymbol{q}_T\boldsymbol{r}_T)\,, \qquad (16)$$

where $q_L = \omega_{fi} + \boldsymbol{q}_T^2/2M$ if $\beta = 1$.

Now let us take into account that the typical value of z in these expressions is of order of the Bohr radius $r_B = 1/\mu\alpha$ and the typical $q_L \sim \omega_{fi} \sim \mu\alpha^2$, thus the product $q_L z$ is of order of α. Then it seems natural to neglect the q_L-dependence of a_{fi}:

$$a_{fi}(\boldsymbol{q}) \approx a_{fi}(\boldsymbol{q}_T)\,. \qquad (17)$$

and consider this case as the zero order approximation to the problem [7]. It corresponds to the choice of the operator $\widehat{A}$ in the form:

$$\begin{aligned}
\widehat{A}(q) = U(\boldsymbol{q}_T)\,\big[&e^{i\boldsymbol{q}_{1T}\boldsymbol{r}_T} - e^{-i\boldsymbol{q}_{2T}\boldsymbol{r}_T} - \\
&(e^{i\boldsymbol{q}_{1T}\boldsymbol{r}_T}/m_1 + e^{-i\boldsymbol{q}_{2T}\boldsymbol{r}_T}/m_2)\boldsymbol{\beta}\widehat{\boldsymbol{p}}\big]\,. \qquad (18)
\end{aligned}$$

Here $\widehat{\boldsymbol{p}} = -i\boldsymbol{\nabla}$ is the momentum operator.

Substituting (18) in (15) results in the following sum rules [7], where the total cross sections is expressed as the sum of the "electric" σ^{el} and "magnetic" σ^{mag} cross sections:

$$\begin{aligned}
\sigma^{\text{tot}} &= \sigma^{\text{el}} + \sigma^{\text{mag}}\,, \qquad (19) \\
\sigma^{\text{el}} &= \int U^2(\boldsymbol{q}_T)M(\boldsymbol{q}_T)d^2\boldsymbol{q}_T\,, \qquad (20) \\
M(\boldsymbol{q}_T) &= 2(1 - S(\boldsymbol{q}_T)) \\
S(\boldsymbol{q}_T) &= \int |\psi(\boldsymbol{r})|^2 e^{i\boldsymbol{q}_T\boldsymbol{r}} d^3r\,; \\
\sigma^{\text{mag}} &= \int U^2(\boldsymbol{q}_T)K(\boldsymbol{q}_T)d^2\boldsymbol{q}_T\,, \qquad (21)
\end{aligned}$$

$$K(\boldsymbol{q}_T) = \int\left[\frac{1}{\mu^2} + \frac{2}{m_1 m_2}(e^{i\boldsymbol{qr}} - 1)\right]|\boldsymbol{\beta}\ \boldsymbol{\nabla}\ \psi_i(\boldsymbol{r})|^2\, d^3r\,.$$

These results differ from the sum rules used in [2] by the additional term σ^{mag}. For beginning let us consider its contribution qualitatively. For this purpose the target atom potential $U(r)$ can be approximated by the screened Coulomb potential:

$$U(r) = \frac{Z\alpha}{r} e^{-\lambda r}, \quad \lambda \sim m_e \alpha Z^{1/3}, \tag{22}$$

where m_e is the electron mass and Z is the atomic number of the target. The pure Coulomb wave function can be used for ψ_i (i.e. the contribution of the strong interaction between the EA components is neglected see [17]). For the ground state it is written as:

$$\psi_i(r) = \frac{\mu \alpha^{3/2}}{\sqrt{\pi}} e^{-\mu\alpha r} \ . \tag{23}$$

Under such assumptions for the ground state the following results can be easy obtained:

$$\sigma^{\rm el} = \frac{8\pi Z^2}{\mu^2} \left[\ln\left(\frac{2\mu}{Z^{1/3} m_e} \right) - \frac{3}{4} \right] \ , \tag{24}$$

$$\begin{aligned} \sigma^{\rm mag} &= \frac{4\pi}{3} \left(\frac{Z\alpha}{\lambda} \right)^2 + O(\alpha^2 \sigma^{\rm el}) \\ &= \frac{4\pi Z^{4/3} \alpha^2}{3 m_e^2} + O(\alpha^2 \sigma^{\rm el}) \ . \end{aligned} \tag{25}$$

It is seen that in spite of α^2 in the numerator of $\sigma^{\rm mag}$ the electron mass square in the denominator makes the contribution of the "magnetic" term in (19) not negligible with respect to the "electric" one, especially for the case of EA consisted of heavy hadrons and low Z values.

To obtain exact numerical values we have precisely repeated the calculations made in [7]. More accurate presentation of the target atom potential, namely, the Moliére parameterization of the Thomas-Fermi potential [18] was used as in [7]:

$$U(r) = Z\alpha \sum_{i=1}^{3} \frac{c_i e^{-\lambda_i r}}{r} \ ; \tag{26}$$

$$c_1 = 0.35, \quad c_2 = 0.55, \quad c_3 = 0.1 \ ;$$

$$\lambda_1 = 0.3\lambda_0, \ \lambda_2 = 1.2\lambda_0, \ \lambda_3 = 6\lambda_0, \ \lambda_0 = m_e \alpha Z^{1/3}/0.885.$$

The values of "electric" (el) and "magnetic" (mag) total cross sections (in units of cm^2) and their ratio (mag/el) are presented in Table I for various EA and target materials. The values published in [7] are given in the parentheses. It is seen that the "electric" cross sections are coincide within the given accuracy, but the "magnetic" ones are underestimated in [7]. It is worth noting that the correct values of $\sigma^{\rm mag}$ does not depend on EA masses as it follows from the simplified approximation result (25). The ratio values confirm the above estimation about the "magnetic" term contribution. Thus inaccuracy in the calculations did not allow the authors of [7] to observe so significant contribution of $\sigma^{\rm mag}$ in their results.

It is clear, that such strong enhancement of the magnetic term in (19) is the consequence of its inverse power dependence (25) on the small screening parameter λ. It is also easily to see that the origin of such unnatural dependence is in the behaviour of the factor $K(\boldsymbol{q}_T)$ at small values of $\boldsymbol{q}_T$ in (21). This factor, contrary to $M(\boldsymbol{q}_T)$ in (20), does not approach to zero at $\boldsymbol{q}_T \to 0$. But at $\beta = 1$ such behaviour of $K(\boldsymbol{q}_T)$ is in contradiction with some general properties of the transition amplitudes (4), which follow from the continuity equation:

TABLE I: The "electric" (el) and "magnetic" (mag) total cross sections in units of cm^2 and their ratio (mag/el) in % for EA consisting of π and K mesons ($A_{2\pi}$, $A_{\pi K}$, A_{2K}) and target materials with the atomic number Z. The values published in [7] are given in the parentheses.

Z		$A_{2\pi}$	$A_{\pi K}$	A_{2K}
6	el	$3.03 \cdot 10^{-22}$	$1.37 \cdot 10^{-22}$	$3.08 \cdot 10^{-23}$
		$(3.1 \cdot 10^{-22})$	$(1.4 \cdot 10^{-22})$	$(3.0 \cdot 10^{-23})$
6	mag	$6.73 \cdot 10^{-24}$	$6.73 \cdot 10^{-24}$	$6.73 \cdot 10^{-24}$
		$(2.5 \cdot 10^{-24})$	$(1.3 \cdot 10^{-24})$	$(0.3 \cdot 10^{-24})$
6	mag/el	2.22%	4.90%	21.9%
13	el	$1.33 \cdot 10^{-21}$	$6.08 \cdot 10^{-22}$	$1.37 \cdot 10^{-22}$
		$(1.3 \cdot 10^{-21})$	$(6.2 \cdot 10^{-22})$	$(1.4 \cdot 10^{-22})$
13	mag	$1.89 \cdot 10^{-23}$	$1.89 \cdot 10^{-23}$	$1.89 \cdot 10^{-23}$
		$(0.96 \cdot 10^{-23})$	$(0.55 \cdot 10^{-23})$	$(0.15 \cdot 10^{-23})$
13	mag/el	1.41%	3.10%	13.7%
29	el	$6.17 \cdot 10^{-21}$	$2.84 \cdot 10^{-21}$	$6.48 \cdot 10^{-22}$
		$(6.1 \cdot 10^{-21})$	$(2.9 \cdot 10^{-21})$	$(6.7 \cdot 10^{-22})$
29	mag	$5.50 \cdot 10^{-23}$	$5.50 \cdot 10^{-23}$	$5.50 \cdot 10^{-23}$
		$(3.6 \cdot 10^{-23})$	$(2.3 \cdot 10^{-23})$	$(0.68 \cdot 10^{-23})$
29	mag/el	0.891%	1.94%	8.49%
47	el	$1.55 \cdot 10^{-20}$	$7.15 \cdot 10^{-21}$	$1.64 \cdot 10^{-21}$
		$(1.5 \cdot 10^{-20})$	$(7.3 \cdot 10^{-21})$	$(1.7 \cdot 10^{-21})$
47	mag	$1.05 \cdot 10^{-22}$	$1.05 \cdot 10^{-22}$	$1.05 \cdot 10^{-22}$
		$(0.79 \cdot 10^{-22})$	$(0.52 \cdot 10^{-22})$	$(0.17 \cdot 10^{-22})$
47	mag/el	0.676%	1.46%	6.37%
82	el	$4.46 \cdot 10^{-20}$	$2.07 \cdot 10^{-20}$	$4.81 \cdot 10^{-21}$
		$(4.4 \cdot 10^{-20})$	$(2.1 \cdot 10^{-20})$	$(5.1 \cdot 10^{-21})$
82	mag	$2.20 \cdot 10^{-22}$	$2.20 \cdot 10^{-22}$	$2.20 \cdot 10^{-22}$
		$(1.9 \cdot 10^{-22})$	$(1.3 \cdot 10^{-22})$	$(0.48 \cdot 10^{-22})$
82	mag/el	0.493%	1.06%	4.58%

$$\omega_{fi} \rho_{fi}(\boldsymbol{q}) - \boldsymbol{q} \boldsymbol{j}_{fi}(\boldsymbol{q}) = 0 \ . \tag{27}$$

(The later can be derived from the Schrödinger equation (9)). Indeed, rewriting the continuity equation in the form:

$$\begin{aligned} &\omega_{fi} \rho_{fi}(\boldsymbol{q}) - q_L \boldsymbol{\beta} \boldsymbol{j}_{fi}(\boldsymbol{q}) - \boldsymbol{q}_T \boldsymbol{j}_{fi}(\boldsymbol{q}) = \\ &\omega_{fi} [\rho_{fi} - \boldsymbol{\beta} \boldsymbol{j}_{fi}(\boldsymbol{q})] - \boldsymbol{q}_T^2 \boldsymbol{\beta} \boldsymbol{j}_{fi}(\boldsymbol{q})/2M - \boldsymbol{q}_T \boldsymbol{j}_{fi}(\boldsymbol{q}) = 0 \ , \end{aligned} \tag{28}$$

it is easily obtain, that

$$\begin{aligned} a_{fi}(\boldsymbol{q}) &= \rho_{fi}(\boldsymbol{q}) - \boldsymbol{\beta} \boldsymbol{j}_{fi}(\boldsymbol{q}) \\ &= \frac{1}{\omega_{fi}} \left[\boldsymbol{q}_T^2 \boldsymbol{\beta} \boldsymbol{j}_{fi}(\boldsymbol{q})/2M + \boldsymbol{q}_T \boldsymbol{j}_{fi}(\boldsymbol{q}) \right] \ . \end{aligned} \tag{29}$$

That is all transition amplitudes become zero at $q_T = 0$. It follows, that any transition cross section (11) can depend on the screening parameter λ at least only logarithmically, but never like inverse power of this parameter. The same is valid for the sum (12) of this quantities, i.e the total cross section.

Since the λ-dependence of the magnetic term in (25) is contradictory to the general result, we must conclude that there is a fallacy in the deriving of sum rules (19) somewhere. To understand the origin of the error, made by authors of [7], let us go back to the quantities (5),(6) and expand them over powers of the longitudinal momentum transfer q_L:

$$\rho_{fi} = \sum_{n=0}^{\infty} \rho_{fi}^{(n)} \, , \quad \rho_{fi}^{(n)} = \frac{q_L^n}{n!}\left(\frac{d^n}{dq_L^n}\rho_{fi}\right)\Bigg|_{q_L=0} \, , \tag{30}$$

$$\boldsymbol{j}_{fi} = \sum_{n=0}^{\infty} \boldsymbol{j}_{fi}^{(n)} \, , \quad \boldsymbol{j}_{fi}^{(n)} = \frac{q_L^n}{n!}\left(\frac{d^n}{dq_L^n}\boldsymbol{j}_{fi}\right)\Bigg|_{q_L=0} . \tag{31}$$

It is easily shown that terms of these expansions obey the following estimation:

$$\rho_{fi}^{(n)} \propto \alpha^n \, , \quad j_{fi}^{(n)} \propto \alpha^{n+1} \, . \tag{32}$$

The additional power of α in the current expansion coefficients, in comparison with the density one, reflects the ordinary relation between the values of current and density in the hydrogen-like atoms.

Expanding the value (4) and taking into account (32) it seems reasonable to group terms with the same order of α rather than q_L as it was done in [7]. Then the successive terms of the a_{fi} expansion over α powers are

$$\begin{aligned} a_{fi} &= \sum_n a_{fi}^{(n)} \\ a_{fi}^{(n)} &= \rho_{fi}^{(n)} - \boldsymbol{\beta}\boldsymbol{j}_{fi}^{(n-1)} \, . \end{aligned} \tag{33}$$

From above it is clear that in the "natural" approximation (17) includes $a_{fi}^{(0)}$ and the only one part of the term $a_{fi}^{(1)}$ of the expansion (33), namely:

$$\boldsymbol{\beta}\boldsymbol{j}_{fi}^{(0)} = -\frac{i}{\mu}\int \psi_f^* E(\boldsymbol{q}_T, \boldsymbol{r}_T)\frac{\partial \psi_i}{\partial z} d^3r \, . \tag{34}$$

While the second one

$$\rho_{fi}^{(1)} = iq_L \int \psi_f E(\boldsymbol{q}_T, \boldsymbol{r}_T) z \psi_i d^3r \tag{35}$$

was omitted according to the reasoning of the approximation (17). In the late equations (34), (35) $E(\boldsymbol{q}_T, \boldsymbol{r}_T)$ denotes:

$$E(\boldsymbol{q}_T, \boldsymbol{r}_T) = \frac{\mu}{m_1} e^{i\boldsymbol{q}_{1T}\boldsymbol{r}_T} + \frac{\mu}{m_2} e^{-i\boldsymbol{q}_{2T}\boldsymbol{r}_T} \, . \tag{36}$$

Let us consider this neglected part in detail. As it is proportional to $q_L = \omega_{fi} + \boldsymbol{q}_T^2/2M$ and therefore explicitly depends on ε_f, one can not use completeness relation (14) to calculate its contribution to the total cross section directly. Before we need to transform it to the form free of such dependence. It can be done with help of the Schrödinger equation (9).

$$\begin{aligned} &\varepsilon_{fi} \int \psi_f^*(\boldsymbol{r}) E(\boldsymbol{q}_T, \boldsymbol{r}_T) z \psi_i(\boldsymbol{r}) d^3r = \\ &\int \psi_f^*(\boldsymbol{r}) \left\{ \varepsilon_f E(\boldsymbol{q}_T, \boldsymbol{r}_T) z - \varepsilon_i E(\boldsymbol{q}_T, \boldsymbol{r}_T) z \right\} \psi_i(\boldsymbol{r}) d^3r = \\ &\qquad \int \psi_f^*(\boldsymbol{r}) [H, E(\boldsymbol{q}_T, \boldsymbol{r}_T) z] \psi_i(\boldsymbol{r}) d^3r \end{aligned} \tag{37}$$

The commutator in this relation is easily calculated and after simple algebra we get the following result:

$$\rho_{fi}^{(1)}(\boldsymbol{q}) = -\frac{i}{\mu}\int \psi_f^*(\boldsymbol{r}) E(\boldsymbol{q}_T, \boldsymbol{r}_T) \frac{\partial \psi_i(\boldsymbol{r})}{\partial z} d^3r + \Delta\rho_{fi}^{(1)}(\boldsymbol{q}) \tag{38}$$

$$\begin{aligned} &\Delta\rho_{fi}^{(1)}(\boldsymbol{q}) = \\ &i \int \psi_f^*(r) \left[\frac{\mu}{m_1} e^{i\boldsymbol{q}_{1T}\boldsymbol{r}_T} \widehat{O}_1 + \frac{\mu}{m_2} e^{-i\boldsymbol{q}_{2T}\boldsymbol{r}_T} \widehat{O}_2 \right] z \psi_i(r) d^3r \end{aligned} \tag{39}$$

$$\widehat{O}_{1,2} = \frac{\boldsymbol{q}_T^2 \pm 2\boldsymbol{q}_T \widehat{\boldsymbol{p}}}{2m_{1,2}} \, , \quad \widehat{\boldsymbol{p}} = -i\boldsymbol{\nabla} \, . \tag{40}$$

It is seen, that "large" (nonvanishing at $\boldsymbol{q}_T = 0$) parts of two terms (34) and (38), contributing to $a_{fi}^{(1)}$, are equal and opposite in sign, so that in the resulting expression they cancel each other, leaving only the term with the "correct" behaviour at small $\boldsymbol{q}_T$:

$$a_{fi}^{(1)} = \Delta\rho_{fi}^{(1)}(\boldsymbol{q}) \tag{41}$$

The same is valid for any $a_{fi}^{(n)}$. Applying the Schrödinger equation (9) to exclude one power of q_L from the expression:

$$\begin{aligned} \rho_{fi}^{(n)}(\boldsymbol{q}) = \frac{(iq_L)^n}{n!} \int \psi_f^*(r) \Bigg[\left(\frac{\mu}{m_1}\right)^n e^{i\boldsymbol{q}_{1T}\boldsymbol{r}_T} + \\ + (-1)^{n+1} \left(\frac{\mu}{m_2}\right)^n e^{-i\boldsymbol{q}_{2T}\boldsymbol{r}_T} \Bigg] z^n \psi_i(r) d^3r \, , \end{aligned} \tag{42}$$

one can represent it in the form:

$$\rho_{fi}^{(n)}(\boldsymbol{q}) = \boldsymbol{\beta}\boldsymbol{j}_{fi}^{(n-1)}(\boldsymbol{q}) + \Delta\rho_{fi}^{(n)}(\boldsymbol{q}) \tag{43}$$

$$\begin{aligned} \Delta\rho_{fi}^{(n)}(\boldsymbol{q}) = &\frac{i(iq_L)^{n-1}}{n!} \int \psi_f^*(r) \Bigg[\left(\frac{\mu}{m_1}\right)^n e^{i\boldsymbol{q}_{1T}\boldsymbol{r}_T} \widehat{O}_1 + \\ &+ \left(\frac{\mu}{m_2}\right)^n e^{-i\boldsymbol{q}_{2T}\boldsymbol{r}_T} \widehat{O}_2 \Bigg] z^n \psi_i(r) d^3r \, . \end{aligned} \tag{44}$$

So that

$$a_{fi}^{(n)} = \Delta\rho_{fi}^{(n)}(\boldsymbol{q}) \, . \tag{45}$$

That confirms the qualitative result (29), derived with help of continuity equation (27).

The remaining ε_f-dependence of right side of (44) can be removed by repeated applying of the Schrödinger equation (9), that allows to represent the transition amplitudes in the form (13).

From z-dependence of the integrand in (44) it is easily to derive, that $a_{fi}^{(2k)} = 0$ for the odd values of Δlm_{fi}, and $a_{fi}^{(2k+1)} = 0$ for even Δlm_{fi} , where $\Delta lm_{fi} = (l_f - l_i) - (m_f - m_i)$, and l_i, l_f, m_i, m_f are the values of the orbital and magnetic quantum numbers of the initial i and final f states (the quantization axis is supposed to be z-axis). Thus "odd" and "even" terms of the expansion (33) do not interfere and therefore in the expansion of the $\sigma^{\rm tot}$ over the powers of α

$$\sigma^{\rm tot} = \sum_{n=0}^{\infty} \sigma^{(n)} \, , \quad \sigma^{(n)} \propto \alpha^n \tag{46}$$

only even powers are present.

The structure of the zero order term of this expansion is well established [see (20)]. In view of the above discussion one may be sure that the higher order terms are numerically negligible and may not be discussed in detail. Nevertheless, for completeness of the consideration we present the expression for contribution of α^2-term to the total cross section which includes $\left|a_{fi}^{(1)}\right|^2$ term and the interference term $a_{fi}^{(0)}\, a_{fi}^{(2)}$.

$$\sigma^{(2)} = -\int U^2(\boldsymbol{q}_T) W(\boldsymbol{q}_T) d^2\boldsymbol{q}_T + O(\alpha^4) \, , \tag{47}$$

$$W(\boldsymbol{q}_T) = \frac{1}{4m_1m_2}\int z^2 \left[q^4 |\psi_i(\boldsymbol{r})|^2 - \right. \\ \left. - \left|2\boldsymbol{q}_T\widehat{\boldsymbol{p}}\psi_i(\boldsymbol{r})\right|^2 \right] e^{i\boldsymbol{qr}} d^3r \, .$$

The "correct" q_T-dependence of the last integrand excludes a possibility of arising some extra λ-dependence, that could dramatically enhance the contribution of this term (like it happened to $\sigma^{\rm mag}$ term in [7]). This can be illustrated by the explicit expression for the case of the screened Coulomb potential (22) and the EA ground state (23):

$$\sigma^{(2)} = -\frac{8\pi(Z\alpha)^2}{5M\mu}\left[\ln\left(\frac{2\mu}{Z^{1/3}m_e}\right) - \frac{4}{5}\right] \, . \tag{48}$$

Because numerical smallness of the value α^2 this term can be successfully neglected compared to (24) in the practical applications.

This result warrants the usage of the simple expression:

$$\sigma^{\rm tot} = 2\int U^2(q_T)\,[1 - S(q_T)]\, d^2q_T \tag{49}$$

for the total cross section calculation in Born approximation in [2] and for the Glauber extensions in [15].

The authors express their gratitude to professors S.Mrówczyński, L.Nemenov and D.Trautmann for helpful discussions.

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