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

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I. INTRODUCTION

The experiment DIRAC [1], now under way at PS CERN's, aims to measure the lifetime of hydrogen-like elementary atoms (EA) consisting of $\pi^+$ and $\pi^-$ mesons ($A_{2\pi}$) with an accuracy of 10%. The interaction of $\pi^+\pi^-$ atoms with target atoms matter is of great importance for the extraction of $A_{2\pi}$ and to measure its lifetime. In the experiment the ratio between 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. The accuracy of the cross sections for interaction 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 with ordinary atoms were considered in different approaches [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16]. In this paper we reconsider corrections of $\alpha^2$ order to the EA total interaction cross sections obtained in [2, 3].

II. GENERAL FORMULAS

As shown in [2, 3] 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 the order of the EA Bohr momentum, in this frame the interaction EA has a non-relativistic velocity and thus the initial and final states of EA can be treated in terms of 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 $A_\mu = (A_0, \mathbf{A})$ with components related to its rest Coulomb potential $U(r)$:

$$A_0 = \gamma U \quad \mathbf{A} = \gamma \beta \mathbf{U}. \quad (1)$$

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

In this paper we consider only EA consisting of spinless particles ($\pi$, $K$-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 one $f$ due to the interaction with $A_\mu$ can be written as:

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

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

$$a_{fi}(q) = \rho_{fi}(q) - \beta j_{fi}(q). \quad (4)$$

The transition densities $\rho_{fi}(q)$ and transition currents $j_{fi}(q)$ are expressed via the the EA wave functions $\psi_i$ and $\psi_f$ for the initial and final states:

$$\rho_{fi}(q) = \int \rho_{fi}(r) (e^{iq\cdot r} - e^{-iq\cdot r}) d^3 r, \quad (5)$$

$$j_{fi}(q) = \int j_{fi}(r) \left( \frac{\mu_1}{m_1} e^{iq\cdot r} + \frac{\mu_2}{m_2} e^{-iq\cdot r} \right) d^3 r, \quad (6)$$

[\text{References and equations continue...}]
\[ \rho_{fi}(r) = \psi_r^*(r)\psi_i(r) \quad (7) \]
\[ j_{fi}(r) = \frac{i}{2\mu} [\psi_i(r)\nabla \psi_r^*(r) - \psi_r^*(r)\nabla \psi_i(r)] . \quad (8) \]

The EA wave functions \( \psi_{i,f} \) and the binding energies \( \varepsilon_{i,f} \) obey the Schrödinger equation
\[ H\psi_{i,f} = \varepsilon_{i,f}\psi_{i,f} \]
\[ H = -\frac{\Delta}{2\mu} + V(r) \] 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, \( q = (q_0, q) \) is the transfer 4-momentum. All other kinematic variables are related by the following equations:
\[ q_1 = \frac{\mu}{m_1} q, \quad q_2 = \frac{\mu}{m_2} q, \quad \mu = \frac{m_1 m_2}{M}, \quad M = m_1 + m_2, \]
\[ q = (q_0, q_L), \quad q = (q_L, q_T), \]
\[ q_0 = \omega_{fi} + \frac{Q^2}{2M} = \beta q_L, \quad \omega_{fi} = \varepsilon_f - \varepsilon_i, \]
\[ Q = \sqrt{Q^2}, \quad Q^2 = q^2 - q_0^2 = q_T^2 + q_L^2(1-\beta^2). \]

The differential and integral cross sections of the EA transition from the initial state \( i \) to the final state \( f \) due to the interaction with the electromagnetic field of the target atom are related to amplitudes \( A_i(q) \):
\[ \frac{d\sigma_{fi}}{d^2q_T} = \frac{1}{\beta^2} |A_{fi}(q)|^2 \]
\[ \sigma_{fi} = \frac{1}{\beta^2} \int |A_{fi}(q)|^2 d^2q_T . \quad (11) \]

Formulas \( \frac{d\sigma_{fi}}{d^2q_T} \) allow to calculate the transition (partial) cross sections in the Born approximation. But for applications (for example see \( \alpha_{fi}^{tot} \)) the total cross sections of the EA interaction with target atoms are also required. Because the Born amplitudes of the EA elastic scattering are pure real values, the optical theorem cannot be used to calculate the total cross sections. Thus they should be calculated as the sum of all partial cross sections:
\[ \sigma_{i}^{tot} = \sum_{fi} \sigma_{fi} . \quad (12) \]

To get a closed expression for the sum of this infinite series (the so-called “sum rule”) the transition amplitudes \( A_{fi}(q) \) are usually rewritten as:
\[ A_{fi}(q) = (f|\hat{A}(q)|i) , \quad (13) \]
where the operator \( \hat{A}(q) \) does not contain explicit dependence on the EA final state variables (for example, its energy \( \varepsilon_f \), see below). Then, using the completeness relation
\[ \sum_f |f\rangle\langle f| = 1 , \quad (14) \]
we can write sum \( \sigma_{i}^{tot} \) in the form:
\[ \sigma_{i}^{tot} = \frac{1}{\beta^2} \int (i|\hat{A}^*(q)\hat{A}(q)|i) d^2q_T . \quad (15) \]

III. SIMPLIFIED APPROACH

One should take some caution when passing from the exact expressions \( \frac{d\sigma_{fi}}{d^2q_T} \) for the transition amplitudes, with explicit dependence on the \( \varepsilon_f \) (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 paper \( \alpha_{fi}^{tot} \) in deriving 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 \( Q^2 = q_T^2 \). Thus \( U(Q) = U(q_T) \) [see \( \alpha_{fi}^{tot} \)] and only \( A_{fi}(q) \) in \( \alpha_{fi}^{tot} \) depends on \( \varepsilon_f \) through the exponential factors \( \exp(iq_T r) \) and \( \exp(-iq_T r) \) in \( \alpha_{fi}^{tot} \) and
\[ q_{1,2}r = \frac{\mu}{m_{1,2}} q r = \frac{\mu}{m_{1,2}} (q_L z + q_T r_T) , \quad (16) \]
where \( q_L = \omega_{fi} + q_T^2/2M \) if \( \beta = 1 \).

Now let us take into account the fact that the typical value of \( z \) in these expressions is of the 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 the order of \( \alpha \). Then it seems natural to neglect the \( q_L \)-dependence of \( a_{fi} \):
\[ a_{fi}(q) \approx a_{fi}(q_T) . \quad (17) \]
and consider this case as the zero order approximation to the problem \( \alpha_{fi}^{tot} \). It corresponds to the choice of the operator \( \hat{A} \) in the form:
\[ \hat{A}(q) = U(q_T) \left[ e^{iq_T z r_T} - e^{-iq_T z r_T} - (e^{iq_T z r_T}/m_1 + e^{-iq_T z r_T}/m_2) \hat{p} \right] . \quad (18) \]

Here \( \hat{p} = -i\nabla \) is the momentum operator.

Substituting \( |q_T\rangle \) in \( \alpha_{fi}^{tot} \) results in the following sum rules \( \alpha_{fi}^{tot} \), where the total cross section is expressed as the sum of the “electric” \( \sigma^{el} \) and “magnetic” \( \sigma^{mag} \) cross sections:
\[ \sigma^{tot} = \sigma^{el} + \sigma^{mag} , \quad (19) \]
\[ \sigma^{el} = \int U^2(q_T) M(q_T)d^2q_T , \quad (20) \]
\[ M(q_T) = 2(1 - S(q_T)) \]
\[ S(q_T) = \int |\psi(r)|^2 e^{iq_T r r} d^3r ; \]
$\sigma^{\text{mag}} = \int U^2(q_T)K(q_T)d^2q_T,$ \hfill (21) \\
$K(q_T) = \int \left[ \frac{1}{\mu^2} + \frac{2}{m_1m_2}(e^{iqr} - 1) \right] |\beta \nabla \psi_i(r)|^2 d^3r.$

These results reproduce the ones obtained in \cite{1} and differ from the sum rules used in \cite{2} by the additional term $\sigma^{\text{mag}}$. 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:

$$U(r) = Z\alpha e^{-\lambda r}, \quad \lambda \sim m_e\alpha Z^{1/3},$$ \hfill (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 $\psi_i$ (i.e. the contribution of the strong interaction between the EA components is neglected, see \cite{17}). For the ground state it is written as:

$$\psi_i(r) = \frac{\mu e^{\lambda r}}{\sqrt{\pi}} e^{-\mu r}.$$ \hfill (23)

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

$$\sigma^{\text{el}} = \frac{8\pi Z^2}{\mu^2} \left[ \ln \left( \frac{2\mu}{Z^{1/3}m_e} \right) - \frac{3}{4} \right],$$ \hfill (24) \\
$$\sigma^{\text{mag}} = \frac{4\pi}{3} \left( \frac{Z\alpha}{\lambda} \right)^2 + O(\alpha^2\sigma^{\text{el}}) =$$

$$= \frac{4\pi Z^4/3}{3m_e^2} + O(\alpha^2\sigma^{\text{el}}).$$ \hfill (25)

It is seen that in spite of $\alpha^2$ in the numerator of $\sigma^{\text{mag}}$ the electron mass square in the denominator makes the contribution of the “magnetic” term in \cite{13} not negligible with respect to the “electric” one, especially for the case of EA consisting of heavy hadrons and low Z values.

To obtain exact numerical values we have precisely repeated the calculations made in \cite{1}. More accurate presentation of the target atom potential, namely, the Molière parametrization of the Thomas-Fermi potential \cite{13} was used as in \cite{1}:

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

$c_1 = 0.35$, \quad $c_2 = 0.55$, \quad $c_3 = 0.1$; \\
$\lambda_1 = 0.3\lambda_0$, \quad $\lambda_2 = 1.2\lambda_0$, \quad $\lambda_3 = 6\lambda_0$, \quad $\lambda_0 = m_e\alpha Z^{1/3}/0.885$.

The values of the “electric” (el) and “magnetic” (mag) total cross sections (in units of cm$^2$) and their ratio (mag/el) are presented in Table \ref{tab1} for various EA and target materials. The values published in \cite{1} are given in parentheses. It is seen that the “electric” cross sections coincide within the given accuracy, but the “magnetic” ones are underestimated in \cite{1}. It is worth noting that the correct values of $\sigma^{\text{mag}}$ do not depend on EA masses as it follows from the simplified approximation result (23). The ratio values confirm the above estimation about the “magnetic” term contribution. Thus, inaccuracy in the calculations did not allow the authors of \cite{1} to observe such a significant contribution of $\sigma^{\text{mag}}$ in their results.

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|}
\hline
\multicolumn{1}{|c|}{Z} & \multicolumn{1}{|c|}{$A_{2e}$} & \multicolumn{1}{|c|}{$A_{2K}$} & \multicolumn{1}{|c|}{$A_{4K}$} \\
\hline
6 & $3.03 \cdot 10^{-22}$ & $1.37 \cdot 10^{-22}$ & $3.08 \cdot 10^{-23}$ \\
& $(3.1 \cdot 10^{-22})$ & $(1.4 \cdot 10^{-22})$ & $(3.0 \cdot 10^{-23})$ \\
6 & $6.73 \cdot 10^{-24}$ & $6.73 \cdot 10^{-24}$ & $6.73 \cdot 10^{-24}$ \\
& $(2.5 \cdot 10^{-24})$ & $(1.3 \cdot 10^{-24})$ & $(0.3 \cdot 10^{-24})$ \\
6 & $2.22\%$ & $4.90\%$ & $21.9\%$ \\
13 & $1.33 \cdot 10^{-21}$ & $6.08 \cdot 10^{-22}$ & $1.37 \cdot 10^{-22}$ \\
& $(1.3 \cdot 10^{-21})$ & $(6.2 \cdot 10^{-22})$ & $(1.4 \cdot 10^{-22})$ \\
13 & $1.89 \cdot 10^{-23}$ & $1.89 \cdot 10^{-23}$ & $1.89 \cdot 10^{-23}$ \\
& $(0.96 \cdot 10^{-23})$ & $(0.55 \cdot 10^{-23})$ & $(0.15 \cdot 10^{-23})$ \\
13 & $1.41\%$ & $3.10\%$ & $13.7\%$ \\
29 & $6.17 \cdot 10^{-21}$ & $2.84 \cdot 10^{-21}$ & $6.48 \cdot 10^{-22}$ \\
& $(6.1 \cdot 10^{-21})$ & $(2.9 \cdot 10^{-21})$ & $(6.7 \cdot 10^{-22})$ \\
29 & $5.50 \cdot 10^{-23}$ & $5.50 \cdot 10^{-23}$ & $5.50 \cdot 10^{-23}$ \\
& $(3.6 \cdot 10^{-23})$ & $(2.3 \cdot 10^{-23})$ & $(0.68 \cdot 10^{-23})$ \\
29 & $0.891\%$ & $1.94\%$ & $8.49\%$ \\
47 & $1.55 \cdot 10^{-20}$ & $7.15 \cdot 10^{-21}$ & $1.64 \cdot 10^{-21}$ \\
& $(1.5 \cdot 10^{-20})$ & $(7.3 \cdot 10^{-21})$ & $(1.7 \cdot 10^{-21})$ \\
47 & $1.05 \cdot 10^{-22}$ & $1.05 \cdot 10^{-22}$ & $1.05 \cdot 10^{-22}$ \\
& $(0.79 \cdot 10^{-22})$ & $(0.52 \cdot 10^{-22})$ & $(0.17 \cdot 10^{-22})$ \\
47 & $0.676\%$ & $1.46\%$ & $6.37\%$ \\
82 & $4.46 \cdot 10^{-20}$ & $2.07 \cdot 10^{-20}$ & $4.81 \cdot 10^{-21}$ \\
& $(4.4 \cdot 10^{-20})$ & $(2.1 \cdot 10^{-20})$ & $(5.1 \cdot 10^{-21})$ \\
82 & $2.20 \cdot 10^{-22}$ & $2.20 \cdot 10^{-22}$ & $2.20 \cdot 10^{-22}$ \\
& $(1.9 \cdot 10^{-22})$ & $(1.3 \cdot 10^{-22})$ & $(0.48 \cdot 10^{-22})$ \\
82 & $0.493\%$ & $1.06\%$ & $4.58\%$ \\
\hline
\end{tabular}
\caption{The “electric” (el) and “magnetic” (mag) total cross sections in units of cm$^2$ and their ratio (mag/el) in % for EA consisting of $\pi$ and $K$ mesons ($A_{2e}$, $A_{2K}$, $A_{4K}$) and target materials with the atomic number $Z$. The values published in \cite{1} are given in parentheses.}
\end{table}

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

$$\omega f_i \rho f_i(q) - q_j f_i(q) = 0.$$ \hfill (27)

(The latter can be derived from the Schrödinger equation \cite{2}). Indeed, rewriting the continuity equation in the
form:
\[
\omega_{fi}\rho_{fi}(q) - q_{L}\beta j_{fi}(q) - q_{T}\dot{j}_{fi}(q) = \\
\omega_{fi}|\rho_{fi} - \beta j_{fi}(q)| - q_{T}^{2}\beta j_{fi}(q)/2M - q_{T}\dot{j}_{fi}(q) = 0,
\]
(28)

it is easy obtain
\[
a_{fi}(q) = \rho_{fi}(q) - \beta j_{fi}(q) = \frac{1}{\omega_{fi}}[q_{T}^{2}\beta j_{fi}(q)/2M + q_{T}\dot{j}_{fi}(q)].
\]
(29)

Thus all transition amplitudes become zero at \(q_{T} = 0\). Therefore, any transition cross section (11) can depend on the screening parameter \(\lambda\) 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.

IV. ACCURATE FORMULAS

Since the \(\lambda\)-dependence of the magnetic term in (24) 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 the authors of [7], let us go back to quantities (5),(6) and expand them in powers of the longitudinal momentum transfer \(q_{L}\):
\[
\rho_{fi} = \sum_{n=0}^{\infty} \rho_{fi}^{(n)} = \rho_{fi}^{(0)}(q_{L}) = \frac{q_{L}^{n}}{n!} \left(\frac{d^{n}}{dq_{L}^{n}} \rho_{fi}\right)_{q_{L} = 0},
\]
(30)
\[
j_{fi} = \sum_{n=0}^{\infty} j_{fi}^{(n)} = j_{fi}^{(0)}(q_{L}) = \frac{q_{L}^{n}}{n!} \left(\frac{d^{n}}{dq_{L}^{n}} j_{fi}\right)_{q_{L} = 0}.
\]
(31)

It is easily shown that terms of these expansions obey the following estimation:
\[
\rho_{fi}^{(n)} \propto a^{n}, \quad j_{fi}^{(n)} \propto a^{n+1}.
\]
(32)

The additional power of \(a\) 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 (11) and taking into account (22) it seems reasonable to group terms with the same order of \(a\) rather than \(q_{L}\) as was done in (12). Then the successive terms of the \(a_{fi}\) expansion in powers of \(a\) are
\[
a_{fi} = \sum_{n=0}^{\infty} a_{fi}^{(n)}
\]
\[
a_{fi}^{(n)} = \rho_{fi}^{(n)} - \beta j_{fi}^{(n-1)}.
\]
(33)

From above it is clear that in the “natural” approximation (17) includes \(a_{fi}^{(0)}\) and only one part of the term \(a_{fi}^{(1)}\) of expansion (22), namely:
\[
\beta j_{fi}^{(0)} = -\frac{i}{\mu} \int \psi_{f}^{*}(q_{T}, r_{T}) \frac{\partial \psi_{i}}{\partial z} d^{3}r,
\]
(34)

while the second one
\[
\rho_{fi}^{(1)} = i q_{L} \int \psi_{f} E(q_{T}, r_{T}) \psi_{i} d^{3}r
\]
(35)

was omitted according to the reasoning of approximation (17). In equations (22), (23) \(E(q_{T}, r_{T})\) denotes:
\[
E(q_{T}, r_{T}) = \frac{\mu}{m_{1}} e^{iq_{T} r_{T}} + \frac{\mu}{m_{2}} e^{-iq_{T} r_{T}}.
\]
(36)

Let us consider this neglected part in detail. As it is proportional to \(q_{L} = \omega_{fi} + q_{T}^{2}/2M\) and therefore explicitly depends on \(\varepsilon_{f}\), one cannot use completeness relation (14) to calculate its contribution to the total cross section directly. First we need to transform it to the form free of such dependence. It can be done with the help of Schrödinger equation (1).
\[
\varepsilon_{f} \int \psi_{f}^{*}(r) E(q_{T}, r_{T}) \psi_{i}(r) d^{3}r = \\
\int \psi_{f}^{*}(r) \left\{ \varepsilon_{f} E(q_{T}, r_{T}) z - \varepsilon_{i} E(q_{T}, r_{T}) z \right\} \psi_{i}(r) d^{3}r = \\
\int \psi_{f}^{*}(r) [H, E(q_{T}, r_{T}) z] \psi_{i}(r) d^{3}r
\]
(37)

The commutator in this relation is easily calculated and after simple algebra we get the following result:
\[
\rho_{fi}^{(1)}(q) = -\frac{i}{\mu} \int \psi_{f}^{*}(r) E(q_{T}, r_{T}) \frac{\partial \psi_{i}}{\partial z} d^{3}r + \Delta \rho_{fi}^{(1)}(q)
\]
(38)
\[
\Delta \rho_{fi}^{(1)}(q) = \\
i \int \psi_{f}^{*}(r) \left[ \frac{\mu}{m_{1}} e^{iq_{T} r_{T}} \hat{O}_{1} + \frac{\mu}{m_{2}} e^{-iq_{T} r_{T}} \hat{O}_{2} \right] \psi_{i}(r) d^{3}r
\]
(39)
\[
\hat{O}_{1,2} = \frac{q_{T}^{2} \pm 2 q_{T} \hat{p}}{2m_{1,2}}, \quad \hat{p} = -i \nabla.
\]
(40)

It is seen that “large” (nonvanishing at \(q_{T} = 0\)) parts of two terms (24) and (25), 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 \(q_{T}\):
\[
a_{fi}^{(1)} = \Delta \rho_{fi}^{(1)}(q)
\]
(41)

The same is valid for any \(a_{fi}^{(n)}\). Applying Schrödinger equation (1) to reduce by one the power of \(q_{L}\) in the expression:
\[
\rho_{fi}^{(n)}(q) = \frac{(iq_{L})^{n}}{n!} \int \psi_{f}^{*}(r) \left[ \left( \frac{\mu}{m_{1}} \right)^{n} e^{iq_{T} r_{T}} + \\
+ (-1)^{n+1} \left( \frac{\mu}{m_{2}} \right)^{n} e^{-iq_{T} r_{T}} \right] z^{n} \psi_{i}(r) d^{3}r,
\]
(42)

one can represent it in the form:
\[
\rho_{fi}^{(n)}(q) = \beta j_{fi}^{(n-1)}(q) + \Delta \rho_{fi}^{(n)}(q)
\]
(43)
\[ \Delta \rho_{f_i}^{(n)}(q) = \frac{i^n}{n!} \int \psi^*_i(r) \left[ \left( \frac{\mu}{m_1} \right)^n e^{iq \cdot r} \hat{O}_1 + \left( \frac{\mu}{m_2} \right)^n e^{-iq \cdot r} \hat{O}_2 \right] z^n \psi_i(r) d^3r. \] 

(44)

Finally one has

\[ a_{f_i}^{(n)} = \Delta \rho_{f_i}^{(n)}(q). \] 

(45)

That confirms the qualitative result \[29\], derived with help of continuity equation \[27\].

The remaining \( \varepsilon_f \)-dependence of right-hand side of \[14\] can be removed by repeatedly applying the Schrödinger equation \[9\], which allows the transition amplitudes to be represented in the form \[12\].

\[ \Delta (lm)_{f_i} = 0 \] for odd \( \Delta (lm)_{f_i} \), and \( a_{f_i}^{(2k+1)} = 0 \) for even \( \Delta (lm)_{f_i} \), where \( \Delta (lm)_{f_i} = (l_f - l_i) - (m_f - m_i) \), and \( l_i, l_f, m_i, m_f \) are 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 expansion \[13\] do not interfere and therefore in the expansion of the \( \sigma^{tot} \) in the powers of \( \alpha \)

\[ \sigma^{tot} = \sum_{n=0}^{\infty} \sigma^{(n)}, \quad \sigma^{(n)} \propto \alpha^n \] 

(46)

only even powers are present.

The structure of the zero order term of this expansion is well established [see \[21\]]. In view of the above discussion one can be assured that the higher order terms are numerically negligible and should not be discussed in detail. Nevertheless, for completeness of the consideration we present the expression for the contribution of the \( \alpha^2 \)-term to the total cross section which includes the term \( a_{f_i}^{(1,2)} \) and the interference term \( a_{f_i}^{(0,2)} \).

\[ \sigma^{(2)} = - \int U^2(q_T) W(q_T) d^2q_T + O(\alpha^4), \] 

(47)

\[ W(q_T) = \frac{1}{4m_1 m_2} \int z^2 |\psi_i(r)|^2 \left| 2q_T \vec{p} \psi_i(r) \right|^2 e^{iqr} d^3r. \]

The “correct” \( q_T \)-dependence of the last integral excludes a possibility of some extra \( \alpha \)-dependence arising, which could dramatically enhance the contribution of this term (as happened to the \( \sigma^{mag} \) term in \[1\]). This can be illustrated by the explicit expression for the case of the screened Coulomb potential \[22\] and the EA ground state \[23\]:

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

(48)

Because of numerical smallness of \( \alpha^2 \) this term can be successfully neglected compared to \[24\].

Thus in most practical applications, in which the required relative accuracy is less than \( 10^{-4} \), only the zero order term, that considers the pure Coulomb interaction and only the transverse transfer momentum, should be taken into account for calculation of the relativistic atom-atom cross sections. This result warrants the usage of the simple expression:

\[ \sigma^{tot} = 2 \int U^2(q_T) \left[ 1 - S(q_T) \right] d^2q_T \] 

(49)

for the total cross section calculation for the Born approximation in \[2\] and for the Glauber extensions in \[3\].

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