Theory of forbidden transitions in light atoms

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Abstract

Forbidden transitions such as intercombination ones, appear due to relativistic effects. In light atoms these effects are usually incorporated through the use of Breit-Pauli Hamiltonian. We show that for some transitions such as $E2$ or $M1$ this treatment is incomplete. There exist additional corrections to the transition amplitude which can be equally significant. We analyze also the role of the anomalous magnetic moment of the electron in some forbidden transitions.

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I. INTRODUCTION

The aim of this work is a readable derivation of relativistic corrections to transition amplitudes in light atoms. In the case of the forbidden transition, such as $M1$: $2^3S_1 \to 1^1S_0$ in the helium, relativistic effects allow this transition to take place [1]. It is commonly accepted in atomic physics that in the so called length gauge, the Breit-Pauli Hamiltonian accounts for leading relativistic effects to the transition amplitude and existing numerical codes and published results [2–5] rely on this assumption, which we claim is not always correct. We note, that fully relativistic approach such as RMBPT [6] gives the correct answer provided negative energy states are included [7]. As it was derived by Feinberg and Sucher in [1] with the help of the Bethe-Salpeter equation, the $2^3S_1 \to 1^1S_0$ amplitude is given by transition matrix elements of something, what can be regarded as a correction to the current $\vec{p}/m$. In our former work apart from rederivation of the Feinberg-Sucher result, we have derived the analogous amplitude for $M1$: $3^3S_1 \to 2^3S_1$ transition and have shown that there is no additional correction to the $E1$ amplitude as written in the length gauge. In this work we generalize former results to the arbitrary light atom. Apart from $E1$, $M1$ and $M2$, we include $E2$ transitions and present the derivation of transition amplitudes including the effect of the anomalous magnetic moment. We show for example, that for the $E2$ amplitude relativistic corrections to the current in the length gauge do not vanish.

II. NONRELATIVISTIC TRANSITION AMPLITUDE

The nonrelativistic few-electron atom interacting with the electromagnetic field is described by the Schrödinger-Pauli Hamiltonian:

$$H = \sum_a \left\{ \frac{(\vec{p}_a - e\,\vec{A}_a)^2}{2\,m} - \frac{Z\,\alpha}{r_a} - \frac{e}{2\,m}\,\vec{\sigma}_a \cdot \vec{B}_a \right\} + \sum_{a>b} \frac{\alpha}{r_{ab}}\,. \tag{1}$$

We use the so called theoretical units, where $\hbar = c = 1$ and α is the fine structure constant $\alpha^{-1} = 137.035\,999\,76(50)$. Moreover, we will use a, b subscripts to count electrons and i, j, k superscripts will denote Cartesian indices. The single photon transition amplitude $\mathcal{T}$ between two eigenstates ϕ and ψ, in the electric dipole approximation is

$$\mathcal{T}^i_{E1} = \langle\phi|\sum_a \frac{p^i_a}{m}|\psi\rangle = i\,\omega\,\langle\phi|\sum_a r^i_a|\psi\rangle\,, \tag{2}$$

where $\omega = E_\phi - E_\psi$, the electric quadrupole transition has the form

$$\mathcal{T}^i_{E2} = \langle\phi|\sum_a \frac{p^i_a}{m}\, i\,\vec{k}\cdot\vec{r}_a|\psi\rangle_{E2} = -\frac{\omega}{2}\,k^j\,\langle\phi|\sum_a\Big(r^i_a\,r^j_a - \frac{\delta^{ij}}{3}\,r^2_a\Big)|\psi\rangle\,, \tag{3}$$

and the magnetic dipole is:

$$\mathcal{T}^i_{M1} = \frac{i}{2\,m}\,\epsilon^{ijl}\,k^l\,\langle\phi|\sum_a\Big(L^j_a + \sigma^j_a\Big)|\psi\rangle\,. \tag{4}$$

The corresponding transition probability $\mathcal{A}$ is

$$\mathcal{A} = 2\,\alpha\,|\omega|\int\frac{d\Omega_k}{4\,\pi}\,\mathcal{T}^i\,\mathcal{T}^{*j}\left(\delta^{ij} - \frac{k^i\,k^j}{k^2}\right). \tag{5}$$

Any transition for which above amplitudes vanish we will call forbidden, for example transitions with the change of total value of the spin, so called intercombination one. These transitions are possible due to various relativistic effects which are derived in the following sections.

III. FOULDY-WOUTHUYSEN TRANSFORMATION AND THE BREIT-PAULI HAMILTONIAN

The purpose of this section is to derive the Breit-Pauli Hamiltonian with the external electromagnetic field. It will serve us for the derivation of transition amplitudes. What is not in the standard approach we include the anomalous magnetic moment. The initial Dirac Hamiltonian for the spin 1/2 particle interacting with the external electromagnetic field including the anomalous magnetic moment κ is [8]:

$$H = \vec{\alpha}\cdot\vec{\pi} + \beta\,m + \frac{e\,\kappa}{2\,m}\,(i\,\beta\,\vec{\alpha}\cdot\vec{E} - \beta\,\vec{\Sigma}\cdot\vec{B})\,, \tag{6}$$

where $\vec{\pi} = \vec{p} - e\,\vec{A}$. The Fouldy-Wouthuysen transformation S [8] leads to a new Hamiltonian

$$H_{FW} = e^{i\,S}\,(H - i\,\partial_t)\,e^{-i\,S}\,, \tag{7}$$

which does not couple upper and lower components of the Dirac wave function up to specified order in the $1/m$ expansion, namely $1/m^3$. The F.W. operator S is a sum of two terms $S = S_0 + \delta S$, where the second one includes an additional transformation required by the presence of the anomalous magnetic moment. These terms are:

$$\begin{aligned} S_0 &= -\frac{i}{2\,m}\left\{\beta\,\vec{\alpha}\cdot\vec{\pi} - \frac{1}{3\,m^2}\,\beta\,(\vec{\alpha}\cdot\vec{\pi})^3 + \frac{1}{2\,m}\,[\vec{\alpha}\cdot\vec{\pi}\,;\,e\,A^0 - i\,\partial_t]\right\}, \\ \delta S &= -\frac{i}{2\,m}\left\{\frac{e\,\kappa}{2\,m}\,i\,\vec{\alpha}\cdot\vec{E} - \frac{e\,\kappa}{4\,m^2}\,[\vec{\alpha}\cdot\vec{\pi}\,;\,\beta\,\vec{\Sigma}\cdot\vec{B}]\right\}. \end{aligned} \tag{8}$$

The F.W. Hamiltonian is expanded in the power series in S

$$\begin{aligned} H_{FW} &= H + [i\,S\,;\,H - i\,\partial_t] + \frac{1}{2!}\,[i\,S\,;\,[i\,S\,;\,H - i\,\partial_t]] \\ &+\frac{1}{3!}\,[i\,S\,;\,[i\,S\,;\,[i\,S\,;\,H - i\,\partial_t]]] + \frac{1}{4!}\,[i\,S\,;\,[i\,S\,;\,[i\,S\,;\,[i\,S\,;\,H - i\,\partial_t]]]] + \ldots \end{aligned} \tag{9}$$

and higher order terms in this expansion, denoted by dots, will not play a role. As a result of these multiple commutations one obtains a nonrelativistic expansion of the Hamiltonian H, namely

$$\begin{aligned} H_{FW} &= \frac{\vec{\pi}^2}{2\,m} + e\,A^0 - \frac{e}{2\,m}\,(1+\kappa)\,\vec{\sigma}\cdot\vec{B} - \frac{\vec{\pi}^4}{8\,m^3} \\ &-\frac{e}{8\,m^2}\,(1+2\,\kappa)\left[\nabla\cdot\vec{E} + \vec{\sigma}\cdot(\vec{E}\times\vec{\pi} - \vec{\pi}\times\vec{E})\right] \\ &+\frac{e}{8\,m^3}\left\{\vec{\sigma}\cdot\vec{B}\,\vec{\pi}^2 + \vec{\pi}^2\,\vec{\sigma}\cdot\vec{B} + \kappa\,[\vec{\pi}\cdot\vec{B}\,\vec{\pi}\cdot\vec{\sigma} + \vec{\pi}\cdot\vec{\sigma}\,\vec{\pi}\cdot\vec{B}]\right\}. \end{aligned} \tag{10}$$

This Hamiltonian sets the ground for further calculations. If one has few electrons interacting through quantum electromagnetic field (Coulomb gauge is used throughout this paper), from the first two lines of Eq. (10) one can derive relativistic corrections to the Hamiltonian of an atom, namely the Breit-Pauli Hamiltonian [9]. It is obtained with the assumption that electric and magnetic fields interacting with the one electron come from the nucleus and the other electrons,

$$H_{BP} = \sum_a H_a + \sum_{a>b} H_{ab}\,. \tag{11}$$

The hydrogenic part H_a is obtained by setting in Eq. (10) $\vec{A} = \vec{B} = 0$, $e\,A^0 = -Z\,\alpha/r_a$, and $e\,\vec{E}_a = -Z\,\alpha\,\vec{r}_a/r_a^3$

$$H_a = \frac{p_a^2}{2\,m} - \frac{Z\,\alpha}{r_a} - \frac{p_a^4}{8\,m^3} + \frac{\pi\,Z\,\alpha}{2\,m^2}\,(1+2\,\kappa)\,\delta^3(r_a) + \frac{(1+2\,\kappa)}{4\,m^2}\,\frac{Z\,\alpha}{r_a^3}\,\vec{\sigma}_a\cdot\vec{r}_a\times\vec{p}_a\,. \tag{12}$$

The electron-electron part is obtained by considering the single photon exchange amplitude (Coulomb + transverse) between two electrons with the vertex as obtained from H_{FW},

$$\begin{aligned} H_{ab} &= \frac{\alpha}{r_{ab}} - \frac{\pi\,\alpha}{m^2}\,(1+2\,\kappa)\,\delta^3(r_{ab}) - \frac{\alpha}{2\,m^2}\,p_a^i\left(\frac{\delta^{ij}}{r_{ab}} + \frac{r_{ab}^i\,r_{ab}^j}{r_{ab}^3}\right)p_b^j \\ &-\frac{2\,\pi\,\alpha}{3\,m^2}\,(1+\kappa)^2\,\vec{\sigma}_a\cdot\vec{\sigma}_b\,\delta^3(r_{ab}) + \frac{\alpha}{4\,m^2}\,(1+\kappa)^2\,\frac{\sigma_a^i\,\sigma_b^j}{r_{ab}^3}\left(\delta^{ij} - 3\,\frac{r_{ab}^i\,r_{ab}^j}{r_{ab}^2}\right) \\ &+\frac{\alpha}{4\,m^2\,r_{ab}^3}\Big[2\,(1+\kappa)\,(\vec{\sigma}_a\cdot\vec{r}_{ab}\times\vec{p}_b - \vec{\sigma}_b\cdot\vec{r}_{ab}\times\vec{p}_a) \\ &\qquad +(1+2\,\kappa)\,(\vec{\sigma}_b\cdot\vec{r}_{ab}\times\vec{p}_b - \vec{\sigma}_a\cdot\vec{r}_{ab}\times\vec{p}_a)\Big]\,. \end{aligned} \tag{13}$$

This Breit-Pauli Hamiltonian gives the leading $O(\alpha^2)$ correction to energy levels in light atoms, such as beryllium. Namely, if we assume that $p \sim m\,\alpha$ and $r \sim 1/(m\,\alpha)$, then H_{BP} contains all $m\,\alpha^4$ terms. H_{BP} can not be applied to heavy systems, with the large Z- charge of the nucleus, because its derivation relies on assumption that Z is small. Moreover, we will treat the Breit-Pauli Hamiltonian in the first order of the perturbation calculus. More precisely, if H_0 is the nonrelativistic Hamiltonian, then

$$H_{BP} = H_0 + \delta H\,, \tag{14}$$

energies and wave functions are calculated up to the first order in δH. We note however, that it will not describe well systems with the relatively large LS configuration mixing.

Let us now construct a general Hamiltonian for few electron atoms interacting with the external electromagnetic field. It will differ from the previous Hamiltonian H_{BP} only by the presence of this additional field A. Again we can start from the H_{FW} and assume that the electromagnetic field is a sum of the external one and the field from the nucleus and other electrons. This Hamiltonian will contain H_{BP}, and as well as H_{FW}. Straightforward derivation leads to:

$$\begin{aligned}
H &= \sum_a H_a + \sum_{a>b} H_{ab}\,, &(15)\\
H_a &= \frac{\vec\pi_a^2}{2\,m} - \frac{Z\,\alpha}{r_a} + e\,A_a^0 - \frac{e}{2\,m}\,(1+\kappa)\,\vec\sigma_a\cdot\vec B_a - \frac{\vec\pi_a^4}{8\,m^3} + \frac{\pi\,Z\,\alpha}{2\,m^2}\,(1+2\,\kappa)\,\delta^3(r_a)\\
&\quad + \frac{Z\,\alpha}{4\,m^2}\,(1+2\,\kappa)\,\vec\sigma_a\cdot\frac{\vec r_a}{r_a^3}\times\vec\pi_a - \frac{e}{8\,m^2}\,(1+2\,\kappa)\left[\nabla\cdot\vec E_a + \vec\sigma_a\,(\vec E_a\times\vec\pi_a - \vec\pi_a\times\vec E_a)\right]\\
&\quad + \frac{e}{8\,m^3}\left\{\vec\sigma_a\cdot\vec B_a\,\vec\pi_a^2 + \vec\pi_a^2\,\vec\sigma_a\cdot\vec B_a + \kappa\,[\vec\pi_a\cdot\vec B_a\,\vec\pi_a\cdot\vec\sigma_a + \vec\pi_a\cdot\vec\sigma_a\,\vec\pi_a\cdot\vec B_a]\right\}, &(16)
\end{aligned}$$

$$\begin{aligned}
H_{ab} &= \frac{\alpha}{r_{ab}} - \frac{\pi\,\alpha}{m^2}\,(1+2\,\kappa)\,\delta^3(r_{ab}) - \frac{\alpha}{2\,m^2}\,\pi_a^i\left(\frac{\delta^{ij}}{r_{ab}} + \frac{r_{ab}^i\,r_{ab}^j}{r_{ab}^3}\right)\pi_b^j\\
&\quad - \frac{2\,\pi\,\alpha}{3\,m^2}\,(1+\kappa)^2\,\vec\sigma_a\cdot\vec\sigma_b\,\delta^3(r_{ab}) + \frac{\alpha}{4\,m^2}\,(1+\kappa)^2\,\frac{\sigma_a^i\,\sigma_b^j}{r_{ab}^3}\left(\delta^{ij} - 3\,\frac{r_{ab}^i\,r_{ab}^j}{r_{ab}^2}\right) + \frac{\alpha}{4\,m^2\,r_{ab}^3}\\
&\quad \times\left[2\,(1+\kappa)\,(\vec\sigma_a\cdot\vec r_{ab}\times\vec\pi_b - \vec\sigma_b\cdot\vec r_{ab}\times\vec\pi_a) + (1+2\,\kappa)\,(\vec\sigma_b\cdot\vec r_{ab}\times\vec\pi_b - \vec\sigma_a\cdot\vec r_{ab}\times\vec\pi_a)\right].
\end{aligned} \tag{17}$$

This is a quite general Hamiltonian of many possible applications, but what has surprised us, we have not found it presented in the literature. This Hamiltonian will serve us here for the derivation of the transition amplitude between various states of the few-electron atom.

If we consider two states ϕ and ψ and the transition amplitude $\mathcal{T}^i$ between them, due to the photon emission or absorption, then:

$$\mathcal{T}^i = \langle\phi|j^i|\psi\rangle + \langle\phi|\, j^i \,\frac{1}{(E_\psi - H)'}\,\delta H\,|\psi\rangle + \langle\phi|\,\delta H\,\frac{1}{(E_\phi - H)'}\, j^i\,|\psi\rangle\,, \tag{18}$$

where δH is defined in Eq. (14). We are interested here in forbidden transitions only, for which matrix elements of first terms in α expansion of the current $\vec{j}$, namely these in Eqs. (20, 21) vanish. This amplitude is frequently treated incompletely in existing numerical codes and will be a subject of the following section.

IV. RELATIVISTIC CORRECTION TO THE TRANSITION AMPLITUDE

The transition current, in the nonrelativistic theory and the dipole limit being $\vec{p}/m$, acquires various relativistic corrections, which could be obtained order by order in α, the fine structure constant

$$\vec{j} = \vec{j}^{(0)} + \vec{j}^{(1)} + \vec{j}^{(2)} + \vec{j}^{(3)}\,, \tag{19}$$

$$\vec{j}^{(0)} = \sum_a \frac{\vec{p}_a}{m}\,, \tag{20}$$

$$\vec{j}^{(1)} = \sum_a \frac{\vec{p}_a}{m}\, i\,\vec{k}\cdot\vec{r}_a + \frac{i\,(1+\kappa)}{2\,m}\,\vec{\sigma}_a\times\vec{k}\,, \tag{21}$$

and higher order corrections $\vec{j}^{(2)}$ and $\vec{j}^{(3)}$ are derived from the general Hamiltonian H. By $\vec{j}^{(i)}$ we denote the order $O(\alpha^i)$ correction to $\vec{p}/m$ with assumption that $k \sim m\,\alpha^2$ and $p \sim 1/r \sim m\,\alpha$. $\vec{j}^{(i)}$ are obtained as a coefficients of the polarization vector $\vec{\epsilon}$ from the vector potential

$$\vec{A}(\vec{r}) = \vec{\epsilon}\, e^{i\vec{k}\cdot\vec{r}} \tag{22}$$

in Hamiltonian in Eqs. (15,16,17). Consistently with this, $\vec{E}$ and $\vec{B}$ fields are

$$\vec{E} = i\,\omega\,\vec{\epsilon}\, e^{i\vec{k}\cdot\vec{r}}\,, \tag{23}$$

$$\vec{B} = i\,\vec{k}\times\vec{\epsilon}\, e^{i\vec{k}\cdot\vec{r}}\,, \tag{24}$$

where in our units $|\omega| = |\vec{k}|$. For $\vec{j}^{(2)}$ we have

$$\begin{aligned}\vec{j}^{(2)} = {} & \sum_a \biggl\{ -\frac{\vec{p}_a}{m}\,\frac{(\vec{k}\cdot\vec{r}_a)^2}{2} - \frac{(1+\kappa)}{2\,m}\,\vec{\sigma}_a\times\vec{k}\,(\vec{k}\cdot\vec{r}_a) - \frac{p_a^2}{2\,m^3}\,\vec{p}_a - \frac{(1+2\,\kappa)}{2\,m^2}\,Z\,\alpha\,\frac{\vec{r}_a}{r_a^3}\times\vec{\sigma}_a \biggr\} \\ & + \sum_{a>b} \biggl\{ \frac{\kappa\,\alpha}{2\,m^2}\,\frac{\vec{r}_{ab}}{r_{ab}^3}\times(\vec{\sigma}_a - \vec{\sigma}_b) - \frac{\alpha}{2\,m^2}\left[\frac{1}{r_{ab}}\,(\vec{p}_a + \vec{p}_b) + \frac{\vec{r}_{ab}}{r_{ab}^3}\,\vec{r}_{ab}\cdot(\vec{p}_a + \vec{p}_b)\right] \biggr\}\,,\end{aligned} \tag{25}$$

where we used the fact that for matrix elements the following identity holds

$$\langle i\,\omega\,\vec{p}_a \times \vec{\sigma}_a\rangle = i\,\langle [H_0, \vec{p}_a \times \vec{\sigma}_a]\rangle\,. \tag{26}$$

Having $\vec{j}^{(2)}$ we transform the transition amplitude to the length form, namely the amplitude

$$\vec{\mathcal{T}}^{(2)} = \langle\phi|\vec{j}^{(2)}|\psi\rangle + \langle\phi|\sum_a \frac{\vec{p}_a}{m}\,\frac{1}{(E_\psi - H)'}\,\delta H\,|\psi\rangle + \langle\phi|\,\delta H\,\frac{1}{(E_\phi - H)'}\,\sum_a \frac{\vec{p}_a}{m}\,|\psi\rangle \tag{27}$$

is transformed with the help of $\vec{p}_a = i\,m\,[H, \vec{r}_a]$ to the following form

$$\vec{\mathcal{T}}^{(2)} = \langle\phi|\vec{j}^{(2)}_L|\psi\rangle + i\,\omega\,\langle\phi|\sum_a \vec{r}_a\,\frac{1}{(E_\psi - H)'}\,\delta H\,|\psi\rangle + i\,\omega\,\langle\phi|\,\delta H\,\frac{1}{(E_\phi - H)'}\,\sum_a \vec{r}_a\,|\psi\rangle\,, \tag{28}$$

where

$$\vec{j}^{(2)}_L = \vec{j}^{(2)} + i\,[\sum_a \vec{r}_a, \delta H] = \sum_a\Big\{-\frac{\kappa}{4\,m}\,k^2\,\vec{r}_a\times\vec{\sigma}_a + \frac{1}{2\,m^2}\,\vec{k}\times\hat{T}_a\cdot\vec{k}\Big\}\,, \tag{29}$$

and

$$T^{ij}_a = m\,(1+\kappa)\Big(\frac{r^i_a\,\sigma^j_a}{2} + \frac{r^j_a\,\sigma^i_a}{2} - \delta^{ij}\,\frac{\vec{r}_a\cdot\vec{\sigma}_a}{3}\Big) + \frac{m}{6}\Big(L^i_a\,r^j_a + r^j_a\,L^i_a + L^j_a\,r^i_a + r^i_a\,L^j_a\Big)\,. \tag{30}$$

We have neglected here the spin-independent electric dipole $E1$ terms, which do not contribute to forbidden transitions, and we also have neglected the whole $E3$ amplitude which will not be treated in this work. For each type of the transition we obtain:

$$\begin{aligned}
\vec{\mathcal{T}}_{M2} &= \frac{1}{2\,m^2}\,\langle\phi|\,\vec{k}\times\sum_a \hat{T}_a\cdot\vec{k}\,|\psi\rangle\,, && (31)\\
\vec{\mathcal{T}}_{E1} &= -\frac{\kappa}{4\,m}\,k^2\,\langle\phi|\,\sum_a \vec{r}_a\times\vec{\sigma}_a\,|\psi\rangle \\
&\quad + i\,\omega\,\langle\phi|\,\sum_a \vec{r}_a\,\frac{1}{(E_\psi - H)'}\,\delta H\,|\psi\rangle + i\,\omega\,\langle\phi|\,\delta H\,\frac{1}{(E_\phi - H)'}\,\sum_a \vec{r}_a\,|\psi\rangle\,. && (32)
\end{aligned}$$

The presence of the first term in $\mathcal{T}_{E1}$ shows that in the length form we have an additional correction proportional to the anomalous magnetic moment κ, beyond that already known, induced by δH. For the intercombination transitions, only few operators from δH contribute, namely the spin dependent one.

The other forbidden transitions are obtained from $\vec{j}^{(3)}$. Since they are already quite small we neglect here the anomalous magnetic moment. From the general Hamiltonian in Eqs. (15,16,17) one derives

$$\begin{aligned}
\vec{j}^{(3)} &= \sum_a\Big\{\frac{i}{4\,m}\,(\vec{k}\cdot\vec{r}_a)^2\,\vec{k}\times\vec{\sigma}_a + \frac{i}{4\,m^3}\,p_a^2\,\vec{k}\times\vec{\sigma}_a + \frac{i}{4\,m^3}\,\vec{k}\cdot\vec{p}_a\,\vec{p}_a\times\vec{\sigma}_a \\
&\quad - \frac{i\,Z\,\alpha}{2\,m^2}\,\vec{k}\cdot\vec{r}_a\,\frac{\vec{r}_a}{r_a^3}\times\vec{\sigma}_a + \frac{\vec{p}_a}{m}\,\frac{(i\,\vec{k}\cdot\vec{r}_a)^3}{3!} - \frac{i}{4\,m^3}\,\vec{p}_a\,\Big(p_a^2\,\vec{k}\cdot\vec{r}_a + \vec{k}\cdot\vec{r}_a\,p_a^2\Big)\Big\} \\
&\quad + \sum_{a\neq b}\Big\{\frac{i\,\alpha}{2\,m^2}\,\vec{k}\cdot\vec{r}_{ab}\,\frac{\vec{r}_{ab}}{r_{ab}^3}\times\vec{\sigma}_a - \frac{\alpha}{2\,m}\,i\,\vec{k}\cdot\vec{r}_a\,\Big(\frac{1}{r_{ab}}\,\vec{p}_b + \frac{\vec{r}_{ab}}{r_{ab}^3}\,\vec{r}_{ab}\cdot\vec{p}_b\Big)\Big\}\,. && (33)
\end{aligned}$$

$\vec{j}^{(3)}$ leads to $M3$, $E2$, $M1$ transitions.

$$\vec{\mathcal{T}}^{(3)} = \langle\phi|\vec{j}^{(3)}|\psi\rangle + \langle\phi|\,\vec{j}^{(1)}\,\frac{1}{(E_\psi - H)'}\,\delta H\,|\psi\rangle + \langle\phi|\,\delta H\,\frac{1}{(E_\phi - H)'}\,\vec{j}^{(1)}\,|\psi\rangle\,. \tag{34}$$

The $M3$ amplitude can be derived as well from Schrödinger-Pauli Hamiltonian and will not be considered any further. The $M1$ amplitude is

$$\begin{aligned}
\vec{\mathcal{T}}_{M1} &= \frac{i\,\vec{k}}{m}\times\langle\phi|\sum_a\{\vec{\sigma}_a\,T_a + \vec{T}_a + \hat{T}_a\cdot\vec{\sigma}_a\}|\psi\rangle \\
&\quad -\frac{i\,\vec{k}}{2\,m}\times\langle\phi|\,\sum_a\{\vec{L}_a+\vec{\sigma}_a\}\,\frac{1}{(E_\psi - H)'}\,\delta H\,|\psi\rangle \\
&\quad -\frac{i\,\vec{k}}{2\,m}\times\langle\phi|\,\delta H\,\frac{1}{(E_\phi - H)'}\,\sum_a\{\vec{L}_a+\vec{\sigma}_a\}|\psi\rangle\,,
\end{aligned} \tag{35}$$

where

$$T_a = \frac{k^2}{12}\,r_a^2 + \frac{p_a^2}{3\,m^2} - \frac{1}{6\,m}\,\frac{Z\,\alpha}{r_a} + \sum_{b,b\neq a}\frac{1}{6\,m}\,\frac{\alpha}{r_{ab}} = \frac{p_a^2}{6\,m^2} - \sum_{b,b\neq a}\frac{\alpha}{6\,m\,r_{ab}^3}\,\vec{r}_{ab}\cdot\vec{r}_b\,, \tag{36}$$

$$\vec{T}_a = \frac{k^2}{20}\,r_a^2\,\vec{L}_a + \frac{1}{4\,m^2}\,p_a^2\,\vec{L}_a + \sum_{b,b\neq a}\frac{\alpha}{2\,m\,r_{ab}^3}\Big(r_{ab}^2\,\vec{r}_a\times\vec{p}_b + \vec{r}_a\times\vec{r}_{ab}\,\vec{r}_{ab}\cdot\vec{p}_b\Big)\,, \tag{37}$$

$$\begin{aligned}
T_a^{ij} &= -\frac{k^2}{20}\,r_a^i\,r_a^j - \frac{1}{8\,m^2}\,p_a^i\,p_a^j + \frac{Z\,\alpha}{4\,m\,r_a^3}\,r_a^i\,r_a^j - \sum_{b,b\neq a}\frac{\alpha}{4\,m\,r_{ab}^3}\,r_{ab}^i\,r_{ab}^j \\
&\quad +\frac{\delta^{ij}}{3}\left[\frac{k^2}{20}\,r_a^2 + \frac{p_a^2}{8\,m^2} - \frac{Z\,\alpha}{4\,m\,r_a} + \sum_{b,b\neq a}\frac{\alpha}{4\,m\,r_{ab}}\right],
\end{aligned} \tag{38}$$

where in Eq. (36) we used the identity

$$k^2 r_a^2 \to [H_0,[H_0,r_a^2]] = \frac{2}{m}\left(\frac{Z\,\alpha}{r_a} - \frac{p_a^2}{m} - \sum_{b,b\neq a}\frac{\alpha}{r_{ab}^3}\,\vec{r}_{ab}\cdot\vec{r}_a\right). \tag{39}$$

The above T terms have been partially derived in the literature, T_a was derived in [1] for the case of $1^1S_o - 2^3S_1$ transition in the helium, but the general form was not known. In published results, for example in [3], all T terms were neglected. The second order terms in Eq. (35) have in fact very simple form here. First of all, the denominator $1/(E_\psi - H)'$ becomes $1/(E_\psi - E_\phi)$, similarly the other one, and the sum over states will involve only these, which may differ from ϕ and ψ correspondingly, by magnetic quantum numbers m_s, m_l.

The electric quadrupole amplitude $E2$ is obtained similarly to $E1$. Here only spin dependent terms will contribute, because we assume that this transition is nonrelativistically forbidden. One uses the identity $\vec{p}_i = i\,m\,[H,\vec{r}_i]$ to transform this amplitude to the length form:

$$\vec{j}_L^{(3)} = \vec{j}^{(3)} - \sum_a\left[\frac{\vec{k}\cdot\vec{r}_a}{2}\,\vec{r}_a,\delta H\right], \tag{40}$$

and $E2$ becomes

$$\begin{aligned}
\mathcal{T}^i_{E2} &= i\,\frac{k^j}{m}\,\sum_a \langle\phi|\sigma^l_a\,[\epsilon^{ikl}\,T^{jk}_a + \epsilon^{jkl}\,T^{ik}_a] + \sigma^j_a\,T^i_a + \sigma^i_a\,T^j_a|\psi\rangle \\
&\quad -\omega\,\frac{k^j}{2}\,\langle\phi|\Big(r^i_a\,r^j_a - \frac{\delta^{ij}}{3}\,r^2_a\Big)\,\frac{1}{(E_\psi - H)'}\,\delta H|\psi\rangle \\
&\quad -\omega\,\frac{k^j}{2}\,\langle\phi|\,\delta H\,\frac{1}{(E_\phi - H)'}\,\Big(r^i_a\,r^j_a - \frac{\delta^{ij}}{3}\,r^2_a\Big)\,|\psi\rangle\,, \qquad (41)\\
T^{ij}_a &= \frac{k^2}{48}\,r^i_a\,r^j_a\,, \qquad (42)\\
T^i_a &= \sum_{b,b\neq a}\frac{1}{16\,m}\,\frac{\alpha}{r^3_{ab}}\,(\vec{r}_a\times\vec{r}_b)^i\,. \qquad (43)
\end{aligned}$$

We observe the existence of additional terms T^i and T^{ij} which contribute to the $E2$ transition amplitude, beyond the well known second order part coming from the Breit-Pauli Hamiltonian.

V. SUMMARY

The purpose of this work was the derivation of complete formulas for amplitudes of forbidden transitions in light atoms, where relativistic effects could be treated perturbatively. This perturbative treatment has several advantages over MCDF and RMBPT with respect to the accuracy of the calculated amplitudes, especially, when correlated basis set are employed. We are currently attempting to calculate the $2^1S_0 - 2^3P_1$ transition in the beryllium like carbon with the use of fully correlated Gaussian basis set, with the hope to resolve the discrepancy between the experiment and the most accurate calculation of Chen, Cheng, and Johnson in [11]. For this reason and probably for many others, we included the anomalous magnetic moment which may contribute to the transition amplitude at the order of 1%. The other motivation was the investigation of parity nonconservation in light atoms through the highly forbidden transitions. Usually one considers heavy systems where parity nonconservation is enhanced by the strong electric field of the nucleus. Light atoms have at least one advantage that any transitions can be calculated with the much higher precision, provided we know the complete matrix element.

The obtained in this work formulas are complete in the leading order of the fine structure constant. We have shown, that apart from corrections from the Breit-Pauli Hamiltonian, there are additional corrections to the amplitude, which we interpret as a relativistic correction to the current. In the case of $E2$ transition these additional corrections are probably numerically small. However, they are significant in the case of the $M1$ amplitude. In our former work in [10] we have confirmed the result of [1] for $1^1S_0 - 2^3S_1$ $M1$ amplitude, together with the calculation of few other forbidden transitions in the helium. Here we generalized formulas for all $E1, E2, M1, M2$ transitions in the arbitrary light atom. As an additional result we derived the relativistic correction to the Hamiltonian of few electron atom interacting with the external electromagnetic field, an analog of the Breit-Pauli Hamiltonian. This general Hamiltonian has many applications and for example can be used in the derivation of relativistic corrections to the interaction potential between light atoms or to Zeeman effect.

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