Long Wavelength Quantum Electrodynamics

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Abstract

The description of few electron atoms interacting with a slowly varying electromagnetic field including relativistic effects is analyzed. Simple and transparent derivations of relativistic and radiative corrections to various atomic properties such as magnetic moments, radiative decay rates, and shielding of the electric dipole moment are presented.

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I. INTRODUCTION

The aim of this work is the reformulation of quantum electrodynamic theory for the description, including relativistic effects, of the interaction of light atomic systems with slowly varying electromagnetic fields with characteristic wavelengths λ much larger than the atomic size. We obtain this in several steps. The first step is the Foldy-Wouthuysen transformation of a Dirac Hamiltonian including the anomalous magnetic moment. The second step is the inclusion of the electron-electron interaction in an external electromagnetic field which leads to a generalized Breit-Pauli Hamiltonian H_{BP}. The third step is the Power-Zienau [1] transformation, followed by an additional transformation of the H_{BP} Hamiltonian of an atom in an external time-varying electromagnetic field, which leads to H_{LW}. These unitary transformations lead to equvalent Hamiltonians, in the sense that matrix elements with asymptotic states are the same. However finite time evolution usually leads to gauge dependent, ill defined matrix elements and this issue is not studied here.

The second quantization of the electromagnetic field interacting with the atom is performed using Feynman integrations by paths [2]. This way of quantization allows for great flexibility in using any transformation of fields, as long as the Jacobian is 1. This approach resembles the Lagrangian of NRQED, first introduced by Caswell and Lepage [3] in the calculation of higher order QED corrections to positronium hyperfine splitting. We use this approach for investigation of three related problems: relativistic and radiative corrections to the magnetic moment of a bound electron, relativistic corrections to transition rates, and relativistic corrections to shielding of the electric dipole moment. We obtain here known and even old results, but present their derivation in a simple and unified way. We obtain also several new results, apart from H_{LW}, such as self-energy corrections to g-factors of 2^3P_J state of helium, and relativistic corrections to some transition rates. This approach, we think, can be used for the calculation of relativistic corrections to the Casimir-Polder potential [4], calculation of two-loop radiative corrections to the bound electron g-factor [5], and of higher order self-energy corrections in few electron atoms, for example to helium Lamb shift [6, 7] and fine structure [8, 9], which currently are of primary interest in high precision tests of QED and fundamental constants determinations.

II. FOLDY-WOUTHUYSEN TRANSFORMATION

The Foldy-Wouthuysen transformation [2] is the nonrelativistic expansion of the Dirac Hamiltonian in an external electromagnetic field. While it is well described in many textbooks, we present here a slightly different and simpler version. Moreover, we include the anomalous magnetic moment and include some higher order terms in this expansion for further applications. In this section we closely follow the former work in [10]. The Dirac Hamiltonian for a spin 1/2 particle [2] interacting with an external electromagnetic field including the anomalous magnetic moment κ is [for electrons $\kappa \approx \alpha/(2\,\pi)$]

$$H = \vec{\alpha}\cdot\vec{\pi} + \beta\, m + e\, A^0 + \frac{e\,\kappa}{2\,m}\,(i\,\beta\,\vec{\alpha}\cdot\vec{E} - \beta\,\vec{\Sigma}\cdot\vec{B})\,, \tag{1}$$

where $\vec{\pi} = \vec{p} - e\,\vec{A}$. The Foldy-Wouthuysen (F.W.) transformation S [2] leads to a new Hamiltonian

$$H_{FW} = e^{i\,S}\,(H - i\,\partial_t)\,e^{-i\,S}\,, \tag{2}$$

which does not couple upper and lower components of the Dirac wave function up to a 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

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

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

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

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 Dirac Hamiltonian H, namely

$$\begin{aligned} H_{FW} &= \frac{\vec{\pi}^2}{2\,m} + e\,A^0 - \frac{e}{2\,m}\,(1+\kappa)\,\vec{\sigma}\cdot\vec{B} - \frac{\vec{\pi}^4}{8\,m^3} \\ &\quad - \frac{e}{8\,m^2}\,(1 + 2\,\kappa)\left[\nabla\cdot\vec{E} + \vec{\sigma}\cdot(\vec{E}\times\vec{\pi} - \vec{\pi}\times\vec{E})\right] \\ &\quad + \frac{e}{8\,m^3}\left\{\vec{\sigma}\cdot\vec{B}\,\vec{\pi}^2 + \vec{\pi}^2\,\vec{\sigma}\cdot\vec{B} + \kappa\,[\vec{\pi}\cdot\vec{B}\,\vec{\pi}\cdot\vec{\sigma} + \vec{\pi}\cdot\vec{\sigma}\,\vec{\pi}\cdot\vec{B}]\right\}. \end{aligned} \tag{5}$$

The Foldy-Wouthuysen transformation, apart for determination of leading relativistic effects, was found to be very convenient in the calculation of higher order corrections to the Lamb shift in hydrogenic systems [11].

III. THE GENERALIZED BREIT-PAULI HAMILTONIAN

Since the one-particle Hamiltonian H_{FW} represents the complete interaction of a charged particle with the electromagnetic field, it allows one to obtain the few-electron, Breit-Pauli Hamiltonian H_{BP} [12]. H_{BP} includes a sum of H_{FW} for all electrons, static Coulomb interactions, and corrections to the electric as well as magnetic interactions between electrons and the nucleus. Corrections to the electron-nucleus interaction are easily accounted for by setting $\vec{E} = -Z\,\alpha\,\vec{r}/r^3$ in Eq. (5) and we assume for simplicity that the nucleus is static and spinless. The derivation of electron-electron interactions is as follows. In the nonrelativistic limit, the few electron Hamiltonian is

$$H_0 = \sum_a \left(\frac{\vec{p}_a^{\,2}}{2\,m} - \frac{Z\,\alpha}{r_a}\right) + \sum_{a>b} \frac{\alpha}{r_{ab}}\,. \tag{6}$$

This Hamiltonian determines the nonrelativistic equal-time two-particle propagator. In quantum field theoretical approach one is able to calculate various corrections to propagators, which inverse leads to some effective Hamiltonian δH. The relativistic correction δH_{ab} to interaction between particles a and b, is obtained from the one photon exchange amplitude

$$\begin{aligned}\langle\phi|\delta H_{ab}|\phi\rangle \;=\; e^2 \int \frac{d^4 k}{(2\,\pi)^4\, i}\, G_{\mu\nu}(k)\, \biggl\{\biggl\langle\phi\biggl|\jmath^\mu_a(k)\, e^{i\,\vec{k}\cdot\vec{r}_a}\, \frac{1}{E_\phi - H_0 - k_0 + i\,\epsilon}\, \jmath^\nu_b(-k)\, e^{-i\,\vec{k}\cdot\vec{r}_b}\biggr|\phi\biggr\rangle \\ +\biggl\langle\phi\biggl|\jmath^\mu_b(k)\, e^{i\,\vec{k}\cdot\vec{r}_b}\, \frac{1}{E_\phi - H_0 + k_0 + i\,\epsilon}\, \jmath^\nu_a(-k)\, e^{-i\,\vec{k}\cdot\vec{r}_a}\biggr|\phi\biggr\rangle\biggr\}\,,\end{aligned} \tag{7}$$

where ϕ is an eigenstate of H_0, $\jmath^\mu_a$ is an electromagnetic current operator for particle a, and $G_{\mu\nu}$ is the photon propagator, for convenience in the Coulomb gauge

$$G_{\mu\nu}(k) = \begin{cases} \frac{1}{\vec{k}^2} & \mu = \nu = 0\,, \\ \frac{1}{k_0^2 - \vec{k}^2 + i\,\epsilon}\left(\delta_{ij} - \frac{k_i k_j}{\vec{k}^2}\right) & \mu = i, \nu = j \end{cases}\,. \tag{8}$$

Since we aim here to derive only leading relativistic corrections, we perform nonretardation approximation, namely set $k_0 = 0$ in the photon propagator $G_{\mu\nu}(k)$ and $\jmath(k)$. Without this approximation Eq. (8) would include higher order terms including Lamb shift, see for details

[13]. The integration with respect to k_0 in Eq. (7), after symmetrization $k_0 \leftrightarrow -k_0$, leads to

$$\langle\phi|\delta H_{ab}|\phi\rangle = e^2 \int \frac{d^3k}{(2\,\pi)^3}\, G_{\mu\nu}(\vec{k}) \left\langle\phi\middle|\jmath^\mu_a(\vec{k})\, e^{i\,\vec{k}\cdot(\vec{r}_a-\vec{r}_b)}\,\jmath^\nu_b(-\vec{k})\,\middle|\phi\right\rangle. \tag{9}$$

It is convenient at this point to recall the Fourier transform of $G(\vec{k})$ in the nonretardation approximation

$$G_{\mu\nu}(\vec{r}) = \int \frac{d^3k}{(2\,\pi)^3} G_{\mu\nu}(\vec{k}) = 4\,\pi \begin{cases} \frac{1}{r}\,, \\ -\frac{1}{2\,r}\left(\delta_{ij} + \frac{r_i r_j}{\vec{r}^{\,2}}\right) \end{cases} . \tag{10}$$

The first term is responsible for the Coulomb interaction and the second one for the magnetic interaction. The electromagnetic current operator $\jmath^\mu(k)$ is defined as a coefficient in front of $e\,A_\mu(k)$ in H_{FW}. The $\jmath^0$ component

$$\jmath^0(\vec{k}) = 1 + \frac{i(1+2\,\kappa)}{4\,m}\,\vec{\sigma}\cdot\vec{k}\times\vec{\pi} - \frac{1+2\,\kappa}{8\,m^2}\vec{k}^{\,2}\,, \tag{11}$$

gives relativistic corrections of the form

$$\delta H_{ab} = -\frac{\pi\,\alpha}{m^2}\,(1+2\,\kappa)\,\delta^3(r_{ab}) + \frac{\alpha}{4\,m^2\,r_{ab}^3}(1+2\,\kappa)\,(\vec{\sigma}_b\cdot\vec{r}_{ab}\times\vec{\pi}_b - \vec{\sigma}_a\cdot\vec{r}_{ab}\times\vec{\pi}_a)\,. \tag{12}$$

The $\vec{\jmath}$ component

$$\vec{\jmath}(\vec{k}) = \frac{\vec{\pi}}{m} + \frac{i(1+\kappa)}{2\,m}\,\vec{\sigma}\times\vec{k}\,, \tag{13}$$

gives the following corrections:

$$\begin{aligned} \delta H_{ab} \;=\; & -\frac{\alpha}{2\,m^2}\,\pi^i_a\left(\frac{\delta^{ij}}{r_{ab}} + \frac{r^i_{ab}\,r^j_{ab}}{r^3_{ab}}\right)\pi^j_b - \frac{2\,\pi\,\alpha}{3\,m^2}\,(1+\kappa)^2\,\vec{\sigma}_a\cdot\vec{\sigma}_b\,\delta^3(r_{ab}) \\ & + \frac{\alpha}{4\,m^2}\,(1+\kappa)^2\,\frac{\sigma^i_a\,\sigma^j_b}{r^3_{ab}}\left(\delta^{ij} - 3\,\frac{r^i_{ab}\,r^j_{ab}}{r^2_{ab}}\right) \\ & + \frac{\alpha}{4\,m^2\,r^3_{ab}} 2\,(1+\kappa)\,(\vec{\sigma}_a\cdot\vec{r}_{ab}\times\vec{\pi}_b - \vec{\sigma}_b\cdot\vec{r}_{ab}\times\vec{\pi}_a)\,. \end{aligned} \tag{14}$$

The sum of H_{FW} for each electron, the electron-nucleus terms, electric and magnetic electron-electron interactions forms the generalized Breit-Pauli Hamiltonian H_{BP}

$$H_{BP} = \sum_a H_a + \sum_{a>b} H_{ab}\,, \tag{15}$$

$$\begin{aligned} H_a \;=\; & \frac{\vec{\pi}^2_a}{2\,m} - \frac{Z\,\alpha}{r_a} + e\,A^0_a - \frac{e}{2\,m}\,(1+\kappa)\,\vec{\sigma}_a\cdot\vec{B}_a - \frac{\vec{\pi}^4_a}{8\,m^3} + \frac{\pi\,Z\,\alpha}{2\,m^2}\,(1+2\,\kappa)\,\delta^3(r_a) \\ & + \frac{Z\,\alpha}{4\,m^2}\,(1+2\,\kappa)\,\vec{\sigma}_a\cdot\frac{\vec{r}_a}{r^3_a}\times\vec{\pi}_a - \frac{e}{8\,m^2}\,(1+2\,\kappa)\left[\nabla\cdot\vec{E}_a + \vec{\sigma}_a\,(\vec{E}_a\times\vec{\pi}_a - \vec{\pi}_a\times\vec{E}_a)\right] \\ & + \frac{e}{8\,m^3}\left\{\vec{\sigma}_a\cdot\vec{B}_a\,\vec{\pi}^2_a + \vec{\pi}^2_a\,\vec{\sigma}_a\cdot\vec{B}_a + \kappa\,[\vec{\pi}_a\cdot\vec{B}_a\,\vec{\pi}_a\cdot\vec{\sigma}_a + \vec{\pi}_a\cdot\vec{\sigma}_a\,\vec{\pi}_a\cdot\vec{B}_a]\right\}, \end{aligned} \tag{16}$$

$$
\begin{aligned}
H_{ab} \; = \; & \frac{\alpha}{r_{ab}} - \frac{\pi\,\alpha}{m^2}\,(1+2\,\kappa)\,\delta^3(r_{ab}) - \frac{\alpha}{2\,m^2}\,\pi^i_a\left(\frac{\delta^{ij}}{r_{ab}} + \frac{r^i_{ab}\,r^j_{ab}}{r^3_{ab}}\right)\pi^j_b \\
& -\frac{2\,\pi\,\alpha}{3\,m^2}\,(1+\kappa)^2\,\vec{\sigma}_a\cdot\vec{\sigma}_b\,\delta^3(r_{ab}) + \frac{\alpha}{4\,m^2}\,(1+\kappa)^2\,\frac{\sigma^i_a\,\sigma^j_b}{r^3_{ab}}\left(\delta^{ij} - 3\,\frac{r^i_{ab}\,r^j_{ab}}{r^2_{ab}}\right) + \frac{\alpha}{4\,m^2\,r^3_{ab}} \\
\times & \Big[2\,(1+\kappa)\,(\vec{\sigma}_a\cdot\vec{r}_{ab}\times\vec{\pi}_b - \vec{\sigma}_b\cdot\vec{r}_{ab}\times\vec{\pi}_a) + (1+2\,\kappa)\,(\vec{\sigma}_b\cdot\vec{r}_{ab}\times\vec{\pi}_b - \vec{\sigma}_a\cdot\vec{r}_{ab}\times\vec{\pi}_a)\Big]\,.
\end{aligned}
\tag{17}
$$

The A, E, B fields are assumed here to be slowly varying along the atomic size. They could represent, for example, external magnetic and electric fields or the field of an emitted or absorbed photon. Let us recall that the Breit-Pauli Hamiltonian can be extended to higher orders of perturbation calculus. It leads however to singular operators, which can be regularized with some cut-off parameters. Within this approach one has obtained energy levels of order $m\,\alpha^6$ for helium atom [6, 7].

IV. POWER-ZIENAU TRANSFORMATION

The Power-Zienau transformation [1] explores the long wavelength of electromagnetic field and is defined by

$$
H' = e^{-i\,\phi}\,H\,e^{i\,\phi} + \partial_t\phi\,, \tag{18}
$$

with phase ϕ given by

$$
\phi = e\int_0^1 du\,\vec{r}\cdot\vec{A}(u\,\vec{r})\,. \tag{19}
$$

The assumption that the A field is slowly varying allows one to perform a Taylor expansion,

$$
A^\mu(\vec{r},t) = A^\mu(0,t) + r^i\,A^\mu_{,i}(0,t) + \frac{1}{2!}\,r^i\,r^j\,A^\mu_{,ij}(0,t) + \frac{1}{3!}\,r^i\,r^j\,r^k\,A^\mu_{,ijk}(0,t) + \ldots \tag{20}
$$

and express derivatives of A in the Hamiltonian in terms of fields $\vec{E}$ and $\vec{B}$. The phase ϕ takes the form

$$
\phi = e\Big[r^i\,A^i + \frac{1}{2!}\,r^i\,r^j\,A^i_{,j} + \frac{1}{3!}\,r^i\,r^j\,r^k\,A^i_{,jk} + \frac{1}{4!}\,r^i\,r^j\,r^k\,r^l\,A^i_{,jkl} + \ldots\Big]\,. \tag{21}
$$

The potential $e\,A^0$ and $\partial_t\,\phi$ combines to

$$
e\,A^0 + \partial_t\,\phi = -e\left[\vec{r}\cdot\vec{E} + \frac{1}{2!}\,r^i\,r^j\,E^i_{,j} + \frac{1}{3!}\,r^i\,r^j\,r^k\,E^i_{,jk} + \ldots\right], \tag{22}
$$

and the transformation of $\vec{\pi}$ is

$$e^{-i\,\phi}\,\pi^j\,e^{i\,\phi} \;=\; p^j + \frac{e}{2!}\,(\vec{r}\times\vec{B})^j + \frac{e}{3!}\,r^l\,r^m\left(\epsilon^{jlk}\,B^k_{,m} + \epsilon^{jmk}\,B^k_{,l}\right) + \frac{e}{4!}\,r^l\,r^m\,r^n\left(\epsilon^{jlk}\,B^k_{,mn} + \epsilon^{jmk}\,B^k_{,ln} + \epsilon^{jnk}\,B^k_{,lm}\right). \tag{23}$$

In the many electron case, the phase ϕ is a sum over all electrons

$$\phi = \sum_a e\int_0^1 du\,\vec{r}_a\cdot\vec{A}(u\,\vec{r}_a)\,. \tag{24}$$

and the Power-Zienau Hamiltonian H_{PZ} being a sum of the transformed Hamiltonians H'_a and H'_{ab} becomes

$$H_{PZ} \;=\; \sum_a H'_a + \sum_{a>b} H'_{ab}\,, \tag{25}$$

$$\begin{aligned}
H'_a \;=\;& \frac{\vec{p}_a^{\,2}}{2\,m} - \frac{Z\,\alpha}{r_a} - \frac{\vec{p}_a^{\,4}}{8\,m^3} + \frac{\pi\,Z\,\alpha}{2\,m^2}\,(1+2\,\kappa)\,\delta^3(r_a) + \frac{Z\,\alpha}{4\,m^2}\,(1+2\,\kappa)\,\frac{\vec{\sigma}_a\cdot\vec{L}_a}{r_a^3}\\
&-e\,\vec{r}_a\cdot\vec{E} - \frac{e}{2\,m}\left[\vec{L}_a + (1+\kappa)\,\vec{\sigma}_a\right]\cdot\vec{B} - \frac{e}{2}\,r_a^i\,r_a^j\,E^i_{,j} + \frac{e^2}{8\,m}\left(\vec{r}\times\vec{B}\right)^2\\
&-\frac{e}{6\,m}\left(L_a^i\,r_a^j + r_a^j\,L_a^i\right)B^i_{,j} - \frac{e}{2\,m}\,(1+k)\,\sigma_a^i\,r_a^j\,B^i_{,j} - \frac{e}{4\,m^2}\,(1+2\,\kappa)\,\vec{\sigma}_a\cdot\vec{E}\times\vec{p}_a\\
&+\frac{e}{4\,m^3}\,\vec{p}_a^{\,2}\,(\vec{L}_a+\vec{\sigma}_a)\cdot\vec{B} + \frac{e\,\kappa}{4\,m^3}\,(\vec{p}_a\cdot\vec{\sigma}_a)\,(\vec{p}_a\cdot\vec{B}) - \frac{e\,(1+2\,\kappa)}{8\,m^2}\,\frac{Z\,\alpha}{r_a^3}\,(\vec{r}_a\times\vec{\sigma}_a)\,(\vec{r}_a\times\vec{B})\\
&-\frac{e^2\,(1+2\,\kappa)}{8\,m^2}\left(\vec{\sigma}_a\times\vec{E}\right)\left(\vec{r}_a\times\vec{B}\right) - \frac{e}{6}\,r_a^i\,r_a^j\,r_a^k\,E^i_{,jk} - \frac{e}{16\,m}\left(L_a^k\,r_a^i\,r_a^j + r_a^i r_a^j\,L_a^k\right)B^k_{,ij}\\
&-\frac{e\,(1+\kappa)}{4\,m}\,\sigma_a^k\,r_a^i\,r_a^j\,B^k_{,ij} + \frac{e\,(1+2\,\kappa)}{8\,m^2}\left[r_a^i\,(\vec{\sigma}_a\times\vec{p}_a)^j + (\vec{\sigma}_a\times\vec{p}_a)^j\,r_a^i\right]E^j_{,i}\\
&-\frac{e}{4!}\,r_a^i\,r_a^j\,r_a^k\,r_a^l\,E^i_{,jkl}\,,
\end{aligned} \tag{26}$$

$$\begin{aligned}
H'_{ab} \;=\;& \frac{\alpha}{r_{ab}} - \frac{\pi\,\alpha}{m^2}\,(1+2\,\kappa)\,\delta^3(r_{ab}) - \frac{\alpha}{2\,m^2}\,p_a^i\left(\frac{\delta^{ij}}{r_{ab}} + \frac{r_{ab}^i\,r_{ab}^j}{r_{ab}^3}\right)p_b^j\\
&-\frac{2\,\pi\,\alpha}{3\,m^2}\,(1+\kappa)^2\,\vec{\sigma}_a\cdot\vec{\sigma}_b\,\delta^3(r_{ab}) + \frac{\alpha}{4\,m^2}\,(1+\kappa)^2\,\frac{\sigma_a^i\,\sigma_b^j}{r_{ab}^3}\left(\delta^{ij} - 3\,\frac{r_{ab}^i\,r_{ab}^j}{r_{ab}^2}\right) + \frac{\alpha}{4\,m^2\,r_{ab}^3}\\
\times&\left[2\,(1+\kappa)\,(\vec{\sigma}_a\cdot\vec{r}_{ab}\times\vec{p}_b - \vec{\sigma}_b\cdot\vec{r}_{ab}\times\vec{p}_a) + (1+2\,\kappa)\,(\vec{\sigma}_b\cdot\vec{r}_{ab}\times\vec{p}_b - \vec{\sigma}_a\cdot\vec{r}_{ab}\times\vec{p}_a)\right]\\
&-\frac{e\,\alpha}{4\,m^2}\left[(\vec{r}_a\times\vec{B})^i\,p_b^j + p_a^i\,(\vec{r}_b\times\vec{B})^j\right]\left(\frac{\delta^{ij}}{r_{ab}} + \frac{r_{ab}^i\,r_{ab}^j}{r_{ab}^3}\right)\\
&+\frac{e\,\alpha}{8\,m^2 r_{ab}^3}\Big\{2\,(1+\kappa)[(\vec{\sigma}_a\times\vec{r}_{ab})\,(\vec{r}_b\times\vec{B}) - (\vec{\sigma}_b\times\vec{r}_{ab})\,(\vec{r}_a\times\vec{B})]\\
&+(1+2\,\kappa)[(\vec{\sigma}_b\times\vec{r}_{ab})\,(\vec{r}_b\times\vec{B}) - (\vec{\sigma}_a\times\vec{r}_{ab})\,(\vec{r}_a\times\vec{B})]\Big\}\,,
\end{aligned} \tag{27}$$

where $\vec{E}=\vec{E}(0)$ and $\vec{B}=\vec{B}(0)$. We have neglected $E^i_{,i}$ and higher order quadratic terms in $\vec{B}$. The Hamiltonian H_{PZ} in Eq. (25) is equivalent to the generalized Breit-Pauli Hamiltonian H_{BP} under the assumption that the electromagnetic field is slowly varying on the scale of atomic size. We perform now the next transformation which leads to H_{LW}, a Hamiltonian in the form most convenient for the calculation of various relativistic effects. This transformation is defined by Eq. (18) with

$$\phi = \sum_a \frac{e(1+2\,\kappa)}{4\,m^2}\int_0^1 dt\,\vec{\sigma}_a\cdot\vec{E}(t\,\vec{r}_a)\times\vec{r}_a = \sum_a \frac{e(1+2\,\kappa)}{4\,m^2}\,\vec{\sigma}_a\,(\vec{E}\times\vec{r}_a+\frac{r_a^i}{2}\,\vec{E}_{,i}\times\vec{r}_a+\ldots). \tag{28}$$

The transformed Hamiltonian H_{LW} is decomposed into three parts

$$H_{LW} = H_0+\delta H+H_I\,, \tag{29}$$

where H_0 is a Schrödinger Hamiltonian of a few electron atom in Eq. (6), δH is a relativistic correction obtained from H_{BP} by neglecting the electromagnetic field, and H_I is an interaction with the electromagnetic field

$$\begin{aligned}
H_I \;=\; & \sum_a\Big\{-e\,\vec{r}_a\cdot\vec{E}-\frac{e}{2\,m}\left[\vec{L}_a+(1+\kappa)\,\vec{\sigma}_a\right]\cdot\vec{B}-\frac{e}{2}\,r_a^i\,r_a^j\,E^i_{,j}+\frac{e^2}{8\,m}\Big(\vec{r}_a\times\vec{B}\Big)^2 \\
& -\frac{e}{6\,m}\Big(L_a^i\,r_a^j+r_a^j\,L_a^i\Big)\,B^i_{,j}-\frac{e}{2\,m}\,(1+k)\,\sigma_a^i\,r_a^j\,B^i_{,j}+\frac{e\,(1+2\,\kappa)}{8\,m^3}\,\sigma_a^i\,L_a^k\,E^k_{,i} \\
& +\frac{e}{4\,m^3}\,\vec{p}_a^{\,2}\,(\vec{L}_a+\vec{\sigma}_a)\cdot\vec{B}+\frac{e\,\kappa}{4\,m^3}\,(\vec{p}_a\cdot\vec{\sigma}_a)\,(\vec{p}_a\cdot\vec{B})-\frac{e\,(1+2\,\kappa)}{8\,m^2}\,\frac{Z\,\alpha}{r_a^3}\,(\vec{r}_a\times\vec{\sigma}_a)\,(\vec{r}_a\times\vec{B}) \\
& -\frac{e^2\,(1+2\,\kappa)}{8\,m^2}\,\Big(\vec{\sigma}_a\times\vec{E}\Big)\,\Big(\vec{r}_a\times\vec{B}\Big)-\frac{e}{6}\,r_a^i\,r_a^j\,r_a^k\,E^i_{,jk}-\frac{e}{16\,m}\Big(L_a^k\,r_a^i\,r_a^j+r_a^i r_a^j\,L_a^k\Big)\,B^k_{,ij} \\
& -\frac{e\,(1+\kappa)}{4\,m}\,\sigma_a^k\,r_a^i\,r_a^j\,B^k_{,ij}+\frac{e\,(1+2\,\kappa)}{4\,m^2}\,\vec{\sigma}_a\cdot\,\dot{\vec{E}}\times\vec{r}_a+\frac{e\,(1+2\,\kappa)}{8\,m^2}\,\epsilon^{ijk}\,\sigma_a^i\,r_a^l\,\dot{E}^j_{,l}\,r_a^k \\
& -\frac{e}{4!}\,r_a^i\,r_a^j\,r_a^k\,r_a^l\,E^i_{,jkl}\Big\}+ \\
& \sum_{a>b}\Big\{-\frac{e\,\alpha}{4\,m^2}\Big[(\vec{r}_a\times\vec{B})^i\,p_b^j+p_a^i\,(\vec{r}_b\times\vec{B})^j\Big]\left(\frac{\delta^{ij}}{r_{ab}}+\frac{r_{ab}^i\,r_{ab}^j}{r_{ab}^3}\right) \\
& +\frac{e\,\alpha}{8\,m^2 r_{ab}^3}\Big\{2\,(1+\kappa)[(\vec{\sigma}_a\times\vec{r}_{ab})\,(\vec{r}_b\times\vec{B})-(\vec{\sigma}_b\times\vec{r}_{ab})\,(\vec{r}_a\times\vec{B})] \\
& +(1+2\,\kappa)[(\vec{\sigma}_b\times\vec{r}_{ab})\,(\vec{r}_b\times\vec{B})-(\vec{\sigma}_a\times\vec{r}_{ab})\,(\vec{r}_a\times\vec{B})]\Big\}\Big\}\,.
\end{aligned} \tag{30}$$

This classical electromagnetic field can now be quantized using the Feynman integration by paths [2], by expressing radiative corrections in terms of Green functions. As a test we have verified the equivalence of the nonrelativistic one-loop, as well as two-loop self-energy in hydrogenic systems as derived from H_{FW} and H_{LW}. The difference is proportional to the linear and quadratic terms in the cut-off Λ, which are eliminated by matching with the contribution coming from high-frequency photons.

V. RELATIVISTIC AND RADIATIVE CORRECTIONS TO THE ZEEMAN EFFECT

One of the interesting applications of H_{LW} is the derivation of relativistic corrections to the Zeeman effect. The Zeeman splitting has been measured very precisely for various atoms and ions, and at present the measurement of the g-factor in hydrogen-like carbon serves as the best determination of the electron mass [5]. We aim here to recall the theory for light few-electron atoms or ions. It has been first investigated by Perl and Hughes in [14] and Van Vleck and co-workers in [15]. A detailed derivation was presented by Hegstrom in [16], and evaluated numerically for several states of helium by Lewis and Hughes in [17], Anthony and Sebastian in [18], and more recently Yan in [19]. The leading relativistic and also radiative corrections can be derived from H_{LW}. This Hamiltonian is similar to that derived by Hegstrom [16], but is more general. In fact we rederive in this section his results, as a simple verification of H_{LW}.

In the nonrelativistic limit, the interaction with a constant magnetic field is given by

$$H_M = \sum_a \mu_B \left[\vec{L}_a + (1+\kappa)\,\vec{\sigma}_a\right]\cdot\vec{B}\,, \tag{31}$$

where $\mu_B = -e/(2\,m)$. Relativistic corrections can be easily obtained for an arbitrary light atom and arbitrary state by taking all the terms which are linear in $\vec{B}$ from Eq. (30),

$$\begin{aligned}
\delta H_M &= \sum_{i=1}^{6} H_i\,, \qquad (32)\\
H_1 &= -\sum_a \frac{\mu_B}{2\,m^2}\,\vec{p}_a^{\,2}\,(\vec{L}_a+\vec{\sigma}_a)\cdot\vec{B}\,,\\
H_2 &= \sum_a \frac{\mu_B\,(1+2\,\kappa)}{4\,m}\,\frac{Z\,\alpha}{r_a^3}\,(\vec{r}_a\times\vec{\sigma}_a)\,(\vec{r}_a\times\vec{B})\,,\\
H_3 &= -\sum_{a>b}\frac{\mu_B\,\alpha}{4\,m\,r_{ab}^3}(1+2\,\kappa)[(\vec{\sigma}_b\times\vec{r}_{ab})\,(\vec{r}_b\times\vec{B})-(\vec{\sigma}_a\times\vec{r}_{ab})\,(\vec{r}_a\times\vec{B})]\,,\\
H_4 &= -\sum_{a>b}\frac{\mu_B\,\alpha}{2\,m\,r_{ab}^3}(1+\kappa)[(\vec{\sigma}_a\times\vec{r}_{ab})\,(\vec{r}_b\times\vec{B})-(\vec{\sigma}_b\times\vec{r}_{ab})\,(\vec{r}_a\times\vec{B})]\,,\\
H_5 &= \sum_{a>b}\frac{\mu_B\,\alpha}{2\,m}\left[(\vec{r}_a\times\vec{B})^i\,p_b^j+p_a^i\,(\vec{r}_b\times\vec{B})^j\right]\left(\frac{\delta^{ij}}{r_{ab}}+\frac{r_{ab}^i\,r_{ab}^j}{r_{ab}^3}\right),\\
H_6 &= -\sum_a \frac{\mu_B\,\kappa}{2\,m^2}\,(\vec{p}_a\cdot\vec{\sigma}_a)\,(\vec{p}_a\cdot\vec{B})\,.
\end{aligned}$$

These terms agree with the former work of Hegstrom in [16]. They were the basis for precise numerical calculations of g-factors for low-lying states of lithium performed by Yan in [20].

We have not considered here recoil and relativistic recoil corrections, which were studied in [16, 18]. However, we obtain below radiative corrections of order α^3 for 2^3P_J states of helium, with the aim of explaining the discrepancy with the experimental value [21].

The self-energy correction to the Zeeman effect, which is of order $\alpha^3\,\mu_B B$, vanishes for S-states, as was found by Hegstrom in [16]. The self-energy correction beyond the anomalous magnetic moment does not vanish only for states with nonzero angular momentum and is of nonrelativistic origin. The nonrelativistic Hamiltonian for the helium atom in the presence of an electromagnetic field in the length gauge is

$$H = H_0 + H_M - e\,\vec{r}_1\cdot\vec{E} - e\,\vec{r}_2\cdot\vec{E} \tag{33}$$

The self-energy correction obtained from Eq. (33) is

$$\Delta E = -\frac{2\,\alpha}{3\,\pi}\int_0^\epsilon d\omega\,\omega^3\,\langle\phi|\,(\vec{r}_1+\vec{r}_2)\,\frac{1}{H_0+H_M-E+\omega}\,(\vec{r}_1+\vec{r}_2)\,|\phi\rangle\,. \tag{34}$$

We assume here that ϕ is an eigenstate of H_0+H_M with energy E. Integration with respect to ω leads to

$$\Delta E = -\frac{2\,\alpha}{3\,\pi}\,\langle\phi|\,(\vec{r}_1+\vec{r}_2)\,(H_0+H_M-E)^3\,\ln|H_0+H_M-E|\,(\vec{r}_1+\vec{r}_2)\,|\phi\rangle\,, \tag{35}$$

where the polynomial terms in ϵ and the logarithmic term $\ln\epsilon$ do not contribute to B field dependence, and thus are omitted. This formula is equivalent to the one presented by Hegstrom in [16]. We now expand Eq. (35) including E in H_M, next neglect nonlogarithmic terms, which do not contribute, and obtain

$$\begin{aligned}\delta E &= -\frac{2\,\alpha}{3\,\pi}\,\langle\phi|\,(\vec{r}_1+\vec{r}_2)\,\Big(H_M-\langle H_M\rangle\Big)(H_0-E)^2\,3\,\ln|H_0-E|\,(\vec{r}_1+\vec{r}_2)\,|\phi\rangle\\ &= -\frac{2\,\alpha}{3\,\pi\,m^2}\,\langle\phi|\,(\vec{p}_1+\vec{p}_2)\,\Big(H_M-\langle H_M\rangle\Big)\,3\,\ln|H_0-E|\,(\vec{p}_1+\vec{p}_2)\,|\phi\rangle\,. \end{aligned}\tag{36}$$

If we assume that the state ϕ has specified value of magnetic quantum numbers m_l and m_s, then $(H_M-\langle H_M\rangle)\,|\phi\rangle = 0$ and

$$(H_M-\langle H_M\rangle)\,(\vec{p}_1+\vec{p}_2)\,|\phi\rangle = \Big[H_M-\langle H_M\rangle,\vec{p}_1+\vec{p}_2\Big]\,|\phi\rangle = \mu_B\,B^j\,i\,\epsilon^{jik}\,(p_1^k+p_2^k)\,|\phi\rangle\,. \tag{37}$$

After using this commutation relation, δE becomes

$$\delta E = -\frac{2\,\alpha}{\pi\,m^2}\,\mu_B\,B^j\,i\,\epsilon^{jik}\,\langle m_l|\,(p_1+p_2)^i\,\ln|H_0-E|\,(p_1+p_2)^k\,|m_l\rangle\,. \tag{38}$$

It is convenient to express the Zeeman effect in terms of the orbital g_l factor, which is defined by $E = \mu_B\, B\, m_l\, g_l$

$$\delta g_l = -\frac{2\,\alpha}{\pi\, m^2}\, i\,\epsilon^{3ik}\, \frac{3}{l(l+1)(2\,l+1)} \sum_{m_l=-l}^{l} m_l \langle m_l|\, (p_1+p_2)^i\, \ln|H_0-E|\, (p_1+p_2)^k\, |m_l\rangle\,. \quad (39)$$

This is a general expression which is valid for any state. We turn now to the particular case of 2^3P states ($l=1$) of helium, and convert this expression to a more convenient form. The factor m_l under the sum is replaced by $m_l\,|m_l\rangle = L_3\,|m_l\rangle$. The resulting sum can be expressed in the Cartesian basis of states $|i\rangle$ as follows

$$\sum_{m_l=-1}^{1} \langle m_l|\hat{Q}|m_l\rangle = 3\sum_{i=1}^{3}\langle i|\hat{Q}|i\rangle\,, \quad (40)$$

with nonstandard normalization $\langle i|j\rangle = \delta^{ij}/3$. The third component of the angular momentum operator acts on state $|i\rangle$ according to $L_3|j\rangle = i\,\epsilon^{3jk}\,|k\rangle$. In this way one obtains the final expression for δg_l

$$\delta g_l = \frac{\alpha^3}{\pi\, m^2}\,(\delta_{in}\,\delta_{kj} - \delta_{ij}\,\delta_{kn})\,\langle n|(p_1+p_2)^i\, \ln|H_0-E|\,(p_1+p_2)^k\,|j\rangle\,. \quad (41)$$

For the numerical calculation we use exponential basis set of functions $\phi = e^{-\alpha r_1 - \beta r_2 - \gamma r_{12}}$ times the angular momentum factor in Cartesian coordinates [22]. The expression in Eq. (41) involves implicit sums over the states with positive parity and angular momenta equal to 0,1,2. We follow here the method for the calculation of Bethe logarithms in helium presented in [22] and more recently in [23], and obtain the result

$$\delta g_l = \frac{\alpha^3}{\pi}\, 0.264\,706(1) \; = 0.032\,742\,4(1)\cdot 10^{-6}\,. \quad (42)$$

This was the last unknown correction to the g_l factor of order α^3 for helium 2^3P state. This self-energy correction has been analyzed in [18] and [24]. Authors of [18] present two numerical results, 0.0179(9) versus 0.0239(9), and Authors of [24] identified a term omitted in [18] which is equal to half of either of these two previous numbers. The result in Eq. (42) is complete and accurate to all digits shown. However, it is too small and of opposite sign to explain the following discrepancy. The theoretical result [19] is

$$g_l' - g_l = [10.719\,291\,348(19) + 0.032\,742\,4(1)]\cdot 10^{-6} = 10.752\,0337\,5(1)\cdot 10^{-6}\,. \quad (43)$$

where we followed notation from Ref. [17], $g_l = 1 - m/m_N$ and the uncalculated higher order terms are not included in the error estimate. The experimental result $g_l' - g_l = 4.9(2.9)\cdot 10^{-6}$

[21] differs by 2 standard deviations from that in Eq. (43). Before going any further in the calculation of higher order corrections to g_l-factor, this experimental value should be confirmed and improved.

VI. RELATIVISTIC CORRECTIONS TO TRANSITION RATES

The long wavelength Hamiltonian H_{LW} is particularly convenient for determination of relativistic corrections to atomic transition rates. The one-photon transition rate $\mathcal{A}$ between two atomic states is

$$\mathcal{A} = 2\,\alpha\,|\omega| \int \frac{d\Omega_k}{4\,\pi} \mathcal{T}^i\,\mathcal{T}^{*j}\left(\delta^{ij} - \frac{k^i\,k^j}{k^2}\right). \tag{44}$$

where $\omega = |\vec{k}|$. If the given atom can be treated in the nonrelativistic approximation, than the transition operator $\mathcal{T}$ is obtained from the Schrödinger-Pauli Hamiltonian

$$\vec{\mathcal{T}} = \langle\phi|\frac{\vec{p}}{m}\,e^{i\,\vec{k}\cdot\vec{r}} + \frac{i}{2\,m}\,\vec{\sigma}\times\vec{k}\,e^{i\,\vec{k}\cdot\vec{r}}|\psi\rangle\,. \tag{45}$$

For heavy atoms and ions, various relativistic approaches are being used, such as RCI, RMBPT or MCDF and one-photon transition rates are obtained from the matrix element of $\alpha\,e^{i\,\vec{k}\cdot\vec{r}}$. As it was pointed out by Johnson in [25], the so called negative energy states can play a significant role for rates of some forbidden transitions, and it is not clear to which extend the commonly used MCDF approach includes them. For light systems one can obtain all relativistic corrections including these negative energy contributions in a systematic approach and derive effective operators which govern a given transition. The Hamiltonian H_{LW} serves for these purposes. We derive complete relativistic corrections $O(\alpha^2)$ to $E1, M1$ and $E2$ transitions and include anomalous magnetic moment for $E1$ transitions. This Section is based on two former works, [26] and [10]. The transition energy (frequency) ω is

$$\omega = \langle\phi|H_0 + \delta H|\phi\rangle - \langle\psi|H_0 + \delta H|\psi\rangle\,. \tag{46}$$

where δH is defined after Eq. (29). The transition current j in the nonrelativistic theory j_0 acquires various relativistic corrections $j = j_0 + \delta j$. The transition amplitude $\mathcal{T}^i$ due to photon emission or absorption is then

$$\mathcal{T}^i = \langle\phi|\delta j^i|\psi\rangle + \langle\phi|\,j_0^i\,\frac{1}{(E_\psi - H_0)'}\,\delta H\,|\psi\rangle + \langle\phi|\,\delta H\,\frac{1}{(E_\phi - H_0)'}\,j_0^i\,|\psi\rangle\,. \tag{47}$$

$\vec{j}$ is obtained from the Hamiltonian H_{LW} as a coefficient of the photon polarization vector $\vec{\epsilon}$ from the vector potential $\vec{A}$

$$\vec{A}(\vec{r}) = \vec{\epsilon}\, e^{i\vec{k}\cdot\vec{r}-i\,\omega\,t}. \tag{48}$$

Consistently with this, $\vec{E}$ and $\vec{B}$ fields are

$$\vec{E} \;=\; i\,\omega\;\vec{\epsilon}\,e^{i\vec{k}\cdot\vec{r}-i\,\omega\,t}, \tag{49}$$

$$\vec{B} \;=\; i\,\vec{k}\times\vec{\epsilon}\,e^{i\vec{k}\cdot\vec{r}-i\,\omega\,t}. \tag{50}$$

For $E1$ transition one obtains

$$\vec{j}_{E1} = i\,k\left[\sum_a \vec{r}_a\left(1-\frac{k^2\,r_a^2}{30}\right)+\frac{i\,k}{12\,m}\left(\vec{L}_a\times\vec{r}_a+\vec{r}_a\times\vec{L}_a\right)+\frac{i\,k\,\kappa}{4\,m}\,\vec{r}_a\times\vec{\sigma}_a\right], \tag{51}$$

where we denote by $k=|\vec{k}|\equiv\omega$ and we used the following decomposition into irreducible parts

$$r^i\,r^j\,r^k = (r^i\,r^j\,r^k)^{(3)}+\frac{r^2}{5}\left(r^i\,\delta^{jk}+r^j\,\delta^{ik}+r^k\,\delta^{ij}\right). \tag{52}$$

It is a remarkable fact that relativistic effects cancel out for $\vec{j}_{E1}$, with the exception for the presence of the anomalous magnetic moment κ. Obviously κ is not a complete radiative correction. There are radiative corrections to energies, wave functions, and the vertex. The complete treatment has recently been performed for hydrogenic atoms in [27], where Authors observed a strong cancellations between various radiative corrections. A similar approach can be applied for few electron atoms when precise values for transition rates become available.

For $E2$ transition one obtains ($\kappa=0$)

$$\begin{aligned} j^i_{E2} \;=\; & \sum_a -\frac{k\,k^j}{2}\left(r^i_a\,r^j_a-\frac{\delta^{ij}}{3}\,r_a^2\right)\left(1-\frac{k^2\,r_a^2}{28}\right)+\frac{i\,k^2}{48\,m}\,k^j\left[r^i_a\,(\vec{r}_a\times\vec{L}_a)^j+r^j_a\,(\vec{r}_a\times\vec{L}_a)^i+\text{h.c.}\right]\\ & +\frac{i\,k^2}{48\,m}\,k^j\left[r^i_a\,(\vec{r}_a\times\vec{\sigma}_a)^j+r^j_a\,(\vec{r}_a\times\vec{\sigma}_a)^i\right]+\frac{k}{16\,m^2}\,k^j\left(\sigma^i_a\,L^j_a+\sigma^j_a\,L^i_a-\frac{2}{3}\,\delta^{ij}\,\vec{\sigma}_a\cdot\vec{L}_a\right) \end{aligned} \tag{53}$$

where we used the following decomposition into irreducible parts

$$r^i\,r^j\,Q^k \;=\; (r^i\,r^j\,Q^k)^{(3)}+\epsilon^{ikl}\,T^{lj}+\epsilon^{jkl}\,T^{li}+\delta^{ik}\,T^j+\delta^{jk}\,T^i+\delta^{ij}T'^k\,, \tag{54}$$

$$T^{ij} \;=\; \frac{1}{6}\left[r^i\,(\vec{r}\times\vec{Q})^j+r^j\,(\vec{r}\times\vec{Q})^i\right], \tag{55}$$

$$T^i \;=\; \frac{1}{10}\left(3\,r^i\,\vec{r}\cdot\vec{Q}-r^2\,Q^i\right), \tag{56}$$

$$T'^i \;=\; \frac{1}{5}\left(2\,r^2\,Q^i-r^i\,\vec{r}\cdot\vec{Q}\right), \tag{57}$$

and

$$r^i\,r^j\,r^k\,r^l \;=\; (r^i\,r^j\,r^k\,r^l)^{(4)} + \frac{r^2}{7}\Big[\delta^{ij}(r^k\,r^l)^{(2)} + \delta^{ik}(r^j\,r^l)^{(2)} + \delta^{il}(r^j\,r^k)^{(2)} + \delta^{jk}(r^i\,r^l)^{(2)} + \delta^{jl}(r^i\,r^k)^{(2)} + \delta^{kl}(r^i\,r^j)^{(2)}\Big] + (r^i\,r^j\,r^k\,r^l)^{(0)}\,. \tag{58}$$

The spin dependent terms have already been derived from H_{BP} in [10]. Here we include the spin independent terms, and present the result in a simpler but equivalent form. It is interesting to note that j_{E2} in the above can be expressed in terms of one-electron operators only.

For $M1$ transition one obtains ($\kappa = 0$)

$$\vec{j}_{M1} \;=\; \frac{i\,\vec{k}}{m}\times\sum_a\Big(\vec{\sigma}_a\,T_a + \vec{T}_a + \hat{T}_a\cdot\vec{\sigma}_a\Big)\,, \tag{59}$$

$$T_a \;=\; -\frac{1}{2} + \frac{k^2}{12}\,r_a^2 + \frac{p_a^2}{3\,m^2} - \frac{1}{6\,m}\,\frac{Z\,\alpha}{r_a} + \sum_{b,b\neq a}\frac{1}{6\,m}\,\frac{\alpha}{r_{ab}}\,, \tag{60}$$

$$\vec{T}_a \;=\; -\frac{\vec{L}_a}{2}\bigg(1 - \frac{k^2\,r_a^2}{10} - \frac{p_a^2}{2\,m^2}\bigg) + \sum_{b,b\neq a}\frac{\alpha}{4\,m\,r_{ab}^3}\Big(r_{ab}^2\,\vec{r}_a\times\vec{p}_b + \vec{r}_a\times\vec{r}_{ab}\,\vec{r}_{ab}\cdot\vec{p}_b\Big)\,, \tag{61}$$

$$T_a^{ij} \;=\; -\frac{k^2}{20}\,r_a^i\,r_a^j - \frac{1}{8\,m^2}\,p_a^i\,p_a^j + \frac{Z\,\alpha}{4\,m\,r_a^3}\,r_a^i\,r_a^j - \sum_{b,b\neq a}\frac{\alpha}{4\,m\,r_{ab}^3}\,r_{ab}^i\,r_{ab}^j + \frac{\delta^{ij}}{3}\bigg[\frac{k^2}{20}\,r_a^2 + \frac{p_a^2}{8\,m^2} - \frac{Z\,\alpha}{4\,m\,r_a} + \sum_{b,b\neq a}\frac{\alpha}{4\,m\,r_{ab}}\bigg]\,, \tag{62}$$

where we used the identity

$$k^2\,r_a^i\,r_a^j \to [H_0,[H_0,r_a^i\,r_a^j]] = -\frac{2}{m^2}\,p_a^i\,p_a^j - \frac{2\,Z\,\alpha}{m}\,\frac{r_a^i\,r_a^j}{r_a^3} - \sum_{b\neq a}\frac{\alpha}{m}\left(\frac{r_{ab}^i\,r_a^j}{r_{ab}^3} + \frac{r_{ab}^j\,r_a^i}{r_{ab}^3}\right), \tag{63}$$

to simplify the results for T_a^{ij} and T_a. j_{M1} has already been presented in the literature. The scalar part T_a was derived by Feinberg and Sucher in [28], the vector $\vec{T}_a$ and tensor T_a^{ij} parts together with the scalar one were derived by us using H_{BP} in [10], however with one mistake. The third term for $\vec{T}_a$ in Eq. (61) had the factor 1/2 instead of 1/4 as in the above. These formulas can be used for the calculations of relativistic corrections to transition rates. They are particularly suited for forbidden transitions, where nonrelativistic matrix elements are exactly equal to zero. Let us investigate in more details the historically important $M1$: $2^3S_1 \to 1^1S_0$ transition in atomic helium. We closely follow here the former work in [26]. The transition current j_{M1} is

$$\vec{j}_{M1} \;=\; \sum_a\frac{i\,\vec{k}}{m}\times\vec{\sigma}_a\left(\frac{k^2}{12}\,r_a^2 + \frac{p_a^2}{3\,m^2} - \frac{1}{6\,m}\,\frac{Z\,\alpha}{r_a} + \sum_{b,b\neq a}\frac{1}{6\,m}\,\frac{\alpha}{r_{ab}}\right)$$

$$\approx \frac{i}{m}\,\vec k\times\frac{(\vec\sigma_1-\vec\sigma_2)}{2}\biggl[\frac{k^2}{12}\,(r_1^2-r_2^2)+\frac{1}{3\,m^2}\,(p_1^2-p_2^2)-\frac{1}{6\,m}\,\biggl(\frac{Z\,\alpha}{r_1}-\frac{Z\,\alpha}{r_2}\biggr)\biggr]\,, \qquad (64)$$

and the $M1$ $2^3S_1\to 1^1S_0$ transition rate is

$$\mathcal{A}_{M1} = 2\,\alpha\,k\int\frac{d\Omega_k}{4\,\pi}\,\biggl(\delta^{ij}-\frac{k^i\,k^j}{k^2}\biggr)\langle j^i_{M1}\rangle\,\langle j^{*j}_{M1}\rangle \qquad (65)$$

$$= \frac{4}{3}\,\alpha\,k^3\,\biggl|\langle 2^3S|\,\frac{k^2}{12}\,(r_1^2-r_2^2)+\frac{1}{3\,m^2}\,(p_1^2-p_2^2)-\frac{1}{6\,m}\,\biggl(\frac{Z\,\alpha}{r_1}-\frac{Z\,\alpha}{r_2}\biggr)\,|1^1S\rangle\biggr|^2. \qquad (66)$$

The matrix element was evaluated in the exponential basis set with the result

$$\langle 2^3S|\,\frac{k^2}{12}\,(r_1^2-r_2^2)+\frac{1}{3\,m^2}\,(p_1^2-p_2^2)-\frac{1}{6\,m}\,\biggl(\frac{Z\,\alpha}{r_1}-\frac{Z\,\alpha}{r_2}\biggr)\,|1^1S\rangle=\alpha^2\,0.318\,985\,2\,, \qquad (67)$$

which together with $k = 0.728\,494\,998\,8$ (in atomic units) leads to a transition rate of $\mathcal{A}_{M1} = \frac{4}{3}\,(2\,R\,c)\,2\,\pi\,\alpha^9\,k^3\,(0.318\,985\,2)^2 = 1.272\,426\cdot 10^{-4}\,s^{-1}$, where physical constants are from [29].

VII. ELECTRODYNAMICS OF EDM

An interesting issue in electrodynamics is the treatment of elementary particles possessing electric dipole moments (EDM). It can be treated almost in the same way as the anomalous magnetic moment. Let us briefly introduce all possible coupling to electromagnetic fields which preserve Lorentz invariance. The electromagnetic current of a spin 1/2 particle can be expressed in terms of 4 Lorentz invariants

$$j^\mu = \bar u(p')\biggl\{F_1(q^2)\,\gamma^\mu-\frac{i}{2\,m}\,F_2(q^2)\,\sigma^{\mu\nu}\,q_\nu$$
$$+\frac{a(q^2)}{m^2}\Bigl(\not q\,q^\mu-q^2\,\gamma^\mu\Bigr)\,\gamma^5-\frac{d(q^2)}{2\,M}\,\sigma^{\mu\nu}\,q_\nu\,\gamma^5\biggr\}\,u(p)\,. \qquad (68)$$

The a formfactor is the anapole moment [30], and breaks invariance under spatial inversions P. d is a dimensionless electric dipole moment [31] which breaks both parity P and time reversal T invariance. While we do not discuss here the origin of d, we investigate the electromagnetic interaction of a charged particle of spin 1/2 having electric dipole moment $\vec D$

$$\vec D = \frac{e\,d}{2\,m}\,\vec\sigma\,. \qquad (69)$$

In the following we neglect the anapole moment a and also neglect the q^2 dependence of formfactors, so we have $F_1 = 1$ and $F_2 = \kappa$, the anomalous magnetic moment. The Dirac

Hamiltonian that includes κ and d is

$$H = \vec{\alpha}\cdot\vec{\pi} + \beta\, m + e\, A^0 + \frac{e\,\kappa}{2\,m}\left(i\,\beta\,\vec{\alpha}\cdot\vec{E} - \beta\,\vec{\Sigma}\cdot\vec{B}\right) - \frac{e\,d}{2\,m}\left(i\,\beta\,\vec{\alpha}\cdot\vec{B} + \beta\,\vec{\Sigma}\cdot\vec{E}\right). \tag{70}$$

We are interested in the nonrelativistic expansion of an interaction of a dipole moment with the electromagnetic field and perform two transformations. The first one, due to Schiff [32], eliminates the leading interaction of a dipole moment with the electric field

$$H' = e^{i\,S}\,(H - i\,\partial_t)\,e^{-i\,S} = H + [i\,S, H - i\,\partial_t]\,, \tag{71}$$

where

$$S = -\frac{d}{2\,m}\,\beta\,\vec{\Sigma}\cdot\vec{\pi}\,. \tag{72}$$

We have assumed that d is small, so quadratic and higher orders term in d are neglected. The transformed Hamiltonian H' is

$$\begin{aligned} H' \;=\; & \vec{\alpha}\cdot\vec{\pi} + \beta\, m + e\, A^0 + \frac{e\,\kappa}{2\,m}\,(i\,\beta\,\vec{\alpha}\cdot\vec{E} - \beta\,\vec{\Sigma}\cdot\vec{B}) \\ & -i\,\frac{d}{m}\,\beta\,\gamma^5\,\pi^2 + i\,\frac{e\,d}{2\,m}\,\beta\,\vec{\alpha}\cdot\vec{B} + \frac{d}{2\,m}\,\frac{e\,\kappa}{2\,m}\Big[\gamma^5\,(\vec{\pi}\cdot\vec{E} + \vec{E}\cdot\vec{\pi}) \\ & +i\,\vec{\alpha}\cdot(\vec{\pi}\times\vec{E} + \vec{E}\times\vec{\pi}) - \vec{\Sigma}\cdot(\vec{\pi}\times\vec{B} - \vec{B}\times\vec{\pi})\Big]\,. \end{aligned} \tag{73}$$

The second transformation is a Foldy-Wouthuysen transformation modified by presence of d. We calculate only the leading terms which are proportional to $1/m^2$, and use standard decomposition of the Hamiltonian into odd and even parts

$$H' = \beta\, m + \Theta + \mathcal{E}. \tag{74}$$

The second transformation is $S = -i\,\beta\,\Theta/(2\,m)$, and the new Hamiltonian H'' becomes

$$H'' = \frac{\beta}{2\,m}\,\Theta^2 + \mathcal{E} = \frac{\pi^2}{2\,m} + e\,A^0 - \frac{e\,(1+\kappa)}{2\,m}\,\vec{\sigma}\cdot\vec{B} + \frac{e\,d\,(1+\kappa)}{4\,m^2}\,(\vec{\pi}\times\vec{\sigma}\cdot\vec{B} + \vec{B}\cdot\vec{\pi}\times\vec{\sigma}). \tag{75}$$

The interaction of a dipole moment with the electric field is eliminated, and only the interaction with the magnetic field remains. This is the modified version of the shielding theorem by Schiff [32]. We assume now that the atomic nucleus has a nonvanishing EDM, and change notation accordingly $e \to -Z\,e, m \to M, \vec{\sigma}/2 \to \vec{I}$. The Hamiltonian H_N of the nucleus is ($I = 1/2$)

$$H_N = \frac{\pi^2}{2\,M} + e\,A^0 + \frac{Z\,e\,(1+\kappa)}{M}\,\vec{I}\cdot\vec{B} - \frac{Z\,e\,d\,(1+\kappa)}{2\,M^2}\,(\vec{\pi}\times\vec{I}\cdot\vec{B} + \vec{B}\cdot\vec{\pi}\times\vec{I})\,. \tag{76}$$

We aim now to derive a PT-odd electron-nucleus interaction, which results from Eq. (76), in the same way as H_{BP} was derived in Eq. (15). The Pauli term $Z\,e\,(1+\kappa)/M\,\vec{I}\cdot\vec{B}$ leads to the interaction Hamiltonian, which is analogous to δH_{ab} in Eq. (14)

$$\delta H_{\rm hfs} = \sum_a \frac{m}{M}\,(1+\kappa)\left[\frac{4}{3}\,\frac{Z\,\alpha}{m^2}\,\vec{I}\cdot\vec{\sigma}_a\,\pi\,\delta^3(r_a)+\frac{Z\,\alpha}{m^2}\,\frac{\vec{r}_a\times\vec{\pi}_a}{r_a^3}\cdot\vec{I}-\frac{Z\,\alpha}{2\,m^2}\,\frac{I^i\,\sigma_a^j}{r_a^3}\left(\delta^{ij}-3\,\frac{r_a^i\,r_a^j}{r_a^2}\right)\right]. \quad (77)$$

The PT-odd interaction Hamiltonian can be obtained from Eq. (77) by the replacement $\vec{I}\cdot\vec{B}\rightarrow -d/(2\,M)\,(\vec{\pi}\times\vec{I}\cdot\vec{B}+\vec{B}\cdot\vec{\pi}\times\vec{I})$, so one obtains

$$\begin{aligned}\delta H_{PT} \;=\; & \sum_{a,b}\frac{d\,(1+\kappa)}{2\,M}\,\frac{Z\,\alpha}{m\,M}\left\{\frac{4}{3}\left[\vec{p}_b\times\vec{I}\cdot\vec{\sigma}_a\,\pi\,\delta^3(r_a)+\pi\,\delta^3(r_a)\,\vec{p}_b\times\vec{I}\cdot\vec{\sigma}_a\right]\right.\\ & +\left[\frac{(\vec{r}_a\times\vec{p}_a)}{r_a^3}\cdot(\vec{p}_b\times\vec{I})+(\vec{p}_b\times\vec{I})\cdot\frac{(\vec{r}_a\times\vec{p}_a)}{r_a^3}\right]\\ & \left.-\frac{1}{2}\left[(\vec{p}_b\times\vec{I})^i\,\frac{\sigma_a^j}{r_a^3}\left(\delta^{ij}-3\,\frac{r_a^i\,r_a^j}{r_a^2}\right)+\left(\delta^{ij}-3\,\frac{r_a^i\,r_a^j}{r_a^2}\right)\frac{\sigma_a^j}{r_a^3}\,(\vec{p}_b\times\vec{I})^i\right]\right\}. \quad (78)\end{aligned}$$

where we set external field to 0, so $\pi_a\rightarrow p_a$ and the momentum of nucleus $p\rightarrow-\sum_b p_b$. This Hamiltonian describes the leading relativistic effects which prevent complete shielding of the nuclear electric dipole for light atoms. The atomic EDM can be obtained in the second order of perturbation calculus

$$\vec{D} = 2\,e\,\langle\phi|\sum_a\vec{r}_a\,\frac{1}{(E-H)'}\,\delta H_{PT}|\phi\rangle\,. \quad (79)$$

For atomic states with total angular momentum $L=0$ and total spin $S=0$ only the second term in δH_{PT} contributes. This term has been originally derived by Schiff in [32],

$$\vec{D} = \vec{I}\,\frac{Z\,e\,d}{2\,M}\,\frac{2\,\alpha\,(1+\kappa)}{3\,m\,M}\,\langle\phi|\sum_c\vec{r}_c\,\frac{1}{(H_0-E)'}\sum_{a,b}\left[\frac{(\vec{p}_a\times\vec{r}_a)}{r_a^3}\times\vec{p}_b+\vec{p}_b\times\frac{(\vec{r}_a\times\vec{p}_a)}{r_a^3}\right]|\phi\rangle\,. \quad (80)$$

It is interesting to note that inspite of this agreement, the original derivation by Schiff relied implicitly on the assumption that there is no relativistic correction to the electron-nucleus interaction coming from the nuclear EDM on the level of Breit-Pauli Hamiltonian. So, it was neglected the coupling of EDM to magnetic field in Eq. (70), which gives such a correction. Moreover, it was omitted the commutator of $-d/(2\,m)\,\vec{\sigma}\cdot\vec{p}$ with the spin-independent electron-nucleus magnetic interaction.

Following Schiff, we summarize this section by the numerical evaluation of atomic EDM for ground state of ^{3}He. The second order matrix element in Eq. (79) is calculated using the exponential basis set [22], with the result $\langle\phi|\ldots|\phi\rangle = m\,\alpha\,15.3209(1)$. Using this result, one obtains for the atomic EDM of ^{3}He

$$\vec{D} = \vec{\sigma}\left[-\frac{Z\,e\,d}{2\,M}\right]\left[-\frac{Z\,e\,(1+\kappa)}{2\,M}\right]\frac{m\,\alpha^2}{Z\,e}\,\frac{2}{3}\,15.320\,9(1) = \vec{\sigma}\,D_h\cdot 1.575\,44(1)\,10^{-7}\,. \tag{81}$$

where the term in the first square brackets is the helion EDM D_h, and the term in the second square brackets is the helion magnetic moment $\mu_h = -2.127\,497\,723(25)\,\mu_N$ (nuclear magneton) [29]. In a similar approach atomic EDM can be calculated for other light atoms. However, for heavy atoms the more significant effect comes from the q^2 dependence of $d(q^2)$ and $F_1(q^2)$, which can be expressed in terms of the so called Schiff moment [31]. Although EDM has not yet been observed, precise measurements [33] have put strong upper limits on it. Moreover new experiments are planned, for example for the Radium atom [34, 35], due to a few enhancements such as accidental degeneracy of two atomic states and the large nuclear charge [36].

VIII. SUMMARY

We have presented an approach to quantum electrodynamics of light few-electron atoms which explores different scales of electron-electron interactions and interaction with the quantum or external electromagnetic fields. We obtain a nonrelativistic expansion using a sequence of transformations which lead to the long wavelength Hamiltonian H_{LW}. As an application of this approach we considered three cases: relativistic and radiative corrections to magnetic moments, relativistic corrections to shielding of the electric dipole moment and relativistic corrections to transition rates. Each case is summarized by an example of numerical calculations. Other possible applications involve dynamic polarizability and related relativistic corrections to the Casimir-Polder potential. For light closed shell atoms, such as helium, the interaction potential can be derived from the Hamiltonian obtained from H_I in Eq. (30) by neglecting spin dependent and higher order terms

$$\begin{aligned} H_I \;\approx\; & \sum_a -e\,\vec{r}_a\cdot\vec{E} - \frac{e}{2}\left(r_a^i\,r_a^j - \frac{\delta^{ij}}{3}\,r_a^2\right)E^i_{,j} - \frac{e}{30}\,r_a^2\,r_a^i\,E^i_{,jj} - \\ & \frac{e}{6\,m}\,(L_a^i\,r_a^j + r_a^j\,L_a^i)\,B^i_{,j} + \frac{e^2}{8\,m^2}\,(\vec{r}_a\times\vec{B})^2\,. \end{aligned} \tag{82}$$

The most recent treatments in the literature [37–39] are rather incomplete and do not include, for example, the 4th term in Eq. (82). The main motivation for developing QED is the precise calculation of higher order corrections in one and few-electron atoms to properties such as energy levels, magnetic moments, polarizabilities, and transition rates. The current experimental precision for helium fine structure of 2^3P_J [40] levels or $2^3S_1 - 2^3P_J$ [41] transition frequency is much larger than theoretical predictions. What is lacking are corrections of order $m\,\alpha^7$, which have been calculated only for hydrogen-like systems. We think the approach presented here can be used to systematically derive QED corrections. Apart from developing QED, one has to be able to calculate accurate nonrelativistic wave functions. For this purpose correlated basis sets such as Hylleraas, Gaussians, and exponential are being developed for few-electron atoms, and several promising results have been obtained recently, for example, calculations of Lamb shift for helium [6, 7], lithium [42, 43], and beryllium atoms [44].

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