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The multipolar Hamiltonian in QED for moving atoms and ions

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Abstract
In this paper we establish a multipolar Hamiltonian in QED for an arbitrary system of moving charges. The particular cases of 2 and 3 charges are considered together with the Breit–Fermi Hamiltonian for two fermions. A scaling analysis shows the perturbative character of the dipole approximation of the multipolar Hamiltonian. The electric-dipole and magnetic-dipole terms of the dilated Hamiltonian are of order 1 and 2, respectively, with respect to the fine structure constant.

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1. Introduction

In this paper we review the multipolar Hamiltonian in QED describing the interaction of a confined system of charges with transverse electromagnetic fields. As usual, the multipolar Hamiltonian is deduced from the conventional one in Coulomb gauge obtained through minimal coupling by applying a canonical transformation (see [CTDRG, CrTh]). In the case of moving atoms or ions we are interested in, the canonical transformation is expressed in terms of the polarization field relative to the centre-of-mass coordinates. Thus we obtain the multipolar Hamiltonian for an arbitrary system of charges in Cartesian coordinates. In the case of a neutral system of charges we then get an obviously gauge invariant Hamiltonian because it is only expressed in terms of the electric and magnetic fields. The canonical transformation is nothing else than a generalized Power–Zienau–Woolley transformation. We only observe that the canonical transformation introduced in [LBBL] to deal with a neutral system of two opposite charges still works in the general case of any system of charges, as far as the centre-of-mass is not considered as a dynamical variable in contrast to [BBL].

Thus, after having established the multipolar Hamiltonian and its dipole approximation, it is easy to introduce new coordinates, as the Jacobi ones, in order to describe more precisely the coupling between the centre-of-mass coordinates and the internal ones due to the transverse electromagnetic fields. Moreover a scaling, i.e. a change of units, initiated by [BFS] and [FFG], exhibits the perturbative character of the Hamiltonian with respect to the fine structure constant α. Writing down an Hamiltonian in the dipole approximation we get the electric-dipole term at first order in α; the Röntgen and the magnetic-dipole terms are obtained at second order in α. The necessity of the Röntgen interaction for moving atoms has been emphasized in [LBBL] and [W]. The magnetic-dipole term is neglected in comparison with the electric-dipole term in [LBBL] (see [BS, p 280]) and it is forgotten in [W]. Nevertheless, according to our scaling analysis, the magnetic-dipole term should be taken into consideration together with the Röntgen one. Furthermore, as far as we are interested in terms of second order in α, an electric-quadrupole term must be added to the electric-dipole, magnetic-dipole and Röntgen terms (see [F]).

The atoms and ions that we consider are moving either freely or in the presence of a static constant magnetic field. Hence we have to introduce an exterior electromagnetic field in the Hamiltonian.

When we consider examples, we restrict ourselves to the case of the two-body and three-body systems. The atoms and ions are non-relativistic. However, we give the example of the relativistic Breit–Fermi Hamiltonian for two fermions.

The paper is organized as follows. We first derive the general multipolar Hamiltonian for any non-relativistic system of charges. We then deduce the dipole approximation for two-body and three-body systems. The Breit–Fermi Hamiltonian for two fermions is also considered. We finally analyse the Hamiltonians by a scaling method, showing that, with respect to the fine structure constant, the magnetic-dipole and Röntgen terms are of higher order than the electric-dipole one.

Finally, in the appendix, we give a detailed proof of the expression of the magnetization fields with respect to the centre-of-mass coordinates.

2. The multipolar Hamiltonian

We consider a system of N charges $(e_\alpha)_{1\leqslant\alpha\leqslant N}$ with respective masses $(m_\alpha)_{1\leqslant\alpha\leqslant N}$ and spins $(S_\alpha)_{1\leqslant\alpha\leqslant N}$. The Hamiltonian for QED in Coulomb gauge is given by

$$H = \sum_{\alpha=1}^{N} \frac{1}{2m_\alpha}(p_\alpha - e_\alpha A(r_\alpha) - e_\alpha A_{\mathrm{ext}}(r_\alpha))^2 + \sum_{\alpha<\beta} \frac{e_\alpha e_\beta}{4\pi\varepsilon_0|r_\alpha - r_\beta|} - \sum_\alpha M_\alpha \cdot B(r_\alpha)$$
$$+ \frac{1}{2}\int \mathrm{d}^3 r \left(\frac{\Pi(r)^2}{\varepsilon_0} + \frac{B(r)^2}{\mu_0}\right) \qquad r_\alpha, r \in \mathbb{R}^3 \tag{1}$$

(see [CTDRG]).

Here $p_\alpha = -\mathrm{i}\hbar\nabla_\alpha$, $M_\alpha = g_\alpha \frac{e_\alpha}{2m_\alpha} S_\alpha$, where g_α is the Landé coefficient of the charge α, $A_{\mathrm{ext}}(\cdot)$ is an exterior vector potential. The units are those of [CTDRG].

Moreover, we have

$$A(r) = \sum_{\lambda=1,2} \int \mathrm{d}^3 k \left(\frac{\hbar}{2\varepsilon_0(2\pi)^3\omega(k)}\right)^{1/2} \left(a_\lambda(k)\varepsilon_\lambda(k)\,\mathrm{e}^{\mathrm{i}k\cdot r} + a_\lambda^*(k)\varepsilon_\lambda(k)\,\mathrm{e}^{-\mathrm{i}k\cdot r}\right) \tag{2}$$

$$B(r) = \mathrm{i} \sum_{\lambda=1,2} \int \mathrm{d}^3k \frac{1}{c} \left(\frac{\hbar\omega(k)}{2\varepsilon_0(2\pi)^3} \right)^{1/2} \left(a_\lambda(k) \left(\frac{k}{|k|} \wedge \varepsilon_\lambda(k) \right) \mathrm{e}^{\mathrm{i}k\cdot r} - a_\lambda^*(k) \left(\frac{k}{|k|} \wedge \varepsilon_\lambda(k) \right) \mathrm{e}^{-\mathrm{i}k\cdot r} \right) \tag{3}$$

$$\Pi(r) = -\mathrm{i} \sum_{\lambda=1,2} \int \mathrm{d}^3k \left(\frac{\hbar\varepsilon_0\omega(k)}{2(2\pi)^3} \right)^{1/2} \left(a_\lambda(k)\varepsilon_\lambda(k)\,\mathrm{e}^{\mathrm{i}k\cdot r} - a_\lambda^*(k)\varepsilon_\lambda(k)\,\mathrm{e}^{-\mathrm{i}k\cdot r} \right) \tag{4}$$

$$E(r) = -\frac{1}{\varepsilon_0}\Pi(r)$$

where $\omega(k) = c|k|$ and $\varepsilon_\lambda(k)$, $\lambda = 1, 2$, are real polarization vectors satisfying

$$\varepsilon_\lambda(k) \cdot \varepsilon_\mu(k) = \delta_{\lambda\mu} \qquad k \cdot \varepsilon_\lambda(k) = 0 \qquad \lambda, \mu = 1, 2.$$

$a_\lambda(k)$, $a_\lambda^*(k)$ are the usual annihilation and creation operators obeying the canonical commutation relations

$$[a_\lambda^\sharp(k), a_\mu^\sharp(k)] = 0 \qquad [a_\lambda(k), a_\mu^*(k')] = \delta_{\lambda\mu}\delta(k-k') \tag{5}$$

where $a^\sharp = a$ or a^*.

Let us remark that $A(r)$ commutes with $B(r)$ but not with $\Pi(r)$.

Let $P(r)$ be the polarization field relative to the centre-of-mass coordinate R:

$$P(r) = \sum_{\alpha=1}^{N} e_\alpha(r_\alpha - R) \int_0^1 \mathrm{d}\lambda\, \delta(r - R - \lambda(r_\alpha - R)) \tag{6}$$

where $R = \frac{1}{M}\sum_{\alpha=1}^{N} m_\alpha r_\alpha$ with $M = \sum_{\alpha=1}^{N} m_\alpha$.

The unitary transformation U to the multipolar Hamiltonian is given by

$$U = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\int \mathrm{d}^3r\, P(r)\cdot A(r)} = \mathrm{e}^{\mathrm{i}S} \tag{7}$$

where

$$S = \frac{1}{\hbar} \int \mathrm{d}^3r\; P(r) \cdot A(r). \tag{8}$$

We then have

$$\begin{aligned} U^{-1} p_\alpha U &= p_\alpha + \mathrm{i}[p_\alpha, S] = p_\alpha + \hbar\nabla_\alpha S \\ &= p_\alpha + e_\alpha A(r_\alpha) - e_T \frac{m_\alpha}{M} A(R) + \int \mathrm{d}^3r\; \Theta_\alpha(r) \wedge B(r) \qquad \alpha = 1, 2, \ldots, N \end{aligned} \tag{9}$$

where $e_T = \sum_{\alpha=1}^{N} e_\alpha$ and

$$\Theta_\alpha(r) = \sum_{\beta=1}^{N} e_\beta \int_0^1 \mathrm{d}\lambda \left(\lambda\delta_{\alpha\beta} - \frac{m_\alpha}{M}(\lambda - 1) \right) (r_\beta - R)\delta(r - R - \lambda(r_\beta - R)) \tag{10}$$

$\Theta_\alpha(r)$, $\alpha = 1, 2, \ldots, N$ are the magnetization fields relative to the centre-of-mass coordinate R.

Furthermore

$$U^{-1}A(r)U = A(r) \tag{11}$$

$$U^{-1}B(r)U = B(r) \tag{12}$$

$$U^{-1}\Pi(r)U = \Pi(r) + P(r). \tag{13}$$

The proof of (9) has been sketched by [LBBL] in the case of $N = 2$ and $e_T = 0$. A different version of Θ_α for an arbitrary system of charges is given in [BBL] to deal with the case where the centre-of-mass is considered as an independent dynamical variable,

(11) follows from

$$[A_i(r), A_j(r')] = 0 \qquad r, r' \in \mathbb{R}^3 \quad i, j = 1, 2, 3$$

(12) follows from

$$[A_i(r), B_j(r')] = 0 \qquad r, r' \in \mathbb{R}^3 \quad i, j = 1, 2, 3$$

(13) is the consequence of

$$[\Pi_i(r), A_j(r')] = -\mathrm{i}\hbar\delta^{\perp}_{ij}(r - r') \qquad r, r' \in \mathbb{R}^3 \quad i, j = 1, 2, 3.$$

For the sake of completeness we give a detailed proof of (9) in the appendix.

2.1. The dipole approximation of the multipolar Hamiltonian

We denote by H_{mult} the multipolar Hamiltonian given by

$$H_{\text{mult}} = U^{-1} H U.$$

By (1) and (9)–(13) we get

$$\begin{aligned} H_{\text{mult}} = \sum_{\alpha=1}^{N} \frac{1}{2m_\alpha}\left(p_\alpha - e_\alpha A_{\text{ext}}(r_\alpha) - e_T \frac{m_\alpha}{M} A(R) + \int \mathrm{d}^3 r\, \Theta_\alpha(r) \wedge B(r)\right)^2 \\ + \sum_{\alpha<\beta} \frac{e_\alpha e_\beta}{4\pi\varepsilon_0 |r_\alpha - r_\beta|} - \sum_\alpha M_\alpha \cdot B(r_\alpha) \\ + \frac{1}{2}\int \mathrm{d}^3 r \left(\frac{(\Pi(r) + P(r))^2}{\varepsilon_0} + \frac{B(r)^2}{\mu_0}\right). \end{aligned} \tag{14}$$

In particular, if $A_{\text{ext}}(\cdot) = 0$ or $A_{\text{ext}}(r_\alpha) = \frac{1}{2} B_0 \wedge r_\alpha$ where B_0 is a constant magnetic field and if the system of charges is neutral, H_{mult} is only expressed in terms of the electric field $E(r) = -\frac{1}{\varepsilon_0}\Pi(r)$ and the magnetic field $B(r)$. In that case H_{mult} is obviously gauge invariant. Let us first consider the case of two charges e_1 and e_2 with a constant magnetic field B_0. We will also consider the case of a free system of two charges.

In the case of an exterior constant magnetic field it is convenient to transform again H_{mult} by introducing a unitary transformation.

Let

$$V = \mathrm{e}^{\mathrm{i}\frac{e_1}{2} r_1 \cdot B_0 \wedge R}\, \mathrm{e}^{\mathrm{i}\frac{e_2}{2} r_2 \cdot B_0 \wedge R}.$$

Let $r = r_1 - r_2$ be the internal coordinate. We have

$$V = \mathrm{e}^{\mathrm{i}\frac{(e_1 m_2 - e_2 m_1)}{2M} r \cdot B_0 \wedge R}.$$

It is well known that

$$V^{-1} p_1 V = p_1 + \frac{e_1 m_2 - e_2 m_1}{2M} B_0 \wedge r_2$$
$$V^{-1} p_2 V = p_2 - \frac{e_1 m_2 - e_2 m_1}{2M} B_0 \wedge r_1$$

(see [GH]).

We then get

$$V^{-1}\left(p_1 - \frac{e_1}{2}B_0 \wedge r_1\right)V = p_1 - \frac{e_1}{2}\,B_0 \wedge r - \frac{m_1}{M}\frac{e_T}{2}\,B_0 \wedge r_2$$
$$V^{-1}\left(p_1 - \frac{e_2}{2}B_0 \wedge r_2\right)V = p_2 + \frac{e_2}{2}\,B_0 \wedge r - \frac{m_2}{M}\frac{e_T}{2}\,B_0 \wedge r_1.$$

Hence

$$\begin{aligned}V^{-1}H_{\text{mult}}V &= H'_{\text{mult}}\\ &= \frac{1}{2m_1}\left(p_1 - \frac{e_1}{2}B_0 \wedge r - \frac{m_1}{M}\frac{e_T}{2}B_0 \wedge R + \left(\frac{m_1}{M}\right)^2 \frac{e_T}{2}B_0 \wedge r\right.\\ &\quad \left. - e_T\frac{m_1}{M}A(R) + \int \mathrm{d}^3r'\Theta_1(r') \wedge B(r')\right)^2 + \frac{1}{2m_2}\left(p_2 + \frac{e_2}{2}B_0 \wedge r\right.\\ &\quad - \frac{m_2}{M}e_T B_0 \wedge R - \left(\frac{m_2}{M}\right)^2 \frac{e_T}{2}B_0 \wedge r - e_T\frac{m_2}{M}A(R)\\ &\quad \left. + \int \mathrm{d}^3r'\Theta_2(r') \wedge B(r')\right)^2 + \frac{e_1e_2}{4\pi\varepsilon_0|r_1 - r_2|} - M_1 \cdot B(r_1)\\ &\quad - M_2 \cdot B(r_2) + \frac{1}{2}\int \mathrm{d}^3r'\left(\frac{\Pi(r')^2}{\varepsilon_0} + \frac{B(r')^2}{\mu_0}\right)\\ &\quad + \int \mathrm{d}^3r'\frac{\Pi(r')\cdot P(r')}{\varepsilon_0} + \frac{1}{2\varepsilon_0}\int \mathrm{d}^3r' P(r')^2. \end{aligned} \tag{15}$$

Let P and p be the canonical variables to the centre-of-mass and internal motion, respectively. We then have

$$\begin{aligned}H'_{\text{mult}} &= \frac{1}{2m_1}\left(p + \frac{m_1}{M}P - \frac{1}{2}\left(e_1 - \left(\frac{m_1}{M}\right)^2 e_T\right)B_0 \wedge r - \frac{m_1}{M}\frac{e_T}{2}B_0 \wedge R\right.\\ &\quad \left. - e_T\frac{m_1}{M}A(R) + \int \mathrm{d}^3r'\Theta_1(r') \wedge B(r')\right)^2 + \frac{1}{2m_2}\left(-p + \frac{m_2}{M}P\right.\\ &\quad + \frac{1}{2}\left(e_2 - \left(\frac{m_2}{M}\right)^2 e_T\right)B_0 \wedge r - \frac{m_2}{M}\frac{e_T}{2}B_0 \wedge R - e_T\frac{m_2}{M}A(R)\\ &\quad \left. + \int \mathrm{d}^3r'\Theta_2(r') \wedge B(r')\right)^2 + \frac{e_1e_2}{4\pi\varepsilon_0|r|} - M_1 \cdot B(r_1) - M_2 \cdot B(r_2)\\ &\quad + \frac{1}{2}\int \mathrm{d}^3r'\left(\frac{\Pi(r')^2}{\varepsilon_0} + \frac{B(r')^2}{\mu_0}\right) + \int \mathrm{d}^3r'\frac{\Pi(r')\cdot P(r')}{\varepsilon_0} + \frac{1}{2\varepsilon_0}\int \mathrm{d}^3r' P(r')^2. \end{aligned} \tag{16}$$

In order to get the dipole approximation of the Hamiltonians (14) and (16), we have to introduce the dipole approximation of $P(r)$ and $\Theta_\alpha(r)$. These approximations are obtained from (6) and (10) by retaining the leading terms in the expansions of the Dirac δ distributions appearing in the vectors $P(r)$ and $\Theta_\alpha(r)$ in powers of $r_\alpha - R$.

Let $P_{\text{dip}}(r)$ and $\Theta_{\alpha,\text{dip}}(r)$ denote the dipole approximations of $P(r)$ and $\Theta_\alpha(r)$, respectively. We have, for any system of N charges,

$$P_{\text{dip}}(r') = \left(\sum_{\alpha=1}^{N} e_\alpha(r_\alpha - R)\right)\delta(r' - R) \tag{17}$$

$$\Theta_{\alpha,\text{dip}}(r') = \left(\sum_{\beta=1}^{N} e_\beta(r_\beta - R)\int_0^1 \mathrm{d}\lambda\left(\lambda\delta_{\alpha\beta} - \frac{m_\alpha}{M}(\lambda - 1)\right)\right)\delta(r' - R). \tag{18}$$

Let

$$d = \sum_{\alpha=1}^{N} e_\alpha (r_\alpha - R) \tag{19}$$

d is the electric-dipole moment vector of the system of N charges. Thus, for $N = 2$, we get $d = \left(\frac{e_1 m_2 - e_2 m_1}{M}\right) r$.

We then have

$$P_{\text{dip}}(r') = d\delta(r' - R) \tag{20}$$

$$\Theta_{\alpha,\text{dip}}(r') = \frac{1}{2}\left(e_\alpha(r_\alpha - R) + \frac{m_\alpha}{M} d\right)\delta(r' - R) \tag{21}$$

$$\frac{1}{\varepsilon_0}\int \mathrm{d}^3 r' \Pi(r') \cdot P_{\text{dip}}(r') = -d \cdot E(R) \tag{22}$$

$$\int \mathrm{d}^3 r' \Theta_{\alpha,\text{dip}}(r') \wedge B(r') = \frac{1}{2} e_\alpha (r_\alpha - R) \wedge B(R) + \frac{1}{2}\frac{m_\alpha}{M} d \wedge B(R). \tag{23}$$

Hence the dipole approximation of H'_{mult}, denoted by $H'_{\text{mult,dip}}$, is given by

$$\begin{aligned}
H'_{\text{mult,dip}} = {} & \frac{1}{2m_1}\left(p + \frac{m_1}{M}P - \frac{1}{2}\left(e_1 - \left(\frac{m_1}{M}\right)^2 e_T\right) B_0 \wedge r\right. \\
& \left. - e_T \frac{m_1}{M} A(R) - \frac{m_1}{M}\frac{e_T}{2} B_0 \wedge R - \frac{e_1}{2}\frac{m_2}{M} B(R) \wedge r - \frac{m_1}{2M} B(R) \wedge d\right)^2 \\
& + \frac{1}{2m_2}\left(-p + \frac{m_2}{M}P + \frac{1}{2}\left(e_2 - \left(\frac{m_2}{M}\right)^2 e_T\right) B_0 \wedge r - \frac{m_2}{M}\frac{e_T}{2} B_0 \wedge R\right. \\
& \left. - e_T \frac{m_2}{M} A(R) + \frac{e_2 m_1}{2M} B(R) \wedge r - \frac{m_2}{2M} B(R) \wedge d\right)^2 + \frac{e_1 e_2}{4\pi\varepsilon_0 |r|} \\
& - (M_1 + M_2) \cdot B(R) + \frac{1}{2}\int \mathrm{d}^3 r' \left(\frac{\Pi(r')^2}{\varepsilon_0} + \frac{B(r')^2}{\mu_0}\right) \\
& + \int \mathrm{d}^3 r' \frac{\Pi(r') \cdot P(r')}{\varepsilon_0} + \frac{1}{2\varepsilon_0}\int \mathrm{d}^3 r' P(r')^2.
\end{aligned} \tag{24}$$

Note that

$$\begin{aligned}
-\frac{e_1 m_2}{2M} B(R) \wedge r - \frac{m_1}{2M} B(R) \wedge d &= \left(-\frac{e_1}{2} + \frac{1}{2}\frac{m_1^2}{M^2} e_T\right) B(R) \wedge r \\
\frac{e_2 m_1}{2M} B(R) \wedge r - \frac{m_2}{2M} B(R) \wedge d &= \left(\frac{e_2}{2} - \frac{1}{2}\frac{m_2^2}{M^2} e_T\right) B(R) \wedge r.
\end{aligned} \tag{25}$$

In the particular case where $B_0 = 0$ we get the following dipole approximation of the multipolar Hamiltonian:

$$\begin{aligned}
H_{\text{mult,dip}} = {} & \frac{P^2}{2M} + \frac{p^2}{2m} - \frac{e^2}{4\pi\varepsilon_0 |r|} + \frac{1}{2}\int \mathrm{d}^3 r' \left(\frac{\Pi(r')^2}{\varepsilon_0} + \frac{B(r')^2}{\mu_0}\right) + \frac{1}{2\varepsilon_0}\int \mathrm{d}^3 r' P(r')^2 \\
& - (M_1 + M_2) \cdot B(R) - er \cdot E(R) - \frac{e}{2M}(P \cdot B(R) \wedge r + B(R) \wedge r \cdot P) \\
& - \frac{e}{4m}\left(1 - \frac{4m}{M}\right)^{1/2} (p \cdot B(R) \wedge r + B(R) \wedge r \cdot p) - \frac{e_T}{4m_2}(p \cdot B(R) \wedge r \\
& + B(R) \wedge r \cdot p) + \frac{e_T}{2M}(P \cdot A(R) + A(R) \cdot P) - e_T \frac{m_1}{M^2}(P \cdot B(R) \wedge r
\end{aligned}$$

$$+ B(R) \wedge r \cdot P) - \frac{e_T}{4M}(p \cdot B(R) \wedge r + B(R) \wedge r \cdot p)$$
$$- \frac{e_T}{2M}\left(e - e_T\frac{m_1}{M}\right)(A(R) \cdot B(R) \wedge r + B(R) \wedge r \cdot A(R)) + \frac{e_T^2}{2M}A(R)^2$$
$$+ \left(\frac{1}{8m_1}\left(e - \frac{m_1^2}{M^2}e_T\right)^2 + \frac{1}{8m_2}\left(e_T\left(1 - \frac{m_2^2}{M^2}\right) - e\right)^2\right)(B(R) \wedge r)^2 \qquad (26)$$

where $m = m_1m_2/M$, $e = e_1$ and $m_2 > m_1$.

In the very particular case where $N = 2$, $e_T = 0$ and $B_0 \neq 0$, we obtain the following dipole approximation:

$$H_{\mathrm{mult,dip}} = \frac{P^2}{2M} + \frac{1}{2m_1}\left(p - \frac{1}{2}B_0 \wedge d\right)^2 + \frac{1}{2m_2}\left(p + \frac{1}{2}B_0 \wedge d\right)^2$$
$$- \frac{e^2}{4\pi\varepsilon_0|r|} + \frac{1}{2}\int \mathrm{d}^3r'\left(\frac{\Pi(r')^2}{\varepsilon_0} + \frac{B(r')^2}{\mu_0}\right) + \frac{1}{2\varepsilon_0}\int \mathrm{d}^2r' P(r')^2$$
$$- (M_1 + M_2) \cdot B(R) - d \cdot E(R) - \frac{1}{2M}(P \cdot B_0 \wedge d + B_0 \wedge d \cdot P)$$
$$- \frac{1}{2M}(P \cdot B(R) \wedge d + B(R) \wedge d \cdot P) - \frac{1}{4m}\left(1 - \frac{4m}{M}\right)^{1/2}(p \cdot B(R) \wedge d$$
$$+ B(R) \wedge d \cdot p) + \frac{1}{8m}(B(R) \wedge d)^2. \qquad (27)$$

When $B_0 = 0$ this is exactly the dipole approximation of the multipolar Hamiltonian which has been obtained by [LBBL] starting from the multipolar Hamiltonian for $N = 2$ and $e_T = 0$ and applying the dipole approximation directly.

In the mathematical study of Hamiltonians in QED we have to introduce cut-off functions $\rho(k)$ in $A(r)$, $B(r)$ and $E(r)$ in order to define a self-adjoint operator in the tensor product of the Hilbert space for the electronic states and of the Fock space for the photonic states.

In the Hamiltonian (1), where the electrons and protons are coupled to the electromagnetic field via minimal coupling, the infrared condition on $\rho(k)$, i.e., the condition to be satisfied by $\rho(k)$ for small $|k|$, is stronger than the one for the multipolar Hamiltonians of neutral systems as (27) (see [BFS] and [FFG]). Nevertheless, for the multipolar Hamiltonians, we have to deal with the behaviour of the electric and magnetic dipoles for large $|r|$. This means that the multipolar Hamiltonians are more convenient for the description of phenomena associated with confined systems of charges with respect to the internal variables.

Let us now consider the three-body system. We restrict ourselves to the case of the helium atom, say H_e^4, for simplicity. Here m_1 is the mass of the electron and m_2 is the mass of the nucleus.

We now introduce the internal variables (r_b, r_a) for the given two-cluster decomposition $\{(1, 2), 3\}$ where $(1, 2)$ corresponds to the two electrons and (3) to the nucleus:

$$r_b = r_3 - \tfrac{1}{2}(r_1 + r_2) \qquad r_a = r_2 - r_1 \qquad (28)$$

which can be expressed in terms of the centre-of-mass coordinate R by

$$r_1 - R = \frac{-m_2}{M}r_b - \frac{1}{2}r_a \qquad r_2 - R = \frac{-m_2}{M}r_b + \frac{1}{2}r_a \qquad r_3 - R = \frac{2m_1}{M}r_b.$$

The corresponding momentum operators are then

$$P = -\mathrm{i}\hbar\nabla_R$$
$$p_b = -\mathrm{i}\hbar\nabla_{r_b} = -\frac{m_2}{M}(p_1 + p_2) + \frac{2m_1}{M}p_3 \qquad (29)$$
$$p_a = -\mathrm{i}\hbar\nabla_{r_a} = \tfrac{-1}{2}p_1 + \tfrac{1}{2}p_2$$

and

$$p_1 = \frac{m_1}{M}P - \frac{1}{2}p_b - p_a \qquad p_2 = \frac{m_1}{M}P - \frac{1}{2}p_b + p_a \qquad p_3 = \frac{m_2}{M}P + \frac{1}{2}p_b$$

gives the reciprocal formulae for the operators of the particles.

We then have

$$\begin{aligned} d &= \sum_{\alpha=1}^{3} e_\alpha(r_\alpha - R) = -2er_b \qquad \frac{1}{2}e_1(r_1 - R) = -\frac{em_2}{2M}r_b - \frac{e}{4}r_a \\ \frac{1}{2}e_2(r_2 - R) &= -\frac{em_2}{2M}r_b + \frac{e}{4}r_a \qquad \frac{1}{2}e_3(r_3 - R) = -\frac{em_1}{2M}r_b. \end{aligned} \tag{30}$$

Then it is straightforward to get the multipolar Hamiltonian for H_e^4 without an exterior electromagnetic field, in the dipole approximation, using (23):

$$\begin{aligned} H_{H_e^4,\text{dip}} = {} & \frac{1}{2m_1}\left(\frac{m_1}{M}P - \frac{1}{2}p_b - p_a - \frac{e}{2}\left(\frac{m_2}{M}r_b + \frac{1}{2}r_a\right) \wedge B(R) - \frac{em_1}{M}r_b \wedge B(R)\right)^2 \\ & + \frac{1}{2m_1}\left(\frac{m_1}{M}P - \frac{1}{2}p_b + p_a - \frac{e}{2}\left(\frac{m_2}{M}r_b - \frac{1}{2}r_a\right) \wedge B(R) - \frac{em_1}{M}r_b \wedge B(R)\right)^2 \\ & + \frac{1}{2m_2}\left(\frac{m_2}{M}P + p_b - \frac{2em_1}{M}r_b \wedge B(R)\right)^2 + \frac{e^2}{4\pi\varepsilon_0|r_a|} - \frac{2e^2}{4\pi\varepsilon_0\left|r_b + \frac{1}{2}r_a\right|} \\ & - \frac{2e^2}{4\pi\varepsilon_0\left|r_b - \frac{1}{2}r_a\right|} - (2M_1 + M_2)\cdot B(R) + \frac{1}{2}\int \mathrm{d}^3r\left(\frac{\Pi^2(r)}{\varepsilon_0} + \frac{B^2(r)}{\mu_0}\right) \\ & + \frac{1}{2\varepsilon_0}\int \mathrm{d}^3r\, P^2(r) - d\cdot E(R). \end{aligned} \tag{31}$$

By expanding the right-hand side of (31) we get

$$\begin{aligned} H_{H_e^4,\text{dip}} = {} & \frac{P^2}{2M} + \frac{p_b}{4m_1m_2/M} + \frac{p_a^2}{m_1} - \frac{e}{M}\left(\frac{M + 2m_1}{M}\right)\{P\cdot(r_b \wedge B) + (r_b \wedge B)\cdot P\} \\ & + \frac{e}{M}\left(\frac{Mm_2 - 4m_1^2}{Mm_1m_2}\right)\{p_b\cdot(r_b \wedge B) + (r_b \wedge B)\cdot p_b\} + \frac{e}{4m_1}\{p_a.(r_a \wedge B) \\ & + (r_a \wedge B)\cdot p_a\} + \frac{e^2}{4m_1}\left\{\frac{m_2M^2 + 8m_1^3}{m_2M^2}\right\}(r_b \wedge B)^2 + \frac{e^2}{4m_1}(r_a \wedge B)^2 \\ & + \frac{e^2}{4\pi\varepsilon_0|r_a|} + \frac{-2e^2}{4\pi\varepsilon_0\left|r_b + \frac{1}{2}r_a\right|} + \frac{-2e^2}{4\pi\varepsilon_0\left|r_a - \frac{1}{2}r_a\right|} - (2M_1 + M_2)\cdot B(R) \\ & + \frac{1}{2}\int \mathrm{d}r^3\left(\frac{\Pi^2(r)}{\varepsilon_0} + \frac{B^2(r)}{\mu_0}\right) + \frac{1}{2\varepsilon_0}\int \mathrm{d}r^3\, P^2(r) + 2er_b\cdot E(R). \end{aligned} \tag{32}$$

2.2. *The Breit–Fermi multipolar Hamiltonian*

Let h_{BF} be the Breit–Fermi Hamiltonian for two fermions:

$$\begin{aligned} h_{BF} = {} & \left(c\alpha_1\cdot p_1 + \beta_1 m_1 c^2\right)\otimes \mathbb{1}_2 + \mathbb{1}_1 \otimes \left(c\alpha_2\cdot p_2 + \beta_2 mc^2\right) + \frac{e_1e_2}{4\pi\varepsilon_0|r|}\mathbb{1}_1\otimes\mathbb{1}_2 \\ & - \frac{e_1e_2}{8\pi\varepsilon_0|r|}\alpha_1\otimes\alpha_2 - \frac{e_1e_2}{8\pi\varepsilon_0|r|}((\alpha_1\cdot\hat{r})\otimes(\alpha_2\cdot\hat{r})) \end{aligned} \tag{33}$$

(see [BS]) where $r = r_1 - r_2$ and $\hat{r} = \frac{r}{|r|}$.

Here α_1 and β_1 (resp. α_2 and β_2) are the 4×4 Dirac matrices for particle 1 (resp. particle 2). $\mathbb{1}_1$ and $\mathbb{1}_2$ are 4×4 unit matrices. h_{BF} is a self adjoint operator in $L^2(\mathbb{R}^3; \mathbb{C}^4) \otimes L^2(\mathbb{R}^3; \mathbb{C}^4)$. $\alpha_1 \otimes \mathbb{1}_2$, $\mathbb{1}_1 \otimes \alpha_2$, $\alpha_1 \otimes \alpha_2$, $\alpha_1 \otimes \alpha_2$ and $\alpha_1 \cdot \hat{r} \otimes \alpha_2 \cdot \hat{r}$ are matrices in $\mathbb{C}^4 \otimes \mathbb{C}^4$.

The Breit–Fermi Hamiltonian in QED, denoted by H_{BF}, is given by

$$\begin{aligned} H_{BF} = {} & \big(c\alpha_1 \cdot (p_1 - e_1 A_{\text{ext}}(r_1) - e_1 A(r_1)) + m_1 c^2 \beta_1\big) \otimes \mathbb{1}_2 \\ & + \mathbb{1}_1 \otimes \big(c\alpha_2 \cdot (p_2 - e_2 A_{\text{ext}}(r_2) - e_2 A(r_2)) + m_2 c^2 \beta_2\big) \\ & + \frac{e_1 e_2}{4\pi\varepsilon_0 |r|} \mathbb{1}_1 \otimes \mathbb{1}_2 - \frac{e_1 e_2}{8\pi\varepsilon_0 |r|} \alpha_1 \otimes \alpha_2 - \frac{e_1 e_2}{8\pi\varepsilon_0 |r|} ((\alpha_1 \cdot \hat{r}) \otimes (\alpha_2 \cdot \hat{r})) \\ & + \frac{1}{2} \int \mathrm{d}^3 r' \left(\frac{\Pi(r')^2}{\varepsilon_0} + \frac{B(r')^2}{\mu_0} \right) \qquad r_1, r_2 \in \mathbb{R}^3. \end{aligned} \tag{34}$$

By applying the unitary transform U (see (7)) to H_{BF} we get the following multipolar Hamiltonian denoted by $H_{BF,\text{mult}}$:

$$\begin{aligned} H_{BF,\text{mult}} = {} & U^{-1} H_{BF} U \\ = {} & \left(c\alpha_1 \cdot \left(p_1 - e_1 A_{\text{ext}}(r_1) - e_T \frac{m_1}{M} A(R) + \int \mathrm{d}^3 r \Theta_1(r) \wedge B(r) \right) \right. \\ & \left. + m_1 c^2 \beta_1 \right) \otimes \mathbb{1}_2 + \mathbb{1}_1 \otimes \left(c\alpha_2 \cdot \left(p_2 - e_2 A_{\text{ext}}(r_1) - e_T \frac{m_2}{M} A(R) \right. \right. \\ & \left. \left. + \int \mathrm{d}^3 r \Theta_2(r) \wedge B(r) \right) + m_2 c^2 \beta_2 \right) - \frac{e^2}{4\pi\varepsilon_0 |r|} \mathbb{1}_1 \otimes \mathbb{1}_2 + \frac{e^2}{8\pi\varepsilon_0 |r|} \alpha_1 \otimes \alpha_2 \\ & + \frac{e^2}{8\pi\varepsilon_0 |r|} ((\alpha_1 \cdot \hat{r}) \otimes (\alpha_2 \cdot \hat{r})) + \frac{1}{2} \int \mathrm{d}^3 r' \left(\frac{\Pi(r')^2}{\varepsilon_0} + \frac{B(r')^2}{\mu_0} \right) \\ & + \frac{1}{\varepsilon_0} \int \mathrm{d}^3 r' \Pi(r') \cdot P(r') + \frac{1}{2\varepsilon_0} \int \mathrm{d}^3 r' P(r')^2. \end{aligned} \tag{35}$$

When $e_T = 0$ and $A_{\text{ext}}(r) = \frac{1}{2} B_0 \wedge r$ it is easy to get the following dipole approximation to $H_{BF,\text{mult}}$:

$$\begin{aligned} H_{BF,\text{dip}} = {} & \left(c\alpha_1 \cdot \left(p + \frac{m_1}{M} P - \frac{1}{2} B_0 \wedge d - \frac{1}{2} B(R) \wedge d \right) + m_1 c^2 \beta_1 \right) \otimes \mathbb{1}_2 \\ & + \mathbb{1}_1 \otimes \left(c\alpha_2 \cdot \left(-p + \frac{m_2}{M} P + \frac{1}{2} B_0 \wedge d + \frac{1}{2} B(R) \wedge d \right) + m_2 c^2 \beta_2 \right) \\ & - \frac{e^2}{4\pi\varepsilon_0 |r|} \mathbb{1}_1 \otimes \mathbb{1}_2 + \frac{e^2}{8\pi\varepsilon_0 |r|} \alpha_1 \otimes \alpha_2 + \frac{e^2}{8\pi\varepsilon_0 |r|} ((\alpha_1 \cdot \hat{r}) \otimes (\alpha_2 \cdot \hat{r})) \\ & + \frac{1}{2} \int \mathrm{d}^3 r' \left(\frac{\Pi(r')^2}{\varepsilon_0} + \frac{B(r')^2}{\mu_0} \right) + \frac{1}{2\varepsilon_0} \int \mathrm{d}^3 r' P(r')^2 - d \cdot E(R) \end{aligned} \tag{36}$$

where $e_1 = e$ and $d = er$.

3. Scaling

In this section we show that a change of units exhibits the perturbative character of the Hamiltonians we are concerned with.

We dilate the electron coordinates and photon momenta independently, $(r, k) \to \left(\frac{r}{\mu}, \eta k\right)$, $\mu > 0$, $\eta > 0$, μ and η are dimensionless constants. This scaling induces a unitary transformation that we now compute.

The dilation $k \to \eta k$ induces an unitary operator in $L^2(\mathbb{R}^3)$ denoted by Γ_η:

$$(\Gamma_\eta f)(k) = \eta^{3/2} f(\eta k) \qquad \eta > 0 \quad k \in \mathbb{R}^3 \tag{37}$$

where $f \in L^2(\mathbb{R}^3)$.

We have

$$\left(\Gamma_\eta^{-1} g\right)(k) = \eta^{-3/2} g\left(\frac{k}{\eta}\right). \tag{38}$$

Let $\mathcal{F}_{ph}$ be the Fock space for transversal photons. We have

$$\mathcal{F}_{ph} = \bigoplus_{n=0}^{\infty} L^2(\mathbb{R}^3, \mathbb{C}^2)^{\otimes_s^n}$$

where $L^2(\mathbb{R}^3, \mathbb{C}^2)^{\otimes_s^0} \equiv \mathbb{C}$, the field of complex numbers. Here $L^2(\mathbb{R}^3, \mathbb{C}^2)^{\otimes_s^n}$ is the symmetrized n-fold tensor product of $L^2(\mathbb{R}^3, \mathbb{C}^2)$.

The vector $\Omega = (1, 0, 0, \ldots, 0 \ldots)$ is the vacuum state. The dilation $k \to \eta k$, $\eta > 0$, induces an unitary operator on $\mathcal{F}_{ph}$ that we still denote by Γ_η. We have

$$\Gamma_\eta^{-1} a_\lambda(k) \Gamma_\eta = \eta^{3/2} a_\lambda(\eta k) \qquad \Gamma_\eta^{-1} a_\lambda^*(k) \Gamma_\eta = \eta^{3/2} a_\lambda^*(\eta k). \tag{39}$$

These formulae can be directly proved from the definitions of $a_\lambda(k)$ and $a_\lambda^*(k)$. We just give a flavour of the proof.

Let N be the number of photon operators. We have

$$N = \sum_{\lambda=1,2} \int \mathrm{d}^3 k \, a_\lambda^*(k) a_\lambda(k).$$

N is obviously invariant by dilation.

Therefore

$$\begin{aligned} \Gamma_\eta^{-1} N \Gamma_\eta &= \sum_{\lambda=1,2} \int \mathrm{d}^3 k \, \Gamma_\eta^{-1} a_\lambda^*(k) \Gamma_\eta \Gamma_\eta^{-1} a_\lambda(k) \Gamma_\eta \\ &= N = \sum_{\lambda=1,2} \int \mathrm{d}^3(\eta k) \, a_\lambda^*(\eta k) a_\lambda(\eta k) \\ &= \sum_{\lambda=1,2} \int \mathrm{d}^3 k \, \eta^3 a_\lambda^*(\eta k) a_\lambda(\eta k). \end{aligned}$$

Thus we have

$$\Gamma_\eta^{-1} a_\lambda(k) \Gamma_\eta = \eta^{3/2} a_\lambda(\eta k) \qquad \Gamma_\eta^{-1} a_\lambda^*(k) \Gamma_\eta = \eta^{3/2} a_\lambda^*(\eta k)$$

because $a_\lambda^*(k)$ is the adjoint of $a_\lambda(k)$.

Note that the right mathematical definition of the energy operator for the photons is given by

$$\frac{1}{2} \int \mathrm{d}^3 r : \frac{\Pi(r)^2}{\varepsilon_0} + \frac{B(r)^2}{\mu_0} :$$

where $: \, :$ is the Wick normal order (see [S]).

Let H_{ph} denote the energy operator for the photons. We then have

$$H_{ph} = \frac{1}{2} \int \mathrm{d}^3 r : \frac{\Pi(r)^2}{\varepsilon_0} + \frac{B(r)^2}{\mu_0} := \sum_{\lambda=1,2} c\hbar \int \mathrm{d}^3 r |k| a_\lambda^*(k) a_\lambda(k).$$

Thus

$$\Gamma_\eta^{-1} H_{ph} \Gamma_\eta = \sum_{\lambda=1,2} c\hbar \int \mathrm{d}^3k |k| \Gamma_\eta^{-1} a_\lambda^*(k) \Gamma_\eta \Gamma_\eta^{-1} a_\lambda(k) \Gamma_\eta$$
$$= \sum_{\lambda=1,2} c\hbar \int \mathrm{d}^3k |k| \eta^3 a_\lambda^*(\eta k) a_\lambda(\eta k)$$
$$= \frac{1}{\eta} \sum_{\lambda=1,2} c\hbar \int \mathrm{d}^3(\eta k) |\eta k| a_\lambda^*(\eta k) a_\lambda(\eta k) = \frac{1}{\eta} H_{ph}. \tag{40}$$

Moreover

$$\Gamma_\eta^{-1} A(r) \Gamma_\eta = \sum_{\lambda=1,2} \int \mathrm{d}^3k \left(\frac{\hbar}{2\varepsilon_0 (2\pi)^3 \omega(k)} \right)^{1/2} \left[\eta^{3/2} (a_\lambda(\eta k) \varepsilon_\lambda(k)\, \mathrm{e}^{\mathrm{i}k\cdot r} + a_\lambda^*(\eta k) \varepsilon_\lambda(k)\, \mathrm{e}^{-\mathrm{i}k\cdot r} \right].$$

Note that $\varepsilon_\lambda(\eta k) = \varepsilon_\lambda(k)$, $\lambda = 1, 2$. We then get

$$\Gamma_\eta^{-1} A(r) \Gamma_\eta = \frac{1}{\eta} \sum_{\lambda=1,2} \int \mathrm{d}^3k \left(\frac{\hbar}{2\varepsilon_0 (2\pi)^3 \omega(\eta k)} \right)^{1/2} \left[(a_\lambda(\eta k) \varepsilon_\lambda(k)\, \mathrm{e}^{\mathrm{i}k\cdot \frac{r}{\eta}} + a_\lambda^*(\eta k) \varepsilon_\lambda(k)\, \mathrm{e}^{-\mathrm{i}k\cdot \frac{r}{\eta}} \right]$$
$$= \frac{1}{\eta} A\left(\frac{r}{\eta}\right).$$

In the same way we get

$$\Gamma_\eta^{-1} B(r) \Gamma_\eta = \frac{1}{\eta^2} B\left(\frac{r}{\eta}\right) \qquad \Gamma_\eta^{-1} E(r) \Gamma_\eta = \frac{1}{\eta^2} E\left(\frac{r}{\eta}\right). \tag{41}$$

We also have, for $r \in \mathbb{R}^3$,

$$\left(\Gamma_\mu^{-1} \frac{\partial}{\partial r_j} \Gamma_\mu \right) \varphi(r) = \mu \frac{\partial \varphi}{\partial r_j}(r).$$

Therefore

$$\Gamma_\mu^{-1} \nabla_r \Gamma_\mu = \mu \nabla_r.$$

Furthermore, for any function $V(r)$, we have

$$\Gamma_\mu^{-1} V(r) \Gamma_\mu = V\left(\frac{r}{\mu}\right). \tag{42}$$

Let us now consider the transformed multipolar Hamiltonian under the scaling $(r_1, r_2, k) \to \left(\frac{r_1}{\mu}, \frac{r_2}{\mu}, \eta k\right)$, $\mu > 0$, $\eta > 0$. Again μ and η are dimensionless constants.

For simplicity, let us consider the dipole approximation of the multipolar Hamiltonian for both $e_T = 0$, $B_0 = 0$ and $M_1 = M_2 = 0$. We have

$$H_{\mathrm{mult,dip}} = \frac{P^2}{2M} + \frac{1}{2m} p^2 - \frac{e^2}{4\pi\varepsilon_0 |r|} + \sum_{\lambda=1,2} c\hbar \int \mathrm{d}^3k |k| a_\lambda^*(k) a_\lambda(k) - d \cdot E(R)$$
$$- \frac{1}{2M} (P \cdot B(R) \wedge d + B(R) \wedge d \cdot P) - \frac{1}{4m} \left(1 - \frac{4m}{M}\right)^{1/2} (p \cdot B(R) \wedge d$$
$$+ B(R) \wedge d \cdot p) + \frac{1}{8m} (B(R) \wedge d)^2. \tag{43}$$

The scaling $(r_1, r_2) \to \left(\frac{r_1}{\mu}, \frac{r_2}{\mu}\right)$, $r_1, r_2 \in \mathbb{R}^3$, induces the scaling $(r, R) \to \left(\frac{r}{\mu}, \frac{R}{\mu}\right)$, $r, R \in \mathbb{R}^3$.

Therefore

$$\left(\Gamma_\mu \otimes \Gamma_\mu \otimes \Gamma_{1/\eta}\right)^{-1} H_{\mathrm{mult,dip}} \left(\Gamma_\mu \otimes \Gamma_\mu \otimes \Gamma_{1/\eta}\right)$$
$$= \mu^2 \frac{P^2}{2M} + \mu^2 \frac{p^2}{2m} - \frac{e^2\mu}{4\pi\varepsilon_0|r|} + \eta \sum_{\lambda=1,2} c\hbar \int \mathrm{d}^3k|k|a_\lambda^*(k)a(k)$$
$$- \frac{\eta^2}{\mu} E\left(\frac{\eta}{\mu}R\right)\cdot d - \frac{1}{2M}\eta^2\left(P\cdot B\left(\frac{\eta}{\mu}R\right)\wedge d + B\left(\frac{\eta}{\mu}R\right)\wedge d\cdot P\right)$$
$$- \frac{1}{4m}\left(1-\frac{4m}{M}\right)^{1/2}\eta^2\left(p\cdot B\left(\frac{\eta}{\mu}R\right)\wedge d + B\left(\frac{\eta}{\mu}R\right)\wedge d\cdot P\right)$$
$$+ \frac{1}{8m}\frac{\eta^4}{\mu^2}\left(B\left(\frac{\eta}{\mu}\right)\wedge d\right)^2. \tag{44}$$

We now suppose that e is the charge of the electron. Let α denote the fine structure constant $\frac{e^2}{4\pi\varepsilon_0\hbar c}$.

Setting

$$\mu^2 = \alpha\mu = \eta$$

we have

$$\mu = \alpha \qquad \text{and} \qquad \eta = \alpha^2. \tag{45}$$

Hence

$$\frac{1}{\alpha^2}\left(\Gamma_\mu \otimes \Gamma_\mu \otimes \Gamma_{1/\eta}\right)^{-1} H_{\mathrm{mult,dip}} \left(\Gamma_\mu \otimes \Gamma_\mu \otimes \Gamma_{1/\eta}\right)$$
$$= \frac{P^2}{2M} + \frac{p^2}{2m} - \frac{\hbar c}{|r|} + \sum_{\lambda=1,2} c\hbar \int \mathrm{d}^3k|k|a_\lambda^*(k)a_\lambda(k) - \alpha E(\alpha R)\cdot d$$
$$- \alpha^2\frac{1}{2M}(P\cdot B(\alpha R)\wedge d + B(\alpha R)\wedge d\cdot P) - \alpha^2\frac{1}{4m}\left(1-\frac{4m}{M}\right)^{1/2}$$
$$\times (p\cdot B(\alpha R)\wedge d + B(\alpha R)\wedge d\cdot p) + \alpha^4\frac{1}{8m}(B(\alpha R)\wedge d)^2. \tag{46}$$

Thus energy eigenvalues of the Hamiltonian (46) are given in units where the ground state energy of a hydrogen atom is $-\frac{1}{2}mc^2$.

This suggests that electric-dipole interaction is a perturbation of order α of the unperturbed Hamiltonian $\frac{P^2}{2M} + \frac{p^2}{2m} - \frac{\hbar c}{|r|} + \sum_{\lambda=1,2} c\hbar \int \mathrm{d}^3k|k|a_\lambda^*(k)a_\lambda(k)$. The two magnetic-dipole terms are then a perturbation of order α^2 and the quadratic term is a much smaller perturbation.

The necessity of the Röntgen term, i.e., the magnetic-dipole term involving P, is emphasized in [LBBL] and [W] in order to describe the interaction between the electromagnetic field and the internal and centre-of-mass motions correctly.

The magnetic-dipole term depending on p is usually neglected. But, according to our analysis, it must be taken into account in order to explain the interaction of the electromagnetic field with a moving neutral atomic system.

Furthermore, as far as we restrict ourselves to perturbations of order α^2, we must add a term coming from the quadrupole approximation of the multipolar Hamiltonian, i.e., a term equal to $-\frac{e}{2}\left(1-\frac{4m}{M}\right)^{1/2} r\cdot(r\cdot\nabla_r)E(r)|_{r=\alpha R}$.

Thus, this scaling analysis allows us to classify the different elements of the perturbation both in terms of the usual dipole, quadrupole and other multipolar moments and in terms of the different powers of the fine structure constant (see [F] for a more complete analysis).

We now compute the transformed three-body multipolar Hamiltonian given by (32) under the scaling

$$(r_1, r_2, r_3, k) \to \left(\frac{r_1}{\mu}, \frac{r_2}{\mu}, \frac{r_3}{\mu}, \eta k\right) \qquad \mu > 0 \quad \eta > 0.$$

As before we get

$$\begin{aligned}
&\left(\Gamma_\mu \otimes \Gamma_\mu \otimes \Gamma_\mu \otimes \Gamma_{1/\eta}\right)^{-1} H_{\mathrm{mult,dip}} \left(\Gamma_\mu \otimes \Gamma_\mu \otimes \Gamma_\mu \otimes \Gamma_{1/\eta}\right) \\
&\quad = \mu^2 \frac{P^2}{2M} + \mu^2 \frac{p_b}{4m_1 m_2/M} + \mu^2 \frac{p_a^2}{m_1} + \frac{e^2\mu}{4\pi\varepsilon_0 |r|} + \frac{-2e^2\mu}{4\pi\varepsilon_0 \left|r_b + \frac{1}{2}r_a\right|} \\
&\qquad + \frac{-2e^2\mu}{4\pi\varepsilon_0 \left|r_b - \frac{1}{2}r_a\right|} + \eta \sum_{\lambda=1,2} c\hbar \int \mathrm{d}^3k |k| a_\lambda^*(k) a_\lambda(k) + \frac{\eta^2}{\mu} 2e r_b \cdot E\left(\frac{\eta}{\mu}R\right) \\
&\qquad + \eta^2 \left[-\frac{e}{M}\left(\frac{M+2m_1}{M}\right)\left\{P \cdot \left(r_b \wedge B\left(\frac{\eta}{\mu}R\right)\right) + \left(r_b \wedge B\left(\frac{\eta}{\mu}R\right)\right) \cdot P\right\}\right. \\
&\qquad + \frac{e}{M}\left(\frac{Mm_2 - 4m_1^2}{Mm_1m_2}\right)\left\{p_b \left(r_b \wedge B\left(\frac{\eta}{\mu}R\right)\right) + \left(r_b \wedge B\left(\frac{\eta}{\mu}R\right)\right) \cdot p_b\right\} \\
&\qquad \left. + \frac{e}{4m_1}\left\{p_a \left(r_a \wedge B\left(\frac{\eta}{\mu}R\right)\right) + \left(r_a \wedge B\left(\frac{\eta}{\mu}R\right)\right) \cdot p_a\right\}\right] \\
&\qquad + \frac{\eta^4}{\mu^2}\left[\frac{e^2}{4m_1}\left(r_a \wedge B\left(\frac{\eta}{\mu}R\right)\right)^2 + \frac{e^2}{4m_1}\left(\frac{m_2M^2 + 8m_1^2}{m_2M^2}\right)\left(r_b \wedge B\left(\frac{\eta}{\mu}R\right)\right)^2\right]
\end{aligned} \tag{47}$$

where we have omitted the spin terms.

Setting as before $\mu^2 = 2\mu\alpha = \eta$, we get $\mu = 2\alpha$ and $\eta = 4\alpha^2$, where again α denotes the fine structure constant $\frac{e^2}{4\pi\varepsilon_0\hbar c}$. Hence we obtain

$$\begin{aligned}
&\frac{1}{4\alpha^2}\left(\Gamma_\mu \otimes \Gamma_\mu \otimes \Gamma_\mu \otimes \Gamma_{1/\eta}\right)^{-1} H_{H_e^4,\mathrm{dip}} \left(\Gamma_\mu \otimes \Gamma_\mu \otimes \Gamma_\mu \otimes \Gamma_{1/\eta}\right) \\
&\quad = \frac{P^2}{2M} + \frac{p_b}{4m_1m_2/M} + \frac{p_a^2}{m_1} + \frac{\hbar c}{2|r_a|} + \frac{-\hbar c}{\left|r_b + \frac{1}{2}r_a\right|} + \frac{-\hbar c}{\left|r_b - \frac{1}{2}r_a\right|} \\
&\qquad + \sum_{\lambda=1,2} c\hbar \int \mathrm{d}^3k |k| a_\lambda^*(k) a_\lambda(k) + 4\alpha e r_b E(2\alpha R) \\
&\qquad + 4\alpha^2 \left[\frac{-e}{M}\left(\frac{M+2m_1}{m}\right)\{P \cdot (r_b \wedge B(2\alpha R)) + (r_b \wedge B(2\alpha R)) \cdot P\}\right. \\
&\qquad + \frac{e}{M}\left(\frac{Mm_2 - 4m_1^2}{Mm_1m_2}\right)\{p_b \cdot (r_b \wedge B(2\alpha R)) + (r_b \wedge B(2\alpha R)) \cdot p_b\} \\
&\qquad \left. + \frac{e}{4m_1}\{p_a \cdot (r_a \wedge B(2\alpha R)) + (r_a \wedge B(2\alpha R)) \cdot p_a\}\right] \\
&\qquad + \alpha^4 \frac{e^2}{4m_1}\left[\frac{m_2M^2 + 8m_1^3}{m_2M^2}(r_b \wedge B(2\alpha R))^2 + (r_a \wedge B(2\alpha R))^2\right].
\end{aligned} \tag{48}$$

Thus the comments in the three-body case are the same as in the two-body case.

In the relativistic case, one easily shows, by a straightforward inspection, that for the dilated Hamiltonian (36) the electric-dipole and magnetic-dipole terms are of the same order with respect to the fine structure constant, in contrast to the non-relativistic case (46).

4. Conclusion

In this paper we have mainly considered a system of moving non-relativistic charges. The dipole Hamiltonian that we have got is essentially valid for a confined system of charges which does not move too fast with respect to the light velocity c. In addition to the Roentgen and quadrupolar electric terms, a Zeeman-like term must be considered in order to explain the emission and absorption of radiation by moving atoms.

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Appendix

In this appendix, we give a detailed proof of the expression for the magnetization fields given by (9). We have

$$\begin{aligned}
\hbar\frac{\partial}{\partial r_{\beta,j}}S &= \frac{\partial}{\partial r_{\beta,j}}\sum_{\substack{\alpha=1\\ i=1,2,3}}^{N} e_\alpha(r_{\alpha,i}-R_i)\int \mathrm{d}^3r\int_0^1 \mathrm{d}\lambda\,\delta(r-R-\lambda(r_\alpha-R))A_i(r)\\
&= \sum_{\substack{\alpha=1\\ i=1,2,3}}^{N} e_\alpha(r_{\alpha,i}-R_i)\int \mathrm{d}^3r\int_0^1 \mathrm{d}\lambda\left(\frac{\partial}{\partial r_{\beta,j}}\delta(r-R-\lambda(r_\alpha-R))\right)A_i(r)\\
&\quad + e_\beta\int \mathrm{d}^3r\int_0^1 \mathrm{d}\lambda\,\delta(r-R-\lambda(r_\beta-R))A_j(r)\\
&\quad - \frac{m_\beta}{M}\sum_{\alpha=1}^{N} e_\alpha\int \mathrm{d}^3r\int_0^1 \mathrm{d}\lambda\,\delta(r-R-\lambda(r_\alpha-R))A_j(r)
\end{aligned} \tag{A.1}$$

and

$$\begin{aligned}
&\sum_{\substack{\alpha=1\\ i=1,2,3}}^{N} e_\alpha(r_{\alpha,i}-R_i)\int \mathrm{d}^3r\int_0^1 \mathrm{d}\lambda\left(\frac{\partial}{\partial r_{\beta,j}}\delta(r-R-\lambda(r_\alpha-R))\right)A_i(r)\\
&\qquad = e_\beta\sum_{i=1}^{3}(r_{\beta,i}-R_i)\int \mathrm{d}^3r\int_0^1 \mathrm{d}\lambda\left(\frac{m_\beta}{M}(\lambda-1)-\lambda\right)\\
&\qquad\quad \times\frac{\partial}{\partial r_j}\delta(r-R-\lambda(r_\beta-R))A_i(r) + \sum_{\substack{\alpha\neq\beta\\ i=1,2,3}}^{N} e_\alpha(r_{\alpha,i}-R_i)\\
&\qquad\quad \times\int \mathrm{d}^3r\int_0^1 \mathrm{d}\lambda\frac{m_\beta}{M}(\lambda-1)\frac{\partial}{\partial r_j}\delta(r-R-\lambda(r_\alpha-R))A_i(r).
\end{aligned} \tag{A.2}$$

We now have to compute the two terms of the rhs of (A.2).

We get for the first term

$$e_\beta \sum_{i=1}^{3}(r_{\beta,i} - R_i) \int \mathrm{d}^3 r \int_0^1 \mathrm{d}\lambda \left(\frac{m_\beta}{M}(\lambda - 1) - \lambda\right) \frac{\partial}{\partial r_j}\delta(r - R - \lambda(r_\beta - R))A_i(r)$$
$$= -e_\beta \int \mathrm{d}^3 r \int_0^1 \mathrm{d}\lambda \left(\frac{m_\beta}{M}(\lambda - 1) - \lambda\right)$$
$$\times \frac{\partial}{\partial r_j}[(r_\beta - R)\cdot A(r)]\delta(r - R - \lambda(r_\beta - R)). \tag{A.3}$$

We have

$$\frac{\partial}{\partial r_j}[(r_\beta - R)\cdot A(r)] = ((r_\beta - R) \wedge (\nabla \wedge A(r)))_j + ((r_\beta - R)\cdot \nabla A(r))_j$$

where

$$((r_\beta - R)\cdot \nabla A(r))_j = \sum_{i=1}^{3}(r_{\beta,i} - R_i)\frac{\partial}{\partial r_i}A_j(r).$$

Thus, since $B(r) = \nabla \wedge A(r)$, we get

$$e_\beta \int \mathrm{d}^3 r \int_0^1 \mathrm{d}\lambda \left(\frac{m_\beta}{M}(\lambda - 1) - \lambda\right) \frac{\partial}{\partial r_j}\delta(r - R - \lambda(r_\beta - R))((r_\beta - R)\cdot A(r))$$
$$= -e_\beta \int \mathrm{d}^3 r \int_0^1 \mathrm{d}\lambda \left(\frac{m_\beta}{M}(\lambda - 1) - \lambda\right) ((r_\beta - R) \wedge B(r))_j \delta(r - R$$
$$- \lambda(r_\beta - R)) - e_\beta \int \mathrm{d}^3 r \int_0^1 \mathrm{d}\lambda \left(\frac{m_\beta}{M}(\lambda - 1) - \lambda\right)$$
$$\times ((r_\beta - R)\cdot \nabla_r A_j(r))\delta(r - R - \lambda(r_\beta - R)). \tag{A.4}$$

We now calculate the second term of the rhs of (A.4). We get

$$-e_\beta \int \mathrm{d}^3 r \int_0^1 \mathrm{d}\lambda \left(\frac{m_\beta}{M}(\lambda - 1) - \lambda\right) ((r_\beta - R)\cdot \nabla_r A_j(r))\delta(r - R - \lambda(r_\beta - R))$$
$$= e_\beta \int \mathrm{d}^3 r \int_0^1 \mathrm{d}\lambda \left(\frac{m_\beta}{M}(\lambda - 1) - \lambda\right)$$
$$\times ([(r_\beta - R)\cdot \nabla_r]\delta(r - R - \lambda(r_\beta - R)))A_j(r)$$
$$= -e_\beta \int \mathrm{d}^3 r \int_0^1 \mathrm{d}\lambda \left(\frac{m_\beta}{M}(\lambda - 1) - \lambda\right) \left(\frac{\mathrm{d}}{\mathrm{d}\lambda}\delta(r - R - \lambda(r_\beta - R))\right) A_j(r).$$

Now, integrating by parts with respect to λ, we get

$$-e_\beta \int \mathrm{d}^3 r \int_0^1 \mathrm{d}\lambda \left(\frac{m_\beta}{M}(\lambda - 1) - \lambda\right) (r_\beta - R)\cdot \nabla_r A_j(r)\delta(r - R - \lambda(r_\beta - R))$$
$$= e_\beta \left(\frac{m_\beta}{M} - 1\right) \int \mathrm{d}^3 r \int_0^1 \mathrm{d}\lambda\, \delta(r - R - \lambda(r_\beta - R))A_j(r)$$
$$+ e_\beta A_j(r_\beta) - \frac{m_\beta}{M} e_\beta A_j(R). \tag{A.5}$$

Finally, from (A.3), (A.4) and (A.5) we obtain

$$e_\beta \sum_{i=1}^{3}(r_{\beta,i} - R_i)\int \mathrm{d}^3r \int_0^1 \mathrm{d}\lambda \left(\frac{m_\beta}{M}(\lambda - 1) - \lambda\right)\frac{\partial}{\partial r_j}\delta(r - R - \lambda(r_\beta - R))A_i(r)$$
$$= -e_\beta \int \mathrm{d}^3r \int_0^1 \mathrm{d}\lambda \left(\frac{m_\beta}{M}(\lambda - 1) - \lambda\right)((r_\beta - R)\wedge B(r))_j$$
$$\times\, \delta(r - R - \lambda(r_\beta - R)) + e_\beta\left(\frac{m_\beta}{M} - 1\right)\int \mathrm{d}^3r \int_0^1 \mathrm{d}\lambda\, \delta(r - R$$
$$- \lambda(r_\beta - R))A_j(r) + e_\beta A_j(r_\beta) - e_\beta \frac{m_\beta}{M}A_j(R). \tag{A.6}$$

We now compute the second term of the rhs of (A.2). We have

$$\sum_{\substack{\alpha\neq\beta\\ i=1,2,3}} e_\alpha(r_{\alpha\cdot i} - R_i)\int \mathrm{d}^3r \int_0^1 \mathrm{d}\lambda \frac{m_\beta}{M}(\lambda - 1)\frac{\partial}{\partial r_j}\delta(r - R - \lambda(r_\alpha - R))A_i(r)$$
$$= -\sum_{\alpha\neq\beta} e_\alpha \int \mathrm{d}^3r \int_0^1 \mathrm{d}\lambda \frac{m_\beta}{M}(\lambda - 1)\frac{\partial}{\partial r_j}[(r_\alpha - R)\cdot A(r)]\delta(r - R - \lambda(r_\alpha - R))$$
$$= -\sum_{\alpha\neq\beta} e_\alpha \int \mathrm{d}^3r \int_0^1 \mathrm{d}\lambda \frac{m_\beta}{M}(\lambda - 1)((r_\alpha - R)\wedge B(r))_j\delta(r - R - \lambda(r_\alpha - R))$$
$$- \sum_{\alpha\neq\beta} e_\alpha \int \mathrm{d}^3r \int_0^1 \mathrm{d}\lambda \frac{m_\beta}{M}(\lambda - 1)\frac{\partial}{\partial \lambda}\delta(r - R - \lambda(r_\alpha - R))A_j(r)$$
$$= -\sum_{\alpha\neq\beta} e_\alpha \int \mathrm{d}^3r \int_0^1 \mathrm{d}\lambda \frac{m_\beta}{M}(\lambda - 1)((r_\alpha - R)\wedge B(r))_j\delta(r - R - \lambda(r_\alpha - R))$$
$$+ \frac{m_\beta}{M}\sum_{\alpha\neq\beta} e_\alpha \int \mathrm{d}^3r \int_0^1 \mathrm{d}\lambda\, \delta(r - R - \lambda(r_\alpha - R))A_j(r)$$
$$- \frac{m_\beta}{M}\left(\sum_{\alpha\neq\beta} e_\alpha\right)A_j(R). \tag{A.7}$$

We finally get from (A.1), (A.6) and (A.7)

$$\hbar\frac{\partial}{\partial r_{\beta,j}}S = e_\beta \int \mathrm{d}^3r \int_0^1 \mathrm{d}\lambda\, \lambda((r_\beta - R)\wedge B(r))_j\delta(r - R - \lambda(r_\beta - R))$$
$$- \sum_{\alpha=1}^{N} e_\alpha \int \mathrm{d}^3r \int_0^1 \mathrm{d}\lambda \frac{m_\beta}{M}(\lambda - 1)((r_\alpha - R)\wedge B(r))_j\delta(r - R - \lambda(r_\beta - R))$$
$$+ e_\beta A_j(r_\beta) - e_T\frac{m_\beta}{M}A_j(R). \tag{A.8}$$

Setting

$$\Theta_\beta(r) = \sum_{\alpha=1}^{N} e_\alpha \int_0^1 \mathrm{d}\lambda \left(\lambda\delta_{\beta\alpha} - \frac{m_\beta}{M}(\lambda - 1)\right)(r_\alpha - R)\delta(r - R - \lambda(r_\alpha - R))$$

we then get

$$\hbar\nabla_{r_\beta}S = e_\beta A(r_\beta) - e_T\frac{m_\beta}{M}A(R) + \int \mathrm{d}^3r\,\Theta_\beta(r)\wedge B(r).$$

Thus (9) is proved.

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