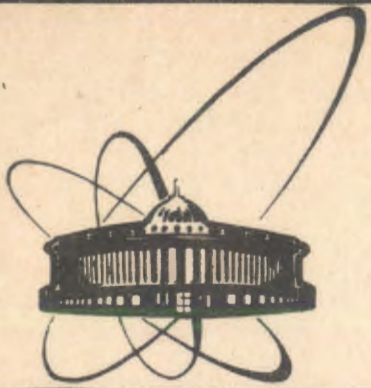

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REGULARIZATION OF THE MULTIPOLAR FORM OF QUANTUM ELECTRODYNAMICS

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I. INTRODUCTION

The multipolar form (MF) of quantum electrodynamics of bound charges has been suggested by Power and Zienau[1] and was developed in subsequent papers, see, e.g.,[2-9]. In this form the interaction term may be expanded in a series of electric and magnetic multipoles (moments) of atoms or molecules. The form can be obtained from the Coulomb gauge electrodynamics by expressing its total Hamiltonian in terms of new electron and photon operators. They are connected with the Coulomb gauge operators by means of unitary transformation, see below Sect.2. I generalize here the form of the transformation given by Atkins and Woolley[2,3], see also[4-9]. Usually MF is defined for the nonrelativistic QED, but it can be also defined for the relativistic case (interacting Dirac and photon fields)[7]. The multipolar electron operators have the important property of being gauge-invariant in a specific sense, see Sect.2. This property is used here as the requirement defining MF.

MF has calculational advantages and is widely used, mainly in the electric dipole approximation when the interaction is reduced to the well-known term $e\vec{q}\vec{E}$. Examples are the multiphoton processes, see, e.g.,[10] and ch.12 in[11]; the quantum theory of molecules[5,9]; the laser theory[11,12]; other collective effects in systems of $N \geq 2$ atoms or molecules, e.g., superradiance, see[13,14]; quantum electronics[15,16]. For many applications it is important that MF does not contain explicitly interatomic Coulomb interactions, see below Sect.6.

But this advantageous formalism has deficiencies which are discussed and overcome here. The first one is that a divergent term is present in the multipolar Hamiltonian. It is an operator and this presents a real trouble. C-number divergent terms arise already when one is dealing with free field Hamiltonian and do not represent a serious problem. This operator term is written usually in the form $\int d^3x |\vec{p}_\perp(\vec{x})|^2$ and is denoted here by $P_\perp$, see Sect.2. Another trouble is that perturbation calculations with the multipolar interaction reveal new additional divergencies as compared to those which arise in the Lorentz or Coulomb gauges. The relation between these two troubles is discussed in Sect.2. I suggest in Sect.3 a regularization of

the above-mentioned unitary transformation. This regularization removes all additional divergencies of MF. Stress that it is not the Hamiltonian which is regularized but the transformation operator. It is shown in Sect.4 that the regularized MF has the same ultraviolet divergencies as the Coulomb gauge electrodynamics.

Electric dipole (long-wave length) approximation needs some additional care in the regularized MF. It is demonstrated in Sect.5 that our regularization must be sufficiently soft in order the electric dipole interaction has the same form $e\vec{q}\vec{E}$ as in the usual MF. Under the same restriction it will be shown in Sect.6 that the regularized MF along with the usual MF has no interatomic Coulomb interactions.

2. MULTIPOLAR HAMILTONIAN AND ITS DIVERGENCIES

2.1. Consider the nonrelativistic spinless charge (electron) bounded by a potential $V(\vec{q})$ and interacting with the quantized electromagnetic field. In the Coulomb gauge its Hamiltonian is

$$H = \frac{1}{2m}[\vec{p} - e\vec{A}(\vec{q})]^2 + V(\vec{q}) + H_{ph}, \quad \mathrm{div}\vec{A} = 0 \tag{1}$$

$$H_{ph} = \frac{1}{2}\int d^3x[\vec{E}_\perp^2(\vec{x}) + \vec{H}^2(\vec{x})]. \tag{2}$$

One can verify that H is invariant under the following gauge transformation:

$$\vec{A}(\vec{x}) \to \vec{A}(\vec{x}) + \vec{\nabla}\chi(\vec{x}), \quad \vec{p} \to \vec{p} + e\vec{\nabla}\chi(\vec{q}). \tag{3}$$

Some comments concerning this transformation must be made.

a) It is the transformation of (electron and field) operators, as is adopted in relativistic spinor electrodynamics. Sometimes, one uses the wave function transformation $\psi(\vec{q},\ldots) \to \psi(\vec{q},\ldots)\exp ie\chi(\vec{q})$ instead of $\vec{p} \to \vec{p} + e\vec{\nabla}\chi$.

b) $\vec{x}$ and $\vec{q}$ values in eq.(3) must belong to a bounded simply connected space region W, not to all space.

The reason is that $\vec{A} \to \vec{A} + \vec{\nabla}\chi$ must conserve A transversality, and therefore, one must have $\Delta\chi(\vec{x}) = 0$. If the equation holds everywhere and the harmonic function χ vanishes at infinity, then $\chi(\vec{x}) \equiv 0$. One assumes that W contains the region where our electron is localized. Owing to this peculiarity the transformation was called quasigradient (quasigauge) in[7]. An

example of such a transformation was discussed in Sect.4.4 of that paper.

2.2. The Hamiltonian (I) has the deficiency that its atomic part $H_A = p^2/2m + V(\vec{q})$ is not invariant under (3). Therefore, H_A can be named the nonphysical operator. To remedy this, let us introduce instead of the canonical variables $\vec{q}, \vec{p}, \vec{A}(\vec{x})$, $\vec{E}_\perp(\vec{x})$ other operators $\vec{q}', \vec{p}', \ldots$ such that the new atomic Hamiltonian $H'_A(p',q')$ will be quasigauge-invariant. If the old variables O and new ones O′ are connected by the transformation $O' = S^{-1}OS$, then the new operators will have canonical commutation relations. One can therefore assume that it is the new operator $\vec{p}'$ which describes the observable electron momentum. Let us consider

$$S = S(\vec{q},\vec{A}) = \exp[-ie\int_r^q d\vec{\ell}\vec{A}(\vec{\ell})]. \qquad (4)$$

The integral in eq.(4) is taken along a line connecting the points $\vec{r}$ and $\vec{q}$, $\vec{r}$ being the centre of the potential $V(\vec{q})$. For details see [2,3,8] and Sect.3 below.

The transformation $O' = S^{-1}OS$ with such S is the usual transformation leading to the multipolar Hamiltonian, see, e.g., [2,3].

As S depends on $\vec{q}$ and $\vec{A}$ only, we have $\vec{q}' = \vec{q}$ and $\vec{A}' = \vec{A}$. Using

$$e^A B e^{-A} = B + [A,B] + \frac{1}{2}[A,[A,B]] + \ldots \qquad (5)$$

one obtains

$$\vec{p}' = S^{-1}\vec{p}S = \vec{p} - e\vec{\nabla}_q\int_r^q d\vec{\ell}\cdot\vec{A}(\vec{\ell}), \qquad (6)$$

$$E'_{\perp m}(\vec{x}) = E_{\perp m}(\vec{x}) + e\int_r^q \Sigma_n\, d\ell_n \delta^\perp_{nm}(\vec{\ell}-\vec{x}), \quad m,n = 1,2,3. \qquad (7)$$

To calculate (7) I used

$$[A_n(\vec{\ell}), E_{\perp m}(\vec{x})] = -i\delta^\perp_{nm}(\vec{\ell}-\vec{x}),$$

$$\delta^\perp_{nm}(\vec{\ell}-\vec{x}) \equiv \delta_{nm}\delta^{(3)}(\vec{\ell}-\vec{x}) - \frac{1}{4\pi}\frac{\partial}{\partial\ell_n}\frac{\partial}{\partial x_m}|\vec{\ell}-\vec{x}|^{-1}. \qquad (8)$$

Now let us show that $\vec{p}'$ is invariant under the transformation (3):

$$p'_m \to p_m + e\,\partial\chi(q)/\partial q_m - e\frac{\partial}{\partial q_m}\int_r^q \Sigma_n\, d\ell_n[A_n(\vec{\ell}) + \partial\chi(\vec{\ell})/\partial\ell_n] =$$

$$= p_m - e\frac{\partial}{\partial q_m}\int_r^q d\vec{\ell}\vec{A} = p'_m. \qquad (9)$$

Here, we used the equation

$$\int_r^q d\vec{\ell}\cdot\vec{\nabla}\chi(\vec{\ell}) = \chi(\vec{q}) - \chi(\vec{r}). \qquad (10)$$

Using eqs.(6) and (7) one can write the Hamiltonian H, see eq.(1), in terms of the new operators, i.e. substituting $\vec{p}' + e\vec{\nabla}\int d\vec{\ell}\vec{A}$ for $\vec{p}$, etc. [6].

$$H = \frac{1}{2m}[\vec{p}' - e\vec{G}(\vec{q})]^2 + V(\vec{q}) + H'_{ph} + e\int_r^q \Sigma_n d\ell_n E'_{\perp n}(\vec{\ell}) + P_\perp. \qquad (11)$$

Here H'_{ph} is the same functional of $\vec{E}'_\perp$ and $\vec{H}' = \vec{H}$ as $H_{ph}(\vec{E}_\perp, \vec{H})$, see eq.(2);

$$\vec{G}(\vec{q}) = \vec{A}(\vec{q}) - \vec{\nabla}_q\int_r^q d\vec{\ell}\vec{A}. \qquad (12)$$

The operator $\vec{G}$ can be represented in terms of the magnetic field [3,7]. The last term $P_\perp$ in eq.(11) originates from $\frac{1}{2}\int\vec{E}^2_\perp(\vec{x})d^3x$ when eq.(7) is used

$$P_\perp = \frac{e^2}{2}\sum_{m,n}\int_r^q d\ell_m\int_r^q d\ell'_n\,\delta^\perp_{m,n}(\vec{\ell}-\vec{\ell}'). \qquad (13)$$

The atomic part is now $H'_A = (\vec{p}')^2/2m + V(\vec{q})$ and is quasigauge-invariant because $\vec{p}'$ is, see eq.(9).

2.3. The term $P_\perp$ will be calculated in the next section for the case when the integral in (4) is taken over the straight line connecting $\vec{r}$ and $\vec{q}$. The result can be represented as

$$\frac{e^2}{4\pi}|\vec{q}-\vec{r}|\int_0^\infty kdk,$$

i.e., the most divergent part of $P_\perp$ is proportional to $|\vec{q}-\vec{r}|$. So $P_\perp$ is the operator of the same type as the potential energy $V(\vec{q})$ but it is quadratically divergent.

Power and Zienau [1] dealt with this divergency in the following manner. Despite the fact that $P_\perp$ has the same nature as $V(\vec{q})$ and is larger than $V(\vec{q})$, they included $P_\perp$ in H'_{int} leaving $V(\vec{q})$ in H'_A: $H = H'_A + H'_{ph} + H'_{int}$. Then, they considered the most divergent part of the radiative correction ΔE_m to the energy E_m of the atomic level m resulting from $e\vec{q}\vec{E}$ in the second order of perturbation theory. It turned out that the part was cancelled by the contribution to E_m resulting from $P_\perp$ in the first order. Woolley (see [5], sect. VIB) noted that Power and Zienau have

done the calculations in the dipole approximation which is not legitimate in this case. He used $e\int_0^q (d\vec{\ell}\cdot\vec{E}_\perp)$ instead of $e\vec{q}\vec{E}_\perp$ and singled out from ΔE_m the most divergent part equal to $(-i)\langle m|P_\perp|m\rangle$, and therefore, cancelled by $P_\perp$ as before.

So in this illogical way the most divergent part of the radiative correction to the level energy is compensated by the divergent potential-like term $P_\perp$ of the multipolar Hamiltonian. All these divergencies are quadratic as compared to the most linear divergency of the Coulomb gauge nonrelativistic electrodynamics /17/.

One may infer that it is the transformation operator S, given by eq.(4), which is the cause of this additional MF divergencies. Indeed, I shall show in the next section that a regularization of S removes them. For this purpose, it is sufficient to consider the above simple case of nonrelativistic Hamiltonian (1) or (11) because all other cases, including the relativistic one, contain the same divergent integral $P_\perp$, see e.g. /7/, Sect.2.

3. REGULARIZED MULTIPOLAR TRANSFORMATION

3.1. The integral in eq.(4) for S is taken over a fixed line connecting the points $\vec{r}$ and $\vec{q}$. The line can be represented, e.g., by the following vector function $\vec{\ell}(\alpha)$ of a parameter α

$$\vec{\ell} = \vec{r} + \alpha(\vec{q} - \vec{r}) + \nu(\alpha)\vec{s}, \quad 0 \le \alpha \le 1. \tag{14}$$

Here the continuous function $\nu(\alpha)$ must vanish at $\alpha=0$ and $\alpha=1$. Then, $\vec{\ell}=\vec{r}$ at $\alpha=0$ and $\vec{\ell}=\vec{q}$ at $\alpha=1$. To define the line a vector $\vec{s}$ is introduced in addition to $\vec{r}$ and $\vec{q}$, see fig.1.

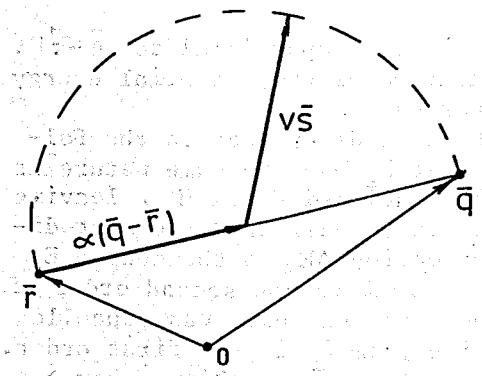

Figure 1. The line of integration is dashed.

It can be shown that $\vec{\ell}(\alpha)$ is a second order algebraic curve if $\nu(\alpha) = \alpha(1-\alpha)$. The most simple case is the straight line when $\vec{s} = 0$.

I suggest the following generalization: an averaging over a set of lines is taken instead of choosing one line. The following set is taken: $\nu(\alpha)$ is a fixed function and $\vec{s}$ runs through all three-dimensional vector space, $\mu(\vec{s})$ being a measure of the particular value $\vec{s}$. So the regularized multipolar transformation is

$$S_R = \exp[-ie\int d^3s\mu(\vec{s})\int_r^q d\vec{\ell}\vec{A}(\vec{\ell})]. \tag{15}$$

The new electron momentum operator is now

$$\vec{p}' = S_k^{-1}\vec{p}S_k = \vec{p} - e\vec{\nabla}_q\int d^3s\mu(\vec{s})\int_r^q d\vec{\ell}\cdot\vec{A}.$$

It remains to be invariant under (3) if

$$\int d^3s\mu(\vec{s}) = 1. \tag{16}$$

Now for multipolar Hamiltonian one obtains eq.(11) in which $\int_r^q \ldots$ must be replaced by $\int d^3s\mu(\vec{s})\int_r^q \ldots$ (and analogously in eqs. (12) and (13)). In particular, the regularized $P_\perp$ is now

$$P_\perp = \frac{e^2}{2}\int d^3s\mu(\vec{s})\int d^3s'\mu(\vec{s}')\sum_{m,n}\int_r^q d\ell_m\int_r^q d\ell'_n\,\delta^\perp_{mn}(\vec{\ell}-\vec{\ell}'). \tag{17}$$

3.2. To calculate $P_\perp$ we replace $\delta^\perp_{mn}$ in eq.(17) by

$$\delta^\perp_{mn}(\vec{\ell}-\vec{\ell}') = (2\pi)^{-3}\int d^3k\,(\delta_{mn} - k_m k_n/k^2)\exp i\vec{k}(\vec{\ell}-\vec{\ell}') =$$

$$= (2\pi)^{-3}\int d^3k\sum_{\lambda=1,2}\epsilon^\lambda_m(\vec{k})\epsilon^\lambda_n(\vec{k})\exp i\vec{k}(\vec{\ell}-\vec{\ell}'),$$

where $\vec{\epsilon}^1(\vec{k})$ and $\vec{\epsilon}^2(\vec{k})$ are two unit vectors, such that $(\vec{\epsilon}^1\vec{k}) = (\vec{\epsilon}^2\vec{k}) = (\vec{\epsilon}^1\vec{\epsilon}^2) = 0$. Changing the order of integration we get

$$P_\perp = \frac{e^2}{2(2\pi)^3}\int d^3k\sum_\lambda |\epsilon^\lambda_m B_m(\vec{k})|^2, \tag{18}$$

$$B_m(\vec{k}) = \int d^3s\mu(\vec{s})\int_r^q d\ell_m \exp i\vec{k}\vec{\ell} = e^{i\vec{k}\vec{r}}\int_0^1 d\alpha\, e^{i\vec{k}(\vec{q}-\vec{r})\alpha}\int d^3s\mu(\vec{s})\times \tag{19}$$

$$\times[q_m - r_m + \nu'(\alpha)s_m]e^{i\nu(\alpha)\vec{k}\vec{s}}.$$

Eq.(14) was used along with

$$d\vec{\ell} = [(\vec{q} - \vec{r}) + \nu'(\alpha)\vec{s}]d\alpha .$$

Now introduce the Fourier transform of μ

$$\tilde{\mu}(\vec{u}) = \int d^3 s \mu(\vec{s}) \exp i\vec{u}\vec{s}. \qquad (20)$$

Let $\mu(\vec{s})$ depend only on $|\vec{s}|$. This means that S_R depends only on $\vec{q}$ and $\vec{r}$ directions. Then, $\tilde{\mu}(\vec{u})$ also depends only on $|\vec{u}|$ and

$$\int d^3 s \mu(s) s_m \exp i\nu\vec{k}\vec{s} = \frac{1}{i\nu} \frac{\partial}{\partial k_m} \tilde{\mu}(\nu k) = -i\frac{\vec{k}}{k}\tilde{\mu}'(\nu k). \qquad (21)$$

Here and below $\tilde{\mu}(\nu k)$ stands for $\tilde{\mu}(|\nu|k)$.

Now we note that expression (21) which enters into eq.(19) does not contribute to $P_\perp$ because $(\vec{\epsilon}^{\lambda}\vec{k}) = 0$. We have

$$\sum_m \epsilon_m^{\lambda} B_m(\vec{k}) = e^{i\vec{k}\vec{r}}\, \vec{\epsilon}^{\lambda}\cdot(\vec{q} - \vec{r}) \int_0^1 d\alpha\, e^{i\alpha\vec{k}(\vec{q}-\vec{r})} \tilde{\mu}(\nu(\alpha)k).$$

Using $\sum_\lambda \epsilon_m^\lambda \epsilon_n^\lambda = \delta_{mn} - k_m k_n/k^2$ one obtains

$$P_\perp = \frac{e^2}{2(2\pi)^3} \int_0^\infty k^2 dk \int d\cos\theta d\phi [x^2 - (\frac{\vec{x}\vec{k}}{k})^2] |\int_0^1 d\alpha e^{i\alpha\vec{k}\vec{x}} \tilde{\mu}(\nu k)|^2. \qquad (22)$$

Here $\vec{x} \equiv \vec{q} - \vec{r}$. If we choose $\mu(s) = \delta^3(\vec{s})$ or $\tilde{\mu} = 1$, see eqs.(20) and (16), then S_R becomes the nonregularized S with the straight line of integration. In this case

$$P_\perp = \frac{e^2 x^2}{2(2\pi)^3} \int k^2 dk \int_{-1}^{+1} dt(1-t^2)[\frac{\sin\frac{1}{2}kxt}{\frac{1}{2}kxt}]^2 =$$

$$= \frac{e^2 x^2}{(2\pi)^2} \int k^2 dk \int_0^{\frac{1}{2}kx} dr \frac{2}{kx}[1 - (\frac{2r}{kx})^2][\frac{\sin r}{r}]^2 \simeq \frac{2e^2|\vec{x}|}{(2\pi)^2} \int_0^\infty kdk \frac{\pi}{2}. \qquad (23)$$

Only the most divergent part of $P_\perp$ is retained here. This result has been used for the discussion in Subsect.2.3.

Now let us show that $P_\perp$ can be made finite by choosing suitable $\tilde{\mu}$ and $\nu(\alpha)$ in eq.(22). Let

$$\tilde{\mu}(\nu k) = \exp(-b\nu(\alpha)k), \quad b > 0, \qquad (24)$$

$$\nu(\alpha) = \begin{cases} \alpha^{\frac{1}{n}}, & 0 \le \alpha \le \frac{1}{2}, \\ (1-\alpha)^{\frac{1}{n}}, & \frac{1}{2} \le \alpha \le 1, \end{cases} \qquad n = 1, 2, 3, \ldots \qquad (25)$$

Then, one may evaluate $|\int d\alpha \ldots|$ in eq.(22):

$$|\int_0^1 d\alpha \exp i\alpha\vec{k}\vec{x}\, \tilde{\mu}(\nu(\alpha)k)| \le \int_0^1 d\alpha |\tilde{\mu}(\nu(\alpha)k)| =$$

$$= \int_0^{1/2} d\alpha \exp(-b\alpha^{\frac{1}{n}}k) + \int_{1/2}^1 d\alpha \exp(-b(1-\alpha)^{\frac{1}{n}}k) = \frac{2n}{(bk)^n} \int_0^L z^{n-1} e^{-z} dz, \quad L \equiv 2^{-\frac{1}{n}} bk. \qquad (26)$$

The change of variables $z = bk\alpha^{1/n}$ was made. The last integral in eq.(26) tends to $(n-1)!$ as $bk \to \infty$. We see that the integral (22) converges surely at large k if $n \ge 2$. There exist other examples of $\tilde{\mu}(\nu k)$ which make $P_\perp$ finite.

3.3. Regularized multipolar Hamiltonian with the chosen μ and $\nu(\alpha)$ now does not contain a divergent operator term. Being finite $P_\perp$ can be now interpreted as an "intramolecular potential energy", see Ref.4 p.238 and Ref.9, p.2639. The approach by Power, Zienau and Woolley discussed in Subsect.2.3. becomes quite legitimate: as $P_\perp$ is finite and proportional to e^2, it can be considered as a small perturbation term. But simultaneously the approach proves the finiteness of the radiation corrections to the level energies which are due to the interaction term

$$e \int d^3 s \mu(s) \int_r^q d\vec{\ell}\vec{E}_\perp'(\vec{\ell}). \qquad (27)$$

Then, a natural question arises: are all radiative corrections finite in the regularized MF? It will be shown in the next section that ultraviolet divergencies in the regularized case are exactly those as in the Coulomb gauge.

3.4. Another possible generalization of the transformation S is to perform an averaging over a set of points $\vec{r}$, replacing $\int_r^q \ldots$ by $\int d^3 r m(r) \int_r^q \ldots$, see Sect.3.3. in /7/. It can be shown that this averaging by itself cannot make $P_\perp$ finite.

4. ULTRAVIOLET DIVERGENCIES IN THE REGULARIZED MULTIPOLAR FORM

Besides (27) another interaction term in the regularized multipolar Hamiltonian is

$$-\frac{e}{2m}[\vec{p}'\vec{\mathcal{A}}(\vec{q}) + \vec{\mathcal{A}}(\vec{q})\vec{p}'] + \frac{e^2}{2m}\vec{\mathcal{A}}^2(\vec{q}), \tag{28}$$

$$\vec{\mathcal{A}}(\vec{q}) \equiv \vec{A}(\vec{q}) - \vec{\nabla}_q \int d^3 s\,\mu(s) \int_r^q d\vec{\ell}\vec{A}(\vec{\ell}). \tag{29}$$

Let us show that the part of the interaction (28) which contains $\vec{\nabla}_q \int \ldots$ gives finite radiative corrections as well as (27). For this purpose insert in $\vec{\nabla}_q \int \ldots$ (see eq.(29)) the standard expansion

$$\vec{A}(\vec{\ell}) = (2\pi)^{-3/2} \int d^3 k (2k)^{-1/2} \Sigma_\lambda \vec{\epsilon}^{\lambda}(\vec{k}) [a_{k\lambda} e^{i\vec{k}\vec{\ell}} + a^+_{k\lambda} e^{-i\vec{k}\vec{\ell}}]. \tag{30}$$

and use (14). Further calculations are similar to those given in Subsect.3.2. for $\vec{\epsilon}^{\lambda}\vec{B}$ (in particular eqs.(20) and $(\vec{\epsilon}^{\lambda}\vec{k}) = 0$ are used). The result can be represented as follows:

$$\vec{\nabla}_q \int d^3 s\,\mu(s) \int_r^q d\vec{\ell}\vec{A}(\vec{\ell}) =$$

$$= (2\pi)^{-3/2} \int d\,k (2k)^{-1/2} \Sigma_\lambda \vec{\epsilon}^{-\lambda}(k) [a_{k\lambda} e^{i\vec{k}\vec{r}} \int_0^1 da\, e^{ia\vec{k}\vec{x}}\, \tilde{\mu}(\nu(a)k) +$$

$$+ a^+_{k\lambda} e^{-i\vec{k}\vec{r}} \int^1 da\, e^{-ia\vec{k}\vec{x}}\, \tilde{\mu}(\nu k)] \sim$$

$$+ (2\pi)^{-3/2} \int d^3 k (2k)^{-1/2} \Sigma_\lambda \vec{k}(\vec{\epsilon}^{-\lambda} \cdot \vec{x})[a_{k\lambda} e^{i\vec{k}\vec{r}} \int_0^1 a\,da\, e^{ia\vec{k}\vec{x}}\, \tilde{\mu}(\nu k) +$$

$$+ a^+_{k\lambda} e^{-i\vec{k}\vec{r}} \int_0^1 a\,da\, e^{-ia\vec{k}\vec{x}}\, \tilde{\mu}(\nu k)]. \tag{31}$$

Here $\vec{x} \equiv \vec{q} - \vec{r}$. We see that (31) contains the transversal part $\sim \vec{\epsilon}^{\lambda}$ along with the longitudinal one $\sim \vec{k}$. Compare the obtained expansion of $\vec{\nabla}_q \int \ldots$ in $a_{k\lambda}$, $a^+_{k\lambda}$ with the expansion (30). The former contains two form factors $\int da\,\tilde{\mu}\exp ia\vec{k}\vec{x}$ and $\int a\,da\,\tilde{\mu}\exp ia\vec{k}\vec{x}$. The first one can be made less than any inverse power of k when $k \to \infty$ by a suitable choice of $\tilde{\mu}(\nu k)$, see Subsect.3.2. above, eq.(26). The same can be proved for the second form factor. Therefore, the part $\vec{\nabla}\int$ of the potential $\vec{\mathcal{A}} = \vec{A} - \vec{\nabla}\int$ cannot lead to divergencies in the radiative corrections. Their divergence is due entirely to the term $\vec{A}$ in $\vec{\mathcal{A}} = \vec{A} - \vec{\nabla}\int$, and therefore, is exactly the same as in the Coulomb gauge.

5. ELECTRIC DIPOLE APPROXIMATION IN THE REGULARIZED MULTIPOLAR FORM

In the usual MF the interaction term $e\int_r^q d\vec{\ell}\vec{E}'_\perp$ turns into $e(\vec{q}-\vec{r})\vec{E}'_\perp$ if $\vec{E}'_\perp(\vec{\ell})$ can be replaced by $\vec{E}'_\perp(\vec{r})$ (remind that $\vec{r}$ is the centre of the potential $V(\vec{q})$ bounding the electron). The replacement can be justified for the matrix elements of the type $\langle \vec{k},\lambda,m|e\int_r^q d\vec{\ell}\vec{E}'_\perp(\vec{\ell})|n\rangle$ if atomic states n and m are localized in the region of $|\vec{q}-\vec{r}|$ values whose dimension is of the order of the atomic radius a and if photon momentum k is small, so that $ka \ll 1$. In the MF one must impose the additional restriction: the line of integration must not go beyond the region a, see fig.2, because $k|\vec{\ell}-\vec{r}| \ll 1$ may be not true for $|\vec{\ell}-\vec{r}| \gg a$.

In the regularized MF one must require that $\mu(s)$ should suppress such lines as shown in fig.2, i.e., suppress large $|\vec{s}|$. For this purpose the parameter b in eq.(24) must not exceed a. Note that $\tilde{\mu}(u) = \exp(-bu)$ corresponds to $\mu(s) = b[\pi^2(b^2+s^2)]^{-1}$. Under this additional requirement one has

$$e\int d^3 s\,\mu(s) \int_r^q d\vec{\ell}\vec{E}'_\perp(\vec{\ell}) = e(\vec{q}-\vec{r})\vec{E}'_\perp(\vec{r}) \int d^3 s\,\mu(s) =$$

$$= e(\vec{q}-\vec{r})\vec{E}'_\perp(\vec{r}).$$

because of eq.(16).

So the regularized MF has the usual main interaction term $e(\vec{q}-\vec{r})\vec{E}_\perp$ for low-energy photons if the regularization is sufficiently soft: $0 < b < a$. I should stress that for hard photons the interaction (28) is important. In particular it must be taken into account when calculating radiative corrections.

6. INTERATOMIC COULOMB INTERACTIONS

It is known that in the usual MF there are no Coulomb interactions between electrons of different atoms or molecules, see, e.g., [3,8,9]. Let us show that this is true also in regularized MF provided the regularization is sufficiently soft. The proof will be given for the simplest case of several neutral atoms, each atom having one electron. In the Coulomb gauge the related Hamiltonian is

$$H = \sum_{j=1}^{N} \frac{1}{2m}[\vec{p}_j - e\vec{A}(\vec{q}_j)]^2 + \Sigma_{ij} V_{ij}(\vec{q}_i - \vec{r}_j) + \frac{e^2}{8\pi} \Sigma_{ij} \frac{1}{|\vec{q}_i - \vec{q}_j|} + H_{ph}. \tag{32}$$

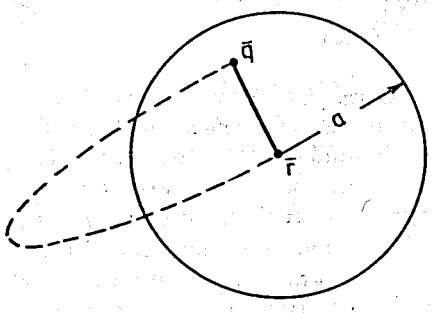

Figure 2. The line of integration is dashed.

Here $\vec{r}_j$ is the centre of the j-th atom. The related regularized transformation to the multipolar form is realized by

$$S_R = \exp[-ie \sum_{j=1}^{N} \int d^3 s_j \mu(s_j) \int_{r_j}^{q_j} d\vec{\ell}_j \vec{A}(\vec{\ell}_j)] \tag{33}$$

$$\vec{\ell}_j = \vec{r}_j + a_j(\vec{q}_j - \vec{r}_j) + \nu(a_j)\vec{s}_j .$$

One may use the same averaging function μ for different atoms. In analogy with Sect.2 I write (32) in terms of the new operators $\vec{p}'_j = S^{-1}\vec{p}_j S$, etc., instead of the old ones. One obtains

$$H = \Sigma_j \frac{1}{2m}[\vec{p}'_j - e\vec{G}_j(\vec{q}_j)]^2 - e\Sigma_j \int d^3 s_j \mu(s_j) \int_{r_j}^{q_j} d\vec{\ell}_j \vec{E}'(\vec{\ell}_j) + \tag{34}$$

$$+ H'_{ph} + \Sigma_{ij}(P_\perp)_{ij} + \Sigma_{ij} V_{ij}(\vec{q}_i - \vec{r}_j) + \frac{e^2}{8\pi} \Sigma_{ij} |\vec{q}_i - \vec{q}_j|^{-1},$$

$$\vec{G}_j(\vec{q}_j) = \vec{A}(\vec{q}_j) - \vec{\nabla}_j \int_{r_j}^{q_j} d\vec{\ell}_j \vec{A}(\vec{\ell}_j), \tag{35}$$

$$(P_\perp)_{ij} = \frac{e^2}{2} \int d^3 s_i \mu(s_i) \int d^3 s'_j \mu(s'_j) \Sigma_{m,n} \int_{r_i}^{q_i} d\ell'_{im} \int_{r_j}^{q_j} d\ell'_{jn} \delta_{mn}(\vec{\ell}_i - \vec{\ell}'_j). \tag{36}$$

The terms $(P_\perp)_{jj}$ were discussed previously. Consider the term $(P_\perp)_{ij}$ with $i \neq j$. Using (8) I represent it as $P_{ij} - (P_{||})_{ij}$, where

$$P_{ij} = \frac{e^2}{2} \int d^3 s_i \mu(s_i) \int d^3 s'_j \mu(s'_j) \int_{r_i}^{q_i} \int_{r_j}^{q_j} d\vec{\ell}_i \, d\vec{\ell}'_j \, \delta^{(3)}(\vec{\ell}_i - \vec{\ell}'_j), \tag{37}$$

$$(P_{||})_{ij} = \frac{e^2}{8\pi} \int d^3 s_i \mu(s_i) \int d^3 s'_j \mu(s'_j) \Sigma_{m,n} \int_{r_i}^{q_i} d\ell_{im} \int_{r_j}^{q_j} d\ell'_j \frac{\partial}{\partial \ell_{im}} \frac{\partial}{\partial \ell'_{jn}} |\vec{\ell}_i - \vec{\ell}'_j|^{-1}.$$

Let the function $\mu(s)$ be supported in the volume whose dimension is of the order of the atom radius a. Suppose that distances between atoms are larger than a. Then, the argument of $\delta^{(3)}(\vec{\ell}_i - \vec{\ell}'_j)$ in (37) cannot be zero and $P_{ij} = 0$ for $i \neq j$.

To calculate $(P_{||})_{ij}$ I use the equation of the type (10). Then

$$\sum_{m,n} \int_{r_i}^{q_i} d\ell_m \int_{r_j}^{q_j} d\ell'_n \frac{\partial}{\partial \ell_m} \frac{\partial}{\partial \ell'_n} |\vec{\ell} - \vec{\ell}'| =$$

$$= |\vec{r}_i - \vec{r}_j|^{-1} - |\vec{q}_i - \vec{r}_j|^{-1} - |\vec{q}_j - \vec{r}_i|^{-1} + |\vec{q}_i - \vec{q}_j|^{-1}. \tag{39}$$

The r.h.s. of eq. (39) does not depend on s_i and s'_j and one can use (16) and obtain that $(P_{||})_{ij}$ is equal to the r.h.s. of eq.(39) multiplied by $e^2/8\pi$. The last term in (39) annihilates with the corresponding term $e^2/8\pi |\vec{q}_i - \vec{q}_j|$ in the Hamiltonian, see eq.(34). The sum $\Sigma_{i \neq j}$ of the second and third terms in (39) annihilates the sum $\Sigma_{i \neq j} V_{ij}(\vec{q}_i - \vec{r}_j)$, see eq.(34), if the potentials V_{ij} are Coulomb: $V_{ij}(\vec{q}_i - \vec{r}_j) = -e^2/4\pi|\vec{q}_i - \vec{r}_j|$ (one must suppose that the nuclear charges are equal to unity, i.e., that atom as a whole is neutral). So all Coulomb interactions are absent in the multipolar Hamiltonian (34). In the multipolar formalism an atom can change the state of another atom only by means of photon exchanges.

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Note added in proof

An example of regularized potential $\hat{P}_\perp$ may be of interest. Let $\nu(a) = (a/\delta)^{1/2}$ at $a < \delta$, $\nu(a) = ((1-a)/\delta)^{1/2}$ at $1-\delta < a \leq 1$ and $\nu(a) = 1$, when $\delta < a < 1-\delta$. Let $\tilde{\mu}(\nu k)$ be represented by eq.(24). Then in the limit $\delta \to 0$, $\hat{P}_\perp$ can be represented by eq.(22), where

$$\left| \int_0^1 da \ldots \right|^2 = \exp(-2bk)\left[\sin\frac{\bar{k}\bar{x}}{2}\right]^2 \left[\frac{\bar{k}\bar{x}}{2}\right]^{-2} ; \quad \bar{k}\bar{x} = kx\cos\theta .$$

The result of integration $\int d\cos\theta$ in eq.(22) contains integral sine function Si(kx) in addition to usual trigonometric functions, but all the subsequent integrals $\int_0^\infty dk \ldots$ can be found in tables of Laplace transforms. The exact result is

$$\lim_{\delta \to 0} \hat{P}_\perp = \frac{2e^2}{(2\pi)^2}\left\{\left[\frac{x}{(2b)^2} + \frac{1}{x}\right]\operatorname{arctg}\frac{x}{2b} - \frac{1}{2b}\right\}, \quad x \equiv |\bar{q} - \bar{r}| .$$

This reduces to $e^2 x^2/(2\pi)^2 6b^3$, when $x \ll b$, and to $\frac{e^2}{4\pi}\left[\frac{x}{(2b)^2} - \frac{2}{\pi b} + 1/x\right]$, when $x \gg b$.