Toroid moment contribution to the problem of multipolar representation of Maxwell's and Schrödinger's equations*

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Quite a lot of works are devoted to the problems given in the title of the paper but the complete solution of them has not been found yet. We propose our treatment of this problem including toroid contributions into consideration.

I. INTRODUCTION

Let us remind a known thing that says *"it is impossible to introduce electrodynamics of matter in general"* (**E. A. Turov, 1983**). For example, different types of crystalline structures of matter lead to the alignment of one or other type of polarizations in the matter considered. So the necessity to introduce in the equations of high tensor polarization is arose. But the most intricate case is the toroid polarization one. The fact is that the ideal static toroid moments do not interact with each other. So the dynamic alignment of toroid moments is impossible thanks to electric and magnetic interactions. But this takes place for example in perovskites [1, 2] and have to be explained. The other case when the local toroid moments can align is connected with their proper oscillations that permit them interact with each other [3] through electric and magnetic fields.

It is noteworthy to remark that toroid moments are the multipole sources of field-free vector potentials. Therefore, electromagnetotoroidic equations we are forced to express in terms of vector potentials. The first part of our report is devoted to introduction of the equations mentioned in Lagrangian formalism. In the second part we introduce toroid moments in Schrödinger equations.

II. TOROID MOMENTS IN LAGRANGIAN FORMALISM

A. Canonical formulation of electrodynamics

We begin with usual canonical formulation of electrodynamics (e.g. [4]). The interacting system of electromagnetic field and non-relativistic charged particles is specified partly by

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a discrete set of variables, namely the coordinates of the charged particles, and partly by a continuous set, which we take to be the values of the vector potential in the Coulomb gauge. The Lagrangian L will thus be a functional of $\mathbf{A}$ and $\dot{\mathbf{A}}$ if the particle coordinates and their velocities are fixed, and a function of the $\mathbf{q}_\alpha$ and $\dot{\mathbf{q}}_\alpha$ if the vector potential and its time derivative are fixed. We write $L = L[\mathbf{A}, \dot{\mathbf{A}}; q\,\dot{q}]$. In the application of Hamilton's principle, the particle and the field coordinates are to be varied independently. The Lagrangian must then be chosen so that variation with respect to the particle coordinates gives Newton's law and variation with respect to the field coordinates (subject to the Coulomb gauge condition) gives the equation of motion for the vector potential. A suitable Lagrangian is obtained by setting (see e.g. [4])

$$L = \frac{1}{2}\sum_\alpha m_\alpha\,\dot{\mathbf{q}}_\alpha^2 - \frac{1}{2}\sum_{\alpha\neq\beta}\frac{e_\alpha\,e_\beta}{|\mathbf{q}_\alpha - \mathbf{q}_\beta|} + \frac{1}{8\pi}\int\big[\frac{\dot{\mathbf{A}}^2}{c^2} - (\mathrm{curl}\,\mathbf{A})^2\big]\,dV + \\ + \,(\frac{1}{c}\int \mathbf{J}(\mathbf{r})\cdot\mathbf{A}(\mathbf{r})\,dV = \sum_\alpha \frac{e_\alpha}{c}\,\dot{\mathbf{q}}_\alpha\cdot\mathbf{A}(q_\alpha,t)). \tag{II.1}$$

Here L_{par} is the Lagrangian appropriate to a system of charged particles interacting solely through instantaneous Coulomb force; it has the simple form of "kinetic energy minus potential energy". L_{rad} is the Lagrangian for a radiation field far removed from the charges and currents, and has the form of "electric field energy minus magnetic field energy". The interaction Lagrangian L_{int} couples the particle variables to the field variables. Since the Coulomb gauge condition is being used as a constraint, the transverse current density $\mathbf{J}^\perp$ has been substituted for the total current density $\mathbf{J}$ without affecting the Lagrangian.

To verify that L given by Equation (2.1) is indeed a suitable Lagrangian, we write down the Euler-Lagrange equations, beginning with those for the particle coordinates. Using the expressions $\mathbf{B} = \mathrm{curl}\mathbf{A}$ and $\mathbf{E}^\parallel = -\mathrm{grad}\phi \quad \mathbf{E}^\perp = -(1/c)\dot{\mathbf{A}}$ with $\phi(\mathbf{r},\,t) = \sum_\alpha \frac{e_\alpha}{|\mathbf{q}_\alpha - \mathbf{r}|}$ for the transverse fields in terms of the vector potentials, we find the second law of Newton with the Lorentz force.

To obtain the field equations, the functional derivatives of L must first be calculated from the Lagrangian density. The Euler–Lagrange field equations in this case give the usual evolution equation for the vector potential in the Coulomb gauge:

$$\mathrm{curl}\,\mathrm{curl}\mathbf{A} + (1/c^2)\,\ddot{\mathbf{A}} = (4\pi/c)\mathbf{J}^\perp. \tag{II.2}$$

The conjugate momenta corresponding to the Lagrangian (2.1) are defined in the usual way as

$$\mathbf{p}_\alpha = \partial L/\partial\dot{\mathbf{q}}_\alpha = m\,\dot{\mathbf{q}}_\alpha + (e_\alpha/c)\,\mathbf{A}(\mathbf{q},\,t), \tag{II.3}$$

$$\mathbf{\Pi}(\mathbf{r}) = \partial L/\partial\dot{\mathbf{A}}(\mathbf{r}) = \dot{\mathbf{A}}(\mathbf{r})/4\pi\,c^2 = -\mathbf{E}(\mathbf{r})/4\pi\,c. \tag{II.4}$$

Proceeding in the conventional way we get

$$H[\mathbf{\Pi},\mathbf{A};p,q] = \sum_\alpha \mathbf{p}_\alpha\cdot\dot{\mathbf{q}}_\alpha + \int \mathbf{\Pi}\cdot\dot{\mathbf{A}}dV - L = \sum_\alpha \frac{1}{2m_\alpha}\big[\mathbf{p}_\alpha - \frac{e_\alpha}{c}\,\mathbf{A}(\mathbf{q},\,t)\big]^2 + \\ + \frac{1}{2}\sum_{\alpha\neq\beta}\frac{e_\alpha\,e_\beta}{|\mathbf{q}_\alpha - \mathbf{q}_\beta|} + \frac{1}{8\pi}\int\big[(4\pi\,c\mathbf{\Pi})^2 + (\mathrm{curl}\,\mathbf{A})^2\big]\,dV \tag{II.5}$$

B. Formation of an equivalent Lagrangian

It is well known that in classical dynamics the addition of a total time derivative to a Lagrangian leads to a new Lagrangian with the equations of motion unaltered. Lagrangians obtained in this manner are said to be equivalent. In general, the Hamiltonians following from the equivalent Lagrangians are different. Even the relationship between the conjugate and the kinetic momenta may be changed.

An equivalent Lagrangian to that of (2.1) is [5]

$$L^{new} \,=\, L \,-\, \frac{1}{c}\frac{d}{dt}\Big[\int \mathbf{P}(\mathbf{r})\cdot\mathbf{A}(\mathbf{r})\,dV\Big]. \tag{II.6}$$

Taking into account the Coulomb gauge condition $\mathrm{div}\mathbf{A} \,=\, 0$ and toroid contribution we may substitute

$$\mathbf{P} \,\Longrightarrow\, \mathbf{P}^{\perp} \,+\, \mathbf{P}^{\parallel} \,+\, \mathrm{curl}\,\mathbf{T}^{e}, \tag{II.7}$$

with the contribution of $\mathbf{P}^{\parallel}$ being vanished.

Thus we have the following equivalent Lagrangian

$$L^{new} \,=\, L \,-\, \frac{1}{c}\frac{d}{dt}\Big[\int (\mathbf{P}^{\perp}(\mathbf{r}) \,+\, \mathrm{curl}\mathbf{T}^{e}(\mathbf{r}))\cdot\mathbf{A}(\mathbf{r})\,dV\Big]. \tag{II.8}$$

The field conjugate to the vector potential $\mathbf{A}$ is now

$$\mathbf{\Pi}(\mathbf{r}) \,=\, -\,\frac{\mathbf{E}^{\perp}(\mathbf{r}) \,+\, 4\pi\,(\mathbf{P}^{\perp}(\mathbf{r}) \,+\, \mathrm{curl}\mathbf{T}^{e}(\mathbf{r}))}{4\pi\,c} \,=:\, -\,\boldsymbol{\mathcal{D}}(\mathbf{r})/4\pi\,c. \tag{II.9}$$

Thus the introduction of additional material field leads to the modification of the first Maxwell equation as

$$\mathrm{curl}\boldsymbol{\mathcal{D}}(\mathbf{r}) \,=\, -\,\frac{1}{c}\,\dot{\mathbf{B}}(\mathbf{r}) \,+\, 4\pi\,(\mathrm{curl}\mathbf{P}(\mathbf{r}) \,+\, \mathrm{curl}\,\mathrm{curl}\mathbf{T}^{e}(\mathbf{r})). \tag{II.10}$$

The new Lagrangian is a function of the variables $\mathbf{q}_{\alpha}$, $\dot{\mathbf{q}}_{\alpha}$ and a functional of the field variables $\mathbf{A}$, $\dot{\mathbf{A}}$, and the equations of motion follow from the variational principle. Applying the Euler-Lagrange equations of motion we obtain

$$\mathrm{curl}\mathbf{B}(\mathbf{r}) \,=\, \frac{1}{c}\dot{\boldsymbol{\mathcal{D}}}(\mathbf{r}) \,+\, 4\pi\big(\mathrm{curl}\mathbf{M}^{\perp}(\mathbf{r}) \,+\, \mathrm{curl}\,\mathrm{curl}\mathbf{T}^{m}(\mathbf{r})\big) \tag{II.11}$$

where the relation $c\,\mathrm{curl}\mathbf{M}^{\perp}(\mathbf{r}) \,=\, \mathbf{J}^{\perp}(\mathbf{r}) \,-\, \dot{\mathbf{P}}^{\perp}(\mathbf{r})$ is used and the following re-notations are introduced

$$\frac{1}{c}\,\dot{\mathbf{T}}^{e,m} \,|_{\Omega} \Longrightarrow \,\mp\,\mathrm{curl}\,\mathbf{T}^{m,e} \,|_{\Omega} \tag{II.12}$$

The relation (2.12) demands some comments. Both $\mathbf{T}^{e}$ and $\mathbf{T}^{m}$ represent themselves in essence closed isolated lines of electric and magnetic fields. So they have to obey the usual differential relations similar to the free Maxwell equations (see in [2] and [6]). However, remark that signs in (2.12) are inverse in comparison with the corresponding Maxwell equations because the direction of electric dipole is accepted to be chosen opposite to its inner electric field [7].

If we define the auxiliary field $\mathbf{H}$ to be $\mathbf{H}(\mathbf{r}) = \mathbf{B}(\mathbf{r}) - 4\pi\,(\mathbf{M}^{\perp}(\mathbf{r}) + \mathrm{curl}\mathbf{T}^{m}(\mathbf{r}))$, then it deduces to

$$\mathrm{curl}\mathbf{H} = (1/c)\dot{\boldsymbol{\mathcal{D}}}. \tag{II.13}$$

But the latter formula is unsatisfactory from the physical point of view. It is easy to image the situation when $\mathbf{B}$ and $\mathbf{M}^{\perp}$ are absent, because the medium may be composed from isolated aligned dipoles $\mathbf{T}^{m}$ [1, 2] and each $\mathbf{T}^{m}$ is the source of free-field (transverse-longitudinal) potential but not $\mathbf{B}$ [3]. The same is justified with respect to (2.10). So the transition to the description by means of potentials, as the entities more inherent than the field strengths more close to Newtonian force conception, is inevitable.

C. Formal deduction of equations of electromagnetotoroidics.

Let us suppose that in an electromagnetic medium there are no free charges and currents. So we may rewrite usual Maxwell equation in the following symmetrical form:

$$\begin{aligned} \mathrm{curl}\,\mathbf{B} &= \frac{1}{c}\dot{\mathbf{D}} + 4\pi\,\mathrm{curl}\,\mathbf{M}, \quad \mathbf{B} = \mathbf{H} + 4\pi\mathbf{M} \text{ in the whole } \Re^3, \\ \mathrm{curl}\,\mathbf{D} &= -\frac{1}{c}\dot{\mathbf{B}} + 4\pi\,\mathrm{curl}\,\mathbf{P}, \quad \mathbf{D} = \mathbf{E} + 4\pi\mathbf{P} \text{ in the whole } \Re^3, \end{aligned} \tag{II.14}$$

being of these equations interchange to each other as before through the self-reciprocal exchanges $\mathbf{B} \to \mp\mathbf{D}$, $\mathbf{D} \to \pm\mathbf{B}$, $\mathbf{M} \to \mp\mathbf{P}$, $\mathbf{P} \to \pm\mathbf{M}$ and the conditions $\mathrm{div}\,\mathbf{B} = 0$ and $\mathrm{div}\,\mathbf{D} = 0$ are fulfilled. Hence is valid the following changes [8]

$$\begin{aligned} \mathbf{B} &\Longrightarrow \mathrm{curl}\,\boldsymbol{\alpha}^{m} + \dot{\boldsymbol{\alpha}}^{e}, \qquad \mathbf{D} \Longrightarrow \mathrm{curl}\,\boldsymbol{\alpha}^{e} - \dot{\boldsymbol{\alpha}}^{m}, \\ \mathrm{curl}\,\mathbf{M} &\Longrightarrow \mathrm{curl}\,\mathbf{M} + \mathrm{curl}\,\mathrm{curl}\,\mathbf{T}^{m} \qquad \mathrm{curl}\,\mathbf{P} \Longrightarrow \mathrm{curl}\,\mathbf{P} + \mathrm{curl}\,\mathrm{curl}\,\mathbf{T}^{e} \end{aligned} \tag{II.15}$$

As a result we obtain for basic equations

$$\mathrm{curl}\,\mathrm{curl}\,\boldsymbol{\alpha}^{m} + \ddot{\boldsymbol{\alpha}}^{m} = 4\pi\,(\mathrm{curl}\,\mathbf{M} + \mathrm{curl}\,\mathrm{curl}\,\mathbf{T}^{m}) \tag{II.16}$$

$$\mathrm{curl}\,\mathrm{curl}\,\boldsymbol{\alpha}^{e} + \ddot{\boldsymbol{\alpha}}^{e} = 4\pi\,(\mathrm{curl}\,\mathbf{P} + \mathrm{curl}\,\mathrm{curl}\,\mathbf{T}^{e}) \tag{II.17}$$

It is necessary to emphasize that the potential descriptions electrotoroidic and magnetotoroidic media are completely separated. The properties of the magnetic and electric potentials $\boldsymbol{\alpha}^{m}$ and $\boldsymbol{\alpha}^{e}$ under the temporal and spatial inversions are opposite [2]. We also see that the substitutions (2.15) in (2.14) produce (2.16) and (2.17) as well.

If $\mathrm{div}\mathbf{D} \neq 0$ and in the medium there does exist free current we have to remember Dirac's approach to the constrained systems and use along for instance [9] its application to electrodynamics of continuous media.

D. Solution to the electromagnetotoroidic equations

Let us solve the equation (2.16). Adding $-\,(4\pi/c^2)\,\ddot{\mathbf{T}}^{m}$ in the both sides of the equation (2.16) for $\mathbf{a}$ we get the wave equation for $\mathbf{a}^{m} = \boldsymbol{\alpha}^{m} + 4\pi\,\mathbf{T}^{m}$

$$\mathrm{curl}\,\mathrm{curl}\mathbf{a}^{m} + \frac{1}{c^2}\,\ddot{\mathbf{a}}^{m} = 4\pi\,\mathrm{curl}\mathbf{M}^{\perp}(\mathbf{r}) - \frac{4\pi}{c^2}\,\ddot{\mathbf{T}}^{m}(\mathbf{r}) \tag{II.18}$$

The solution to this equation can be written as [10]

$$\mathbf{a}^m \;=\; -\frac{1}{4\pi}\int\limits_{all\ space} \frac{\left[-\nabla'(\nabla'\cdot\mathbf{T}^{m\,\prime}) \;-\; 4\pi\,\nabla'\times\mathbf{M}'\right) \;+\; (4\pi/c^2)\ddot{\mathbf{T}}^{m\,\prime}\right]}{|\mathbf{r}\;-\;\mathbf{r}'|}\,dV' \tag{II.19}$$

here $\mathbf{M}'$ denotes $\mathbf{M}(\mathbf{r}')$. One can obtain the solution to the equation (2.17) inserting $\mathbf{a}^e$, $\mathbf{P}$ and $\mathbf{T}^e$ instead of $\mathbf{a}^m, \mathbf{M}$ and $\mathbf{T}^m$. Under the Coulomb gauge the substitution $\mathrm{div}\,\mathbf{a}^{m,e} = -4\pi\,\mathrm{div}\,\mathbf{T}^{m,e}$ is valid. The brackets [] in the above equations are the "retardation symbol". This symbol indicates a special space and time dependence of the quantities to which it is applied and is defined by the identity

$$[f] \;\equiv\; f(x', y', z', t - r/c).$$

III. INTRODUCING OF MULTIPOLAR INTERACTIONS INTO SCHRödINGER EQUATIONS

A large number of works have been devoted to this problem. Unfortunately most of them are confusing. We demonstrate it on the basis of detail but incorrect paper by K. Haller and R. B. Sohn [11]. The matter is that they begin with the expression independent of the scalar-longitudinal contributions $(\rho, \mathrm{div}\mathbf{j})$ and after the integrations by parts in the final expression restore them. It is a very common methodical error.

A. Description of non-relativistic interaction of electrons and photons

Here we proceed and set the problem in terms used in [11]. The Hamiltonian that describes the interaction between photons and non-relativistic Schrödinger electrons is given by

$$H_c \;=\; H_0 \;-\; \int \mathbf{J}(\mathbf{r})\cdot\mathbf{A}^T(\mathbf{r})\,d\mathbf{r} \;+\; \frac{e}{2m}\int \rho(\mathbf{r})\mathbf{A}^T(\mathbf{r})\cdot\mathbf{A}^T(\mathbf{r})\,d\mathbf{r} \;+$$
$$+\;\int \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{8\pi|\mathbf{r}\;-\;\mathbf{r}'|}\,d\mathbf{r}\,d\mathbf{r}', \tag{III.1}$$

where $\mathbf{A}^T$ is the transverse vector potential with $\mathrm{div}\,\mathbf{A}^T \;=\; 0$. H_0 is the Hamiltonian for noninteracting electrons and photons that can be represented by $H_0 \;=\; H_0(e) \;+\; H_0(\gamma)$, where

$$H_0(e) \;=\; \int \psi^+(\mathbf{r})[-(2m)^{-1}\,\nabla^2 \;+\; V(\mathbf{r})]\psi(\mathbf{r})d\mathbf{r} \tag{III.2}$$

with $V(\mathbf{r})$ representing an external short-range potential (for example, the shielded Coulomb potential of a static nucleus). $H_0(\gamma)$ is the Hamiltonian for free transverse photons and is given by

$$H_0(\gamma) \;=\; \frac{1}{2}\int [\mathbf{E}^T(\mathbf{r})^2 \;+\; \mathbf{B}(\mathbf{r})^2]d\mathbf{r}, \tag{III.3}$$

where $\mathbf{E}^T(\mathbf{r})$ and $\mathbf{B}(\mathbf{r})$ represent the transverse electric and magnetic field, respectively. In equation (3.1) $\rho(\mathbf{r})$ and $\mathbf{J}(\mathbf{r})$ are the standard quantum mechnical charge and current and hold the usual quantum mechanical commutation rules. The current $\mathbf{J}(\mathbf{r})$ is conserved under the time dependence provided by the Hamiltonian so that

$$\operatorname{div}\mathbf{J}(\mathbf{r}) \;=\; -i[H_0, \rho(\mathbf{r})]. \tag{III.4}$$

The current $\mathbf{j}(\mathbf{r}) \;=\; \mathbf{J}(\mathbf{r}) \;-\; (e/m)\,\rho(\mathbf{r})\,\mathbf{A}^T(\mathbf{r})$ is conserved under the time dependence provided by the Hamiltonian so that

$$\operatorname{div}\mathbf{j}(\mathbf{r}) \;=\; -i[H_c, \rho(\mathbf{r})]. \tag{III.5}$$

Now H_c may be expressed by (3.1) substituting $\mathbf{J}(\mathbf{r}) \to \mathbf{J}(\mathbf{r}) \;+\; \mathbf{j}(\mathbf{r})$.

B. Introduction of toroid moments

A formal procedure was first proposed by E. G. P. Rowe [12] permits to obtain the complete solution to the problem of multipole expansion of electromagnetic current [3], which consists of the replacing of some vector function of current by the three (in general unlimited) series of multipole parameters. The multipole parametrization of interaction Hamiltonian of an arbitrary system with external fields under the Coulomb gauge has the form [3]

$$\begin{aligned} H_c \;=\; & -\sum_{l=1}^{\infty}\sum_{m=-l}^{l}\sum_{n=0}^{\infty}\frac{(2l\;+\;1)!!}{2^n\,n!(2l+2n+1)!!}\sqrt{\frac{2l+1}{4\pi}}\;\times \\ & \times\;\{l^{-1}M_{lm}^{(2n)}(t)Y_{lm}(\nabla)\triangle^n(\mathbf{r}\cdot\mathbf{B})|_{r=0} + \\ & +\;l_{-1}[\dot{Q}_{lm}(t)\delta_{n,0}\triangle^{-1} - T_{lm}^{2n}(t)]Y_{lm}(\nabla)\triangle^n[(1/c)\mathbf{r}\cdot\dot{\mathbf{D}} + (4\pi/c)\mathbf{r}\cdot\mathbf{j}]_{r=0}\}. \end{aligned} \tag{III.6}$$

where $\dot{Q}_{lm}(t)$, connected with Coulomb multipole moments of the charge distribution of the system are

$$\dot{Q}_{lm}(t) \;=\; \sqrt{4\pi l}\int r^{l-1}\,Y^*_{l\,l-1\,m}(\hat{r})\,\mathbf{j}(\mathbf{r},t)\,d\mathbf{r}, \tag{III.7}$$

$M_{lm}^{(2n)}(t)$ are the magnetic multipole moments or their radii

$$M_{lm}^{(2n)}(t) \;=\; \frac{-i}{c}\sqrt{\frac{l}{l+1}}\sqrt{\frac{4\pi}{2l+1}}\int r^l\,Y^*_{ll m}(\hat{r})\,\mathbf{j}(\mathbf{r},t)\,d\mathbf{r}, \tag{III.8}$$

and $T_{lm}^{(2n)}(t)$ are third family of multipole moments [13], the toroid moments and their radii, namely

$$T_{lm}^{(2n)}(t) = -\frac{\sqrt{\pi}l}{c(2l+1)}\int r^{l+2n+1}[Y^*_{l\,l-1\,m}(\hat{r}) + \frac{2\sqrt{l/l+1}}{2l+3}Y^*_{l\,l+1\,m}(\hat{r})]\cdot\mathbf{j}(\mathbf{r},t)\,d\mathbf{r}, \tag{III.9}$$

In the case considered by Haller and Sohn [11] we have to substitute into (3.15)

$$\dot{Q}_{lm}(t) \;\equiv\; \frac{\partial\,Q_{lm}}{\partial t} \;=\; i[H_c, Q_{lm}] \quad\text{and}\quad \mathbf{j} \;=\; \mathbf{J} \;-\; e\rho\,\mathbf{A}, \tag{III.10}$$

in the formulas (3.6), (3.7), (3.8) and (3.9). In this approach there does not appear any longitudinal contributions that are fictitious (mutually cancelled out) in the expression, deduced by Haller and Sohn. The formulas (3.7 - 3.9) obtained by us give correct multipole parametrization for the interaction energy transverse degrees of freedom of a non-relativistic system with radiation field.

C. Toroid moments in Schrödinger equation

Now suppose that we consider some electron involved in the molecular structure. We may introduce a coordinate system [see Fig.1] such that the Schrödinger equation for this electron interacting with external sources of electromagnetic fields has the following form [14]

$$i\hbar\dot{\phi}(\mathbf{q}) \;=\; \Big[-\frac{\hbar^2}{2m}(\nabla^{(q)})^2 \,+\, V(\mathbf{q}) \,+\, e^2\int \frac{\bar{\phi}(\mathbf{q}')\phi(\mathbf{q}')}{|\mathbf{q}\,-\,\mathbf{q}'|}\,d\mathbf{q} \,-\, \int \mathbf{P}(\mathbf{r},\,\mathbf{q})\cdot\mathbf{E}^{\perp}(\mathbf{r})\,d\mathbf{r} \,-$$
$$-\,\int \mathbf{M}(\mathbf{r},\,\mathbf{q})\cdot\mathbf{B}^{\perp}(\mathbf{r})\,d\mathbf{r} \,+\, \frac{1}{2mc^2}\Big[\int \mathbf{n}(\mathbf{r},\,\mathbf{q})\times\mathbf{B}(\mathbf{r})\,d\mathbf{r}\Big]^2\Big]\phi(\mathbf{q}), \qquad \text{(III.11)}$$

with $\mathbf{n}(\mathbf{r},\,\mathbf{q}) \,=\, -\frac{e}{2}(\mathbf{q}\,-\,\mathbf{R})\,\delta(\mathbf{r}\,-\,\mathbf{R})$.

There are two ways to introduce here the toroid contributions. The first one is straightforward to use the substitution (2.16) Then we obtain

$$\int \mathbf{P}\cdot\mathbf{E}^{\perp}\,d\mathbf{r} \Longrightarrow \int \mathbf{P}\cdot\mathbf{E}^{\perp}\,d\mathbf{r} + \int \mathrm{curl}\mathbf{T}^{e}\cdot\mathbf{E}^{\perp}\,d\mathbf{r} \,=\, \int \mathbf{P}\cdot\mathbf{E}^{\perp}\,d\mathbf{r} + \int \mathbf{T}^{e}\cdot\mathrm{curl}\mathbf{E}^{\perp}\,d\mathbf{r}, \quad \text{(III.12)}$$

$$\int \mathbf{M}\cdot\mathbf{B}\,d\mathbf{r} \Longrightarrow \int \mathbf{M}\cdot\mathbf{B}\,d\mathbf{r} \,+\, \int \mathbf{T}^{m}\cdot\mathrm{curl}\mathbf{B}\,d\mathbf{r}. \qquad \text{(III.13)}$$

More reasonable approach is developed in [2]. It goes back to the classic multipolar description of quasimolecular structure [9, 15]. According to it we may use immediately the multipole expansion of the densities $\mathbf{P}(\mathbf{r},\,\mathbf{q})$ and $\mathbf{M}(\mathbf{r},\,\mathbf{q})$ as follows [2]:

$$W^{e} \,=\, -\int \mathbf{d}(\mathbf{r},\,\mathbf{q})\cdot\mathbf{E}^{\perp}(\mathbf{r})\,d\mathbf{r} \,=\! -\mathbf{Q}\cdot\mathbf{E}^{\perp} \,-\, \mathbf{T}^{e}\cdot\mathrm{curl}\mathbf{E} \,-$$
$$-\hat{\mathbf{P}}^{e}\cdot\mathrm{curl}\,\mathrm{curl}\mathbf{E} \,-\, \frac{1}{2}Q_{ij}(\nabla_i\mathbf{E}^{\perp}_j \,+\, \nabla_j\mathbf{E}^{\perp}_i) \,-\, T^{e}_{ij}\nabla_i(\mathrm{curl}\mathbf{E}^{\perp})_i - \cdots \qquad \text{(III.14)}$$

where $\mathbf{Q} \,=\, \int \mathbf{d}(\mathbf{r})\,d\mathbf{r}$ is the conventional total electric dipole moment of the system, $\mathbf{T}^{e} \,=\, \frac{1}{2}\int \mathbf{r}\times\mathbf{d}(\mathbf{r})\,d\mathbf{r}$ is the axial toroid moment and (see [14])

$$\mathbf{P}(\mathbf{r},\,\mathbf{q}) \,=\, -e\Big\{(\mathbf{q}\,-\,\mathbf{R}) \,-\, \frac{1}{2}(\mathbf{q}\times\mathbf{R}) \,-$$
$$-\frac{e}{2}\big[(q\,-\,R)_i\,(q\,-\,R)_j \,-\, \frac{2}{3}(q\,-\,R)^2\,\delta_{ij}\big] \,+\, \cdots\Big\}\,\delta(\mathbf{r}\,-\,\mathbf{R}). \qquad \text{(III.15)}$$

Analogically for $\mathbf{M}(\mathbf{r},\,\mathbf{q})$.

Let us now define the axial toroid moment. From the classical point of view on the **origin** of electric dipoles we see that the multipole expansion of the distribution density $\mathbf{P}(\mathbf{r},t)$ contents generally three kinds of dipole moments (see Formula (3.14)). Working within the scope of classical framework after Power a. o. [5] we see that $\mathbf{T}^{e} \,=\, 0$ for a separate "atom". Really, all the electric dipoles are characterized by its space vectors, with the origins lying in the origin of the coordinate system (center mass of the system considered) and the endpoints in the electron coordinates. The sum of these vectors characterizes the total electric dipole moment of the system. To demonostrate the forementioned conclusion we consider the following example.

Let us have a system containing N atoms where each j-atom itself forms a subsystem [see Fig.2]. Let "O" be the center-mass of the system as a whole. If the system contains only one atom, say "A", which on his part consists of one nuclei and n electrons, the electric dipole moment of this system relating to the point "O" can be written as

$$\mathbf{Q} \,=\, -e\sum_{i=1}^{n}(\mathbf{R}-\mathbf{q}_i), \quad \mathbf{d} \,=\, \mathbf{Q}\,\delta(\mathbf{r}-\mathbf{R}). \tag{III.16}$$

Then the axial toroid moment of the such a system with respect to its proper center-mass is

$$\mathbf{T}^{(d)} \,=\, \frac{1}{2}\int \mathbf{d}\times\mathbf{r}\,d\mathbf{r} \,=\, \frac{e}{2}\sum_{i=1}^{n}(\mathbf{R}-\mathbf{q}_i)\times(\mathbf{R}-\mathbf{q}_i) \,=\, 0, \tag{III.17}$$

as $\mathbf{r}_i \,=\, \mathbf{R}-\mathbf{q}_i$ and $\mathbf{R}$ is fixed. If the molecule contains N atoms then we define the total toroid moment of the molecule $\mathbf{T}^{(d)}$ as a whole [16] with respect to its center-mass by the following formula

$$\mathbf{T}^{(d)} \,=\, \frac{e}{2}\sum_{j=1}^{N}\sum_{i=1}^{n}(\mathbf{R}_j-\mathbf{q}_{ij})\times\mathbf{R}_j \,=\frac{e}{2}\sum_{j=1}^{N}\sum_{i=1}^{n}[\mathbf{q}_{ij}\times\mathbf{R}_j] \,\neq 0, \tag{III.18}$$

although the axial toroid moment $\mathbf{T}_j^{(d)}$ for each separate j-atom with respect to its proper center-mass is equal to zero as before.

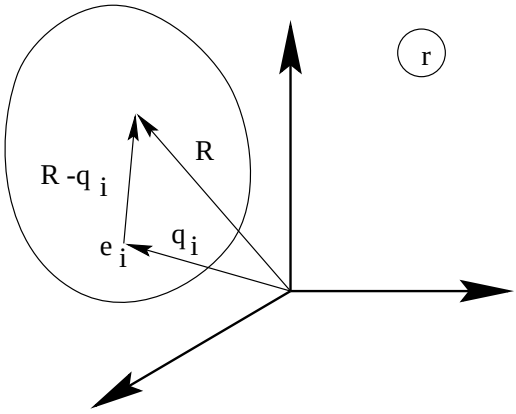

FIG. 1:

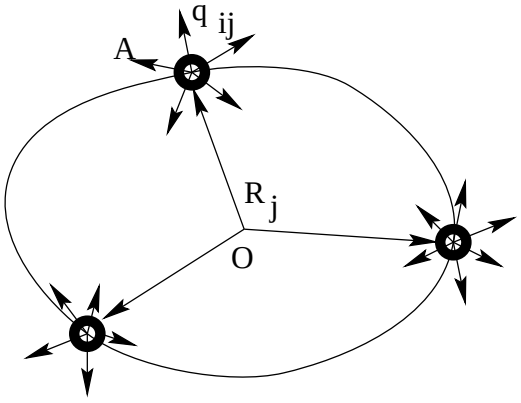

FIG. 2:

As a particular example where electromagnetic properties of molecules are described by the axial toroid moment, we point out the phenomenon of "aromagnetism" [17, 18]. The molecular orbitals ψE_{2g} and ψE_{1u} with this symmetry are built [18]. The molecules in this state are shown to have axial toroid moment.

IV. CONCLUSION

Now let us remember that there are two electric fields those differ by properties [9]. That, which appears in transverse part, is radiation field, unlike the longitudinal part that can be

connected with the evolution of scalar one in Lorentz gauge $\mathrm{div}\mathbf{A} = -(1/c)\,\dot{\varphi}$. In connection with this we should notice the terminological ambiguity. In the framework of electrodynamics of continuous media, where may be realized the situation when $\mathrm{div}\mathbf{j} = 0$, the moments $\dot{Q}_{lm}$ are the functions, independent to Coulomb moments Q_{lm}, because there is no free charges in the system considered. So $\dot{Q}_{lm}$ cannot be restored as a result of the measurement of Coulomb moments by means of permanent electric field. We will illustrate it doing inverse transformation, i.e. adding in the current part of multipole expansion the transverse and longitudinal contributions, for simplicity $\dot{Q}_{1m}$:

$$l^{-1}\big[\dot{Q}_{lm}\triangle^{-1}Y_{lm}(r\dot{\mathbf{D}}) - \dot{Q}_{lm}Y_{lm}(\nabla)\triangle^{n-1}\mathrm{div}\,\mathbf{A}\big]_{l=1,n=0} \Longrightarrow$$

$$\Longrightarrow \dot{\mathbf{Q}}\triangle^{-1}\big(\frac{1}{c}\dot{\mathbf{D}} - \nabla\mathrm{div}\mathbf{A}\big) = \dot{\mathbf{Q}}\triangle^{-1}\big(\mathrm{curl}\,\mathrm{curl}\mathbf{A} - \nabla\mathrm{div}\mathbf{A}\big) =$$

$$= -\dot{\mathbf{Q}}\triangle^{-1}\triangle\mathbf{A} = -\dot{\mathbf{Q}}\,\mathbf{A} = \mathbf{Q}\dot{\mathbf{A}} - \frac{d}{dt}\mathbf{Q}\mathbf{A} \Longrightarrow -\mathbf{Q}\mathbf{E} \qquad \text{(IV.1)}$$

Here we take into account that $\frac{1}{c}\dot{\mathbf{E}} = \mathrm{curl}\,\mathbf{B} = \mathrm{curl}\,\mathrm{curl}\,\mathbf{A}$. Naturally, these expressions are nonzero and can be justified only if the system is described but by a charge density and $\dot{\mathbf{Q}} = \int \mathbf{j}\,d\mathbf{r}$ (see e.g. [9]). Note that in quantum mechanics of atoms and moluclues there are always isolated charges and the moments $\dot{Q}_{lm}$ and Q_{lm} are connected by the evolution equation (3.10) i.e. $\dot{Q}_{lm} = i[H_c, Q_{lm}]$.

The Coulomb gauge is generally not applied if a system in consideration contains some free charges. Therefore we give the multipole expansion of $\rho(\mathbf{r},\,t)$ for the completeness of consideration [3, 11]

$$\rho(\mathbf{r},t) = \sum_{l,m,n=0} \frac{(2l+1)!!}{2^n n!(2l+2n+1)!!}\sqrt{\frac{4\pi}{2l+1}}Q^{(2n)}_{lm}(t)\triangle^n\delta_{lm}(\mathbf{r}), \qquad \text{(IV.2)}$$

$$Q_{lm}(t) = \sqrt{\frac{4\pi}{2l+1}}\int r^{l+2n}Y^*_{lm}(\hat{r})\rho(\mathbf{r},t)\,d\mathbf{r}. \qquad \text{(IV.3)}$$

Naturally, the Coulomb dipole moments, inherent to (4.1–4.3), interact with electric field as usual $H = -\mathbf{QE}$. Had we used the Dirac's analysis of constrained Hamiltonian system developed within the scope of our problem in [19, 20] we would have been in need of the fixation of Coulomb gauge [21] (see also [9]).

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