Multipolar Representation of Maxwell and Schr$\ddot{o}$dinger Equations: Lagrangian and Hamiltonian Formalisms: Examples*

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Development of quantum engineering put forward new theoretical problems. Behavior of a single mesoscopic cell (device) we may usually describe by equations of quantum mechanics. However if experimentators gather hundreds of thousands of similar cells there arises some artificial medium that one already needs to describe by means of new electromagnetic equations. The same problem arises when we try to describe e.g. a sublattice structure of such complex substances like perovskites. It is demonstrated that the inherent primacy of vector potential in quantum systems leads to a generalization of the equations of electromagnetism by introducing in them toroid polarizations. To derive the equations of motion the Lagrangian and the Hamiltonian formalisms are used. Some examples where electromagnetic properties of molecules are described by the toroid moment are pointed out.

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1. INTRODUCTION

Let us recall 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 types of polarizations in the matter considered. 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 to interact with each other [3], [4], [5] 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.

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The first part of our report is devoted to the introduction of the equations mentioned in Lagrangian formalism. In the second part we introduce toroid moments in Schrödinger equations.

2. TOROID MOMENTS IN LAGRANGIAN FORMALISM

A. Canonical formulation of electrodynamics

We begin with usual canonical formulation of electrodynamics (e.g. [6]). The interacting system of electromagnetic field and non-relativistic charged particles is specified partly by 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 varied independently. The Lagrangian must then be chosen so that variation with respect to the particle coordinates gives Newton's law

$$m_\alpha\, \ddot{\mathbf{q}}_\alpha = e_\alpha \big(\mathbf{E} + \frac{1}{c}\dot{\mathbf{q}}_\alpha \times \mathbf{B}\big)$$

and variation with respect to the field coordinates (subject to the Coulomb gauge condition) gives the equation of motion

$$\nabla^2 \mathbf{A} - \frac{1}{c^2}\, \ddot{\mathbf{A}} = -\frac{4\pi}{c}\, \mathbf{J}^\perp$$

for the vector potential. A suitable Lagrangian is obtained by setting (see e.g. [6])

$$L = L_{par} + L_{rad} + L_{int} \tag{2.1}$$

with

$$L_{par} = \frac{1}{2} \sum_\alpha m_\alpha\, \dot{\mathbf{q}}_\alpha^2 - \frac{1}{2} \sum_{\alpha\neq\beta} \frac{e_\alpha\, e_\beta}{|\mathbf{q}_\alpha - \mathbf{q}_\beta|} \tag{2.2}$$

$$L_{rad} = \frac{1}{8\pi} \int \big[\frac{\dot{\mathbf{A}}^2}{c^2} - (\mathrm{curl}\, \mathbf{A})^2\big]\, dV \tag{2.3}$$

and

$$L_{int} = \frac{1}{c} \int \mathbf{J}(\mathbf{r}) \cdot \mathbf{A}(\mathbf{r})\, dV = \sum_\alpha \frac{e_\alpha}{c}\, \dot{\mathbf{q}}_\alpha \cdot \mathbf{A}(q_\alpha, t). \tag{2.4}$$

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. The part of the Lagrangian that involves the vector potential can be written as the integral over a Lagrangian density $\mathcal{L}$,

$$\mathcal{L} = \frac{1}{8\pi} \big[\frac{\dot{\mathbf{A}}^2}{c^2} - (\mathrm{curl}\, \mathbf{A})^2\big] + \frac{1}{c}\, \mathbf{J}^\perp(\mathbf{r}) \cdot \mathbf{A}(\mathbf{r}) \tag{2.5}$$

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.

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_{\alpha i}} - \frac{\partial L}{\partial q_{\alpha i}} = 0.$$

In this particular case we have

$$m_\alpha \ddot{q}_{\alpha i} - e_\alpha \Big[\sum_{\beta\neq\alpha} \frac{e_\beta}{|\mathbf{q}_\alpha - \mathbf{q}_\beta|^3}(q_{\alpha i} - q_{\beta i}) - \frac{1}{c}\dot{a}_i\Big] - \frac{e_\alpha}{c}\dot{q}_{\alpha j}\Big(\frac{\partial a_j}{\partial q_{\alpha i}} - \frac{\partial a_i}{\partial q_{\alpha j}}\Big) = 0. \tag{2.6}$$

Using the expressions $\mathbf{B} = \mathrm{curl}\mathbf{A}$ and $\mathbf{E}^{\parallel} = -\mathrm{grad}\phi$, $\mathbf{E}^{\perp} = -\frac{1}{c}\dot{\mathbf{A}}$ 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 that

$$m_\alpha \ddot{\mathbf{q}}_\alpha = e_\alpha \mathbf{E}(\mathbf{q}_\alpha, t) + \frac{e_\alpha}{c}\dot{\mathbf{q}}_\alpha \times \mathbf{B}(\mathbf{q}_\alpha, t) \tag{2.7}$$

which is nothing but 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 $\mathcal{L}$. The Euler–Lagrange field equations

$$\frac{\partial}{\partial t}\frac{\delta L}{\delta \dot{A}_i} - \frac{\delta L}{\delta A_i} = 0$$

in this case give

$$\mathrm{curl}\,\mathbf{B} = \frac{1}{c}\dot{\mathbf{E}} + \frac{4\pi}{c}\mathbf{J}^{\perp}$$

which leads to the usual evolution equation for the vector potential in the Coulomb gauge:

$$\mathrm{curl}\,\mathrm{curl}\mathbf{A} + \frac{1}{c^2}\ddot{\mathbf{A}} = \frac{4\pi}{c}\mathbf{J}^{\perp}. \tag{2.8}$$

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

$$\mathbf{p}_\alpha = \frac{\partial L}{\partial \dot{\mathbf{q}}_\alpha} = m\,\dot{\mathbf{q}}_\alpha + \frac{e_\alpha}{c}\mathbf{A}(\mathbf{q}, t) \tag{2.9}$$

and

$$\mathbf{\Pi}(\mathbf{r}) = \frac{\partial L}{\partial \dot{\mathbf{A}}(\mathbf{r})} = \frac{\dot{\mathbf{A}}(\mathbf{r})}{4\pi c^2}(= -\mathbf{E}(\mathbf{r})/4\pi c). \tag{2.10}$$

Proceeding in the conventional way we get

$$\begin{aligned} H[\mathbf{\Pi}, \mathbf{A}; p, q] &= \sum_\alpha \mathbf{p}_\alpha \cdot \dot{\mathbf{q}}_\alpha + \int \mathbf{\Pi}\cdot\dot{\mathbf{A}}dV - L \\ &= \sum_\alpha \frac{1}{2m_\alpha}\big[\mathbf{p}_\alpha - \frac{e_\alpha}{c}\mathbf{A}(\mathbf{q}, t)\big]^2 + \frac{1}{2}\sum_{\alpha\neq\beta}\frac{e_\alpha e_\beta}{|\mathbf{q}_\alpha - \mathbf{q}_\beta|} \\ &+ \frac{1}{8\pi}\int \big[(4\pi c\mathbf{\Pi})^2 + (\mathrm{curl}\,\mathbf{A})^2\big]\,dV \end{aligned} \tag{2.11}$$

The Hamiltonian equations reproduce the equations of motions (2.7) and (2.8) as they must be. The pair of equations

$$\dot{q}_{\alpha i} = \frac{\partial H}{\partial p_{\alpha i}}, \quad \dot{A}_i = \frac{\delta H}{\delta \Pi_i}$$

are equivalent to the relations between the canonical momenta and Lagrangian velocities, where as the equations

$$\dot{p}_{\alpha i} = -\frac{\partial H}{\partial q_{\alpha i}}, \quad \dot{\Pi}_i = -\frac{\delta H}{\delta A_i}$$

yield once again the Lorentz force law (2.7) and the inhomogeneous wave equation (2.8) for the vector potential with the transverse current density as source.

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.

Moreover, let us notice that the basic equations of any new theory cannot be introduced strictly deductively. Usually, either they are postulated in differential form based on the partial integral conservation laws or transformations of basic dynamical variables, whose initial definitions usually have some analogs in mechanics. Let us remark that we need to do so not only by inertia of thinking but also because of the fact that most of our measurements have its objects as individual particles or use them as test one. The situation is the same in electromagnetism and in gravitation. In general geometrical interpretation of dynamical variables plays the crucial role. Even the slight modifications of electrodynamic equations that we performed here, demands to be clarified. As a simple most example we will consider the "geometrization" of momenta in non-relativistic quantum theory when the external classical electromagnetic field, acting on free particle, is available. Let us begin with the classical Lagrangian:

$$\mathcal{L}(\mathbf{r}, \mathbf{v}; t) = \frac{1}{2} m\mathbf{v}^2 - q[\phi(\mathbf{r}; t) - \mathbf{v} \cdot \mathbf{A}(\mathbf{r}; t)],$$

that leads to the equations of motion of particle with charge q and mass m, moving under the influence of electric and magnetic potentials ϕ and $\mathbf{A}$. To move up to Hamiltonian formalism, more closer to the quantum one, let us find the canonical momenta of the particle:

$$\mathbf{p} := \delta_v \mathcal{L}(\mathbf{r}, \mathbf{v}; t) = m\mathbf{v} + q\mathbf{A}(\mathbf{r}; t). \tag{$\star$}$$

The Hamiltonain in this case is defined as:

$$H := \mathbf{p}\mathbf{v} - \mathcal{L} = \frac{1}{2m}[\mathbf{p} - q\mathbf{A}]^2 + q\phi. \tag{$\star\star$}$$

Let us use the initially defined mechanical momenta $\boldsymbol{\pi} := m\mathbf{v}$ (gauge invariant quantity that can be directly measured!) to write the expression in square bracket in ($\star\star$). We find

$$[\mathbf{p} - q\mathbf{A}]^2 = [m\mathbf{v} + q\mathbf{A} - q\mathbf{A}]^2 = \boldsymbol{\pi}^2.$$

It is of course the simplest tautology, however introducing electromagnetic field in Schrödinger equation leads to some subtlety. Quantum physicists randomly say or write that the gauge invariant introduction of external electromagnetic field in Schrödinger equation occurs by extended momenta (of particle), implying the substitution $\mathbf{p} \to \mathbf{p} - q\mathbf{A}$. In fact the operation to move up from the classical description to the quantum one with the introduction of electromagnetic potential we imply the following substitutions:

$$\boldsymbol{\pi} := m\mathbf{v} = \nabla \qquad \text{to} \qquad \mathbf{p} = \boldsymbol{\pi} + q\mathbf{A} \to \nabla$$

and

$$H = \frac{1}{2m}[\nabla - q\mathbf{A}]^2.$$

In this the mathematical expectation of meansquare deviation between "geometrized" momenta (operator of spatial displacement of particle) and field (potential) angular moment of the particle $q\mathbf{A}$ are equated to the quantum mechanical expectation of evolution operator of the particle considered:

$$i\hbar\Psi^+\frac{\partial}{\partial t}\Psi \;=\; \frac{1}{2m}\Psi^+\big[(i\hbar\nabla + q\mathbf{A})^2 + q\phi\big]\Psi. \qquad (\star\star\star)$$

Power a.o. [7] (see also [17]) introduced the electrical polarization in Schrödinger equation starting with the equivalent Lagrangian. An equivalent Lagrangian to that of (2.1) is [7]

$$L^{new} \;=\; L \,-\, \frac{1}{c}\frac{d}{dt}\big[\int \mathbf{P}(\mathbf{r})\cdot\mathbf{A}(\mathbf{r})\,dV\big]. \qquad (2.12)$$

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

$$\mathbf{P} \;\Longrightarrow\; \mathbf{P}^\perp \,+\, \mathrm{curl}\,\mathbf{T}^e, \qquad (2.13)$$

where $\mathbf{T}^e$ is axial toroid moment (ATM), which, as will be shown later, is electrical by nature. Thus we have the following equivalent Lagrangian

$$L^{new} \;=\; L \,-\, \frac{1}{c}\frac{d}{dt}\big[\int (\mathbf{P}^\perp(\mathbf{r}) \,+\, \mathrm{curl}\mathbf{T}^e(\mathbf{r}))\cdot\mathbf{A}(\mathbf{r})\,dV\big]. \qquad (2.14)$$

Writing it in the explicit form we get

$$\begin{aligned} L^{new} \;&=\; L_{par} \,+\, L_{rad} \,+\, \frac{1}{c}\int \big(\mathbf{J}^\perp(\mathbf{r}) \,-\, \dot{\mathbf{P}}^\perp(\mathbf{r}) \,-\, \mathrm{curl}\dot{\mathbf{T}}^e(\mathbf{r})\big)\cdot\mathbf{A}(\mathbf{r})\,dV \;- \\ &-\; \frac{1}{c}\int (\mathbf{P}^\perp(\mathbf{r}) \,+\, \mathrm{curl}\mathbf{T}^e(\mathbf{r}))\cdot\dot{\mathbf{A}}(\mathbf{r})\,dV \end{aligned} \qquad (2.15)$$

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

$$\mathbf{\Pi}(\mathbf{r}) \;=\; \frac{\partial L^{new}}{\partial \dot{\mathbf{A}}(\mathbf{r})} \;=\; -\,\frac{\mathbf{E}^\perp(\mathbf{r}) \,+\, 4\pi\,(\mathbf{P}^\perp(\mathbf{r}) \,+\, \mathrm{curl}\mathbf{T}^e(\mathbf{r}))}{4\pi\,c} \qquad (2.16)$$

In fact, if we define the new vector field in a medium $\boldsymbol{\mathcal{D}}$ by the relation

$$\boldsymbol{\mathcal{D}}(\mathbf{r}) \;=\; \mathbf{E}^\perp(\mathbf{r}) \,+\, 4\pi\,(\mathbf{P}^\perp(\mathbf{r}) \,+\, \mathrm{curl}\mathbf{T}^e(\mathbf{r})) \;=\; \mathbf{D}^\perp(\mathbf{r}) \,+\, 4\pi\,\mathrm{curl}\mathbf{T}^e(\mathbf{r}) \qquad (2.17)$$

for the conjugate field we get

$$\mathbf{\Pi}(\mathbf{r}) \,=\, -\,\frac{\boldsymbol{\mathcal{D}}(\mathbf{r})}{4\pi\, c} \tag{2.18}$$

Now from the definition of $\boldsymbol{\mathcal{D}}$ we get

$$\mathrm{curl}\boldsymbol{\mathcal{D}}(\mathbf{r}) \,=\, -\,\frac{1}{c}\,\dot{\mathbf{B}}(\mathbf{r}) \,+\, 4\pi\,(\mathrm{curl}\mathbf{P}(\mathbf{r}) \,+\, \mathrm{curl}\,\mathrm{curl}\mathbf{T}^{e}(\mathbf{r})), \tag{2.19}$$

under $\mathrm{curl}\mathbf{E}(\mathbf{r}) \,=\, -\frac{1}{c}\,\dot{\mathbf{B}}(\mathbf{r})$, since only the free field $\mathbf{E}$ is generated due to the change of magnetic field $\mathbf{B}$ as before. 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. We have

$$\frac{\partial L^{new}}{\partial \mathbf{A}(\mathbf{r})} \,=\, \frac{1}{c}\,\big(\mathbf{J}^{\perp}(\mathbf{r}) \,-\, \dot{\mathbf{P}}^{\perp}(\mathbf{r}) \,-\, \mathrm{curl}\dot{\mathbf{T}}^{e}(\mathbf{r})\big) \,=\, \frac{1}{c}\,\big(c\,\mathrm{curl}\mathbf{M}^{\perp}(\mathbf{r}) \,-\, \mathrm{curl}\dot{\mathbf{T}}^{e}(\mathbf{r})\big), \tag{2.20}$$

$$\frac{\partial L^{new}}{\partial(\partial \mathbf{A}_i(\mathbf{r})/\partial x_j)} \,=\, \frac{1}{4\pi}\,\varepsilon_{ijk}\,B_k \tag{2.21}$$

as usual. Note that in (2.20) we put

$$c\,\mathrm{curl}\mathbf{M}^{\perp}(\mathbf{r}) \,=\, \mathbf{J}^{\perp}(\mathbf{r}) \,-\, \dot{\mathbf{P}}^{\perp}(\mathbf{r})$$

as it is physically sensible to devide the current due to bound electrons into electric polarization and magnetization currents [7]. Applying the Euler-Lagrange equations of motion

$$\frac{\partial}{\partial t}\,\frac{\partial L^{new}}{\partial \dot{\mathbf{A}}_i(\mathbf{r})} \,+\, \sum_j \frac{\partial}{\partial x_j}\,\frac{\partial L^{new}}{\partial(\partial \mathbf{A}_i(\mathbf{r})/\partial x_j)} \,-\, \frac{\partial L^{new}}{\partial \mathbf{A}_i(\mathbf{r})} \,=\, 0 \tag{2.22}$$

we obtain

$$-\,\frac{\dot{\boldsymbol{\mathcal{D}}}(\mathbf{r})}{4\pi\, c} \,+\, \frac{1}{4\pi}\,\mathrm{curl}\mathbf{B}(\mathbf{r}) \,-\, \frac{1}{c}\,\big(c\,\mathrm{curl}\mathbf{M}^{\perp}(\mathbf{r}) \,-\, \mathrm{curl}\dot{\mathbf{T}}^{e}(\mathbf{r})\big) \,=\, 0. \tag{2.23}$$

Introducing the following re-notations, corresponding to the initial identification by Maxwell for local relation between the derivatives of electric and magnetic fields:

$$\frac{1}{c}\,\dot{\mathbf{T}}^{e,m}\,|_{\Omega} \Longrightarrow\, \mp\,\mathrm{curl}\,\mathbf{T}^{m,e}\,|_{\Omega} \tag{2.24}$$

we may rewrite (2.23) as

$$\mathrm{curl}\mathbf{B}(\mathbf{r}) \,=\, \frac{1}{c}\dot{\boldsymbol{\mathcal{D}}}(\mathbf{r}) \,+\, 4\pi\big(\mathrm{curl}\mathbf{M}^{\perp}(\mathbf{r}) \,+\, \mathrm{curl}\,\mathrm{curl}\mathbf{T}^{m}(\mathbf{r})\big) \tag{2.25}$$

The relation (2.24) demands some comments. Both $\mathbf{T}^{e}$ and $\mathbf{T}^{m}$ represent the 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 [8]). However, remark that signs in (2.24) are opposite to the corresponding one in Maxwell equations because the direction of electric dipole is accepted to be chosen opposite to its inner electric field [9]. If we define the auxiliary field $\mathbf{H}$ to be

$$\mathbf{H}(\mathbf{r}) \,=\, \mathbf{B}(\mathbf{r}) \,-\, 4\pi\,(\mathbf{M}^{\perp}(\mathbf{r}) \,+\, \mathrm{curl}\mathbf{T}^{m}(\mathbf{r})), \tag{2.26}$$

then it deduces to

$$\mathrm{curl}\mathbf{H} \;=\; \frac{1}{c}\dot{\boldsymbol{\mathcal{D}}}.$$

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]. So the transition to the description by means of potentials is inevitable.

C. Hamiltonian for new Lagrangian

Proceeding as before we get

$$\begin{aligned} H^{new}[\mathbf{\Pi}, \mathbf{A}; p, q] \;&=\; \sum_{\alpha} \mathbf{p}_{\alpha}\cdot\dot{\mathbf{q}}_{\alpha} + \int \mathbf{\Pi}\cdot\dot{\mathbf{A}}dV \;-\; L^{new} \\ &=\; \sum_{\alpha}\frac{1}{2m_{\alpha}}\big[\mathbf{p}_{\alpha} \,-\, \frac{e_{\alpha}}{c}\,\mathbf{A}(\mathbf{q},\,t)\big]^2 + \frac{1}{2}\sum_{\alpha\neq\beta}\frac{e_{\alpha}\,e_{\beta}}{|\mathbf{q}_{\alpha}\,-\,\mathbf{q}_{\beta}|} \\ &+\; \frac{1}{8\pi}\int\big\{[4\pi(\mathbf{P}+\mathrm{curl}\,\mathbf{T}^e) - \boldsymbol{\mathcal{D}}]^2 \,+\, (\mathrm{curl}\,\mathbf{A})^2\big]\,dV \\ &+\; \frac{1}{c}\int\big(\dot{\mathbf{P}}^{\perp} \,+\, \mathrm{curl}\dot{\mathbf{T}}^{e}\big)\cdot\mathbf{A}\,dV. \end{aligned} \tag{2.27}$$

Taking into account $\frac{1}{c}\dot{\mathbf{P}}^{\perp} = \frac{1}{c}\mathbf{J}^{\perp} \,-\, \mathrm{curl}\mathbf{M}^{\perp}$ and the relation (2.24) and also $\mathrm{div}[\mathbf{M}\times\mathbf{A}] = \mathbf{A}\cdot\mathrm{curl}\,\mathbf{M} + \mathbf{M}\cdot\mathrm{curl}\,\mathbf{A}$ the fourth term of the foregoing equality can be reconstructed after integration and H can be presented as

$$\begin{aligned} H^{new}[\mathbf{\Pi}, \mathbf{A}; p, q] \;&=\; \sum_{\alpha}\frac{1}{2m_{\alpha}}\big[\mathbf{p}_{\alpha} \,-\, \frac{e_{\alpha}}{c}\,\mathbf{A}(\mathbf{q},\,t)\big]^2 + \frac{1}{2}\sum_{\alpha\neq\beta}\frac{e_{\alpha}\,e_{\beta}}{|\mathbf{q}_{\alpha}\,-\,\mathbf{q}_{\beta}|} \\ &+\; \frac{1}{8\pi}\int\big\{[4\pi(\mathbf{P}+\mathrm{curl}\,\mathbf{T}^e) - \boldsymbol{\mathcal{D}}]^2 \,+\, (\mathrm{curl}\,\mathbf{A})^2\big\}\,dV \\ &+\; \frac{1}{c}\int\mathbf{J}^{\perp}\cdot\mathbf{A}\,dV \,-\, \int\mathbf{M}\cdot\mathbf{B}\,dV \,-\, \int\mathbf{B}\cdot\mathrm{curl}\,\mathbf{T}^m\,dV. \end{aligned} \tag{2.28}$$

The Hamiltonian equations in this case give

$$\dot{q}_{\alpha i} \,=\, \frac{\partial H}{\partial p_{\alpha i}} \,=\, \sum_{\alpha}\frac{1}{m_{\alpha i}}\big(p_{\alpha i} - \frac{e_{\alpha i}}{c}A_i(\mathbf{q}_{\alpha}, t)\big), \quad \dot{A}_i \,=\, \frac{\delta H}{\delta \Pi_i} \,=\, c[4\pi(\mathbf{P}+\mathrm{curl}\,\mathbf{T}^e) - \boldsymbol{\mathcal{D}}]_i$$

which together with

$$\dot{\Pi}_i = -\,\frac{\delta H}{\delta A_i} = \sum_{\alpha}\frac{e_{\alpha}}{c\,m_{\alpha i}}\big(p_{\alpha i} - \frac{e_{\alpha i}}{c}A_i(\mathbf{q}_{\alpha}, t)\big) - \frac{1}{c}(\dot{\mathbf{P}} + \mathrm{curl}\,\dot{\mathbf{T}}^{e})_i - \frac{1}{4\pi}[\nabla\times(\nabla\times\mathbf{A})]_i,$$

$$\dot{p}_{\alpha i} = -\,\frac{\partial H}{\partial q_{\alpha i}} = \sum_{\alpha}\frac{e_{\alpha}}{c\,m_{\alpha i}}\big(p_{\alpha i} - \frac{e_{\alpha i}}{c}A_i(\mathbf{q}_{\alpha}, t)\big)\Big(\frac{\partial A_j}{\partial q_{\alpha i}} - \frac{\partial A_i}{\partial q_{\alpha j}}\Big) - \frac{1}{2}\sum_{\alpha}\frac{e_{\alpha}\,e_{\beta}}{|\mathbf{q}_{\alpha} - \mathbf{q}_{\beta}|}(q_{\alpha} - q_{\beta})$$

once again yield the Lorentz force law (2.7) and the inhomogeneous wave equation (2.8) for the vector potential.

D. Canonical quantization

Let us now draw the Schrödinger picture operators corresponding to the quantities obtained above. To do so we need to interpret the coordinates $\mathbf{q}_\alpha$ of the particles together with their conjugate momenta $\mathbf{p}_\alpha$ and the *coordinates* $\mathbf{A}(\mathbf{r})$ of the field together with their conjugate momenta $\mathbf{\Pi}(\mathbf{r})$ as operators in Hilbert space. Thus we have six operators $q_{\alpha i}$ and $p_{\alpha i}$, $(i = 1, 2, 3)$ associated with each particle α and six operators $A_i(\mathbf{r})$ and $\Pi_i(\mathbf{r})$, $(i = 1, 2, 3)$ associated with each field point $\mathbf{r}$. These operators are Schrödinger picture operators since they are time-independent. The corresponding Heisenberg picture operators may be written as $\mathbf{q}_\alpha(t)$, $\mathbf{p}_\alpha(t)$, $\mathbf{A}(\mathbf{r}, t)$, $\mathbf{\Pi}(\mathbf{r}, t)$ respectively. The Schrödinger operators satisfy the following canonical commutation relations, precisely

$$\begin{aligned} [q_{\alpha i}, q_{\beta j}] &= 0, \quad [p_{\alpha i}, p_{\beta j}] = 0 \\ [q_{\alpha i}, p_{\beta j}] &= i\hbar\, \delta_{\alpha\beta}\, \delta ij \end{aligned} \tag{2.29}$$

for the particle variables and

$$\begin{aligned} [A_i(\mathbf{r}), A_j(\mathbf{r}')] &= 0, \quad [\Pi_i(\mathbf{r}), \Pi_j(\mathbf{r}')] = 0 \\ [A_i(\mathbf{r}), \Pi_j(\mathbf{r}')] &= i\hbar\, \delta_{ij}^{\perp}(\mathbf{r} - \mathbf{r}') \end{aligned} \tag{2.30}$$

for the field variables. These equations are held for all α and β and all i and j. The commutator bracket of any particle variable with any field variable vanishes. The canonical commutation relations are also satisfied by the Heisenberg dynamical variables, provided all operators are evaluated at the same time t. These follows from the equations (2.29) and (2.30) and the relation between two pictures:

$$\Omega(t) = e^{(i/\hbar)\, Ht}\, \Omega e^{-(i/\hbar)\, Ht} \tag{2.31}$$

where H is the hamiltonian operator and $\Omega(t)$ is the Heisenberg operator corresponding to the Schrödinger operator Ω. The operator $\Omega(t)$ satisfies the Heisenberg equation

$$\dot{\Omega}(t) = \frac{1}{i\hbar}\, [\Omega(t), H], \tag{2.32}$$

while the Schrödinger picture operator corresponding to $\dot{\Omega}(t)$ is given by

$$\dot{\Omega} = \frac{1}{i\hbar}\, [\Omega, H]. \tag{2.33}$$

Taking the expression (2.28) for the Hamiltonian one can easily verify that the equation (2.32) together with the commutation relations leads to the expected equations of motion.

E. 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:

$$\begin{aligned} \operatorname{curl} \mathbf{B} &= \frac{1}{c}\dot{\mathbf{D}} + 4\pi \operatorname{curl} \mathbf{M}, \quad \mathbf{B} = \mathbf{H} + 4\pi\mathbf{M} \text{ in the whole } \Re^3, \\ \operatorname{curl} \mathbf{D} &= -\frac{1}{c}\dot{\mathbf{B}} + 4\pi \operatorname{curl} \mathbf{P}, \quad \mathbf{D} = \mathbf{E} + 4\pi\mathbf{P} \text{ in the whole } \Re^3. \end{aligned} \tag{2.34}$$

One can easily see that these equations transform into each other and the conditions $\operatorname{div}\mathbf{B} = 0$ and $\operatorname{div}\mathbf{D} = 0$ are fulfilled if the following substitutions are performed: $\mathbf{B} \to \mp\mathbf{D}$, $\mathbf{D} \to \pm\mathbf{B}$, $\mathbf{M} \to \mp\mathbf{P}$, $\mathbf{P} \to \pm\mathbf{M}$. The conditions $\operatorname{div}\mathbf{B} = 0$ and $\operatorname{div}\mathbf{D} = 0$ together with $\operatorname{div}\boldsymbol{\alpha}^{e,m} = 0$ allow us to rewrite $\mathbf{B}$ and $\mathbf{D}$ as follows [10]

$$\mathbf{B} \Longrightarrow \operatorname{curl}\boldsymbol{\alpha}^m + \dot{\boldsymbol{\alpha}}^e, \qquad \mathbf{D} \Longrightarrow \operatorname{curl}\boldsymbol{\alpha}^e - \dot{\boldsymbol{\alpha}}^m. \tag{2.35}$$

If now we use the substitutions, implied canonically in the foregoing paragraphs i.e.

$$\operatorname{curl}\mathbf{M} \Longrightarrow \operatorname{curl}\mathbf{M} + \operatorname{curl}\operatorname{curl}\mathbf{T}^m \qquad \operatorname{curl}\mathbf{P} \Longrightarrow \operatorname{curl}\mathbf{P} + \operatorname{curl}\operatorname{curl}\mathbf{T}^e,$$

we obtain for basic equations

$$\begin{aligned} \operatorname{curl}\operatorname{curl}\boldsymbol{\alpha}^m + \ddot{\boldsymbol{\alpha}}^m &= 4\pi\,(\operatorname{curl}\mathbf{M} + \operatorname{curl}\operatorname{curl}\mathbf{T}^m), \\ \operatorname{curl}\operatorname{curl}\boldsymbol{\alpha}^e + \ddot{\boldsymbol{\alpha}}^e &= 4\pi\,(\operatorname{curl}\mathbf{P} + \operatorname{curl}\operatorname{curl}\mathbf{T}^e). \end{aligned} \tag{2.36}$$

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 (2.28) in (2.25) produce (2.34) as well. If $\operatorname{div}\mathbf{D} \neq 0$ and there does exist free current in the medium we have to use the direct method for finding all constrains in the theory suggested by Dirac. Dirac applied his method to electrodynamics and found that electromagnetic potentials have only two degrees of freedom described by transverse components of vector potential. This method was developed by Dobovik and Shabanov [11], where classical and quantum dynamics of a system of non-relativistic charged particles were considered.

F. Solution to the electromagnetotoroidic equations

Let us first solve the static equations. In this case we write

$$\operatorname{curl}\operatorname{curl}(\boldsymbol{\alpha}^m - 4\pi\mathbf{T}^m) =: \operatorname{curl}\operatorname{curl}\mathbf{a}^m = 4\pi\operatorname{curl}\mathbf{M}^{\perp}(\mathbf{r}), \tag{2.37}$$

$$\operatorname{curl}\operatorname{curl}(\boldsymbol{\alpha}^e - 4\pi\mathbf{T}^e) =: \operatorname{curl}\operatorname{curl}\mathbf{a}^e = 4\pi\operatorname{curl}\mathbf{P}^{\perp}(\mathbf{r}), \tag{2.38}$$

here $\mathbf{a}$ is an analog of $\mathbf{H}$. From the vector analysis we can see

$$\operatorname{curl}\operatorname{curl}\mathbf{a}^m = \operatorname{grad}\ \operatorname{div}\mathbf{a}^m - \nabla^2\mathbf{a}^m = -4\pi\operatorname{grad}\operatorname{div}\mathbf{T}^m - \nabla^2\mathbf{a}^m \tag{2.39}$$

where we use the condition $\operatorname{div}\boldsymbol{\alpha}^m = 0$. The solutions of the equations (2.37) and (2.38) can be written as

$$\mathbf{a}^m = \int \frac{\operatorname{curl}'\mathbf{M}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}\,dV' + \nabla\int \frac{\operatorname{div}'\mathbf{T}^m(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}\,dV' \tag{2.40}$$

Analogically we get

$$\mathbf{a}^e = \int \frac{\operatorname{curl}'\mathbf{P}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}\,dV' + \nabla\int \frac{\operatorname{div}'\mathbf{T}^e(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}\,dV' \tag{2.41}$$

Now let us return to the general case. Adding $-(4\pi/c^2)\,\ddot{\mathbf{T}}^{m,e}$ to both sides of the equations (2.35) and (2.36) for $\mathbf{a}$ we get the wave equations

$$\mathrm{curl\,curl}\mathbf{a}^m + \frac{1}{c^2}\,\ddot{\mathbf{a}}^m = 4\pi\,\mathrm{curl}\mathbf{M}^{\perp}(\mathbf{r}) - \frac{4\pi}{c^2}\,\ddot{\mathbf{T}}^m(\mathbf{r}) \tag{2.42}$$

and

$$\mathrm{curl\,curl}\mathbf{a}^e + \frac{1}{c^2}\,\ddot{\mathbf{a}}^e = 4\pi\,\mathrm{curl}\mathbf{P}^{\perp}(\mathbf{r}) - \frac{4\pi}{c^2}\,\ddot{\mathbf{T}}^e(\mathbf{r}) \tag{2.43}$$

The solutions to these equations can be written as [12]

$$\mathbf{a}^m = -\frac{1}{4\pi}\int\limits_{all\ space}\frac{\left[-\nabla'(\nabla'\cdot\mathbf{T}^{m\prime}) - 4\pi\,\nabla'\times\mathbf{M}') + (4\pi/c^2)\ddot{\mathbf{T}}^{m\prime}\right]}{|\mathbf{r}-\mathbf{r}'|}\,dV' \tag{2.44}$$

$$\mathbf{a}^e = -\frac{1}{4\pi}\int\limits_{all\ space}\frac{\left[-\nabla'(\nabla'\cdot\mathbf{T}^{e\prime})) - 4\pi\,\nabla'\times\mathbf{P}') + (4\pi/c^2)\ddot{\mathbf{T}}^{e\prime}\right]}{|\mathbf{r}-\mathbf{r}'|}\,dV' \tag{2.45}$$

here $\mathbf{M}'$ denotes $\mathbf{M}(\mathbf{r}')$. 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

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

It is obvious from the foregoing solutions that the quantities that an experimentator measures are $\boldsymbol{\alpha}$ and $\mathbf{a}$ and the fields, they generate, differ from the old ones. It leads to the fact that we no longer work with $\mathbf{B}$ and $\mathbf{D}$ but with some new quantities which need to be defined differently. So instead of (2.35) we should now write

$$\boldsymbol{\beta} = \mathrm{curl}\,\boldsymbol{\alpha}^m + \dot{\boldsymbol{\alpha}}^e, \qquad \boldsymbol{\delta} = \mathrm{curl}\,\boldsymbol{\alpha}^e - \dot{\boldsymbol{\alpha}}^m. \tag{2.46}$$

Note that the quantities $\boldsymbol{\beta}$ and $\boldsymbol{\delta}$ may be measured and possess physical significance. For example, let us imagine the situation when the experimentator measures magnetic field in a needle-like hole. Let the hole that is not along the principal axis of magnetization, be dug in magnetic media. In the case mentioned above, beside the contribution of Ampere current of magnetization curl$\mathbf{M}$ the experimentator measures the contribution of inhomogeneous toroidazation that is obvious from (2.44) and (2.45). Thus introduction of potential and magnetic field based on the magnetization of media only, generally speaking is incorrect [3].

3. MULTIPOLAR INTERACTIONS IN 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 the detailed paper by K. Haller and R. B. Sohn [13]. The matter is that they begin with the expression independent of the scalar-longitudinal contributions (ρ, 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 the terms used in [13], [14]. The Hamiltonian that describes the interaction between photons and non-relativistic Schrödinger electrons is given by

$$\begin{aligned} H_c \;&=\; H_0 - \int \mathbf{J}(\mathbf{r}) \cdot \mathbf{A}^T(\mathbf{r})\, d\mathbf{r} + \frac{e}{2m} \int \rho(\mathbf{r}) \mathbf{A}^T(\mathbf{r}) \cdot \mathbf{A}^T(\mathbf{r})\, d\mathbf{r} \;+ \\ &+ \int \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{8\pi|\mathbf{r} - \mathbf{r}'|}\, d\mathbf{r}\, d\mathbf{r}', \end{aligned} \tag{3.1}$$

where $\mathbf{A}^T$ is the transverse vector potential with $\operatorname{div} \mathbf{A}^T = 0$. H_0 is the Hamiltonian for noninteracting electrons and photons that can be represented by

$$H_0 \;=\; H_0(e) + H_0(\gamma), \tag{3.2}$$

where

$$H_0(e) \;=\; \int \psi^+(\mathbf{r})[-(2m)^{-1}\nabla^2 + V(\mathbf{r})]\psi(\mathbf{r}) d\mathbf{r} \tag{3.3}$$

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

$$H_0(\gamma) \;=\; \frac{1}{2} \int [\mathbf{E}^T(\mathbf{r})^2 + \mathbf{B}(\mathbf{r})^2] d\mathbf{r}, \tag{3.4}$$

where $\mathbf{E}^T(\mathbf{r})$ and $\mathbf{B}(\mathbf{r})$ represent the transverse electric and magnetic field, respectively. In equation (3.1) $\rho(\mathbf{r})$ represents the charge density $\rho(\mathbf{r}) = e\,\psi^+(\mathbf{r})\psi(\mathbf{r})$ and $\mathbf{J}(\mathbf{r})$ represents a current

$$\mathbf{J}(\mathbf{r}) \;=\; \frac{ie}{2m}[\nabla\psi^+(\mathbf{r})\,\psi(\mathbf{r}) - \psi^+(\mathbf{r})\,\nabla\psi(\mathbf{r})]. \tag{3.5}$$

The commutation rules of these fields are

$$\{\psi^+(\mathbf{r}), \psi(\mathbf{r}')\} \;=\; \delta(\mathbf{r} - \mathbf{r}') \tag{3.6}$$

for the electron field; for the photon field, $-\mathbf{A}^T(\mathbf{r})$ has the transverse electric field $\mathbf{E}^T(\mathbf{r})$ as its conjugate momentum, so that the nonlocal commutation rule for the transverse components is given by

$$[A_i^T(\mathbf{r}), E_j^T(\mathbf{r}')] \;=\; -\big(\delta_{i,j}\,\delta(\mathbf{r} - \mathbf{r}') + \frac{\partial}{\partial r_i}\frac{\partial}{\partial r_j}\frac{1}{4\pi|\mathbf{r} - \mathbf{r}'|}\big). \tag{3.7}$$

The current $\mathbf{J}(\mathbf{r})$ is conserved under the time dependence provided by the Hamiltonian so that

$$\operatorname{div} \mathbf{J}(\mathbf{r}) \;=\; -i[H_0, \rho(\mathbf{r})]. \tag{3.8}$$

The current

$$\mathbf{j}(\mathbf{r}) \;=\; \mathbf{J}(\mathbf{r}) - (e/m)\,\rho(\mathbf{r})\,\mathbf{A}^T(\mathbf{r}) \tag{3.9}$$

is conserved under the time dependence provided by the Hamiltonian so that

$$\operatorname{div} \mathbf{j}(\mathbf{r}) \;=\; -i[H_c, \rho(\mathbf{r})]. \tag{3.10}$$

H_c may be expressed as

$$H_c \,=\, H_0 \,-\, \int [\mathbf{J}(\mathbf{r}) \,+\, \mathbf{j}(\mathbf{r})] \cdot \mathbf{A}^T(\mathbf{r})\, d\mathbf{r} \,+\, \int \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{8\pi|\mathbf{r} \,-\, \mathbf{r}'|}\, d\mathbf{r}\, d\mathbf{r}'. \tag{3.11}$$

When ψ is quantized in orbitals that are solutions of

$$[-(2m)^{-1}\,\nabla^2 \,+\, V(\mathbf{r}) \,-\, \omega_i]\, U_i \,=\, 0, \tag{3.12}$$

(where U_i includes both bound and continuum states), $H_0(e)$ is given by

$$H_0(e) \,=\, \sum_n e_n^+\, e_n\, \omega_n, \tag{3.13}$$

where e_n^+ and e_n designate creation and annihilation operators, respectively, for electrons in the n orbitals. $H_0(\gamma)$ can be represented as

$$H_0(\gamma) \,=\, \sum_{i=1,2} \int d\mathbf{k}\, |\mathbf{k}| \mathbf{a}^+_{\epsilon(i)}(\mathbf{k})\, \mathbf{a}_{\epsilon(i)}(\mathbf{k}), \tag{3.14}$$

and describes free photons in the two polarization modes.

B. Introduction of toroid moments

A formal procedure was first proposed by E. G. P. Rowe [15] which permits to obtain the complete solution to the problem of multipole expansion of electromagnetic current [3], which consists of replacing 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]

$$\begin{aligned} H_c \,=\, &-\sum_{l=1}^{\infty}\sum_{m=-l}^{l}\sum_{n=0}^{\infty} \frac{(2l\,+\,1)!!}{2^n\, n!(2l+2n+1)!!}\sqrt{\frac{2l+1}{4\pi}} \times \\ &\times\, \{l^{-1} M_{lm}^{(2n)}(t) Y_{lm}(\nabla)\triangle^n(\mathbf{r}\cdot\mathbf{B})|_{r=0} + \\ &+\, l_{-1}[\dot{Q}_{lm}(t)\delta_{n,0}\triangle^{-1} - T_{lm}^{2n}(t)] Y_{lm}(\nabla)\triangle^n[(1/c)\mathbf{r}\cdot\dot{\mathbf{D}} + (4\pi/c)\mathbf{r}\cdot\mathbf{j}]_{r=0}\}. \end{aligned} \tag{3.15}$$

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

$$\dot{Q}_{lm}(t) \,=\, \sqrt{4\pi l}\int r^{l-1}\, Y^*_{l\,l-1\,m}(\hat{r})\, \mathbf{j}(\mathbf{r},t)\, d\mathbf{r}, \tag{3.16}$$

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

$$M_{lm}^{(2n)}(t) \,=\, \frac{-i}{c}\sqrt{\frac{l}{l+1}}\sqrt{\frac{4\pi}{2l+1}}\int r^l\, Y^*_{llm}(\hat{r})\, \mathbf{j}(\mathbf{r},t)\, d\mathbf{r}, \tag{3.17}$$

and $T_{lm}^{(2n)}(t)$ are third family of multipole moments [16], the toroid moments and their radii, namely

$$T_{lm}^{(2n)}(t) = -\frac{\sqrt{\pi}l}{c(2l+1)}\int r^{l+2n+1}[Y^*_{l\,l-1\,m}(\hat{r}) + \frac{2\sqrt{l/l+1}}{2l+3} Y^*_{l\,l+1\,m}(\hat{r})]\cdot\mathbf{j}(\mathbf{r},t)\, d\mathbf{r}, \tag{3.18}$$

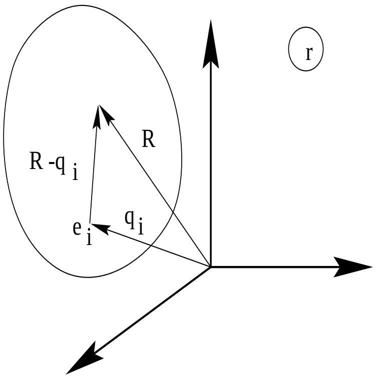

FIG. 1:

In the case considered by Haller and Sohn [13] we have to substitute into (3.15)

$$\dot{Q}_{lm}(t) \equiv \frac{\partial\, Q_{lm}}{\partial t} = i[H_c, Q_{lm}] \tag{3.19}$$

and

$$\mathbf{j} = \mathbf{J} - e\rho\,\mathbf{A} \tag{3.20}$$

in the formulas (3.15), (3.16), (3.17) and (3.18). In this approach no longitudinal contributions appear that are fictitious (mutually cancelled out) in the expression, deduced by Haller and Sohn. The formulas (3.16 - 3.18) 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 Schr$\ddot{o}$dinger equation

Let us now consider a system of some electrons involved in the molecular structure. We may introduce a coordinate system as in Fig. 1. Then it may be shown that the Schr$\ddot{o}$dinger equation for this electron interacting with external sources of electromagnetic fields has the following form [17]

$$\begin{aligned} i\hbar\dot{\phi}(\mathbf{q}) = \Big[&-\frac{\hbar^2}{2m}(\nabla^{(q)})^2 + V(\mathbf{q}) + e^2 \int \frac{\bar{\phi}(\mathbf{q}')\phi(\mathbf{q}')}{|\mathbf{q} - \mathbf{q}'|}\, d\mathbf{q}' - \\ &- \int \big(\mathbf{P}(\mathbf{r}, \mathbf{q}) \cdot \mathbf{E}^{\perp}(\mathbf{r})\big)\, d\mathbf{r} - \int \big(\mathbf{M}(\mathbf{r}, \mathbf{q}) \cdot \mathbf{B}(\mathbf{r})\big)\, d\mathbf{r} + \\ &+ \frac{1}{2mc^2}\Big[\int \mathbf{n}(\mathbf{r}, \mathbf{q}) \times \mathbf{B}(\mathbf{r})\, d\mathbf{r}\Big]^2\Big]\phi(\mathbf{q}), \end{aligned} \tag{3.21}$$

with $\mathbf{n}(\mathbf{r}, \mathbf{q}) = -\frac{e}{2}(\mathbf{q} - \mathbf{R})\,\delta(\mathbf{r} - \mathbf{R})$. To get the Schr$\ddot{o}$dinger equation (3.21) Power a.o. used the following substitutions in the Lagrangian for an electron field uncoupled from the radiation field: $\nabla^{(q)}$ is replaced by $\nabla^{(q)} + \frac{ie}{\hbar c}\mathbf{A}(\mathbf{q})$ and the wave function describing electron field initially is transformed according to

$$\psi(\mathbf{q}) = e^{-S(\mathbf{q})}\,\phi(\mathbf{q}),$$

where $S(\mathbf{q})$ is given by

$$S(\mathbf{q}) = \frac{1}{\hbar c}\int \mathbf{P}(\mathbf{r},\mathbf{q})\cdot\mathbf{A}^{\perp}(\mathbf{r})d\mathbf{r}.$$

There are two ways to introduce here the toroid contributions. The first one is to substitute (2.13) into (3.21). Then we obtain

$$\int \mathbf{P}\cdot\mathbf{E}^{\perp}\,d\mathbf{r} \Longrightarrow \int \mathbf{P}\cdot\mathbf{E}^{\perp}\,d\mathbf{r} + \int \mathrm{curl}\mathbf{T}^{e}\cdot\mathbf{E}^{\perp}\,d\mathbf{r} = \int \mathbf{P}\cdot\mathbf{E}^{\perp}\,d\mathbf{r} + \int \mathbf{T}^{e}\cdot\mathrm{curl}\mathbf{E}^{\perp}\,d\mathbf{r}. \quad (3.22)$$

Analogically

$$\int \mathbf{M}\cdot\mathbf{B}\,d\mathbf{r} \Longrightarrow \int \mathbf{M}\cdot\mathbf{B}\,d\mathbf{r} + \int \mathbf{T}^{m}\cdot\mathrm{curl}\mathbf{B}\,d\mathbf{r}. \quad (3.23)$$

A more reasonable approach is developed in [15]. It goes back to the classic multipolar description of quasimolecular structure [11], [18]. 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]:

$$W^{e} = -\int \mathbf{d}(\mathbf{r},\,\mathbf{q})\cdot\mathbf{E}^{\perp}(\mathbf{r})\,d\mathbf{r} = -\mathbf{Q}\cdot\mathbf{E}^{\perp} - \mathbf{T}^{e}\cdot\mathrm{curl}\mathbf{E} -$$
$$-\mathbf{P}^{e}\cdot\mathrm{curl}\,\mathrm{curl}\mathbf{E} - \frac{1}{2}Q_{ij}(\nabla_i\mathbf{E}_j^{\perp} + \nabla_j\mathbf{E}_i^{\perp}) - T_{ij}^{e}\nabla_i(\mathrm{curl}\mathbf{E}^{\perp})_i - \cdots \quad (3.24)$$

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 $\mathbf{P}^{e} = \frac{1}{10}\int \left[\mathbf{r}(\mathbf{r}\cdot\mathbf{d}) - 2r^2\,\mathbf{d}\right]d\mathbf{r}$ the polar poloidal one. For the case, illustrated in *Figure* 1 we have (compare with [17] and Appendix)

$$\mathbf{d}(\mathbf{r},\,\mathbf{q}) = -e\Big\{(\mathbf{q} - \mathbf{R}) - \frac{1}{2}(\mathbf{q}\times\mathbf{R}) -$$
$$-\frac{e}{2}\left[(q - R)_i\,(q - R)_j - \frac{2}{3}(q - R)^2\,\delta_{ij}\right] + \cdots\Big\}\,\delta(\mathbf{r} - \mathbf{R}). \quad (3.25)$$

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 in general the multipole expansion of the distribution density $\mathbf{d}(\mathbf{r},t)$ contents three kinds of dipole moments (see expression (3.24)). Working within the scope of classical framework after Power a. o. [7] 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

$$\mathbf{Q} = -e\sum_{i=1}^{n}(\mathbf{R} - \mathbf{q}_i), \quad \mathbf{d} = \mathbf{Q}\,\delta(\mathbf{r} - \mathbf{R}). \quad (3.26)$$

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

$$\mathbf{T}^{(e)} = \frac{1}{2}\int \mathbf{d}\times\mathbf{r}\,d\mathbf{r} = \frac{e}{2}\sum_{i=1}^{n}(\mathbf{R} - \mathbf{q}_i)\times(\mathbf{R} - \mathbf{q}_i) = 0, \quad (3.27)$$

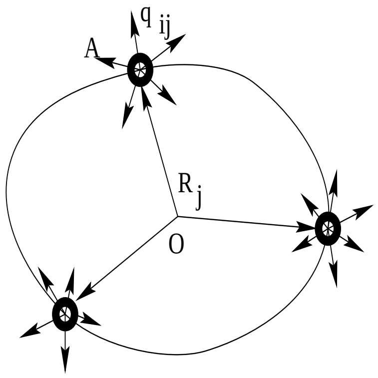

FIG. 2:

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 $\mathbf{T}^{(e)}$ as a whole [19] with respect to its center-mass by the following formula

$$\mathbf{T}^{(e)} = \frac{e}{2}\sum_{j=1}^{N}\sum_{i=1}^{n}(\mathbf{R}_j - \mathbf{q}_{ij}) \times \mathbf{R}_j = \frac{e}{2}\sum_{j=1}^{N}\sum_{i=1}^{n}[\mathbf{q}_{ij} \times \mathbf{R}_j] \neq 0, \tag{3.28}$$

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

As a particular example where electromagnetic properties of molecules are described by the axial toroid moment, we point out the phenomenon of "aromagnetism" [20]. There exists substances with closed chains of atoms like benzol ring. In the experiment, the microcrystals of the aromatic series substances (antrazen, fenantren etc.), suspended either in water or in other liquids, were reoriented by an alternating magnetic field so that the modulation of polarized light, propagating through the media given, was observed. This reorientation can be easily explained if the aromatic molecules are considered to possess axial toroid moment $\mathbf{T}^{(e)}$ (see Fig. 3) as an electromagnetic order parameter. The latter can be clarified as follows. All molecular wave functions Ψ of the benzol ring, being the main fragment of aromatic molecules, are first classified through the irreducible representations of the point group symmetry D_{6h} and then the asymmetric representations (E_{2g} and E_{1u}) are selected among them. When such molecules are packed into a molecular crystal, the parallel orientation of their axial toroid moments are preferred and the crystal as a whole can possess a macroscopic axial toroid moment [21].

Here is a fragment of an aromatic molecule where C_i is a carbon atom, X_i is a hydrogen atom or its substitute with C_i. The vectors $\mathbf{d}_i$ denotes the electric dipole moments, being due to the molecular orbital with the symmetry E_{2g} of the representation of the point group D_{6h}. The molecular wave functions ΨE_{2g} and ΨE_{1u} with this symmetry are built [21]. The molecules in this states are shown to have the axial toroid moment.

Now let us see what "aromagnetism" is? Microscopic crystals of aromatics like anthracene, penthacene, phenanthrene and others were suspended in water or some other liquids. When alternating or rotating magnetic field was applied to the suspension the change of orientation of microcrystals was observed. This new magnetic property of aromatic substances was named "aromagnetism" [20]. This phenomena cannot be explained by

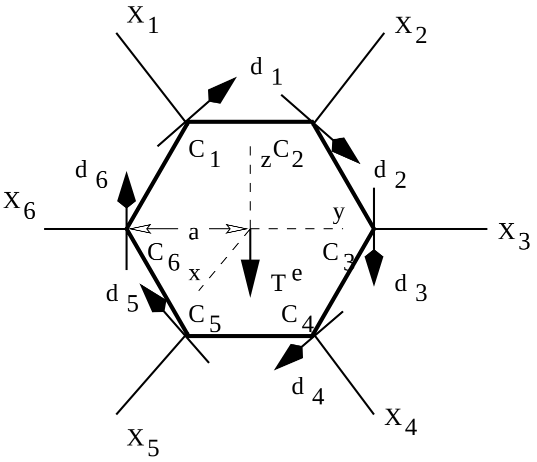

FIG. 3: A fragment of an aromatic molecule

the standard way like ferromagnetism since the organic molecules do not possess magnetic moments neither orbital nor spin origin. The theory of aromagnetism origin was proposed in [21]. It was assumed there that the sample of aromagnetic substance possesses an axial toroid moment $\mathbf{T}^e$ (ATM). This moment describes the vortex distribution of the electrical dipoles $\mathbf{d}$ deposited at points $\mathbf{r}$ and equal to

$$\mathbf{T}^e = (1/2)\sum[\mathbf{r}\times\mathbf{d}],$$

where the sum is taken over the whole sample. Electrodynamics theory of ATM was developed in [22]. The energy of ATM in external field is equal to

$$\boldsymbol{\mathcal{E}} = -\mathbf{T}^e\,\mathrm{curl}\,\mathbf{E} = \mathbf{T}^e\,\frac{\partial\mathbf{H}}{\partial ct}.$$

Thus toroid moment $\mathbf{T}^e$, electrical by its nature, can interact with alternating magnetic field $\mathbf{H}(t)$. In the following we consider as 'aromagnetic' any molecule or macroscopic sample that possesses toroid moment $\mathbf{T}^e$. The main feature that singles out aromagnetics among the other magnetics is their interaction with magnetic field time derivative $\partial\mathbf{H}/\partial t$ (not with magnetic field $\mathbf{H}$ itself). The theory previously given in [21] may be extended so that new substances with aromagnetic properties can be predicted. Indeed it was shown (see [21]) that the cause of molecular aromagnetism is the existence of quantum molecular electronic states (MO) where the quantum mean value of toroid moment $< \mathbf{T}^e >$ of molecule is not equal to zero. In [21] only molecules with group symmetry D_{6h} were considered. It is obvious that molecules with the other symmetry groups may be examined. The scheme of the examination is the following. Toroid moment is a pseudovector and for any given group we know the irreps of its transformation under the group operations. For example in the group D_{4h} the irreps of pseudovector are : A_{2g} for T^e_z and E_g for T^e_x and T^e_y components of $\mathbf{T}^e$. Considering direct products of this irreps (A_{2g} and E_g in a given case) with the other irreps of this group it is possible to find out the symmetry of MO where the mean value of toroid moment is not zero (E_g or E_u for group D_{4h}). Then it is possible to find these MO in explicit form and calculate the mean value $< \mathbf{T}^e >$, as it was described in [21]. Toroid polarization coefficients of the molecule can also be calculated in an analogous way.

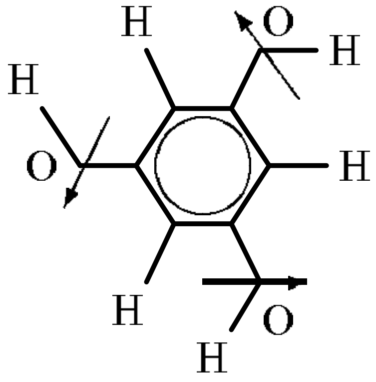

FIG. 4: Distribution of dipole moments of oxygen atoms of the molecule phloroglycine. It can be estimated from this figure that molecule has axial toroid moment.

The other important case of molecular aromagnetism is the vortex distribution of dipole moments of oxygen or nitrogen atoms. In the Figure 4 the stereomer of the molecule of phloroglycine is represented and dipole moments of the oxygen atoms are shown. The stability of this stereomer was demonstrated by numerical calculation by standard molecular dynamic method. It follows from the picture that vortex distribution of the electrical dipole moments on the oxygen atoms exists and that this stereomer of phloroglycine is an aromagnetic one. The other examples of organic molecules with the same kind of aromagnetism are given here. To explain structural aromagnetism let us consider molecular crystal of indandion-1,3 pyridine-betaine (IPB) polar intramolecular salt (Figure 5, left). Due to charge transfer this molecule has electrical dipole moment. The fundamental unit of the crystal of IPB is shown in Figure 5 (to draw the Figure 5 the picture 1.9 from the book [23] is used) and on the figure we show the dipole moments of the molecules. It can be seen from the figure that toroid moment of the crystal cell is not equal to zero, i.e. this substance has aromagnetic properties which we call structural aromagnetism.

Let us see one more example. In a cubic perovskite the crystallographic plane $(1,1,1)$ contains triangular sublattice of oxygen atoms [24], [25], [26] (see Figure 6). Magnetic moments of these atoms can be in two states of orientating symmetry that are separated by temperatural phase transition.

4. CONCLUSION

It was shown in [11] that the longitudinal degree of freedom of an electromagnetic field contains the information about the Coulomb interaction of charges. The perfect confirmation of this statement can be found in quantum theory of charged particle. Here one has to stress that the longitudinal component $\mathbf{E}^{\|}$ of $\mathbf{E}$ is represented by the gradient of a scalar function φ such that $\mathbf{E}^{\|} = -\nabla\varphi$. This function may be called Coulomb potential. But from the dynamical point of view, the quantities $\mathbf{A}_0$ and φ have different physical meaning and cannot be identified. Notice that by construction the Coulomb potential is gauge-invariant. On the other hand for the transverse part $\mathbf{E}^{\perp}$ of $\mathbf{E}$ one gets $\mathbf{E}^{\perp} = -\frac{1}{c}\frac{\partial \mathbf{A}}{\partial t}$. Thus we see that

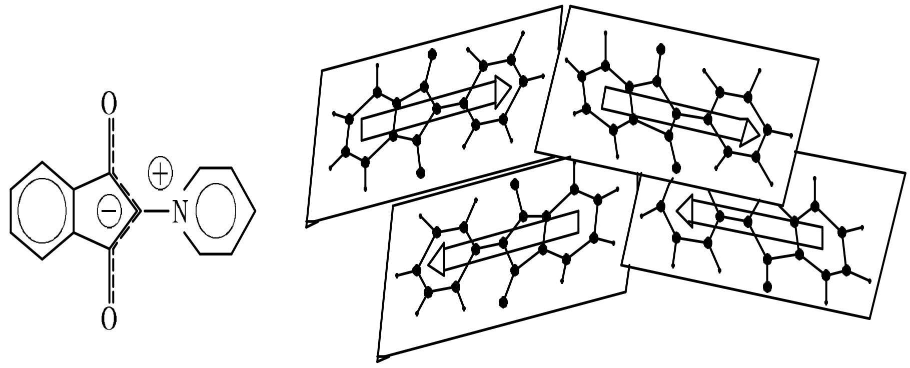

FIG. 5: Structure of IPB molecule (left). Deposition of IPB molecules in fundamental crystal unit (right). The electric dipole moments of the IPB molecules are shown that demonstrates it vortex (toroid) distribution.

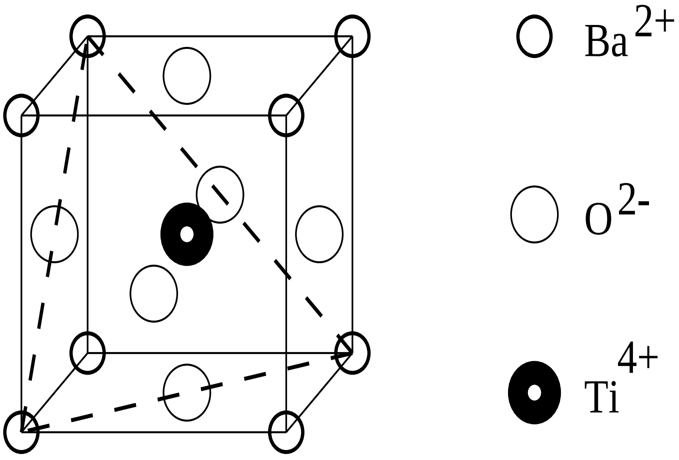

FIG. 6: Structure of type perovskite-type compound Barium Titanate $BaTiO_3$. In reality atoms fill up the major part of space. Here the position of their center is shown only.

the two components of electric fields are physically distinct from each other [11]. 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

$$\mathrm{div}\mathbf{A} =_{1} -\frac{1}{c}\,\dot{\varphi}. \tag{4.1}$$

In connection with this we should notice the terminological ambiguity. In the framework of electrodynamics of continuous media, 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 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.

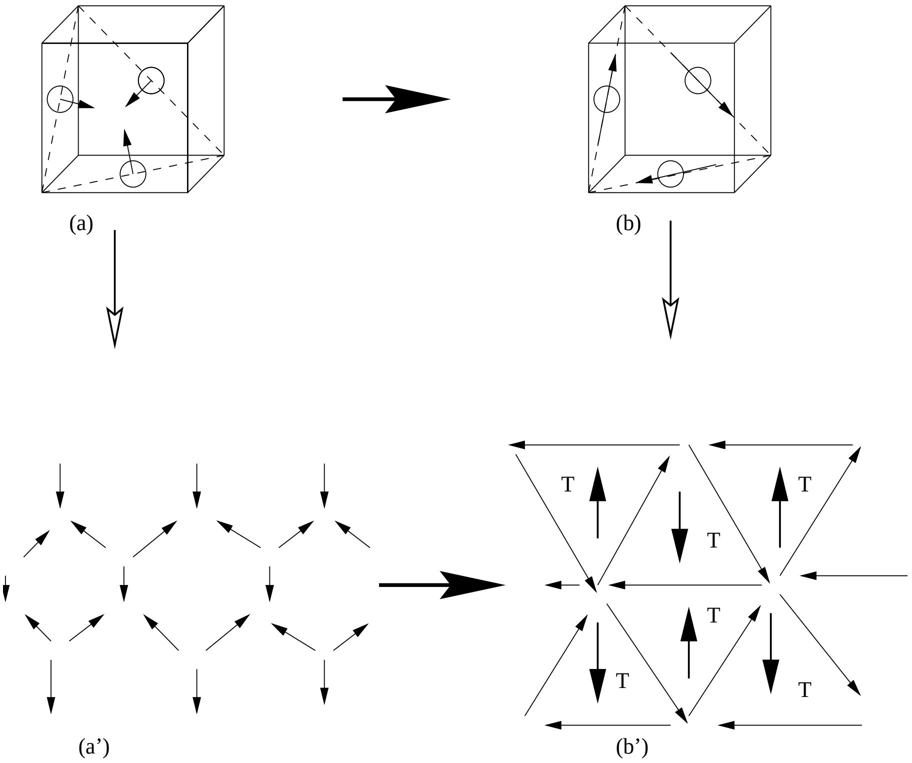

FIG. 7: Magnetic moments of oxygen atoms are orientated in such a way that they generate in each triangle toroid moment directed "up" or "down" by turns and thus build up anti-toroic [(a) and (a')]. Triangular anti-regulation of meansquare radii of magnetic moments of each domain in $(1, 1, 1)$ plane [(b) and (b')].

adding in the current part of multipole expansion the transverse and longitudinal contributions, for simplicity $\dot{Q}_{1m}$:

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

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

$$= -\dot{\mathbf{Q}}\triangle^{-1}\triangle\mathbf{A} = -\dot{\mathbf{Q}}\,\mathbf{A} = \mathbf{Q}\dot{\mathbf{A}} - \frac{d}{dt}\mathbf{Q}\mathbf{A} \Longrightarrow -\mathbf{Q}\mathbf{E} \qquad (4.2)$$

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. [11]). 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 (3.19) 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 [13], [2]

$$\rho(\mathbf{r}, t) = \sum_{l,m,n=0} \frac{(2l+1)!!}{2^n n!(2l+2n+1)!!}\sqrt{\frac{4\pi}{2l+1}}Q_{lm}^{(2n)}(t)\triangle^n\delta_{lm}(\mathbf{r}), \qquad (4.3)$$

$$Q_{lm}(t) \,=\, \sqrt{\frac{4\pi}{2l+1}} \int r^{l+2n} Y^{*}_{lm}(\hat{r}) \rho(\mathbf{r}, t)\, d\mathbf{r}. \tag{4.4}$$

Naturally, the Coulomb dipole moments, inherent to (4.24), 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 [27], [28] we would have been in need of the fixation of Coulomb gauge [29] (see also [11]).

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5. APPENDIX

According to the definition the current density, corresponding to one dipole moment in the proper system of coordinates (see Fig. 1) is equal (see e.g. [16]) to

$$\mathbf{J}^{\alpha}(\mathbf{q}^{\alpha}, \mathbf{R}) \,=\, \dot{\mathbf{Q}}^{\alpha}\, \delta(\mathbf{q}^{\alpha} \,-\, \mathbf{R}). \tag{$A.1$}$$

where value of dipole is defined as $\mathbf{Q}^{\alpha} \,=\, -e\,(\mathbf{q}^{\alpha} \,-\, \mathbf{R})$. We may introduce the total point-like current $\sum_{\alpha} \dot{\mathbf{q}}^{\alpha}$ considered to be localized in the fixed point R in the coordinate system $\mathbf{r}$ and attach it to the fixed point $\mathbf{R}$ (Fig. 1):

$$\mathbf{J}(\mathbf{r}) \,:=\, \sum_{\alpha} \dot{\mathbf{q}}^{\alpha}\, \delta(\mathbf{r} \,-\, \mathbf{R}), \tag{$A.2$}$$

where the proper dipoles $\mathbf{Q}^{\alpha} \,=\, -e\,(\mathbf{q}^{\alpha} \,-\, \mathbf{R})$ as before, but $\dot{\mathbf{Q}}^{\alpha} \,=\, \dot{\mathbf{q}}^{\alpha}$. Certainly we may obtain the last definition from the exact definition of the total current density of all electrons in the system of coordinates $\mathbf{r}$ using dipole approximation:

$$\mathbf{J}(\mathbf{r}) \,=\, \sum_{\alpha} \dot{\mathbf{q}}^{\alpha} \delta(\mathbf{r} - \mathbf{q}^{\alpha}) \approx \sum_{\alpha} \dot{\mathbf{q}}^{\alpha} \delta(\mathbf{r} - \mathbf{R}), \tag{$A.3$}$$

as far as

$$\delta(\mathbf{r} - \mathbf{q}^{\alpha}) \,=\, \delta(\mathbf{r} - \mathbf{R} + \mathbf{R} - \mathbf{q}^{\alpha})|_{\mathbf{R} \to \mathbf{q}^{\alpha}} \approx \delta(\mathbf{r} - \mathbf{R}) + (\mathbf{R} - \mathbf{q}^{\alpha}) \nabla \delta(\mathbf{r} - \mathbf{R}) + \cdots$$

But in the system $\mathbf{r}$, the polarization vector field of the molecular system can be represented as [17]

$$\mathbf{P}(\mathbf{r}, \mathbf{q}^{\alpha}) \Longrightarrow \sum_{\alpha} \mathbf{p}(\mathbf{q}^{\alpha}) \delta(\mathbf{r} - \mathbf{q}^{\alpha}) \,=\, \sum_{\alpha} \mathbf{p}(\mathbf{q}^{\alpha}) \delta(\mathbf{r} - \mathbf{R} + \mathbf{R} - \mathbf{q}^{\alpha})|_{\mathbf{R} \to \mathbf{q}^{\alpha}} \approx \sum_{\alpha} \mathbf{p}(\mathbf{q}^{\alpha}) \delta(\mathbf{r} - \mathbf{R}) + \cdots \tag{$A.4$}$$

where $\sum_{\alpha} \mathbf{p}^{\alpha}$ is the sum of dipoles of all electrons. From here the polarization current is found as

$$\mathbf{J}(\mathbf{r}) \,:=\, \frac{\partial \mathbf{P}}{\partial t} \Longrightarrow \sum_{\alpha} \dot{\mathbf{p}}(\mathbf{q}^{\alpha}) \delta(\mathbf{r} - \mathbf{R}). \tag{$A.5$}$$

Comparing (A.5) with (A.2) we conclude that

$$\mathbf{P}(\mathbf{r}, \mathbf{q}^{\alpha}) \,=\, -e\,(\mathbf{q}^{\alpha} \,-\, \mathbf{R})\, \delta(\mathbf{r} \,-\, \mathbf{R}) \,+\, \cdots \tag{$A.6$}$$

Now to define the quadrupole moment we use the following expression

$$Q_{ij} = \frac{1}{2}\int \Big[\mathbf{P}_i\mathbf{r}_j + \mathbf{r}_i\mathbf{P}_j - \frac{2}{3}\big(\mathbf{r}\cdot\mathbf{P}\big)\delta_{ij}\Big]\, d\mathbf{r}. \qquad (A.7)$$

Putting the value $\mathbf{P}$ from (A.6) we obtain

$$Q_{ij} = -\frac{e}{2}\Big[\mathbf{q}_i^\alpha\mathbf{r}_j + \mathbf{r}_i\mathbf{q}_j^\alpha - 2\mathbf{r}_i\mathbf{r}_j + \frac{2}{3}\mathbf{r}(\mathbf{q}-\mathbf{r})\delta_{ij}\Big]. \qquad (A.8)$$

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