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Reply to "The gauge-invariant lagrangian, the Power-Zienau-Woolley picture, and the choices of field momenta in nonrelativistic quantum electrodynamics." by A. Vuckis *et al.*

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ABSTRACT

In a recent paper¹, we have shown that:

(α) The Power-Zienau-Woolley hamiltonian²⁻⁶ cannot be derived from the minimal-coupling hamiltonian with the help of a gauge transformation.

This result is the opposite to a few papers^{3,7} and many textbooks^{4-6,8} where it was shown the opposite, namely that the Power-Zienau-Woolley hamiltonian effectively derived from the minimal-coupling hamiltonian with the help of a gauge transformation.

Based on a detailed discussion, we have then shown¹ that:

(β) The Power-Zienau-Woolley hamiltonian mixes two gauge conditions. Indeed, the kinetic-energy term is written in the Poincaré gauge^{9,10} whereas the electromagnetic-energy term is written in the Coulomb gauge.

This ill-defined gauge condition has consequences at the quantum level. Indeed,

(γ) As an operator the Power-Zienau-Woolley hamiltonian creates non-physical photons¹.

As a comment to our paper, A. Vukics *al.*¹¹ claim that the Power-Zienau-Woolley hamiltonian can be derived from the minimal-coupling lagrangian (or hamiltonian) without referring to any gauge transformation: (quote) "the Power-Zienau-Woolley picture of the electrodynamics of nonrelativistic neutral particles (atoms) can be derived from a gauge-invariant Lagrangian without making reference to any gauge whatsoever in the process.". Note that, their claim does not contradict our conclusion(α). Moreover, A. Vukics *al.* do not discuss **nor refute** our conclusions (β) and (γ).

This paper is organized as follows.

In section (1) we summarize the main assumptions done by A. Vukics *et al.* to derive the Power-Zienau-Woolley hamiltonian.

In section (2), we prove unambiguously that A. Vukics *et al.* calculations are actually performed in the Coulomb gauge. As a consequence they are not gauge-independent on the opposite to their claim.

In section (3) we hopefully end the debate by proving that the Power-Zienau-Woolley Hamiltonian is not equivalent to the minimal-coupling hamiltonian. Indeed the correct dynamical equations for the charged particles can not be obtained from this hamiltonian. This discrepancy is related to our initial claims (β) that the Power-Zienau-Woolley Hamiltonian mixes different gauge conditions.

Finally, in section(4), we question the validity of the assumptions done by A. Vukics *et al.* to model the interaction of punctual charges with the electromagnetic field. We conclude that A. Vukics *al.* miss the harmonic forms because of incorrect assumptions to model the physical system under consideration.

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1 Introduction: A. Vukics *al.* assumptions

In their comment, A. Vukics *al.*¹¹ claim to have exhibited:

(i) A lagrangian and a hamiltonian formulation of the light-matter coupling that is gauge-independent. The corresponding Hamiltonian is the Power-Zienau-Woolley Hamiltonian.

Their calculations are based on the following assumptions:

- (ii) The fields are defined on \mathbb{R}^3 and
- (iii) Vanish faster than $1/|r|$ as $|r| \rightarrow +\infty$.

As a consequence of these assumptions, any vector field $\mathbf{V}(\mathbf{x}, t)$ can be uniquely decomposed as the sum of a transverse component $\mathbf{V}^\perp(\mathbf{x}, t)$ and a longitudinal component $\mathbf{V}^\parallel(\mathbf{x}, t)$, *i.e.* $\mathbf{V}(\mathbf{x}, t) = \mathbf{V}^\perp(\mathbf{x}, t) + \mathbf{V}^\parallel(\mathbf{x}, t)$. This is the Helmholtz-Hodge decomposition in \mathbb{R}^3 .

Within this assumptions, A. Vuckis *et al.* derive the Power-Zienau-Woolley hamiltonian from the minimal-coupling lagrangian. To do so, they have to:

(iv) consider the transverse component of the vector potential $\mathbf{A}^\perp(\mathbf{x}, t)$ and the transverse component of the electric field $\mathbf{E}^\perp(\mathbf{x}, t)$ as the only dynamical variables for the electromagnetic field.

As a consequence:

- (v) They have to postulate the value of the longitudinal-part of the electric field, $\mathbf{E}^\parallel(\mathbf{x}, t)$. This is done from the knowledge of its value in the Coulomb gauge. It is worth emphasizing that on the opposite to the minimal-coupling hamiltonian the longitudinal-part of the electric field **cannot be found** from the Power-Zienau-Woolley hamiltonian.
- (vi) Nothing is said concerning the longitudinal part of the vector potential $\mathbf{A}^\parallel(\mathbf{x}, t)$. *A minima*, one can only speculate that it remains undetermined but irrelevant for the charged-particles and the electromagnetic-field dynamics.

2 Gauge-independent calculations ?

A. Vukics *et al.*¹¹ claim that their calculations are gauge independent. We do not agree with this statement. We prove in the following that the starting point of A. Vukics *al.*¹¹, namely eq.(VKD-13) in their paper, is actually written in the Coulomb gauge. [We have added their initial "VKD" before the equations number related to their paper.] As a consequence, **the lagrangian written by A. Vukics *al.* and the following calculations are not gauge-invariant. They are written and done in the Coulomb gauge.**

We follow their reasoning. The starting point is the minimal-coupling lagrangian:

$$L = \sum_{\alpha=0}^Z \frac{m_\alpha}{2} \dot{\mathbf{x}}_\alpha(t) + \int_{\mathbb{R}^3} d^3x \left[\frac{\epsilon_0}{2} \mathbf{E} \cdot \mathbf{E} - \frac{1}{2\mu_0} \mathbf{B} \cdot \mathbf{B} \right] + \int_{\mathbb{R}^3} d^3x \mathbf{j} \cdot \mathbf{A} - \int_{\mathbb{R}^3} d^3x \phi \rho \quad (\text{VKD-11})$$

We follow their assumptions and we assume that the fields are defined on \mathbb{R}^3 [assumption (ii)] and vanishes faster than $1/|r|$ as $|r| \rightarrow +\infty$ [assumption (iii)]. These assumptions lead to the following decomposition for the vector fields: $\mathbf{E} = \mathbf{E}^\perp + \mathbf{E}^\parallel$, $\mathbf{A} = \mathbf{A}^\perp + \mathbf{A}^\parallel$, and $\mathbf{j} = \mathbf{j}^\perp + \mathbf{j}^\parallel$, where \mathbf{E} , \mathbf{A} and \mathbf{j} are respectively the electric field, the vector potential and the current density. This decomposition is unique.

The following relations are satisfied:

$$\int_{\mathbb{R}^3} d^3x \mathbf{E}^\perp \cdot \mathbf{E}^\parallel = 0, \int_{\mathbb{R}^3} d^3x \mathbf{A}^\perp \cdot \mathbf{j}^\parallel = 0, \int_{\mathbb{R}^3} d^3x \mathbf{j}^\perp \cdot \mathbf{A}^\parallel = 0 \quad (1)$$

With these equations, the equation (VKD-11) reads:

$$L = \sum_{\alpha=0}^Z \frac{m_\alpha}{2} \dot{\mathbf{x}}_\alpha(t) + \frac{\epsilon_0}{2} \int_{\mathbb{R}^3} d^3x \mathbf{E}^\parallel \cdot \mathbf{E}^\parallel + \int_{\mathbb{R}^3} d^3x \left[\frac{\epsilon_0}{2} \mathbf{E}^\perp \cdot \mathbf{E}^\perp - \frac{1}{2\mu_0} \mathbf{B} \cdot \mathbf{B} \right] + \int_{\mathbb{R}^3} d^3x \mathbf{j}^\parallel \cdot \mathbf{A}^\parallel + \int_{\mathbb{R}^3} d^3x \mathbf{j}^\perp \cdot \mathbf{A}^\perp - \int_{\mathbb{R}^3} d^3x \phi \rho$$

Following A. Vukics *al.*¹¹, the dynamical variables for the electromagnetic-field are assumed to be the transverse part of the vector potential $\mathbf{A}^\perp(\vec{x}, t)$. As an immediate consequence, **as written above, the longitudinal component has then to be postulated.** A. Vukics *al.* assume the value of the longitudinal component to be $\mathbf{E}^\parallel(\mathbf{x}, t) = -\nabla\phi_c(\mathbf{x})$ where

$$\phi_c(\mathbf{x}; \mathbf{x}_m) = \frac{1}{4\pi\epsilon_0} \sum_{\alpha=1}^Z \frac{q_m}{|\mathbf{x} - \mathbf{x}_m(t)|} \quad (2)$$

is the scalar potential in the Coulomb gauge, $x_\alpha(t)$ being the position for the $\alpha \in \{1, \dots, Z\}$ particle. Since the electric field is gauge invariant so is its longitudinal part.

With this assumption, we have:

$$\int_{\mathbb{R}^3} d^3x \mathbf{E}^\parallel \cdot \mathbf{E}^\parallel = \int_{\mathbb{R}^3} d^3x (\nabla\phi_c)^2 = - \int_{\mathbb{R}^3} d^3x \phi_c \Delta\phi_c = \int_{\mathbb{R}^3} d^3x \phi_c(\mathbf{x}, t; \mathbf{x}_m) \frac{\rho(\mathbf{x}, t; \mathbf{x}_n)}{\epsilon_0} \quad (3)$$

Where $\rho(\mathbf{x}, t; \mathbf{x}_n) = \sum_{n=1}^Z q_n \delta(\mathbf{x} - \mathbf{x}_n(t))$ is the charge density.

With the help of equation (3), we can write the lagrangian as

$$L = \sum_{\alpha=1}^Z \frac{m_\alpha}{2} \dot{\mathbf{x}}_\alpha(t) + \int_{\mathbb{R}^3} d^3x \left[\frac{\epsilon_0}{2} \mathbf{E}^\perp \cdot \mathbf{E}^\perp - \frac{1}{2\mu_0} \mathbf{B} \cdot \mathbf{B} \right] + \int_{\mathbb{R}^3} d^3x \mathbf{j}^\perp \cdot \mathbf{A}^\perp + \int_{\mathbb{R}^3} d^3x \mathbf{j}^\parallel \cdot \mathbf{A}^\parallel + \int_{\mathbb{R}^3} d^3x \left(\frac{1}{2} \phi_c - \phi \right) \rho \quad (4)$$

This expression has to be compared with the eq:(VKD-13):

$$L_{V,K,D} = \sum_{\alpha=1}^Z \frac{m_\alpha}{2} \dot{\mathbf{x}}_\alpha(t) + \int_{\mathbb{R}^3} d^3x \left[\frac{\epsilon_0}{2} \mathbf{E}^\perp \cdot \mathbf{E}^\perp - \frac{1}{2\mu_0} \mathbf{B} \cdot \mathbf{B} \right] + \int_{\mathbb{R}^3} d^3x \mathbf{j}^\perp \cdot \mathbf{A}^\perp - \int_{\mathbb{R}^3} d^3x \frac{1}{2} \phi_c \rho \quad (\text{VKD-13})$$

To make easier the comparison between the eq:(VKD-13) and the eq:(4), we have used the following relation:

$$\frac{1}{2} \int_{\mathbb{R}^3} d^3x \phi_c(\mathbf{x}, t; \mathbf{x}_m) \rho(\mathbf{x}, t; \mathbf{x}_n) = \frac{1}{2} \frac{1}{4\pi\epsilon_0} \sum_{m=1}^Z \sum_{n=1}^Z \frac{q_m q_n}{|\mathbf{x}_n(t) - \mathbf{x}_m(t)|} = \frac{1}{4\pi\epsilon_0} \sum_{m=1}^Z \sum_{n=\alpha+1}^Z \frac{q_m q_n}{|\mathbf{x}_n(t) - \mathbf{x}_m(t)|}$$

Our result eq:(4) differs from A. Vukics *al.* result eq:(VKD-13) by the last two terms. Without fixing the gauge, one has the generic result that $\mathbf{A}^\parallel \neq 0$ and $\phi \neq \phi_c$. So equation (4) does not reduce to equation eq:(VKD-13). **As a consequence, we conclude that equation (VKD-13) assumes $\mathbf{A}^\parallel = 0$ and $\phi = \phi_c$, which is nothing else than the Coulomb-gauge condition.** Equation eq:(VKD-13) being the starting point for the derivation of the Power-Zienau-Woolley hamiltonian, this theory cannot be claimed to be gauge independent.

This conclusion is strengthened by a comment explaining that the scalar potential does not depend on the gauge. Indeed, the author wrote [11, p.6]: "In fact, we could have solved the electrostatic part of the problem in any gauge, and arrive at the same Lagrangian. The reason why the Coulomb gauge was invoked is solely because it is in this gauge that the electrostatic problem is the easiest."

The precise meaning of their sentences is hard to pin down. It seems like the authors identify the scalar potential to its value in the Coulomb gauge $\phi = \phi_c$. However it is only in the Coulomb gauge that the scalar potential satisfies the Poisson equation. Moreover they wrote:

$$\mathbf{E}^\parallel(\mathbf{x}, t) = -\nabla\phi_c(\mathbf{x}, t)$$

But this is specific to the Coulomb gauge and in the generic case (gauge-independent case), it reads:

$$\mathbf{E}^\parallel(\mathbf{x}, t) = -\nabla\phi(\mathbf{x}, t) - \partial_t \mathbf{A}^\parallel(\mathbf{x}, t)$$

This confirms that they assume that the vector potential is transverse $\mathbf{A}^{\parallel} = 0$ and $\phi = \phi_c$.

As a consequence, they exclude *de facto* any other solutions than the Coulomb gauge solutions.

In the gauge-independent case, the longitudinal component of the vector potential compensates the contribution of the scalar potential leading to the expected result $\mathbf{E}^{\parallel}(\mathbf{x}, t) = -\nabla\phi(\mathbf{x}, t) - \partial_t\mathbf{A}^{\parallel}(\mathbf{x}, t) = -\nabla\phi_c(\mathbf{x}, t)$. In the literature a similar error was done in¹² where the authors report a lagrangian formulation of light-matter interaction alleged to be gauge-independent. Actually they also did the calculations in the Coulomb gauge as proved in a subsequent comment¹³.

3 The equations of motion for the charged-particles from the Power-Zienau-Woolley hamiltonian

We now compute the equations of motion for the charged particles $\alpha = 1, \dots, Z$ from the Hamilton equations and the Power-Zienau-Woolley Hamiltonian [eq.(VKD-32) in A. Vukics *et al.* paper¹¹]:

$$H_{PZW} = \sum_{\alpha=1}^Z \left\{ \frac{1}{2m_{\alpha}} [\mathbf{p}_{\alpha} + q_{\alpha}\mathbf{x}_{\alpha} \times \int_0^1 ds s \mathbf{B}(s\mathbf{x}_{\alpha}, t)]^2 + \int_{\mathbb{R}^3} d^3x \left[\frac{1}{2\epsilon_0} \mathbf{D}^2(\mathbf{x}, t) + \frac{1}{2\mu_0} \mathbf{B}^2(\mathbf{x}, t) \right] - \int_{\mathbb{R}^3} d^3x \left[\frac{1}{\epsilon_0} \mathbf{P}^{\perp}(\mathbf{x}, t) \cdot \mathbf{D}^{\perp}(\mathbf{x}, t) + \int_{\mathbb{R}^3} d^3x \left[\frac{1}{2\epsilon_0} \mathbf{P}^2(\mathbf{x}, t) \right] \right\} \quad (\text{VKD-32})$$

In the following we prove that the equations of motion for the charged particles are not the ones expected from Newton equation.

The first Hamilton equation reads as

$$\dot{\mathbf{x}}_{\alpha} = \frac{\partial}{\partial \mathbf{p}_{\alpha}} H_{pzw} = \frac{1}{m_{\alpha}} [\mathbf{p}_{\alpha} + q_{\alpha}\mathbf{x}_{\alpha} \times \int_0^1 ds \mathbf{B}(s\mathbf{x}_{\alpha})] = \frac{1}{m_{\alpha}} [\mathbf{p}_{\alpha} - q_{\alpha} \mathbf{Y}(\mathbf{x}_{\alpha}, t)] \quad (5)$$

In order to simplify the notations, we have defined

$$\mathbf{Y}(\mathbf{x}_{\alpha}, t) = -\mathbf{x}_{\alpha} \times \int_0^1 ds s \mathbf{B}(s\mathbf{x}_{\alpha}, t) \quad (6)$$

The equation of motion eq:(5) for the particle "α" velocity is the expected one if and only if one identifies the quantity $\mathbf{Y}(\mathbf{x}_{\alpha}, t)$ to the vector potential [14, p.299]. **This is then the vector potential in the Poincaré gauge $\mathbf{Y}(\mathbf{x}_{\alpha}, t) \equiv \mathbf{A}_p(\mathbf{x}_{\alpha}, t)$.** The longitudinal part of this vector potential $\mathbf{A}_p^{\parallel}(\mathbf{x}_{\alpha}, t)$ is not null but its value cannot be found from the PZW-theory since the perpendicular component is the only dynamical variable. Moreover the quantity $\mathbf{A}_p(\mathbf{x}_{\alpha}, t)$ appears in the hamiltonian H_{PZW} eq:(VKD-32). Therefore contrarily to the claim by Vukics *et al.* p.12 that: (The PWZ hamiltonian) "is free from an electric A-square term (the magnetic contribution to the particle kinetic term is the so-called Röntgen term that vanishes in electric-dipole order)", eq:(VKD-32) has a A^2 -term just as to the minimal-coupling hamiltonian.

Now we want to compute the second Hamilton equation $\dot{\mathbf{p}}_{pzw, \alpha} = -\frac{\partial}{\partial \mathbf{x}_{\alpha}} H_{pzw}$.

In order to simplify the calculations, we shown that the following term simplifies as eq:(8):

$$T = \int_{\mathbb{R}^3} d^3x \left[\frac{1}{2\epsilon_0} \mathbf{D}^2 + \frac{1}{2\mu_0} \mathbf{B}^2 \right] - \frac{1}{\epsilon_0} \int_{\mathbb{R}^3} d^3x \mathbf{D} \cdot \mathbf{P} + \frac{1}{2\epsilon_0} \int_{\mathbb{R}^3} d^3x \mathbf{P}^2 \quad (7)$$

To see that, first note that:

$$\frac{1}{2\epsilon_0} \int_{\mathbb{R}^3} d^3x \mathbf{P}^2 = \frac{1}{2\epsilon_0} \int_{\mathbb{R}^3} d^3x \mathbf{P}^{\perp 2} + \frac{1}{2\epsilon_0} \int_{\mathbb{R}^3} d^3x \mathbf{P}^{\parallel 2}$$

Then using the definition of $\mathbf{D}(\mathbf{x}, t) = \epsilon_0 \mathbf{E}^{\perp}(\mathbf{x}, t) + \mathbf{P}^{\perp}(\mathbf{x}, t)$ [eq.(KVD-iv) in Vukics *et al.*¹¹], we obtain:

$$-\frac{1}{\epsilon_0} \int_{\mathbb{R}^3} d^3x \mathbf{D} \cdot \mathbf{P} = -\int_{\mathbb{R}^3} d^3x \mathbf{E}^{\perp} \cdot \mathbf{P}^{\perp} - \frac{1}{\epsilon_0} \int_{\mathbb{R}^3} d^3x \mathbf{P}^{\perp 2}$$

And:

$$\int_{\mathbb{R}^3} d^3x \frac{1}{2\epsilon_0} \mathbf{D}^2 = \int_{\mathbb{R}^3} d^3x \left[\frac{\epsilon_0}{2} \mathbf{E}^{\perp 2}(\mathbf{x}, t) + \mathbf{E}^{\perp} \cdot \mathbf{P}^{\perp} + \frac{1}{2\epsilon_0} \mathbf{P}^{\perp 2}(\mathbf{x}, t) \right]$$

As a consequence, the term T simplifies as:

$$T = \int_{\mathbb{R}^3} d^3x \left[\frac{\epsilon_0}{2} \mathbf{E}^{\perp 2}(\mathbf{x}, t) + \frac{1}{2\mu_0} \mathbf{B}^2 \right] + \frac{1}{2\epsilon_0} \int_{\mathbb{R}^3} d^3x \mathbf{P}^{\parallel 2} \quad (8)$$

From the Maxwell-Gauss equation $\nabla \cdot \mathbf{E}(\mathbf{x}, t) = \rho(\mathbf{x}, t)/\epsilon_0$ and the Polarization field as defined by Vukics *et al.* satisfying $\nabla \cdot \mathbf{P}(\mathbf{x}, t) = -\rho(\mathbf{x}, t)$, one concludes that $\mathbf{P}^{\parallel}(\mathbf{x}, t) = -\epsilon_0 \mathbf{E}^{\parallel}(\mathbf{x}, t)$. As a consequence, the following equality holds:

$$\frac{1}{2\epsilon_0} \int_{\mathbb{R}^3} d^3x \mathbf{P}^{\parallel 2}(\mathbf{x}) = \frac{\epsilon_0}{2} \int_{\mathbb{R}^3} d^3x \mathbf{E}^{\parallel 2}(\mathbf{x}) = \frac{1}{2} \int_{\mathbb{R}^3} d^3x \phi_c(\mathbf{x}; \mathbf{x}_\alpha) \rho(\mathbf{x}; \mathbf{x}_n) = \frac{1}{2} \frac{1}{4\pi\epsilon_0} \sum_{\alpha=1}^Z \sum_{n=1}^Z \frac{q_\alpha q_n}{|\mathbf{x}_\alpha - \mathbf{x}_n|}$$

We can now compute the time evolution of the canonical momentum \mathbf{p}_α for the particle α from the Power-Zienau-Woolley hamiltonian H_{pzw} given by:

$$H_{pzw} = \sum_{\alpha=1}^Z \left\{ \frac{1}{2m_\alpha} [\mathbf{p}_\alpha + q_\alpha \mathbf{x}_\alpha \times \int_0^1 ds ds \mathbf{B}(s\mathbf{x}_\alpha, t)]^2 + \int_{\mathbb{R}^3} d^3x \left[\frac{\epsilon_0}{2} \mathbf{E}^{\perp 2}(\mathbf{x}, t) + \frac{1}{2\mu_0} \mathbf{B}^2 \right] + \frac{1}{2} \sum_{n=1}^Z \frac{q_\alpha q_n}{|\mathbf{x}_n - \mathbf{x}_\alpha|} \right\}$$

The Hamilton equation reads:

$$\dot{\mathbf{p}}_\alpha = -\frac{\partial}{\partial \mathbf{x}_\alpha} H_{pzw}$$

The component "i" reads:

$$\dot{p}_\alpha^i = \frac{q_\alpha}{m_\alpha} [\mathbf{p} - q_\alpha \mathbf{Y}(\mathbf{x}_\alpha, t)] \cdot \nabla_{\mathbf{x}_\alpha}^i \mathbf{Y}(\mathbf{x}_\alpha, t) - q_\alpha \nabla_{\mathbf{x}_\alpha}^i \left[\frac{1}{4\pi\epsilon_0} \sum_{n=1}^Z \frac{q_n}{|\mathbf{x}_\alpha - \mathbf{x}_n|} \right] \quad (9)$$

where $\nabla_{\mathbf{x}_\alpha}^i = \frac{\partial}{\partial x_\alpha^i}$. In the following we will write $\phi_c(\mathbf{x}_\alpha) = \frac{1}{4\pi\epsilon_0} \sum_{n=1}^Z \frac{q_n}{|\mathbf{x}_\alpha - \mathbf{x}_n|}$ that is the expression of the scalar potential in the Coulomb gauge.

Taking the time-derivative of the expression $\dot{\mathbf{x}}_\alpha = \frac{1}{m_\alpha} [\mathbf{p}_\alpha - q_\alpha \mathbf{Y}_\alpha(\mathbf{x}_\alpha, t)]$ leads to:

$$\frac{d}{dt} p_\alpha^i = m_\alpha \frac{d^2 x_\alpha^i}{dt^2} + q_\alpha \frac{d}{dt} Y^i(\mathbf{x}_\alpha, t) \quad (10)$$

We can equate eq:(9) and eq:(10) and find:

$$m_\alpha \frac{d^2 x_\alpha^i}{dt^2} + q_\alpha \frac{d}{dt} Y^i(\mathbf{x}_\alpha, t) = \frac{q_\alpha}{m_\alpha} [\mathbf{p} - q_\alpha \mathbf{Y}(\mathbf{x}_\alpha, t)] \cdot \nabla_{\mathbf{x}_\alpha}^i \mathbf{Y}(\mathbf{x}_\alpha, t) - q_\alpha \nabla_{\mathbf{x}_\alpha}^i [\phi_c(\mathbf{x}_\alpha)]$$

The "i" component of the linear momentum $m_\alpha \frac{d^2 x_\alpha^i}{dt^2}$ then reads:

$$m_\alpha \frac{d^2 x_\alpha^i}{dt^2} = \frac{q_\alpha}{m_\alpha} [\mathbf{p} - q_\alpha \mathbf{Y}(\mathbf{x}_\alpha, t)] \cdot \nabla_{\mathbf{x}_\alpha}^i \mathbf{Y}(\mathbf{x}_\alpha, t) - q_\alpha \nabla_{\mathbf{x}_\alpha}^i [\phi_c(\mathbf{x}_\alpha)] - q_\alpha \frac{d}{dt} Y^i(\mathbf{x}_\alpha, t)$$

Since $\frac{d}{dt} \mathbf{Y}(\mathbf{x}_\alpha, t) = \frac{\partial}{\partial t} \mathbf{Y}(\mathbf{x}_\alpha, t) + (\dot{\mathbf{x}}_\alpha \cdot \nabla_{\mathbf{x}_\alpha}) \mathbf{Y}(\mathbf{x}_\alpha, t)$ and $\frac{1}{m_\alpha} [\mathbf{p}_\alpha - q_\alpha \mathbf{Y}_\alpha(\mathbf{x}_\alpha, t)] = \dot{\mathbf{x}}_\alpha$, we can write:

$$m_\alpha \frac{d^2 x_\alpha^i}{dt^2} = q_\alpha \dot{\mathbf{x}}_\alpha \cdot \nabla_{\mathbf{x}_\alpha}^i \mathbf{Y}(\mathbf{x}_\alpha, t) - q_\alpha \nabla_{\mathbf{x}_\alpha}^i [\phi_c(\mathbf{x}_\alpha)] - q_\alpha \frac{\partial}{\partial t} Y^i(\mathbf{x}_\alpha, t) - q_\alpha (\dot{\mathbf{x}}_\alpha \cdot \nabla_{\mathbf{x}_\alpha}) Y^i(\mathbf{x}_\alpha, t)$$

With the help of the relation $\nabla(\dot{\mathbf{x}} \cdot \mathbf{Y}) - (\dot{\mathbf{x}} \cdot \nabla) \mathbf{Y} = \dot{\mathbf{x}} \times (\nabla \times \mathbf{Y})$, the equation of motion of the electric charge is:

$$m_\alpha \frac{d^2 x_\alpha^i}{dt^2} = q_\alpha \{ \dot{\mathbf{x}}_\alpha \times [\nabla_{\mathbf{x}_\alpha} \times \mathbf{Y}(\mathbf{x}_\alpha, t)] \}_i - q_\alpha \nabla_{\mathbf{x}_\alpha}^i [\phi_c(\mathbf{x}_\alpha)] - q_\alpha \frac{\partial}{\partial t} Y^i(\mathbf{x}_\alpha, t)$$

A direct computation⁹ shows that $\nabla_{\mathbf{x}_\alpha} \times \mathbf{Y}(\mathbf{x}_\alpha, t) = \mathbf{B}(\mathbf{x}_\alpha, t)$

$$m_\alpha \frac{d^2 \mathbf{x}_\alpha^i}{dt^2} = q_\alpha \{ \dot{\mathbf{x}}_\alpha \times \mathbf{B}(\mathbf{x}_\alpha, t) \}_i - q_\alpha \nabla_{\mathbf{x}_\alpha}^i [\phi_c(\mathbf{x}_\alpha)] - q_\alpha \frac{\partial}{\partial t} Y_p^i(\mathbf{x}_\alpha, t)$$

From the ref.⁹, $-\frac{\partial}{\partial t} Y_p^i(\mathbf{x}_\alpha, t) = E^i(\mathbf{x}_\alpha, t) - \nabla_{\mathbf{x}_\alpha}^i \left[\int_0^1 ds \mathbf{x}_\alpha \cdot \mathbf{E}(s\mathbf{x}_\alpha, t) \right] = E^i(\mathbf{x}_\alpha, t) + \nabla_{\mathbf{x}_\alpha}^i \phi_p(\mathbf{x}_\alpha, t)$, where we have defined $\phi_p(\mathbf{x}_\alpha, t) = -\int_0^1 ds \mathbf{x}_\alpha \cdot \mathbf{E}(s\mathbf{x}_\alpha, t)$
Finally the equation of motion for the particle α reads:

$$m_\alpha \frac{d^2 \mathbf{x}_\alpha^i}{dt^2} = q_\alpha \{ \dot{\mathbf{x}}_\alpha \times \mathbf{B}(\mathbf{x}_\alpha, t) \}_i + q_\alpha E^i(\mathbf{x}_\alpha, t) + q_\alpha \nabla_{\mathbf{x}_\alpha}^i [\phi_p(\mathbf{x}_\alpha, t) - \phi_c(\mathbf{x}_\alpha)]$$

We can now make a few remarks:

1. This is not the expected equation of motion because $\phi_p(\mathbf{x}_\alpha, t) - \phi_c(\mathbf{x}_\alpha) \neq 0$. In the Power-Zienau-Woolley theory, the longitudinal part of the vector potential is not compensated in the appropriate way by the scalar potential. As a consequence, the term $\phi_p(\mathbf{x}_\alpha, t) - \phi_c(\mathbf{x}_\alpha)$ appears in the equations of motion.
2. If we disregard the contribution $\phi_p(\mathbf{x}_\alpha, t) - \phi_c(\mathbf{x}_\alpha) \neq 0$, we can note that the Lorentz-force term $q_\alpha \{ \dot{\mathbf{x}}_\alpha \times \mathbf{B}(\mathbf{x}_\alpha, t) \}_i + q_\alpha E^i(\mathbf{x}_\alpha, t)$, i.e. the interaction term, arises from the term $\frac{1}{2m_\alpha} [\mathbf{p}_\alpha + q_\alpha \mathbf{x}_\alpha \times \int_0^1 ds \mathbf{B}(s\mathbf{x}_\alpha)]^2$ and not from the term $-\frac{1}{\epsilon_0} \int_{\mathbb{R}^3} d^3 \mathbf{x} \mathbf{D} \cdot \mathbf{P}$. Our conclusion is that $\mathbf{Y}(\mathbf{x}_\alpha, t) = -\mathbf{x}_\alpha \times \int_0^1 ds s \mathbf{B}(s\mathbf{x}_\alpha, t) = \mathbf{A}_p(\mathbf{x}_\alpha, t)$ is the vector potential in the Poincaré gauge and describes the interaction of light and matter.

The statement p.12 in¹¹: "the familiar PZW hamiltonian accounts for the light-matter interaction in the form of the $\mathbf{D} \cdot \mathbf{P}$ term" is then incorrect.

To conclude, the Power-Zienau-Woolley hamiltonian can not be said to be equivalent to the minimal-coupling hamiltonian since it does not reproduce the correct equations of motion.

4 The domain of definition of the fields and the Helmholtz-Hodge decomposition

We now comment on the set of assumptions (ii) and (iii) to model the interaction of charged particles with the electromagnetic field.

Vukics *et al.*¹¹ assume that the fields are defined on \mathbb{R}^3 in order to write the Helmholtz theorem as $\mathbf{V}(\mathbf{x}, t) = \mathbf{V}^\perp(\mathbf{x}, t) + \mathbf{V}^\parallel(\mathbf{x}, t)$. They model the electric charges as Dirac distributions, the charge density being $\rho(\mathbf{x}, t; \mathbf{x}_n) = \sum_{\alpha=1}^Z q_n \delta(\mathbf{x} - \mathbf{x}_\alpha(t))$ in their model. As a consequence, the electromagnetic fields are not defined at the positions of the charges \mathbf{x}_α . Therefore, the domain of definition of the fields is $\mathbb{R}^3 \setminus \{ \mathbf{x}_\alpha \}$ and not \mathbb{R}^3 as assumed by Vukics *et al.*

The sets \mathbb{R}^3 and $\mathbb{R}^3 \setminus \{ \mathbf{x}_\alpha \}$ are not topologically equivalent. The Helmholtz-Hodge decomposition that these authors used $\mathbf{V}(\mathbf{x}, t) = \mathbf{V}^\perp(\mathbf{x}, t) + \mathbf{V}^\parallel(\mathbf{x}, t)$ is valid only in \mathbb{R}^3 , which is a space whose cohomology ring is trivial, while $H^p(\mathbb{R}^3 \setminus \{ \mathbf{x}_\alpha \}) = \mathbb{R}$ when $p = 0, 2$ (H^p denotes the p th de Rahm cohomology space).

A more general theorem is (theorem 13 in¹⁵):

A smooth vector field $\mathbf{V}(\mathbf{x})$ defined on a bounded or an unbounded domain, can be uniquely decomposed into three components: 1) an irrotational component $\mathbf{V}^\perp(\mathbf{x})$, which is normal to the boundary, 2) an incompressible component $\mathbf{V}^\parallel(\mathbf{x})$, which is parallel to the boundary, and 3) a harmonic component $\mathbf{h}(\mathbf{x})$:

$$\mathbf{V}(\mathbf{x}, t) = \mathbf{V}^\perp(\mathbf{x}, t) + \mathbf{V}^\parallel(\mathbf{x}, t) + \mathbf{h}(\mathbf{x}) \quad (11)$$

Harmonic components are both irrotational and incompressible vectors satisfying $\nabla \times \mathbf{h}(\mathbf{x}) = \mathbf{0}$ and $\nabla \cdot \mathbf{h}(\mathbf{x}) = 0$. Harmonic fields are null in case of compact space¹⁵.

Vukics *et al.*¹¹ assume that the longitudinal part of the electric field is $\mathbf{E}^\parallel(\mathbf{x}) = \frac{1}{4\pi\epsilon_0} \sum_{m=1}^Z q_m \frac{\mathbf{x}(t) - \mathbf{x}_m}{|\mathbf{x}(t) - \mathbf{x}_m|^3}$. Actually this is not the longitudinal part of the electric field but the harmonic form related to the Helmholtz-Hodge decomposition in $\mathbb{R}^3 \setminus \{ \mathbf{x}_\alpha \}$.

Indeed, $\nabla \times \left[\frac{1}{4\pi\epsilon_0} \sum_{m=1}^Z q_m \frac{\mathbf{x}(t) - \mathbf{x}_m}{|\mathbf{x}(t) - \mathbf{x}_m|^3} \right] = \mathbf{0}$ is obvious since it derives from the scalar potential in there Coulomb gauge.

Moreover $\frac{\partial}{\partial x_i} \left[\sum_{m=1}^Z \frac{\mathbf{x}(t) - \mathbf{x}_m}{|\mathbf{x}(t) - \mathbf{x}_m|^3} \right] = \sum_{m=1}^Z \left[\frac{3(x^i(t) - x_m^i)}{|\mathbf{x}(t) - \mathbf{x}_m|^5} - \frac{1}{|\mathbf{x}(t) - \mathbf{x}_m|^3} \right]$ for each component "i". So in $\mathbb{R}^3 \setminus \{ \mathbf{x}_\alpha \}$, $\nabla \cdot \left[\frac{1}{4\pi\epsilon_0} \sum_{m=1}^Z q_m \frac{\mathbf{x}(t) - \mathbf{x}_m}{|\mathbf{x}(t) - \mathbf{x}_m|^3} \right] = 0$.

$\mathbf{h}(\mathbf{x}) = \frac{1}{4\pi\epsilon_0} \sum_{m=1}^Z q_m \frac{\mathbf{x}(t) - \mathbf{x}_m}{|\mathbf{x}(t) - \mathbf{x}_m|^3}$ is a harmonic form in $\mathbb{R}^3 \setminus \{ \mathbf{x}_\alpha \}$ not the longitudinal component of a vector.

To conclude, the Helmholtz-Hodge decomposition used by Vukics *et al.*¹¹ is not correct and misses the harmonic forms. **The set of assumptions (ii) and (iii) are not in adequacy with the physical system to be modeled.** The theory presented by Vukics *et al.*¹¹ to recover the Power-Zienau-Woolley hamiltonian leaves indeterminate both the value of the longitudinal part of the electric-field $\mathbf{E}^{\parallel}(\mathbf{x})$ and its harmonic form $\mathbf{h}(\mathbf{x})$. One can postulate their values but such ambiguities are of course absent from the minimal-coupling hamiltonian indicating the inequivalence between both hamiltonians.

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Author contributions statement

DF initiated this work. ER did the calculations. ER and DF have discussed the results and reviewed the manuscript.

Additional information

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