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Reply to "The equivalence of the Power-Zineau-Woolley picture and the Poincaré gauge from the very first principles" by G. Kónya *et al.*¹

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ABSTRACT

This note is a reply to the paper¹ arXiv:1801.0559: "The equivalence of the Power-Zineau-Woolley picture and the Poincaré gauge from the very first principles" by G. Kónya *et al.*

The error as summarized by G. Kónya al. would be: "The canonical field momentum is not gauge invariant. Equivalent transformations of the Lagrangian do change the momentum. In field theories, gauge transformations are special cases of such transformations. The electric field \vec{E} is gauge invariant, but its capacity of being the canonical momentum is not."

The wrong emphasis as summarized by G. Kónya al. would be: "The use of the canonical coordinate/momentum pair \vec{A}_p and \vec{E} in Poincaré gauge is presented as mandatory in Rousseau and Felbacq paper, whereas as there is a certain freedom of choice in selecting this pair. Also in Poincaré gauge it is possible to use \vec{A}_c as canonical coordinate, in which case the conjugate momentum will be \vec{D} . This is the most convenient choice in terms of the set of nontrivial Dirac brackets. Cf. Table 1 in G. Kónya al. paper¹ for possible choices."

We do not share these conclusions and show in this reply that these statements are incorrect. Specifically, we show that under a gauge transformation, the canonical momentum $\pi(\vec{x},t)$ conjugated to the vector potential $\vec{A}(\vec{x},t)$ is given by $\pi(\vec{x},t) = -\varepsilon_0 \vec{E}(\vec{x},t)$.

This happens because the Lagrangian does not contains terms proportional to $\partial_t \phi(\vec{x},t)$ where $\phi(\vec{x},t)$ is the scalar potential. Moreover our choice of canonical variables was challenged. Actually, our set of independent variables is exactly the same as in G. Kónya *al.*¹ except that we do not write explicitly the dependent variables in term of the independent ones. This is one great advantage of the Dirac procedure for constrained hamiltonian [8, p.347].

1 The canonical momentum conjugated to $\vec{A}_p/\vec{A}_p^{\perp}$ is $-\varepsilon_0 \vec{E}$

In order to recover the Power-Zienau-Woolley Hamiltonian, it is mandatory to find that the canonical momentum $\vec{\pi}$ conjugated to the vector potential is the displacement vector \vec{D} , *i.e.* $\vec{\pi} = -\vec{D}$. We show in the following that cannot be correct. We do the calculations in two ways. The first one follows the comment by G. Kónya *al.*¹ in writing the explicit dependence between the dynamical variables (see subsection 1.1). The second way (subsection 1.2) follows the Dirac procedure for constraint hamiltonians. This method highlights unambiguously the contribution of the constraint $\partial_t \pi_{\phi} = 0$. In both ways, we show that the canonical momentum $\vec{\pi}$ equal the electric field $\vec{\pi} = -\varepsilon_0 \vec{E}$ because of the constraints $\pi_{\phi} = 0$ and $\partial_t \pi_{\phi} = 0$ coming from the fact that the Lagrangian is free from $\partial_t \phi(\vec{x}, t)$ -term.

For completeness let us first recall our main assumptions and the starting points share by G. Kónya $al.^1$ and our work². We consider one single electron with position \vec{r} and electric charge q evolving in a binding potential $V(\vec{r})$. The electron interacts with the electromagnetic field. The electromagnetic-field dynamical-variables are the vector potential $\vec{A}(\vec{x},t)$ and the scalar potential $\phi(\vec{x},t)$. The gauge is fixed to the Poincaré gauge defined by $\vec{x}.\vec{A}_p(\vec{x},t) = 0$ for all points \vec{x} in space.

In the Poincaré gauge the Lagrangian reads as

In a recent paper², we have shown that the Power-Zienau-Woolley Hamiltonian does not derived from the minimal-coupling hamiltonian with the help of a gauge transformation. This result has been challenged by G. Kónya *al.* in a comment¹ where the authors claim the equivalence between the Power-Zienau-Woolley hamiltonian^{3–7} and the minimal-coupling hamiltonian in the Poincaré gauge. They claim that we have made one error and one wrong emphasis in our paper:

Physical quantities	Rousseau and Felbacq ²	Kónya <i>et al</i> . ¹
Lagrangian	The same given by eq.(1-3)	
Constraint; $\chi_1 = \pi_{\phi} = 0$	Yes	Yes
Constraint; $\chi_2 = \partial_t \pi_{\phi}$	Yes	No
$\chi_2 = -[q\delta(\vec{x} - \vec{r}) + \vec{\nabla}.\vec{\pi}(\vec{x}, t)] = 0$		
Constraint;	Yes	Yes, through vector potential equation;
$\chi_3 = \vec{x}.\vec{A}(\vec{x},t) = 0$		eq.(4)
Constraint; $\chi_4 = \vec{x} \cdot \partial_t \vec{A}(\vec{x}, t)$	Yes	Yes, through scalar potential equation
$\chi_4 = \vec{x} \cdot \left[\frac{\vec{\pi}}{\varepsilon_0} - \vec{\nabla}\phi(\vec{x}, t)\right] = 0$		eq.(5)
	Dirac procedure	Explicit writing of the constraints
methods for constrained hamiltonian	and	at the Lagrangian level
	Dirac Brackets	
Discrepancy:	$-\boldsymbol{\varepsilon}_{0}\vec{E}(\vec{x},t)$	$-ec{D}(ec{x},t)$
Canonical momentum $\vec{\pi}$		
	electric field	displacement field

Table 1. Similarities and differences in Rousseau and Felbacq results² and in Kónya *et al.*¹. The main difference lyies in the method used to get the hamiltonian. Rousseau and Felbacq² used the Dirac theory for constrained hamiltonien whereas Kónya *et al.*¹ wrote explicitly the constraints at the level of the Lagrangian.

$$L_p(\vec{r}, \vec{A}_p, \phi_p) = \frac{1}{2}m\dot{\vec{r}}^2 - V(\vec{r})$$
(1)

+
$$\int d\vec{x} \frac{1}{2} \varepsilon_0 [(\partial_t \vec{A}_p(\vec{x},t) + \nabla \phi_p(\vec{x},t))^2 - \frac{1}{2\mu_0} (\vec{\nabla} \times \vec{A}_p(\vec{x},t))^2]$$
 (2)

$$+ q\dot{\vec{r}} \cdot \vec{A}_p(\vec{r},t) - q\phi_p(\vec{r}) \tag{3}$$

This is the eq.(38) in ref.¹ except that these authors have expressed the potentials with their values in the Poincaré gauge:

$$\vec{A}_{p}(\vec{r},t) = -\vec{r} \times \int_{0}^{1} u du \vec{B}(u\vec{r}) = -\vec{r} \times \int d\vec{x} \int_{0}^{1} u du \vec{B}(\vec{x}) \delta(\vec{x}-u\vec{r})$$

$$\tag{4}$$

$$\phi(\vec{r},t)_{p} = -\vec{r}.\int_{0}^{1} du\vec{E}(u\vec{r}) = -\vec{r}.\int d\vec{x} \int_{0}^{1} du\vec{E}(\vec{x})\delta(\vec{x}-u\vec{r})$$
(5)

To understand the discrepancies between G.Kónya *et al.* results¹ and our results² one should have in mind the similarities and the differences between our two works. Our approach² is based on the Dirac procedure for constrained hamiltonians^{9,10} whereas the approach by Kónya *et al.*¹ writes explicitly the constraints between the dynamical variables. Similarities and discrepancies are summarized in the table (1). This table shows that the two approaches share similar inputs except one constraint that is missing in Kónya *et al.*¹. This constraint imposes that the canonical momentum π_{ϕ} associated to the scalar potential ϕ has to remain null at any time. *This is the origin of the discrepancy between our results*.

Although, both papers share lots of similarities, the final results are different: this comes from a different canonical momentum $\vec{\pi}$. In order to understand the origin of the discrepancy let us emphasize the main advantages of Dirac theory. In this theory, although the dynamical variables may be dependent upon each other, they are considered as being independent variables, while their interdependences are taken into account through constraints used to compute the Dirac Brackets. The Dirac brackets add corrective terms to the Poisson brackets, these corrective terms arising from the constraints. Among several advantages, the Dirac theory is algorithmic in the sense that the procedure is based on theorems¹⁰. If the procedure is done in a correct way, a unique solution exists for the transformation from the Lagrangian formalism to the Hamiltonian formalism^{9,10}. On another hand, from a more a concrete point of view, an important consequence of the theory is that the dynamical variables are considered as being independent from each other. As a consequence, one has not "to use explicit expressions for the dependent variables in terms of the independent ones" [8, p.347]. In such a way, taking the functional derivative of any quantity can be done safely without having to take into account for the constraints between the variables.

When computing the canonical momentum conjugated to the vector potential, using Dirac theory as we have done, we can compute the functional derivative safely since all dynamical variables are assumed to be independent from each other. In other

words, in Dirac theory, the functional derivative has to be understood as $\frac{\delta L_p}{\delta \partial_t A_p} = \frac{\delta L_p}{\delta \partial_t A_p} \Big|_{\phi_p = cst}$. The previous notation means that the scalar potential ϕ_p is considered as a constant with respect to the functional derivative. In such a case, we found²:

$$\vec{\pi} = \frac{\delta L_p}{\delta \partial_t A_p} \bigg|_{\phi_p = cst} = -\varepsilon_0 \vec{E}$$
(6)

In G. Kónya *et al.*'s approach the difficulty is to perform variations in phase-space only on the manifold allowed by the constraints. Following their approach, the transverse part of the vector potential \vec{A}_p^{\perp} is the dynamical variable. The longitudinal part of the vector potential \vec{A}_p^{\parallel} and the scalar potential ϕ_p are considered as functions of the transverse part. Concerning the canonical momentum, they found:

$$\vec{\pi}' = -\varepsilon_0 \vec{E} - q\vec{r} \int_0^1 du \delta(\vec{x} - u\vec{r}) \tag{7}$$

As in our result, the first term originates from variations of the term $\frac{\varepsilon_0}{2}\vec{E}^2$ in the Lagrangian. The second term arises from variation of the term $-\vec{r} \cdot \int_0^1 du\vec{E}(u\vec{r})$ that is nothing else but the scalar potential in the Poincaré gauge [see eq.(5)]. Indeed $q \frac{\delta}{\delta \partial_t A_p^\perp} [-\vec{r} \cdot \int_0^1 du\vec{E}(u\vec{r})] = q \int_0^1 du\delta(\vec{x} - u\vec{r})$. To summarize, the canonical momentum $\vec{\pi}'$ computed by Kónya *et al.*¹ includes also variations along the scalar potential variable.

$$\vec{\pi}' = \frac{\delta L_p}{\delta \partial_t A_p^{\perp}} \bigg|_{\phi_p = cst} + \frac{\delta L_p}{\delta \phi_p} \bigg|_{A_p^{\perp} = cst} \frac{\delta \phi_p [A_p^{\perp}]}{\delta \partial_t A_p^{\perp}}$$

In the next subsection, we compute the canonical momentum $\vec{\pi}'$ one the manifold allowed by the constraints.

1.1 Calculation of the canonical momentum conjugated to \vec{A} with an explicit writing of the constraints

To do so, we consider the Lagrangian given by the set of equations (1-3). The scalar potential $\phi_p(\vec{x},t)$ is expressed with the help of the equation (5). The longitudinal part of the vector potential $\vec{A_p}$ is given in the Poincaré gauge by the gauge-generating function. It reads $\vec{A_p} = -\vec{\nabla} \int_0^1 du \vec{x} \cdot \vec{A_p}(u\vec{x},t)$. We are actually assuming a transition from the Coulomb gauge to the Poincaré gauge. As a consequence, we consider the transverse part of the vector potential $\vec{A_p}(\vec{x},t)$ as the only dynamical variable for the electromagnetic field. Here we are mimicking Kónya *et al.*¹. We are assuming an explicit dependence of the longitudinal part of the vector potential $\vec{A_p}(\vec{A_p})$ with the transverse part of the vector potential.

$$\vec{\pi}' = \frac{\delta L_p}{\delta \partial_t A_p^{\perp}} \bigg|_{\phi_p = cst} + \frac{\delta L_p}{\delta \phi_p} \bigg|_{A_p^{\perp} = cst} \frac{\delta \phi_p [A_p^{\perp}]}{\delta \partial_t A_p^{\perp}}$$

The functional derivative occurs along a path for which the action is extremal. Then the Euler-Lagrange equation holds

$$\left. \frac{\delta L_p}{\delta \phi} \right|_{A_p^\perp = cst} = \partial_t \left. \frac{\delta L_p}{\partial_t \delta \phi} \right|_{A_p^\perp = cst}$$

One finds $\frac{\delta L_p}{\delta \phi}\Big|_{A_p^{\perp}=cst} = -\varepsilon_0 \vec{\nabla} . (\partial_t \vec{A}_p + \vec{\nabla} \phi_p) - q \delta(\vec{x} - \vec{r}) = 0$. This is the Maxwell-Gauss equation. But, most importantly for our purpose, this equation is a consequence of the first constraint $\chi_1 = \pi_{\phi} = 0$. Indeed since this constraint has to hold at any time $\partial_t \pi_{\phi} = \partial_t \frac{\delta L_p}{\partial \delta \phi}\Big|_{A_p^{\perp}=cst} = 0$. If one wishes that the system remains on the surface defined by $\pi_{\phi} = 0$ at any time, one must have $\frac{\delta L_p}{\delta \phi}\Big|_{A_p^{\perp}=cst} = 0$. The canonical momentum conjugated to A_p^{\perp} is then:

$$ec{\pi}' = rac{\delta L_p}{\delta \partial_t A_p^\perp} igg|_{\phi_p = cst} = ec{\pi}$$

It reduces to the same equation as ours [eq:(6)]. As a consequence of the constraint $\partial_t \pi_{\phi} = 0$, the functional derivative must be evaluated as if the scalar potential is a constant. The result $\vec{\pi}' = \vec{\pi} = -\varepsilon_0 \vec{E}$ is recovered as in our paper² but following Kónya *et al.*¹ method. Because the scalar potential and the transverse part of the vector potential are coupled through the equation (5) a small variation $\delta \partial_t \vec{A}_p^{\perp}$ induces a variation of the time derivative of the scalar potential $\delta \partial_t \phi_p$. In the hamiltonian formalism this last variation $\partial_t \delta \phi_p$ implies a variation of the canonical momentum $\delta \pi_{\phi}$. But π_{ϕ} and its variations are constrained. So $\delta \pi_{\phi}$ must be null, *i.e.* $\delta \pi_{\phi} = 0$. This is the error done by Kónya *et al.*¹. They did not realize that the term $-q \int_0^1 du \delta(\vec{x} - u\vec{r})$ arises from variations of the scalar potential. They have differentiated the term arising from the scalar potential in the Pioncaré gauge as if it were an independent term, which is not.

To be exhaustif, as noted by G. Kónya $al.^1$, there is an ambiguity in the definition of the canonical momentum $\vec{\pi}(\vec{x},t)$ [see also ref. [8, p.348] for more details]. As a matter of fact, changing $\partial_t \vec{A_p}(\vec{x},t)$ by the amount $\delta \partial_t \vec{A_p}(\vec{x},t)$ changes the Lagrangian by the quantity $\delta L_p[\partial_t \vec{A}^{\perp} \rightarrow \partial_t \vec{A}^{\perp} + \delta \partial_t \vec{A}^{\perp}] = \int d\vec{x} \vec{\pi}(\vec{x},t) \cdot \delta \partial_t \vec{A_p}(\vec{x},t)$. But since we change only the transverse part of the vector potential, we must have $\vec{\nabla} \cdot \delta \partial_t \vec{A_p}(\vec{x},t) = 0$. So we can add to $\vec{\pi}(\vec{x},t)$ the gradient of a scalar function $f(\vec{x},t)$ without changing the variations δL_p . Indeed,

$$\begin{split} \delta L_p[\partial_t \vec{A}^{\perp} \to \partial_t \vec{A}^{\perp} + \delta \partial_t \vec{A}^{\perp}] &= \int d\vec{x} (\vec{\pi}(\vec{x},t) + \vec{\nabla} f(\vec{x},t)) \cdot \delta \partial_t \vec{A_p^{\perp}}(\vec{x},t) \\ &= \int d\vec{x} [\vec{\pi}(\vec{x},t) \cdot \delta \partial_t \vec{A_p^{\perp}}(\vec{x},t) - f(\vec{x},t)) \vec{\nabla} \cdot \delta \partial_t \vec{A_p^{\perp}}(\vec{x},t)] \\ &= \int d\vec{x} \vec{\pi}(\vec{x},t) \cdot \delta \partial_t \vec{A_p^{\perp}}(\vec{x},t) \end{split}$$

The most general solution is $\vec{\pi}(\vec{x},t) = -\varepsilon_0 \vec{E}(\vec{x},t) + \vec{\psi}(\vec{x},t)$ with $\vec{\psi}(\vec{x},t) = \vec{\nabla} f(\vec{x},t)$. As shown in the following, the vector field $\vec{\psi}(\vec{x},t)$ is not a dynamical variable since it does not modify the equations of motion. The vector field $\vec{\psi}(\vec{x},t)$ contributes to a shift of the total energy. Fixing the reference of the energy to zero when all fields are null leads to the condition $\vec{\psi}(\vec{x},t) = \vec{0}$. Then $\vec{\pi}(\vec{x},t) = -\varepsilon_0 \vec{E}(\vec{x},t)$ as it is found in our paper² or in many books^{8–11}.

1.2 Calculation of the canonical momentum conjugated to \vec{A} following Dirac procedure for constrained Hamiltonian

As explained above, the Dirac procedure for constrained hamiltonian considers dynamical variables as being independent from each other⁹ [10, p.29] [8, p.347]. Relationships are taken into account by a set a constraints denoted χ_i with i = 1, ..., 4in our paper². For completeness, they are recalled in the table (1). This table shows that except for the constraint χ_2 forgotten by G. Kónya *al.*¹ both results include the same list of constraints. Particularly, in our result also, the scalar and the vector potential are respectively given by the eq.(4) and the eq.(5). Consequently, the independent degrees of freedom are exactly the same in both papers. As demonstrated above, the difference lies in the constraint χ_2 which has not been taken into account in G. Kónya *al.*¹ but not from the consideration of different dynamical variables.

Using the Dirac formalism for constrained hamiltonian, we show in the following that the proposition $\vec{\pi}' = -\varepsilon_0 \vec{E} - q\vec{r} \int_0^1 du \delta(\vec{x} - u\vec{r})$ as a momentum is excluded. From the set of equations (1-3) the canonical momentum conjugated to the vector potential is given by :

$$\pi_i(\vec{x},t) = \frac{\delta L_p(\vec{r},\vec{A}_p,\phi_p)}{\delta \partial_t A_p^i} = \varepsilon_0[\partial_t A_i(\vec{x},t) + \partial_i \phi(\vec{x},t)] = -\varepsilon_0 E_i(\vec{x},t)$$
(8)

As noted by G. Kónya *al.*¹ there is an ambiguity in the definition of the canonical momentum $\vec{\pi}(\vec{x},t)$ see also ref. [8, p.348] for more details.

Changing $\partial_t \vec{A}(\vec{x},t)$ by the amount $\delta \partial_t \vec{A}(\vec{x},t)$ changes the Lagrangian by the quantity $\delta L = \int d\vec{x} \vec{\pi}(\vec{x},t) \cdot \delta \partial_t \vec{A}(\vec{x},t)$. But since variations must also satisfy the gauge constraints, for example in the Coulomb gauge, we can add the gradient of a scalar function $f(\vec{x},t)$ without changing the variations δL_c . Indeed,

$$\delta L_c = \int d\vec{x} [\vec{\pi}(\vec{x},t) + \vec{\nabla} f(\vec{x},t)] \cdot \delta \partial_t \vec{A}_c(\vec{x},t) = \int d\vec{x} \vec{\pi}(\vec{x},t) \cdot \delta \partial_t \vec{A}_c(\vec{x},t)$$

In a similar fashion, in the Poincaré gauge, the vector-potential satisfies $\vec{x} \cdot \delta \vec{A}(\vec{x},t) = x\vec{e}_r \cdot \delta \vec{A}(\vec{x},t) = \delta A_r(\vec{x},t) = 0$ where $A_r(\vec{x},t)$ is the component along the basis vector \vec{e}_r . So we can add any radial vector-field $\vec{\psi}(\vec{r}) = f(\vec{r})\vec{e}_r$ without changing the Lagrangian variations δL_p :

$$\delta L_p = \int d\vec{x} [\vec{\pi}(\vec{x},t) + f(\vec{r})\vec{e}_r] \cdot \delta \partial_t \vec{A}_p(\vec{x},t) = \int d\vec{x} \vec{\pi}(\vec{x},t) \cdot \delta \partial_t \vec{A}_p(\vec{x},t)$$

Since the previous conditions have to hold at any time, we must have $\partial_t \vec{\psi}(\vec{r},t) = 0$ in both case. The field $\vec{\psi}(\vec{r})$ depends only on space variables.

At this stage, neither in the Coulomb gauge nor in the Poincaré gauge, the canonical momentum π is uniquely defined by the eq.(8). In the Poincaré gauge, in a generic way, it reads $\vec{\pi}(\vec{x},t) = \varepsilon_0[\partial_t \vec{A}_p(\vec{x},t) + \vec{\nabla}\phi_p(\vec{x},t)] + \vec{\psi}(\vec{r})$ where $\vec{\psi}(\vec{r})$ is a radial vector-field.

We can specify the vector-field $\vec{\psi}(\vec{x},t)$ with the help of the constraints and the Maxwell-Gauss equation. First, we need to find the Hamiltonian:

$$\begin{aligned} H_{p}(\vec{r},\vec{A}_{p},\phi_{p}) &= \vec{\mathscr{P}}\cdot\vec{r} + \int d\vec{x}\vec{\pi}(\vec{x},t).\partial_{t}\vec{A}_{p}(\vec{x},t) - L_{p}(\vec{r},\vec{A}_{p},\phi_{p}) \\ &= \frac{1}{2m}[\vec{\mathscr{P}}-q\vec{A}_{p}(\vec{x},t)]^{2} + V(\vec{r}) + q\phi_{p}(\vec{r},t) \\ &+ \int d\vec{x}\{\frac{1}{2\varepsilon_{0}}[2\vec{\pi}^{2}(\vec{x},t) - (\vec{\pi}(\vec{x},t) - \vec{\psi}(\vec{x},t))^{2}] + \frac{1}{2\mu_{0}}\vec{B}^{2}(\vec{x},t) - \vec{\pi}(\vec{x},t).[\vec{\nabla}\phi_{p}(\vec{x},t) + \frac{\vec{\psi}(\vec{x},t)}{\varepsilon_{0}}]\} \end{aligned}$$
(9)

where $\vec{\mathscr{P}}$ is the canonical momentum associated to the particle position \vec{r} .

To obtain this expression one writes $\partial_t \vec{A}_p(\vec{x},t) = \left[\frac{1}{\epsilon_0} \vec{\pi}(\vec{x},t) - \vec{\nabla} \phi_p(\vec{x},t) - \frac{1}{\epsilon_0} \vec{\psi}(\vec{x})\right]$

At this step, all dynamical variables $\vec{A}_p(\vec{x},t)$, $\vec{\pi}(\vec{x},t)$, $\phi(\vec{x},t)$, $\pi_{\phi}(\vec{x},t)$ are assumed to be independent. Since $\frac{\delta L}{\delta \partial_t \phi} = \pi_{\phi} = 0$, we have found one constraint that applies to the dynamics. This constraint has to hold at any time. So, the following should hold:

$$\partial_t \vec{\pi}_{\phi}(\vec{x},t) = \{\pi_{\phi}, H_p\} = -\frac{\delta \pi_{\phi}}{\delta \pi_{\phi}} \frac{\delta H_p}{\delta \phi} = -[q\delta(\vec{x}-\vec{r}) + \vec{\nabla}.\vec{\pi}(\vec{x},t)] = 0$$
(10)

The Hamiltonian H_p is given by the equation (9).

On the other hand, the Maxwell-Gauss equation has to hold too: $q\delta(\vec{x}-\vec{r}) - \varepsilon_0 \vec{\nabla}.\vec{E}(\vec{x},t) = 0$ leading to the constraint $\vec{\nabla}.\vec{\psi}(\vec{x}) = 0$ for the field $\vec{\psi}(\vec{x})$.

To conclude, there is a freedom in the choice of the canonical momentum associated to the vector potential but with some constraints as summarized in table (2).

Poincaré gauge	Coulomb gauge
$ec{\pi}(ec{x},t) = -arepsilon_0ec{E}_p(ec{x},t) + ec{\psi}(ec{x})$	$\vec{\pi}(\vec{x},t) = -\varepsilon_0 \vec{E}_p(\vec{x},t) + \vec{\psi}(\vec{x})$
	with $\vec{\psi}(\vec{r}) = \vec{\nabla}f(\vec{x})$, $\partial_t \vec{\psi}(\vec{x}) = 0$
and $\vec{ abla}.ec{\psi}(ec{x})=0$	and $\vec{\nabla}.\vec{\psi}(\vec{x})=0$

Table 2. Conditions satisfied by the vector field $\vec{\psi}$ in the Poincaré and in the Coulomb gauge.

The condition $\vec{\nabla} \cdot \vec{\psi}(\vec{x}) = 0$ does not depend on the chosen gauge. It results from $\partial_t \pi_{\phi} = 0$. As a consequence there is here an additional argument against G. Kónya $al.^1$ proposition [eq:(7)] as a canonical momentum $\vec{\pi}$. The vector field $\vec{\psi}(\vec{x}) = -q\vec{r}\int_0^1 du\delta(\vec{x}-u\vec{r})$ that they proposed is not divergence-free. So the constraint χ_2 given by the eq.(10) excludes this solution. Again, the constraint $\partial_t \pi_{\phi} = 0$ excludes G. Kónya $al.^1$ result as a valid solution for the canonical momentum $\vec{\pi}$.

For completeness we specify a bit more the radial field $\vec{\psi}$ and show that it does only change the reference of the energy. For this we need the Hamiltonian. The Dirac procedure for constrained hamiltonian can be continued as in our paper². The Dirac brackets can be computed². After these computations the constraints act effectively. The hamiltonian can be simplify by taking all the constraints into account. After, integration by part, it reads:

$$\begin{split} H_{p}(\vec{r},\vec{A}_{p},\phi_{p}) &= \frac{1}{2m} [\vec{\mathscr{P}} - q\vec{A}_{p}(\vec{x},t)]^{2} + V(\vec{r}) \\ &+ \int d\vec{x} \{ \frac{\vec{\pi}^{2}(\vec{x},t)}{2\epsilon_{0}} + \frac{\vec{\pi}(\vec{x},t).\vec{\psi}(\vec{x},t)}{\epsilon_{0}} - \frac{\vec{\psi}^{2}(\vec{x},t)}{2\epsilon_{0}}] - \frac{\vec{\pi}(\vec{x},t).\vec{\psi}(\vec{x},t)}{\epsilon_{0}} + \frac{1}{2\mu_{0}} \vec{B}^{2}(\vec{x},t)] \} \\ &+ \int d\vec{x} \phi_{p}(\vec{x},t) [\vec{\nabla}.\vec{\pi}(\vec{x},t) + q\delta(\vec{x} - \vec{r})] \end{split}$$

It can be simplified with the help of the constraint χ_2 [eq:(10)].

$$H_{p}(\vec{r}, \vec{A}_{p}, \phi_{p}) = \frac{1}{2m} [\vec{\mathscr{P}} - q\vec{A}_{p}(\vec{x}, t)]^{2} + V(\vec{r}) + \int d\vec{x} \{ \frac{\vec{\pi}^{2}(\vec{x}, t)}{2\epsilon_{0}} + \frac{1}{2\mu_{0}} \vec{B}^{2}(\vec{x}, t) \} - \int d\vec{x} \frac{\vec{\psi}^{2}(\vec{x}, t)}{2\epsilon_{0}}$$
(11)

This last expression shows that the field $\vec{\psi}(\vec{x},t)$ is not a dynamical variable. It does not contribute to any equations of motion. Actually, it just adds up a constant contribution to the total energy. But the energy can only be defined up to a constant. If we make the usual choice H = 0 as the origin of the energy when there is no electromagnetic field then $\vec{\psi}(\vec{x},t) = 0$. we recover then the usual results:

$$H_p(\vec{r}, \vec{A}_p, \phi_p) = \frac{1}{2m} [\vec{\mathscr{P}} - q\vec{A}_p(\vec{x}, t)]^2 + V(\vec{r}) + \int d\vec{x} \{ \frac{\vec{\pi}^2(\vec{x}, t)}{2\varepsilon_0} + \frac{1}{2\mu_0} \vec{B}^2(\vec{x}, t) \}$$
(12)

$$\vec{\pi}(\vec{x},t) = -\varepsilon_0[\partial_t \vec{A}_p(\vec{x},t) + \vec{\nabla}\phi_p(\vec{x},t)] = -\varepsilon_0 \vec{E}(\vec{x},t)$$
(13)

As a conclusion, the Power-Zienau-Woolley hamiltonian is not the minimal-coupling hamiltonian written in the Poincaré gauge. As previously shown¹², it remains form-invariant through a gauge transformation.

2 Inserting $A_p^{\perp} = A_C$ and A_p^{\parallel} in our result does not lead to the Power-Zienau-Woolley Hamiltonian

On the contrary to Kónya *et al.*¹ we do not consider that our choice of dynamical variables is mandatory. It just considers the vector potential as a whole quantity. Nevertheless as in Kónya *et al.*¹ paper the transverse part of the vector potential is the only independent variable. Nonetheless once our result is known one is always free to exhibit the only independent variable and can write $\vec{A}_p = \vec{A}_p^{\perp} + \vec{A}_p^{\parallel} [\vec{A}_p^{\perp}]$. So we do not share the conclusion that our choice of variable is an "awkward choice". It has been described as an "awkward choice" by Kónya *et al.* based on a quote from Weinberg's book¹¹. In fact, Kónya *et al.* quotation of Weinberg writings is approximative and changes its very meaning. Page 15 of their manuscript¹, they wrote: "As explained by Weinberg in Section 11.3 of his book [13], $\Pi'_C = -\varepsilon_0 E$ is "an awkward choice" (quote: Weinberg) for the canonical field momenta because when quantized, it does not commute with the particle momenta"

Here is the exact citation [11, p.315-316]: There is an awkward feature about the canonical commutation relations in Coulomb gauge, that we have not yet uncover. Although the commutators of the particle coordinates x_{nj} with A_i and Π_i all vanish, the particle momenta p_{nj} have non-vanishing commutators with Π_i . According to the Dirac prescription and Eqs. (11.3.8)-(11.3.11), this commutator is [not zero]. We can avoid this complication by introducing as a replacement for Π_i its solenoidal part.

The "awkward feature" is actually not related to the choice of the dynamical variables but to a transition to the interaction picture. Weinberg made another statement in Ref. [8, p.348-349] confirming our understanding of his previous citation: Although the commutation relations (8.3.5) [commutation relations with A and II involving the Dirac-transverse distribution] are reasonably simple, we must face the complication that II does not commute with matter fields and the canonical conjugates. If F is any functional of these matter degrees of freedom, then its Dirac bracket with A vanishes, but its Dirac brackets with II is [not zero]...In order to facilitate the transition to the interaction picture, instead of expressing the Hamiltonian in terms of A and Π_{\perp} , where Π_{\perp} is the solenoidal part of Π .

Weinberg then expresses the dynamical variables in terms of the longitudinal and transverse part. He then writes $\vec{A} = \vec{A}^{\perp} + \vec{A}^{\parallel}$ and $\vec{\pi} = \vec{\pi}^{\perp} + \vec{\pi}^{\parallel}$ and inserts these expressions into the commutators and the hamiltonian previously derived.

So can the Power-Zienau-Woolley hamiltonian be obtained by writing $\vec{A}_p = \vec{A}_p^{\perp} + \vec{A}_p^{\parallel}$ and $\vec{\pi}_p = \vec{\pi}_p^{\perp} + \vec{\pi}_p^{\parallel}$ in our Hamiltonian [eq.(8) of the main manuscript or equation (12) in these paper]?

Of course not. If we do the same procedure as Weinberg's and write $\vec{A}_p = \vec{A}_p^{\perp} + \vec{A}_p^{\parallel}$ and $\vec{\pi}_p = \vec{\pi}_p^{\perp} + \vec{\pi}_p^{\parallel}$, we do not recover the Power-Zienau-Woolley hamiltonian since $\vec{\pi}_p^{\perp} = -\varepsilon_0 \vec{E}^{\perp} \neq \vec{D}$ where \vec{D} is the displacement vector as shown previously.

As a conclusion, the Power-Zienau-Woolley hamiltonian <u>cannot</u> be derived from the minimal-coupling hamiltonian through a gauge transformation.

3 Some weaknesses of the Power-Zienau-Woolley hamiltonian

The Power-Zienau-Woolley hamiltonian reads:

$$H_{PZW} = \frac{1}{2m} [\mathscr{P} + q\vec{r} \times \int_0^1 du d\vec{B}(u\vec{r}, t)]^2$$
(14)

$$+ \int d^3x \frac{1}{2\epsilon_0} \vec{D}^2(\vec{x}, t) + \frac{1}{2\mu_0} \vec{B}^2(\vec{x}, t)$$
(15)

$$- -\frac{1}{\varepsilon_0} \int d^3x \, \vec{D}(\vec{x},t) \cdot \vec{P}(\vec{x},t) \tag{16}$$

$$+ + \frac{1}{2\varepsilon_0} \int d^3x \, \vec{P}^2(\vec{x}, t) \tag{17}$$

This is the equation eq:(46) in Kónya *et al.* comment [1, p.14] and according to them this is also the minimal coupling hamiltonian in the Poincaré gauge. They made the following comments quote in italic:

1. The PZW Hamiltonian is free from the A-square term,

Maybe it is here a question of semantic. But it can not be said that the PZW hamiltonian is free from the A-square term since precisely $\vec{r} \times \int_0^1 du d\vec{B}(d\vec{r},t) = -\vec{A}_p(\vec{r},t)$ is the vector potential in the Poincaré gauge. This term is usually neglected in the so-called electric-dipole approximation but it does contribute in the complete theory.

- 2. accounts for the light-matter interaction in the form of the $\vec{D}(\vec{x},t).\vec{P}(\vec{x},t)$ term,
- 3. contains a P-square term.

By definition $\vec{D}(\vec{x},t) = \varepsilon_0 \vec{E}(\vec{x},t) + \vec{P}(\vec{x},t)$. Replacing this definition into the set of equations (1-4), one can remark that the so-called light-matter interaction term and the P-square term cancel out. It is dramatic in the electric-dipole approximation since there is then no interaction term. Indeed, the Power-Zienau-Woolley Hamiltonian reduces to:

$$H_{PZW} \simeq \frac{1}{2m} \mathscr{P}^2 + \int d^3x \, \frac{1}{2\varepsilon_0} \vec{E}^2(\vec{x},t) + \frac{1}{2\mu_0} \vec{B}^2(\vec{x},t)$$

Those criticisms previously raised in our paper weaken strongly the validity of the Power-Zienau-Woolley Hamiltonian. Nevertheless Kónya *et al.* did not comment on them.

Conclusion

To conclude, we have shown that if all the constraints are taken into account correctly then the canonical momentum $\vec{\pi}(\vec{x},t)$ conjugated to the vector potential is $-\varepsilon_0 \vec{E}(\vec{x},t)$ provided that the reference of the energy is taken to be null. This result has been derived following Kónya *et al.* methodology [1, p.14] where all quantities are written with the help of the independent dynamical variable $\vec{A}_p^{\perp}(\vec{x},t)$. We have shown that the constraint $\partial_t \pi_{\phi} = 0$ leads to this result. We have also recalled our derivation based on the Dirac theory for constrained hamiltonian. We have obtained the same result $\vec{\pi}(\vec{x},t) = -\varepsilon_0 \vec{E}(\vec{x},t)$ based on the same argument $\partial_t \pi_{\phi} = 0$. Moreover, this derivation allowed us to conclude that the following proposition for the momentum $\vec{\pi}'(\vec{x},t) = -\varepsilon_0 \vec{E}(\vec{x},t) - q\vec{r} \int_0^1 du \delta(\vec{x} - u\vec{r})$ cannot be considered as correct since $-q\vec{r} \int_0^1 du \delta(\vec{x} - u\vec{r})$ is not divergence-free. We have also explained that the differences between our both results cannot be attributed to the consideration

of different dynamical variables since they are similar in both papers. The independent dynamical variables are taken into account explicitly in Kónya *et al.*¹ work and implicitly in our work through the constraints χ_i . Nevertheless they are exactly the same.

In order to obtain the Power-Zienau-Woolley hamiltonian one needs $\vec{\pi}'(\vec{x},t) = -\vec{D}(\vec{x},t)$, which is impossible as we have demonstrated. As a consequence, we conclude that this hamiltonian cannot be derived from the minimal-coupling hamiltonian. We ended these notes in highlighting some weaknesses of the Power-Zienau-Woolley hamiltonian. More weaknesses can be found in our paper. Particularly the physical meaning of the term $\frac{1}{2\epsilon_0}\vec{D}^2(\vec{x},t) + \frac{1}{2\mu_0}\vec{B}^2(\vec{x},t)$ is questionable since this is neither the electromagnetic-field energy-density in vacuum nor in matter. As far as we know, the weaknesses of the Power-Zienau-Woolley hamiltonian have never been commented (and answered) into the literature.

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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

The authors declare no competing financial interests.

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