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1985 J. Phys. A: Math. Gen. 18 377

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# The path-dependent electrodynamics of bound charges: QED of spinors in an external Coulomb field

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Received 16 February 1984

**Abstract.** The manifestly gauge invariant relativistic electrodynamics of neutral atoms is derived from a path-dependent Lagrangian. A second quantised spinor field is used for the description of electrons, while the infinitely heavy nucleus is represented by a static Coulomb field. Classical Lagrangian formalism is constructed. Generalised Poisson brackets are obtained from canonical formalism. Canonical quantisation is performed. The whole description is without any reference to the electromagnetic potentials. A comparison with other formulations is given.

## 1. Introduction

The very first formulation of quantum electrodynamics (Dirac 1927a,b) was used for the description of the interaction of neutral atoms with the electromagnetic field. Already in these fundamental papers two different forms of the interaction Hamiltonian were used. The first one was based on the following description of the interaction energy

$$H_1 = e(\boldsymbol{\xi} - \boldsymbol{\xi}_0) \cdot \mathbf{e}(\boldsymbol{\xi}_0) \quad (1.1)$$

where  $\boldsymbol{\xi}$  is the position of the electron,  $\boldsymbol{\xi}_0$  the position of the nucleus,  $\mathbf{e}(\boldsymbol{\xi}_0)$  the vector of the electric field. The second one was based on the minimal coupling principle, i.e. substitution of the canonical momentum  $\mathbf{p}$  of the non-interacting particle by  $\mathbf{p} - (e/c)\mathbf{a}(\boldsymbol{\xi})$  where  $\mathbf{a}$  is the vector potential in the Coulomb gauge.

After the discovery of the Dirac equation for electrons, the construction of the relativistic version of the theory became the main aim of most papers on QED. The interaction was usually introduced by employing the minimal coupling method. This method employs potentials as basic dynamical variables describing the electromagnetic fields and thus, since potentials are not observables, is associated with the problems connected with gauges. The question of the gauge invariance of QED is far more complicated than that for the classical case. A survey of these problems can be found in Haller (1975).

QED has a local and covariant form only in the Lorentz gauge. However, one has to introduce unphysical states normalised with respect to an indefinite metric. The basic alternative is to use the Coulomb gauge. No unphysical states appear, but the components of the vector potential do not form a four-vector. The commutation rules have a non-local form. The Coulomb interaction, which replaces the fourth component of the vector potential, also has a non-local form, and propagates with an infinite

velocity. Despite the behaviour of the potentials, the real observables of the EM field, i.e. the components of  $f_{\mu\nu}$ , have a covariant character. An important feature of the Coulomb gauge is the non-quantised description of the Coulomb field, and that corresponds closely with the physical reality, since photons are associated only with radiation.

A method of avoiding these complications is based on an observation that the gauge problems can be avoided if the description involves only gauge-independent quantities. One can treat the tensor  $f_{\mu\nu}$  as the set of dynamical variables for the electromagnetic field. The potentials, if introduced at all, are functionals of  $f_{\mu\nu}$ , and serve only as mathematical aids which simplify the field equations.

QED based on the above observations was constructed by Belinfante and Lomont (1951). In the early sixties De Witt (1962) and Mandelstam (1962) constructed QED without potentials, in the so-called path-dependent formulation. The basic variables of the theory are the components of  $f_{\mu\nu}$  for the EM field, and  $\Phi(x, P)$  and  $\Phi^*(x, P)$  for the charged particles. The latter ones are related to the conventional gauge-dependent operators  $\tilde{\Phi}$  and  $\tilde{\Phi}^*$  by the formula

$$\Phi(x, P) = \Phi(x) \exp\left(ie \int_{-\infty}^x d\xi^\mu a_\mu(\xi)\right) \quad (1.2)$$

and its adjoint. The integral on the right-hand side of (1.2) is to be taken over a spacelike path joining the point  $x$  with spatial infinity. The operators  $\Phi(x, P)$  are path-dependent (Mandelstam 1962). If the path  $P$  is deformed infinitesimally, close to a point  $z$ , while the end-point remains fixed, this changes the operators by

$$\delta_2 \Phi(x, P) = ie \Phi(x, P) \div f_{\mu\nu}(z) d\sigma^{\mu\nu} \quad (1.3)$$

where  $d\sigma_{\mu\nu}$  is an infinitesimal surface element spanned between the curve  $P$  and its deformation. This feature is the source of the name of the theory. It should be noted that the word 'path' means here an abstract line in the Minkowski space without any direct physical interpretation. The arbitrariness of the choice of paths is a manifestation of the freedom of the fixing of the phase factors in the operators of charged fields.

This version of QED was further studied in the works of Sarker (1963) and Mandelstam (1968). Białynicki-Birula (1963) adapted the formalism to suit Yang-Mills fields. Belinfante (1962) showed that after averaging over all straight spatial lines, the theory is concurrent with that of Belinfante and Lomont (1951). Rohrlich and Strocchi (1965) performed an average over all possible straight paths, including the timelike ones. They showed that this procedure is equivalent to the introduction of gauge-invariant and path-independent quantities  $\mathcal{A}_\mu$ , which behave as potentials in the Landau gauge:

$$[\mathcal{A}_\mu(x), \mathcal{A}_\nu(x')] = -i(g_{\mu\nu} - \partial_\mu \partial_\nu / \square) D(x - x'). \quad (1.4)$$

These operators fulfil the Lorentz condition  $\partial_\mu \mathcal{A}^\mu = 0$ , since they are functionals of the fields  $f_{\mu\nu}$ :

$$\mathcal{A}_\mu(x) = \int f_{\mu\nu}(x+y) \partial / \partial y_\nu D_i(y) d^4 y \quad (1.5)$$

where  $D_i$  is a Green function of the inhomogeneous d'Alembert equation. The Lorentz condition is consistent with the commutation rules and is an operator equation. Thus, there is no need for the indefinite metric.

From the above review one can conclude that the construction of QED without potentials is always associated with the introduction of a certain non-locality into the theory. Indeed, in a theory without potentials this non-locality is necessary for the description of the Aharonov-Bohm effect. The non-locality is often thought to be a serious drawback of the path-dependent theory, especially when compared with the apparent locality of a theory with potentials, e.g. Aharonov and Bohm (1961, 1962). However, from the theorem of Strocchi and Wightman (1974) on the charge superselection rule, one can infer that there are no local charged states in QED. This means that the non-local nature is intrinsic to the theory, and cannot be avoided even in the apparently local formulations. Thus, the charge carrying operators of the path-dependent theories, e.g. (1.2), must have a non-local form.

There has been renewed interest in the QED of atoms and molecules because of the development of quantum optics. The gauge-independent form of the non-relativistic QED of molecules and atoms is well known. It is associated with the so-called multipolar Hamiltonian. However, for many years the relationship of this theory with the Coulomb gauge QED was not clear. Also the complete form of the multipolar Hamiltonian was not known. These problems were first solved by Power and Zienau (1957, 1959). They obtained the final form of the unitary transformation leading to the multipolar formalism, and presented the full form of the Hamiltonian, including, for the first time, the term

$$\frac{1}{2} \int \mathbf{p}^{\perp 2}(\mathbf{x}) d^3 \mathbf{x}, \quad (1.6)$$

where  $\mathbf{p}^{\perp}$  is the transverse part of the polarisation operator. The Power-Zienau unitary operator has the form

$$U = \exp \left( i \int d^3 \mathbf{x} \mathbf{p}(\mathbf{x}) \cdot \mathbf{a}(\mathbf{x}) \right) \quad (1.7)$$

where, in the original papers,  $\mathbf{p}(\mathbf{x})$  was expressed by the first terms of the multipolar expansion. The Hamiltonian of Power and Zienau has a gauge-independent form for the neutral atom. The electromagnetic fields are represented by vectors  $\mathbf{b}$  and  $\boldsymbol{\varepsilon}^{\perp} = \mathbf{e}^{\perp} + \mathbf{p}^{\perp}$ . However, as the canonical variables the authors used the vector potential in the Coulomb gauge and the field  $\boldsymbol{\varepsilon}^{\perp}$ .

Fiutak (1963) introduced a new representation of the multipolar Hamiltonian, and of the unitary transformation. This representation uses path integrals, and thus is closely related with the path-dependent electrodynamics of De Witt (1962) and Mandelstam (1962). The Fiutak approach was later developed in many papers, e.g. Woolley (1971, 1980), Fiutak and Engels (1973), Babiker (1975), Babiker *et al* (1974), Healy (1977a, b), Fiutak and Żukowski (1978, 1981), Power and Thirunamachandran (1980a).

The correct interpretation of the dynamical variables of the multipolar Hamiltonian has been a very controversial problem. In many papers the multipolar Hamiltonian has been treated as a result of a unitary transformation of the total Coulomb gauge Hamiltonian. Such an interpretation leads to an incorrect interpretation of the field variables, which in turn gives the Heisenberg picture equations of motion which do not correspond with the Maxwell equations (Mandel 1979, and the comments by Power and Thirunamachandran 1980b, 1982, Healy 1980, 1982 and Haller 1982).

The correct interpretation of the field  $\boldsymbol{\varepsilon}^{\perp}$  has been given by Babiker *et al* (1974), Fiutak and Engels (1975), and Healy (1977a). This field is the transverse electric

induction vector  $\mathbf{d}^\perp$ , and in the case of neutral atoms  $\mathbf{d} = \mathbf{d}^\perp$ . This is the field which after averaging gives the macroscopic electric induction vector (de Groot 1969).

In the works of Fiutak and Żukowski (1978, 1981) and Rzążewski and Wódkiewicz (1980) a completely gauge-independent set of canonical variables has been introduced. For the electromagnetic fields these are  $\mathbf{b}$  and  $\mathbf{d}$ . Thus the vector  $\mathbf{a}$  is eradicated from the theory of the multipolar Hamiltonian.

The basic aim of this paper is the construction of a gauge-invariant theory of the quantised radiation field and the Dirac electron field interacting with a nucleus of charge  $Ze$  represented by a static field. The total charge carried by the electron field is  $-Ze$ , thus in the case of bound states we get a neutral atom. We aim at a formally covariant theory, so that the Feynman-Dyson diagrammatic technique could be used. Nevertheless, the very introduction of the static field creates a privileged reference system.

The electrodynamics presented in § 2 is a classical theory. However, one can perform the canonical quantisation thanks to the generalised Poisson brackets introduced in § 3. In the construction of the Lagrangian and the canonical formalism the emphasis is directed at the definition of the variables for both formulations.

In § 4 we compare the path-dependent bound state electrodynamics with other formulations. This is given here in the context of the  $S$ -matrix. The theory can be shown to be completely equivalent with other formulations of bound state QED. However, applications of a physical theory are always associated with certain approximations. These approximations may lead to discrepancies when different Hamiltonians are used, see e.g. Rzążewski (1978), Davidovich and Nussenzweig (1978), Fried (1973), Bassani *et al* (1977), Reiss (1979). Thus despite the equivalence of the full  $S$ -matrices, the use of a truncated perturbation series may lead to different results for different versions of the theory.

The multipolar form of the bound state spinor QED was first given by Babiker (1975). In contradistinction from Babiker's treatment of this problem, in this paper the stress is laid on the gauge invariance of the description, and the Lagrangian formalism is formally covariant. The main thesis is that one can discard the potentials and use the tensor  $f_{\mu\nu}$  as the full set of Lagrange's variables for the electromagnetic fields. However, in order to derive Maxwell's equations from the principle of least action one cannot use the familiar text-book methods. This is because Maxwell's equations, when expressed in terms of fields rather than potentials, do not have the form of Euler-Lagrange equations. Therefore the present work is based on a modified version of the Lagrangian formalism presented by Fiutak and Żukowski (1981). The canonical formalism presented here does not employ the potentials either. The canonical variables for the fields are  $\mathbf{b}$  and  $\mathbf{d}$ .

## 2. The Lagrangian and equations of motion

The theory of the external field is a branch of QED. It is based on the separation of the total radiation field into two parts, one of which is treated classically, and the other describes the quantum effects.

The classical field and the current density of its source are described by the  $c$ -number quantities  $f_{\mu\nu}^{\text{ex}}$  and  $j_\mu^{\text{ex}}$ . These are related by the equation

$$\partial^\nu f_{\mu\nu}^{\text{ex}} = j_\mu^{\text{ex}}, \quad (2.1)$$

or, employing the electromagnetic potential,

$$\partial^\nu \partial_{[\mu} a_{\nu]}^{\text{ex}} \stackrel{\text{df}}{=} \partial^\nu (\partial_\mu a_\nu^{\text{ex}} - \partial_\nu a_\mu^{\text{ex}}) = j_\mu^{\text{ex}}. \quad (2.2)$$

In the standard versions of the electrodynamics of spinor fields, the interaction of the electromagnetic field and particles is commonly introduced through the 'minimal coupling' interaction Lagrangian, in which an electromagnetic potential is linked to the current density four-vector. The potential and its derivatives are employed as Lagrange variables for the electromagnetic field. The action integral is then given by

$$W[a, \psi, \bar{\psi}; \sigma_1, \sigma_2] = W = - \int_{\sigma_1}^{\sigma_2} d^4x [\bar{\psi}(\gamma^\mu \partial_\mu + m + ie\gamma^\mu a_\mu)\psi + \frac{1}{4}f_{\mu\nu}f^{\mu\nu}], \quad (2.3)$$

where the symbols have their usual meaning, e.g. Jauch and Rohrlich (1976). There are two equivalent methods of introducing the external field to the theory with potentials (Schwinger 1949). Either the interaction with an external source can be described by the current  $j_\mu^{\text{ex}}$  associated with it, and this amounts to adding to (2.3) the following term

$$\Delta W_{(1)} = \int_{\sigma_1}^{\sigma_2} d^4x j_\mu^{\text{ex}} a^\mu \quad (2.4a)$$

or the interaction is introduced through the field of the external source,  $f_{\mu\nu}^{\text{ex}} = \partial_{[\mu} a_{\nu]}^{\text{ex}}$ , and the additional term in the action integral is then given by

$$\Delta W_{(2)} = -ie \int_{\sigma_1}^{\sigma_2} d^4x \bar{\psi} \gamma^\mu a_\mu^{\text{ex}} \psi. \quad (2.4b)$$

The action integral  $W + \Delta W_{(1)}$  implies the following equations of motion

$$\partial_\nu f^{\mu\nu} = j_{\text{ex}}^\mu - ie\bar{\psi}\gamma^\mu\psi, \quad (2.5)$$

$$(\gamma^\mu \partial_\mu + ie\gamma^\mu a_\mu + m)\psi = 0, \quad (2.6)$$

whereas  $W + \Delta W_{(2)}$  gives

$$\partial_\mu f^{\mu\nu} = ie\bar{\psi}\gamma^\nu\psi \quad (2.5a)$$

$$(\gamma^\mu \partial_\mu + ie\gamma^\mu (a_\mu + a_\mu^{\text{ex}}) + m)\psi = 0. \quad (2.6a)$$

One can propose studying another action integral for a neutral system consisting of a spinor field and an infinitely heavy nucleus interacting with the electromagnetic fields. This integral may be written in the form

$$\begin{aligned} W' &= \int_{\sigma_1}^{\sigma_2} d^4x \mathcal{L}'[x] = W'[f_{\mu\nu}, \bar{\psi}_p, \psi_p; \sigma_1, \sigma_2] \\ &= \int_{\sigma_1}^{\sigma_2} d^4x (-\bar{\psi}_p \gamma^\mu \partial_\mu \psi_p - \bar{\psi}_p \psi_p m - \frac{1}{4}f_{\mu\nu}f^{\mu\nu} + \frac{1}{2}f_{\mu\nu}m^{\mu\nu}[x; \psi_p]), \end{aligned} \quad (2.7)$$

where the coupling term is expressed in terms of the electromagnetic field tensor  $f_{\mu\nu}$ , and the polarisation tensor  $m^{\mu\nu}[x; \psi]$ . The latter is an antisymmetric solution of the equation

$$\partial_\beta m^{\alpha\beta}[x; \psi] = -ie\bar{\psi}\gamma^\alpha\psi + j_{\text{ex}}^\alpha = j^\alpha + j_{\text{ex}}^\alpha, \quad (2.8)$$

with one additional condition that the total charge of the system is equal to zero, i.e.

$$\int_{\sigma} d\sigma^{\mu} (-ie\bar{\psi}\gamma_{\mu}\psi + j_{\mu}^{\text{ex}}) = 0. \tag{2.9}$$

The new spinor field is denoted as  $\psi_p$  in order to stress that, as we shall see further, it differs from the gauge-dependent  $\psi$ . Since the current  $j_{\mu}^{\text{ex}}$  has to represent an infinitely heavy nucleus, we shall define it as

$$j_{\mu}^{\text{ex}}(z) = Ze \int_{-\infty}^{+\infty} (\delta^{(4)}(z - R) dR_{\mu}/ds) ds, \tag{2.10}$$

where  $R_{\mu}$  is the four-dimensional trajectory of the nucleus, which in turn is assumed to be at rest in a privileged reference frame; the parameter  $s$  is defined by  $ds = dR^{\mu} dR_{\mu}$ . This reference frame is defined by a unit time-like vector  $n_{\mu} = dR_{\mu}/ds$ . The polarisation tensor is a bivector composed of the electric polarisation  $p^i = m^{i0}$  and the magnetisation  $m^i = \frac{1}{2}\epsilon^{ijk}m^{jk}$ , where the latin indices denote the three spatial dimensions. The polarisation tensor describes the distribution of the multipole moments of the system.

One has to construct an explicit form for the polarisation tensor. This may be done by adopting a path-dependent solution of (2.8) valid for all points between two spacelike hyperplanes  $\sigma_1$  and  $\sigma_2$  normal to  $n^{\mu}$ :

$$m^{\alpha\beta}(z) = \int_{\sigma_1}^{\sigma_2} F^{\alpha\beta}_{\rho}(z|x) j^{\rho}(x) d^4x, \tag{2.11}$$

where the kernel is given by

$$F^{\alpha\beta}_{\rho}(z|x) = \int_{R(x)}^x d\xi^{\lambda} \delta^{(4)}(z - \xi) \partial\xi^{\beta 1}/\partial x^{\rho} \tag{2.12}$$

(Żukowski 1985). The path  $\xi$  joins the point  $R(x)$  with  $x$ .  $R(x)$  is the position of the charge carried by  $j_{\mu}^{\text{ex}}$ . Its dependence on  $x$  can be defined by the following invariant condition

$$(x^{\alpha} - R^{\alpha}(x)) dR_{\alpha}(x)/ds = 0,$$

which means that  $R(x)$  is the point of the intersection of a hyperplane  $\sigma$ , which is normal to  $n_{\mu}$  and contains the event point  $x_{\mu}$ , with the trajectory of the nucleus  $R_{\mu}(s)$ .

The path in (2.12) is a spacelike one, with  $\xi_0 = x_0$  in the rest frame of the nucleus. The simplest choice is a straight line.

One must stress here that arbitrary spacelike paths can be used in a more general description. However, such a generalisation seems to be of no practical value, except for a possible theoretical discussion of the invariance properties of the theory. For such a case one should suitably change the domain of integration in the action integral.

The polarisation and magnetisation fields associated with the  $m^{\alpha\beta}$  of (2.11)-(2.12), are given in § 4, formulae (4.25)-(4.26).

The difference between the form of the new action integral (2.7) and  $W + \Delta W_{(1)}$ , can be thought of as arising from a phase transformation of the spinor variables, namely by going over from  $\psi$  of  $W + \Delta W_{(1)}$  to  $\psi_p$ . This transformation is given by

$$\psi_p(x) = \psi(x) \exp\left(ie \int_{R(x)}^x a_{\mu}(\xi) d\xi^{\mu}\right). \tag{2.13a}$$

However, the condition (2.9) has been used explicitly when passing from  $W + \Delta W_{(1)}$  to (2.7). These operations have the following influence on the form of the action integral  $W + \Delta W_{(1)}$ :

$$\begin{aligned}
 W[a, \bar{\psi}_p, \psi_p; \sigma_1, \sigma_2] + W_{(1)}[a; \sigma_1, \sigma_2] + \int_{\sigma_1}^{\sigma_2} d^4x \partial_\mu (a_\nu m^{\mu\nu}[x, \psi_p]) \\
 = W'[f_{\mu\nu}, \bar{\psi}_p, \psi_p; \sigma_1, \sigma_2].
 \end{aligned}
 \tag{2.13b}$$

The four divergence in (2.13b) can be rewritten in the form

$$\int_{\sigma_1}^{\sigma_2} d^4x \left( \frac{1}{2} f_{\mu\nu} m^{\mu\nu}[x; \psi_p] - (j_\nu + j_\nu^{ex}) a^\nu \right).
 \tag{2.13c}$$

The expression  $a_\nu m^{\mu\nu}$  is a functional of  $a_\nu, \bar{\psi}_p$  and  $\psi_p$  but not their derivatives. Thus, when Hamilton's principle is employed, the variations of the action integrals  $W + W_{(1)}$  and  $W'$  are identical and the equations of motion associated with them are equivalent.

The difference between both integrals can be considered as of more profound nature than merely the relation (2.13b). Namely, in the case of  $W'$ , as we shall see, one can choose the tensor  $f_{\mu\nu}$  as the full set of Lagrange's variables for the electromagnetic fields.

We shall apply the procedure of Lagrangian QFT, see e.g. Jauch and Rohrlich (1976), especially the section S1-1. We treat the fields in the functional  $W'$  as classical ones. With the action principle we can derive the equations of motion and the energy-momentum tensor. This tensor enables us to define the energy functional, which becomes the Hamiltonian for the canonical formulation. We firstly define the generalised Poisson brackets. Then the procedure of canonical quantisation is applied.

Since the interaction term in  $W'$  has a non-local form the expression for  $W'$  can be written as

$$\begin{aligned}
 W' &= \int_{\sigma_1}^{\sigma_2} d^4x \mathcal{L}''[x] \\
 &= \int_{\sigma_1}^{\sigma_2} d^4x \left( -\bar{\psi}_p(x) \gamma^\mu \partial_\mu \psi(x) - \frac{1}{2} i e \bar{\psi}_p(x) \gamma^\rho \psi_p(x) \right. \\
 &\quad \left. \times \int_{\sigma_1}^{\sigma_2} d^4y f_{\mu\nu}(y) F^{\mu\nu}(y|x) - \bar{\psi}_p(x) \psi_p(x) m - \frac{1}{4} f_{\mu\nu} f^{\mu\nu} \right).
 \end{aligned}
 \tag{2.14}$$

When analysing the invariance of the theory with respect to the choice of paths, we shall use the Lagrangian density in the form of  $\mathcal{L}''$ .

The electrodynamics based on the action integral  $W'$  is an example of a theory of a charged field interacting with the electromagnetic fields. As we are free to fix the phase factors of the charged operators, in the conventional theory with potentials the description of the interaction is associated with gauge transformations of the potentials, which compensate the changes of the phase of the charged field. The action integral is invariant with respect to such coupled transformations, and this is a manifestation of the conservation of charge.

According to Mandelstam (1962) the path-dependent theories are a consequence of a specified method of defining the phase of charged fields at points separated by a finite distance. One fixes the phase at one point, here  $R(x)$ , and then chooses a path  $P$  joining this point with another point  $x$ . The phase is defined as equal on the whole path, and in that way one fixes it at the point  $x$ . This procedure can be path-independent



only when the electromagnetic fields are absent. The fields introduce a 'phase curvature' (an analogy with Riemannian geometry).

Arbitrary changes of the kernel  $F^{\alpha\beta}_\rho$  can be expressed by

$$\Delta F^{\mu\nu}_\rho(y|x) = \oint d\xi^{[\mu} \partial \xi^{\nu]} / \partial x^\rho \delta^{(4)}(y - \xi), \tag{2.15}$$

where the integration is over a closed line formed from the old path  $P$  and the new path  $P'$  both joining  $R(x)$  and  $x$ . The direction of the integration is obvious. For any  $x$  belonging to the region of spacetime between the hypersurfaces  $\sigma_1$  and  $\sigma_2$ , and for the fields  $f_{\mu\nu}$  satisfying the first pair of the Maxwell equations, i.e.

$$\varepsilon^{\alpha\beta\gamma\delta} \partial_\gamma f_{\alpha\beta} = 0, \tag{2.16}$$

we have

$$\begin{aligned} & \frac{1}{2} \int_{\sigma_1}^{\sigma_2} d^4y f_{\mu\nu}(y) \Delta F^{\mu\nu}_\rho(y|x) \\ &= \frac{1}{2} \oint d\xi^{[\alpha} \partial \xi^{\gamma]} / \partial x^\rho f_{\alpha\gamma}(\xi) = -\frac{\partial}{\partial x^\rho} \left( \frac{1}{2} \int_{\sigma(x)} f_{\alpha\gamma} d\sigma^{\alpha\gamma} \right), \end{aligned} \tag{2.17}$$

where  $\sigma(x)$  is an arbitrary surface spanned between  $P$  and  $P'$ . The last equation can be proved as follows: let  $a^\mu$  be an arbitrary vector potential, then we have

$$\begin{aligned} & -\frac{\partial}{\partial x^\mu} \int_{R(x)}^x a_\gamma(\xi) d\xi^\gamma \\ &= -\frac{\partial}{\partial x^\mu} \int_0^1 dl a_\gamma(\xi(x, l)) \frac{d\xi^\gamma(x, l)}{dl} = -\int_0^1 dl \left( \frac{\partial \xi^\alpha}{\partial x^\mu} \right) \left( \frac{\partial}{\partial \xi^\alpha} \right) a_\gamma(\xi) \left( \frac{d\xi^\gamma}{dl} \right) \\ & \quad + \int_0^1 dl \left( \frac{d\xi^\alpha}{dl} \right) \left( \frac{\partial}{\partial \xi^\alpha} \right) a_\gamma(\xi) \left( \frac{\partial \xi^\alpha}{\partial x^\mu} \right) - \left|_0^1 a_\gamma(\xi(x, l)) \frac{\partial \xi^\gamma(x, l)}{\partial x^\mu} \right. \\ &= \int_0^1 \frac{d\xi^\alpha}{dl} \frac{\partial \xi^\gamma}{\partial x^\mu} f_{\alpha\gamma}(\xi) dl - \left|_0^1 a_\gamma(\xi(x, l)) \frac{\partial \xi^\mu}{\partial x^\mu} \right., \end{aligned} \tag{2.18}$$

where for the parametrisation  $\xi^\mu(x, l)$  we have  $\xi^\mu(x, 1) = x$  and  $\xi^\mu(x, 0) = R(x)$ . The formula is formally identical for both paths  $P$  and  $P'$ , thus one can infer that

$$-\frac{\partial}{\partial x^\mu} \oint a_\gamma(\xi) d\xi^\gamma = \frac{1}{2} \oint d\xi^\alpha \frac{\partial \xi^\gamma}{\partial x^\mu} f_{\alpha\gamma}(\xi). \tag{2.19}$$

Finally the relation  $f_{\mu\nu} = \partial_{[\mu} a_{\nu]}$  and the use of the Stokes theorem give (2.17). It should be noted that the use of potentials is not necessary for the proof of (2.17), but enables one to achieve the aim in the shortest way. However, the first pair of the Maxwell equations is a necessary condition for the validity of (2.17), since otherwise the right-hand side would have been defined ambiguously, due to the arbitrariness of  $\sigma(x)$ .

From (2.17) one can infer that the action integral is invariant with respect to the changes of path in the kernel  $F^{\alpha\beta}_\rho$  coupled with the following phase transformation

$$\psi_p(x) \rightarrow \psi_{p'}(x) = \psi_p(x) \exp\left( ie \frac{1}{2} \int_{\sigma(x)} f_{\alpha\beta} d\sigma^{\alpha\beta} \right), \tag{2.20a}$$

$$\bar{\psi}_p(x) \rightarrow \bar{\psi}_{p'}(x) = \bar{\psi}_p(x) \exp\left( -ie \frac{1}{2} \int_{\sigma(x)} f_{\alpha\beta} d\sigma^{\alpha\beta} \right). \tag{2.20b}$$

The transformation (2.20) is a result of a change in the phase fixing procedure associated with the detour from the original path.

Reversing the argument, one can see that the path-dependence of the charged operators due to the phase fixing procedure proposed by Mandelstam, together with the arbitrariness of the paths in the kernel  $F^{\alpha\beta}{}_{\rho}$ , requires the imposition of the first pair of the Maxwell equations as constraints, rather than as equations of motion.

As the surface  $\sigma(x)$  in (2.20) is arbitrary, one can choose it to be inside a hypersurface of constant time. Thus only the magnetic induction vector plays a role in the phase fixing. The Aharonov-Bohm effect is a direct consequence of this fact.

One can obtain the equations of motion for the electromagnetic fields from the principle of stationary action, if one chooses the variations of these fields,  $\delta_0 f_{\mu\nu}$ , which are of bounded support in the region of spacetime  $\Omega$  between the hypersurfaces  $\sigma_1$  and  $\sigma_2$ . This condition guarantees that the variations  $\delta_0 f_{\mu\nu}$  vanish at  $\sigma_1$  and  $\sigma_2$ . It is sufficient to use variations which are infinitely differentiable, i.e. those belonging to the class of functions usually denoted as  $C_0^\infty(\Omega)$ . The condition for the field equations reads

$$\delta W' = \frac{1}{2} \int_{\sigma_1}^{\sigma_2} \frac{\partial \mathcal{L}'}{\partial f_{\mu\nu}} \delta_0 f_{\mu\nu} d^4x = 0. \quad (2.21)$$

However, the electromagnetic fields obey the constraint relations (2.16), and therefore the variations  $\delta_0 f_{\mu\nu}$  cannot be arbitrary. In fact  $\delta_0 f_{\mu\nu}$  satisfy

$$\varepsilon^{\alpha\beta\gamma\delta} \partial_\gamma \delta_0 f_{\alpha\beta} = 0. \quad (2.22)$$

Before proceeding further one has to analyse the relation between (2.21) and (2.22). The expression  $\partial \mathcal{L}' / \partial f_{\mu\nu}$  in (2.21) is an antisymmetric tensor. Let us assume that (2.22) is satisfied, and  $\varphi^{\alpha\beta}$  is an arbitrary antisymmetric tensor. This implies that

$$\int_{\sigma_1}^{\sigma_2} \varphi^{\alpha\beta} \delta_0 f_{\alpha\beta} d^4x = 0 \quad (2.23)$$

for arbitrary  $\delta_0 f_{\alpha\beta}$  belonging to  $C_0^\infty(\Omega)$ , if and only if

$$\partial_\alpha \varphi^{\alpha\beta} = 0. \quad (2.24)$$

This theorem stems from the generalisation of the Helmholtz theorem to the antisymmetric tensors of the Minkowski space, e.g. Plebański (1970), which says that any antisymmetric tensor  $\varphi^{\alpha\beta}$  can be split in the following way

$$\varphi^{\alpha\beta} = \varepsilon^{\alpha\beta\gamma\delta} \partial_\gamma A_\delta + \partial^{[\alpha} B^{\beta]} = \varphi_A^{\alpha\beta} + \varphi_B^{\alpha\beta} \quad (2.25)$$

with

$$\partial_\alpha \varphi_A^{\alpha\beta} = 0 \quad \text{and} \quad \varepsilon^{\alpha\beta\gamma\delta} \partial_\gamma (\varphi_B)_{\alpha\beta} = 0. \quad (2.26)$$

As a consequence of (2.23)-(2.24) we get

$$\partial_\alpha (\partial \mathcal{L}' / \partial f_{\alpha\beta}) = 0 \quad (2.27)$$

as a condition for (2.21). This is the equation of motion for the fields, i.e. the second pair of the Maxwell equations. The tensor  $\partial \mathcal{L}' / \partial f_{\alpha\beta}$  is usually denoted as  $h_{\alpha\beta}$ . The equations (2.27) do not have the traditional form of the Euler-Lagrange equations, and this fact was often thought to imply the necessity of the introduction of the potentials to the Lagrangian formalism. One can note that the method presented above is a general one and can be applied in other branches of electrodynamics;

especially the derivation of the equation of motion for the electrodynamics of point particles, given by Fiutak and Żukowski (1981), can be rewritten according to the above scheme, and thus one could dispel any doubts that the potentials are there introduced to the Lagrangian formalism by backdoor methods.

In the case of the spinor field  $\psi_p$  the derivation of the equations of motion is obvious, and gives

$$m\psi_p(x) + \gamma^\mu \partial_\mu \psi_p(x) + \frac{1}{2}ie \int_{R(x)}^x d\xi^{[\mu} f_{\mu\nu}(\xi) \frac{\partial \xi^{\nu]}}{\partial x^\rho} \gamma^\rho \psi_p(x) = 0. \quad (2.28)$$

The equation for  $\bar{\psi}(x)$  can be obtained by conjugation of (2.28).

### 3. The energy-momentum tensor

We shall give here the explicit expressions for the energy-momentum tensor and angular energy-momentum tensor. This will be achieved using the method based on the work of Fiutak and Żukowski (1981).

To this end let us consider an infinitesimal Lorentz transformation

$$(Ax)^\mu = x'^\mu = x^\mu + \varepsilon^\mu + a^{\mu\nu} x_\nu = x^\mu + \delta x^\mu. \quad (3.1)$$

For the fields we have

$$f^{\alpha\beta}(x) \rightarrow f'^{\alpha\beta}(x') = f^{\alpha\beta}(x) + a^{\alpha\gamma} f_\gamma^\beta(x) + a^{\beta\gamma} f^\alpha_\gamma(x) = f^{\alpha\beta} + \delta f^{\alpha\beta}, \quad (3.2)$$

$$\psi_p(x) \rightarrow \psi'_p(x') = \psi_p(x) + \frac{1}{4}a^{\mu\nu} \gamma_\mu \gamma_\nu \psi_p(x) = \psi_p + \delta \psi_p. \quad (3.3)$$

The action integral is changed by an amount

$$\begin{aligned} \delta W' &= \int_{A(\sigma_1)}^{A(\sigma_2)} \mathcal{L}'[Ax] d^4x - \int_{\sigma_1}^{\sigma_2} \mathcal{L}'[x] d^4x = \int_{\sigma_1}^{\sigma_2} d^4x \partial_\mu (\delta x^\mu \mathcal{L}'[x]) \\ &+ \int_{\sigma_1}^{\sigma_2} d^4x \left[ \frac{1}{2} \frac{\delta W'}{\delta f^{\mu\nu}(x)} (\delta f^{\mu\nu}(x) - \delta x^\alpha \partial_\alpha f^{\mu\nu}(x)) \right] + \int_{\sigma_1}^{\sigma_2} d^4x \\ &\times \left[ \frac{\delta W'}{\delta \psi_p(x)} (\delta \psi_p(x) - \delta x^\alpha \partial_\alpha \psi_p(x)) + \frac{\delta W'}{\delta \bar{\psi}_p(x)} (\delta \bar{\psi}_p(x) - \delta x^\alpha \partial_\alpha \bar{\psi}_p(x)) \right. \\ &\left. + \frac{\delta W'}{\delta (\partial_\mu \psi_p(x))} (\delta (\partial_\mu \psi_p(x)) - \delta x^\alpha \partial_\alpha \partial_\mu \psi_p(x)) \right], \end{aligned} \quad (3.4)$$

where the symbols of the type  $\delta W / \delta \psi_p$  denote functional derivatives.

Using the equations of constraints (2.16) we can get

$$a^{\alpha\gamma} f_\gamma^\beta + a^{\beta\gamma} f^\alpha_\gamma - \delta x^\mu \partial_\mu f^{\alpha\beta} = \partial^\alpha (f^{\beta\mu} \delta x_\mu) + \partial^\beta (f^{\mu\alpha} \delta x_\mu). \quad (3.5)$$

The equations of motion together with (3.4)-(3.5) finally give

$$\delta W' = \left( \int_{\sigma_1} d\sigma_\mu - \int_{\sigma_2} d\sigma_\mu \right) (t^{\mu\alpha} \varepsilon_\mu + \frac{1}{2} a_{\alpha\beta} m^{\mu\alpha\beta}), \quad (3.6)$$

where the energy-momentum tensor  $t^{\mu\nu}$  is given by

$$t^{\mu\alpha} = \partial \mathcal{L}' / \partial f_{\mu\nu} f_\nu^\alpha + g^{\mu\alpha} \mathcal{L}' + \bar{\psi}_p \gamma^\mu \partial^\alpha \psi_p, \quad (3.7)$$

and the angular energy-momentum tensor by

$$m^{\rho\mu\nu} = x^\mu t^{\rho\nu} - x^\nu t^{\rho\mu} - \frac{1}{4} \bar{\psi}_p \gamma^\rho [\gamma^\mu, \gamma^\nu] \psi_p. \quad (3.8)$$

The electromagnetic field part of  $t^{\mu\nu}$  is symmetric. The full  $t^{\mu\nu}$  can be symmetrised using the standard procedures, see e.g. Rzewuski (1964).

The energy density of the system is defined as the component of the energy-momentum tensor

$$t^{00} = \partial \mathcal{L}' / \partial f_{0\nu} f_\nu^0 - \mathcal{L}' + \bar{\psi}_p \gamma^0 \partial^0 \psi_p. \quad (3.9)$$

We can conclude that the formalism presented here verifies the thesis, that the Lagrange variables for the electromagnetic fields are vectors  $\mathbf{e}$  and  $\mathbf{b}$ .

#### 4. Canonical formalism

In this section we shall present an approach which enables us to introduce the Poisson brackets, without any reference to the potentials. We shall establish the set of the canonical variables of the theory. These will be chosen in such a way that the Poisson brackets of the variables for the EM fields with their counterparts for the electron field vanish.

The canonical formalism cannot be expressed in a covariant form, owing to the fact that the time translations play a special role in it. Therefore, we shall construct this formalism in the rest frame of the nucleus.

The total energy of the system  $P^0$  is a functional of the fields  $f_{\mu\nu}$ ,  $\bar{\psi}_p$  and  $\psi_p$ . It is given by

$$P^0 = \int d^3\mathbf{x} t^{00} = \int d^3\mathbf{x} (\mathbf{d} \cdot \mathbf{e} + \bar{\psi}_p \gamma_0 \partial_0 \psi_p - \mathcal{L}') \quad (4.1)$$

where

$$d_i = \partial \mathcal{L}' / \partial f_{0i} = h^{0i} = \partial \mathcal{L}' / \partial e_i; \quad (4.2)$$

the form of (4.1) suggests that as the set of canonical variables one should choose  $\mathbf{b}$ ,  $\mathbf{d}$ ,  $\psi_p$  and  $\bar{\psi}_p \gamma_0$ .

The functional of energy (4.1), when expressed by these variables, is, as we shall see, the Hamiltonian of the system, i.e. the generator of the time translations:

$$H = P^0[\mathbf{d}, \mathbf{b}, \bar{\psi}_p \gamma_0, \psi_p]. \quad (4.3)$$

Taking the variation of  $P^0$  expressed by (4.1) we obtain:

$$\begin{aligned} \delta P^0 = \int d^3\mathbf{x} \left( \delta \mathbf{d}(\mathbf{x}) \cdot \mathbf{e}(\mathbf{x}) + \mathbf{d}(\mathbf{x}) \cdot \delta \mathbf{e}(\mathbf{x}) \right. \\ \left. - \frac{\partial \mathcal{L}'}{\partial \mathbf{e}(\mathbf{x})} \cdot \delta \mathbf{e}(\mathbf{x}) - \frac{\partial \mathcal{L}'}{\partial \mathbf{b}(\mathbf{x})} \cdot \delta \mathbf{b}(\mathbf{x}) - \frac{\delta L'}{\delta (\bar{\psi}_p \gamma_0)} \delta (\bar{\psi}_p \gamma_0(\mathbf{x})) \right. \\ \left. - \frac{\delta L'}{\delta \psi_p(\mathbf{x})} \delta \psi_p(\mathbf{x}) + \delta \bar{\psi}_p(\mathbf{x}) \gamma_0 \partial_0 \psi_p(\mathbf{x}) + \psi_p(\mathbf{x}) \gamma_0 \delta (\partial_0 \psi_p(\mathbf{x})) \right), \end{aligned} \quad (4.4)$$

where

$$L' = \int d^3\mathbf{x} \mathcal{L}'[\mathbf{x}]. \quad (4.5)$$

The definition of the functional derivative enables us to treat  $\nabla \psi$  as a variable dependent

on  $\psi$ . On the other hand

$$\delta H = \int d^3x \left( \frac{\delta H}{\delta \mathbf{d}(\mathbf{x})} \cdot \delta \mathbf{d}(\mathbf{x}) + \frac{\delta H}{\delta \mathbf{b}(\mathbf{x})} \cdot \delta \mathbf{b}(\mathbf{x}) + \frac{\delta H}{\delta (\psi_p(\mathbf{x}) \gamma_0)} \delta (\bar{\psi}_p(\mathbf{x}) \gamma_0) + \frac{\delta H}{\delta \psi_p(\mathbf{x})} \delta \psi_p(\mathbf{x}) \right). \quad (4.6)$$

Let us now concentrate on the method of obtaining the Hamilton equations for the electromagnetic fields, because for the spinors the procedure is well known.

The variations  $\delta \mathbf{d}$  and  $\delta \mathbf{b}$  are not unconstrained. The path dependence of the variables in  $H$  imposes additional conditions. As we work in the privileged reference frame, the condition

$$\operatorname{div} \mathbf{b} = 0 \quad (4.7)$$

is enough to guarantee that the transformations (2.15), (2.20) leave the Hamiltonian invariant. On the other hand, as the motion of the sources is described by polarisation and magnetisation vectors, and formally there are no free charges, this gives for the electric induction the transversality condition

$$\operatorname{div} \mathbf{d} = 0. \quad (4.8)$$

The equations (4.7) and (4.8) will serve as constraints for the canonical formulation.

Taking into account only the variations of the electromagnetic fields, and comparing (4.4), (4.6) and (4.2), from the requirement  $\delta P^0 = \delta H$ , we get

$$\int d^3x \left[ \delta \mathbf{d}(\mathbf{x}) \cdot \left( \mathbf{e}(\mathbf{x}) - \frac{\delta H}{\delta \mathbf{d}(\mathbf{x})} \right) + \delta \mathbf{b}(\mathbf{x}) \cdot \left( \mathbf{h}(\mathbf{x}) - \frac{\delta H}{\delta \mathbf{b}(\mathbf{x})} \right) \right]. \quad (4.9)$$

The constraints enable us to put

$$\delta_c d_i(\mathbf{x}) = \int \delta_{ij}^+(x-y) \delta_r d_j(\mathbf{y}) d^3y \quad (4.10)$$

with the same relation for  $\delta_c \mathbf{b}$ . The variation  $\delta_c \mathbf{d}$  satisfies the constraint relation (4.8), whereas the 'free' one  $\delta_r \mathbf{d}$  does not have to. The transverse delta function is given by

$$\delta_{ij}^+(\mathbf{x}) = \delta(\mathbf{x}) \delta_{ij} + (1/4\pi) \partial^2 / \partial x_i \partial x_j (1/|\mathbf{x}|). \quad (4.11)$$

From (4.10) and (4.9) we are led to

$$\int d^3y \left( e_i(\mathbf{x}) - \frac{\delta H}{\delta d_i(\mathbf{x})} \right) \delta_{ij}^+(\mathbf{x}-\mathbf{y}) = 0, \quad (4.12a)$$

$$\int d^3y \left( h_i(\mathbf{x}) - \frac{\delta H}{\delta b_i(\mathbf{x})} \right) \delta_{ij}^+(\mathbf{x}-\mathbf{y}) = 0, \quad (4.12b)$$

and this in turn implies that

$$\nabla \times (\mathbf{e}(\mathbf{x}) - \delta H / \delta \mathbf{b}(\mathbf{x})) = 0 = \nabla \times (-\mathbf{h}(\mathbf{x}) + \delta H / \delta \mathbf{b}(\mathbf{x})). \quad (4.13)$$

Finally the equations of the Lagrangian formalism enable us to put

$$\dot{\mathbf{b}}(\mathbf{x}) = -\nabla \times (\delta H / \delta \mathbf{d}(\mathbf{x})), \quad \dot{\mathbf{d}}(\mathbf{x}) = \nabla \times (\delta H / \delta \mathbf{b}(\mathbf{x})). \quad (4.14a, b)$$

These formulae, together with

$$\dot{\psi}_p(\mathbf{x}) = \delta H / \delta(\bar{\psi}_p(\mathbf{x})\gamma_0), \quad \dot{\bar{\psi}}_p(\mathbf{x})\gamma_0 = -\delta H / \delta\psi_p(\mathbf{x}) \quad (4.15a, b)$$

constitute the complete set of Hamilton equations for the theory.

If one introduces the generalised Poisson brackets defined as

$$\begin{aligned} \{\mathcal{F}, \mathcal{G}\} = \int d^3x \left[ \frac{\delta\mathcal{F}}{\delta\mathbf{d}(\mathbf{x})} \cdot \left( \nabla \times \frac{\delta\mathcal{G}}{\delta\mathbf{b}(\mathbf{x})} \right) - \frac{\delta\mathcal{G}}{\delta\mathbf{d}(\mathbf{x})} \cdot \left( \nabla \times \frac{\delta\mathcal{F}}{\delta\mathbf{d}(\mathbf{x})} \right) \right. \\ \left. + \frac{\delta\mathcal{F}}{\delta\psi_p(\mathbf{x})} \frac{\delta\mathcal{G}}{\delta(\bar{\psi}_p(\mathbf{x})\gamma_0)} - \frac{\delta\mathcal{F}}{\delta(\bar{\psi}_p(\mathbf{x})\gamma_0)} \frac{\delta\mathcal{G}}{\delta\psi_p(\mathbf{x})} \right] \end{aligned} \quad (4.16)$$

the equations (4.14)-(4.15) can be treated as examples of a general law of evolution for any observable dependent only on the canonical variables:

$$\dot{\mathcal{F}} = \{\mathcal{F}, H\}. \quad (4.17)$$

The explicit form of the Hamiltonian is given by

$$\begin{aligned} H = \int d^3x \left( \frac{1}{2}\mathbf{d}^2(\mathbf{x}) + \frac{1}{2}\mathbf{b}^2(\mathbf{x}) - \mathbf{p}(\mathbf{x}) \cdot \mathbf{d}(\mathbf{x}) + \frac{1}{2}\mathbf{p}^2(\mathbf{x}) - \mathbf{m}(\mathbf{x}) \cdot \mathbf{b}(\mathbf{x}) \right. \\ \left. + \bar{\psi}_p(\mathbf{x})\boldsymbol{\gamma} \cdot \boldsymbol{\partial}\psi_p(\mathbf{x}) + m\bar{\psi}_p(\mathbf{x})\psi_p(\mathbf{x}) \right). \end{aligned} \quad (4.18)$$

The total momentum of the electrons and photons can be written as

$$\mathbf{P} = \mathbf{P}_f + \mathbf{P}_m \quad (4.19)$$

where

$$\mathbf{P}_f = \int d^3x (\mathbf{d}(\mathbf{x}) \times \mathbf{b}(\mathbf{x})) \quad (4.20)$$

and

$$\mathbf{P}_m = \int d^3x \bar{\psi}_p(\mathbf{x})\boldsymbol{\gamma}^0\nabla\psi_p(\mathbf{x}). \quad (4.21)$$

For the angular momentum we have

$$\mathbf{M} = \mathbf{M}_f + \mathbf{M}_m \quad (4.22)$$

$$\mathbf{M}_f = \int d^3x \mathbf{x} \times (\mathbf{d}(\mathbf{x}) \times \mathbf{b}(\mathbf{x})) \quad (4.23)$$

$$\mathbf{M}_m = \int d^3x [\mathbf{x} \times (\bar{\psi}_p(\mathbf{x})\boldsymbol{\gamma}^0\nabla\psi_p(\mathbf{x})) - \frac{1}{2}i\bar{\psi}_p(\mathbf{x})\boldsymbol{\gamma}^0\boldsymbol{\Sigma}\psi_p(\mathbf{x})] \quad (4.24)$$

where the matrix  $\boldsymbol{\Sigma}$  is defined by  $\Sigma_i = -i\epsilon_{ijk}\gamma^j\gamma^k$ . The functionals (4.19)-(4.24) are the canonical generators of translations and rotations. The splittings (4.19) and (4.22) can be called canonical, because for example, the generators  $\mathbf{P}_f$  and  $\mathbf{M}_f$  govern the rotations and translations of the canonical variables for the EM fields.

In the rest frame of the nucleus the polarisation and magnetisation vectors are given by formulae (4.25)-(4.26). If one puts  $\mathbf{R} = 0$ , these read

$$p^i(z) = \int d^3x \int_0^x d\xi^1 \delta^{(3)}(z - \boldsymbol{\xi})(-ie\bar{\psi}_p(\mathbf{x})\boldsymbol{\gamma}^0\psi_p(\mathbf{x})), \quad (4.25)$$

$$m^i(\mathbf{z}) = \int d^3\mathbf{x} \int_0^x d\xi^j \frac{\partial \xi^k}{\partial x^m} \varepsilon^{ijk} \delta^{(3)}(\mathbf{z} - \boldsymbol{\xi}) (-ie\bar{\psi}(\mathbf{x}) \gamma^m \psi(\mathbf{x})). \quad (4.26)$$

As a result one can rewrite the Hamiltonian in the following way

$$\begin{aligned} H = & \int d^3\mathbf{z} \left( \frac{1}{2} \mathbf{d}^2(\mathbf{z}) + \frac{1}{2} \mathbf{b}^2(\mathbf{z}) + \bar{\psi}_p(\mathbf{z}) \boldsymbol{\gamma} \cdot \nabla \psi_p(\mathbf{z}) + m\bar{\psi}(\mathbf{z})\psi(\mathbf{z}) \right. \\ & + ie \int_0^z d\xi \cdot \mathbf{d}(\boldsymbol{\xi}) \bar{\psi}_p(\mathbf{z}) \gamma^0 \psi_p(\mathbf{z}) + ie \int_0^z d\xi^j \varepsilon^{ijk} \frac{\partial \xi^k}{\partial x^m} b^i(\boldsymbol{\xi}) \bar{\psi}_p(\mathbf{z}) \gamma^m \psi_p(\mathbf{z}) \left. \right) \\ & - \frac{1}{2} e^2 \int d^3\mathbf{z}_1 \int d^3\mathbf{z}_2 (\bar{\psi}_p(\mathbf{z}_1) \gamma^0 \psi_p(\mathbf{z}_1)) (\bar{\psi}_p(\mathbf{z}_2) \gamma^0 \psi_p(\mathbf{z}_2)) (4\pi|\mathbf{z}_1 - \mathbf{z}_2|)^{-1} \\ & + \int d^3\mathbf{z} [(-iZe^2 \bar{\psi}_p(\mathbf{z}) \gamma^0 \psi_p(\mathbf{z})) (4\pi|\mathbf{z}|)^{-1} + \frac{1}{2} \mathbf{p}^{\perp 2}(\mathbf{z})], \end{aligned} \quad (4.27)$$

where we have used the properties of the  $\delta^+$  function. Using the new form of the Hamiltonian one can write down the explicit form of Hamilton's equations

$$\dot{\mathbf{d}}(\mathbf{x}) = \nabla \times (\mathbf{b} - \mathbf{m}), \quad (4.28)$$

$$\dot{\mathbf{b}}(\mathbf{x}) = -\nabla \times (\mathbf{d} - \mathbf{p}), \quad (4.29)$$

$$\begin{aligned} \gamma_0 \partial_0 \psi_p(\mathbf{x}) = & \boldsymbol{\gamma} \cdot \nabla \psi_p(\mathbf{x}) + m\psi_p(\mathbf{x}) + ie \int_0^x d\xi \cdot \mathbf{d}(\boldsymbol{\xi}) \gamma^0 \psi_p(\mathbf{x}) \\ & - ie \int_0^x d\xi \cdot \mathbf{p}^{\perp}(\boldsymbol{\xi}) \gamma^0 \psi(\mathbf{x}) + ie \int_0^x d\xi^j \frac{\partial \xi^k}{\partial x^m} \varepsilon^{ijk} b^i(\boldsymbol{\xi}) \gamma^m \psi_p(\mathbf{x}) \\ & - e^2 \int d^3\mathbf{z} (\bar{\psi}_p(\mathbf{z}) \gamma^0 \psi_p(\mathbf{z})) (4\pi|\mathbf{z} - \mathbf{x}|)^{-1} \gamma^0 \psi_p(\mathbf{x}) \\ & - ie^2 Z (4\pi|\mathbf{x}|)^{-1} \gamma^0 \psi_p(\mathbf{x}). \end{aligned} \quad (4.30)$$

The equation for  $\bar{\psi}_p$  can be obtained by conjugation of (4.30). In the non-relativistic limit of the equation (4.30) one can show that the term with the field  $\mathbf{b}$  describes interaction of  $\mathbf{b}$  with the orbital and spin angular momentum.

The equations (4.28)–(4.30) agree with the equations (2.16), (2.27) and (2.28) for the Lagrangian formalism. The last two terms of (4.30) can be written together as

$$-ie \int_0^x d\xi \cdot \mathbf{p}^{\parallel}(\boldsymbol{\xi}) \gamma^0 \psi(\mathbf{x}), \quad (4.31)$$

whereas

$$\mathbf{e}(\mathbf{x}) = \mathbf{d}(\mathbf{x}) - \mathbf{p}^{\perp}(\mathbf{x}) - \mathbf{p}^{\parallel}(\mathbf{x}). \quad (4.32)$$

The quantisation of the theory can be performed by associating the Poisson brackets of the canonical variables with commutators. The structure of the general definition of the Poisson brackets gives the following set of non-vanishing commutators and anticommutators

$$[\mathbf{b}_i(\mathbf{x}), \mathbf{d}_j(\mathbf{y})] = i\varepsilon_{ijk} \partial/\partial \mathbf{x}_k \delta(\mathbf{x} - \mathbf{y}) \quad (4.33)$$

$$[\psi_p(\mathbf{x}), \bar{\psi}_p(\mathbf{y})]_{+} = i\gamma^0 \delta(\mathbf{x} - \mathbf{y}). \quad (4.34)$$

One should stress here that the commutators of the spinors with  $\mathbf{d}$  and  $\mathbf{b}$  are zero. It is a clear contradistinction of this formulation with that of Mandelstam, where the EM field variables were not commuting with the spinors.

As a consistency requirement for the sign of the anticommutators one can demand that the Heisenberg picture equations, calculated with the ordering of the Hamiltonian as in (4.27), should be formally identical with the Hamilton equations.

The discussion presented in this section shows that the fields  $\mathbf{b}$  and  $\mathbf{d}$  are the canonical variables for the EM field. For the spinors we have  $\psi_p$  and  $\bar{\psi}_p$ . The fields  $\mathbf{d}$ ,  $\psi_p$  and  $\bar{\psi}_p$  are path dependent. The multipolar Hamiltonian should be expressed in terms of these fields, rather than  $\mathbf{b}$  and  $\mathbf{e}^\perp$  plus the spinors, as it is often done. The formalism is gauge independent from the outset.

### 5. Comparison with the Coulomb gauge formulation

QED of atoms and molecules is usually formulated in the Coulomb gauge. In this gauge the electric field is split into its longitudinal  $\mathbf{e}^\parallel$  and transversal part  $\mathbf{e}^\perp$ , i.e.

$$\mathbf{e}(\mathbf{x}) = \mathbf{e}^\perp(\mathbf{x}) + \mathbf{e}^\parallel(\mathbf{x}), \tag{5.1}$$

which are defined by the equations

$$\dot{\mathbf{a}}(\mathbf{x}) = \mathbf{e}^\perp(\mathbf{x}) \tag{5.2}$$

$$\text{div } \mathbf{e}^\parallel(\mathbf{x}) = \rho(\mathbf{x}). \tag{5.3}$$

Equation (5.3) has many solutions. However we choose the longitudinal one which enables us to express the Coulomb energies by

$$\frac{1}{2} \int d^3\mathbf{x} \mathbf{e}^\parallel(\mathbf{x}) \cdot \mathbf{e}^\parallel(\mathbf{x}). \tag{5.4}$$

The transverse field is expressed by a Fourier decomposition into creation and annihilation operators, i.e. by (5.2) and

$$\mathbf{a}(\mathbf{x}) = \sum_{\lambda=1}^2 \int d^3\mathbf{k} (2k(2\pi)^3)^{-1/2} \boldsymbol{\epsilon}_\lambda(\mathbf{k}) a_\lambda(\mathbf{k}) \exp(i\mathbf{k} \cdot \mathbf{x}) + a_\lambda^\dagger(\mathbf{k}) \exp(-i\mathbf{k} \cdot \mathbf{x}). \tag{5.5}$$

The symbols used here have their standard meaning, e.g. Kroll (1968). For the creation and annihilation operators we have

$$[a_\lambda(\mathbf{k}), a_{\lambda'}^\dagger(\mathbf{k}')] = \delta_{\lambda\lambda'} \delta^{(3)}(\mathbf{k} - \mathbf{k}'), \tag{5.6}$$

$$[a_\lambda(\mathbf{k}), a_\lambda(\mathbf{k}')] = [a_\lambda^\dagger(\mathbf{k}), a_\lambda^\dagger(\mathbf{k}')] = 0. \tag{5.7}$$

The Power-Zienau type transformation leading to the multipolar version of the theory is given by

$$U = \exp\left(i \int d^3\mathbf{x} \mathbf{p}(\mathbf{x}) \cdot \mathbf{a}(\mathbf{x})\right) \tag{5.8}$$



with  $\mathbf{p}(\mathbf{x})$  defined by the formula (4.25), with  $\bar{\psi}_p$  and  $\psi_p$  now replaced by the path-independent Coulomb gauge spinor operators. The relation between the path-dependent and Coulomb gauge variables is given by

$$\mathbf{d}(\mathbf{x}) = U\mathbf{e}^\perp(\mathbf{x})U^{-1} = \mathbf{e}^\perp(\mathbf{x}) + \mathbf{p}^\perp(\mathbf{x}), \tag{5.9}$$

$$\psi_p(\mathbf{x}) = U\psi(\mathbf{x})U^{-1}, \tag{5.10}$$

$$\bar{\psi}_p(\mathbf{x}) = U\bar{\psi}(\mathbf{x})U^{-1}. \tag{5.11}$$

The spinor operators of the path-dependent theory are marked by the letter  $p$ , to distinguish them from the Coulomb gauge ones.

When adopting the notion of canonical transformations to quantum mechanics, one must be very careful in order to avoid confusion. In the author's view one should comply with the remarks of Dirac (1958). The analogy between the canonical transformations in classical mechanics and the unitary transformations in quantum mechanics is that both are applied to the canonical variables of the theories. The Hamiltonian, for the time-independent transformations, is left intact, but re-expressed in the new variables. Many authors treat the unitary transformation  $H' = U^{-1}HU$  as a canonical transformation. Such an approach demands great care, because with this transformation is associated a change in the Heisenberg equations of motion, i.e.

$$[q, U^{-1}HU] \neq [q, H] = \dot{q} \tag{5.13}$$

(see e.g. Mandel (1979) and the comments listed in the introduction).

In the perturbation calculus we split the total Hamiltonian into a 'free'  $H_0$  part and an interaction part  $H_{INT}$ . The  $H_0$  is always a simple one, and in the case of the Coulomb gauge it reads

$$H_0 = \int d^3x \left[ \left( \frac{1}{2} \mathbf{e}^{\perp 2}(\mathbf{x}) + \frac{1}{2} \mathbf{b}^2(\mathbf{x}) \right) + \bar{\psi}(\mathbf{x}) \boldsymbol{\gamma} \cdot \nabla \psi(\mathbf{x}) \right. \\ \left. + m\bar{\psi}(\mathbf{x})\psi(\mathbf{x}) - iZe^2(4\pi|\mathbf{x}|)^{-1} \bar{\psi}(\mathbf{x}) \boldsymbol{\gamma}^0 \psi(\mathbf{x}) \right] \tag{5.14}$$

(for the Furry picture). It is clear that  $UH_0U^{-1}$  should be used as a new 'free' part  $H'_0$  for the path-dependent case. It has the same form as (5.14) with  $\mathbf{e}^\perp$ ,  $\bar{\psi}$  and  $\psi$  replaced by  $\mathbf{d}$ ,  $\bar{\psi}_p$  and  $\psi_p$ . The eigenstates of the respective 'free' Hamiltonian will be denoted as  $|s\rangle$  and  $|s'\rangle$ .

When interpreting the relation between both formulations one should also note that the definition of the photon is not identical for both cases. The Coulomb gauge transverse field is given by

$$\mathbf{e}^\perp(\mathbf{x}) = i \sum_{\lambda=1}^2 \int d^3\mathbf{k} \sqrt{k} (2(2\pi)^3)^{-1/2} \hat{\mathbf{e}}_\lambda(\mathbf{k}) (a_\lambda(\mathbf{k}) \exp(i\mathbf{k} \cdot \mathbf{x}) \\ - a_\lambda^\dagger(\mathbf{k}) \exp(-i\mathbf{k} \cdot \mathbf{x})). \tag{5.15}$$

For the path-dependent description we have a different situation. The field  $\mathbf{e}(\mathbf{x})$  is split in the following way

$$\mathbf{e}(\mathbf{x}) = \mathbf{d}(\mathbf{x}) - \mathbf{p}(\mathbf{x}) \tag{5.16}$$

where  $-\mathbf{p}(\mathbf{x})$ , just as the field  $\mathbf{e}^\parallel(\mathbf{x})$ , is a solution of the equation

$$\text{div}(-\mathbf{p}(\mathbf{x})) = \rho(\mathbf{x}) \tag{5.17}$$

but this time given by the path-dependent form (4.25). The field  $d(\mathbf{x})$  can be expressed by redefined creation and annihilation operators

$$d(\mathbf{x}) = i \sum_{\lambda=1}^2 \int d^3\mathbf{k} \sqrt{k} (2(2\pi)^3)^{-1/2} \hat{\epsilon}_\lambda(\mathbf{k}) (a'_\lambda(\mathbf{k}) \exp(i\mathbf{k} \cdot \mathbf{x}) - a'^{+\lambda}(\mathbf{k}) \exp(-i\mathbf{k} \cdot \mathbf{x})), \quad (5.18)$$

where

$$a'_\lambda(\mathbf{k}) = U a_\lambda(\mathbf{k}) U^{-1} = a_\lambda(\mathbf{k}) - e [2k(2\pi)^3]^{-1/2} \int d^3z \int_0^z d\xi \cdot \hat{\epsilon}_\lambda(\mathbf{k}) \times \exp(-i\mathbf{k} \cdot \boldsymbol{\xi}) \bar{\psi}_p(\mathbf{z}) \gamma^0 \psi_p(\mathbf{z}), \quad (5.19)$$

and

$$a'^{+\lambda}(\mathbf{k}) = U a_\lambda^+(\mathbf{k}) U^{-1} = (a'_\lambda(\mathbf{k}))^+. \quad (5.20)$$

The equations (5.18)–(5.19) show that the word ‘photon’ has, at least formally, different meaning for both theories. As it was pointed out by Rzążewski (1978) and Rzążewski and Żakowicz (1980) the state of photon vacuum, for the non-interacting fields, is associated with a different total electric field, i.e.

$$\langle 0 | e(\mathbf{x}) | 0 \rangle \neq \langle 0' | e(\mathbf{x}) | 0' \rangle. \quad (5.21)$$

Nevertheless, Healy and Wooley (1978) have shown that the  $S$ -matrix elements, which one obtains with the use of the multipolar path-dependent Hamiltonian of point charges are equivalent to those for the Coulomb Hamiltonian. The proof was up to the order  $e^2$ , and can be easily rewritten for the spinor QED. However, in their approach the equivalence means that processes  $|i\rangle \rightarrow |f\rangle$  and  $|i'\rangle = U|i\rangle \rightarrow |f'\rangle = U|f\rangle$  have the same  $S$ -matrix elements. The authors did not give any clear interpretation of the relation between the eigenstates of the different ‘free’ Hamiltonians.

The equivalence of the  $S$ -matrices up to all orders in perturbation theory was shown by Haller and Landovitz (1970). However, this has been done in a different context. Since the derivation given in this work was quite general it has been applied to the problem which we discuss here by Haller and Sohn (1979), see also Aharonov and Au (1979). However, the equivalence has been shown only up to the interpretation questions mentioned in the previous paragraph.

These difficulties are associated with the unrealistic situation that the eigenstates of ‘free’ Hamiltonian describe. The photons are totally unlocalised, and the atom is decoupled from the radiation. If one introduces wavepackets for the description of photons, and works only with the eigenstates of the full Hamiltonian, these difficulties can be avoided.

In the work of Żukowski (1982) such procedure was proposed. The  $S$ -matrix theory can be based on Kroll’s (1968) adaptation of the formalism of Wick (1955). The whole derivation of Żukowski can be very easily adopted to the case discussed in this paper. The only basic difference is that now the creation and annihilation operators are given by (5.18)–(5.19). From the analysis one can conclude the eigenstates of  $H_0$  and  $U H_0 U^{-1}$  can be interpreted as completely equivalent, if they are related by  $|s'\rangle = U|s\rangle$ . For the details see Żukowski (1982).

## Acknowledgment

This work has been supported by Ministerstwo Szkolnictwa Wyższego, Nauki i Techniki, Project MR.I.7.

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