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Minimally nonlocal quantum electrodynamics without potentials for bound electrons

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Abstract. In the formulation of QED which does not use potentials the charged field ψ interacts nonlocally with the electromagnetic fields $\boldsymbol{E}$ and $\boldsymbol{H}$. The suggested formulation in the case of bound electrons has a minimally nonlocal interaction as compared with the other known formulations without potentials. Some applications of the new formulation are discussed.

1. Introduction

As is well known, one ought to use the Coulomb gauge and not the Lorentz one when considering bound electrons (see e.g. Heitler 1954). The Coulomb gauge is an example of the QED formulations in which the charged field ψ interacts nonlocally with the electromagnetic fields $\boldsymbol{E}$ and $\boldsymbol{H}$, and the gauge group is absent. Indeed, the transverse potential $\boldsymbol{A}_\perp$ can be replaced by

$$\boldsymbol{A}_\perp(\boldsymbol{x}) = \frac{1}{4\pi}\int \mathrm{d}^3 y \, \frac{\operatorname{rot} \boldsymbol{H}(\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|} \tag{1}$$

(see Belinfante 1962). Other formulations of this type are given in e.g. DeWitt (1962), Mandelstam (1962) and Ogievetsky *et al* (1962). They can be characterised as formulations without potentials (WP formulations).

All these formulations are strongly nonlocal theories. Thus, in the Coulomb gauge, both the Coulomb interaction of the charges and their interaction with the magnetic field by means of (1) can be characterised by the 'form factor' $1/|\boldsymbol{x}-\boldsymbol{y}|$ which has infinite range. An analogous situation holds in other WP formulations (see § 2 below).

We suggest in § 2 one more WP form of QED which, for bound charges, turns out to be the least nonlocal as compared with all the known WP formulations. Its range of nonlocality coincides with the bound-charge localisation region.

Some variants and generalisations of the new form are given in § 3. Possible applications and connections with other approaches are discussed in § 4.

In the Appendix we stress a difference between the DeWitt (1962) and Mandelstam (1962) approaches which is essential for the derivation of the important equation (8).

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2. Minimally nonlocal WP form of the QED

2.1.

The new form will be constructed starting with the Coulomb gauge. The electrons and positrons will be described by the new spinor field

$$\psi'(\boldsymbol{x}) = \psi(\boldsymbol{x}) \exp\left(-ie \int_{\boldsymbol{r}}^{\boldsymbol{x}} (\boldsymbol{A}_\perp \cdot \mathrm{d}\boldsymbol{\xi})\right). \tag{2}$$

Here ψ, $\boldsymbol{A}_\perp$, ψ' are the Schrödinger operators, the integral

$$\int (\boldsymbol{A}_\perp \cdot \mathrm{d}\boldsymbol{\xi}) = \int [A_{\perp x}(\boldsymbol{\xi})\, \mathrm{d}\xi_x + A_{\perp y}(\boldsymbol{\xi})\, \mathrm{d}\xi_y + A_{\perp z}(\boldsymbol{\xi})\, \mathrm{d}\xi_z]$$

is taken along the straight line connecting a point $\boldsymbol{r}$ with the point $\boldsymbol{x}$. We set $c = 1$ and $h = 1$. A new element $\boldsymbol{r}$ is introduced in the theory by (2). If electrons of the physical system under construction are localised somehow in a certain volume V, then one can take for $\boldsymbol{r}$ the centre of V. An external potential U is introduced in the theory to produce such a localisation.

Constructions of the type (2) are known, see e.g. Dirac (1934, 1955), Capps *et al* (1955), DeWitt (1962) and Mandelstam (1962). But here the purpose of (2) is not to obtain the gauge-invariant charge field (both ψ and ψ' in (2) are such fields), the intention of (2) is to get a less nonlocal WP theory†.

2.2.

We shall represent (2) as a canonical transformation of the type $\psi' = S^\dagger \psi S$ and introduce, besides ψ', new operators $\boldsymbol{E}'$, $\boldsymbol{H}'$ for the photons. Then the equal-time commutators for ψ', $\boldsymbol{E}'$, $\boldsymbol{H}'$ will be the same as for ψ, $\boldsymbol{E}$, $\boldsymbol{H}$ and new electron operators will be independent of the (new) photon operators. Let

$$S = \exp\left(-ie \int \mathrm{d}^3x' \rho(\boldsymbol{x}') \int_{\boldsymbol{r}}^{\boldsymbol{x}'} (\boldsymbol{A}_\perp \cdot \mathrm{d}\boldsymbol{\xi})\right). \tag{3}$$

Here $\rho = \psi^\dagger \psi$ is the charge density, the integral $\int \mathrm{d}^3x'$ is over the whole space. With the help of the equation

$$\mathrm{e}^A B \mathrm{e}^{-A} = B + [A, B] + \tfrac{1}{2}[A, [A, B]] + \ldots \tag{4}$$

one can verify that the equation $\psi' = S^\dagger \psi S$ (calculated by means of the equal-time commutators) coincides with (2). We have $\boldsymbol{A}'_\perp = \boldsymbol{A}_\perp$ and $\boldsymbol{H}' = \boldsymbol{H}$ so that S changes, besides ψ, only the electric transverse field $\boldsymbol{E}_\perp$

$$E'_{\perp m}(\boldsymbol{x}) = S^\dagger E_{\perp m} S = E_{\perp m} + e \int \mathrm{d}^3x' \rho(\boldsymbol{x}') \int_{\boldsymbol{r}}^{\boldsymbol{x}'} \sum_n \mathrm{d}\xi_n\, \mathrm{d}\xi_n \delta^{\mathrm{tr}}_{nm}(\boldsymbol{\xi} - \boldsymbol{x}) \tag{5}$$

† Our motive for (2) can be described in terms which will be introduced in § 4: we look for the quasigradient-invariant charge field (see (27) below).

where $m, n = 1, 2, 3$. To obtain (5) we use (4) and the commutator

$$[A_{\perp k}(\boldsymbol{y}), E_{\perp m}(\boldsymbol{x})]$$

$$= -\mathrm{i}\delta^{\mathrm{tr}}_{km}(\boldsymbol{y}-\boldsymbol{x}) \equiv -\mathrm{i}\left(\delta_{km}\delta^{(3)}(\boldsymbol{y}-\boldsymbol{x}) - \frac{1}{4\pi}\frac{\partial}{\partial y_k}\frac{\partial}{\partial x_m}\frac{1}{|\boldsymbol{y}-\boldsymbol{x}|}\right), \tag{6}$$

see e.g. (14.17) in Bjorken and Drell (1965).

2.3.

Now our aim is to rewrite the Coulomb gauge Hamiltonian H in terms of the new operators. We take H from § 15.2 in Bjorken and Drell (1965):

$$H = \tfrac{1}{2}\int \mathrm{d}^3x\,(\boldsymbol{H}^2(\boldsymbol{x}) + \boldsymbol{E}_\perp^2(\boldsymbol{x})) + \int \mathrm{d}^3x\,\psi^\dagger(\boldsymbol{x})[\boldsymbol{\alpha}(-\mathrm{i}\boldsymbol{\nabla} - e\boldsymbol{A}_\perp(\boldsymbol{x})) + \beta m]\psi(\boldsymbol{x})$$

$$+ \frac{e^2}{8\pi}\int \mathrm{d}^3x \int \mathrm{d}^3x' \frac{\rho(\boldsymbol{x})\rho(\boldsymbol{x}')}{|\boldsymbol{x}-\boldsymbol{x}'|} - e\int \mathrm{d}^3x\,\psi^\dagger(\boldsymbol{x})\gamma_0\gamma_\mu U_\mu(\boldsymbol{x})\psi(\boldsymbol{x}). \tag{7}$$

The last term contains the external potential U, see above. In appendix A the following equation is derived:

$$\frac{\partial}{\partial x_k}\int_r^x (\boldsymbol{A}_\perp \cdot \mathrm{d}\boldsymbol{\xi}) = A_{\perp k}(\boldsymbol{x}) - \mathscr{A}_k(\boldsymbol{x}) \tag{8}$$

$$\mathscr{A}(\boldsymbol{x}) \equiv -\int_0^1 \alpha\,\mathrm{d}\alpha\,(\boldsymbol{x}-\boldsymbol{r}) \times \boldsymbol{H}(\boldsymbol{r} + \alpha(\boldsymbol{x}-\boldsymbol{r})) \tag{9}$$

($\times$ means the vector product). Using (8) we get

$$\boldsymbol{\nabla}\psi'(\boldsymbol{x}) = \exp\left(-\mathrm{i}e\int_r^x (\boldsymbol{A}_\perp \cdot \mathrm{d}\boldsymbol{\xi})\right)[\boldsymbol{\nabla} - \mathrm{i}e(\boldsymbol{A}_\perp - \mathscr{A})]\psi(\boldsymbol{x}). \tag{10}$$

Let us multiply both sides of (10) by $\psi'^\dagger = \psi^\dagger \exp(\mathrm{i}e\int)$ and write the result in the form

$$\psi^\dagger(-\mathrm{i}\boldsymbol{\nabla} - e\boldsymbol{A}_\perp(\boldsymbol{x}))\psi = \psi'^\dagger(-\mathrm{i}\boldsymbol{\nabla} - e\mathscr{A}(\boldsymbol{x}))\psi'. \tag{11}$$

Further using (5), (6) and the equation $\operatorname{div} \boldsymbol{E}'_\perp = 0$ we obtain

$$\int \boldsymbol{E}_\perp^2(\boldsymbol{x})\,\mathrm{d}^3x$$

$$= \int \boldsymbol{E}_\perp'^2(\boldsymbol{x})\,\mathrm{d}^3x - 2e\int \rho(\boldsymbol{y})\,\mathrm{d}^3y \int_r^y (\boldsymbol{E}'_\perp(\boldsymbol{\xi}) \cdot \mathrm{d}\boldsymbol{\xi})$$

$$+ e^2 \iint \mathrm{d}^3y\,\mathrm{d}^3y'\,\rho(\boldsymbol{y})\rho(\boldsymbol{y}') \int_r^y \int_r^{y'} \delta^{(3)}(\boldsymbol{\xi}-\boldsymbol{\xi}')(\mathrm{d}\boldsymbol{\xi} \cdot \mathrm{d}\boldsymbol{\xi}')$$

$$- \frac{e^2}{4\pi}\iint \mathrm{d}^3y\,\mathrm{d}^3y'\frac{\rho(\boldsymbol{y})\rho(\boldsymbol{y}')}{|\boldsymbol{y}-\boldsymbol{y}'|} + 2\int \mathrm{d}^3y \frac{Qe\rho(\boldsymbol{y})}{4\pi|\boldsymbol{y}-\boldsymbol{r}|} - \frac{Q^2}{4\pi|\boldsymbol{r}-\boldsymbol{r}|}. \tag{12}$$

Here $Q \equiv e\int \mathrm{d}^3x\psi'^\dagger(\boldsymbol{x})\psi'(\boldsymbol{x})$ is the total-charge operator. The next to last term is the Coulomb interaction of the electron field with a point charge of magnitude Q at point $\boldsymbol{r}$. The last term is infinite and describes the Coulomb self-interaction of this charge. It will be omitted for the same reason as the Coulomb self-interaction in the Coulomb gauge.

2.4.

Inserting (11) and (12) into (7) one gets the desired expression for H in terms of ψ', $\boldsymbol{E}'_\perp$, $\boldsymbol{H}' = \boldsymbol{H}$:

$$H = \tfrac{1}{2}\int \mathrm{d}^3x(\boldsymbol{H}'^2 + \boldsymbol{E}'^2_\perp) + \int \mathrm{d}^3x\, \psi'^\dagger[\boldsymbol{\alpha}(-\mathrm{i}\boldsymbol{\nabla} - e\mathscr{A}) + \beta m]\psi'$$
$$- e\int \rho(\boldsymbol{x})\,\mathrm{d}^3x \int_r^x (\boldsymbol{E}'_\perp \cdot \mathrm{d}\boldsymbol{\xi}) - e\int \mathrm{d}^3x\, \psi'^\dagger \gamma_0\gamma_\mu U_\mu \psi'$$
$$+ \tfrac{1}{2}e^2 \iint \mathrm{d}^3x\, \mathrm{d}^3x'\, \rho(\boldsymbol{x})\rho(\boldsymbol{x}') \int_r^x \int_r^{x'} \delta^{(3)}(\boldsymbol{\xi} - \boldsymbol{\xi}')(\mathrm{d}\boldsymbol{\xi} \cdot \mathrm{d}\boldsymbol{\xi}')$$
$$+ \int \frac{Qe\rho(\boldsymbol{x})\,\mathrm{d}^3x}{4\pi|\boldsymbol{x} - \boldsymbol{r}|}. \tag{13}$$

The Coulomb interaction term in (7) disappears (it is cancelled by the fourth term of (12)) and the last two terms in (13) substitute for it. The field ψ' interacts with the magnetic field by means of $\mathscr{A}(\boldsymbol{x})$, see (9), and with the transverse electric field $\boldsymbol{E}'_\perp$ by means of

$$e\int \rho(\boldsymbol{x})\,\mathrm{d}^3x \int_r^x (\boldsymbol{E}'_\perp(\boldsymbol{\xi}) \cdot \mathrm{d}\boldsymbol{\xi})$$
$$= e\int \rho(\boldsymbol{x})\,\mathrm{d}^3x \int_0^1 \mathrm{d}\alpha\, (\boldsymbol{x} - \boldsymbol{r}) \cdot \boldsymbol{E}'_\perp(\boldsymbol{r} + \alpha(\boldsymbol{x} - \boldsymbol{r})). \tag{14}$$

Both these interactions are nonlocal: $\psi'(\boldsymbol{x})$ interacts with $\boldsymbol{H}'(\xi)$ and $\boldsymbol{E}'_\perp(\xi)$ taken at the points $\boldsymbol{\xi}$ of the straight line, connecting $\boldsymbol{x}$ with $\boldsymbol{r}$. If the electrons are localised in a volume V, the region of nonlocality is confined to V.

In the De Witt (1962) formulation, the charge field at the point $\boldsymbol{x}$ interacts with $\boldsymbol{E}$ and $\boldsymbol{H}$ taken at the points of a line going from $\boldsymbol{x}$ to infinity. The Mandelstam (1962) formulation has the same type of nonlocality (see, e.g., his equations (3.11)). The Coulomb gauge nonlocality was characterised in § 1.

The WP formulations by Ogievetsky and Polubarinov (1962), Levy (1964) and Rohrlich and Strocchi (1965) are still more nonlocal (not only in space but also in time).

So, in the form of QED obtained, the interaction is minimally nonlocal as compared with the other WP forms and it seems that still less nonlocal forms do not exist. We conclude this section with two notes.

2.5.

The relation between ψ', $\mathscr{A}$ and ψ, $\boldsymbol{A}_\perp$ can be written in the form of the (operator) gauge transformation

$$\psi' = \psi(\boldsymbol{x}, t)\exp(\mathrm{i}e\Lambda(\boldsymbol{x}, t)), \qquad \mathscr{A}(\boldsymbol{x}, t) = \boldsymbol{A}_\perp(\boldsymbol{x}, t) + \boldsymbol{\nabla}\Lambda(\boldsymbol{x}, t)$$
$$\Lambda(\boldsymbol{x}, t) \equiv -\int_r^x (\boldsymbol{A}_\perp(\xi, t) \cdot \mathrm{d}\boldsymbol{\xi}). \tag{15}$$

Indeed, (15) is merely equations (2) and (8) written in terms of the Heisenberg

operators. Note that the total electric field is the same in the new and the Coulomb gauge but in the former it should be expressed in terms of $\boldsymbol{E}'_\perp$: $\boldsymbol{E}_\perp$ in $\boldsymbol{E} = \boldsymbol{E}_\perp - \nabla \int [\mathrm{d}^3 y\, \rho(\boldsymbol{y})/(4\pi|\boldsymbol{x}-\boldsymbol{y}|)]$ must be replaced by $\boldsymbol{E}'_\perp$ using (5). Instead of the condition $\operatorname{div} \boldsymbol{A}_\perp = 0$ the new gauge is characterised by the equation

$$\int_r^x (\mathscr{A}(\boldsymbol{\xi}) \cdot \mathrm{d}\boldsymbol{\xi}) = 0, \qquad \forall \boldsymbol{x}. \tag{16}$$

It can be verified by taking the integral (16) of the equation $\mathscr{A} = \boldsymbol{A}_\perp + \nabla\Lambda$ (see (15)) or of (9).

2.6.

Let us show that the results of calculations with (13) do not depend upon the parameter $\boldsymbol{r}$, which is explicitly present in the interaction terms of (13). Consider the interaction term (14).

As the commutators between ψ', $\boldsymbol{E}'_\perp$, $\boldsymbol{H}'$ are the same as in the Coulomb gauge we can assume for ψ', $\boldsymbol{E}'_\perp$, $\boldsymbol{H}'$ the usual expansion in the creation–annihilation operators of the electron–positrons pairs a', $a'^\dagger$, b', $b'^\dagger$ and the transverse photons c', $c'^\dagger$. Of course, (2) means that a', $a'^\dagger$, when expanded over the Coulomb gauge operators, will contain old photon operators c, $c^\dagger$.

For ψ' we must use the expansion over the proper functions of the Dirac equation Hamiltonian with the external potential U. They depend in fact upon $\boldsymbol{x}-\boldsymbol{r}$, if $\boldsymbol{r}$ is a centre of U. Therefore the matrix element $\langle|\rho|\rangle$ of the operator $\rho(\boldsymbol{x})$ in (14) should depend upon $\boldsymbol{x}-\boldsymbol{r}$: $\langle|\rho|\rangle \equiv M(\boldsymbol{x}-\boldsymbol{r})$. The integral

$$\int \mathrm{d}^3 x\, M(\boldsymbol{x}-\boldsymbol{r}) \int_0^1 \mathrm{d}\alpha\, (\boldsymbol{x}-\boldsymbol{r}) \cdot \boldsymbol{E}'_\perp(\boldsymbol{r} + \alpha(\boldsymbol{x}-\boldsymbol{r})) \tag{17}$$

after the variable change $\boldsymbol{x}' = \boldsymbol{x} - \boldsymbol{r}$ turns into

$$\int \mathrm{d}^3 x'\, M(\boldsymbol{x}') \int_0^1 \mathrm{d}\alpha\, \boldsymbol{x}' \cdot \boldsymbol{E}'_\perp(\boldsymbol{r} + \alpha\boldsymbol{x}). \tag{18}$$

The operator $\boldsymbol{E}'_\perp(\boldsymbol{x})$ can be expanded not over $\exp(\mathrm{i}\boldsymbol{\kappa}_0\boldsymbol{x})$ but over $\exp[\mathrm{i}\boldsymbol{\kappa}_0(\boldsymbol{x}-\boldsymbol{r})]$:

$$\boldsymbol{E}'_\perp(\boldsymbol{x}) = \frac{\mathrm{i}}{(2\pi)^{3/2}} \int \mathrm{d}^3\kappa \sum_{\lambda=1,2} (\tfrac{1}{2}\kappa)^{1/2} \boldsymbol{e}_\lambda(\kappa)(\mathrm{e}^{\mathrm{i}\boldsymbol{\kappa}_0(\boldsymbol{x}-\boldsymbol{r})} c'(\boldsymbol{\kappa}, \lambda) - \mathrm{HC}). \tag{19}$$

This expansion is convenient for calculations in the dipole approximation, when $\boldsymbol{E}'_\perp(\boldsymbol{\xi})$ in (14) or in (18) is replaced by $\boldsymbol{E}'_\perp(\boldsymbol{r})$. As the left-hand side of (19) does not depend upon $\boldsymbol{r}$, we must assume that $c'(\boldsymbol{\kappa}, \lambda)$ in the right-hand side does depend upon $\boldsymbol{r}$. If the expansion (19) is adopted, $\boldsymbol{E}'_\perp(\boldsymbol{r} + \alpha\boldsymbol{x}')$ will depend upon $\boldsymbol{r}$ only via $c'(\boldsymbol{\kappa}, \lambda)$. We see that matrix elements of (14) do not depend explicitly upon $\boldsymbol{r}$. Its implicit $\boldsymbol{r}$-dependence through the creation–annihilation operators does not influence the result if one chooses for these operators the same Fock representation, irrespective of concrete values of $\boldsymbol{r}$.

The consideration is applicable for all other $\boldsymbol{r}$-dependent terms of (13). So, the physical consequences of (13) do not depend upon $\boldsymbol{r}$ as they should for isolated physical systems.

3. Modifications and generalisations

3.1.

Instead of taking $\int \boldsymbol{A}_\perp \cdot \mathrm{d}\boldsymbol{\xi}$ along the straight line we may integrate along a curved path. But the theory then acquires additional parameters besides $\boldsymbol{r}$, e.g. the path curvature.

3.2.

The points $\boldsymbol{\xi}$ in $\int \boldsymbol{A}_\perp(\boldsymbol{\xi}) \cdot \mathrm{d}\boldsymbol{\xi}$ have the same time coordinates. Space-like paths can be introduced. But this generalisation would look more natural if one were to obtain the new form from the covariant Lorentz gauge rather than from the Coulomb one. Starting with the former would have both virtues and demerits, the latter being related to dealing with the Lorentz condition $\partial_\mu A_\mu \Phi = 0$.

3.3.

One can perform an averaging over a set of points $\boldsymbol{r}$. For this purpose one can insert $\int \mathrm{d}^3 r\, m(\boldsymbol{r})$ in front of the integral $\int_{\boldsymbol{r}}^{\boldsymbol{x}}$ in each place in § 2 where $\int_{\boldsymbol{r}}^{\boldsymbol{x}}$ appears. The measure function $m(\boldsymbol{r})$ must be normalised to unity. If the averaging set is in the electron localisation region V, the minimal nonlocality of the interaction will not be spoiled. In particular, one can assume the boundary of V to be this set. If one averages uniformly over the minimal sphere containing V, the last term in (13) turns into Q^2/R, R being the sphere radius. It becomes a c-number, in fact, and can be omitted. So, the interaction of the electrons with the fictitious charge Q vanishes if Q is spread over the sphere. It is possible to show that when $R \to \infty$ the transformation S (see (3)) tends to 1, and the new form turns into the Coulomb gauge.

3.4. Mixed gauge

The integral over $\boldsymbol{x}'$ in (3) is taken over the finite volume V, where the electrons are localised, rather than over the whole space. In this case the Hamiltonian density has a different appearance outside and inside V.

3.5.

The electrons can be localised not in one but in several disjoint regions $V_1, V_2, \ldots$. Then the minimally nonlocal form will be obtained by dividing the whole space into the parts $W_1, W_2, \ldots$ such that $V_n \subset W_n$ (and $\Sigma\, W_n$ is all space) and putting

$$S = \exp\left(-\mathrm{i}e \int_{W_n} \mathrm{d}^3 x\, \rho(\boldsymbol{x}) \int_{\boldsymbol{r}_n}^{\boldsymbol{x}} (\boldsymbol{A}_\perp \cdot \mathrm{d}\boldsymbol{\xi})\right)$$

if one transforms a field at the point $\boldsymbol{x} \in W_n$ ($\boldsymbol{r}_n$ is a centre of V_n). The other form for S is

$$S = \exp\left(-\mathrm{i}e \int \mathrm{d}^3 x \sum_n \Pi_n \rho(\boldsymbol{x}) \int_{\boldsymbol{r}_n}^{\boldsymbol{x}} (\boldsymbol{A}_\perp \cdot \mathrm{d}\boldsymbol{\xi})\right) \tag{20}$$

where $\Pi_n = 1$ if $\boldsymbol{x} \in W_n$ and $\Pi_n = 0$ if $\boldsymbol{x}$ is out of W_n. The following different definition of Π_n is possible: $\Pi_n = 1$ if $\boldsymbol{x} \in V_n$ and $\Pi_n = 0$ if $\boldsymbol{x} \notin V_n$. In this case a generalisation of § 3.4 is obtained.

3.6.

Quantum electrodynamics with several charged fields. If one has two fields, electron ψ_e and proton ψ_p, then

$$S = \exp\left(-ie \int d^3x(\rho_e(x) - \rho_p(x)) \int_r^x (\boldsymbol{A}_\perp \cdot d\boldsymbol{\xi})\right). \tag{21}$$

This form of S gives minimally nonlocal interaction when both electrons and protons are localised in the same region V (e.g. in a crystal).

4. Applications

We discuss applications of the new form, taking as an example one nonrelativistic spinless charged particle (the name 'electron' will be retained) interacting with the quantised electromagnetic field. The Coulomb gauge Hamiltonian is

$$H = (\boldsymbol{p} - e\boldsymbol{A}_\perp(\boldsymbol{q}))^2/2m + U(\boldsymbol{q} - \boldsymbol{r}) + \tfrac{1}{2}\int d^3x(\boldsymbol{H}^2 + \boldsymbol{E}_\perp^2). \tag{22}$$

The replacement $\boldsymbol{p} - e\boldsymbol{A}_\perp \to \boldsymbol{p}' - e\mathscr{A}$ (compare (11)) is accomplished by the transformation

$$S = \exp\left(-ie \int_0^q (\boldsymbol{A}_\perp \cdot d\boldsymbol{\xi})\right) \tag{23}$$

where $\boldsymbol{q}$ is the electron coordinate. When expressed in terms of $\boldsymbol{p}' = S^\dagger \boldsymbol{p} S$ and $\boldsymbol{E}'_\perp = S^\dagger \boldsymbol{E}_\perp S$ the Hamiltonian (22) is recorded as follows:

$$H = (\boldsymbol{p}' - e\mathscr{A}(\boldsymbol{q}))^2/2m + U(\boldsymbol{q} - \boldsymbol{r}) + (1/8\pi)\int d^3x(\boldsymbol{H}'^2 + \boldsymbol{E}'^2_\perp)$$
$$- e\int_r^q (\boldsymbol{E}'_\perp(\boldsymbol{\xi}) \cdot d\boldsymbol{\xi}) + \tfrac{1}{2}e^2 \sum_m \int_r^q d\xi_m \int_r^q d\xi'_m \delta^{(3)}(\boldsymbol{\xi} - \boldsymbol{\xi}') + \frac{e^2}{4\pi|\boldsymbol{q} - \boldsymbol{r}|}. \tag{24}$$

The last term is the Coulomb interaction of the electron with the fictitious charge Q, which is now equal to e (compare (13)).

4.1.

In the dipole approximation when $\boldsymbol{E}'_\perp(\boldsymbol{\xi})$ and $\boldsymbol{H}(\boldsymbol{\xi})$ in $\mathscr{A}$ (see (9)) are replaced by $\boldsymbol{E}'_\perp(\boldsymbol{r})$ and $\boldsymbol{H}(\boldsymbol{r})$ one has

$$\int_r^q (\boldsymbol{E}_\perp(\boldsymbol{\xi}) \cdot d\boldsymbol{\xi}) = \boldsymbol{E}'_\perp(\boldsymbol{r})(\boldsymbol{q} - \boldsymbol{r}), \qquad \mathscr{A} = -\tfrac{1}{2}(\boldsymbol{q} - \boldsymbol{r}) \times \boldsymbol{H}(\boldsymbol{r}). \tag{25}$$

Let $\boldsymbol{r} = 0$ in the following. If one also takes into account the next terms of the $\boldsymbol{E}'_\perp(\boldsymbol{\xi})$ and $\boldsymbol{H}(\boldsymbol{\xi})$ multipole expansions, one gets from (24) the Hamiltonian (78) of Power and Zienau (1959) (for the case of a single electron). The authors arrived at (78) from the Coulomb gauge using a unitary transformation, which can be obtained from (23) by replacing $\boldsymbol{A}_\perp(\boldsymbol{\xi})$ by its expansion in the Maclaurin series.

4.2.

The dipole–Coulomb-gauge interaction terms are effectively replaced in the new WP form by $\boldsymbol{E}'_{\perp}\boldsymbol{q}$ (the nonrelativistic electron interaction with $\boldsymbol{H}$ by means of $\mathscr{A}$, see the first term of (24), can be neglected). The interaction $\boldsymbol{E}_{\perp}\boldsymbol{q}$ became famous in connection with the problem of the hydrogen $2^2S_{1/2}$ level shape†. The shape obtained in the Lamb experiments did not agree with the usual calculation using $-\boldsymbol{pA}/m$, but did agree with the one using $\boldsymbol{Eq}$. This problem is important for the Lamb shift theory: the shift is much less than the level width and one must find the line centre precisely. Detailed discussion and references can be found in Fried (1973). It was there shown that a more accurate calculation of the level shape using $-\boldsymbol{pA}/m$ tends to agree with the $\boldsymbol{Eq}$ calculation, but the latter possesses the advantage of simplicity. Let us remind ourselves in this connection that the new and Coulomb formulations differ only by the gauge change (15). But we are going to discuss another problem where the equivalence turns out to be a more delicate question.

4.3.

Consider the physical system which is described by the Hamiltonian (22), the potential U localising the electron inside V. Let the system be in a stationary state till an external current J is switched on at an instant t_0, inside the remote region W (H acquires the additional term $\int d^3x\, JA$). Then the fields $\boldsymbol{E}$ and $\boldsymbol{H}$ change at the instant $t > t_0$ only inside the 'light front', i.e. inside the region W_t, whose boundary is at a distance $c(t-t_0)$ from the W boundary. It was shown in Shirokov (1978) that the Heisenberg operator $\boldsymbol{A}_{\perp}$ under these conditions changes outside W_t, acquiring a gradient

$$\boldsymbol{A}_{\perp}(\boldsymbol{x}, t) \to \boldsymbol{A}_{\perp}(\boldsymbol{x}, t) + \nabla\lambda(\boldsymbol{x}, t). \tag{26}$$

This 'acausal' behaviour follows from (1). The function $\lambda(\boldsymbol{x}, t)$ is harmonic, $\Delta\lambda = 0$, but only outside W_t‡. The electron momentum also changes outside W_t: $\boldsymbol{p} \to \boldsymbol{p} + e\nabla\lambda$. Note that the electron velocity $\partial q/\partial t = (p - eA(q))/m$ behaves causally (see e.g. § 3 in Shirokov (1978)) as does the quantised field ψ: $\psi \to \psi \exp(ie\lambda)$. Instead of the momentum change one can speak about the electron wavefunction change: $\phi(\boldsymbol{q}) \to \phi(\boldsymbol{q}) \exp(ie\lambda)$. These changes were called quasigradient transformations in Shirokov (1978), because they have the form of gauge (gradient) transformations but only outside W_t. They must not entail any observable effects in the region V at the insant t, if the distance R between W and V is greater than $c(t-t_0)$.

However, the transformation $\phi(\boldsymbol{q}) \to \phi(\boldsymbol{q}) \exp(ie\lambda(\boldsymbol{q}))$ does not reduce to a phase change in the momentum representation. It entails a change in the momentum distribution $|\tilde{\phi}(\boldsymbol{p})|^2$ which must also be considered as nonobservable (fictitious). At the instants t when W_t partially covers V, the $|\tilde{\phi}(\boldsymbol{p})|^2$ change turns out to be only partially fictitious. So does the electron energy distribution, if the energy operator is $\boldsymbol{p}^2/2m + U(\boldsymbol{q})$. In other words, a part of the electron excitation probability in the Coulomb gauge may be fictitious under the described conditions.

The absence of the stated difficulty is the advantage of the new WP form. For instance, when $\psi(\boldsymbol{x}) \to \psi(\boldsymbol{x}) \exp(ie\lambda(\boldsymbol{x}))$ and $\boldsymbol{A}_{\perp}(\boldsymbol{x}) \to \boldsymbol{A}_{\perp}(\boldsymbol{x}) + \nabla\lambda(\boldsymbol{x})$ the operator ψ' (see

† The $\boldsymbol{Eq}$ interaction was known long ago, but for the case when $\boldsymbol{E}$ is an external field (not quantised as in Power and Zienau (1959) and here). In particular, it was used in the Stark effect calculation. This case has also been discussed in the recent papers by Kuo (1976) and Forney *et al* (1977).

‡ If λ were harmonic everywhere and $\boldsymbol{A}_{\perp}$ is to vanish at infinity, then $\nabla\lambda = 0$ everywhere. For this reason the gauge group is absent in the Coulomb gauge.

(2)) acquires only the phase multiplier which does not depend upon $\boldsymbol{x}$

$$\psi'_{(\boldsymbol{x})} \to \psi'_{(\boldsymbol{x})} \exp(\mathrm{i}e\lambda(\boldsymbol{r})). \tag{27}$$

This transformation changes neither the coordinate nor the momentum distributions. One can directly show that $\boldsymbol{p}' = \boldsymbol{S}^{\dagger}\boldsymbol{p}\boldsymbol{S}$, unlike $\boldsymbol{p}$, does not change when W_t does not cover the electron localisation region V.

So, we shall get the same results in the Coulomb gauge and in the new WP form only if we are able to get rid of the fictitious parts of the Coulomb gauge calculations.

Acknowledgment

I am grateful to V Ogievetsky for discussions.

Appendix

We stress that the Mandelstam (1962) and DeWitt (1962) WP formulations differ essentially, in spite of the formal resemblance of the starting expressions $\psi' = \psi \exp(-ie\int A_\mu \,\mathrm{d}\xi_\mu)$. In the Mandelstam paper the integration path is not fixed and ψ' depends upon the path variation, see (2.8). Due to the definition (2.11) of the 'gauge-invariant derivative' one has

$$\frac{\partial}{\partial x_\mu}\int_{-\infty}^{x} \boldsymbol{A}\,.\,\mathrm{d}\boldsymbol{\xi} = \lim_{\Delta x_\mu \to 0}\left(\int_{-\infty}^{x+\Delta x_\mu} \boldsymbol{A}\,.\,\mathrm{d}\boldsymbol{\xi} - \int_{-\infty}^{x} \boldsymbol{A}\,.\,\mathrm{d}\boldsymbol{\xi}\right)(\Delta x_\mu)^{-1} = A_\mu(x)$$

where $\int_{-\infty}^{x+\Delta x_\mu}$ is defined as the sum $\int_{-\infty}^{x} + \int_{x}^{x+\Delta x_\mu}$, the latter integral being taken over the straight line, connecting x and $x + \Delta x_\mu$.

We adhere to the DeWitt approach in which the integration path is fixed. The coordinates ξ_m of a point of the path leading from $\boldsymbol{r}$ to $\boldsymbol{x}$ are functions $\phi_m(\boldsymbol{x}, \alpha)$ which depend on one parameter α: $\boldsymbol{\xi} = \boldsymbol{\phi}(\boldsymbol{x}, \alpha)$. We have $\phi_m(\boldsymbol{x}, 0) = r_m$ and $\phi_m(\boldsymbol{x}, 1) = x_m$. The most simple path is a straight line $\boldsymbol{\xi} = \boldsymbol{r} + \alpha(\boldsymbol{x} - \boldsymbol{r})$.

Now the derivative $(\partial/\partial x_k)\int \boldsymbol{A}\,.\,\mathrm{d}\boldsymbol{\xi}$ must be defined and calculated as follows:

$$\begin{aligned}\lim_{\Delta\to 0}\frac{1}{\Delta}&\left(\int_{r}^{x+\mathbf{e}_k\Delta} \boldsymbol{A}\,\mathrm{d}\xi - \int_{r}^{x} \boldsymbol{A}\,\mathrm{d}\xi\right)\\ &= \lim\frac{1}{\Delta}\left(\int_{r}^{x+\mathbf{e}_k\Delta} + \int_{x+\mathbf{e}_k\Delta}^{x} + \int_{x}^{r} - \int_{x+\mathbf{e}_k\Delta}^{x}\right)\\ &= \lim\frac{1}{\Delta}\oint \boldsymbol{A}\,\mathrm{d}\xi + A_k(\boldsymbol{x}).\end{aligned} \tag{A.1}$$

Here $\boldsymbol{e}_k$ is the unit vector along kth axis. We have added and subtracted the integral $\int_{x}^{x+\mathbf{e}_k\Delta}(\boldsymbol{A}\,.\,\mathrm{d}\boldsymbol{\xi}) \cong A_k(\boldsymbol{x})\Delta$. The integral $\oint$ is taken over the closed path $\boldsymbol{r} \to \boldsymbol{x} + \boldsymbol{e}_k\Delta \to \boldsymbol{x} \to \boldsymbol{r}$ (see figure 1). According to the Stokes formula

$$\begin{aligned}\oint(\boldsymbol{A}\,.\,\mathrm{d}\boldsymbol{\xi}) &= \tfrac{1}{2}\iint\sum_{m,n}\left(\frac{\partial}{\partial\xi_m}A_n - \frac{\partial}{\partial\xi_n}A_m\right)\mathrm{d}\xi_m\,\mathrm{d}\xi_n\\ &= \tfrac{1}{2}\iint\sum_{mn}F_{mn}(\boldsymbol{\xi})\,\mathrm{d}\xi_m\,\mathrm{d}\xi_n.\end{aligned} \tag{A.2}$$

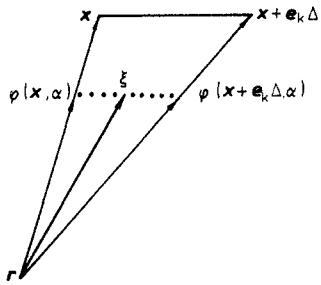

Figure 1.

The point $\boldsymbol{\xi}$ of the integration surface in $\iint$ is the sum of the vectors $\boldsymbol{\phi}(\boldsymbol{x}, \alpha)$ and $\beta \boldsymbol{a} \equiv \beta[\boldsymbol{\phi}(\boldsymbol{x}+\boldsymbol{e}_k\Delta, \alpha) - \boldsymbol{\phi}(\boldsymbol{x}, \alpha)]$. The vector $\boldsymbol{a}$ is shown by the dotted line in figure 1. When β changes from 0 to 1, $\boldsymbol{\xi}$ goes from $\boldsymbol{\phi}(\boldsymbol{x}, \alpha)$ to $\boldsymbol{\phi}(\boldsymbol{x}+\boldsymbol{e}_k\Delta, \alpha)$:

$$\boldsymbol{\xi} = \boldsymbol{\phi}(\boldsymbol{x}, \alpha) + \beta(\boldsymbol{\phi}(\boldsymbol{x}+\boldsymbol{e}_k\Delta, \alpha) - \boldsymbol{\phi}(\boldsymbol{x}, \alpha))$$

$$= \boldsymbol{\phi}(\boldsymbol{x}, \alpha) + \beta\Delta \frac{\partial}{\partial x_k} \boldsymbol{\phi}(\boldsymbol{x}, \alpha). \tag{A.3}$$

Neglecting terms of the order Δ^2 we have

$$\frac{\mathscr{D}(\xi_m, \xi_n)}{\mathscr{D}(\alpha, \beta)} \cong \left(\frac{\partial \phi_m}{\partial \alpha}\frac{\partial \phi_n}{\partial x_k} - \frac{\partial \phi_n}{\partial \alpha}\frac{\partial \phi_m}{\partial x_k}\right)\Delta. \tag{A.4}$$

The argument $\boldsymbol{\xi}$ of F_{mn} in (A.2) can be put equal to $\boldsymbol{\phi}(\boldsymbol{x}, \alpha)$, see (A.3), so that

$$\oint (\boldsymbol{A} \cdot \mathrm{d}\xi) = \frac{1}{2}\int_0^1 \mathrm{d}\alpha\, F_{mn}(\boldsymbol{\phi}(\boldsymbol{x}, \alpha))\left(\frac{\partial \phi_m}{\partial \alpha}\frac{\partial \phi_n}{\partial x_k} - \frac{\partial \phi_n}{\partial \alpha}\frac{\partial \phi_m}{\partial x_k}\right)\Delta \int_0^1 \mathrm{d}\beta$$

$$= \Delta \int_0^1 \mathrm{d}\alpha\, F_{mn}\frac{\partial \phi_m}{\partial \alpha}\frac{\partial \phi_n}{\partial x_k}. \tag{A.5}$$

Using $F_{mn} = -F_{nm}$, one gets from (A.1), (A.2) and (A.5)

$$\frac{\partial}{\partial x_k}\int_r^x (\boldsymbol{A} \cdot \mathrm{d}\boldsymbol{\xi}) = \int_0^1 \mathrm{d}\alpha\, F_{mn}\frac{\partial \phi_m}{\partial \alpha}\frac{\partial \phi_n}{\partial x_k} + A_k(\boldsymbol{x}) \tag{A.6}$$

If $\boldsymbol{\xi} = \boldsymbol{\phi}(\boldsymbol{x}, \alpha) = \boldsymbol{r} + \alpha(\boldsymbol{x} - \boldsymbol{r})$ we have

$$\int_0^1 \mathrm{d}\alpha \sum_{m,n} F_{mn} \cdot (\boldsymbol{x}-\boldsymbol{r})_m \delta_{nk}\alpha = -\int_0^1 \alpha\, \mathrm{d}\alpha[(\boldsymbol{x}-\boldsymbol{r}) \times \boldsymbol{H}]_k. \tag{A.7}$$

Inserting (A.7) into (A.6) gives equation (8) of § 2.

Capps and Holladay (1955) also introduce $\int \boldsymbol{A} \cdot \mathrm{d}\boldsymbol{\xi}$ over a finite line, but equation (16) from (Capps and Holladay 1955) for $\nabla \int \boldsymbol{A} \cdot \mathrm{d}\boldsymbol{\xi}$ is wrong. This is the reason for the above derivation. Note that our result is consistent with the DeWitt (1962) equation (7).

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