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1980 J. Phys. A: Math. Gen. 13 2795

(http://iopscience.iop.org/0305-4470/13/8/027)

J. Phys. A: Math. Gen. 13 (1980) 2795–2805. Printed in Great Britain

Gauge invariant wave mechanics and the Power–Zienau–Woolley transformation

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Received 19 July 1979

Abstract. The wave mechanical formulation of quantum electrodynamics is investigated in an explicitly gauge invariant form and this leads to the connection between manifest charge conservation and the Power–Zienau–Woolley transformation.

1. Introduction

The existence of gauge transformations in electrodynamics has held a special fascination ever since the first quantum mechanical discussions of gauge invariance (Dirac 1931). In a quantum theory, the gauge symmetry implies a superselection rule that explains the empirical fact that charge cannot be created or destroyed, i.e. matrix elements connecting states belonging to different charge eigenvalues necessarily vanish (charge conservation). Manifestly gauge invariant formulations of relativistic QED have been proposed by many workers (Dirac 1955, Mandelstam 1962, Goldberg 1965, Białynicki-Birula 1970, Menikoff and Sharp 1977) and in that context the subject of gauge invariance has been much studied. At the same time non-relativistic QED, which deals with the interactions between quantised radiation and atoms (molecules), has become a topic of renewed interest largely because of the developments in laser spectroscopy and the experimental realisation of a wide range of multiphoton processes. Manifest covariance is not possible here and non-relativistic QED is usually formulated in wave-mechanical language i.e. in the canonical formalism, with the evolution of the system described by the Schrödinger equation,

$$i\hbar(\partial\Psi/\partial t) = \hat{H}\Psi. \tag{1.1}$$

The Hamiltonian operator $\hat{H}$ for a closed system of atoms and radiation can be decomposed into three parts,

$$\hat{H} = \hat{H}^{\text{atom}} + \hat{H}^{\text{int}} + \hat{H}^{\text{rad}}, \tag{1.2}$$

and there is considerable freedom in the choice of these three terms consistent with a total Hamiltonian that describes a definite physical system, not least because of the gauge symmetry. The connection between the Coulomb gauge Hamiltonian $\hat{H}_c$ and the generalised 'multipole' Hamiltonian $\hat{\tilde{H}}$ is given by means of a path-dependent unitary transformation. This is the Power–Zienau–Woolley transformation (Power and Zienau

0305-4470/80/082795+11$01.50

1959, Woolley 1971, Babiker *et al* 1974) for which the transformation operator has the form

$$\hat{U} = \exp\left\{\frac{\mathrm{i}}{\hbar}\int \mathrm{d}^3x\, \hat{\boldsymbol{P}}(\boldsymbol{x}) \cdot \hat{\boldsymbol{A}}(\boldsymbol{x})\right\}, \qquad \boldsymbol{\nabla} \cdot \hat{\boldsymbol{A}}(\boldsymbol{x}) = 0 \tag{1.3}$$

and one then has

$$\hat{H} = \hat{H}_{\mathrm{c}}^{\mathrm{atom}} + \hat{H}_{\mathrm{c}}^{\mathrm{int}} + \hat{H}_{\mathrm{c}}^{\mathrm{rad}} \tag{1.4}$$

$$= \hat{\tilde{H}}^{\mathrm{atom}} + \hat{\tilde{H}}^{\mathrm{int}} + \hat{\tilde{H}}^{\mathrm{rad}} \tag{1.5}$$

with

$$\hat{\tilde{H}}^{\mathrm{rad}} = \hat{U}\hat{H}_{\mathrm{c}}^{\mathrm{rad}}\hat{U}^{-1} \tag{1.6}$$

$$\hat{\tilde{H}}^{\mathrm{atom}} = \hat{U}\hat{H}_{\mathrm{c}}^{\mathrm{atom}}\hat{U}^{-1} \tag{1.7}$$

but

$$\hat{\tilde{H}}^{\mathrm{int}} \neq \hat{U}\hat{H}_{\mathrm{c}}^{\mathrm{int}}\hat{U}^{-1} \tag{1.8}$$

because $\hat{H}$ is not invariant under the action of $\hat{U}$ ($[\hat{H}, \hat{U}] \neq 0$) (Healy 1977, Healy and Woolley 1978), and

$$|\bar{\Psi}\rangle = \hat{U}|\Psi_{\mathrm{c}}\rangle. \tag{1.9}$$

The non-locality of $\hat{U}$ arises from the 'polarisation' field $\hat{\boldsymbol{P}}(\boldsymbol{x})$ which is a solution of the linear equation

$$\boldsymbol{\nabla} \cdot \hat{\boldsymbol{P}}(\boldsymbol{x}) = -\hat{\rho}(\boldsymbol{x}) \tag{1.10}$$

where $\hat{\rho}(\boldsymbol{x})$ is the charge-density operator. One can use the constraint (Woolley 1974)

$$\int \mathrm{d}^3x\, \hat{\boldsymbol{P}}(\boldsymbol{x}) \cdot \hat{\boldsymbol{A}}(\boldsymbol{x}) \equiv 0 \tag{1.11}$$

as a gauge condition (choose $\hat{\boldsymbol{A}}(\boldsymbol{x})$ orthogonal to $\hat{\boldsymbol{P}}(\boldsymbol{x})$), and in that way one can set up the canonical formalism with the Hamiltonian fixed, but with the non-locality incorporated in the associated Poisson-bracket algebra of the dynamical variables: this approach can also give the usual Coulomb gauge theory by choosing the polarisation field $\hat{\boldsymbol{P}}(\boldsymbol{x})$ in (1.11) to be purely longitudinal.

The aim of this paper is to investigate the gauge invariant formulation of wave mechanics starting directly from the canonical equations and thus show how the Power–Zienau–Woolley transformation emerges in a natural way. We shall see that the requirement that the quantum mechanical formalism be gauge invariant forces the result that gauge invariant wavefunctions necessarily contain the non-local phase $\hat{U}$, equation (1.3), multiplied into a gauge-dependent wavefunction, so that the usual theories involving gauge-dependent quantities can be obtained by invoking equation (1.11) with specific choices for $\boldsymbol{P}(\boldsymbol{x})$ as a (gauge) condition on the vector potential ($\hat{U} \to \hat{1}$).

2. The canonical equations

The classical Hamiltonian may be obtained from the Lagrangian for a closed system of charged particles and the electromagnetic field using a familiar argument (Woolley

1975), and we only quote the final equations from which the redundant conjugate field variables $(\phi(\boldsymbol{x}), \pi_0(\boldsymbol{x}))$ have been eliminated. The Hamiltonian takes the familiar form,

$$H \approx \tfrac{1}{2}\sum_i (\boldsymbol{P}_i - e_i\boldsymbol{A}(\boldsymbol{q}_i))^2 + \tfrac{1}{2}\epsilon_0 \int \mathrm{d}^3\boldsymbol{x}\, \{\epsilon_0^{-2}\boldsymbol{\pi}(\boldsymbol{x}) \cdot \boldsymbol{\pi}(\boldsymbol{x}) + c^2\boldsymbol{B}(\boldsymbol{x}) \cdot \boldsymbol{B}(\boldsymbol{x})\} \tag{2.1}$$

where $\boldsymbol{P}_i$ is the canonical momentum conjugate to $\boldsymbol{q}_i$, $\boldsymbol{\pi}(\boldsymbol{x})$ is the field variable conjugate to the vector potential $\boldsymbol{A}(\boldsymbol{x})$, and the motion generated by H is subject to a non-integrable equation of constraint

$$\Omega(\boldsymbol{x}) = \rho(\boldsymbol{x}) + \boldsymbol{\nabla} \cdot \boldsymbol{\pi}(\boldsymbol{x}) \approx 0. \tag{2.2}$$

The $\approx$ sign is Dirac's (1952) 'weak' equality symbol. The Poisson-bracket of H and $\Omega(\boldsymbol{x})$ vanishes strongly

$$\{H, \Omega(\boldsymbol{x})\} = 0 \tag{2.3}$$

and so $\Omega(\boldsymbol{x})$ is recognised as a symmetry of the system—it is the generator of gauge transformations. Since $\boldsymbol{\pi}(\boldsymbol{x})$ is essentially the electric field strength $(\boldsymbol{\pi}(\boldsymbol{x}) = -\epsilon_0\boldsymbol{E}(\boldsymbol{x}))$ the equation of constraint, when interpreted as a 'strong' i.e. ordinary equation, provides the Maxwell equation relating the sources to the longitudinal electric field. The magnetic field $\boldsymbol{B}(\boldsymbol{x})$ is related to the canonical variable $\boldsymbol{A}(\boldsymbol{x})$ by $\boldsymbol{B}(\boldsymbol{x}) = \boldsymbol{\nabla} \times \boldsymbol{A}(\boldsymbol{x})$, which implies the second Maxwell equation $\boldsymbol{\nabla} \cdot \boldsymbol{B}(\boldsymbol{x}) = 0$, and the remaining two Maxwell equations emerge from the equations of motion. The dynamical variables satisfy canonical (local) Poisson-bracket relations.

$$\{q_i^r, P_j^t\} = \delta_{ij}\,\delta_{rt} \tag{2.4}$$

$$\{\boldsymbol{A}(\boldsymbol{x})_r, \pi(\boldsymbol{x}')_t\} = \delta_{rt}\,\delta^3(\boldsymbol{x} - \boldsymbol{x}') \tag{2.5}$$

with all other brackets zero.

3. Quantisation

The formal quantisation of the classical canonical scheme summarised in § 2 follows the usual lines with the Poisson-bracket algebra reinterpreted as a commutator algebra between operators,

$$[\hat{\boldsymbol{A}}(\boldsymbol{x})_r, \hat{\boldsymbol{\pi}}(\boldsymbol{x}')_t] = \mathrm{i}\hbar\delta_{rt}\delta(\boldsymbol{x} - \boldsymbol{x}') \tag{3.1}$$

$$[\hat{q}_i^r, \hat{P}_j^t] = \mathrm{i}\hbar\delta_{ij}\delta_{rt} \tag{3.2}$$

and $\hat{H}$ and $\hat{\Omega}(\boldsymbol{x})$ are operators expressed in terms of the fundamental canonical operators $(\hat{\boldsymbol{q}}_i, \hat{\boldsymbol{P}}_i, \hat{\boldsymbol{A}}(\boldsymbol{x}), \hat{\boldsymbol{\pi}}(\boldsymbol{x}))$. This prescription leads to a Heisenberg representation with a state vector fixed in time, and the dynamics described by the coupled equations of motion for the operators, provided only that we can find a consistent interpretation of the classical equation of constraint (2.2). It is convenient to pass to a Schrödinger representation in which the operators have no explicit time dependence, and the time evolution of the system is described by the Schrödinger equation

$$\mathrm{i}\hbar\,\partial|\Psi_n\rangle/\partial t = \hat{H}|\Psi_n\rangle. \tag{3.3}$$

The equation of constraint can be handled in two ways: one obvious procedure is to

require that the physical solutions of equation (3.3) be those for which

$$\hat{\Omega}(\boldsymbol{x})|\Psi_n\rangle = 0 \tag{3.4}$$

so that the Maxwell equation holds as a condition on the physical states. This procedure is not usual in non-relativistic QED; rather it is customary to impose a definite gauge condition on the vector potential, and then look for the conditions that allow one to interpret the constraint equation $\Omega \approx 0$ as a strong i.e. ordinary equality (Dirac 1952). In the quantum theory we would then have

$$\hat{\Omega}(\boldsymbol{x}) = 0 \tag{3.5}$$

holding as an operator identity. We have previously shown how the gauge condition (1.11) with special choices of the polarisation field $\hat{\boldsymbol{P}}(\boldsymbol{x})$ lead to the Coulomb gauge and 'multipole' Hamiltonian theories (Woolley 1971, 1974, 1975). In the present context, however, it is of interest to discuss the constraint equation (3.4) which, written out in full, is

$$\nabla \cdot \hat{\boldsymbol{\pi}}(\boldsymbol{x}) + \hat{\rho}(\boldsymbol{x})|\Psi_n\rangle = 0. \tag{3.6}$$

Let us choose a representation that is diagonal in the particle coordinates $\{\hat{\boldsymbol{q}}_i\}$, so that we can replace the operator $\hat{\rho}(\boldsymbol{x})$ by the c-number expression $\rho(\boldsymbol{x})$, the classical charge density. If we now use equation (1.10) we can write

$$\nabla \cdot \{\hat{\boldsymbol{\pi}}(\boldsymbol{x}) - \boldsymbol{P}(\boldsymbol{x})\}|\Psi_n\rangle = 0 \tag{3.7}$$

where $\boldsymbol{P}(\boldsymbol{x})$ is a function of the particle coordinates but has no dependence on the field potential operator $\hat{\boldsymbol{A}}(\boldsymbol{x})$. In general the physical solutions of the Schrödinger equation (3.3) cannot be expected to be eigenfunctions of $\hat{\boldsymbol{\pi}}(\boldsymbol{x})$ with eigenvalue $\boldsymbol{P}(\boldsymbol{x})$: however, equation (3.7) will be satisfied if we can write

$$\hat{\boldsymbol{\pi}}(\boldsymbol{x})|\Psi_n\rangle = \boldsymbol{P}(\boldsymbol{x})|\Psi_n\rangle + \boldsymbol{T}_n[\hat{\boldsymbol{A}}(\boldsymbol{x})] \tag{3.8}$$

where $\boldsymbol{T}_n$, a functional of $\hat{\boldsymbol{A}}(\boldsymbol{x})$, is transverse, i.e.

$$\nabla \cdot \boldsymbol{T}_n[\hat{\boldsymbol{A}}(\boldsymbol{x})] = 0. \tag{3.9}$$

We use square brackets to indicate functional dependence. According to the commutation relation (3.1), $\hat{\boldsymbol{\pi}}(\boldsymbol{x})$ can be represented as a functional derivative operator,

$$\hat{\boldsymbol{\pi}}(\boldsymbol{x}) \to -\mathrm{i}\hbar\, \delta/\delta\hat{\boldsymbol{A}}(\boldsymbol{x}), \tag{3.10}$$

and so equation (3.8) can be written as

$$\{\delta/\delta\hat{\boldsymbol{A}}(\boldsymbol{x}) - \mathrm{i}\boldsymbol{P}(\boldsymbol{x})/\hbar\}\Psi_n[\hat{\boldsymbol{A}}(\boldsymbol{x})] = \mathrm{i}\boldsymbol{T}_n[\hat{\boldsymbol{A}}(\boldsymbol{x})]/\hbar \tag{3.11}$$

or

$$\delta/\delta\hat{\boldsymbol{A}}(\boldsymbol{x})\left\{\exp\left(-(\mathrm{i}/\hbar)\int \mathrm{d}^3\boldsymbol{x}'\, \boldsymbol{P}(\boldsymbol{x}') \cdot \hat{\boldsymbol{A}}(\boldsymbol{x}')\right)\Psi_n[\hat{\boldsymbol{A}}(\boldsymbol{x})]\right\} = \hat{\boldsymbol{S}}[\hat{\boldsymbol{A}}(\boldsymbol{x})] \tag{3.12}$$

where

$$\hat{\boldsymbol{S}}[\hat{\boldsymbol{A}}(\boldsymbol{x})] = (\mathrm{i}/\hbar)\boldsymbol{T}_n[\hat{\boldsymbol{A}}(\boldsymbol{x})]\exp\left(-(\mathrm{i}/\hbar)\int \mathrm{d}^3\boldsymbol{x}'\, \boldsymbol{P}(\boldsymbol{x}') \cdot \hat{\boldsymbol{A}}(\boldsymbol{x}')\right). \tag{3.13}$$

The requirement that $\hat{\boldsymbol{S}}(\boldsymbol{x})$ be the functional derivative of the expression in braces in (3.12) strongly restricts the form of the functional $\boldsymbol{T}_n$, for if we write (3.12) in the form

$$\hat{\boldsymbol{S}}[\hat{\boldsymbol{A}}(\boldsymbol{x})] = \delta V[\hat{\boldsymbol{A}}(\boldsymbol{x})]/\delta\hat{\boldsymbol{A}}(\boldsymbol{x}) \tag{3.14}$$

then we must have

$$\delta\hat{S}[\hat{\boldsymbol{A}}(\boldsymbol{x})]/\delta\hat{\boldsymbol{A}}(\boldsymbol{y}) = \delta\hat{S}[\hat{\boldsymbol{A}}(\boldsymbol{y})]/\delta\hat{\boldsymbol{A}}(\boldsymbol{x}) \tag{3.15}$$

(the integrability condition), and this requires that

$$\boldsymbol{T}_n[\hat{\boldsymbol{A}}(\boldsymbol{x})] = t_n(\hat{\boldsymbol{A}}(\boldsymbol{x}))\exp\Big(+(\mathrm{i}/\hbar)\int \mathrm{d}^3x'\,\boldsymbol{P}(\boldsymbol{x}')\,.\,\hat{\boldsymbol{A}}(\boldsymbol{x}')\Big) \tag{3.16}$$

where t_n is a transverse vector *function* of $\hat{\boldsymbol{A}}(\boldsymbol{x})$. Thus we must have

$$\Psi_n[\hat{\boldsymbol{A}}(\boldsymbol{x})] = \exp\Big(+(\mathrm{i}/\hbar)\int \mathrm{d}^3x'\,\boldsymbol{P}(\boldsymbol{x}')\,.\,\hat{\boldsymbol{A}}(\boldsymbol{x}')\Big)\int^{\hat{\boldsymbol{A}}(\boldsymbol{x})} \delta\hat{\boldsymbol{A}}'(\boldsymbol{x})\,.\,t_n(\hat{\boldsymbol{A}}'(\boldsymbol{x})) \tag{3.17}$$

$$= \exp\Big(+(\mathrm{i}/\hbar)\int \mathrm{d}^3x'\,\boldsymbol{P}(\boldsymbol{x}')\,.\,\hat{\boldsymbol{A}}(\boldsymbol{x}')\Big)\Phi_n(\{\boldsymbol{q}_i\}, \hat{\boldsymbol{A}}(\boldsymbol{x})) \tag{3.18}$$

in an obvious notation (cf equations (1.3) and (1.9)). In the next section we shall study the gauge symmetry and show explicitly that gauge-invariant wavefunctionals have the form of equation (3.18).

4. Gauge symmetry

In this section we investigate the gauge symmetry of the Hamiltonian implied by the commutator

$$[\hat{H}, \hat{\Omega}(\boldsymbol{x})] = 0. \tag{4.1}$$

In order to construct a unitary gauge transformation operator we integrate $\hat{\Omega}(\boldsymbol{x})$ against a suitably smooth test function $f(\boldsymbol{x})$, so that

$$\hat{\Omega}[f] = \int \mathrm{d}^3x\;\hat{\Omega}(\boldsymbol{x})f(\boldsymbol{x}) \tag{4.2}$$

$$= \hat{\rho}[f] - \hat{\pi}[\nabla f] \tag{4.3}$$

where

$$\hat{\rho}[f] = \int \mathrm{d}^3x\,\hat{\rho}(\boldsymbol{x})f(\boldsymbol{x}) \tag{4.4}$$

$$\hat{\pi}[\nabla f] = \int \mathrm{d}^3x\,\hat{\boldsymbol{\pi}}(\boldsymbol{x})\,.\,\nabla f(\boldsymbol{x}), \tag{4.5}$$

after an integration by parts. Since $\hat{\Omega}(\boldsymbol{x})$ is Hermitian we can construct a unitary operator $\hat{G}[f]$,

$$\hat{G}[f] = \exp(\mathrm{i}\hat{\Omega}[f]/\hbar), \tag{4.6}$$

with the multiplication law of an Abelian group,

$$\hat{G}[f]\hat{G}[g] = \hat{G}[f+g] = \hat{G}[g]\hat{G}[f], \tag{4.7}$$

that is isomorphic to $U(1)$, the unitary unimodular group of complex numbers. If we apply $\hat{G}$ to the basic canonical operators we see that $\hat{\boldsymbol{q}}_i$ and $\hat{\boldsymbol{\pi}}(\boldsymbol{x})$ are invariant since they

commute with $\hat{\Omega}(\boldsymbol{x})$, but that

$$\hat{\boldsymbol{P}}_i' = \hat{G}[f]\boldsymbol{P}_i\hat{G}[f]^{-1} = \hat{\boldsymbol{P}}_i + e_i\nabla f(\hat{\boldsymbol{q}}_i) \tag{4.8}$$

$$\hat{\boldsymbol{A}}'(\boldsymbol{x}) = \hat{G}[f]\hat{\boldsymbol{A}}(\boldsymbol{x})\hat{G}[f]^{-1} = \hat{\boldsymbol{A}}(\boldsymbol{x}) - \nabla f(\boldsymbol{x}). \tag{4.9}$$

In view of these equations we have

$$\hat{H}(\{\hat{\boldsymbol{P}}_i\}, \{\hat{\boldsymbol{q}}_i\}, [\hat{\boldsymbol{A}}(\boldsymbol{x})], [\hat{\boldsymbol{\pi}}(\boldsymbol{x})]) \xrightarrow{G[f]} \hat{H}'(\{\hat{\boldsymbol{P}}_i'\}, \{\hat{\boldsymbol{q}}_i'\}, [\hat{\boldsymbol{A}}'(\boldsymbol{x})], [\hat{\boldsymbol{\pi}}'(\boldsymbol{x})])$$
$$\equiv \hat{H}(\{\hat{\boldsymbol{P}}_i\}, \{\hat{\boldsymbol{q}}_i\}, [\hat{\boldsymbol{A}}(\boldsymbol{x})], [\hat{\boldsymbol{\pi}}(\boldsymbol{x})]) \tag{4.10}$$

consistent with (4.1). A general wavefunction ϕ that is not subject to the constraint equation (3.4), however, is *not* invariant: if we choose a 'coordinate' representation for the particle and field variables, we easily compute the transformed wavefunction ϕ_f' to be

$$\phi_f' = \hat{G}[f]\phi(\{\boldsymbol{q}_i\}, [\boldsymbol{A}(\boldsymbol{x})])$$
$$\equiv \exp((\mathrm{i}/\hbar)\rho[f])\phi(\{\boldsymbol{q}_i\}, [\boldsymbol{A}'(\boldsymbol{x})]) \tag{4.11}$$

in terms of the transformed vector potential $\boldsymbol{A}'(\boldsymbol{x})$, equation (4.9). These equations justify our interpretation of $\hat{G}[f]$ as the gauge transformation operator.

Instead of working with gauge-dependent wavefunctions we may insist that the formalism should be based solely on manifestly gauge invariant quantities, since all physical quantities are gauge-invariant. Wavefunctions that are invariant under the action of $\hat{G}[f]$ may be constructed as follows. Let $\hat{U}[\hat{\boldsymbol{P}}]$ be a unitary operator,

$$\hat{U}[\hat{\boldsymbol{P}}] = \exp((\mathrm{i}/\hbar)\hat{A}[\hat{\boldsymbol{P}}]) \tag{4.12}$$

where

$$\hat{A}[\hat{\boldsymbol{P}}] = \int \mathrm{d}^3\boldsymbol{x}\, \hat{\boldsymbol{P}}(\boldsymbol{x}) \cdot \hat{\boldsymbol{A}}(\boldsymbol{x}) \tag{4.13}$$

for some vector field $\hat{\boldsymbol{P}}(\boldsymbol{x})$ which is to be determined (for simplicity, the notation here anticipates the final result). If we define

$$|\psi[\hat{\boldsymbol{P}}]\rangle = \hat{U}[\hat{\boldsymbol{P}}]|\phi\rangle \tag{4.14}$$

where the wavefunctional $|\phi\rangle$ is a functional of the vector potential $\hat{\boldsymbol{A}}(\boldsymbol{x})$ in the same gauge as in the integral (4.13), then $\psi[\hat{\boldsymbol{P}}]$ will be *gauge-invariant* provided that the gauge symmetry operator $\hat{G}[f]$ acts trivially on $\psi[\hat{\boldsymbol{P}}]$ i.e. if $\psi[\hat{\boldsymbol{P}}]$ is a representation of the gauge group with character $+1$. The vector field $\hat{\boldsymbol{P}}(\boldsymbol{x})$ is thus to be determined by the requirement that

$$\hat{G}[f]|\psi[\hat{\boldsymbol{P}}]\rangle \equiv |\psi[\hat{\boldsymbol{P}}]\rangle, \tag{4.15}$$

so that using (4.14) we must have

$$(\hat{G}[f]\hat{U}[\hat{\boldsymbol{P}}] - \hat{U}[\hat{\boldsymbol{P}}])|\phi\rangle = 0 \tag{4.16}$$

for any $|\phi\rangle$ calculated in the gauge of the vector potential $\hat{\boldsymbol{A}}(\boldsymbol{x})$. Now according to equations (4.2)–(4.5), $\Omega[f]$ consists of the sum of two commuting operators and we may write

$$\hat{G}[f] = \exp((\mathrm{i}/\hbar)\hat{\rho}[f])\exp(-(\mathrm{i}/\hbar)\hat{\pi}[\nabla f]). \tag{4.17}$$

$\hat{U}[\hat{\boldsymbol{P}}]$ must therefore be a solution of the operator equation,

$$\exp(-(\mathrm{i}/\hbar)\hat{\pi}[\nabla f])\hat{U}[\hat{\boldsymbol{P}}] = \exp(-(\mathrm{i}/\hbar)\hat{\rho}[f])\hat{U}[\hat{\boldsymbol{P}}]. \tag{4.18}$$

If we combine equations (3.10) and (4.18) and note that $\hat{\pi}[\nabla f]$ generates a 'translation' of ∇f on $\hat{\boldsymbol{A}}(\boldsymbol{x})$, we obtain

$$\hat{A}[\hat{\boldsymbol{P}}] - \nabla f[\hat{\boldsymbol{P}}] = -\hat{\rho}[f] + \hat{A}[\hat{\boldsymbol{P}}] \tag{4.19}$$

which gives the following condition for $\boldsymbol{P}(\boldsymbol{x})$,

$$\int \mathrm{d}^3\boldsymbol{x}\, \hat{\boldsymbol{P}}(\boldsymbol{x}) \,.\, \nabla f(\boldsymbol{x}) - \int \mathrm{d}^3\boldsymbol{x}\, \hat{\rho}(\boldsymbol{x}) f(\boldsymbol{x}) = 0. \tag{4.20}$$

Thus after an integration by parts and the neglect of surface integral we see that $\hat{\boldsymbol{P}}(\boldsymbol{x})$ satisfies an inhomogeneous linear differential equation at all points $\boldsymbol{x}$,

$$\nabla \,.\, \hat{\boldsymbol{P}}(\boldsymbol{x}) = -\hat{\rho}(\boldsymbol{x}): \tag{4.21}$$

this is the defining equation for the 'polarisation' field $\hat{\boldsymbol{P}}(\boldsymbol{x})$, (1.10), originally introduced into non-relativistic QED by analogy with classical dielectric theory (Power and Zienau 1959). The gauge-invariant wavefunction (4.14) is of exactly the same form as equation (3.18) for the physical states on which Maxwell's equation $\epsilon_0 \nabla \,.\, \boldsymbol{E}(\boldsymbol{x}) = \rho(\boldsymbol{x})$ holds, and (4.14) is the same equation as the Power–Zienau–Woolley transformation equation (1.9) if $|\phi\rangle$ and $\hat{U}[\hat{\boldsymbol{P}}]$ are evaluated with the Coulomb gauge vector potential $\hat{\boldsymbol{A}}^{\mathrm{c}}$.

5. Physics of the Power–Zienau–Woolley transformation

In the previous sections we have shown that the form of gauge-invariant wavefunctionals is determined entirely by the structure of quantum electrodynamics once gauge invariance is demanded, and the Power–Zienau–Woolley transformation is a device for transforming the usual (gauge-dependent) Coulomb gauge theory into this explicitly gauge-invariant form. It is thus of interest to enquire what physical interpretation can be given to gauge-invariant wave mechanics: the following discussion focusses on the fundamental law of nature that electrical charge cannot be created or destroyed. The conventional motivation for the Power–Zienau–Woolley transformation, namely that it displays atomic (molecular) multipoles explicitly in the transformed Hamiltonian, is gratuitous, not least because a separation into electric and magnetic multipoles cannot be carried out in a unique or invariant fashion.

In order to take account of charge conservation explicitly in the description of electrodynamic processes one must consider the additional currents that flow during every experiment in which beams of charged particles are involved. These additional currents, which flow between the source and the detector of charged particles, have been called compensating currents because they compensate for the charge lost by the source and gained by the detector (Bialynicki-Birula and Białynicki-Birula 1975). Taking into account the compensating currents one simply has the separation and subsequent recombination of charges instead of 'creation' and 'destruction', and this is in full accord with the observation that the natural state of all matter under terrestrial conditions is an electrically neutral state.

The simplest approach to the incorporation of compensating currents in quantum electrodynamics is to ignore all dynamical aspects of these currents so that the

compensating current can be described by a set of four given c-number functions, $J^\mu(z)$ ($\mu = 0, 1, 2, 3$), of the space–time coordinates ($z = \boldsymbol{x}, t$). The propagator describing the creation of electrons from the vacuum at the points $y_1, \ldots, y_n$ and their subsequent annihilation at $x_1, \ldots, x_n$ (or the converse interpretation for positrons) in either a prescribed c-number or fully quantised electromagnetic field, described by a field potential $A_\mu(z)$ ($A_\mu = \boldsymbol{A}, \phi$), can be written symbolically as

$$T[x_1, \ldots x_n, y_n, \ldots y_1|\mathscr{A}]. \tag{5.1}$$

This propagator depends on the gauge of the four-potential $A_\mu(z)$: it can be shown that a propagator that is invariant under gauge transformations of the potentials,

$$A_\mu(z) \to A_\mu(z) + \partial_\mu \Lambda(z), \tag{5.2}$$

can be defined using the compensating current $J^\mu(z)$,

$$T[x_1, \ldots x_n, y_n, \ldots y_1|\mathscr{A}, J] = \exp\Big((\mathrm{i}/\hbar)\int \mathrm{d}^4 z\, J^\mu(z) A_\mu(z)\Big) T[x_1, \ldots x_n, y_n, \ldots y_1], \tag{5.3}$$

provided that $J^\mu(z)$ satisfies the following inhomogeneous continuity equation (Białynicki-Birula and Białynicki-Birula 1975),

$$\partial_\mu J^\mu(z : x_1, \ldots x_n, y_1, \ldots y_n) = e \sum_{i=1}^{n} \{\delta^4(z - y_i) - \delta^4(z - x_i)\}. \tag{5.4}$$

In the wave-mechanical formulation of electrodynamics we work with dynamical variables on a space-like three-dimensional surface in space–time and see how they are connected with the dynamical variables on a neighbouring surface: the connections constitute the equations of motion. For simplicity consider the electrodynamics of a single charged particle for which the particle-field Hamiltonian is $\hat{H}$ (cf § 1). The Schrödinger equation (1.1) describes the change in the state ψ in the infinitesimal time Δt as due to the action of a unitary operator $\exp(-\mathrm{i}\hat{H}\Delta t/\hbar)$. One can also ask, if $\Psi(x_1, t_1)$ is the wavefunction at x_1, t_1 what is the wavefunction at time $t_2 > t_1$? This is obtained from the propagator T,

$$\Psi(\boldsymbol{x}_2, t_2) = \int \mathrm{d}^3 \boldsymbol{x}_1\, T(\boldsymbol{x}_2, t_2; \boldsymbol{x}_1, t_1)\Psi(\boldsymbol{x}_1, t_1) \tag{5.5}$$

where T is the causal Green function for the Schrödinger equation,

$$[\mathrm{i}\hbar(\partial/\partial t_2) - \hat{H}_2]T(z_2, z_1) = \mathrm{i}\hbar\delta^4(z_2 - z_1). \tag{5.6}$$

$T(z_2, z_1)$ has a bilinear representation in terms of the eigenfunctions of $\hat{H}$ (Feynman 1949)

$$T(z_2, z_1) = \begin{cases} \sum_n \Psi_n(\boldsymbol{x}_2)\Psi_n(\boldsymbol{x}_1)^* \exp[-(\mathrm{i}/\hbar)E_n(t_2 - t_1)] & t_2 > t_1 \\ 0 & t_2 < t_1. \end{cases} \tag{5.7}$$

In these equations the state vectors Ψ are to be understood as functionals of the electromagnetic field variables, as well as functions of the particle variables. We may choose the wavefunctions in equation (5.7) to be gauge invariant wavefunctions carrying the phase-factor $\hat{U}$ as in § 4, so that for example

$$\Psi_n(\boldsymbol{x}_2) = \exp\Big((\mathrm{i}/\hbar)\int \mathrm{d}^3 \boldsymbol{x}\, \boldsymbol{P}(\boldsymbol{x}) \cdot \hat{\boldsymbol{A}}(\boldsymbol{x})\Big)\phi_n(\boldsymbol{x}_2) \tag{5.8}$$

with

$$\nabla \cdot \boldsymbol{P}(\boldsymbol{x}, \boldsymbol{x}_2) = -e\delta^3(\boldsymbol{x} - \boldsymbol{x}_2) \tag{5.9}$$

and hence the gauge-invariant propagator T carries the phase

$$\exp\Big((\mathrm{i}/\hbar) \int \mathrm{d}^3\boldsymbol{x}\, \boldsymbol{J}(\boldsymbol{x}) \cdot \hat{\boldsymbol{A}}(\boldsymbol{x})\Big) \tag{5.10}$$

where

$$\boldsymbol{J}(\boldsymbol{x}) = \boldsymbol{P}(\boldsymbol{x}, \boldsymbol{x}_2) - \boldsymbol{P}(\boldsymbol{x}, \boldsymbol{x}_1) \tag{5.11}$$

and

$$\nabla \cdot \boldsymbol{J}(\boldsymbol{x}) = e[\delta^3(\boldsymbol{x} - \boldsymbol{x}_1) - \delta^3(\boldsymbol{x} - \boldsymbol{x}_2)]. \tag{5.12}$$

This is the expected result, since the construction of the Hamiltonian for electrodynamics involves the elimination of the zero-component of the four-potential A_μ (i.e. the scalar potential $A_0 = \phi$), and hence we expect the phase-factor in the propagator for the Schrödinger equation, due to a compensating current of electrons, to be of the form (5.10) with no time-integration, and with the vector field $\boldsymbol{J}(\boldsymbol{x})$ satisfying the spatial part of the inhomogeneous continuity equation, (5.4),

$$\nabla \cdot \boldsymbol{J}(\boldsymbol{x}; \boldsymbol{x}_1, \ldots \boldsymbol{x}_n, \boldsymbol{y}_1, \ldots \boldsymbol{y}_n) = e \sum_{i=1}^{n} (\delta^3(\boldsymbol{x} - \boldsymbol{y}_i) - \delta^3(\boldsymbol{x} - \boldsymbol{x}_i)). \tag{5.13}$$

Recall that the divergence of a vector field is interpreted physically as the outward flux of the field from a volume V in the limit $V \to 0$, and this observation motivated the interpretation of the kernel $\boldsymbol{J}(\boldsymbol{x})$ as an electrical current between the points $\{\boldsymbol{y}_i\}$, $\{\boldsymbol{x}_i\}$.

At this point we may make contact between the idea of compensating currents and the analogy Power and Zienau (1959) made with classical dielectric theory when they introduced the 'electric polarisation field' $\boldsymbol{P}(\boldsymbol{x})$ through equations (1.3), (1.10) in their discussion of non-relativistic QED. If we consider a volume V in the dielectric, the net charge δq that flows out of the volume across an element $\mathrm{d}\boldsymbol{S}$ of its surface is $\boldsymbol{P} \cdot \mathrm{d}\boldsymbol{S}$ (i.e. the flux of $\boldsymbol{P}(\boldsymbol{x})$), so that the total flux Q flowing out of V is given by:

$$Q = \int_S \delta q = \int_S \boldsymbol{P} \cdot \mathrm{d}\boldsymbol{S}. \tag{5.14}$$

In order to maintain electrical neutrality we must have a charge $-Q$ remaining in the volume V. If $\rho(\boldsymbol{x})$ is the volume density of the charge remaining within this volume then

$$-Q = \int_V \rho(\boldsymbol{x})\, \mathrm{d}^3\boldsymbol{x} = -\int_S \boldsymbol{P} \cdot \mathrm{d}\boldsymbol{S} = -\int_V (\nabla \cdot \boldsymbol{P})\, \mathrm{d}^3\boldsymbol{x} \tag{5.15}$$

by Green's theorem, and since this is true for all V we must have

$$\nabla \cdot \boldsymbol{P}(\boldsymbol{x}) = -\rho(\boldsymbol{x}) \tag{5.16}$$

at all points $\boldsymbol{x}$, i.e. equation (1.10). Similarly, integration of equations (5.12), (5.13) over a volume containing the points $(\boldsymbol{x}_1, \boldsymbol{x}_2)$, $(\boldsymbol{x}_i, \boldsymbol{y}_i)$ respectively yields zero, consistent with the law of conservation of charge. The Power–Zienau–Woolley transformation

deals with the wavefunctional Ψ at a given instant in time, and gives Ψ a phase that ensures the correct form for the compensating current $\boldsymbol{J}(\boldsymbol{x})$, which in turn makes explicit local conservation of charge.

The form of the solutions of equation (5.16) is well known. The purely longitudinal solution $\boldsymbol{P}(\boldsymbol{x})^{\parallel}$ describes the Coulomb field of the charges: on the other hand, the Power–Zienau–Woolley transformation is generally discussed in terms of line integral representations of the polarisation field (Healy and Woolley 1978), in which each charged particle has its own integration path. One may ask whether the different possible choices of polarisation field $\boldsymbol{P}(\boldsymbol{x})$ have any physical content. If one confines attention to the electrodynamics of a specified number of charges and electromagnetic field considered as a closed system with Hamiltonian $\hat{H}$, equation (1.2), there is no reason to distinguish between the different phase-factors $\hat{U}$, equations (4.12) and (4.13), that can be given to gauge-invariant wavefunctions associated with a system with charge density $\rho(\boldsymbol{x})$. However, the discussion of compensating currents and charge conservation at the start of this section indicates that in principle the 'isolation' of such a system is not possible quite apart from practical considerations. The experimental arrangement or apparatus used in the measurement must therefore be described by a Hamiltonian operator $\lambda\hat{V}$ which is to be added to the system Hamiltonian $\hat{H}$. We ignore any dynamical consequences of the compensating current ($\boldsymbol{J}(\boldsymbol{x})$ is a c-number vector field) which means that we are dealing with the limit of $\lambda \to 0$, and we can suppose that the gauge-invariant quantum states associated with $\hat{H}$ give a satisfactory description. In this case only the symmetry of the perturbation operator $\lambda\hat{V}$ is of importance, and we simply use wavefunctionals $\Psi(\boldsymbol{x})$ of the form (§ 4)

$$\Psi_\alpha(\boldsymbol{x}) = \exp(\mathrm{i}\varphi_\alpha/\hbar)\phi(\boldsymbol{x}) \tag{5.17}$$

$$\varphi_\alpha = \int \mathrm{d}^3\boldsymbol{x}'\, \boldsymbol{P}(\boldsymbol{x}') \cdot \hat{\boldsymbol{A}}(\boldsymbol{x}') \tag{5.18}$$

with the phase φ_α chosen so as to match the symmetry of $\hat{V}$. Thus in principle one should expect the appropriate compensating current, and thus also the polarisation field $\boldsymbol{P}(\boldsymbol{x})$ (e.g. through the choice of paths C) to be chosen for every experimental situation. According to equation (1.6) the two commonly used radiation field Hamiltonians $\hat{H}_{\mathrm{c}}^{\mathrm{rad}}$, $\hat{H}^{\mathrm{rad}}$, that describe the 'free field' in perturbation theory, are related by the Power–Zienau–Woolley transformation, and so the vectors in their associated Fock spaces are of the form (Healy 1977, Healy and Woolley 1978), for photons with momentum $\boldsymbol{k}_i$, polarisation λ_i, (or $\bar{\boldsymbol{k}}_i$, $\bar{\lambda}_i$)

$$|i\rangle = |\boldsymbol{k}_i, \lambda_i\rangle \qquad |\bar{i}\rangle = |\bar{\boldsymbol{k}}_i, \bar{\lambda}_i\rangle \tag{5.19}$$

$$|\bar{i}\rangle = \hat{U}|i\rangle \tag{5.20}$$

with $\hat{U}$ given by equation (1.3), and these photon states may be thought of as being physically distinct by virtue of the above 'broken symmetry' argument.

Acknowledgments

It is a pleasure to acknowledge stimulating discussion with Iwo Białynicki-Birula at the 1978 LMS Symposium in Durham, England where this work was started. The financial support of an SRC Advanced Fellowship is gratefully acknowledged.

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