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Gauge-invariant non-relativistic limit of an electron in a time-dependent electromagnetic field

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Abstract. The Dirac equation for a charged particle in a time-dependent electromagnetic field is reduced to the Pauli equation in the non-relativistic limit by making a time-dependent Foldy–Wouthuysen transformation in a completely gauge-invariant way. In a time-dependent field, the expectation value of the Hamiltonian is dependent on the gauge, and so it cannot be the energy. The energy is obtained by taking the expectation value of the energy operator, the time rate of change of which is the average of the quantum mechanical power operator. The Hamiltonian formulation of a charged particle in a time-dependent external electromagnetic field is satisfactory when this distinction between the Hamiltonian, which describes the time evolution of the system, and the energy operator, which is gauge invariant, is made.

1. Introduction

For an electron in a time-dependent electromagnetic field, Goldman (1977) and Nieto (1977), using a time-dependent Foldy–Wouthuysen (FW) transformation (Foldy and Wouthuysen 1950, Pryce 1948, Tani 1951, Kurşunoğlu 1956, Osch 1977, Cohen 1971) have recently re-examined the non-relativistic reduction of the Dirac equation to the Pauli equation (Pauli 1927). They showed that the non-relativistic reduction of a Hamiltonian unitarily equivalent to the Dirac Hamiltonian gives the Pauli Hamiltonian plus some additional gauge-dependent relativistic corrections. Both Goldman (1977) and Nieto (1977) assume that in the presence of a *time-dependent* electromagnetic field the expectation value of the Dirac Hamiltonian is the physically meaningful energy. In the non-relativistic limit there thus appears to be a conflict between physical meaning and gauge invariance, that is, in the non-relativistic limit the physical energy is apparently given by the expectation value of a gauge-dependent operator.†

According to Goldman and Nieto this conflict arises because of the Hamiltonian formulation of an external field problem in a gauge theory. Goldman shows that the Hamiltonian for the system composed of the electromagnetic field and a charged particle is gauge invariant, but that the reduction to an external field problem produces a gauge-dependent Hamiltonian. He explains this situation by saying that changing the gauge 'shifts some energy from the interactions with the external field to the (ignored) structure of the field itself, or vice versa' (Goldman 1977 § IV). Since changes in energy

† Nieto (1977 Note 4) says that the FW transformation affects the gauge in this external field problem, and this is the reason for the lack of a gauge-invariant non-relativistic Hamiltonian.

are observable, they should not be dependent on the choice of gauge. According to Goldman (1977 § V), however, the FW transformation which reduces the Dirac Hamiltonian to the Pauli Hamiltonian is an operator gauge transformation (OGT), which "has 'gauged-in' something that was defined as part of the external field." Presumably, this something that is 'gauged-in' by making the FW transformation is energy that was transferred to the particle from the field, or vice versa. However, it is clear that making a unitary transformation on an equation should not change physical quantities.

In this paper the physical interpretation of a wave equation for a particle in a *time-dependent* external field is clarified by making the distinction between the Hamiltonian and the *energy operator*.† The Hamiltonian, which is not form invariant under gauge transformations, describes the time evolution of the states. In contrast, the energy operator, which is form invariant under gauge transformations, is defined such that the time rate of change of its expectation value is the expectation value of the power operator (Yang 1976). The expectation value of the energy operator, not the Hamiltonian, is the physical energy for the time-dependent case. When the expectation value of the energy operator in the Dirac theory is compared with the expectation value of the energy operator in the Pauli theory, they are equal to a given order in v/c. The problem formulated by Goldman (1977) and Nieto (1977) arises because they have not distinguished in the *time-dependent case* between the Hamiltonian and the *energy operator.*

In the next section the form invariance of the Dirac equation under local gauge transformations is briefly reviewed to establish notation, and the distinction between the Hamiltonian and the energy operator is made. Time-dependent unitary transformations are considered in § 3. The gauge-invariant reduction of the Dirac equation to the Pauli equation using the FW transformation is made in § 4. The non-relativistic reduction of the Dirac power operator to the Pauli power operator is given in § 5. In § 6 a gauge-invariant perturbation theory for the Dirac equation is developed and shown to reduce to a gauge-invariant perturbation theory for the Pauli equation. The conclusion is given in § 7. The Appendix discusses operator gauge transformations for the electromagnetic potentials.

2. Gauge transformations

The form invariance of the Schrödinger equation and the Dirac equation under local gauge transformations is well known (Bohm 1951), but is reviewed here to establish the notation. The expectation values of observables must be gauge invariant. Consequently, the distinction is made between the Hamiltonian, for which the expectation value is not gauge invariant, and the energy operator, for which the expectation value is. The time rate of change of the average of the energy operator is shown to be equal to the average of the quantum mechanical power operator (Yang 1976).

† Nieto (1977 p 1043) states: 'When one uses a particular external-field Hamiltonian in a Schrödinger (-like) equation, one is saying that this Hamiltonian—*and this Hamiltonian alone* (italics added) (up to time-dependent transformations)—gives both the time development of the Schrödinger (-like) equation and the object to consider for *exact* physical matrix elements'. The diagonal matrix elements would then be the energy, and so Nieto does not make the distinction between Hamiltonian and energy operator in the time-dependent case.

2.1. Local gauge transformations

The Dirac equation for a particle of mass m and charge q in a classical time-dependent electromagnetic radiation field described by the vector and scalar potentials, $\boldsymbol{A}$ and A_0 respectively, is (Bjorken and Drell 1964)

$$H(\boldsymbol{A}, A_0)\psi = \mathrm{i}\,\partial\psi/\partial t. \tag{2.1}$$

The Hamiltonian $H(\boldsymbol{A}, A_0)$ is defined as

$$H(\boldsymbol{A}, A_0) = \boldsymbol{\alpha}\,.\,(\boldsymbol{p} - q\boldsymbol{A}) + \beta m + qA_0 + qV, \tag{2.2}$$

where the momentum operator is $\boldsymbol{p} = -\mathrm{i}\nabla$. The Dirac matrices $\boldsymbol{\alpha}$ and β satisfy the anticommutation relations

$$\{\alpha_i, \alpha_j\} = 2\delta_{ij} \tag{2.3}$$

and

$$\{\beta, \alpha_i\} = 0, \tag{2.4}$$

where δ_{ij} is the Kronecker delta and $\beta^2 = 1$. The problem we consider is one in which there can also be an electrostatic potential V, for example, the static field of the proton in the hydrogen atom. In this case qV is a potential energy, since $-\nabla qV = q\boldsymbol{E}_0$, the electrostatic force acting on the electron. By definition potential energy is a quantity whose negative gradient is a force. In practical problems there is no difficulty in making this separation between the electrostatic potential energy and the scalar potential of the time-dependent electromagnetic radiation field.

A local gauge transformation can be made on the wavefunction ψ which transforms it into†

$$\psi' = \exp(\mathrm{i}q\Lambda)\psi, \tag{2.5}$$

where $\Lambda = \Lambda(x)$ is a function of the spatial coordinates and time $x = x^\mu = (x^0, x^1, x^2, x^3)$, and $x^0 = t$. The Dirac equation in equation (2.1) is form invariant under the transformation in equation (2.5), since it becomes

$$H(\boldsymbol{A}', A_0')\psi' = \mathrm{i}\,\partial\psi'/\partial t. \tag{2.6}$$

The new vector and scalar potentials, $\boldsymbol{A}'$ and A_0' respectively, in equation (2.6) must be related to the old potentials by

$$\boldsymbol{A}' = \boldsymbol{A} + \nabla\Lambda \tag{2.7}$$

and

$$A_0' = A_0 - \partial\Lambda/\partial t, \tag{2.8}$$

which are the usual gauge transformations of electromagnetic theory. Under these transformations the radiation electric field

$$\boldsymbol{E} \doteq -\nabla A_0 - \partial\boldsymbol{A}/\partial t \tag{2.9}$$

† There is considerable confusion regarding the terminology of gauge transformations. Pauli (1941) called equation (2.5) a 'gauge transformation of the first kind' and equations (2.7) and (2.8) 'gauge transformations of the second kind'. When Λ depends on the space and time, the gauge transformation is called 'local', while if Λ is a constant the gauge transformation is called 'global'. This terminology was used by Kobe and Smirl (1978). On the other hand, Abers and Lee (1973) call the case where Λ is a constant a 'gauge transformation of the first kind' and the case where Λ depends on space and time, which includes equations (2.5), (2.7) and (2.8), a 'gauge transformation of the second kind.' To avoid confusion, the terminology of 'gauge transformations of the first and second kind' is not used here.

and the magnetic induction

$$B = \nabla \times A \tag{2.10}$$

are invariant. Invariance of the Dirac equation under local gauge transformations is thus exactly the same as the invariance of the Schrödinger equation (Bohm 1951).

2.2. *Gauge invariance of operators*

For an operator to correspond to an observable, its expectation value cannot be dependent on the gauge (Yang 1976, Kobe and Smirl 1978). An arbitrary operator θ corresponding to an observable can in general depend on the potentials, so $\theta = \theta(A, A_0)$. However, the expectation value of an observable should be gauge invariant in the sense that

$$\langle\psi|\theta(A, A_0)\psi\rangle = \langle\psi'|\theta(A', A_0')\psi'\rangle. \tag{2.11}$$

In other words, the same number should be obtained if the wavefunction ψ and potentials A and A_0 are used to calculate the expectation value, or if the wavefunction ψ' given in equation (2.5) and the potentials A' and A_0' given in equations (2.7) and (2.8) are used. However, for all operators it is true that

$$\langle\psi|\theta(A, A_0)\psi\rangle = \langle\psi'|\theta'(A, A_0)\psi'\rangle, \tag{2.12}$$

where the operator θ' is defined as

$$\theta'(A, A_0) = \exp(iq\Lambda)\theta(A, A_0) \exp(-iq\Lambda). \tag{2.13}$$

Equation (2.13) is a unitary transformation on the operator $\theta(A, A_0)$, and is defined here as a 'gauge transformation on the operator.' The prime is used on all operators to denote the transformation of equation (2.13), *except* for the vector and scalar potentials where the prime denotes the gauge transformations of electrodynamics in equations (2.7) and (2.8). From a comparison of equations (2.11) and (2.12), for an operator to correspond to an observable, it must satisfy

$$\theta'(A, A_0) = \theta(A', A_0'). \tag{2.14}$$

In other words, when $\theta(A, A_0)$ is transformed by a gauge transformation on the operator, the electromagnetic potentials on which the operator depends undergo a gauge transformation. If an operator has the property given in equation (2.14), it is said to be *form invariant* under gauge transformations. A necessary and sufficient condition for an operator to have a gauge invariant expectation value is that it is form invariant under gauge transformations. In common language, we refer to an operator as being gauge invariant when it is form invariant under gauge transformations.

In order to make clear the definition of the form invariance of an operator under gauge transformations, some examples are given. The operator $p - qA$ is form invariant under gauge transformation on the operator in equation (2.13), since

$$(p - qA)' = p - qA', \tag{2.15}$$

where A' is given by equation (2.7). Likewise, the operator $i\,\partial/\partial t - qA_0$ is also form invariant under gauge transformation on the operator in equation (2.13), since

$$(i\,\partial/\partial t - qA_0)' = i\,\partial/\partial t - qA_0', \tag{2.16}$$

where A_0' is given by equation (2.8). However, the Hamiltonian $H(A, A_0)$ is not form invariant under gauge transformation on the operator in equation (2.13), since

$$H'(\boldsymbol{A}, A_0) = H(\boldsymbol{A}', A_0) = H(\boldsymbol{A}', A_0') + q\, \partial\Lambda/\partial t. \tag{2.17}$$

The Hamiltonian for a particle in a time-dependent electromagnetic field cannot therefore be the energy operator since its expectation value is gauge dependent. The Hamiltonian depends on the gauge in such a way that the Dirac equation in equation (2.1) is gauge invariant, that is, is form invariant under gauge transformation. Thus the Hamiltonian governs the temporal development of the wavefunction ψ through a gauge-invariant dynamical equation.

2.3. *Energy operator*

In order for an operator to correspond to the energy it is necessary for it to have (i) a gauge-invariant expectation value, and (ii) the time derivative of its expectation value equal to the average power transferred to the particle. Since the lack of gauge invariance of the Hamiltonian in equation (2.17) is due to the scalar potential A_0 of the time-dependent field, let us consider the operator $H(\boldsymbol{A}, 0)$ which is defined as

$$H(\boldsymbol{A}, 0) = H(\boldsymbol{A}, A_0) - qA_0. \tag{2.18}$$

In this time-dependent case it is shown here that $H(\boldsymbol{A}, 0)$, the Hamiltonian without the scalar potential of the time-dependent electromagnetic field, is the *energy operator* for the charged particle, *not* the Hamiltonian $H(\boldsymbol{A}, A_0)$. In the *time-dependent* case qA_0 is *not* a potential energy, since the electric force $q\boldsymbol{E}$ is not $-q\nabla A_0$, but instead is given by $-q\nabla A_0 - q\, \partial\boldsymbol{A}/\partial t$ from equation (2.9). For the electrostatic field the electric force is $q\boldsymbol{E}_0 = -q\nabla V$, so qV is a true potential energy. There is thus a fundamental difference between the time-dependent and time-independent cases (Yang 1976). Of course, the potential energy is not a Lorentz invariant concept, but nevertheless it can be useful. For example, in the hydrogen atom problem it is natural to choose the frame in which the proton is at rest. Then the interaction between the proton and the electron is a static Coulomb potential.

The operator $H(\boldsymbol{A}, 0)$ satisfies condition (i) that its expectation value is gauge invariant. The operator $H(\boldsymbol{A}, 0)$ is form invariant under gauge transformation on the operator, since

$$H'(\boldsymbol{A}, 0) = H(\boldsymbol{A}', 0). \tag{2.19}$$

By equation (2.14) its expectation value is therefore independent of the gauge.

In order to show more definitively that $H(\boldsymbol{A}, 0)$ is the energy operator for the particle, the correspondence principle can be used. If $H(\boldsymbol{A}, 0)$ is the energy operator, then according to the condition (ii) the time rate of change of its expectation value is (Yang 1976)

$$\mathrm{d}\langle\psi|H(\boldsymbol{A}, 0)\psi\rangle/\mathrm{d}t = \langle\psi|P\psi\rangle, \tag{2.20}$$

where P is the power operator for the particle. Using the equation of motion in equation (2.1), the time rate of change of the average value of $H(\boldsymbol{A}, 0)$ is

$$\mathrm{d}\langle\psi|H(\boldsymbol{A}, 0)\psi\rangle/\mathrm{d}t = -\mathrm{i}\langle\psi|[H(\boldsymbol{A}, 0), H(\boldsymbol{A}, A_0)]\psi\rangle + \langle\psi|\partial H(\boldsymbol{A}, 0)/\partial t|\psi\rangle. \tag{2.21}$$

The last term in equation (2.21) can be rewritten as

$$\langle\psi|\partial H(\boldsymbol{A}, 0)/\partial t|\psi\rangle = \mathrm{i}\langle\psi|[-\mathrm{i}\,\partial/\partial t, H(\boldsymbol{A}, 0)]\psi\rangle. \tag{2.22}$$

When equations (2.18) and (2.22) are substituted into equation (2.21), equation (2.20) is obtained with the power operator given by

$$P = \mathrm{i}[qA_0 - \mathrm{i}\,\partial/\partial t, H(\boldsymbol{A}, 0)]. \tag{2.23}$$

Because of equations (2.16) and (2.19) this operator is gauge invariant, as all physical observables must be. If the Dirac energy operator $H(\boldsymbol{A}, 0)$, obtained from equations (2.2) and (2.18), is used in equation (2.23), the power operator

$$P = q\boldsymbol{\alpha} \cdot \boldsymbol{E} = q\boldsymbol{v} \cdot \boldsymbol{E} \tag{2.24}$$

is obtained, where equation (2.9) has been used for the electric field of the electromagnetic radiation. The velocity operator $\boldsymbol{v}$ in the Dirac theory is $\boldsymbol{\alpha}$, expressed in units of the speed of light (Bjorken and Drell 1964). Since equation (2.24) is the same form as the classical power, our assumption that $H(\boldsymbol{A}, 0)$ is the energy operator for the particle is verified. To emphasise the importance of the energy operator, it is denoted by

$$\mathscr{E}(\boldsymbol{A}) = H(\boldsymbol{A}, 0) \tag{2.25}$$

in the following sections.

3. Time-dependent unitary transformations

When a unitary transformation is made on the wave equation in equation (2.1) the resulting equation is equivalent to it. However, in the case of a time-dependent unitary transformation a distinction must be made, just as in the last section, between the new Hamiltonian, which describes the temporal development of the transformed state, and the transformed energy operator. Since the original equation is invariant under gauge transformations, the unitarily transformed equation is also, as long as the unitary operator itself is gauge invariant. The point of view that considers an arbitrary unitary transformation as an operator gauge transformation (Goldman 1977) is discussed in the Appendix.

The Dirac equation in equation (2.1) can be transformed by an arbitrary unitary operator U, which gives

$$H_U(\boldsymbol{A}, A_0)\psi_U = \mathrm{i}\,\partial\psi_U/\partial t. \tag{3.1}$$

The unitarily transformed wavefunction is

$$\psi_U = U\psi, \tag{3.2}$$

and the new Hamiltonian is

$$H_U(\boldsymbol{A}, A_0) = UH(\boldsymbol{A}, A_0)U^{-1} - \mathrm{i}U\,\partial U^{-1}/\partial t. \tag{3.3}$$

The presence of the last term in equation (3.3) destroys the unitary equivalence between the new Hamiltonian and the old one, as Nieto (1977) has pointed out. It is the new Hamiltonian that describes the time evolution of the new wavefunction, but in the time-dependent case it is not the energy.

The energy operator $\mathscr{E}(\boldsymbol{A})$ of equation (2.25) can be unitarily transformed,

$$\mathscr{E}_U(\boldsymbol{A}) = U\mathscr{E}(\boldsymbol{A})U^{-1}. \tag{3.4}$$

The average energy of the system is thus unchanged under unitary transformation, since it is given by

$$\langle\psi|\mathscr{E}(\boldsymbol{A})\psi\rangle = \langle\psi_U|\mathscr{E}_U(\boldsymbol{A})\psi_U\rangle. \tag{3.5}$$

The unitarily transformed problem is thus completely equivalent to the original problem.

If a gauge transformation is made on the unitarily transformed equation, the equations are form invariant provided the unitary operator U is form invariant under gauge transformations. In general U can depend on $\boldsymbol{A}$ and A_0. The operator $U = U(\boldsymbol{A}, A_0)$ is gauge invariant as defined in equation (2.14) if it is form invariant under gauge transformations on the operator U,

$$U'(\boldsymbol{A}, A_0) = U(\boldsymbol{A}', A_0'), \tag{3.6}$$

where

$$U'(\boldsymbol{A}, A_0) = \exp(\mathrm{i}q\Lambda)U(\boldsymbol{A}, A_0)\exp(-\mathrm{i}q\Lambda) \tag{3.7}$$

as defined in equation (2.13). For U to be form invariant under gauge transformations, it must involve the form-invariant operators in equations (2.15) and (2.16) or not act on the space and time variables.

Under gauge transformation equation (3.1) is form invariant in the sense that

$$H_{U'}(\boldsymbol{A}', A_0')\psi'_{U'} = \mathrm{i}\,\partial\psi'_{U'}/\partial t. \tag{3.8}$$

The gauge-transformed new Hamiltonian is defined as in equation (3.3) with U, $\boldsymbol{A}$ and A_0 replaced by U', $\boldsymbol{A}'$ and A_0' respectively. The gauge-transformed new wavefunction is defined as in equation (3.2) with U and ψ replaced by U' and ψ' respectively. The gauge-transformed new energy operator is

$$\mathscr{E}_{U'}(\boldsymbol{A}') = U'\mathscr{E}'(\boldsymbol{A})U'^{-1}. \tag{3.9}$$

When the expectation value of this operator is taken in the state $\psi'_{U'}$, the value given in equation (3.5) is obtained. The importance of the gauge invariance of the unitarily transformed Dirac equation is shown in § 4 where the Foldy–Wouthuysen transformation is made.

4. Foldy–Wouthuysen transformation

The Foldy–Wouthuysen (FW) transformation (Foldy and Wouthuysen 1950) can be made on the Dirac equation to put it in a form in which the reduction to the non-relativistic Pauli equation can be made more easily (Bjorken and Drell 1964 ch 4, Kurşunoğlu 1962 pp 302–5). For a particle in a time-dependent electromagnetic field, the general FW transformation is a time-dependent unitary transformation of the kind discussed in the last section. The distinction is made in this section between the Hamiltonian with relativistic corrections, which describes the time development of the non-relativistic two-component spinor wavefunction, and the energy operator in the Pauli theory.

The reduction of the Dirac equation to the Pauli equation can be made without using the FW transformation (Pauli 1958, Löwdin 1964, Moss 1971). The four-component spinor in the Dirac equation can be separated into two equations involving the large and small components. One of the equations can be solved for the small component in terms of the large, and substituted into the other. This procedure can be performed in a completely gauge-invariant way, to any order in v/c. Consequently, it would be expected that the reduction based on the FW transformation could also be done in a gauge-invariant way. In this section the gauge invariance of the reduction is emphasised.

A good discussion of the FW transformation has been given by Bjorken and Drell (1964 ch 4). In order to remove the 'odd' terms to order m^{-3} in the Hamiltonian, it is necessary to make a succession of three unitary transformations. The unitary operator U of § 3 can be written as

$$U = U_3 U_2 U_1 \tag{4.1}$$

where

$$U_1 = \exp\{\beta\boldsymbol{\alpha}\cdot\boldsymbol{\pi}/2m\}, \tag{4.2}$$

$$U_2 = \exp\left\{\frac{\mathrm{i}\boldsymbol{\alpha}\cdot q(\boldsymbol{E}_0+\boldsymbol{E})}{4m^2} - \frac{\beta(\boldsymbol{\alpha}\cdot\boldsymbol{\pi})^3}{6m^3}\right\}, \tag{4.3}$$

and

$$U_3 = \exp\left\{\frac{-\beta\boldsymbol{\alpha}\cdot q\,\partial\boldsymbol{E}/\partial t}{8m^3}\right\}. \tag{4.4}$$

The electric field of the radiation $\boldsymbol{E}$ is given by equation (2.9) and the electrostatic field is $\boldsymbol{E}_0 = -\nabla V$, the negative gradient of the electrostatic potential V in equation (2.2). The operator $\boldsymbol{\pi}$ is the kinematical momentum operator,

$$\boldsymbol{\pi} = \boldsymbol{p} - q\boldsymbol{A}, \tag{4.5}$$

which is gauge invariant according to equation (2.15). Since the unitary operators in equations (4.2)–(4.4) involve only $\boldsymbol{\pi}$ or $\boldsymbol{E}$, they are gauge invariant in the sense given in equations (3.6) and (3.7).

The unitary transformation in equation (4.1) can be used in equation (3.3), or the unitary transformations in equations (4.2)–(4.4) can be applied successively, with the same results. The transformed Hamiltonian in equation (3.3) becomes†

$$\begin{aligned} H_U(\boldsymbol{A}, A_0) = {} & m\beta - m + \beta(\boldsymbol{\alpha}\cdot\boldsymbol{\pi})^2/2m + qA_0 + qV - (q/8m^2)\nabla\cdot(\boldsymbol{E}_0+\boldsymbol{E}) \\ & + (q/8m^2)\boldsymbol{\Sigma}\cdot[\boldsymbol{\pi}\times(\boldsymbol{E}_0+\boldsymbol{E}) - (\boldsymbol{E}_0+\boldsymbol{E})\times\boldsymbol{\pi}] + \mathrm{O}(m^{-3}), \end{aligned} \tag{4.6}$$

where the 4×4 matrix $\boldsymbol{\Sigma}$ is defined as

$$\boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix}, \tag{4.7}$$

and $\boldsymbol{\sigma}$ are the 2×2 Pauli matrices. The electrostatic field is $\boldsymbol{E}_0 = -\nabla V$.

The Pauli equation can be obtained by applying the projection operators

$$P_\pm = \tfrac{1}{2}(1\pm\beta) \tag{4.8}$$

(which form a resolution of the identity) to the unitarily transformed Dirac equation in equation (3.1). The Pauli equation is

$$H^{\mathrm{P}}(\boldsymbol{A}, A_0)\psi^{\mathrm{P}} = \mathrm{i}\,\partial\psi^{\mathrm{P}}/\partial t \tag{4.9}$$

† A trivial gauge transformation on the wavefunction of $\exp(-\mathrm{i}mt)$ can be made in equation (2.1) which results in the subtraction of the rest energy in equation (4.6).

where the Pauli wavefunction is $\psi^{\mathrm{P}} = P_+\psi_U$ and the Pauli Hamiltonian is $H^{\mathrm{P}}(\boldsymbol{A}, A_0) = P_+H_U(\boldsymbol{A}, A_0)P_+$. In the space of 2×2 matrices the Pauli Hamiltonian is

$$H^{\mathrm{P}}(\boldsymbol{A}, A_0) = (1/2m)(\boldsymbol{\sigma}\cdot\boldsymbol{\pi})^2 + qA_0 + qV - (q/8m^2)\boldsymbol{\nabla}\cdot(\boldsymbol{E}_0+\boldsymbol{E}) - (q/8m^2)\boldsymbol{\sigma}\cdot[(\boldsymbol{E}_0+\boldsymbol{E})\times\boldsymbol{\pi} - \boldsymbol{\pi}\times(\boldsymbol{E}_0+\boldsymbol{E})] + \mathrm{O}(m^{-3}), \tag{4.10}$$

which is the operator that describes the time evolution of the wavefunction by equation (4.9). The relativistic corrections in equation (4.10) are manifestly gauge invariant.†

The Hamiltonian in equation (4.10) is not gauge invariant because of the qA_0 term in it, although the relativistic corrections are manifestly gauge invariant. Goldman (1977) interprets the Dirac Hamiltonian as the energy operator. He is then concerned because in equation (4.10) the $-\partial\boldsymbol{A}/\partial t$ part of $\boldsymbol{E}$ in equation (2.9) comes from the last term in equation (3.3), which he says gives a spurious contribution to the energy. According to him the correct energy operator for the Pauli equation would be obtained by omitting the last term in equation (3.3) which would make it unitarily equivalent to the Dirac Hamiltonian. Then the Pauli energy operator would be equation (4.10) with $\boldsymbol{E}$ replaced by $-\nabla A_0$, which is gauge dependent. He writes, 'It seems as if we have run into a direct conflict between physical meaning in terms of unitary equivalence and in terms of explicit gauge invariance . . .' (Goldman 1977). According to Goldman (1977) the source of this problem is 'the Hamiltonian formulation of an external field problem in a gauge theory.' The problem is actually due to his incorrect identification of the Dirac Hamiltonian $H(\boldsymbol{A}, A_0)$ with the energy operator in the time-dependent case.

As we have seen in § 2, the Hamiltonian $H(\boldsymbol{A}, A_0)$ is not the same as the energy operator $\mathscr{E}(\boldsymbol{A}) = H(\boldsymbol{A}, 0)$ when a time-dependent external field is applied. The unitarily transformed energy operator in equation (3.4) becomes the energy operator for the non-relativistic problem when the FW of equation (4.1) is used and the positive energy part is projected out. The Pauli energy operator $\mathscr{E}^{\mathrm{P}} = P_+U\mathscr{E}(\boldsymbol{A})U^{-1}P_+$ is

$$\mathscr{E}^{\mathrm{P}} = (1/2m)(\boldsymbol{\sigma}\cdot\boldsymbol{\pi})^2 + qV - (q/8m^2)\boldsymbol{\nabla}\cdot\boldsymbol{E}_0 - (q/8m^2)\boldsymbol{\sigma}\cdot(\boldsymbol{E}_0\times\boldsymbol{\pi} - \boldsymbol{\pi}\times\boldsymbol{E}_0). \tag{4.11}$$

The energy operator is thus the Hamiltonian in equation (4.10) without the scalar potential of the time-dependent field A_0, and without the time-dependent radiation electric field $\boldsymbol{E}$. It is this operator $\mathscr{E}^{\mathrm{P}}$ which should be used to calculate the energy expectation value in equation (3.5), not equation (4.10). It is also the operator whose eigenstates are the basis functions for perturbation theory. In § 5 the non-relativistic limit of the power operator in equation (2.24) is obtained.

5. Non-relativistic limit of the power operator

In this section we show that the expectation value of the Pauli energy operator $\mathscr{E}^{\mathrm{P}}$ in equation (4.11) satisfies the condition that its time rate of change is equal to the average power transferred to the particle. This expression is the analogue for the Pauli energy operator of equation (2.20) for the Dirac energy operator.

If equation (2.20) is unitarily transformed it becomes

$$\mathrm{d}\langle\psi_U|\mathscr{E}_U(\boldsymbol{A})\psi_U\rangle/\mathrm{d}t = \langle\psi_U|P_U\psi_U\rangle \tag{5.1}$$

† Goldman (1977), Nieto (1977) and Bjorken and Drell (1964 ch 4) have the term $\boldsymbol{E}\times\boldsymbol{p}$ in their Hamiltonian instead of $\boldsymbol{E}\times\boldsymbol{\pi}$. The term $\boldsymbol{E}\times\boldsymbol{p}$ is not form invariant under a gauge transformation on the operator in equation (2.13).

where the unitarily transformed Dirac power operator P defined in equation (2.24) is

$$P_U = UPU^{-1}. \tag{5.2}$$

If we insert into equation (5.1) the resolution of the identity

$$P_+ + P_- = 1, \tag{5.3}$$

where $P_\pm$ is given in equation (4.8), and neglect terms of $O(m^{-3})$, we obtain

$$(\mathrm{d}/\mathrm{d}t)\langle\psi^{\mathrm{P}}|\mathscr{E}^{\mathrm{P}}\psi^{\mathrm{P}}\rangle = \langle\psi^{\mathrm{P}}|P^{\mathrm{P}}\psi^{\mathrm{P}}\rangle. \tag{5.4}$$

The Pauli power operator P^{P} is defined as

$$P^{\mathrm{P}} = P_+ P_U P_+, \tag{5.5}$$

when the unitary transformation U given in equation (4.1) is used. Equation (5.4) can be derived by using the fact that the negative energy part of the spinor wavefunction is $P_-\psi_U = O(m^{-3})\psi^{\mathrm{P}}$, which follows by applying P_- to equation (3.1) and using equation (4.11).

The projection operators in equation (5.5) eliminate the odd terms which appear in P_U and we obtain to order m^{-3} for the Pauli power operator

$$P^{\mathrm{P}} = (q/2m)(\boldsymbol{\pi}\cdot\boldsymbol{E} + \boldsymbol{E}\cdot\boldsymbol{\pi}) - (q/2m)\boldsymbol{\sigma}\cdot(\partial\boldsymbol{B}/\partial t) - (q^2/2m^2)(\boldsymbol{\sigma}\times\boldsymbol{E}_0)\cdot\boldsymbol{E}, \tag{5.6}$$

where $\boldsymbol{E}$ is the radiation electric field in equation (2.9) and $\boldsymbol{E}_0$ is the electrostatic field, $\boldsymbol{E}_0 = -\nabla V$.

In the Pauli theory the velocity operator $\boldsymbol{v}$ is

$$\begin{aligned}\boldsymbol{v} &= (\mathrm{i}\hbar)^{-1}[\boldsymbol{r}, H^{\mathrm{P}}(\boldsymbol{A}, A_0)] \\ &= (\boldsymbol{\pi}/m) - (q/4m^2)\boldsymbol{\sigma}\times(\boldsymbol{E}_0 + \boldsymbol{E}).\end{aligned} \tag{5.7}$$

Therefore equation (5.6) for the Pauli power operator can be written as

$$P^{\mathrm{P}} = (q/2)(\boldsymbol{v}\cdot\boldsymbol{E} + \boldsymbol{E}\cdot\boldsymbol{v}) - (q/2m)\boldsymbol{\sigma}\cdot(\partial\boldsymbol{B}/\partial t) - (q^2/4m^2)[\boldsymbol{\sigma}\times(\boldsymbol{E}_0 + \boldsymbol{E})]\cdot\boldsymbol{E}. \tag{5.8}$$

The first term on the right-hand side of equation (5.8) is the usual Hermitian power operator involving the velocity operator (Yang 1976). The middle term on the right-hand side is the power absorbed due to the particle having a magnetic moment given by $\boldsymbol{\mu} = 2(q/2m)(\frac{1}{2}\boldsymbol{\sigma})$ which results in an energy $-\boldsymbol{\mu}\cdot\boldsymbol{B}$ in the magnetic field $\boldsymbol{B}$. To obtain this result Faraday's law is used. The last term is due to the spin–orbit interaction in equation (4.10). For a classical interpretation of all these terms see Yang and Hirschfelder (1979). Therefore the operator $\mathscr{E}^{\mathrm{P}}$ is the appropriate Pauli energy operator, since the time rate of change of its average value is the average power transferred to the electron.

6. Perturbation theory

In order to solve the Dirac equation in equation (2.1), it is usually necessary to use perturbation theory. In this section a gauge-invariant perturbation theory is developed†, which is also shown to be invariant under arbitrary unitary transformations. In particular, the FW transformation of § 4 can be used for the unitary transformation and in the non-relativistic limit the resulting equation is the same as

† For the non-relativistic case see Yang (1976) and Kobe and Smirl (1978).

would have been obtained by using the Pauli equation in equation (4.9). Therefore it makes no difference whether the perturbation theory for the Dirac equation is solved in the non-relativistic limit, or whether the non-relativistic Pauli equation is solved by perturbation theory.

To develop a gauge-invariant perturbation theory (Yang 1976), it is necessary to use the eigenstates ψ_n of the energy operator. For the Dirac equation in equation (2.1) the energy operator is $\mathscr{E}(\boldsymbol{A}) = H(\boldsymbol{A}, 0)$ which satisfies the eigenvalue problem

$$\mathscr{E}(\boldsymbol{A})\psi_n = \epsilon_n \psi_n, \tag{6.1}$$

with eigenvalues ϵ_n. Since the vector potential is a function of time, the eigenstates ψ_n and eigenvalues ϵ_n will also be functions of time. Equation (6.1) is form invariant under the gauge transformation in equation (2.5). The solutions to equation (2.1) can be expanded in terms of the complete set of states $\{\psi_n\}$,

$$\psi = \sum_n c_n \psi_n, \tag{6.2}$$

where c_n is the gauge-invariant probability amplitude for finding the system in the state ψ_n with energy ϵ_n. If equation (6.2) is substituted into equation (2.1), the resulting gauge-invariant equation for the probability amplitudes is

$$(\mathrm{i}\,\partial/\partial t - \epsilon_n)c_n = \sum_m \langle \psi_n | (qA_0 - \mathrm{i}\,\partial/\partial t)\psi_m \rangle c_m. \tag{6.3}$$

Equation (6.3) can be rewritten in terms of the power operator in equation (2.23) in the non-degenerate case as (Yang 1976)

$$(\mathrm{i}\,\partial/\partial t - \tilde{\epsilon}_n)c_n = \sum_{m \neq n} \mathrm{i}(\epsilon_n - \epsilon_m)^{-1} \langle \psi_n | P\psi_m \rangle c_m. \tag{6.4}$$

The dressed energy $\tilde{\epsilon}_n$ in equation (6.4) is defined as

$$\tilde{\epsilon}_n = \epsilon_n + \langle \psi_n | (qA_0 - \mathrm{i}\,\partial/\partial t)\psi_n \rangle, \tag{6.5}$$

and is gauge invariant. It is therefore the gauge-invariant power operator in equation (6.4) that induces the transitions between states. For the Dirac equation the power operator is given in equation (2.24).

Not only is the perturbation theory invariant under gauge transformations, it is also invariant under the time-dependent unitary transformations discussed in § 3. Under the unitary transformation U, equation (6.1) becomes

$$\mathscr{E}_U(\boldsymbol{A})\psi_{nU} = \epsilon_n \psi_{nU}, \tag{6.6}$$

where the energy operator is defined in equation (3.4) and the state is defined in equation (3.2). The expansion of the wavefunction in equation (6.2) becomes

$$\psi_U = \sum_n c_n \psi_{nU}. \tag{6.7}$$

The coefficients c_n and the eigenenergies ϵ_n are unchanged under the unitary transformation. Equation (6.3) for the coefficients c_n becomes

$$(\mathrm{i}\,\partial/\partial t - \epsilon_n)c_n = \sum_m \langle \psi_{nU} | U(qA_0 - \mathrm{i}\,\partial/\partial t)U^{-1}\psi_{mU} \rangle c_m. \tag{6.8}$$

Equation (6.4) for the coefficients also has the same form after the unitary transformation,

$$(\mathrm{i}\,\partial/\partial t-\tilde{\epsilon}_n)c_n=\sum_{m\neq n}\mathrm{i}(\epsilon_n-\epsilon_m)^{-1}\langle\psi_{mU}|P_U\psi_{mU}\rangle c_m, \tag{6.9}$$

where $\tilde{\epsilon}_n$ is given by equation (6.5) with the states and operator in the matrix element unitarily transformed and P_U is defined in equation (5.2).

The unitary operator U for the FW transformation is given by equation (4.1). The unperturbed eigenvalue problem in equation (6.6) then becomes

$$\mathscr{E}^{\mathrm{P}}\psi_n^{\mathrm{P}}=\epsilon_n\psi_n^{\mathrm{P}}, \tag{6.10}$$

in which the energy operator is given by equation (4.11) and where $\psi_n^{\mathrm{P}}=P_+\psi_{nU}$. The negative energy part of the wavefunction $P_-\psi_{nU}=\mathrm{O}(m^{-3})\psi_n^{\mathrm{P}}$ is neglected here. Equation (6.8) then becomes

$$(\mathrm{i}\,\partial/\partial t-\epsilon_n)c_n=\sum_m\langle\psi_n^{\mathrm{P}}|\{qA_0-\mathrm{i}\,\partial/\partial t-(q/8m^2)\boldsymbol{\nabla}\cdot\boldsymbol{E}$$
$$-(q/8m^2)\boldsymbol{\sigma}\cdot(\boldsymbol{E}\times\boldsymbol{\pi}-\boldsymbol{\pi}\times\boldsymbol{E})\}\psi_m^{\mathrm{P}}\rangle c_m, \tag{6.11}$$

when equation (4.1) is used. Equation (6.11) is the equation we would obtain if we treated the terms in the Hamiltonian in equation (4.10) by perturbation theory†. Likewise equation (6.9) becomes

$$(\mathrm{i}\,\partial/\partial t-\tilde{\epsilon}_n)c_n=\sum_{m\neq n}\mathrm{i}(\epsilon_n-\epsilon_m)^{-1}\langle\psi_n^{\mathrm{P}}|P^{\mathrm{P}}\psi_m^{\mathrm{P}}\rangle c_m, \tag{6.12}$$

on neglecting the negative energy contribution to the matrix element and using the Pauli power operator in equation (5.5). The dressed energy is

$$\tilde{\epsilon}_n=\epsilon_n+\langle\psi_n^{\mathrm{P}}|\{qA_0-\mathrm{i}\,\partial/\partial t-(q/8m^2)\boldsymbol{\nabla}\cdot\boldsymbol{E}-(q/8m^2)\boldsymbol{\sigma}\cdot(\boldsymbol{E}\times\boldsymbol{\pi}-\boldsymbol{\pi}\times\boldsymbol{E})\}\psi_n^{\mathrm{P}}\rangle, \tag{6.13}$$

where the matrix element is the diagonal element of the interaction terms in equation (4.10). The Pauli power operator in this case up to order m^{-3} is given in equation (5.6).

In most cases the eigenvalue problem in equation (6.10) must be solved by perturbation theory for the eigenstates ψ_n^{P} and eigenvalues ϵ_n. These would then be used in equation (6.11) or (6.12) to obtain the probability amplitudes c_n for transitions. The advantage of this procedure is that it is manifestly gauge invariant, so that gauge-invariant results are guaranteed.

7. Conclusion

In this paper we have shown that in the case of an electron in an external time-dependent electromagnetic field, the Dirac theory reduces in a completely gauge-invariant way to the Pauli theory. Although in each case the Hamiltonian is not form invariant under gauge transformations, the energy operator is. The use of the energy operator resolves the problem formulated by Goldman (1977) and Nieto (1977) that the energy, which is an observable, is given by the expectation value of a gauge-dependent operator.

† The term $-\mathrm{i}\,\partial/\partial t$ on the right-hand side of equation (6.11) would not be obtained if the perturbation were time independent, and occurs in our case because the state ψ_m^{P} can be time dependent.

In a time-dependent external electromagnetic field, the Hamiltonian determines the time evolution of the state vector. Its expectation value is gauge dependent, and thus cannot be the energy. On the other hand, the energy operator is an operator which has a gauge-invariant expectation value whose time rate of change is the average power transferred to the particle by the external field.

Since the FW transformation is a unitary transformation which is form invariant under gauge transformation, it preserves the gauge invariance of the expectation value of the Dirac energy operator. The Dirac energy reduces to the Pauli energy to a given order in v/c. There is therefore no gauge problem in the reduction of the Dirac theory to the Pauli theory. The physics of a slowly moving electron should not depend on whether it is described by the Dirac equation or the Pauli equation, or in what gauge it is described. The theory presented here is in keeping with these general principles of physics.

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Appendix. Operator gauge transformation on electromagnetic potentials

If it is demanded that under an *arbitrary* unitary transformation the transformed equations (3.1) have the same form as the original Dirac equation in equation (2.1), the electromagnetic potentials must undergo an operator gauge transformation (OGT)†. In the external field problem considered here, the electromagnetic field is unquantised. Thus the only physically meaningful transformations of the potentials are the gauge transformations in equations (2.7) and (2.8). Otherwise the electric and magnetic fields would not be obtained from equations (2.9) and (2.10). However, there is no physical reason for demanding form invariance under *arbitrary* unitary transformations that do not correspond to basic symmetry principles.

To be more specific, let us consider the conceptual difficulties which arise when it is demanded that equation (2.1) be form invariant under any arbitrary unitary transformation in the sense that

$$H(\tilde{A}^i, \tilde{A}^0)\tilde{\psi} = \mathrm{i}\, \partial\tilde{\psi}/\partial t \tag{A1}$$

where $i = 1, 2, 3$, $A^0 = A_0$, and $\tilde{\psi} \equiv \psi_U$. But from equation (3.3) the operator describing

† A distinction should be made between different types of operator gauge transformations. The type considered by Goldman (1977) are not the same as gauge transformations on the vector potential operator in QED (Corinaldesi and Roman 1965, Gaisser 1966).

the time development of $\psi_U = \tilde{\psi}$ is

$$\tilde{H}(A^i, A^0) = UH(A^i, A^0)U^{-1} - \mathrm{i}U\,\partial U^{-1}/\partial t. \qquad \text{(A2)}$$

As we have seen, this operator is not the transformed energy operator, which is $\mathscr{E}_U(\boldsymbol{A})$. The demand for form invariance between equations (2.1) and (A1) requires that the operator $\tilde{H}$ in equation (A2) be written in the same form as equation (2.2),

$$\tilde{H}(A_i, A^0) = H(\tilde{A}_i, \tilde{A}^0) = \tilde{\alpha}_i(p_i + q\tilde{A}_i) + \tilde{\beta}m + q\tilde{A}_0 + q\tilde{V}, \qquad \text{(A3)}$$

where the Einstein summation convention is used.† The operator gauge transformed potentials $\tilde{A}_\mu = (\tilde{A}^0, -\tilde{A}^1, -\tilde{A}^2, -\tilde{A}^3)$ are defined as

$$\tilde{A}_\mu = UA_\mu U^{-1} - \mathrm{i}q^{-1}U\,\partial U^{-1}/\partial x^\mu. \qquad \text{(A4)}$$

The Dirac matrices in equation (A3) are also transformed:

$$\tilde{\alpha}_i = U\alpha_i U^{-1}, \qquad \tilde{\beta} = U\beta U^{-1}, \qquad \text{(A5)}$$

as well as the electrostatic potential

$$\tilde{V} = UVU^{-1}. \qquad \text{(A6)}$$

However, these transformations are only of a formal significance unless equation (A4) reduces to equations (2.7) and (2.8). In general, the quantities $\tilde{A}_\mu$ are no longer electromagnetic potentials in the usual sense. In particular, when equation (A4) is substituted into the right-hand side of equations (2.9) and (2.10) the result is not the electric and magnetic fields, unless U is the gauge transformation in equation (2.5). Therefore the condition of form invariance under an arbitrary unitary transformation is physically meaningless in this case.

Although there is a formal similarity between equation (A4) and gauge transformations in non-Abelian gauge theories, the similarity has no physical content. The electromagnetic field here is unquantised and the group U(1) for electromagnetism is Abelian. It is only when the unitary operator U is a representation of U(1) that the transformation in equation (A4) makes physical sense for electromagnetism (Abers and Lee 1973 equations (1.23) and (1.36)).

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† The minus sign in equation (2.2) occurs because $\boldsymbol{A}$ has contravariant components, whereas covariant components A_i are used in equation (A3).

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