Foldy–Wouthuysen transformation, scalar potentials and gravity

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Abstract
We show that care is required in formulating the nonrelativistic limit of generalized Dirac Hamiltonians which describe particles and antiparticles interacting with static electric and/or gravitational fields. The Dirac–Coulomb and the Dirac–Schwarzschild Hamiltonians, and the corrections to the Dirac equation in a non-inertial frame, according to general relativity, are used as example cases in order to investigate the unitarity of the standard and ‘chiral’ approaches to the Foldy–Wouthuysen transformation, and spurious parity-breaking terms. Indeed, we find that parity-violating terms can be generated by unitary pseudo-scalar transformations (‘chiral’ Foldy–Wouthuysen transformations). Despite their interesting algebraic properties, we find that ‘chiral’ Foldy–Wouthuysen transformations change fundamental symmetry properties of the Hamiltonian and do not conserve the physical interpretation of the operators. Supplementing the discussion, we calculate the leading terms in the Foldy–Wouthuysen transformation of the Dirac Hamiltonian with a scalar potential (of the $1/r$-form and of the confining radially symmetric linear form), and obtain compact expressions for the leading higher-order corrections to the Dirac Hamiltonian in a non-inertial rotating reference frame (‘Mashhoon term’).

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1. Introduction

A (generalized) Dirac Hamiltonian describes the quantum dynamics of a spin-1/2 particle including all relativistic corrections, in the presence of external fields. Examples include the Dirac–Coulomb (DC) Hamiltonian [1–3], which describes the motion of a particle bound to the Coulomb field of a nucleus (in the non-recoil approximation), and the Dirac–Schwarzschild (DS) Hamiltonian [4–6], which describes the motion of a particle in the curved space-time around a planet or black hole. The Foldy–Wouthuysen transformation [1] of the Dirac Hamiltonian identifies the nonrelativistic limit and the relativistic correction terms. Let us briefly recall the basic properties. A static, noninteracting Dirac particle is described by the Hamiltonian

$$\beta m,$$

where $\beta$ is the Dirac $\beta$ matrix with eigenvalues $\pm 1$, and $m$ is the particle mass. The energy eigenvalues at rest are thus given as $\pm m$, where the positive sign describes particles, and the negative sign describes antiparticles (we set $\hbar = c = \epsilon_0 = 1$ in this paper). The nonrelativistic kinetic energy reads as $\vec{p}^2/(2m)$. Relativistic corrections of order $\vec{p}^4$ and higher in the momenta can be derived from the Foldy–Wouthuysen transformation. The most important property of the Foldy–Wouthuysen transformation consists in the disentanglement of the particle and antiparticle terms and the identification of ‘effective’ Hamiltonians which govern the quantum dynamics of the particles and antiparticles.

The hierarchy of the terms in the Foldy–Wouthuysen leads to a consistent perturbative formalism. The so-called Thomas precession of a spinning particle bound to a Coulomb field [1–3], or the Fokker precession of a spinning particle in a gravitational field [6–9], can be calculated on the basis of the Foldy–Wouthuysen transformation. In higher orders, the calculation of the Foldy–Wouthuysen transformation can be difficult, notably, when corrections to the transition current have to be included [6, 10]. Thus, alternative approaches to the calculation of the Foldy–Wouthuysen transformation have been considered, with the eventual hope of simplifying the calculation substantially (see [4, 11, 12] and references therein). Typically, the alternative approaches involve chiral transformations, still unitary, with the Dirac $\gamma^5$ matrix. In principle, the alternative approach, which is based on interesting algebraic identities [4, 11, 12], has the potential of fundamentally simplifying the approach to obtaining the relativistic correction terms and could potentially simplify quantum electrodynamic bound-state calculations. Here, we compare the original Foldy–Wouthuysen approach, and the chiral approach, using a number of example calculations based on the Dirac Hamiltonians in the Coulomb field, in the Schwarzschild metric, in a non-inertial frame, and for a Dirac particle bound in a scalar potential (SP). The physical problems studied here are introduced in section 2, together with a brief explanation of the standard and chiral Foldy–Wouthuysen (CFW) transformations, whereas concrete calculations are reserved for section 3. Conclusions are drawn in section 4. The interpretation of the spin operator in the context of the chiral method is discussed in the appendix.

2. Relativistic formalism: outline of the problem

2.1. Generalized Dirac Hamiltonians

We shall investigate the Dirac equation for spin-1/2 particles, $i\hbar \dot{\psi}(t, \vec{r}) = H\psi(t, \vec{r})$, where $H$ is a (generalized) Dirac Hamiltonian, $t$ is the time coordinate, and $\psi$ is a four-component (bispinor) wave function. The Hamiltonian $H$ is a $(4 \times 4)$ matrix in spinor space. The free Dirac Hamiltonian is given by the expression

$$H_\psi = \vec{\alpha} \cdot \vec{p} + \beta m.$$  (1)
The momentum operator is $\vec{p}$ and the mass of the particle is denoted as $m$. The Dirac matrices $\gamma^i = \gamma^0 \gamma^i$ (for $i = 1, 2, 3$) and $\beta = \gamma^0$ are used in the Dirac representation,

$$\gamma^0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \vec{\gamma} = \begin{pmatrix} 0 & \vec{\sigma} \\ -\vec{\sigma} & 0 \end{pmatrix}, \quad \gamma^5 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \quad (2)$$

These matrices fulfil the relation $\{\gamma^\mu, \gamma^\nu\} = 2g^\mu{}^\nu$ in ‘West-coast’ conventions with $g^{\mu\nu} = \text{diag}(1, -1, -1, -1)$. The DC Hamiltonian is given by the expression

$$H_{\text{DC}} = \vec{\alpha} \cdot \vec{p} + \beta m - \frac{Z\alpha}{r}, \quad (3)$$

where $Z$ is the nuclear charge number, $\alpha$ is the fine-structure constant, and $r = |\vec{r}|$ is the distance from the nucleus. By contrast, the SP multiplies the $\beta$ matrix,

$$H_{\text{SP}} = \vec{\alpha} \cdot \vec{p} + \beta \left( m - \frac{\lambda}{r} \right), \quad (4)$$

where $\lambda$ is a coupling parameter. The Hamiltonian (4) can be used as a rough approximation to nuclear attractive forces, mediated by meson exchange [13]. The Dirac Hamiltonian with a radially symmetric, linear confining potential is

$$H_{\text{LC}} = \vec{\alpha} \cdot \vec{p} + \beta \left( m + 2\alpha^2 r \right), \quad (5)$$

where $\alpha$ is a symbolic parameter governing the expansion about the nonrelativistic limit. Namely, for the Foldy–Wouthuysen transformation to be physically meaningful, the term $\beta m$ in the Hamiltonian needs to dominant in the nonrelativistic limit. This implies that the linear confining potential must be shallow or the bound particle is always relativistic, in which case the Foldy–Wouthuysen transform should not be applied. If we then expand in the momenta $p_i \sim \alpha$ and distances $r \sim \alpha^{-1}$, we obtain a meaningful expansion about the nonrelativistic limit.

The DS Hamiltonian reads as follows [4–6],

$$H_{\text{DS}} = \frac{1}{2} \left\{ \vec{\alpha} \cdot \vec{p}, \left( 1 - \frac{r^2}{r_s^2} \right) \right\} + \beta m \left( 1 - \frac{r_s}{2r} \right), \quad (6)$$

where $\{., .\}$ denotes the anticommutator. The Schwarzschild radius is given as $r_s = 2GM$, where $G$ is Newton’s gravitational constant, and $M$ is the mass of the planet or gravitational centre. The Dirac Hamiltonian in a non-inertial frame [14, 15] reads as

$$H_{\text{SF}} = (1 + \vec{\alpha} \cdot \vec{r})\beta m + \frac{1}{2} \left( 1 + \vec{\alpha} \cdot \vec{r}, \vec{\alpha} \cdot \vec{p} \right) - \vec{\omega} \cdot \left( \vec{L} + \frac{1}{2} \vec{\Sigma} \right), \quad (7)$$

where $\vec{\alpha}$ is the acceleration with respect to the inertial reference frame. The term involving the proper angular rotation frequency $\vec{\omega}$ is otherwise known as the Mashhoon term [16].

### 2.2. Standard Foldy–Wouthuysen transformation

For the Foldy–Wouthuysen transformation [1] one divides a Dirac Hamiltonian $H$ into even and odd (in spinor space) parts, canonically denoted as $\mathcal{E}$ and $\mathcal{O}$. The even and odd parts of a general operator $H$ are defined as follows,

$$\{H\} = \frac{1}{2} \left( H + \beta H \beta \right), \quad \{H\}_{\text{odd}} = \frac{1}{2} \left( H - \beta H \beta \right). \quad (8)$$

One identifies

$$\mathcal{E} = \{H\}_{\text{even}}, \quad \mathcal{O} = \{H\}_{\text{odd}}. \quad (9)$$

For the free Dirac–Hamiltonian (1), one writes

$$\mathcal{E} = \beta m, \quad \mathcal{O} = \vec{\alpha} \cdot \vec{p}. \quad (10)$$
In the Dirac representation, the $\beta$ matrix anticommutes with any odd operator, and the term $\beta m$, which describes a nonrelativistic particle at rest, actually is retained upon iterating the Foldy–Wouthuysen transformation [1, 2, 6]. One defines the Hermitian operator $S$ and the unitary transformation $U$ as follows,

$$S = -i\frac{\beta}{2m}O, \quad U = \exp(iS).$$

The Foldy–Wouthuysen transformation is calculated as the multi-commutator expansion

$$H' = UHU^+ = \exp(iS)H \exp(-iS)$$

$$= H + i[S, H] + \frac{i^2}{2!}[S, [S, H]] + \cdots,$$

and it is easy to check that the first commutator $i[S, H] \approx i[S, \beta m] = -O$

generates a term which eliminates the odd operator $O$ from the transformed Hamiltonian $H'$. However, many more (possibly odd) terms are generated by the higher-order terms in the Foldy–Wouthuysen Hamiltonian, which may have to be eliminated using subsequent transformations $U, U', U''$, and so on, until all odd operators are eliminated up to a given order in the perturbative expansion. One usually defines a perturbative parameter (e.g., the power of the momentum operator, or, in classical terms, the velocity of the particle expressed in units of the speed of light) and keeps terms only up to a specified order in this parameter.

2.3. Chiral Foldy–Wouthuysen transformation

In [4, 11, 12], an alternative variant of the ‘Foldy–Wouthuysen’ transformation is proposed, which we would like to refer to as the ‘chiral’ Foldy–Wouthuysen transformation because it actually contains ‘chiral’ $\gamma^5$ matrices. At face value, the proposed method leads to an exact separation of the input Hamiltonian into even and odd contributions, which are straightforward to expand in the perturbative parameters. The proposed rotation contains a combination of two unitary transformations, which are both chiral,

$$U = U_2U_1, \quad U_1 = \frac{1}{\sqrt{2}}(1 + J\Lambda), \quad U_2 = \frac{1}{\sqrt{2}}(1 + \beta J).$$

The operators $\Lambda$ and $J$ are Hermitian roots of unity,

$$\Lambda = \frac{H}{\sqrt{H^2}}, \quad \Lambda^+ = \Lambda, \quad J = i\gamma^5 \beta, \quad J^+ = J, \quad \Lambda^2 = J^2 = 1.$$}

Of course, $H$ is the Hamiltonian that we are trying to transform, and it is understood that the square root of its square, $\sqrt{H^2}$, can be expanded easily in terms of the perturbative parameters. For the chiral transformation to work, it is essential that

$$\{\Lambda, J\} = [H, J] = \{\sqrt{H^2}, J\} = 0.$$

The following proof of the unitarity of $U$ depends on the property (16),

$$UU^+ = U_2U_1U_1^+U_2^+ = U_2\frac{1}{2}(1 + J\Lambda)(1 + \Lambda J)U_2^+$$

$$= \frac{1}{2}U_2(2 + J\Lambda + \Lambda J)U_2^+$$

$$= \frac{1}{2}(1 + \beta J)(2 + J\Lambda + \Lambda J)(1 + J\beta)$$

$$= \frac{1}{2}(2 + 2\beta J + J\Lambda + \beta J + \Lambda J + \beta J\Lambda J + 2J\beta + 2\beta JJ\beta + J\Lambda J + \beta J\Lambda J + \beta J\Lambda J + \beta J\Lambda J)$$

$$+ \beta \Lambda J + \Lambda JJ + \beta JJ\beta).$$
Taking notice of the properties (15) and (16), as well as the relation \( J\beta = -\beta J \), one can show that all terms in equation (17) mutually cancel except for
\[
UU^+ = \frac{1}{4} (2 + 2\beta JJ\beta) = 1.
\] (18)

The following surprisingly simple and elegant result \([4, 12]\) (after some manipulations which we give in detail) is central to the CFW transformation,
\[
UHU^+ = U_2 U_1 H U_1^+ U_2^+ = \frac{1}{4} U_2 (H + JA + J\lambda H + J\lambda J) U_2^+ = U_2 J\lambda H U_2^+ = \frac{1}{2} (1 + \beta J) J\lambda H (1 + J\beta)
= \frac{1}{2} (J\lambda H + \beta \lambda H + \lambda H \beta - \beta \lambda H \beta J)
= \frac{1}{2} \beta (\sqrt{H^2} + \beta \sqrt{H^2} \beta) + \frac{1}{2} (\sqrt{H^2} - \beta \sqrt{H^2} \beta) J
= \{\sqrt{H^2}\}_{\text{even}} \beta + \{\sqrt{H^2}\}_{\text{odd}} J.
\] (19)

The operator \( J \) is odd in spinor space, and both terms in the last line of equation (19) constitute even expressions in spinor space. One might thus assume that the CFW transformation considerably simplifies the identification of the nonrelativistic limit of generalized Dirac Hamiltonians. The transformed Hamiltonian is even in spinor space, and the (relativistic) expansion of the square root of the square of the ‘input’ Hamiltonian \( H \) is generally accomplished easily. The CFW transformation might thus completely eliminate the need for the complicated evaluation of multiple commutators, as would otherwise be the case for the standard Foldy–Wouthuysen (SFW) transformation. Conceivably, the CFW transformation would thus lead to a much simplified identification of higher-order terms in the Breit–Pauli Hamiltonian for atoms interacting with external fields, and quantization radiation fields, where considerable effort has been invested in recent years \([17–21]\) in the identification of the general \((Z\alpha)^6\) higher-order correction terms for bound systems.

3. Application to the Hamiltonians

3.1. Free Dirac and Dirac–Coulomb Hamiltonian

For the free Dirac Hamiltonian \( H_F = \vec{\alpha} \cdot \vec{p} + \beta m \) defined in equation (1), it is easy to verify that
\[
\{\vec{\alpha} \cdot \vec{p}, \ i\gamma^5 \beta\} = 0, \quad \{\beta m, \ i\gamma^5 \beta\} = 0, \quad \{H_F, J\} = 0.
\] (20)

The conditions for the application of the CFW transformation are thus fulfilled. One calculates
\[
H_F^2 = \vec{p}^2 + m^2, \quad \sqrt{H_F^2} = m + \frac{\vec{p}^2}{2m} - \frac{\vec{p}^4}{8m^3} + \cdots,
\] (21)

where the expansion is carried out in ascending powers of the momenta, and thus \( \{\sqrt{H_F^2}\}_{\text{even}} = \sqrt{H_F^2} \) while \( \{\sqrt{H_F^2}\}_{\text{odd}} \) vanishes. Formula (19) immediately leads to the result
\[
H_F^{(\text{CFW})} = \beta \left( m + \frac{\vec{p}^2}{2m} - \frac{\vec{p}^4}{8m^3} + \cdots \right),
\] (22)

where by the superscript CFW we denote the result of the CFW transformation. It is well known \([1, 2]\) that the SFW transformation leads to the same result,
\[
H_F^{(\text{SFW})} = H_F^{(\text{CFW})} = \beta \sqrt{\vec{p}^2 + m^2},
\] (23)
The first two terms fulfill the condition (16) (see equation (20)), but the third term fulfills

\[
[V, J] = \left[ -\frac{Z\alpha}{r}, i\gamma^5\beta \right] = 0,
\]

instead of the corresponding relation with the anticommutator. Therefore, strictly speaking, the conditions for the application of the CFW transformation are not fulfilled. A rather famous, yet distant, example is the use of asymptotic mathematical method leads to consistent results, even if the corresponding conditions, strictly speaking, are not fulfilled. A rather famous, yet distant, example is the use of asymptotic expansions in the non-asymptotic regime, which lead to perfectly consistent results if they are combined with suitable resummation prescriptions [22–24].

It is thus more than an academic exercise to apply the formalism of the CFW transformation to the DC Hamiltonian, and to investigate the results. We first square the DC Hamiltonian to find

\[
H_{\text{DC}}^2 = m^2 + \vec{p}^2 - \left\{ \vec{a} \cdot \vec{p}, \frac{Z\alpha}{r} \right\} - 2\beta m \frac{Z\alpha}{r} + \frac{Z^2 \alpha^2}{r^2}.
\]

It is easy to expand the square root of \(H_{\text{DC}}^2\) to second order in \(Z\alpha\),

\[
\sqrt{H_{\text{DC}}^2} \approx m + \frac{\vec{p}^2}{2m} - \frac{iZ\alpha}{2m^2} \vec{a} \cdot \vec{r} - \frac{Z\alpha}{mr} \vec{a} \cdot \vec{p} - \frac{Z\alpha^2}{r^2}.
\]

We here suppress the term \(\frac{Z^2 \alpha^2}{r^2}\) on the right-hand side because it is of order \((Z\alpha)^4 m\) (we recall that for atomic systems, \(\vec{p} \sim Z\alpha m\) and \(r \sim 1/(Z\alpha m)\), see [25, 26]). The two terms in equation (19) are then identified as follows,

\[
\sqrt{H_{\text{DC}}^2}\bigg|_{\text{even}} = \beta \left( m + \frac{\vec{p}^2}{2m} \right) - \frac{Z\alpha}{r},
\]

\[
\sqrt{H_{\text{DC}}^2}\bigg|_{\text{odd}} = -\frac{Z\alpha}{2m} \vec{\beta} \vec{\Sigma} \cdot \vec{r} - i\frac{Z\alpha}{mr} \vec{\beta} \vec{\Sigma} \cdot \vec{p}.
\]

Here, the vector of \((4 \times 4)\)-spin matrices has the representation \(\vec{\Sigma}^i = \gamma^5 \gamma^i \gamma^4\). The CFW transformation of the DC Hamiltonian,

\[
H_{\text{DC}}^{(\text{CFW})} = \beta \left( m + \frac{\vec{p}^2}{2m} \right) - \frac{Z\alpha}{r} + \frac{Z\alpha}{2m} \beta \vec{\Sigma} \cdot \vec{r} - i\frac{Z\alpha}{mr} \vec{\beta} \vec{\Sigma} \cdot \vec{p},
\]

is different from the result of the SFW transformation (see [1–3, 10, 26]), which reads as

\[
H_{\text{DC}}^{(\text{SFW})} \approx \beta \left( m + \frac{\vec{p}^2}{2m} \right) - \frac{Z\alpha}{r} + \frac{Z\alpha}{2m^2} \delta^{(3)}(\vec{r}) + \frac{Z\alpha}{4m^2 r^3} \vec{\Sigma} \cdot \vec{L}.
\]

to fourth order in \(Z\alpha\). In the latter result, the zitterbewegung term, and the Thomas precession term (spin–orbit coupling) are consistently taken into account. One may observe that the CFW transformation fails to reproduce the known result for the DC Hamiltonian, as a consequence of the fact that the condition for its application is not fulfilled, as shown in equation (25). Because the CFW is a one-step, ‘exact’ process, there is no possibility that the spurious terms
in equation (29) are eliminated upon the consideration of ‘higher orders’ in the transformation. One may also point out that the last term in the transformed Hamiltonian (29) is not even Hermitian, as a consequence of an application of the chiral transformation beyond its range of applicability. The manifest failure of the chiral method for the phenomenologically important case of the DC Hamiltonian indicates that the range of applicability of chiral transformation might be somewhat limited.

3.2. Dirac Hamiltonian with scalar \((1/r)\)-potential

In contrast to the DC Hamiltonian, the Dirac Hamiltonian with a SP, given in equation (4),

\[
H_{SP} = \bar{\alpha} \cdot \bar{p} + \beta \left( m - \frac{\lambda}{r} \right),
\]

fulfills the criteria for the application of the chiral transformation, because the anticommutator \([H_{SP}, J]\) vanishes. We recall that the name ‘SP’ is derived from the covariant representation of the corresponding Dirac equation,

\[
(i\gamma^\mu \partial_\mu - m + \lambda/r) \psi(t, \vec{r}) = 0,
\]

where the potential enters as a Lorentz scalar (the Einstein summation convention is used for the sum over \(\mu\)). We obtain for the square of the Hamiltonian,

\[
H_{SP}^2 \approx \bar{p}^2 + m^2 + \beta \left[ \bar{\alpha} \cdot \bar{p}, \frac{\lambda}{r} \right] - 2m\frac{\lambda}{r},
\]

where we ignore higher-order terms of order \(\lambda\) and terms beyond second order in the momentum. To second order in the momenta and first order in \(\lambda\), we thus have

\[
\sqrt{H_{SP}^2} \approx m + \frac{\bar{p}^2}{2m} + \frac{i\lambda\beta}{2m} \bar{\alpha} \cdot \frac{\bar{r}}{r^3} - \frac{\lambda}{r}.
\]

For the SP, the two terms in equation (19) are thus identified as follows,

\[
\left\{ \sqrt{H_{SP}^2} \right\}_{\text{even}} \beta = \beta \left( m + \frac{\bar{p}^2}{2m} - \frac{\lambda}{r} \right),
\]

\[
\left\{ \sqrt{H_{SP}^2} \right\}_{\text{odd}} J = -\frac{\lambda}{2m} \frac{\vec{\Sigma} \cdot \vec{r}}{r^3}.
\]

The result of the chiral transformation of the Dirac Hamiltonian with a SP thus is

\[
H_{SP}^{(CFW)} = \beta \left( m + \frac{\bar{p}^2}{2m} - \frac{\lambda}{r} \right) - \frac{\lambda}{2m} \frac{\vec{\Sigma} \cdot \vec{r}}{r^3}.
\]

The occurrence of the first term proportional to the \(\beta\) matrix had to be expected, but the second (pseudo-scalar) term breaks parity, even though the ‘input’ Hamiltonian \(H_{SP}\) is parity invariant. The Hamiltonian (35) is Hermitian, as it should be, because the chiral transformation is unitary in the case of a SP (we have \([H_{SP}, J] = 0\)).

Within the SFW procedure, the transformation of the Dirac Hamiltonian with a SP follows the lines of the standard method outlined in section 2.2. To second order in the momenta, the result reads as \(H_{SP}^{(SFW)} \approx \beta(m + \bar{p}^2/2m - \lambda/r)\) and needs to be compared with equation (35). To fourth order in the momenta, we have

\[
H_{SP}^{(SFW)} = \beta \left( m + \frac{\bar{p}^2}{2m} - \frac{\lambda}{r} + \frac{\lambda}{8m^3} - \frac{\lambda}{4m^2} \right) + \frac{\pi\lambda}{2m^2} \bar{\delta}^{(3)}(\vec{r}) - \frac{\lambda}{4m^2} \frac{\vec{\Sigma} \cdot \vec{L}}{r^3}.
\]

We obtain the spin–orbit coupling term (proportional to \(\vec{\Sigma} \cdot \vec{L}\)) and the zitterbewegung term (proportional to the Dirac-\(\delta\)). All the terms in the result (36) are parity-invariant, as they should be, because we started from the parity-invariant Hamiltonian (4). (Both the spin as well as the
orbital angular momenta are pseudo-vectors.) The scalar character of the potential is manifest in the universal prefactor $\beta$ in the Foldy–Wouthuysen transformed Hamiltonian (36), which ensures that both particles as well as antiparticles are attracted by the potential proportional to $\beta \lambda / r$. This is in contrast to the Coulomb potential, which is attractive for electrons (positive-energy eigenstates of the DC Hamiltonian, but repulsive for negative-energy solutions to the DC Hamiltonian). The physical interpretation of the $\vec{\Sigma}$ spin matrices is preserved under the standard approach [1].

### 3.3. Dirac Hamiltonian with scalar confining potential

We consider the Hamiltonian (5)

$$H_{\text{LC}} = \vec{\alpha} \cdot \vec{p} + \beta (m + \alpha^2 m^2 r),$$

(37)

where we distinguish the vector $\vec{\alpha} = \gamma_0 \vec{\gamma}$ of Dirac matrices from the coupling parameter $\alpha$. The potential $W = \beta \alpha^2 m^2 r$ anticommutes with $J$,

$$\{W, J\} = \{\beta \alpha^2 m^2 r, i \beta \gamma^5\} = 0,$$

(38)

and the condition for the applicability of the chiral method is thus fulfilled. One finds

$$H_{\text{LC}}^2 = m^2 + \vec{p}^2 - \beta \{\vec{\alpha} \cdot \vec{p}, \alpha^2 m^2 r\} + 2\alpha^2 m^3 r + \frac{1}{2} \alpha^4 m^3 r^2.$$

(39)

In the regime where $p' \sim \alpha$, and $r \sim 1/\alpha$, one finds to second order in $\alpha$,

$$\sqrt{H_{\text{LC}}^2} \approx m + \frac{\vec{p}^2}{2m} + \frac{\beta m}{2} [\vec{\alpha} \cdot \vec{p}, \alpha^2 m^2 r] + \alpha^2 m^3 r + \frac{1}{2} \alpha^4 m^3 r^2,$$

(40)

$$= m + \frac{\vec{p}^2}{2m} - \frac{i \alpha^2}{2r} \beta m \vec{\alpha} \cdot \vec{r} + \alpha^2 m^3 r + \frac{1}{2} \alpha^4 m^3 r^2,$$

(41)

and thus

$$\sqrt{H_{\text{LC}}^2} \text{even} = \beta \left(m + \frac{\vec{p}^2}{2m} + \alpha^2 m^3 r + \frac{1}{2} \alpha^4 m^3 r^2\right),$$

(42a)

$$\sqrt{H_{\text{DC}}^2} \text{odd}^2 = \frac{\alpha^2 m \vec{\Sigma} \cdot \vec{r}}{2r}.$$

(42b)

The CFW transformation of the DC Hamiltonian with a scalar, confining potential thus reads as

$$H_{\text{LC}}^{\text{CFW}} = \beta \left(m + \frac{\vec{p}^2}{2m} + \alpha^2 m^3 r + \frac{1}{2} \alpha^4 m^3 r^2\right) - \frac{\alpha^2 m \vec{\Sigma} \cdot \vec{r}}{2r}.$$

(43)

Two last terms in equation (43) are again pseudo-scalar and break parity (spin is a pseudo-vector, while $\vec{r}$ is a vector). Within the standard approach to the Foldy–Wouthuysen transformation, the spin–orbit coupling here enters at order $\alpha^3$, and we have

$$H_{\text{LC}}^{\text{SFW}} = \beta \left(m + \frac{\vec{p}^2}{2m} + \alpha^2 m^3 r - \frac{\alpha^2}{4} \{r, \vec{p}^2\} - \frac{\alpha^2 m \vec{\Sigma} \cdot \vec{L}}{4r}\right).$$

(44)

Again, we obtain an anticommutator term of the binding potential with the operator $\vec{p}^2$, and we recover full particle-antiparticle symmetry (overall prefactor $\beta$).
3.4. Dirac–Schwarzschild Hamiltonian

We now turn our attention to the DS Hamiltonian (6), which we recall for convenience,

\[
H_{DS} = \frac{1}{2} \left( \vec{\alpha} \cdot \vec{p} - \frac{\beta m}{2r} \left( 1 - \frac{GM}{r} \right) \right) + \beta \frac{m}{r} \left( 1 - \frac{GM}{r} \right),
\]

(45)

replacing the Schwarzschild radius from equation (6) according to \( r_s = 2 GM \). With the identification \( \lambda = GM \), the scalar ‘potential’ in the mass term in equation (45) is exactly equal to the SP in equation (4), but the kinetic term also is affected in equation (45). Because \([H_{DS}, J] = 0\), the conditions for the application of the CFW method are fulfilled.

The result from equation (31) of [4], rewritten in terms of the gravitational constant \( G \) and the mass \( M \) of the planet, reads as

\[
H_{DS}^{(\text{CFW})} = \beta \left( m + \frac{\vec{p}^2}{2m} - \frac{GmM}{r} + \frac{2\pi GM}{m} \delta^{(3)}(\vec{r}) + \frac{GM \vec{\Sigma} \cdot \vec{L}}{m r^3} \right) = \frac{GM \vec{\Sigma} \cdot \vec{r}}{2m r^3}. \]

(46)

As compared to equation (31) of [4], we here leave the leading gravitational interaction term proportional to \( GmM/r \) in an unexpanded form (it is written as \( m \vec{g} \cdot \vec{x} \) for a small displacement \( \vec{x} \) from the position \( \vec{r} \), where \( \vec{g} \) is the acceleration due to gravity). We thus confirm that the formalism of the chiral CFW has been consistently applied in [4] in order to obtain the result given in equation (46). The term proportional to \( \vec{\Sigma} \cdot \vec{r} \) in equation (46) indicates that the symmetry of the problem has been altered. The ‘input’ Hamiltonian (6) is parity-even, while the term proportional to \( \vec{\Sigma} \cdot \vec{r} \) in the result of the CFW transformation (46) constitutes a pseudo-scalar. The parity-breaking term is spurious and indicates that the physical interpretation of the spin operator \( \vec{\Sigma} \) has been altered [15].

By contrast, the SFW transformation leads to a different result [6, 15, 27], given recently in manifestly Hermitian form [6],

\[
H_{DS}^{(\text{SFW})} = \beta \left( m + \frac{\vec{p}^2}{2m} - \frac{GmM}{r} + \frac{3\pi GM}{4m} \left( \frac{3}{r} + \frac{1}{r^2} \right) + \frac{3GM \vec{\Sigma} \cdot \vec{L}}{4mr^3} \right). \]

(47)

The leading gravitational interaction is consistently obtained with the prefactor \( \beta \) in both approaches (46) and (47). The gravitational spin–orbit coupling term in equation (47) is in agreement with classical physics [7–9].

3.5. Dirac Hamiltonian in a non-inertial frame

We recall the Dirac Hamiltonian in a non-inertial frame from equation (7),

\[
H_{NF} = (1 + \alpha \cdot \vec{r}) \beta m + \frac{1}{2} (1 + \alpha \cdot \vec{r}, \alpha \cdot \vec{p}) - \alpha \cdot (\vec{L} + \frac{1}{2} \vec{\Sigma}).
\]

(48)

This Hamiltonian is valid for an accelerated frame of reference accelerated with a uniform acceleration vector \( \vec{a} \). Because of the spatially uniform acceleration, the magnitude of the coordinate \( \vec{r} \) is not bound by any dimension of the system. It is therefore indicated to carry out the perturbative program of the Foldy–Wouthuysen transformation as an expansion in powers of the parameter \( \xi \), where \( \vec{p} \sim \xi \) and \( \vec{r} \sim 1 \), i.e., the spatial coordinate is treated as a quantity of order unity. Furthermore, in all calculations below, we keep the acceleration vector \( \vec{a} \) and the angular rotation frequency vector \( \vec{\omega} \) only to first order.

Using the operator identity

\[
[A, B]^2 - 2[A^2, B^2] = 3 [A, B] [B, A],
\]

(49)

which is valid provided \([A, [A, B]] = [B, [A, B]] = 0\), with \( A = \frac{1}{2} (1 + \alpha \cdot \vec{r}) \) and \( B = \alpha \cdot \vec{p} \), one verifies the relation

\[
H_{NF} \approx (1 + 2 \alpha \cdot \vec{r}) m^2 + \frac{1}{2} \{1 + 2 \alpha \cdot \vec{r}, \vec{p}^2\} + i \beta m \alpha \cdot \vec{a} - 2 \beta m \vec{a} \cdot \vec{L} \left( 1 + \frac{1}{2} \vec{\Sigma} \right),
\]

(50)
where quadratic terms in the parameter \( \vec{a} \) and \( \omega \) have been neglected. Therefore,
\[
\sqrt{H_{SFW}^2} \approx m (1 + \vec{a} \cdot \vec{r}) + \frac{\vec{p}^2}{2m} + \frac{1}{2m} (\vec{a} \cdot \vec{r}, p^2) + \frac{\beta}{2} \vec{a} \cdot \vec{a} - \beta \vec{\omega} \cdot \left( \vec{L} + \frac{1}{2} \vec{\Sigma} \right). \tag{51}
\]

The CFW transform therefore reads as follows,
\[
H_{\text{CFW}} = \beta \left( m (1 + \vec{a} \cdot \vec{r}) + \frac{\vec{p}^2}{2m} + \frac{1}{2m} (\vec{a} \cdot \vec{r}, p^2) \right) - \vec{\omega} \cdot \left( \vec{L} + \frac{1}{2} \vec{\Sigma} \right) + \frac{1}{2} \vec{\Sigma} \cdot \vec{a}. \tag{52}
\]

The pseudo-scalar term proportional to \( \vec{\Sigma} \cdot \vec{a} \) has the same structure as the corresponding term in equation (46), if we identify the acceleration due to gravity \( \vec{g} = -GM\vec{r}/r^3 \) with \( \vec{a} \).

The SFW transformation leads to a different result. We would like to investigate terms up to fourth order in the momenta. In the sense of section 2.2, one then has to perform a four-fold Foldy–Wouthuysen transformation (four iterated transformations of the form given in equation (11)), to obtain the result
\[
H_{\text{NF}}^{(\text{SFW})} = \beta \left( m + \frac{\vec{p}^2}{2m} - \frac{\vec{p}^4}{8m^3} + m \vec{a} \cdot \vec{r} + \frac{1}{4m} (\vec{p}^2, \vec{a} \cdot \vec{r}) - \frac{1}{16m} (\vec{p}^4, \vec{a} \cdot \vec{r}) \right) + \beta [\vec{\Sigma} \cdot (\vec{a} \times \vec{p})] \left( \frac{1}{4m} - \frac{\vec{p}^2}{16m^3} \right) - \vec{\omega} \cdot \left( \vec{L} + \frac{1}{2} \vec{\Sigma} \right). \tag{53}
\]

This result fully conserves parity. It is in agreement with equation (20) of [14] but adds higher-order terms (in the momenta). In order to verify consistency with equation (20) of [14], one notices that \( [p^i, [p^j, \vec{a} \cdot \vec{r}]] = 0 \), where the \( p^i \) denote the Cartesian components of the momentum vector. Our result (53) also is in agreement with various other recent investigations [15, 28, 29] in appropriate limits, and with equation (5.14) of [30]. The results in [15, 28–30] are obtained within a conceptually different approach to the Foldy–Wouthuysen transformation. The result (53) confirms that the Mashhoon term receives no relativistic corrections up to the relative order \( \vec{p}^4 \), and indicates the leading fourth-order (in the momenta) relativistic corrections to the spin–orbit coupling in the accelerated frame, in compact form.

### 4. Conclusions

We have contrasted the standard and the chiral method for the Foldy–Wouthuysen transformation of generalized Dirac Hamiltonians. The chiral method is based on surprising and perhaps, quite fascinating operator identities discussed in section 2.3. A somewhat ‘hidden’ assumption of the chiral method implies that the input Hamiltonian anticommutes with the chiral operator \( J = i\gamma^5 \beta \). We confirm that the chiral method leads to a consistent result for the free Dirac Hamiltonian (see section 3.1). However, the Dirac–Coulomb Hamiltonian (see section 3.1), for scalar \((1/r)\)-potentials and scalar confining potential (see sections 3.2 and 3.3), as well as for the Dirac–Schwarzschild Hamiltonian (see section 3.4), and for a Dirac particle moving in an accelerated reference frame (see section 3.5).

The eventual goal of the ‘chiral’ transformation is the calculation of an ‘exact’ Foldy–Wouthuysen transformation, which disentangles the particle and antiparticle degrees of freedom, without the restrictions set forth by a perturbative formalism. Such calculations may eventually be possible [12, 15, 31–33], but they rely on additional mathematical relations fulfilled by the Hamiltonian at hand and cannot be generalized as easily. When the method is generalized to more complicated configurations [32], one has to resort to additional approximations such as the neglect to of terms proportional to the square of the field strengths (see the text preceding equation (21) of [32]). The latter terms, however, are important in higher-order Lamb shift calculations [19, 20].
This situation raises a pertinent question. Let us suppose now that $[H, J] = 0$ and that all the conditions for the application of the chiral method are fulfilled (section 2.3). In that case, the outcome of both the standard as well as the chiral method are unitary transformations. One could argue that the ‘input’ Hamiltonian, as well as the ‘output’ Hamiltonians of the chiral and standard methods, are Hermitian Hamiltonians connected via a unitary transformation: they should be equivalent. Why, then, would the results contain conflicting terms and fulfil conflicting symmetry relations? The reason is to be found in the transformation $U_2$, defined in equation (14), which breaks parity and constitutes a chiral transformation which fundamentally alters the symmetry properties of the Hamiltonian (see also the appendix). This leads to problems, both in regard to the physical interpretation of the transformed wave functions, and also, in terms of the symmetry properties of the transformed operators.

While the ‘chiral’ transformed Hamiltonian thus is Hermitian and is obtained from the ‘input’ Hamiltonian by a unitary transformation, the operators are obtained in nonequivalent representations. Unfortunately, this implies that the realm of applicability of the otherwise elegant and concise ‘chiral’ Foldy–Wouthuysen transformation, which is described in section 2.3, remains very limited. For the free Dirac Hamiltonian, the result of the chiral method coincides with the one obtained using the standard approach (while of course the wave function still receives a nontrivial transformation, see [15, 33] and the appendix). For more complicated ‘input’ Hamiltonians, spurious terms are obtained which break fundamental physical symmetries of the system. It appears as though the standard approach to the Foldy–Wouthuysen transformation, while technically more involved and perhaps less elegant than the ‘chiral’ or ‘exact’ approach, remains the most reliable ansatz for the relativistic corrections which result from a generalized Dirac Hamiltonian.

Beside these considerations, which aim to clarify the formal properties of chiral, unitary transformations in the context of generalized Dirac Hamiltonians, we here obtain two results which, to the best of our knowledge, have not appeared in the literature before. The first of these concerns the Foldy–Wouthuysen transformation of the Dirac Hamiltonian with a scalar potential, given in equation (36), which contains a somewhat surprising anticommutator term proportional to $\{\vec{p}^2, 1/r\}$ which is not present in the Dirac–Coulomb case. The result given in equation (36) exhibits particle-antiparticle symmetry (global prefactor $\beta$). The same is true for a confining, scalar potential (see equation (44)). We also give a compact analytic formula for the leading fourth-order (in the momenta) relativistic corrections to the Dirac Hamiltonian in a non-inertial and rotating frame (see equation (53)).

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**Appendix. Parity violation and spin operators**

The results of the CFW transformations in equations (35), (46), and (52) contain terms which manifestly break parity symmetry. In order to understand this phenomenon, we first note that matrix elements are only invariant under unitary transformations if the wave functions also is transformed, according to the formula

$$M_{\psi\phi} = \langle \psi | H | \phi \rangle = \langle U \psi | U H U^\dagger | U \phi \rangle = \langle \psi' | H' | \phi' \rangle,$$

(A.1)
where $|\psi\rangle = U |\psi\rangle$, $|\phi\rangle = U |\phi\rangle$, and $\mathcal{H}' = U \mathcal{H} U^\dagger$. In our case, the transformation $U = U_2 = \exp(-i \frac{\gamma}{2} \gamma^5)$ does not correspond to a spinor transformation which can be reached from the identity transformation, within the proper orthochronous Lorentz group: it is a chiral transformation which changes the physical interpretation of the wave function and alters the symmetry properties of the Hamiltonian. Related problem have been considered in the context of gauge transformations of atomic transition rates, with regard to the ‘length’ and ‘velocity’ gauge forms of the interaction [34–37] (see also the now famous remark on p 268 of [38]).

Let us supplement this argument by some remarks on the unitary transformations of the operators, which also clarify the relation of the transformations to the original paper [1]. The unitary operator which transforms the free Dirac Hamiltonian into the Foldy–Wouthuysen form, can be expressed in closed form as follows [1, 2],

$$U^{(\text{SFW})} = \frac{E_p + m + \beta \, \vec{a} \cdot \vec{p}}{\sqrt{2E_p (E_p + m)}}, \quad E_p = \sqrt{p^2 + m^2}. \quad (A.2)$$

One has the relation $U^{(\text{SFW})} \, (\vec{a} \cdot \vec{p} + \beta m) \, [U^{(\text{SFW})}]^\dagger = \beta \, E_p$. The spin matrix transforms as follows,

$$U^{(\text{SFW})} \, \Sigma \, [U^{(\text{SFW})}]^\dagger = \tilde{\Sigma} + \frac{i \beta}{E_p} \, (\vec{a} \times \vec{p}) = \frac{1}{E_p (E_p + m)} \left[ \vec{p} \times (\tilde{\Sigma} \times \vec{p}) \right]. \quad (A.3)$$

This equation corresponds to the entries in row 7 of table 1 of [1]. We note that $U^{(\text{SFW})} \, \Sigma \, [U^{(\text{SFW})}]^\dagger$ is a Hermitian operator. In particular, we have $\left[ i \beta \, (\vec{a} \times \vec{p}) \right]^\dagger = -i \left( \vec{a} \times \vec{p} \right)$, $\beta = i \beta (\vec{a} \times \vec{p})$. The inverse operator $[U^{(\text{SFW})}]^\dagger$ is obtained from $U^{(\text{SFW})}$ by the replacement $i \rightarrow -i$. Hence,

$$U^{(\text{SFW})} \left( \tilde{\Sigma} - \frac{i \beta}{E_p} \, (\vec{a} \times \vec{p}) - \frac{1}{E_p (E_p + m)} \left[ \vec{p} \times (\tilde{\Sigma} \times \vec{p}) \right] \right) [U^{(\text{SFW})}]^\dagger = \tilde{\Sigma}. \quad (A.4)$$

One defines, according to row 11 of table 1 of [1], the ‘mean’ spin operator as

$$\Sigma_{\text{mean}} = \tilde{\Sigma} - \frac{i \beta}{E_p} \, (\vec{a} \times \vec{p}) - \frac{1}{E_p (E_p + m)} \left[ \vec{p} \times (\tilde{\Sigma} \times \vec{p}) \right]. \quad (A.5)$$

We then have the relation, $U^{(\text{SFW})} \, \Sigma_{\text{mean}} \, [U^{(\text{SFW})}]^\dagger = \tilde{\Sigma}$, i.e. the spin matrix $\Sigma$ can be identified as the relevant physical spin operator in the Foldy–Wouthuysen representation. The identification as a ‘mean’ operator is motivated by the fact that, in the nonrelativistic picture, the zitterbewegung term describes the influence of the ‘quiver’ motion of the electron on its quantum trajectory in the mean, i.e., without the influence of the instantaneous velocity operator which has the eigenvalues of the $\vec{a}$ matrix. The leading nonrelativistic kinetic term is $\vec{p}^2/(2m)$, which implies that all the operators after the Foldy–Wouthuysen transformation can be interpreted as ‘mean’ operators. We note that the all terms in the mean spin operator $\Sigma_{\text{mean}}$ constitute pseudovectors. Under parity, we have $\Sigma \rightarrow \Sigma$, $\vec{p} \rightarrow -\vec{p}$, and $\vec{a} \rightarrow -\vec{a}$. The total angular momentum $J = \vec{L} + \frac{1}{2} \Sigma$ commutes with the Dirac Hamiltonians investigated here in equations (3), (4), (6) and (7), and with their (standard) Foldy–Wouthuysen transforms given in equations (30), (36), (44), (47) and (53).

One may transform the spin operator $\tilde{\Sigma}$ into the Eriksen–Kolsrud (‘chiral’) representation [11], using the unitary transformation $U^{(\text{CWF})} \, [U^{(\text{SFW})}]^{-1}$. In this case, one obtains, according to equation (10) of [15], terms proportional to $\vec{p} \times \Sigma$, which transform as vectors under parity ($\vec{p} \rightarrow -\vec{p}$, but $\Sigma \rightarrow \Sigma$). This implies that the spin operator in the chiral representation cannot be consistently identified with the spin matrix $\Sigma$, not even in the nonrelativistic limit. This consideration affords an alternative view on the generation of the parity-breaking terms.
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