Comparative analysis of direct and step-by-step FoldyWouthuysen transformation methods

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Abstract

Relativistic methods for the FoldyWouthuysen transformation of the step-by-step type already at the first step give an expression for the Hamilton operator not coinciding with the exact result determined by the Eriksen method. The methods agree for the zeroth and first orders in the Planck constant terms but do not agree for the second and higher-order terms. We analyze the benefits and drawbacks of various methods and establish their applicability boundaries.

Keywords: Foldy-Wouthuysen transformation, unitary transformations, relativistic quantum mechanics

INTRODUCTION

Because the FoldyWouthuysen (FW) representation [1] has some unique properties, it holds a special place in quantum mechanics. In this representation, quantum mechanical operators for relativistic particles in an external field have the same form as in the nonrelativistic quantum theory. In particular, the position operator [2] and momentum operator are equal to $\boldsymbol{r}$ and $\boldsymbol{p} = -i\hbar\nabla$, and the polarization operator for spin-1/2 particles is expressed by the Dirac matrix $\mathbf{\Pi}$. In other representations, much more cumbersome formulas are used to write these operators (see [1, 3]). The relations between the operators in the FW representation are analogous to the relations between the corresponding classical quantities. The simple form of operators corresponding to classical observables is a great advantage of this representation. These properties of the FWrepresentation allow using it successfully for passing to the semiclassical approximation and the classical limit of relativistic quantum mechanics [1, 4]. We note that the Hamiltonian and all other operators are diagonal in two spinors (block-diagonal) in this representation.

When the FW representation is used, the passage to the classical limit is usually accomplished by simply replacing the operators in the expressions for the Hamiltonian and in the operator equations for the dynamics with the corresponding classical quantities. The possibility of such a replacement, explicitly or implicitly used in practically all works devoted to the relativistic FW transformation, was recently rigorously proved in [5]. This possibility radically simplifies interpreting the basic quantum mechanics equations, especially in the relativistic case.

For practical purposes, the Hamilton operator in the FW representation must be derived up to terms of the order $\hbar^2$. The contribution to the Hamilton operator provided by the scalar electric and magnetic polarizability and for spin $s > 1/2$ particles also by the quadrupole interaction and tensor electric and magnetic polarizability has exactly this order of magnitude. We note that the terms characterizing the polarizability are of the second order in the field. As an example showing the importance of such interaction analysis for modern experimental physics, we mention the need to take the tensor polarizability into account in experiments seeking the electric dipole moment of the deuteron. In these experiments, the tensor polarizability of the deuteron can be successfully measured (see [6–8] and the references therein).

The importance of the FW representation for modern quantum mechanics and elementary particle physics makes the problem of passing to this representation quite relevant. The basic methods for the passage are direct, which allows passing to the FW representation in a single transformation, and step by step (iterative methods). Here, we analyze these methods comparatively and establish their applicability boundaries.

We use the $c = 1$ system of units. At the same time, the Planck constant $\hbar$ is included in the equations.

METHODS FOR PASSING TO THE FW REPRESENTATION

Passing to the FW representation is a highly nontrivial problem. It was noted relatively early that such a passage is by no means identical to bringing Hamiltonian to a block-diagonal form (see [9] and the references therein). In particular, as shown in [10], even the classical method, developed by Foldy and Wouthuysen [1], strictly speaking, does not lead to this representation. In [1], passing to the blockdiagonal form is done step by step, in successive iterations, each of which results in removal of odd (non-block-diagonal) terms of the highest order. But the operator U_{FW} of the *exact* FW transformation U_{FW} ($\Psi_{FW} = U_{FW}\Psi$) for spin-1/2 particles should satisfy the Eriksen condition [11]

$$\beta U_{FW} = U_{FW}^{\dagger}\beta, \tag{1}$$

where β is a Dirac matrix. With the operator U_{FW} represented in the exponential form

$$U_{FW} = \exp(iS) \tag{2}$$

condition (1) is equivalent to the requirement that the exponent S should be Hermitian and odd [10]. In view of the Hausdorff theorem [12]

$$\exp(A)\exp(B) = \exp\left(A + B + \frac{1}{2}[A, B] + \text{higher order commutators}\right),$$
$$\exp(A)\exp(B) \neq \exp(B)\exp(A). \tag{3}$$

If $A = iS_1$ and $B = iS_2$, where S_1 and S_2 are odd Hermitian operators, then the operator $[A, B]$ is odd, and $\exp(A)\exp(B)$ does not satisfy Eriksen condition (1) [10]. Therefore, the classical FW method [1] and other methods of step-by-step type do not satisfy the oddness condition for the operator S and can consequently provide only an approximate passage to

the FW representation. Because Dirac matrices do not commute, the operator $[S_1, S_2]$ can be of the same order as S_2. In this case, even the second iteration is useless. But formula (3) does not allow estimating the error coming from iterative methods quantitatively.

Eriksen found a general form for the operator of the exact transformation to the FW representation (the FW transformation) in the static case [11]. The initial Hamiltonian for spin-1/2 particles can be represented in the general form

$$\mathcal{H}_D = \beta m + \mathcal{E} + \mathcal{O}, \quad \beta\mathcal{E} = \mathcal{E}\beta, \quad \beta\mathcal{O} = -\mathcal{O}\beta, \tag{4}$$

where $\mathcal{E}$ and $\mathcal{O}$ are even and odd operators. The operator found by Eriksen is defined by the expression

$$U_{FW} = \frac{1}{2}(1+\beta\lambda)\left[1 + \frac{1}{4}(\beta\lambda + \lambda\beta - 2)\right]^{-1/2}, \tag{5}$$

where $\lambda = \mathcal{H}_D \Big/ \sqrt{\mathcal{H}_D^2}$. The quantity λ takes the respective values $+1$ and -1 for states with positive and negative energies. It is important that [11]

$$\lambda^2 = 1, \quad [\beta\lambda, \lambda\beta] = 0, \tag{6}$$

and the operator $\beta\lambda + \lambda\beta$ is even:

$$[\beta, (\beta\lambda + \lambda\beta)] = 0. \tag{7}$$

Even operators are block-diagonal and do not mix upper and lower spinors. Formula (5) can also be written in the form [9]

$$U_{FW} = \frac{1+\beta\lambda}{\sqrt{(1+\beta\lambda)^\dagger(1+\beta\lambda)}}. \tag{8}$$

The two operator factors in the radicand commute.

The operator U_{FW} annihilates the respective lower or upper spinor of any eigenfunction of Dirac Hamiltonian for positive or negative energy. This transformation is done in one step.

Other direct methods for the FW transformation were developed in [13–15]. We limit ourself to considering the Eriksen method because it was thoroughly justified in [16].

But it easily seen that it is problematic to effectively use the Eriksen method with the goal of obtaining relativistic formulas for particles in an external field because general formula (5) is extremely cumbersome and contains square roots of Dirac matrices. The most general

expression for the Hamiltonian operator in the FW representation, found by the Eriksen method in [16], represents this operator as a series of relativistic corrections in powers of the operators $\mathcal{E}/m$ and $\mathcal{O}/m$. This expansion gives a good solution of the problem for nonrelativistic particle velocities. In particular, it can be used for electrons in atoms (except heavy atoms) because $|v/c| \sim \sqrt{Z}\alpha \ll 1$. But the Eriksen method, for example, does not allow passing to the FW representation for fast particles moving in external fields (in accelerators and storage rings). For $\mathcal{O}^2/m^2 \approx \boldsymbol{p}^2/m^2 \geq 1$, the relativistic correction series does not converge at all. We therefore cannot use the Eriksen method to find compact relativistic expressions for the Hamilton operator in this representation.

In contrast to the Eriksen method, some of the iterative methods give the sought relativistic expressions [3, 17–22]. We note that the method developed in [18] is applicable to particles with any spin. Because all these methods are approximate, we must determine their applicability boundaries. Obviously, the simplest, most reliable way to do this is to compare relativistic Hamiltonians in the FW representation obtained by methods of the step-by-step type with the exact power series given in [16]. This problem is extremely important, in particular, because the terms proportional to the second derivatives of the field potentials and to the squared field strengths are checked. As indicated above, taking them into account can be necessary in considering effects due to scalar and tensor polarizability.

Here, we compare results obtained by the three methods developed in [17], in [3, 18] and in [19–22]. These methods have the most fundamental justification among the methods of the step-by-step type. We then compare these results with results of the Eriksen method and draw conclusions about the precision of the FW transformations given by these methods.

COMPARISON OF RESULTS OBTAINED BY DIFFERENT METHODS OF THE STEP-BY-STEP TYPE

To compare the results, certainly, we need to use Eqs. (4) as the initial and formal expression for the Hamiltonian in the FW representation in terms of the operators $\mathcal{E}$ and $\mathcal{O}$. The transformed Hamiltonian was represented in precisely this form in [10, 11, 16, 23]. Although some fairly general problems were considered in [17, 19–22], the above form was not used there. On the other hand, a concrete form of the Hamiltonian operator in the FW representation was obtained in [3] in the weak-field approximation, i.e., with only first-

order terms in field potentials and their derivatives taken into account. We therefore first determine this operator with the precision needed for comparison, using general equation (31) in [3]. This equation has the form

$$\mathcal{H}_{FW} = \beta\epsilon + \mathcal{E}' + \frac{1}{4}\beta\left\{\frac{1}{\epsilon}, \mathcal{O}'^2\right\}, \quad \epsilon = \sqrt{m^2 + \mathcal{O}^2}, \tag{9}$$

where $\{\dots, \dots\}$ denotes the anticommutator and $\mathcal{E}'$ and $\mathcal{O}'$ are the even and odd operators after the first step of the transformation, defined by the expressions [3]:

$$\begin{aligned}
\mathcal{E}' = \mathcal{E} &- \frac{1}{4}\left[\frac{\epsilon+m}{\sqrt{2\epsilon(\epsilon+m)}}, \left[\frac{\epsilon+m}{\sqrt{2\epsilon(\epsilon+m)}}, \mathcal{F}\right]\right] \\
&+\frac{1}{4}\left[\frac{\beta\mathcal{O}}{\sqrt{2\epsilon(\epsilon+m)}}, \left[\frac{\beta\mathcal{O}}{\sqrt{2\epsilon(\epsilon+m)}}, \mathcal{F}\right]\right], \\
\mathcal{O}' = &\frac{\beta\mathcal{O}}{\sqrt{2\epsilon(\epsilon+m)}}\mathcal{F}\frac{\epsilon+m}{\sqrt{2\epsilon(\epsilon+m)}} \\
&-\frac{\epsilon+m}{\sqrt{2\epsilon(\epsilon+m)}}\mathcal{F}\frac{\beta\mathcal{O}}{\sqrt{2\epsilon(\epsilon+m)}},
\end{aligned} \tag{10}$$

where

$$\mathcal{F} = \mathcal{E} - i\hbar\frac{\partial}{\partial t}.$$

Deriving the Hamiltonian in the FW representation with a fixed precision in the Planck constant and writing the initial Hamiltonian formally as in (4), we must use the following a priori information. Every commutation of the operator $\boldsymbol{p}$ with some function $f(\boldsymbol{r})$ of coordinates (e.g., with the scalar potential), compared with the product $\boldsymbol{p}f(\boldsymbol{r})$, adds a factor of the order $\hbar/S_0$, where S_0 is some value with the dimension of action. When the condition $\lambda_B \ll l$ of small de Broglie wavelength $\lambda_B = \hbar/p$ compared with the characteristic size l of the external field inhomogeneity region (or the particle localization region) is satisfied, the commutator of the operators is smaller in order of magnitude than their product:

$$\frac{|[\boldsymbol{p}, f(\boldsymbol{r})]|}{|pf(\boldsymbol{r})|} \sim \frac{\hbar}{lp} = \frac{\lambda_B}{l} \ll 1. \tag{11}$$

To find the order of S_0, we use an estimate of the means of the corresponding Hamiltonian terms. It follows from (11) that $S_0 = lp$. For particle beams in accelerators and storage rings, this value is equal to the angular momentum ($S_0 = rp = L$, where r is the ring radius), and the condition $\hbar/S_0 \ll 1$ is automatically satisfied. Certainly, this condition is not satisfied in all cases. In particular, very often (whenis automatically satisfied. Certainly, this condition is not satisfied in all cases. In particular, very often (when $rp \sim \hbar$, where r

is the electron orbit radius), it does not hold for electrons in atoms. At the same time, the compact character of an interaction (electro-weak, for example), as the analysis in [24] shows, does not preclude a correct description of relativistic effects using the FW transformation.

One more standard reason why the operators $\mathcal{O}$ and $\mathcal{E}$ do not commute is the noncommutativity of different components of the kinetic momentum operator $\boldsymbol{\pi} = \boldsymbol{p} - e\boldsymbol{A}$: $[\pi_i, \pi_j] = iee_{ijk}B_k$. In this case, we have the estimate for relativistic particles

$$\frac{|[\pi_i, \pi_j]|}{|\pi_i \pi_j|} \sim \frac{\hbar}{S_0} = \frac{|e|\hbar B}{\epsilon^2},$$

where ϵ is the total kinetic energy including the rest energy. This absence of commutativity usually leads to spin-dependent terms appearing in the Hamilton operator in the FW representation, and $S_0 = \epsilon^2/(|e|B)$ is significantly greater than $\hbar$ as a rule.

In the general case, the order of magnitude of the commutator $[\mathcal{O}, \mathcal{E}]$ is determined by the commutator of the operator $\boldsymbol{p}$ with a function of coordinates or by their commutators with matrices contained in the operator $\mathcal{O}$ if the operator $\mathcal{E}$ contains even matrices $\boldsymbol{\Sigma}$ or $\boldsymbol{\Pi}$. For example, for spin-1/2 particles in homogenous electric and magnetic fields [3], we have

$$\mathcal{E} = e\Phi - \mu' \boldsymbol{\Pi} \cdot \boldsymbol{B}, \quad \mathcal{O} = \boldsymbol{\alpha} \cdot \boldsymbol{\pi} + i\mu' \boldsymbol{\gamma} \cdot \boldsymbol{E}.$$

In this case,

$$[\mathcal{O}, \mathcal{E}] = ie\hbar \boldsymbol{\alpha} \cdot \boldsymbol{E} - 2\beta\gamma^5 \mu' \boldsymbol{\pi} \cdot \boldsymbol{B} - 2i\gamma^5 \mu'^2 \boldsymbol{E} \cdot \boldsymbol{B}. \tag{12}$$

Because $\mu' = (g-2)e\hbar/(4mc)$, the second term in the right-hand side of (12), resulting from the noncommutativity of the matrices $\boldsymbol{\alpha}$ and $\boldsymbol{\Pi}$, is also proportional to $\hbar$. If the order of magnitude of $\mathcal{E}$ is determined by the scalar potential and $|g-2| \sim 1$, then $S_0 = m|\Phi|/B$ for this term. With $B \sim E$ for relativistic particles, it has the same order of magnitude as the first term.

The operator $\mathcal{O}$, being odd (non-block-diagonal), contains the Dirac matrices γ_1, γ_2, and γ_3. In accordance with the properties of these matrices, multiple commutators of the form $[\mathcal{O}, [\mathcal{O}, \ldots [\mathcal{O}, \mathcal{E}] \ldots]]$ have the order of magnitude $\hbar/S_0$ with respect to the operator product $\mathcal{O}\mathcal{O} \ldots \mathcal{O}\mathcal{E}$ with the factor $\hbar$ already appearing in the result of the first commutation. In contrast, commutators of the forms $[\mathcal{O}^2, [\mathcal{O}, \mathcal{E}]]$, $[\mathcal{O}^2, [\mathcal{O}^2, \mathcal{E}]]$, and $[[\mathcal{O}, \mathcal{E}], \mathcal{E}]$ are of the order $(\hbar/S_0)^2$ (with respect to the product of the operators appearing in them). This property follows because $\mathcal{O}^2$ and $\mathcal{E}$ are even operators and do not contain the Dirac matrices γ_1, γ_2, and γ_3 which are non-block-diagonal.

Determining the order of magnitude, we indicate the smallest possible degree in $\hbar$. For example, the commutator $[\mathcal{O},\mathcal{E}]$ with the nominal order $\hbar/S_0$ can, as in (12), contain terms of the orders $(\hbar/S_0)^2, (\hbar/S_0)^3, \dots$, can have an order higher than one in $\hbar/S_0$ (see Sec.), or can just be zero.

In [3], the expressions for $\mathcal{H}_{FW}$ were computed only for concrete problems, and the weak-field approximation was used. But using general formulas (9),(10), we can easily determine the form of this operator up to terms of the order $(\hbar/S_0)^2$:

$$\begin{gathered}\mathcal{H}_{FW}=\beta\epsilon+\mathcal{E}-\frac{1}{8}\left\{\frac{1}{\epsilon(\epsilon+m)},[\mathcal{O},[\mathcal{O},\mathcal{F}]]\right\}\\+\frac{1}{64}\left\{\frac{2\epsilon^2+2\epsilon m+m^2}{\epsilon^4(\epsilon+m)^2},[\mathcal{O}^2,[\mathcal{O}^2,\mathcal{F}]]\right\}\\-\frac{1}{16}\beta\left\{\frac{1}{\epsilon^3},([\mathcal{O},\mathcal{F}])^2\right\}+\frac{1}{64}\beta\left\{\frac{1}{\epsilon^5},\left([\mathcal{O}^2,\mathcal{F}]\right)^2\right\}.\end{gathered}\tag{13}$$

To compare results obtained by different methods of the step-by-step type, we consider Dirac particles in an inhomogeneous electrostatic field. In this case, in formula (13), obtained by the method developed in [3, 18], we have $\mathcal{E}=e\Phi$ and $\mathcal{O}=\boldsymbol{\alpha}\cdot\boldsymbol{p}$, where Φ is the scalar potential and $\boldsymbol{\alpha}$ is a Dirac matrix. We note that the expression for $\mathcal{E}$ and $\mathcal{O}$ is nontrivial, which excludes the possibility of random coincidence. Equation (13) becomes

$$\begin{gathered}\mathcal{H}_{FW}=\beta\epsilon'+e\Phi\\+\frac{e\hbar}{8}\left\{\frac{1}{\epsilon'(\epsilon'+m)},\left[\boldsymbol{\Sigma}\cdot(\boldsymbol{p}\times\boldsymbol{E})-\boldsymbol{\Sigma}\cdot(\boldsymbol{E}\times\boldsymbol{p})+\hbar\Delta\Phi\right]\right\}\\-\frac{e\hbar^2}{16}\left\{\frac{2\epsilon'^2+2\epsilon' m+m^2}{\epsilon'^4(\epsilon'+m)^2},(\boldsymbol{p}\cdot\nabla)(\boldsymbol{p}\cdot\nabla)\Phi\right\}\\+\frac{e^2\hbar^2}{16}\beta\left\{\frac{1}{\epsilon'^3},\boldsymbol{E}^2\right\}-\frac{e^2\hbar^2}{64}\beta\left\{\frac{1}{\epsilon'^5},(\boldsymbol{p}\cdot\boldsymbol{E}+\boldsymbol{E}\cdot\boldsymbol{p})^2\right\},\end{gathered}\tag{14}$$

where $\epsilon'=\sqrt{m^2+\boldsymbol{p}^2}$ and $\boldsymbol{E}=-\nabla\Phi$.

The result shown above coincides with corresponding expressions obtained in [17, 22] (the magnetic field was also taken into account in the first of them). An analysis of the methods being compared shows that this coincidence is perfectly natural. All three methods are relativistic, and the FW transformation is realized in them with the same scheme. The transformation operators are chosen such that they annihilate the total odd operator $(\mathcal{O},\mathcal{O}',\mathcal{O}'',\dots)$ under the condition that it commutes with the total even operator $(\mathcal{E},\mathcal{E}',\mathcal{E}'',\dots)$, in the first and subsequent stages (steps) and also with the operator ϵ, the operators ϵ'', etc. in the second and subsequent stages. Such commutativity is absent in general, and we therefore obtain a converging series of corrections defining the transformed Hamilton operator. All three

methods should lead to equivalent results because their difference consists in using different quantum mechanics formalisms. In the method proposed in [17], unitary transformations are not used. It is based on the Moyal quantum mechanics (see [25] and the references therein), where quantum mechanical operators are associated with classical distributions in the phase space. Quantum mechanical evolution is described using Moyal brackets, corresponding to commutators in ordinary quantum mechanics, while observable quantities are characterized by functions on the phase space. In the original method proposed in [19–22], unitary transformations are also not used. The quantum mechanical system Hamiltonian is represented as a matrix $H_0(\boldsymbol{P}, \boldsymbol{R})$, whose elements are operators depending on the pair of canonical variables $\boldsymbol{P}$ and $\boldsymbol{R}$. This method determines a diagonalization procedure based on formal series in powers of the Planck constant $\hbar$ and can be used for a wide class of Hamiltonians, for which Berry phase corrections are essential. Unlike these methods, the ordinary form of quantum mechanical operators was used in [3, 18] and the FW transformation is accomplished using unitary transformations.

But the agreement of the results obtained by the three methods only means that in the framework of these methods, the initial Hamiltonian is transformed to the same representation but not that this representation is indeed the FW representation. We also note that this agreement is an additional confirmation of the correctness of the quantum mechanics formalisms used in [17, 19–22].

Some other methods for the relativistic FW transformation, in particular, the method proposed in [24, 26], based on one variant of the exclusion method developed by Akhiezer, Berestetskii, and Landau [27, 28], also lead to correct results in computing terms of the zeroth and first orders in $\hbar/S_0$. The method used in [29]. also gives correct expressions. At the same time, some relativistic methods, including those proposed for passing to the FW representation, yield incorrect results even in the first order in $\hbar/S_0$ (see examples in [9]).

Comparing the three methods under consideration leads to the following conclusion. The most cumbersome computations are needed in the method in [19–22], while using the traditional mathematical apparatus of quantum mechanics (in [3, 18]) allows passing to the FW representation most easily. Writing the initial Hamiltonian in form (4) and using general formula (13) simplifies the computations even more. We note that the easiest way to derive the relativistic Hamilton operator in the traditional operator framework is to compute with formula (19) below, where, compared with (13), terms of the order $(\hbar/S_0)^2$, not computable

by iterative methods, are omitted. But we should note that the need for substantially more computation when using the methods developed in [17, 19–22] to a large extent results from the need to switch between different quantum mechanics formalisms in the initial and final expressions. We also note importance of the results obtained in [19–22, 30] (also see the references therein) in studying effects due to Berry phases.

COMPARISON OF HAMILTONIANS OBTAINED BY THE ERIKSEN METHOD AND METHODS OF THE STEP-BY-STEP TYPE

To determine the precision of methods of the step-by-step type, we must compare Eq. (13) with the Hamilton operator expansion in the FW representation in powers of the operators $\mathcal{E}$ and $\mathcal{O}$ and their products containing sufficiently large powers obtained by the Eriksen method. Such an expansion was found in [16]. But the result there, obtained using symbolic computer computations, is represented in a form very inconvenient for this comparison. Reducing the Hamiltonian operator found in [16] by writing it via multiple commutators leads to the expression

$$\begin{aligned}\mathcal{H}_{FW}^{(1)} &= \beta\left(m+\frac{\mathcal{O}^2}{2m}-\frac{\mathcal{O}^4}{8m^3}+\frac{\mathcal{O}^6}{16m^5}-\frac{5\mathcal{O}^8}{128m^7}\right)\\ &+\mathcal{E}-\frac{1}{128m^6}\left\{(8m^4-6m^2\mathcal{O}^2+5\mathcal{O}^4),[\mathcal{O},[\mathcal{O},\mathcal{E}]]\right\}\\ &+\frac{1}{512m^6}\left\{(2m^2-\mathcal{O}^2),[\mathcal{O}^2,[\mathcal{O}^2,\mathcal{E}]]\right\}\\ &+\frac{1}{16m^3}\beta\left\{\mathcal{O},[[\mathcal{O},\mathcal{E}],\mathcal{E}]\right\}-\frac{1}{32m^4}\left[\mathcal{O},[[[\mathcal{O},\mathcal{E}],\mathcal{E}],\mathcal{E}]\right]\\ &+\frac{11}{1024m^6}\left[\mathcal{O}^2,\left[\mathcal{O}^2,[\mathcal{O},[\mathcal{O},\mathcal{E}]]\right]\right]+A_{24},\end{aligned} \tag{15}$$

where

$$\begin{aligned}A_{24}=\frac{1}{256m^5}\beta\Big(&24\left\{\mathcal{O}^2,([\mathcal{O},\mathcal{E}])^2\right\}-11\left([\mathcal{O}^2,\mathcal{E}]\right)^2\\ &-14\left\{\mathcal{O}^2,\left[[\mathcal{O}^2,\mathcal{E}],\mathcal{E}\right]\right\}-4\left[\mathcal{O},\left[\mathcal{O},\left[[\mathcal{O}^2,\mathcal{E}],\mathcal{E}\right]\right]\right]\\ &+\frac{9}{2}\left[\left[\mathcal{O},\left[\mathcal{O},\left[\mathcal{O}^2,\mathcal{E}\right]\right]\right],\mathcal{E}\right]+\frac{5}{2}\left[\mathcal{O}^2,[\mathcal{O},[[\mathcal{O},\mathcal{E}],\mathcal{E}]]\right]\Big).\end{aligned}$$

In A_{24}, the first and second subscripts indicate the respective numbers of $\mathcal{E}$ and $\mathcal{O}$ operators in the product. The two preceding terms in Eq. (15), defining A_{32} and part of A_{16}, have the order of magnitude $(\hbar/S_0)^3$ and can be discarded. Neglecting these operators and

also terms of the third degree in $\hbar$ in A_{24}, we obtain

$$\begin{aligned}\mathcal{H}_{FW}^{(1)} &= \beta\left(m+\frac{\mathcal{O}^2}{2m}-\frac{\mathcal{O}^4}{8m^3}+\frac{\mathcal{O}^6}{16m^5}-\frac{5\mathcal{O}^8}{128m^7}\right)\\ &+\mathcal{E}-\frac{1}{128m^6}\left\{(8m^4-6m^2\mathcal{O}^2+5\mathcal{O}^4),[\mathcal{O},[\mathcal{O},\mathcal{E}]]\right\}\\ &+\frac{1}{512m^6}\left\{(2m^2-\mathcal{O}^2),[\mathcal{O}^2,[\mathcal{O}^2,\mathcal{E}]]\right\}\\ &+\frac{1}{16m^3}\beta\left\{\mathcal{O},[[\mathcal{O},\mathcal{E}],\mathcal{E}]\right\}+\frac{1}{256m^5}\beta\Bigg(24\left\{\mathcal{O}^2,([\mathcal{O},\mathcal{E}])^2\right\}\\ &-11\left([\mathcal{O}^2,\mathcal{E}]\right)^2-14\left\{\mathcal{O}^2,\left[[\mathcal{O}^2,\mathcal{E}],\mathcal{E}\right]\right\}\Bigg).\end{aligned} \tag{16}$$

To compare (13) with the exact solution, we must write it in the static case and also represent it as a series of relativistic corrections in powers of the operators $\mathcal{E}/m$ and $\mathcal{O}/m$. In this case, it becomes

$$\begin{aligned}\mathcal{H}_{FW} &= \mathcal{H}_{FW}^{(2)} = \beta\left(m+\frac{\mathcal{O}^2}{2m}-\frac{\mathcal{O}^4}{8m^3}\right.\\ &\left.+\frac{\mathcal{O}^6}{16m^5}-\frac{5\mathcal{O}^8}{128m^7}\right)+\mathcal{E}\\ &-\frac{1}{128m^6}\left\{(8m^4-6m^2\mathcal{O}^2+5\mathcal{O}^4),[\mathcal{O},[\mathcal{O},\mathcal{E}]]\right\}\\ &+\frac{1}{512m^6}\left\{(10m^2-19\mathcal{O}^2),[\mathcal{O}^2,[\mathcal{O}^2,\mathcal{E}]]\right\}\\ &-\frac{1}{8m^3}\beta\left([\mathcal{O},\mathcal{E}]\right)^2+\frac{1}{32m^5}\beta\left([\mathcal{O}^2,\mathcal{E}]\right)^2.\end{aligned} \tag{17}$$

If we consider the nonstationary case, change the criterion for estimating the magnitude of the terms in Eqs. (13) and (17), and represent these equations as an expansion in powers of $\mathcal{F}/m$, and $\mathcal{O}/m$, limiting ourself to terms of the third order in the inverse mass, then the indicated relations lead to an expression coinciding with those obtained in [10] by the classical FW method [1]:

$$\begin{aligned}\mathcal{H}_{FW} &= \mathcal{H}_{FW}^{(3)} = \beta\left(m+\frac{\mathcal{O}^2}{2m}-\frac{\mathcal{O}^4}{8m^3}\right)+\mathcal{E}\\ &-\frac{1}{8m^2}[\mathcal{O},[\mathcal{O},\mathcal{F}]]-\frac{1}{8m^3}\beta\left([\mathcal{O},\mathcal{F}]\right)^2.\end{aligned} \tag{18}$$

This also shows that the results obtained by the different iterative methods agree. But we note that for terms of higher order in the inverse mass in the power series in $\mathcal{F}/m$ and $\mathcal{O}/m$, the results derived using the classical method [1] and relativistic methods of the step-by-step type differ.

Comparing terms in expressions (16) and (17), we can easily establish that they do not completely agree. Complete agreement occurs for only two terms, determining the series

expansion of the operator $\beta\epsilon$ and first of the anticommutators in Eq. (13), which in turn is the result of transforming the second double commutator in (10). These two terms are respectively of the zeroth and first orders in $\hbar/S_0$. Subsequent terms in (16) and (17) do not coincide. There is a disagreement even for operators proportional to $[\mathcal{O}^2,[\mathcal{O}^2,\mathcal{E}]]$. It is very important that the operators corresponding to them in formulas (13) and (17) already appear in the result of the *first* transformation step, and they must be taken into account in the framework of the weak-field approximation ($\mathcal{E} \ll m$) when considering terms of the order $(\hbar/S_0)^2$. They arise as a result of transforming the first double commutator in Eq. (10). The term A_{22} in (16), also of the order $(\hbar/S_0)^2$, can be transformed as

$$\frac{1}{16m^3}\beta\left\{\mathcal{O},[[\mathcal{O},\mathcal{E}],\mathcal{E}]\right\} = \frac{1}{16m^3}\beta\left[[\mathcal{O}^2,\mathcal{E}],\mathcal{E}\right] - \frac{1}{8m^3}\beta\left([\mathcal{O},\mathcal{E}]\right)^2.$$

Its significant difference from the corresponding term in (17) is obvious, as is the difference between the expressions for the operators A_{24} in the two equations.

In summary, using the relativistic methods of the step-by-step type in [3, 17–22], allows determining the correct relativistic form of the terms of the zeroth and first orders in $\hbar/S_0$, but the terms of the order $(\hbar/S_0)^2$ differ from the corresponding terms in the FW representation. Their difference determines the degree to which the resulting transformation operator obtained by methods of the step-by-step type and equal to the product of the operators of the successive transformations differs from exact FWtransformation operator (5). The Hamilton operators obtained by the Eriksen method and the methods of the step-by-step type do not agree even for terms of the order $(\hbar/S_0)^2$. Some terms of the order $(\hbar/S_0)^2$ arise after the first transformation step and are proportional to the first power of the operator $\mathcal{E}$, i.e., they correspond to the weak-field approximation. Even for them, the Hamilton operators obtained by the Eriksen method and the methods of the step-by-step type do not agree. Such agreement exists if and only if the terms of second and higher orders in $\hbar/S_0$ under consideration arise as a result of computing the operator $\beta\epsilon$ or the first anticommutator in (13). For example, the Eriksen method and the iterative methods lead to mutually consistent results in computing the Darwin interaction, which is of the order $(\hbar/S_0)^2$. This interaction is determined by the term proportional to $\Delta\Phi$ in (14)and arises as a result of computing the above mentioned anticommutator.

From results of this study, we can conclude that the iterative methods agree excellently

with each other. Even the nonrelativistic method proposed by Foldy and Wouthuysen [1], with only basic relativistic corrections taken into account gives expression (18), which is also obtained by the relativistic methods of the step-by-step type (such an agreement does not occur for terms of higher orders in the inverse mass). The difference between the results obtained from the iterative methods and the results of the Eriksen method, which realizes the direct FW transformation, is substantially stronger.

According to the analysis of initial Hamilton operator (4), the relativistic FW transformation methods give the form of the transformed Hamiltonian

$$\mathcal{H}_{FW} = \beta\epsilon + \mathcal{E} - \frac{1}{8}\left\{\frac{1}{\epsilon(\epsilon+m)}, [\mathcal{O}, [\mathcal{O}, \mathcal{F}]]\right\}. \tag{19}$$

This Hamiltonian contains exactly determined terms of the zeroth and first orders in $\hbar/S_0$. Terms of the second and higher orders in $\hbar/S_0$, if they do not arise as a result of computing Hamiltonian (19), cannot be determined using methods of the step-by-step type.

EXAMPLE: RELATIVISTIC PARTICLES IN A UNIFORM FIELD

As an example showing the importance of methods for the FW transformation of the step-by-step type for relativistic particles, we determine the energy spectrum of spin-0, -1/2, and -1 particles moving in a plane orthogonal to a uniform magnetic field. For spin-0 particles, the Hamilton operator in the FW representation has the form [31]:

$$\mathcal{H}_{FW} = \beta\sqrt{m^2 + \boldsymbol{\pi}^2}, \tag{20}$$

and for spin-1/2 particles and the anomalous magnetic moment (AMM) [3, 32, 33], this operator has the form

$$\mathcal{H}_{FW} = \beta\sqrt{m^2 + \boldsymbol{\pi}^2 - e\hbar\boldsymbol{\Sigma}\cdot\boldsymbol{B}} - \mu'\boldsymbol{\Pi}\cdot\boldsymbol{B}. \tag{21}$$

Equations (20) and (21) are exact.

If a magnetic field is directed along the z, axis and the particle motion is transverse (the eigenvalues of the operators p_z and π_z are zero), then $p_z = -i\hbar(\partial/\partial z)$ commutes with the Hamiltonian and has eigenvalues $\mathcal{P}_z = \text{const}$. Consequently, considering the particular case $\mathcal{P}_z = 0$ is well justified [3, 33]. At the same time, the problem of particle motion with an arbitrary nonzero eigenvalue $\mathcal{P}_z$ reduces to this case by a coordinate transformation.

The energy spectrum of scalar particles is defined by the formula

$$E = \sqrt{m^2 + (2n+1)|e|\hbar B}, \quad n = 0, 1, 2, \ldots. \tag{22}$$

We note that for relativistic particles, the two terms in the radicand have the same order of magnitude, which as a rule requires the condition $n \gg 1$.

The energy spectrum and eigenfunctions of AMM particles in constant, uniform magnetic fields were first found in the Dirac representation [34]. This problem was also successfully solved in the FW representation [35]. For $\mathcal{P}_z = 0$, the formula for the energy spectrum has the form

$$\begin{gathered} E = \sqrt{m^2 + (2n+1)|e|\hbar B - \lambda e\hbar B} - \lambda\mu' B, \\ n = 0, 1, 2, \ldots, \quad \lambda = \pm 1. \end{gathered} \tag{23}$$

Relations (20)–(23) show the effectiveness of the relativistic FW transformation by methods of the step-by-step type [3] (it is exact in this case). In contrast, the Eriksen method and other direct FW transformation methods allow representing equations for the Hamiltonian and energy spectrum only by expanding square roots appearing in them in powers of the operator $|\boldsymbol{\pi}|/m$.

Under the same conditions, we now find the energy spectrum of spin-1 particles whose magnetic moment has not only the normal part $\mu_0 = e\hbar/m$ corresponding to $g = 2$ but also the anomalous part $\mu' = e\hbar(g-2)/(2m)$. The initial Hamilton operator in the Sakata-Taketani representation [36], derived in [37] (see also [38]), in the case under consideration is most conveniently represented as [39]:

$$\begin{gathered} \mathcal{H} = \rho_3\mathcal{M} + \mathcal{E} + \mathcal{O}, \quad \rho_3\mathcal{E} = \mathcal{E}\rho_3, \quad \rho_3\mathcal{O} = -\mathcal{O}\rho_3, \\ \mathcal{M} = m + \frac{\boldsymbol{\pi}^2}{2m} - \frac{e\hbar}{m}\boldsymbol{S}\cdot\boldsymbol{B}, \quad \mathcal{E} = -\rho_3\frac{e\hbar(g-2)}{2m}\boldsymbol{S}\cdot\boldsymbol{B}, \\ \mathcal{O} = i\rho_2\left[\frac{\boldsymbol{\pi}^2}{2m} - \frac{(\boldsymbol{\pi}\cdot\boldsymbol{S})^2}{m} + \frac{e\hbar(g-2)}{2m}\boldsymbol{S}\cdot\boldsymbol{B}\right]. \end{gathered} \tag{24}$$

Here, the Hamilton operator acts on six-component wave functions $\Psi = \begin{pmatrix} \phi \\ \chi \end{pmatrix}$, which are analogues of bispinors, ϕ and χ are three-component analogues of spinors, $\boldsymbol{S}$ is a 3×3 spin matrix for spin-1 particles, ρ_i are Pauli matrices, and $\rho_i\boldsymbol{S}$ denotes the direct product of matrices, for example, $\rho_1\boldsymbol{S} \equiv \begin{pmatrix} 0 & \boldsymbol{S} \\ \boldsymbol{S} & 0 \end{pmatrix}$. In the case under consideration, $[\mathcal{M}, \mathcal{E}] = [\mathcal{M}, \mathcal{O}] = 0$, and we can use formulas (13) and (15) replacing m with $\mathcal{M}$. In these formulas, the Dirac matrix β corresponds to the direct product of ρ_3 and the 3×3 identity matrix.

For particles without an AMM, the FW transformation is exact, and the obtained Hamiltonian is given by [38]:

$$\mathcal{H}_{FW} = \rho_3\sqrt{m^2 + \boldsymbol{\pi}^2 - 2e\hbar\boldsymbol{S}\cdot\boldsymbol{B}}. \tag{25}$$

The energy spectrum has the form

$$E = \sqrt{m^2 + (2n+1)|e|\hbar B - 2\lambda e\hbar B}, \quad n = 0, 1, 2, \ldots, \quad \lambda = -1, 0, +1. \tag{26}$$

For particles with an AMM, the corresponding Hamiltonian was derived in [38, 40] up to terms linear in the field. To find the spectrum for $\mathcal{P}_z = 0$, it is convenient to write the Hamiltonian in the form

$$\mathcal{H}_{FW} = \rho_3\sqrt{m^2 + \boldsymbol{\pi}^2 - 2e\hbar\boldsymbol{S}\cdot\boldsymbol{B}} - \rho_3\frac{e\hbar(g-2)}{2m}\boldsymbol{S}\cdot\boldsymbol{B}. \tag{27}$$

With the indicated precision, the energy spectrum is defined by

$$\begin{gathered} E = \sqrt{m^2 + (2n+1)|e|\hbar B - 2\lambda e\hbar B} - \frac{\lambda e\hbar(g-2)}{2m}B, \\ n = 0, 1, 2, \ldots, \quad \lambda = -1, 0, +1. \end{gathered} \tag{28}$$

In the case under consideration, the relativistic FW transformation can be accomplished with high precision, although it is an approximation. The operators in (24) satisfy the relations

$$\begin{gathered} [\mathcal{O}^2, \mathcal{E}] = 0, \quad [\mathcal{O}, \mathcal{E}] = \rho_1\frac{e^2\hbar^2(g-1)(g-2)}{2m^2}(\boldsymbol{S}\cdot\boldsymbol{B})^2, \\ \{\mathcal{O}, [[\mathcal{O}, \mathcal{E}], \mathcal{E}]\} = -\frac{e^4\hbar^4(g-1)^2(g-2)^2}{2m^4}B^2(\boldsymbol{S}\cdot\boldsymbol{B})^2, \\ ([\mathcal{O}, \mathcal{E}])^2 = \frac{e^4\hbar^4(g-1)^2(g-2)^2}{4m^4}B^2(\boldsymbol{S}\cdot\boldsymbol{B})^2. \end{gathered} \tag{29}$$

In (24), among the terms with a nominal order $(\hbar/S_0)^2$, only two, which are proportional to $\{\mathcal{O}, [[\mathcal{O}, \mathcal{E}], \mathcal{E}]\}$ and $([\mathcal{O}, \mathcal{E}])^2$, are nonzero, and they are in fact of the fourth order in $\hbar$ and B. Because $S_0 = \epsilon^2/(|e|B) \sim m^2/(|e|B)$ in the considered case, the relativistic FW transformation allows determining the Hamiltonian for spin-1 particles up to terms of the order $(|e|\hbar B)^3/m^5$ inclusively. With these terms taken into account, the Hamiltonian becomes

$$\begin{gathered} \mathcal{H}_{FW} = \rho_3\epsilon - \rho_3\frac{e\hbar(g-2)}{2m}\boldsymbol{S}\cdot\boldsymbol{B} \\ +\rho_3\frac{e^2\hbar^2(g-1)(g-2)}{16m^3}\left\{\frac{1}{\epsilon(\epsilon+m)}, \left(B^2(\boldsymbol{S}\cdot\boldsymbol{\pi})^2\right.\right. \\ \left.\left. -[\boldsymbol{S}\cdot(\boldsymbol{\pi}\times\boldsymbol{B})]^2 - e\hbar(g-1)B^2(\boldsymbol{S}\cdot\boldsymbol{B})\right)\right\}, \\ \epsilon = \sqrt{m^2 + \boldsymbol{\pi}^2 - 2e\hbar\boldsymbol{S}\cdot\boldsymbol{B} - \frac{e^2\hbar^2 g(g-2)}{4m^2}(\boldsymbol{S}\cdot\boldsymbol{B})^2}. \end{gathered} \tag{30}$$

We note that the effects due to the tensor electric and magnetic polarizability indicated in the introduction are determined by spin-dependent terms of the second order in $\hbar$ and B. For these terms, we have the equality

$$B^2(\boldsymbol{S}\cdot\boldsymbol{\pi})^2+[\boldsymbol{S}\cdot(\boldsymbol{\pi}\times\boldsymbol{B})]^2+\boldsymbol{\pi}^2(\boldsymbol{S}\cdot\boldsymbol{B})^2=2(\boldsymbol{\pi}\times\boldsymbol{B})^2.$$

The term in the right-hand side characterizes the scalar electric polarizability of a moving particle.

The definition of the Hamiltonian and energy spectrum for spin-1 particles with an AMM in a homogenous magnetic field is also a demonstration of the possibilities provided by the iterative methods for the FW transformation. Neither in the SakataTaketani representation nor with other transformation methods (see [32, 41]) this problem has been solved. Moreover, the problem of consistency of the quantum mechanics of spin particles had been discussed for several years (see [32, 42, 43] and the references therein).

DISCUSSION AND CONCLUSIONS

Comparing the results obtained by the Eriksen method and by methods of the step-by-step type leads to an important and rather surprising conclusion. Relativistic FW transformation methods of the step-by-step type already after the *first* transformation step (let alone the subsequent steps) give an expression for the Hamiltonian inconsistent with the exact result determined from a series of relativistic corrections computed by the Eriksen method.

The disagreement between the Eriksen method realizing the direct FW transformation and methods of the step-by-step type occurs for terms of the second and higher orders in $\hbar/S_0$, if they do not arise as a result of computing the operator $\beta\epsilon$ or the first anticommutator in (13). The exact Eriksen method and the relativistic methods of the step-by-step type developed in [3, 17–22] lead to fully consistent results only for terms arising as a result of computing these operators, including all terms of the zeroth and first orders in $\hbar/S_0$.

The Eriksen method allows representing the transformed Hamiltonian as an expansion in powers of the operators $\mathcal{E}/m$ and $\mathcal{O}/m$. Therefore, it is convenient to use it to solve nonrelativistic problems (e.g., in atomic physics) when relativistic corrections must be taken into account. For relativistic methods of the step-by-step type, the operators $\mathcal{E}$ and $\mathcal{O}$ are

not considered small, and the expansion is based on the assumption that the commutator of these operators is small in order of magnitude compared with their products. The validity of this assumption depends on the problem considered. It is quite often invalid in atomic physics but is always valid in the quantum mechanical description of particle beams in accelerators, storage rings, and Penning traps. On the other hand, the Eriksen method not only does not allow deriving compact relativistic expressions for the Hamiltonian in the FW representation but plainly gives a divergent series of relativistic corrections when $\boldsymbol{p}^2/m^2 \geq 1$. Therefore, there is currently no alternative to iterative methods for describing relativistic particles.

In particular, with adequate precision, iterative methods describe spin effects for relativistic particles including spin affecting the motion trajectory (determined by the respective Stern-Gerlach and Mathisson forces for electromagnetic and gravitational interactions [3, 18, 44, 45]). These effects are determined by terms of the order $\hbar/S_0$. There are some indirect arguments for extending this conclusion to spin-($s \neq 1/2$) particles. Terms linear in the spin and Planck constant in the FW representation Hamiltonian derived in [40] (see also [38]) by a method of the step-by-step type for spin-1 particles lead to an operator equation for the spin motion that corresponds to the Thomas-Bargmann-Michele-Telegdi equation and consequently correctly describes spin effects. The effectiveness of iterative methods was shown in Sec. 5 in the example of relativistic spin-0, -1/2, and -1 particles in a homogenous magnetic field. Using the results obtained here, we determined the precision provided by methods of the step-by-step type in that case.

In the general case, the problem of correctly defining the contributions to the Hamiltonian determined by the quadrupole interaction and tensor magnetic and electric polarizability of spin-($s > 1/2$) particles and having the order $(\hbar/S_0)^2$ by a method of the step-by-step type needs separate study. Additional analysis is needed because the initial Proca-Corben-Schwinger equation and similar equations for higher-spin particles characterize structureless point particles.

A comparison of the three methods of the step-by-step type [3, 17–22] with the most fundamental justification showed the principal commonality of the approaches used. At each step, a transformation operator is chosen that would realize the exact transformation if the even and odd operators commute. This commonality leads to agreement of the results of the three methods. But a substantial difference in quantum mechanics formalisms used in these

methods leads to differences in the amount of computation needed to obtain the final results. The simplest way to derive the Hamiltonian is to use the traditional operator formalism and unitary transformations [3, 18] computing in accordance with (19) and estimating the computational precision (determining the order of magnitude) by computing the neglected terms in accordance with (16). An example of this approach was given in Sec. 5, and this example also showed the possibility of using the method for particles with spins other than 1/2.

The precision estimation allows detecting the difference of iterative methods from Eriksens formal expansion of the Hamiltonian and shows their applicability boundaries. We note that computing by (19) requires much fewer computational steps than using the other two iterative methods analyzed here. Nevertheless, the method developed and applied in [19–22, 30] is the best for studying effects determined by Berry phases. We also note a successful use of a similar method in [29], also for the analysis of Berry phases.

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