Foldy-Wouthyusen wave functions and conditions of transformation between Dirac and Foldy-Wouthuysen representations

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Abstract

The block-diagonalization of the Hamiltonian is not sufficient for the transformation to the Foldy-Wouthuysen (FW) representation. The conditions enabling the transition from the Dirac representation to the FW one are formulated and proved. The connection between wave functions in the two representations is derived. The results obtained allows calculating expectation values of operators corresponding to main classical quantities.

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I. INTRODUCTION

The Foldy-Wouthuysen representation introduced in Ref. [1] occupies a special place in the quantum theory. This is mainly due to the fact that the FW representation provides the best possibility of obtaining a meaningful classical limit of the relativistic quantum mechanics [1, 2, 3, 4]. The Hamiltonian and all operators in this representation are block-diagonal (diagonal in two spinors). The basic advantages of the FW representation are investigated in Refs. [1, 2, 3, 4] and shortly described in Sec. II.

There are many methods of the FW transformation considered in Refs. [3, 4, 5, 6, 7, 8] (see also below). However, some of them are rather intuitive. Therefore, conditions of the FW transformation and main properties of the FW representation should be determined.

In the present work, the basic properties of wave functions in the FW representation are investigated and the connection between wave functions in the Dirac and FW representations is found. Such a connection has been determined in Ref. [9] in the particular case when the FW transformation is exact.

We also establish conditions of the transformation from the Dirac representation to the FW one. The action of these conditions is illustrated by several examples. In particular, the obtained result allows calculating the expectation values of operators corresponding to the basic classical quantities. Explicit forms of these operators for relativistic particles in external fields can be determined in the FW representation but not in the Dirac one.

II. FOLDY-WOUTHUYSEN REPRESENTATION

The use of the FW representation possesses the important advantages investigated in Refs. [1, 2, 3]. The relations between the operators in the FW representation are similar to those between the respective classical quantities. Only the FW representation possesses these properties considerably simplifying the transition to the semiclassical description. The Hamiltonian for a free particle fully agrees with that of classical physics in contrast with the Hamiltonian in the Dirac representation [1].

We use the system of units $\hbar = c = 1$ and denote matrices as follows.

$$\boldsymbol{\alpha} = \beta\boldsymbol{\gamma} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}, \quad \beta \equiv \gamma^0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix}, \quad \boldsymbol{\Pi} = \beta\boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & -\boldsymbol{\sigma} \end{pmatrix}$$

are the Dirac matrices; σ^i are the Pauli matrices. $\psi_D(x)$, $\psi_{FW}(x)$ are four-component wave functions in the Dirac and FW representation, respectively. The scalar product of four-vectors is taken in the form $xy \equiv x^\mu y_\mu \equiv x^0 y^0 - x^k y^k$, $\mu = 0,1,2,3$, $k = 1,2,3$; $p^\mu = i(\partial/\partial x_\mu)$.

The position operator in the FW representation is $\boldsymbol{r}$. It is given by the cumbersome expression in the Dirac representation [10]:

$$\boldsymbol{r}_D = \boldsymbol{r} + \frac{i\beta\boldsymbol{\alpha}}{2E} - \frac{i\beta(\boldsymbol{\alpha}\cdot\boldsymbol{p})\boldsymbol{p} + [\boldsymbol{\Sigma}\times\boldsymbol{p}]|\boldsymbol{p}|}{2E(E+m)|\boldsymbol{p}|}, \quad E = \sqrt{m^2+\boldsymbol{p}^2}.$$

For free particles, the momentum and velocity operators are expressed in a normal, close to classical, way, $\boldsymbol{p} = -i\nabla$ and $\boldsymbol{v} = \boldsymbol{p}/E$ ($\boldsymbol{v} = \boldsymbol{\alpha}$ in the Dirac representation).

In the FW representation, the problem of "*Zitterbewegung*" motion never arises [2, 10]. The operators $\boldsymbol{l} = \boldsymbol{r}\times\boldsymbol{p}$ and $\boldsymbol{\Sigma}/2$ define the angular momentum and the spin for a free particle, respectively. In this representation, unlike the Dirac one, each of them is a constant of motion (see Ref. [1]). The corresponding operators conserving in the Dirac representation are known only for free particles and are expressed by cumbersome formulae (see Refs. [1, 3]). The FW representation is very convenient for describing the particle polarization. In this representation, polarization operators have simple forms. The three-dimensional polarization operator is equal to the matrix $\boldsymbol{\Pi}$ [11, 12]. In the Dirac representation, this operator depends on the particle momentum [3, 11, 12]. For particles interacting with external fields, it also depends on external field parameters [12].

Thus, in the Dirac representation all operators corresponding to the basic classical quantities are defined by cumbersome expressions. Moreover, these operators should also depend on the external field parameters for particles interacting with external fields. Therefore, explicit forms of such operators in the Dirac representation are usually unknown. We can conclude that the preferable employment of the FW representation is evident, although the relativistic wave equations are more complicated in this representation.

The use of the FW representation permits to reduce the number of components of the bispinor wave function because one of the FW spinors is zero.

Note also that the derivation of the relativistic Hamiltonian $\mathcal{H}_{FW}$ in Ref. [7] made it possible to treat quantum-field processes in the FW representation within the framework of the perturbation theory [8].

Equations for the wave function in the FW representation have a non-covariant form, and the FW Hamiltonians are non-local and block-diagonal (they contain infinite sets of differential operators and are diagonal in two spinors).

III. METHODS OF THE FOLDY-WOUTHUYSEN TRANSFORMATION

In this Section, we give an overview of known methods of the FW transformation.

In the presence of time-dependent external fields, transformation to the FW representation described by the wave function ψ_{FW} is performed with the unitary operator U_{FW}:

$$\psi_{FW} = U_{FW}\psi_D = e^{iS}\psi_D,$$

where $\psi_D = A\begin{pmatrix}\phi\\ \chi\end{pmatrix}$ is the wave function (bispinor) in the Dirac representation.

The Hamilton operator in the FW representation takes the form [1, 13]:

$$\mathcal{H}_{FW} = U_{FW}\mathcal{H}_D U_{FW}^{-1} - iU_{FW}\frac{\partial U_{FW}^{-1}}{\partial t}. \tag{III.1}$$

The Dirac Hamiltonian can be split into operators commuting and noncommuting with the operator β:

$$\mathcal{H}_D = \beta m + \mathcal{E} + \mathcal{O}, \quad \beta\mathcal{E} = \mathcal{E}\beta, \quad \beta\mathcal{O} = -\mathcal{O}\beta. \tag{III.2}$$

The Hamiltonian $\mathcal{H}_D$ is Hermitian. We assume that both operators $\mathcal{E}$ and $\mathcal{O}$ are also Hermitian.

In the classical work by Foldy and Wouthuysen [1], the exact transformation for free relativistic particles and the approximate transformation for nonrelativistic particles in electromagnetic fields have been carried out.

For free Dirac particles, $\mathcal{E} = 0,\ \mathcal{O} = \boldsymbol{\alpha}\cdot\boldsymbol{p}$.

The FW Hamiltonian $(\mathcal{H}_0)_{FW}$ and the FW wave function $\psi_{FW}(x)$ are related to the Dirac Hamiltonian for free particles,

$$(\mathcal{H}_0)_D = \beta m + \boldsymbol{\alpha}\cdot\boldsymbol{p}, \tag{III.3}$$

and to the Dirac wave function $\psi_D(x)$ by the unitary transformation

$$(\mathcal{H}_0)_{FW} = U_0(\mathcal{H}_0)_D U_0^\dagger = \beta E, \quad \psi_{FW}(x) = U_0\psi_D(x), \quad U_0 = \sqrt{\frac{E+m}{2E}}\left(1 + \frac{\beta\boldsymbol{\alpha}\cdot\boldsymbol{p}}{E+m}\right). \tag{III.4}$$

The FW equation for the free motion of a quantum mechanical particle with the spin 1/2 takes the following form:

$$p_0\psi_{FW}(x) = (\mathcal{H}_0)_{FW}\psi_{FW}(x) = \beta E\psi_{FW}(x). \tag{III.5}$$

Solutions of Eq. (III.5) are plane waves with positive and negative energy [1]:

$$\psi^{(+)}_{FW}(x) = \frac{1}{(2\pi)^{3/2}}\mathcal{U}e^{-ipx}, \quad \psi^{(-)}_{FW}(x) = \frac{1}{(2\pi)^{3/2}}\mathcal{V}e^{ipx}, \quad p_0 = E = \sqrt{m^2+\boldsymbol{p}^2}. \tag{III.6}$$

In Eq. (III.6), $\mathcal{U} = \begin{pmatrix}\phi\\ 0\end{pmatrix}$ and $\mathcal{V} = \begin{pmatrix}0\\ \chi\end{pmatrix}$, ϕ and χ are two-component normalized Pauli spin functions.

For $\mathcal{U}$ and $\mathcal{V}$, the following orthonormality and completeness conditions are true:

$$\begin{gathered}\mathcal{U}^\dagger_s\mathcal{U}_{s'} = \mathcal{V}^\dagger_s\mathcal{V}_{s'} = \delta_{ss'}, \quad \mathcal{U}^\dagger_s\mathcal{V}_{s'} = \mathcal{V}^\dagger_s\mathcal{U}_{s'} = 0,\\ \sum_s(\mathcal{U}_s)_\gamma(\mathcal{U}^\dagger_s)_\delta = \frac{1}{2}(1+\beta)_{\gamma\delta}, \quad \sum_s(\mathcal{V}_s)_\gamma(\mathcal{V}^\dagger_s)_\delta = \frac{1}{2}(1-\beta)_{\gamma\delta}.\end{gathered} \tag{III.7}$$

In expressions (III.6), (III.7), γ, δ belong to spinorial indices and s to spin indices. Further, the sum sign and the indices themselves are not shown, when summing is performed in the spinorial indices.

It has been shown in Ref. [3] that the exact FW transformation can be fulfilled with the operator

$$U_{FW} = \sqrt{\frac{E+m}{2E}}\left(1+\frac{\beta\mathcal{O}}{E+m}\right), \quad E = \sqrt{m^2+\mathcal{O}^2} \tag{III.8}$$

on condition that the operators $\mathcal{E}$ and $\mathcal{O}$ commute:

$$[\mathcal{E},\mathcal{O}] = 0. \tag{III.9}$$

In this case, the FW Hamiltonian is given by

$$\mathcal{H}_{FW} = \beta E + \mathcal{E}. \tag{III.10}$$

Eq. (III.10) agrees with formula (III.5) for free particles.

Condition (III.9) is satisfied for the Dirac equation at a presence of the static external magnetic field $\boldsymbol{B} = \text{rot}\,\boldsymbol{A}$ (exact transformation by Case [14]) and also of some other interactions described in Refs. [3, 15]. In the general case of interaction of a fermion with an arbitrary boson field, condition (III.9) is not satisfied and the problem of transition between the Dirac and FW representations becomes much more complicated.

The general form of the exact FW transformation has been found by Eriksen [5] for stationary external fields. The Eriksen transformation operator is given by [5]

$$U_E = U_{FW} = \frac{1}{2}(1+\beta\lambda)\left[1+\frac{1}{4}(\beta\lambda+\lambda\beta-2)\right]^{-1/2}, \quad \lambda = \frac{\mathcal{H}_D}{(\mathcal{H}_D^2)^{1/2}}, \tag{III.11}$$

where $\mathcal{H}_D$ is the Hamiltonian in the Dirac representation. $\lambda = +1$ and -1 for the positive-energy and negative-energy solutions, respectively. It is important that [5]

$$\lambda^2 = 1, \quad [\beta\lambda, \lambda\beta] = 0 \tag{III.12}$$

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

$$[\beta, (\beta\lambda + \lambda\beta)] = 0. \tag{III.13}$$

Any even operator is block-diagonal and does not mix the upper and lower components of the wave function.

The validity of the Eriksen transformation has been argued in Ref. [6]. It has been shown that the Eriksen transformation directly leads to the FW representation. We can give an additional argument which follows from the fact that the use of Eqs. (III.12),(III.13) reduces transformation operator (III.11) to the form

$$U_E = (2+\beta\lambda+\lambda\beta)^{-1/2}(1+\beta\lambda). \tag{III.14}$$

Since two factors in the right hand side of Eq. (III.14) commutate and the first factor defines an even operator, an action of U_E on any eigenfunction of the Dirac Hamiltonian nullifies either the lower spinor or the upper one. Eq. (III.14) can also be transformed to the form

$$U_E = \frac{1+\beta\lambda}{\sqrt{(1+\beta\lambda)^\dagger(1+\beta\lambda)}}. \tag{III.15}$$

The Eriksen operator brings the Dirac wave function and the Dirac Hamiltonian to the FW representation in one step. However, it is difficult to use the Eriksen method because the general final formula is very cumbersome and contains roots of Dirac matrix operators.

Another direct way to obtain the FW transformation has been proposed in Ref. [7] (see also overview [8]). The transformation operator U_{FW} and the relativistic Hamiltonian $\mathcal{H}_{FW}$ (III.1), obtained for the general case with arbitrary external boson field as a power series in coupling constant q, have the following form:

$$\begin{aligned} U_{FW} &= U_0(1+q\delta_1+q^2\delta_2+q^3\delta_3+\dots), \\ \mathcal{H}_{FW} &= \beta E + qK_1 + q^2K_2 + q^3K_3 + \dots \end{aligned} \tag{III.16}$$

In expressions (III.16), U_0 is the FW transformation operator for free Dirac particles defined by Eq. (III.4) and δ_i, K_i are some operators. The Hamiltonian $\mathcal{H}_{FW}$ (III.16) can be used, in particular, to consider field quantum theory issues [8].

Along with direct derivation of the block-diagonal Hamiltonians, there is a lot of step-by-step methods to obtain Hamiltonians free of odd operators. In particular, one of such methods has been used in the classical work by Foldy and Wouthuysen [1] to derive the Hamilatonian $\mathcal{H}_{FW}$ in the presence of an external electromagnetic field as a power series in $1/m$. In the next section, we compare step-by-step and direct methods of transition to the FW representation.

IV. COMPARISON OF DIRECT AND STEP-BY-STEP METHODS OF THE FOLDY-WOUTHYUSEN TRANSFORMATION

The transformation of the Hamiltonian to a block-diagonal form may not be equivalent to the FW transformation. There are infinitely many representations that differ from the FW representation despite the block-diagonal form of the Hamiltonian [16]. As an example, one can indicate the Eriksen-Kolsrud method [17] which variants have been used in Refs. [18, 19, 20, 21]. It has been proved in Ref. [16] (see also below) that these transformations are not equivalent to the FW transformation. The same conclusion will be made for the Melosh transformation [22].

One should draw special attention to the step-by-step method initially proposed in the classical work by Foldy and Wouthuysen [1] and widely used in many applications. De Vries and Jonker [6] and later the author of Ref. [7] have shown that the step-by-step removal of odd operators being the main distinguishing feature of step-by-step methods does not result in the FW representation. The Hamiltonians transformed to the FW representation by the Eriksen method [5] and the method developed in Ref. [7] differ from the Hamiltonian obtained by the original FW method [1]. A reason is a noncommutativity of unitary transformations [7, 8]. Formula (III.1) can be re-written as

$$\mathcal{H}_{FW} = U_{FW}\left(\mathcal{H}_D - i\frac{\partial}{\partial t}\right)U_{FW}^{-1} + i\frac{\partial}{\partial t}.$$

Any unitary transformation operator can be presented in the exponential form

$$U_{FW} = e^{iS}.$$

For direct methods [5, 7]

$$\mathcal{H}_{FW} = e^{iS}\left(\mathcal{H}_D - i\frac{\partial}{\partial t}\right)e^{-iS} + i\frac{\partial}{\partial t}. \tag{IV.1}$$

For step-by-step methods

$$\mathcal{H}_{FW} = \dots e^{iS_n}\dots e^{iS_2}e^{iS_1}\left(\mathcal{H}_D - i\frac{\partial}{\partial t}\right)e^{-iS_1}e^{-iS_2}\dots e^{-iS_n}\dots + i\frac{\partial}{\partial t}. \tag{IV.2}$$

Hamiltonians (IV.1), (IV.2) are equivalent only when

$$e^{iS} = e^{i(S_1+S_2+\dots S_n+\dots)} = \dots e^{iS_n}\dots e^{iS_2}e^{iS_1}. \tag{IV.3}$$

However, equality (IV.3) is valid only for the trivial case of commuting S_i's. Such a situation almost never takes place in applications.

According to the theorem of F. Haussdorff [23],

$$\exp A\cdot\exp B = \exp\left(A + B + \frac{1}{2}[A,B] + \textit{higher order commutators}\right) \neq \exp B\cdot\exp A. \tag{IV.4}$$

The noncommutativity of unitary transformations leads to a dependence of the resulting operator of the FW transformation

$$U = U_{FW} = \dots U_n\dots U_2U_1U_0 \tag{IV.5}$$

on a specific method of this transformation [7, 8]. This circumstance does not mean that the exact FW representation cannot be reached in several steps. If the step-by-step transformation has been carried out with operator (IV.5), the Hamiltonian obtained can be brought to the exact FW form with the unitary operator $U' = U_EU^{-1}$, where U_E is given by Eq. (III.11). Evidently, the exact FW representation needs one of the exact methods even in this case.

It has been shown in Refs. [6, 7] that the original step-by-step transformation [1] does not exactly lead to the FW representation. The same situation takes place for the methods developed in Ref. [3, 4]. Thus, step-by-step methods are approximate and the exact FW representation cannot be obtained with these methods.

However, step-by-step methods are rather helpful, when one can restrict oneself to several leading orders of a FW Hamiltonian expansion in a chosen small parameter. As a rule, this level of accuracy is quite sufficient, in particular, when one uses the weak field approximation or the nonrelativistic one. Eqs. (IV.2),(IV.4) show that a difference between Hamiltonians obtained by the exact and step-by-step methods is defined by the commutator $[S_1, S_2]$. Therefore, this difference appears for the first time only for the third step.

For example, the expansion in powers of $1/m$ in the nonrelativistic approximation carried out in Ref. [1] gives an accuracy up to $1/m^2$ and can be restricted to S_1 and S_2. In this case, $e^{iS_2}e^{iS_1} \approx e^{i(S_1+S_2)}$, since $[S_1, S_2] \sim 1/m^3$.

An essential advantage of the step-by-step methods consists in the relative simplicity of computations they offer. On the contrary, the use of direct methods leads to cumbersome derivations.

The differences between the FW Hamiltonians obtained by the direct and step-by-step methods are beyond the weak field approximation and even beyond the leading terms of expansion in the Planck constant. The latter statement is illustrated by the correspondence between the quantum-mechanical motion equations obtained by the method proposed in Ref. [4] and respective classical relativistic equations.

In addition to the aforesaid, any transformation that diagonalizes the Hamiltonian and claims to enable the transition to the FW representation should be tested for the wave function reduction condition. The formulation and proof of this condition is provided in the next section.

V. CONNECTION BETWEEN WAVE FUNCTIONS IN THE DIRAC AND FOLDY-WOUTHYUSEN REPRESENTATIONS. PROOF OF THE WAVE FUNCTION REDUCTION CONDITION FOR THE FOLDY-WOUTHYUSEN TRANSFORMATION

Diagonalization of the Hamiltonian relative to the upper and lower components of the wave function $\psi_D(x)$ is the necessary condition for the transformation from the Dirac representation to the FW representation (the FW transformation).

The second condition for the FW transformation consists in the nullification of either upper or lower components of the bispinor wave function

$$\psi_D(\boldsymbol{x}, t) = A \begin{pmatrix} \phi(\boldsymbol{x}, t) \\ \chi(\boldsymbol{x}, t) \end{pmatrix}$$

and the transformation of the normalization operator of the wave function $\psi_D(x)$ into the unit operator. Let us call this the "wave function reduction condition". For the case when the Dirac Hamiltonian is independent of time (the free case or the case of static external fields) this condition can be represented in the following form

$$\begin{gathered}\psi_D^{(+)}(\boldsymbol{x},t)=e^{-iEt}A_+\begin{pmatrix}\phi^{(+)}(\boldsymbol{x})\\ \chi^{(+)}(\boldsymbol{x})\end{pmatrix}\rightarrow\psi_{FW}^{(+)}(\boldsymbol{x},t)=e^{-iEt}\begin{pmatrix}\phi^{(+)}(\boldsymbol{x})\\ 0\end{pmatrix};\\ \psi_D^{(-)}(\boldsymbol{x},t)=e^{iEt}A_-\begin{pmatrix}\phi^{(-)}(\boldsymbol{x})\\ \chi^{(-)}(\boldsymbol{x})\end{pmatrix}\rightarrow\psi_{FW}^{(-)}(\boldsymbol{x},t)=e^{iEt}\begin{pmatrix}0\\ \chi^{(-)}(\boldsymbol{x})\end{pmatrix}.\end{gathered}\tag{V.1}$$

In this equation, E is the module of the particle energy operator; A_+ and A_- are normalization operators, which may differ, in general, for solutions with positive and negative energies. Definition of the operators A_+ and A_- implies that the wave functions $\psi_D^{(+)}(\boldsymbol{x},t),\psi_D^{(-)}(\boldsymbol{x},t)$ and the spinors $\phi^{(+)}(\boldsymbol{x}),\chi^{(-)}(\boldsymbol{x})$ are normalized to 1:

$$\int\psi_D^{(\pm)\dagger}(\boldsymbol{x},t)\psi_D^{(\pm)}(\boldsymbol{x},t)dV=1,\quad\int\phi^{(+)\dagger}(\boldsymbol{x})\phi^{(+)}(\boldsymbol{x})dV=1,\quad\int\chi^{(-)\dagger}(\boldsymbol{x})\chi^{(-)}(\boldsymbol{x})dV=1.$$

Pluses and minuses denote positive and negative energy states, respectively.

For a free particle,

$$E=\sqrt{m^2+\boldsymbol{p}^2},\quad A_+=A_-=\sqrt{\frac{E+m}{2E}}.\tag{V.2}$$

$\phi^{(+)}(\boldsymbol{x})=e^{i\boldsymbol{p}\cdot\boldsymbol{x}}\phi$ and $\chi^{(-)}(\boldsymbol{x})=e^{-i\boldsymbol{p}\cdot\boldsymbol{x}}\chi$ for the positive and negative energy solutions, respectively. ϕ and χ are the two-component Pauli spin functions [see Eq. (III.6)].

Functions $\psi_D^{(\pm)}(\boldsymbol{x},t)$ and $\psi_{FW}^{(\pm)}(\boldsymbol{x},t)$ are the appropriate solutions of the initial Dirac equation and the equation transformed to the FW representation for a free particle and a particle moving in static external fields. The reduction condition implies transformation of the Dirac wave functions to the form $\psi_{FW}^{(\pm)}(\boldsymbol{x},t)$ with the unit normalization operator.

In general, the Dirac and FW Hamiltonians depend on time. In this case, the reduction condition (V.1) has the same meaning. We use expansions in the Dirac equation solutions obtained either for free motion of particles, or for a motion in the presence of static external fields when solving specific problems of physics (at least, with the use of the perturbation theory).

The reduction condition can be proved with the Eriksen transformation [5], which is the exact FW transformation of the time-independent Hamiltonian $\mathcal{H}_D$. Let us consider the positive energy solutions. Since $\lambda\psi_D^{(\pm)}(\boldsymbol{x},t)=\pm\psi_D^{(\pm)}(\boldsymbol{x},t)$, Eriksen transformation operator (III.14) transforms the Dirac wave function to the form

$$\psi_{FW}^{(+)}(\boldsymbol{x},t)=e^{-iEt}\left[\frac{1}{2}+\frac{1}{4}\left(\beta\lambda+\lambda\beta\right)\right]^{-1/2}A_+\begin{pmatrix}\phi^{(+)}(\boldsymbol{x})\\ 0\end{pmatrix}. \qquad (\mathrm{V.3})$$

The wave function normalization requirement can be written as

$$\int\psi_{FW}^{(+)\dagger}(\boldsymbol{x},t)\psi_{FW}^{(+)}(\boldsymbol{x},t)dV=\int\phi^{(+)\dagger}(\boldsymbol{x})A_+\left[\frac{1}{2}+\frac{1}{4}\left(\beta\lambda+\lambda\beta\right)\right]^{-1}A_+\phi^{(+)}(\boldsymbol{x})dV=1. \qquad (\mathrm{V.4})$$

Eq. (V.4) is valid only when the following condition is satisfied:

$$A_+\left[\frac{1}{2}+\frac{1}{4}\left(\beta\lambda+\lambda\beta\right)\right]^{-1}A_+=1. \qquad (\mathrm{V.5})$$

Multiplying the left-hand and right-hand sides of equation (V.5) by the operator A_+^{-1} and extracting a root square results in

$$\left[\frac{1}{2}+\frac{1}{4}\left(\beta\lambda+\lambda\beta\right)\right]^{-1/2}=A_+^{-1}$$

and

$$A_+=\left[\frac{1}{2}+\frac{1}{4}\left(\beta\lambda+\lambda\beta\right)\right]^{1/2}. \qquad (\mathrm{V.6})$$

Eqs. (V.3),(V.6) prove the reduction condition (V.1). An explicit form of the operator A_+ has been determined in Ref. [9] in the particular case when the FW transformation is exact.

Similar derivation proves Eq. (V.1) for the negative energy solutions. In this case

$$A_-=A_+=\left[\frac{1}{2}+\frac{1}{4}\left(\beta\lambda+\lambda\beta\right)\right]^{1/2}. \qquad (\mathrm{V.7})$$

VI. VERIFICATION OF METHODS OF THE FOLDY-WOUTHUYSEN TRANSFORMATION

The reduction condition can be successfully used for the verification of methods of the Foldy-Wouthuysen transformation. The validity of the Eriksen method [5] has been proved in the precedent section. Next subsection is devoted to the method proposed in Ref. [7] and discussed in Ref. [8].

A. Particle in a static electric field

For a particle in a static electric field, we can demonstrate that the condition (V.1) is satisfied up to linear terms on e and quadratic terms on v/c in the expansion of U_{FW} in powers of charge e [7]. This procedure can, apparently, be applied up to any order of expansion on e and v/c using the mathematical technique of Ref. [7].

We obtain with denotations used in [7] and within the accepted accuracy that

$$
\begin{gathered}
\mathcal{H}_D = \beta m + \boldsymbol{\alpha}\cdot\boldsymbol{p} + eA_0(\boldsymbol{x}),\\
U_{FW} = (1+\delta_1^0+\delta_1^e)U_0 = 1 + \frac{\beta\boldsymbol{\alpha}\cdot\boldsymbol{p}}{2m} - \frac{p^2}{8m^2} - \frac{ie}{4m^2}(\boldsymbol{\alpha}\cdot\nabla A_0)\\
-\frac{ie\beta}{16m^3}\left[(\boldsymbol{\alpha}\cdot\boldsymbol{p})(\boldsymbol{\alpha}\cdot\nabla A_0) - (\boldsymbol{\alpha}\cdot\nabla A_0)(\boldsymbol{\alpha}\cdot\boldsymbol{p})\right],\\
\mathcal{H}_{FW} = \beta E, \quad E = m + \frac{p^2}{2m} + e\beta\left\{A_0 + \frac{i}{8m^2}\left[(\boldsymbol{\alpha}\cdot\boldsymbol{p})(\boldsymbol{\alpha}\cdot\nabla A_0) - (\boldsymbol{\alpha}\cdot\nabla A_0)(\boldsymbol{\alpha}\cdot\boldsymbol{p})\right]\right\},\\
\psi_D^{(+)}(\boldsymbol{x},t) = e^{-iEt}\Big\{1 - \frac{p^2}{8m^2} - \frac{ie}{16m^3}\left[(\boldsymbol{\sigma}\cdot\boldsymbol{p})(\boldsymbol{\sigma}\cdot\nabla A_0)\right.\\
\left.-(\boldsymbol{\sigma}\cdot\nabla A_0)(\boldsymbol{\sigma}\cdot\boldsymbol{p})\right]\Big\}\begin{pmatrix}\phi^{(+)}(\boldsymbol{x})\\ \left(\frac{\boldsymbol{\sigma}\cdot\boldsymbol{p}}{2m} + \frac{ie\boldsymbol{\sigma}\cdot\nabla A_0}{4m^2}\right)\phi^{(+)}(\boldsymbol{x})\end{pmatrix},\\
\psi_{FW}^{(+)}(\boldsymbol{x},t) = U_{FW}\psi_D^{(+)}(\boldsymbol{x},t) = e^{-iEt}\begin{pmatrix}\phi^{(+)}(\boldsymbol{x})\\ 0\end{pmatrix},\\
\psi_D^{(-)}(\boldsymbol{x},t) = e^{iEt}\Big\{1 - \frac{p^2}{8m^2} + \frac{ie}{16m^3}\left[(\boldsymbol{\sigma}\cdot\boldsymbol{p})(\boldsymbol{\sigma}\cdot\nabla A_0)\right.\\
\left.-(\boldsymbol{\sigma}\cdot\nabla A_0)(\boldsymbol{\sigma}\cdot\boldsymbol{p})\right]\Big\}\begin{pmatrix}-\left(\frac{\boldsymbol{\sigma}\cdot\boldsymbol{p}}{2m} - \frac{ie\boldsymbol{\sigma}\cdot\nabla A_0}{4m^2}\right)\chi^{(-)}(\boldsymbol{x})\\ \chi^{(-)}(\boldsymbol{x})\end{pmatrix},\\
\psi_{FW}^{(-)}(\boldsymbol{x},t) = U_{FW}\psi_D^{(-)}(\boldsymbol{x},t) = e^{iEt}\begin{pmatrix}0\\ \chi^{(-)}(\boldsymbol{x})\end{pmatrix}.
\end{gathered}
\tag{VI.1}
$$

In Eq. (VI.1), $\boldsymbol{p}$ and functions of $\boldsymbol{p}$ imply the corresponding operators; $\phi^{(+)}(\boldsymbol{x})$ and $\chi^{(-)}(\boldsymbol{x})$ are two-component spinors.

It follows from (VI.1) that reduction condition (V.1) is satisfied and, therefore, the obtained unitary transformation is the FW one.

The method described in Refs. [7, 8] can also be checked by means of its comparing with the Eriksen method [5]. In the case considered (see Ref. [24])

$$\lambda = \frac{\mathcal{H}_D}{\sqrt{\mathcal{H}_D^2}} = \frac{\beta m + \boldsymbol{\alpha}\cdot\boldsymbol{p}}{p_0} - \frac{1}{2}\mathcal{B} + \frac{1}{2p_0}(\beta m + \boldsymbol{\alpha}\cdot\boldsymbol{p})\mathcal{B}(\beta m + \boldsymbol{\alpha}\cdot\boldsymbol{p})\frac{1}{p_0},$$

$$p_0 = \sqrt{m^2+\boldsymbol{p}^2}, \quad p_0\mathcal{B} + \mathcal{B}p_0 = -2eA_0.$$

Since

$$\mathcal{B} = -\frac{eA_0}{m} + \frac{e(p_0^2A_0 + A_0p_0^2)}{2m^3}$$

to within terms of order of p^2/m^2, then

$$\lambda = \beta + \frac{\boldsymbol{\alpha}\cdot\boldsymbol{p}}{m} - \beta\frac{p^2}{2m^2} - \frac{i\beta e}{2m^2}\boldsymbol{\alpha}\cdot\nabla A_0 + \frac{ie}{4m^3}\left[(\boldsymbol{\alpha}\cdot\nabla A_0)(\boldsymbol{\alpha}\cdot\boldsymbol{p}) - (\boldsymbol{\alpha}\cdot\boldsymbol{p})(\boldsymbol{\alpha}\cdot\nabla A_0)\right],$$

$$\left(\frac{\beta\lambda+\lambda\beta}{4}+\frac{1}{2}\right)^{-1/2} = 1 + \frac{p^2}{8m^2} + \frac{i\beta e}{16m^3}\left[(\boldsymbol{\alpha}\cdot\boldsymbol{p})(\boldsymbol{\alpha}\cdot\nabla A_0) - (\boldsymbol{\alpha}\cdot\nabla A_0)(\boldsymbol{\alpha}\cdot\boldsymbol{p})\right],$$

$$U_E = 1 + \frac{\beta\boldsymbol{\alpha}\cdot\boldsymbol{p}}{2m} - \frac{p^2}{8m^2} - \frac{ie}{4m^2}\boldsymbol{\alpha}\cdot\nabla A_0 - \frac{i\beta e}{16m^3}\left[(\boldsymbol{\alpha}\cdot\boldsymbol{p})(\boldsymbol{\alpha}\cdot\nabla A_0) - (\boldsymbol{\alpha}\cdot\nabla A_0)(\boldsymbol{\alpha}\cdot\boldsymbol{p})\right].$$

The latter expression for U_E coincides with the expression (VI.1) for the FW transformation operator U_{FW} obtained by the method described in Refs. [7, 8].

B. Super-algebra in the Dirac equation with static external fields

In Ref. [15], supersymmetric quantum mechanics was applied to a wide range of interactions between a Dirac particle and external static fields that provides a closed form of a block-diagonal Hamiltonian. The authors of Ref. [15] considered the $SU(2)$ transformation of the Dirac Hamiltonian as the FW transformation.

It is interesting to determine whether reduction condition (V.1) is satisfied for this transformation. Using denotations from [15], we have

$$\mathcal{H}_D = Q + Q^\dagger + \Lambda, \tag{VI.2}$$

where Λ is a Hermitian operator, Q and $Q^\dagger$ are two fermion operators satisfying the following requirements:

$$Q^2 = {Q^\dagger}^2 = 0, \quad \{Q,\Lambda\} = \{Q^\dagger,\Lambda\} = 0. \tag{VI.3}$$

$\{\dots,\dots\}$ denotes an anticommutator.

Then, the Hermitian operators of $SU(2)$ algebra are introduced as follows:

$$J_1 = \frac{Q+Q^\dagger}{2(\{Q,Q^\dagger\})^{1/2}}, \quad J_2 = \frac{-i\Lambda(Q+Q^\dagger)}{2(\Lambda^2\{Q,Q^\dagger\})^{1/2}}, \quad J_3 = \frac{\Lambda}{2(\Lambda^2)^{1/2}}, \quad [J_i,J_j] = ie_{ijk}J_k.$$

The transformation operator is

$$U_{FW}=e^{iJ_2\theta}=\cos\frac{\theta}{2}+2iJ_2\sin\frac{\theta}{2}=\sqrt{\frac{1}{2}\left(1+\cos\theta\right)}+\frac{\Lambda(Q+Q^\dagger)}{(\Lambda^2\{Q,Q^\dagger\})^{1/2}}\sqrt{\frac{1}{2}\left(1-\cos\theta\right)}. \quad \text{(VI.4)}$$

In contrast to Ref. [15], the exponent of $iJ_2\theta$ in Eq. (VI.4) is taken with the positive sign. This is a necessary step to be in agreement with the reduction condition (V.1) (see below). Since

$$\mathcal{H}_{FW}=e^{iJ_2\theta}\mathcal{H}_De^{-iJ_2\theta}=(Q+Q^\dagger)\cos\theta+2iJ_2\Lambda\sin\theta+\Lambda\cos\theta+2iJ_2(Q+Q^\dagger)\sin\theta \quad \text{(VI.5)}$$

and

$$\sin\theta=\frac{\{Q,Q^\dagger\}^{1/2}}{(\{Q,Q^\dagger\}+\Lambda^2)^{1/2}},\quad \cos\theta=\frac{(\Lambda^2)^{1/2}}{(\{Q,Q^\dagger\}+\Lambda^2)^{1/2}},\quad \tan\theta=\frac{\{Q,Q^\dagger\}^{1/2}}{(\Lambda^2)^{1/2}},$$

expression (VI.5) is reduced to the diagonal form

$$\mathcal{H}_{FW}=\frac{\Lambda}{(\Lambda^2)^{1/2}}\left(\{Q,Q^\dagger\}+\Lambda^2\right)^{1/2}. \quad \text{(VI.6)}$$

If

$$\Lambda=\beta m,\quad Q=\begin{pmatrix}0&0\\M&0\end{pmatrix},\quad Q^\dagger=\begin{pmatrix}0&M^\dagger\\0&0\end{pmatrix} \quad \text{(VI.7)}$$

and

$$M=\boldsymbol{\sigma}\cdot(\boldsymbol{p}+\boldsymbol{C})-iC_5,\quad C_i=A_i-i\varepsilon_i,\quad i=1,2,3,5,$$

the Dirac Hamiltonian $\mathcal{H}_D$ is given by

$$\mathcal{H}_D=\beta m+\boldsymbol{\alpha}\cdot\boldsymbol{\pi}+i\beta\gamma_5\pi_5,\quad \pi_i=p_i+A_i(\boldsymbol{x})+i\beta\varepsilon_i(\boldsymbol{x}),\quad i=1,2,3,5,\quad p_5=0. \quad \text{(VI.8)}$$

The following interactions are described using these denotations: i) A_5 is the pseudo-scalar potential, ii) ε_5 is the time component of the axial-vector potential, iii) $\boldsymbol{\varepsilon}$ is the "electrical" component of interaction of the anomalous magnetic moment of the particle, iv) $\boldsymbol{A}$ is the minimum magnetic interaction; v) if $A_5=0$, $\varepsilon_5=0$, $\boldsymbol{A}=0$, $\boldsymbol{\varepsilon}=\boldsymbol{r}$, the Hamiltonian $\mathcal{H}_D$ reduces to the Hamiltonian of the Dirac oscillator. All of the above interactions admit a closed transformation to the diagonal form (VI.6).

Let us check whether the $SU(2)$ transformation (VI.4) satisfies the reduction condition

(V.1) and is the FW transformation. In the case defined by Eq. (VI.7),

$$
\begin{gathered}
\mathcal{H}_{FW}=\beta E=\beta(\{Q,Q^\dagger\}+m^2)^{1/2},\quad E^2=\{Q,Q^\dagger\}+m^2=\begin{pmatrix} M^\dagger M+m^2 & 0\\ 0 & MM^\dagger+m^2\end{pmatrix},\\
U_{FW}=\sqrt{\frac{E+m}{2E}}\left[1+\frac{\beta(Q+Q^\dagger)}{E+m}\right],\\
\psi_D^{(+)}(\boldsymbol{x},t)=e^{-iEt}\sqrt{\frac{E+m}{2E}}\begin{pmatrix}\phi^{(+)}(\boldsymbol{x})\\ \dfrac{1}{E+m}M\phi^{(+)}(\boldsymbol{x})\end{pmatrix},\quad \psi_{FW}^{(+)}(\boldsymbol{x},t)=e^{-iEt}\begin{pmatrix}\phi^{(+)}(\boldsymbol{x})\\ 0\end{pmatrix},\\
\psi_D^{(-)}(\boldsymbol{x},t)=e^{iEt}\sqrt{\frac{E+m}{2E}}\begin{pmatrix}-\dfrac{1}{E+m}M^\dagger\chi^{(-)}(\boldsymbol{x})\\ \chi^{(-)}(\boldsymbol{x})\end{pmatrix},\quad \psi_{FW}^{(-)}(\boldsymbol{x},t)=e^{iEt}\begin{pmatrix}0\\ \chi^{(-)}(\boldsymbol{x})\end{pmatrix}.
\end{gathered}
\tag{VI.9}
$$

Expressions (VI.9) show that, indeed, the reduction condition (V.1) is fulfilled for $SU(2)$ transformation [15] (with the changed sign in the exponential factor $iJ_2\theta$). Thus, this is a FW transformation. If the authors' sign in this factor [15] remains unchanged ($e^{-iJ_2\theta}$), the transformation operator U_{FW} in Eq. (VI.9) takes the form

$$
U=\sqrt{\frac{E+m}{2E}}\left[1-\frac{\beta(Q+Q^\dagger)}{E+m}\right].
$$

In this case, the reduction condition (V.1) is violated despite the block-diagonalization of the Hamiltonian.

C. Eriksen-Kolsrud transformation

The Eriksen-Kolsrud (EK) transformation [17] was used in many works (see, e.g., Refs. [18, 19, 20, 21, 25]). It is fulfilled in two stages defined by the operators U_1 and U_2. The unitary operator of resulting transformation is given by [17]

$$
\begin{gathered}
U_{EK}=U_1U_2,\quad U_1=\frac{1}{\sqrt{2}}\left(1+J\lambda\right),\quad U_2=\frac{1}{\sqrt{2}}\left(1+\beta J\right),\\
J=i\gamma_5\beta,\quad \lambda=\frac{\mathcal{H}_D}{(\mathcal{H}_D^2)^{1/2}}.
\end{gathered}
\tag{VI.10}
$$

There are many examples of the exact EK transformation. It is often claimed that this transformation is equivalent to the FW one. It has been proved in Ref. [16] that this statement is incorrect. We can show that the EK transformation does not satisfy reduction condition (V.1).

For a free particle, $\mathcal{H}_{EK}=\beta E$ and

$$\begin{gathered}\psi^{(+)}_{EK}(\boldsymbol{x},t)=U_{EK}\psi^{(+)}_{D}(\boldsymbol{x},t)=e^{-iEt}\sqrt{\frac{E+m}{2E}}\left(\begin{array}{c}\left(1+\frac{i\boldsymbol{\sigma}\cdot\boldsymbol{p}}{E+m}\right)\phi^{(+)}(\boldsymbol{x})\\ 0\end{array}\right),\\ \psi^{(-)}_{EK}(\boldsymbol{x},t)=e^{iEt}\sqrt{\frac{E+m}{2E}}\left(\begin{array}{c}0\\ \left(1-\frac{i\boldsymbol{\sigma}\cdot\boldsymbol{p}}{E+m}\right)\chi^{(-)}(\boldsymbol{x})\end{array}\right).\end{gathered}\tag{VI.11}$$

It can be seen from Eq. (VI.11) that Eq. (V.1) is not satisfied and one needs to perform additional transformation [16]

$$U_{EK\rightarrow FW}=\sqrt{\frac{E+m}{2E}}\left(1-\frac{i\beta\boldsymbol{\sigma}\cdot\boldsymbol{p}}{E+m}\right)\tag{VI.12}$$

which does not change the form of the Hamiltonian ($\mathcal{H}_{EK}=\mathcal{H}_{FW}$).

Let us consider a Dirac particle in an external gravitational field defined by the static metric $ds^2=V^2(\boldsymbol{x})(dx^0)^2-W^2(\boldsymbol{x})d\boldsymbol{x}^2$. This problem was investigated in Refs. [16, 18, 19, 20]. In the considered case, the EK transformation is exact [18, 19].

The Dirac Hamiltonian is given by [18, 19]

$$\mathcal{H}_D=\beta mV+\frac{1}{2}\{\boldsymbol{\alpha}\cdot\boldsymbol{p},\mathcal{F}\},\quad \mathcal{F}=\frac{V}{W}.\tag{VI.13}$$

Similarly to Refs. [16, 18, 19], we take into account the first-order terms for the potentials $(V-1)$, $(\mathcal{F}-1)$ and their first-order spatial derivatives. We use the method proposed in Refs. [7, 8]. We perform the expansion in a power series in $|\boldsymbol{p}|/m$ and take into account terms up to p^2/m^2.

In this case

$$\begin{gathered}U_{FW}=1+\frac{\beta\boldsymbol{\alpha}\cdot\boldsymbol{p}}{2m}-\frac{p^2}{8m^2}+\frac{\beta}{4m}\left\{(\mathcal{F}-V),\boldsymbol{\alpha}\cdot\boldsymbol{p}\right\}\\ -\frac{1}{16m^2}\left[(\mathcal{F}-V)p^2+2\boldsymbol{\alpha}\cdot\boldsymbol{p}\,(\mathcal{F}-V)\,\boldsymbol{\alpha}\cdot\boldsymbol{p}+p^2(\mathcal{F}-V)\right]\end{gathered}$$

and

$$\begin{gathered}\mathcal{H}_{FW}=\beta m+\frac{\beta p^2}{2m}+\beta m(V-1)-\frac{\beta}{4m}\left\{p^2,(V-1)\right\}+\frac{\beta}{2m}\left\{p^2,(\mathcal{F}-1)\right\}\\ -\frac{\beta}{8m}\left[2\boldsymbol{\Sigma}\cdot(\boldsymbol{\phi}\times\boldsymbol{p})+\nabla\cdot\boldsymbol{\phi}\right]+\frac{\beta}{4m}\left[2\boldsymbol{\Sigma}\cdot(\boldsymbol{f}\times\boldsymbol{p})+\nabla\cdot\boldsymbol{f}\right],\end{gathered}\tag{VI.14}$$

where $\boldsymbol{\phi}=\nabla V$, $\boldsymbol{f}=\nabla\mathcal{F}$. Eq. (VI.14) coincides with the corresponding equation obtained in Ref. [16].

It can be shown that the FW wave functions satisfy Eq. (V.1). The EK transformation operator can be written as

$$U_{EK}=\frac{1}{2}\Biggl\{1+i\gamma_5-\frac{\beta\gamma_5}{2}\{\mathbf{\Sigma}\cdot\boldsymbol{p},\mathcal{F}\}\frac{1}{mV}-\frac{i\gamma_5}{4m^2}\left(\frac{1}{W}p^2\mathcal{F}+\mathcal{F}p^2\frac{1}{W}\right)\frac{1}{V}$$
$$-\frac{i\gamma_5}{4m^2}\left[2\mathbf{\Sigma}\cdot(\boldsymbol{f}\times\boldsymbol{p})+\nabla\cdot\boldsymbol{f}\right]-\frac{i\gamma_5\beta}{2m}\mathbf{\Sigma}\cdot\boldsymbol{\phi}-\frac{\gamma_5}{4m^2}\{\mathbf{\Sigma}\cdot\boldsymbol{p},\mathcal{F}\}\mathbf{\Sigma}\cdot\boldsymbol{\phi}\Biggr\}(1-i\gamma_5). \tag{VI.15}$$

The EK wave functions are given by

$$\psi_{EK}^{(+)}(\boldsymbol{x},t)=e^{-iEt}\Biggl\{1-\frac{p^2}{8m^2}-\frac{1}{16m^2}\left[(\mathcal{F}-V)p^2+2\mathbf{\Sigma}\cdot\boldsymbol{p}\,(\mathcal{F}-V)\mathbf{\Sigma}\cdot\boldsymbol{p}+p^2(\mathcal{F}-V)\right]$$
$$+\frac{i}{4}\{\mathbf{\Sigma}\cdot\boldsymbol{p},\mathcal{F}\}\frac{1}{mV}-\frac{1}{4m}\mathbf{\Sigma}\cdot\boldsymbol{\phi}\Biggr\}\begin{pmatrix}\phi^{(+)}(\boldsymbol{x})\\ 0\end{pmatrix},$$
$$\psi_{EK}^{(-)}(\boldsymbol{x},t)=e^{iEt}\Biggl\{1-\frac{p^2}{8m^2}-\frac{1}{16m^2}\left[(\mathcal{F}-V)p^2+2\mathbf{\Sigma}\cdot\boldsymbol{p}\,(\mathcal{F}-V)\mathbf{\Sigma}\cdot\boldsymbol{p}+p^2(\mathcal{F}-V)\right]$$
$$-\frac{i}{4}\{\mathbf{\Sigma}\cdot\boldsymbol{p},\mathcal{F}\}\frac{1}{mV}-\frac{1}{4m}\mathbf{\Sigma}\cdot\boldsymbol{\phi}\Biggr\}\begin{pmatrix}0\\ \chi^{(-)}(\boldsymbol{x})\end{pmatrix}. \tag{VI.16}$$

In Eq. (VI.16), E is the module of the Dirac particle energy in the external gravitational field which Hamiltonian is defined by Eq. (VI.13).

Thus, reduction condition (V.1) is not satisfied for the EK wave functions. This conclusion remains valid for the EK transformation performed in Ref. [21] for Dirac particles interacting with a plane gravitational wave and a constant uniform magnetic field.

A closed transformation of the EK type was applied in Ref. [20] to Hamiltonian (VI.13) using the supersymmetric quantum mechanics methods. The resultant Hamiltonian coincides with the transformed one obtained in Refs. [18, 19] in any order of the expansion in powers of $1/m$.

The transformation operator used in Ref. [20] is

$$U=\frac{1}{\sqrt{2}}\left(1+\beta\frac{Q}{(Q^2)^{1/2}}\right)\frac{1}{\sqrt{2}}(1-i\gamma_5),\quad Q=\frac{1}{2}\{\boldsymbol{\alpha}\cdot\boldsymbol{p},\mathcal{F}\}+i\gamma_5\beta mV. \tag{VI.17}$$

Expanding Eq. (VI.17) in a series up to the terms of the first order in the potentials $(V-1)$, $(\mathcal{F}-1)$ and their first spatial derivatives and taking into account only terms up to $\sim 1/m^2$, one can prove that formulas (VI.15) and (VI.17) for the transformation operator coincide within the accepted accuracy. Similarly to the transformation applied in Ref. [18], reduction condition (V.1) is not satisfied. Hence, the transformation constructed in Ref. [20] is not the FW one.

D. Generalized Melosh transformation

The Melosh transformation [22] is often used in the strong interaction theory. It has been independently proposed by Tsai [26] to describe interactions of particles with spins 1/2 and 1 with the magnetic field. For free particles, the exponential operator transforming Dirac Hamiltonian (III.3) is given by [26]

$$U_1 = \exp\left(-\frac{1}{2}\arctan\frac{\boldsymbol{\gamma}\cdot\boldsymbol{p}_\perp}{m}\right), \quad \boldsymbol{p}_\perp = p_x\boldsymbol{e}_x + p_y\boldsymbol{e}_y. \tag{VI.18}$$

This transformation operator can be expressed in the equivalent form

$$U_1 = \frac{\epsilon + m + \boldsymbol{\gamma}\cdot\boldsymbol{p}_\perp}{\sqrt{2\epsilon(\epsilon+m)}}, \quad \epsilon = \sqrt{m^2 + \boldsymbol{p}_\perp^2}. \tag{VI.19}$$

The transformed Hamiltonian is [22, 26]

$$\mathcal{H}_1 = \beta(\epsilon + \gamma_z p_z). \tag{VI.20}$$

This Hamiltonian is not block-diagonal. To bring it to the block-diagonal form, one can perform the second transformation. Since the form of Hamiltonian (VI.20) is covered by the condition of exact FW transformation (III.9), the second transformation operator is equal to

$$U_2 = \frac{E + \epsilon + \gamma_z p_z}{\sqrt{2E(E+\epsilon)}}, \quad E = \sqrt{\epsilon^2 + p_z^2} = \sqrt{m^2 + \boldsymbol{p}^2}. \tag{VI.21}$$

The resultant transformation operator is given by

$$U_M = U_2 U_1. \tag{VI.22}$$

It brings initial Dirac Hamiltonian (III.3) to the form

$$\mathcal{H}_M = \beta\sqrt{m^2 + \boldsymbol{p}^2} = \beta E. \tag{VI.23}$$

Despite the block-diagonality of generalized Melosh transformation (VI.22), it is not equivalent to the FW one. The connection between the generalized Melosh transformation and the FW one is given by

$$\begin{gathered} U_{M\to FW} = \frac{\sqrt{(E+\epsilon)(\epsilon+m)} + i\sqrt{(E-\epsilon)(\epsilon-m)}R}{\sqrt{2\epsilon(E+m)}}, \\ U_{FW\to M} = \frac{\sqrt{(E+\epsilon)(\epsilon+m)} - i\sqrt{(E-\epsilon)(\epsilon-m)}R}{\sqrt{2\epsilon(E+m)}}, \quad R = \frac{p_x\sigma_y - p_y\sigma_x}{\sqrt{p_x^2+p_y^2}}. \end{gathered} \tag{VI.24}$$

The wave functions in the generalized Melosh representation are equal to

$$\begin{aligned}
\psi_M^{(+)}(\boldsymbol{x},t) = U_M\psi_D^{(+)}(\boldsymbol{x},t) = e^{-iEt}\frac{\sqrt{(E+\epsilon)(\epsilon+m)}-i\sqrt{(E-\epsilon)(\epsilon-m)}R}{\sqrt{2\epsilon(E+m)}}\begin{pmatrix}\phi^{(+)}(\boldsymbol{x})\\ 0\end{pmatrix},\\
\psi_M^{(-)}(\boldsymbol{x},t) = U_M\psi_D^{(-)}(\boldsymbol{x},t) = e^{iEt}\frac{\sqrt{(E+\epsilon)(\epsilon+m)}-i\sqrt{(E-\epsilon)(\epsilon-m)}R}{\sqrt{2\epsilon(E+m)}}\begin{pmatrix}0\\ \chi^{(-)}(\boldsymbol{x})\end{pmatrix}.
\end{aligned} \tag{VI.25}$$

Therefore, these wave functions do not satisfy reduction condition (V.1).

VII. APPLICATIONS OF CONNECTION BETWEEN THE DIRAC AND FOLDY-WOUTHUYSEN WAVE FUNCTIONS

The Hamiltonian for relativistic particles in the FW representation contains a square root of operators (see Refs. [1, 3]). Therefore, the Dirac representation is usually more convenient than the FW one for finding wave eigenfunctions and eigenvalues of the Hamilton operator. Many exact solutions of relativistic wave equations have been found just in the Dirac representation [27]. Nevertheless, a derivation of equations of motion is much more difficult in this representation than in the FW one [2, 3].

The use of connection between wave functions in the Dirac and FW representations defined by Eq. (V.1) is very important. One can calculate wave eigenfunctions in the Dirac representation and then obtain corresponding eigenfunctions in the FW representation. After that, one can determine expectation values of needed operators corresponding to certain classical quantities and derive quantum and semiclassical equations of motion. When the semiclassical approximation is not admissible, quantum formulae describing the evolution of the operators can be derived. Semiclassical evolution of classical quantities corresponding to these operators can be obtained by averaging the operators in the solutions. An example of such an evolution is time dependence of average energy and momentum in a two-level system. Another example is the spin dynamics in external fields. It is very difficult to solve these problems in the Dirac representation. It is important that Eq. (V.1) is exact because one can solve the above mentioned problems with any desirable accuracy. The example of description of spin evolution in the FW representation has been given in Ref. [9].

In the Dirac representation, the connection between operators and classical quantities is rather complicated and sometimes not clear. Explicit expressions for the operators that correspond to certain classical quantities are known only for free relativistic particles (see. [1]). It is clear that the expressions for these operators in the general case must depend on the parameters that characterize the external field. The FW transformation if free of this drawback. Main operators including the operators of position, momentum, and spin have the same form as in the nonrelativistic quantum theory. The determination of the FW wave function allows calculating, e.g., expectation values of operators of the root-mean-square radius $\sqrt{\langle r^2\rangle}$, electric and magnetic dipole moments, kinetic energy and so on. In particular, the operators of the electric and magnetic dipole moments are equal to $\partial\mathcal{H}_{FW}/\partial\boldsymbol{E}$ and $\partial\mathcal{H}_{FW}/\partial\boldsymbol{B}$, respectively. The use of the FW representation for this purpose can be effective not only in the atomic physics but also in the nuclear and particle physics.

VIII. SUMMARY

The paper formulates and proves the conditions enabling the transition from the Dirac representation to the FW one. An exact correlation between wave functions in both representations has been established. It has been demonstrated that the block-diagonalization of the Hamiltonian is often insufficient (see Refs. [18, 19, 20, 21, 22]) for its transformation to the FW representation. Such a transformation becomes possible, if the reduction condition (V.1) is satisfied. The results obtained enable unambiguous transition to the FW transformation and calculation of matrix elements and expectation values of the operators that correspond to the major classical quantities. It is possible because the exact form of such operators in the FW representation – as opposed to the Dirac representation – can be established quite easily.

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