

CONNECTION BETWEEN WAVE FUNCTIONS IN THE DIRAC AND FOLDY–WOUTHUYSEN REPRESENTATIONS

*A. J. Silenko*¹

Institute of Nuclear Problems, Belarusian State University, Minsk, Belarus

When the Foldy–Wouthuysen (FW) transformation is exact and the particle energy is positive, upper spinors in the Dirac and FW representations differ only by a constant factor and lower spinors in the FW representation are zero. Deducing FW wave eigenfunctions directly from Dirac wave eigenfunctions allows one to use the FW representation for a calculation of expectation values of needed operators and a derivation of quantum and semiclassical equations of motion.

Когда преобразование Фолди–Ваутхойзена (ФВ) является точным и энергия частиц положительна, верхние спиноры в представлениях Дирака и ФВ различаются только постоянными множителями, а нижние спиноры в представлении ФВ равны нулю. Вывод собственных волновых функций в представлении ФВ непосредственно из собственных волновых функций в представлении Дирака позволяет использовать представление ФВ для вычисления собственных значений требуемых операторов и вывода квантовых и квазиклассических уравнений движения.

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INTRODUCTION

The Foldy–Wouthuysen (FW) representation [1] occupies a special place in the quantum theory thanks to its unique properties. In this representation, the Hamiltonian and all operators are block-diagonal (diagonal in two spinors). Relations between operators in the FW representation are similar to those between the respective classical quantities. For relativistic particles in external fields, the operators have the same form as in the nonrelativistic quantum theory. For example, the position operator is \mathbf{r} , the momentum one is $\mathbf{p} = -i\nabla$, the orbital angular momentum operator is $\mathbf{l} = \mathbf{r} \times \mathbf{p}$, and the spin momentum operator is $\Sigma/2$ (Σ is the Dirac matrix) [1]. Only the FW representation possesses these properties considerably simplifying the transition to the semiclassical description. In the Dirac representation, all corresponding operators are defined by cumbersome expressions and depend on external field parameters [1,2]. As a result, the FW representation provides the best possibility of obtaining a meaningful classical limit of the relativistic quantum mechanics [3]. In particular, the FW representation is very useful to derive semiclassical equations of particle and spin motion [2]. The basic advantages of the FW representation are described in [1–3].

¹E-mail: silenko@inp.minsk.by

The Hamiltonian for relativistic particles in the FW representation contains a square root of operators (see [1,2]). 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 were found just in the Dirac representation [4]. Nevertheless, a derivation of equations of motion is much more difficult in this representation than in the FW one [2,3].

Therefore, the use of connection between wave functions in the Dirac and FW representations 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 and derive quantum and semiclassical equations of motion.

In the present work, we calculate the explicit connection between wave functions in the Dirac and FW representations at condition that the FW transformation (transformation to the FW representation) is exact.

Throughout the work we use the system of units $\hbar = c = 1$ and generally accepted designations of Dirac matrices (see [1]).

1. FOLDY–WOUTHUYSEN TRANSFORMATION FOR RELATIVISTIC PARTICLES IN EXTERNAL FIELDS

In the general case, the transformation to a new representation described by the wave function Ψ' is performed with the unitary operator U :

$$\Psi' = U\Psi,$$

where $\Psi = \begin{pmatrix} \phi \\ \chi \end{pmatrix}$ is the wave function (bispinor) in the Dirac representation. The Hamilton operator in the new representation takes the form [1,5]

$$\mathcal{H}' = U\mathcal{H}U^{-1} - iU\frac{\partial U^{-1}}{\partial t}.$$

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

$$\mathcal{H} = \beta m + \mathcal{E} + \mathcal{O}, \quad \beta\mathcal{E} = \mathcal{E}\beta, \quad \beta\mathcal{O} = -\mathcal{O}\beta, \quad (1)$$

where the operators \mathcal{E} and \mathcal{O} designate the sums of even and odd operators, respectively, and m is the particle mass. We suppose that the operator \mathcal{E} is multiplied by the unit matrix I which is everywhere omitted.

The FW transformation has been justified in the best way. 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. There exist several other nonrelativistic transformation methods which give the same results (see [2] and references therein).

The method of the FW transformation for relativistic spin-1/2 particles in external fields has been elaborated in [2]. In the general case, the FW Hamiltonian has been obtained as a

power series in external field potentials and their derivatives. The first stage of transformation is performed with the operator [2]

$$U = \frac{\epsilon + m + \beta\mathcal{O}}{\sqrt{2\epsilon(\epsilon + m)}}, \quad U^{-1} = \frac{\epsilon + m - \beta\mathcal{O}}{\sqrt{2\epsilon(\epsilon + m)}}, \quad \epsilon = \sqrt{m^2 + \mathcal{O}^2}. \quad (2)$$

As a result, the following Hamiltonian can be found:

$$\mathcal{H}' = \beta\epsilon + \mathcal{E}' + \mathcal{O}', \quad \beta\mathcal{E}' = \mathcal{E}'\beta, \quad \beta\mathcal{O}' = -\mathcal{O}'\beta. \quad (3)$$

The odd operator \mathcal{O}' is now comparatively small:

$$\begin{aligned} \mathcal{E}' &= i\frac{\partial}{\partial t} + \frac{\epsilon + m}{\sqrt{2\epsilon(\epsilon + m)}} \left(\mathcal{E} - i\frac{\partial}{\partial t} \right) \frac{\epsilon + m}{\sqrt{2\epsilon(\epsilon + m)}} - \\ &\quad - \frac{\beta\mathcal{O}}{\sqrt{2\epsilon(\epsilon + m)}} \left(\mathcal{E} - i\frac{\partial}{\partial t} \right) \frac{\beta\mathcal{O}}{\sqrt{2\epsilon(\epsilon + m)}}, \quad (4) \\ \mathcal{O}' &= \frac{\beta\mathcal{O}}{\sqrt{2\epsilon(\epsilon + m)}} \left(\mathcal{E} - i\frac{\partial}{\partial t} \right) \frac{\epsilon + m}{\sqrt{2\epsilon(\epsilon + m)}} - \frac{\epsilon + m}{\sqrt{2\epsilon(\epsilon + m)}} \left(\mathcal{E} - i\frac{\partial}{\partial t} \right) \frac{\beta\mathcal{O}}{\sqrt{2\epsilon(\epsilon + m)}}. \end{aligned}$$

The second stage of transformation leads to the approximate equation for the FW Hamiltonian:

$$\mathcal{H}_{\text{FW}} = \beta\epsilon + \mathcal{E}' + \frac{1}{4}\beta \left\{ \mathcal{O}'^2, \frac{1}{\epsilon} \right\}. \quad (5)$$

To reach a better precision, additional transformations can be used [2].

When

$$[\mathcal{E}, \mathcal{O}] = 0 \quad (6)$$

and an external field is stationary, the considered FW transformation is exact [2]. The transformation operator is defined by Eq. (2). The exact FW Hamiltonian takes the form

$$\mathcal{H}_{\text{FW}} = \beta\epsilon + \mathcal{E}, \quad (7)$$

where ϵ is given by Eq. (2).

Equation (6) is a sufficient but not necessary condition of the exact transformation.

2. FOLDY-WOUTHUYSEN TRANSFORMATION OF SOME OPERATORS

Since the external field is stationary, the FW transformation of some operators retains them unchanged. Hereinafter, the index «FW» designates FW-transformed operators: $A_{\text{FW}} = UAU^{-1}$. It follows from Eqs. (6), (7) that the operators \mathcal{O}^2, ϵ , and \mathcal{E} commute with the FW Hamiltonian \mathcal{H}_{FW} . Therefore, wave eigenfunctions in the FW representation are also eigenfunctions of the operators \mathcal{O}^2, ϵ , and \mathcal{E} .

As appears from Eqs. (2), (6) and the time independence of the external field, some operators remain unchanged after the FW transformation:

$$\mathcal{E}_{\text{FW}} = \mathcal{E}, \quad \left(i\frac{\partial}{\partial t} \right)_{\text{FW}} = i\frac{\partial}{\partial t}, \quad \epsilon_{\text{FW}} = \epsilon. \quad (8)$$

Evidently, the operators \mathcal{E} and ϵ commute with Dirac Hamiltonian (1). Therefore, they have the eigenvalues, \mathcal{E}_0 and ϵ_0 :

$$\mathcal{E}\Psi = \mathcal{E}_0\Psi, \quad \epsilon\Psi = \epsilon_0\Psi. \quad (9)$$

The operators \mathcal{E}_{FW} and ϵ_{FW} commute with FW Hamiltonian (7) and their eigenvalues are defined by

$$\mathcal{E}_{\text{FW}}\Psi_{\text{FW}} = \mathcal{E}_0\Psi_{\text{FW}}, \quad \epsilon_{\text{FW}}\Psi_{\text{FW}} = \epsilon_0\Psi_{\text{FW}}. \quad (10)$$

Since the quantities \mathcal{E}_0 and ϵ_0 in Eq.(9) and the corresponding quantities in Eq.(10) designate the eigenvalues of the same operators, they do not depend on a representation. Similar relations for the Hamilton operator have the form

$$i\frac{\partial\Psi}{\partial t} = \mathcal{H}\Psi = E\Psi, \quad i\frac{\partial\Psi_{\text{FW}}}{\partial t} = \mathcal{H}_{\text{FW}}\Psi_{\text{FW}} = E\Psi_{\text{FW}}. \quad (11)$$

The particle energy, E , is also independent of a representation.

Equations (7), (10), (11) define the connection between the considered eigenvalues:

$$E = \pm\epsilon_0 + \mathcal{E}_0. \quad (12)$$

The particle energy can be positive and negative and ϵ_0 is always positive. Therefore,

$$\epsilon_0 = |E - \mathcal{E}_0|. \quad (13)$$

The operator $\beta m + \mathcal{O}$ commutes with the Dirac Hamiltonian and has the eigenvalue $\pm\epsilon_0$:

$$(\beta m + \mathcal{O})\Psi = (E - \mathcal{E}_0)\Psi = \pm\epsilon_0\Psi. \quad (14)$$

3. CONNECTION BETWEEN WAVE FUNCTIONS

The connection between the initial and final wave functions has the form

$$\Psi_{\text{FW}} = U\Psi = \frac{\epsilon + \beta(\beta m + \mathcal{O})}{\sqrt{2\epsilon(\epsilon + m)}}\Psi. \quad (15)$$

Formulae (9), (14), (15) lead to the relation

$$\Psi_{\text{FW}} = \frac{\epsilon_0 \pm \beta\epsilon_0}{\sqrt{2\epsilon_0(\epsilon_0 + m)}}\Psi. \quad (16)$$

As appears from Eqs. (12), (13), and (16), the FW wave function is given by

$$\Psi_{\text{FW}} = \sqrt{\frac{2\epsilon_0}{\epsilon_0 + m}} \begin{pmatrix} \phi \\ 0 \end{pmatrix}, \quad (17)$$

when the particle energy E is positive, and

$$\Psi_{\text{FW}} = \sqrt{\frac{2\epsilon_0}{\epsilon_0 + m}} \begin{pmatrix} 0 \\ \chi \end{pmatrix}, \quad (18)$$

when the particle energy is negative. It can be proved that wave functions (17) and (18) are normalized to unit.

Since the energy of real particles is positive, we consider only Eq.(17). To avoid a calculation of ϵ_0 , one can use another form of this equation:

$$\Psi_{\text{FW}} = \frac{1}{\int \phi^\dagger \phi dV} \begin{pmatrix} \phi \\ 0 \end{pmatrix}. \quad (19)$$

It follows from Eqs. (17) and (19) that upper spinors in the Dirac and FW representations differ only by a constant factor and lower spinors in the FW representation are equal to zero.

4. EXAMPLE: PARTICLE IN A UNIFORM MAGNETIC FIELD

The FW transformation is exact for particles with an anomalous magnetic moment (AMM) moving in the plane orthogonal to a static uniform magnetic field [2]. The magnetic field is supposed to be upward. In this case, the operator $p_z = -i(\partial/\partial z)$ commutes with the Hamilton operator and has eigenvalues $P_z = \text{const.}$ Therefore, the consideration of the particular case $P_z = 0$ is quite reasonable [2].

The Hamilton operator in the Dirac representation satisfies Eq. (1), where

$$\mathcal{E} = -\mu' \mathbf{\Pi} \cdot \mathbf{H}, \quad \mathcal{O} = \boldsymbol{\alpha} \cdot \boldsymbol{\pi}, \quad \boldsymbol{\pi} = \mathbf{p} - e\mathbf{A}. \quad (20)$$

μ' is the AMM; \mathbf{A} is the vector potential, and \mathbf{H} is the magnetic field strength. The matrix $\mathbf{\Pi}$ is the polarization operator in the FW representation [6]. Since $P_z = 0$, the operators \mathcal{E} and \mathcal{O} commute.

In this case, the Hamilton operator in the FW representation is equal to [7]

$$\mathcal{H}_{\text{FW}} = \beta \sqrt{\boldsymbol{\pi}^2 + m^2} - e\boldsymbol{\Sigma} \cdot \mathbf{H} - \mu' \mathbf{\Pi} \cdot \mathbf{H}, \quad (21)$$

where $\pi_z \Psi_{\text{FW}} = P_z \Psi_{\text{FW}} = 0$ and

$$\epsilon = \sqrt{\boldsymbol{\pi}^2 + m^2 - e\boldsymbol{\Sigma} \cdot \mathbf{H}} = \sqrt{\boldsymbol{\pi}_\perp^2 + m^2 - e\boldsymbol{\Sigma} \cdot \mathbf{H}}.$$

The sign « \perp » designates a component orthogonal to \mathbf{H} .

The Dirac wave eigenfunctions of spin-1/2 particles possessing the AMM and interacting with the uniform magnetic field were derived in [9].

The eigenvalues of the operators are defined by [8,9]

$$\epsilon_0 = \sqrt{m^2 + (2n+1)|e|H - \lambda eH}, \quad \mathcal{E}_0 = -\lambda \mu' H, \quad (22)$$

$$n = 0, 1, 2, \dots, \quad \lambda = \pm 1.$$

Therefore, the connection between the wave functions is given by Eq. (19), where ϕ is the upper spinor in the Dirac representation and ϵ_0 is defined by Eq. (22).

Hamiltonian (21) commutes with the operators $\boldsymbol{\pi}_\perp^2$ and Π_z . As a result, the wave eigenfunction Ψ_{FW} is also an eigenfunction of these operators and can be given by

$$\Psi_{\text{FW}} = \psi \zeta,$$

where ψ is a coordinate wave function and ζ is an eigenfunction of operator Π_z :

$$\Pi_z \zeta = \lambda \zeta, \quad \lambda = \pm 1.$$

Since the lower spinors are zero, $\zeta^+ = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$, when $\lambda = 1$, and $\zeta^- = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$, when $\lambda = -1$.

We should take into account that z -components of the spin and the orbital angular momentum have definite values. When z -component of the total angular momentum is equal to M , the wave eigenfunctions take the form

$$\begin{aligned} \Psi_{\text{FW}}^+ &= \frac{\exp[i(M-1/2)\varphi]}{\sqrt{2\pi}} R_{|M-1/2|}(\rho) \zeta^+, \\ \Psi_{\text{FW}}^- &= \frac{\exp[i(M+1/2)\varphi]}{\sqrt{2\pi}} R_{|M+1/2|}(\rho) \zeta^-, \end{aligned} \quad (23)$$

where $R_{|M\pm 1/2|}(\rho)$ are the well-known radial eigenfunctions of operator π_\perp^2 and the signs «+» and «-» mean positive and negative projections of the spin, respectively. The wave eigenfunctions of spin-1/2 particles possessing the AMM have been derived in [9].

When the FW transformation is exact, the use of the FW representation makes it possible to calculate exact expectation values of main operators and derive exact equations of particle and spin motion. It is very difficult to solve these problems in the Dirac representation.

The FW Hamiltonian can be linearized in the spin operator [11]. The linearized Hamiltonian has the form

$$\begin{aligned} \mathcal{H}_{\text{FW}} &= \frac{\beta}{2}(K_+ + K_-) - \frac{1}{2}(K_+ - K_-) \frac{\mathbf{\Pi} \cdot \mathbf{H}}{H} - \mu' \mathbf{\Pi} \cdot \mathbf{H}, \\ K_+ &= \sqrt{\pi_\perp^2 + m^2 + eH}, \quad K_- = \sqrt{\pi_\perp^2 + m^2 - eH}. \end{aligned} \quad (24)$$

As an example, we can calculate the eigenvalues of the kinetic energy operator $T = \beta(K_+ + K_-)/2$:

$$T_0 = \frac{1}{2} \left(\sqrt{m^2 + 2(n+1)|e|H} + \sqrt{m^2 + 2n|e|H} \right). \quad (25)$$

One can also use the FW representation for a description of spin evolution. If an initial spin state is a superposition of spin-up and spin-down states, the particle polarization depends on time. We utilize Hamiltonian (24) and the matrix Hamilton equation for a determination of evolution of the spin wave function:

$$i \frac{d\Psi}{dt} = H\Psi, \quad \Psi = \begin{pmatrix} C_1(t) \\ C_2(t) \end{pmatrix}, \quad H_{ij} = \langle i | \mathcal{H} | j \rangle, \quad (26)$$

where H is a 2×2 matrix; H_{ij} are matrix elements of \mathcal{H} ; Ψ is the two-component spin wave function (spinor) [12]. The wave function $|i\rangle$ is defined by $C_i = 1$ and $i, j = 1, 2$. The

upper and lower components of Ψ define the amplitudes of spin-up and spin-down states, respectively.

When we take into account a possible decay of particles, the matrix Hamiltonian takes the form

$$H = \begin{pmatrix} E_0 + \mathcal{A} - i\frac{\Gamma}{2} & 0 \\ 0 & E_0 - \mathcal{A} - i\frac{\Gamma}{2} \end{pmatrix}, \quad (27)$$

where Γ is the decay constant, E_0 is the zero energy level, and

$$\mathcal{A} = -\frac{1}{2}(K_+ - K_-) - \mu' H. \quad (28)$$

It can be easily checked that the real part of matrix Hamiltonian (27) coincides with Hamilton operator (24) expressed in the matrix form. This coincidence results from the fact that the considered Hamilton operator is independent of coordinates.

The general solution of Eqs. (26)–(28) is given by

$$\Psi = \exp\left(-iE_0 t - \frac{\Gamma t}{2}\right) \begin{pmatrix} \exp(-i\mathcal{A}t)C_1(0) \\ \exp(i\mathcal{A}t)C_2(0) \end{pmatrix}. \quad (29)$$

The spin evolution can also be exhaustively described with the polarization vector \mathbf{P} , which is defined by

$$\mathbf{P} = \Psi^\dagger \boldsymbol{\sigma} \Psi, \quad P_x = C_1 C_2^* + C_1^* C_2, \quad P_y = i(C_1 C_2^* - C_1^* C_2), \quad P_z = C_1 C_1^* - C_2 C_2^*. \quad (30)$$

In the case considered

$$\begin{aligned} P_x(t) &= [P_x(0) \cos(2\mathcal{A}t) - P_y(0) \sin(2\mathcal{A}t)] \exp(-\Gamma t), \\ P_y(t) &= [P_x(0) \sin(2\mathcal{A}t) + P_y(0) \cos(2\mathcal{A}t)] \exp(-\Gamma t), \\ P_z(t) &= P_z(0) \exp(-\Gamma t). \end{aligned} \quad (31)$$

In agreement with [7], Eqs. (30), (31) describe the spin rotation in the horizontal plane with the angular frequency

$$\Omega = 2\mathcal{A} = -(K_+ - K_-) - 2\mu' H. \quad (32)$$

This expression for Ω is exact.

5. DISCUSSION AND SUMMARY

When the FW transformation is exact, the connection between wave functions in the Dirac and FW representations is very simple. When the particle energy is positive, upper spinors in two representations differ only by the constant factor given by Eq. (17) and lower spinors in the FW representation are zero. The result obtained makes it possible to deduce the FW wave eigenfunctions directly from the Dirac wave eigenfunctions. In principle, one can solve the inverse problem and derive the Dirac wave eigenfunctions from the FW wave eigenfunctions.

It is possible because the lower Dirac spinor can be expressed in terms of the upper one. However, this possibility is much less important because the exact solutions of relativistic wave equations can be easier obtained just in the Dirac representation.

The FW representation is very useful to determine the expectation values of needed operators and derive the operator equations of motion of particles and their spins. Solutions of these equations define the quantum evolution of main operators. 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 above-discussed spin dynamics in external fields.

Thus, one can use wave eigenfunctions previously calculated in the Dirac representation and then obtain corresponding eigenfunctions in the FW representation. After that, the quantum and semiclassical evolution of main operators can be found in the latter representation. The determination of their evolution directly in the Dirac representation is confronted by some difficulties (see [2] and references therein).

The equations derived can also be used in the more general case [10] when the particle mass m is replaced with the even operator \mathcal{M} and the initial Hamiltonian takes the form

$$\mathcal{H} = \beta\mathcal{M} + \mathcal{E} + \mathcal{O}, \quad \beta\mathcal{M} = \mathcal{M}\beta, \quad \beta\mathcal{E} = \mathcal{E}\beta, \quad \beta\mathcal{O} = -\mathcal{O}\beta. \quad (33)$$

Equations (17) and (18) remain valid on condition that the operator \mathcal{M} substituted for m commutes with the operators \mathcal{E} and \mathcal{O} .

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