Exact form of the exponential Foldy-Wouthuysen transformation operator for an arbitrary-spin particle

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The exact exponential Foldy-Wouthuysen transformation operator applicable for a particle with an arbitrary spin is derived. It can be successfully utilized for verifying any Foldy-Wouthuysen transformation method based on the exponential operator. When a verified method is relativistic, the relativistic exponential operator should be expanded in the semirelativistic power series. The obtained exponential operator can be also used for a derivation of the Foldy-Wouthuysen Hamiltonian and its comparison with Hamiltonians found by other methods. This procedure makes it possible to check the validity of any other method of the Foldy-Wouthuysen transformation.

The Foldy-Wouthuysen (FW) transformation [1] restoring the Schrödinger form of relativistic wave equations is one of the basic methods of contemporary quantum mechanics (QM). An importance of the FW transformation for physics has significantly increased nowadays due to the great progress of the art of analytic computer calculations. A great advantage of the FW representation is the simple form of operators corresponding to classical observables. In this representation, the Hamiltonian and all operators are even, i.e., block diagonal (diagonal in two spinors). The passage to the classical limit usually reduces to a replacement of the operators in quantum-mechanical Hamiltonians and equations of motion with the corresponding classical quantities. The possibility of such a replacement, explicitly or implicitly used in practically all works devoted to the FW transformation, has been rigorously proved for the stationary case in Ref. [2]. Thanks to these properties, the FW representation provides the best possibility of obtaining a meaningful classical limit of relativistic QM not only for the stationary case [1–4] but also for the nonstationary one [5,6].

Various properties and applications of the FW method have been considered in Refs. [7–9]. The FW transformation is widely used in electrodynamics [10,11], quantum field theory [12], optics [13–15], condensed matter physics [16], nuclear physics [6,17], gravity [18–20], in the theory of the weak interaction [21], and also in quantum chemistry (see the books [22,23] and the reviews [24–31]). It is applicable not only for Dirac fermions but also for particles with any spins [13,32–38].

The general form of an initial Hamiltonian for arbitrary-spin particles is given by [39]

$$\mathcal{H} = \beta\mathcal{M} + \mathcal{E} + \mathcal{O}, \quad \beta\mathcal{M} = \mathcal{M}\beta, \quad \beta\mathcal{E} = \mathcal{E}\beta,$$
$$\beta\mathcal{O} = -\mathcal{O}\beta. \tag{1}$$

The even operators $\mathcal{M}$ and $\mathcal{E}$ and the odd operator $\mathcal{O}$ are diagonal and off-diagonal in two spinors, respectively. Equation (1) is applicable for a particle with any spin if the number of components of a corresponding wave function is equal to $2(2s+1)$, where s is the spin quantum number. For a

Dirac particle, the $\mathcal{M}$ operator usually reduces to the particle rest energy mc^2:

$$\mathcal{H}_D = \beta mc^2 + \mathcal{E} + \mathcal{O}. \tag{2}$$

The Hamiltonian $\mathcal{H}$ is Hermitian for fermions and pseudo-Hermitian (more exactly, β-pseudo-Hermitian, $\mathcal{H} = \mathcal{H}^\ddagger \equiv \beta\mathcal{H}^\dagger\beta$) for bosons. We assume that the operators $\beta\mathcal{M},\mathcal{E}$, and $\mathcal{O}$ also possess this property. The transformation operator for bosons is therefore β-pseudounitary ($U^\dagger = \beta U^{-1}\beta$). We mention the existence of bosonic symmetries of the Dirac equation [40].

The FW transformation operator can be presented in the two forms, nonexponential (U_{FW}) and exponential (S_{FW}):

$$\Psi_{\mathrm{FW}} = U_{\mathrm{FW}}\Psi, \quad U_{\mathrm{FW}} = \exp\left(iS_{\mathrm{FW}}\right). \tag{3}$$

This operator transforms the initial Hamiltonian $\mathcal{H}$ to the FW representation:

$$\mathcal{H}_{\mathrm{FW}} = i\hbar\frac{\partial}{\partial t} + U_{\mathrm{FW}}\left(\mathcal{H} - i\hbar\frac{\partial}{\partial t}\right)U_{\mathrm{FW}}^{-1}. \tag{4}$$

The FW Hamiltonian obtained with this operator is even. The FW transformation vanishes either lower or upper spinor for positive and negative energy states, respectively.

There is an infinite set of representations different from the FW representation whose distinctive feature is a block-diagonal form of the Hamiltonian. The FW transformation is *uniquely* defined by the condition that the exponential operator S_{FW} is *odd*,

$$\beta S_{\mathrm{FW}} = -S_{\mathrm{FW}}\beta, \tag{5}$$

and Hermitian [41,42] (β-pseudo-Hermitian for bosons). This condition is equivalent to [41,42]

$$\beta U_{\mathrm{FW}} = U_{\mathrm{FW}}^\dagger\beta. \tag{6}$$

Eriksen [41] has found the exact expression for the nonexponential FW transformation operator. It is convenient to present this expression in the form [4],

$$U_E = U_{\mathrm{FW}} = \frac{1 + \beta\lambda}{\sqrt{2 + \beta\lambda + \lambda\beta}}, \quad \lambda = \frac{\mathcal{H}}{(\mathcal{H}^2)^{1/2}}. \tag{7}$$

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The initial Hamiltonian operator $\mathcal{H}$ is arbitrary. It is easy to see that [41]

$$\lambda^2 = 1, \quad [\beta\lambda, \lambda\beta] = 0, \quad [\beta, (\beta\lambda + \lambda\beta)] = 0, \quad (8)$$

where $[\dots, \dots]$ means a commutator.

The equivalent form of the operator U_E [4] shows that it is properly unitary (β-pseudounitary for bosons):

$$U_E = \frac{1 + \beta\lambda}{\sqrt{(1 + \beta\lambda)^\dagger(1 + \beta\lambda)}}. \quad (9)$$

The Eriksen formula is an important achievement of the theory of the FW transformation. However, the FW transformation method proposed by Eriksen [41] is semirelativistic. We use the term "semirelativistic" for methods applying an expansion of a derived block-diagonal Hamiltonian in a series of even terms of ascending order in $1/c$. For the semirelativistic and the relativistic methods, the zeroth order Hamiltonian is the Schrödinger one and the relativistic FW Hamiltonian of a free particle, respectively. The Eriksen method is not practically used in specific calculations. Since the exact equation (7) contains the square roots of Dirac matrices, it excludes a possibility to obtain a series of relativistic terms with the relativistic FW Hamiltonian of a free particle [1] as the zero-order approximation (see Ref. [43] for more details). Contemporary methods of the FW transformation are relativistic. The use of all semirelativistic methods is restricted due to their divergence at large momenta, when $p/(mc) > 1$. In this case (which takes place for an electron near a nucleus), the semirelativistic methods become inapplicable [44] (see also Ref. [43]).

Nevertheless, the calculation of the FW Hamiltonian by the perfectly substantiated Eriksen method [45–47] is very important for checking results obtained by other semirelativistic and relativistic methods (see the examples given in Ref. [43]).

We should mention that the condition (5) is used much more often than the condition (6) to check the correspondence of the final Hamiltonian to the FW representation. For example, this is one of the basic conditions for the generalized Douglas-Kroll-Hess method which is rather widely applied in quantum chemistry [31,44,48,49]. This fact obviously demonstrates the importance of the exact derivation of the exponential FW transformation operator. However, the problem of the exact form of S_{FW} was never investigated. In the present study, we solve this problem.

Evidently, the exact form of S_{FW} should be based on the operator λ. It is convenient to use the following relations (see, e.g., Ref. [47]):

$$S_{FW} = -i\beta\Theta,$$
$$U_{FW} = \cos S_{FW} + i \sin S_{FW} = \cos\Theta + \beta\sin\Theta. \quad (10)$$

To obtain an explicit expression for S_{FW}, it is instructive to consider the special case $[\mathcal{O}, \mathcal{M}] = [\mathcal{O}, \mathcal{E}] = [\mathcal{M}, \mathcal{E}] = 0$. When the operators $\mathcal{M}, \mathcal{E}$, and $\mathcal{O}$ do not explicitly depend on time and

$$\tan 2\Theta = \frac{\mathcal{O}}{\mathcal{M}}, \quad (11)$$

the odd terms are eliminated and the Hamiltonian $\mathcal{H}$ is transformed to the FW representation [47]. In the considered

special case,

$$(\mathcal{H}^2)^{1/2} = \epsilon + \frac{(\beta\mathcal{M} + \mathcal{O})\mathcal{E}}{\epsilon},$$
$$\mathcal{H} = (\beta\mathcal{M} + \mathcal{O})\left[1 + \frac{(\beta\mathcal{M} + \mathcal{O})\mathcal{E}}{\epsilon^2}\right],$$
$$\epsilon = \sqrt{\mathcal{M}^2 + \mathcal{O}^2},$$

and the operator λ is determined exactly [50]:

$$\lambda = \frac{\beta\mathcal{M} + \mathcal{O}}{\epsilon}. \quad (12)$$

Equation (11) has two solutions, Θ_1 and Θ_2, differing in $\pi/2$ [10]. Since

$$\tan 2\Theta = \frac{2\tan\Theta}{1 - \tan^2\Theta}, \quad \tan\Theta = \frac{\tan 2\Theta}{1 \pm \sqrt{1 + \tan^2 2\Theta}},$$

they are defined by the relations,

$$\tan\Theta_1 = \frac{\mathcal{O}}{\epsilon + \mathcal{M}}, \quad \tan\Theta_2 = -\frac{\mathcal{O}}{\epsilon - \mathcal{M}}. \quad (13)$$

As

$$\cos 2\Theta = \frac{1 - \tan^2\Theta}{1 + \tan^2\Theta}, \quad \sin 2\Theta = \tan 2\Theta\cos 2\Theta, \quad (14)$$

the needed trigonometrical operators are given by

$$\cos 2\Theta_1 = \frac{\mathcal{M}}{\epsilon}, \quad \cos 2\Theta_2 = -\frac{\mathcal{M}}{\epsilon}, \quad \sin 2\Theta_1 = \frac{\mathcal{O}}{\epsilon},$$
$$\sin 2\Theta_2 = -\frac{\mathcal{O}}{\epsilon}. \quad (15)$$

This equation shows that $\cos 2\Theta_1 > 0$, $\cos 2\Theta_2 < 0$.

Thus, there are two unitary transformations of the operator $\mathcal{H}$ to an even form. They are characterized by the angles Θ_1 and Θ_2, where the angle Θ_1 corresponds to the FW transformation. As a result of both transformations, one of the spinors (lower for Θ_1 and upper for Θ_2) becomes zero as for free particles [10]. Since we consider the FW transformation, $\Theta = \Theta_1$.

A comparison with Eq. (11) shows that

$$\sin 2\Theta = \tfrac{1}{2}(\lambda - \beta\lambda\beta). \quad (16)$$

The corresponding exponential FW transformation operator is given by

$$S_{FW} = -\frac{i\beta}{2}\arcsin\frac{\lambda - \beta\lambda\beta}{2}. \quad (17)$$

Let us check that Eqs. (16) and (17) obtained in the above-mentioned special case remain valid in the general case of a relativistic particle in arbitrary stationary fields. We can utilize the operator relations (cf. Ref. [47]),

$$\sin\Theta = \frac{\sin 2\Theta}{\sqrt{2(1 + \cos 2\Theta)}} = \frac{\sin 2\Theta}{\sqrt{2(1 + \sqrt{1 - \sin^2 2\Theta})}}, \quad (18)$$

$$\cos\Theta = \frac{1 + \cos 2\Theta}{\sqrt{2(1 + \cos 2\Theta)}} = \frac{1 + \sqrt{1 - \sin^2 2\Theta}}{\sqrt{2(1 + \sqrt{1 - \sin^2 2\Theta})}}. \quad (19)$$

These relations repeat the corresponding trigonometrical ones. We can mention that the FW transformation operator U_{FW} is equal to unit when the initial Hamiltonian does not contain odd terms ($\mathcal{O} = 0$).

As follows from Eq. (10), the nonexponential FW transformation operator reads

$$U_{\mathrm{FW}} = \frac{1 + \sqrt{1 - \sin^2 2\Theta} + \beta \sin 2\Theta}{\sqrt{2(1 + \sqrt{1 - \sin^2 2\Theta})}}. \tag{20}$$

Equations (8) and (16) result in

$$1 - \sin^2 2\Theta = \tfrac{1}{4}(\beta\lambda + \lambda\beta)^2. \tag{21}$$

The use of Eqs. (16) and (21) shows the equivalence of Eqs. (7) and (20). This equivalence rigorously proves the validity of Eq. (17) in the general case.

Equation (17) cannot be used for a derivation of the FW Hamiltonian in the *relativistic* case because the operator S_{FW} contains the square root of Dirac matrices (or corresponding matrices for particles with other spins). However, this equation opens a wonderful possibility to check a validity of semirelativistic and relativistic methods of the FW transformation. Indeed, a calculation of a *semirelativistic* series for the exponential operator is straightforward.

The numerator and denominator in the formula for λ commute. Therefore, it is convenient to present this quantity in the form,

$$\lambda = \tfrac{1}{2}\{\mathcal{H},(\mathcal{H}^2)^{-1/2}\}, \tag{22}$$

where $\{\ldots,\ldots\}$ means an anticommutator. Then, we apply the expansion of the square root in the power series. It is important that this procedure can be performed for arbitrary-spin particles because the initial Hamiltonians can be presented in the form (2). For example, the operator $\mathcal{M}$ for a spin-1 particle in a magnetic field reads [38,46]

$$\mathcal{M} = mc^2 + \frac{\boldsymbol{\pi}^2}{2m} - \frac{e\hbar}{mc}\boldsymbol{S} \cdot \boldsymbol{B}, \tag{23}$$

where $\boldsymbol{S}$ is the spin matrix for the spin-1 particle, $\boldsymbol{\pi} = \boldsymbol{p} - (e/c)\boldsymbol{A}$ is the kinetic momentum operator, $\boldsymbol{A}$ is the vector potential, and e is the charge of a particle. For the electron, it is negative ($e = -|e|$). The two last terms in Eq. (23) can be added to the operator $\mathcal{E}$ and therefore the operator $\mathcal{M}$ can be reduced to mc^2.

For analytic calculations with computer, one can use the formula,

$$\sqrt{\mathcal{H}^2} = mc^2\sqrt{1 + \frac{\mathcal{H}^2 - m^2c^4}{m^2c^4}}$$
$$= mc^2\sqrt{1 + \frac{2\beta mc^2\mathcal{E} + \mathcal{O}^2 + \mathcal{E}^2 + \{\mathcal{O},\mathcal{E}\}}{m^2c^4}}, \tag{24}$$

and the well-known expansions,

$$(1 + x)^{-1/2} = 1 - \frac{1}{2}x + \frac{1 \times 3}{2 \times 4}x^2 - \frac{1 \times 3 \times 5}{2 \times 4 \times 6}x^3 + \cdots,$$

$$\arcsin x = x + \frac{1}{2 \times 3}x^3 + \frac{1 \times 3}{2 \times 4 \times 5}x^5$$
$$+ \frac{1 \times 3 \times 5}{2 \times 4 \times 6 \times 7}x^7 + \cdots \tag{25}$$

The result of the expansion in the power series can be written as follows:

$$(\mathcal{H}^2)^{-1/2} = \frac{1 + q_{\mathcal{E}} + q_{\mathcal{O}}}{mc^2}, \quad \beta q_{\mathcal{E}} = q_{\mathcal{E}}\beta, \quad \beta q_{\mathcal{O}} = -q_{\mathcal{O}}\beta, \tag{26}$$

where $q_{\mathcal{E}}$ and $q_{\mathcal{O}}$ denote the sums of even and odd terms, respectively. The resulting expansion of the operator $(\lambda - \beta\lambda\beta)/2$ in the semirelativistic power series is given by

$$\frac{\lambda - \beta\lambda\beta}{2} = \frac{1}{2mc^2}[2\mathcal{O} + \{\mathcal{E},q_{\mathcal{O}}\} + \{\mathcal{O},q_{\mathcal{E}}\}]. \tag{27}$$

The final equation for the exponential FW transformation operator takes the form,

$$S_{\mathrm{FW}} = -\frac{i\beta}{2} \arcsin\left(\frac{1}{2mc^2}[2\mathcal{O} + \{\mathcal{E},q_{\mathcal{O}}\} + \{\mathcal{O},q_{\mathcal{E}}\}]\right). \tag{28}$$

This operator can be calculated with any necessary precision while the computational effort depends on this precision.

Equation (28) gives one a wonderful opportunity to verify any FW transformation method based on the exponential operator. If the checked FW transformation method is relativistic, one needs to expand all terms of the relativistic series for S_{FW} in powers of $\mathcal{E}/(mc^2), \mathcal{O}/(mc^2)$. Comparison with an explicit form of Eq. (28) verifies the checked method. Of course, any expansion can be performed only if the semirelativistic series is convergent (see Refs. [43,44]).

We should also add that the FW Hamiltonian can be calculated with the exponential operator as follows (cf. Ref. [1]):

$$\mathcal{H}_{\mathrm{FW}} = \mathcal{H} + i[S_{\mathrm{FW}},\mathcal{G}] + \frac{i^2}{2!}[S_{\mathrm{FW}},[S_{\mathrm{FW}},\mathcal{G}]]$$
$$+ \frac{i^3}{3!}[S_{\mathrm{FW}},[S_{\mathrm{FW}},[S_{\mathrm{FW}},\mathcal{G}]]] + \cdots, \tag{29}$$

where

$$\mathcal{G} = \mathcal{H} - i\hbar\frac{\partial}{\partial t}, \quad \left[S_{\mathrm{FW}},\frac{\partial}{\partial t}\right] \equiv -\frac{\partial S_{\mathrm{FW}}}{\partial t}. \tag{30}$$

Unlike the original FW approach [1], this approach needs not subsequent iterations.

This result allows one to verify any other FW transformation method which is not based on the exponential operator. For this purpose, one has to expand all terms of the relativistic series for the FW Hamiltonian calculated by the checked method in powers of $\mathcal{E}/(mc^2), \mathcal{O}/(mc^2)$ and then has to compare the obtained expression with the FW Hamiltonian given by Eqs. (29) and (30). The computational effort, of course, grows when the maximum powers increase. However, any error usually manifests itself in noncoincidence of the first few terms (see, for example, Refs. [43,51]).

Let us verify the original method by Foldy and Wouthuysen [1] as an example of the application of Eqs. (24)–(28). A calculation of the exponential FW transformation operator in the stationary case with allowance for all terms up to the order

of m^{-4} results in

$$S_{\text{FW}} = -\frac{i}{2mc^2}\beta\mathcal{O} - \frac{i}{4m^2c^4}[\mathcal{O},\mathcal{E}] + \frac{i}{6m^3c^6}\beta\mathcal{O}^3$$

$$- \frac{i}{8m^3c^6}\beta[[\mathcal{O},\mathcal{E}],\mathcal{E}] + \frac{3i}{16m^4c^8}\{\mathcal{O}^2,[\mathcal{O},\mathcal{E}]\}$$

$$- \frac{i}{16m^4c^8}[[[\mathcal{O},\mathcal{E}],\mathcal{E}],\mathcal{E}]. \tag{31}$$

The original method [1] belongs to iterative methods. The result of successive iterations expressed by the equation,

$$U = \dots \exp(iS^{(n)}) \dots \exp(iS''') \exp(iS'') \exp(iS') \exp(iS), \tag{32}$$

can be presented in the exponential form with the use of the Baker-Campbell-Hausdorff formula (see Ref. [43] and references therein). This formula defines the product of two exponential operators:

$$\exp(A)\exp(B) = \exp\left(A + B + \tfrac{1}{2}[A,B] + \tfrac{1}{12}[A,[A,B]]\right.$$

$$- \tfrac{1}{12}[B,[A,B]] - \tfrac{1}{24}[A,[B,[A,B]]]$$

$$\left. + \text{ higher order commutators}\right). \tag{33}$$

To verify the original method [1], it is sufficient to take into account three first iterations and to hold terms up to the order of m^{-3}. In the considered stationary case, they are given by [7,9,43]

$$S = -\frac{i}{2mc^2}\beta\mathcal{O}, \quad S' = -\frac{i}{4m^2c^4}[\mathcal{O},\mathcal{E}] + \frac{i}{6m^3c^6}\beta\mathcal{O}^3,$$

$$S'' = -\frac{i\beta}{8m^3c^6}[[\mathcal{O},\mathcal{E}],\mathcal{E}]. \tag{34}$$

The result of these iterations can be approximately presented as follows (see Ref. [43]):

$$U = \exp(iS'')\exp(iS')\exp(iS) = \exp(i\mathfrak{S}),$$

$$\mathfrak{S} = S'' + S' + S - \frac{i}{2}[S,S'] = -\frac{i}{2mc^2}\beta\mathcal{O} - \frac{i}{4m^2c^4}[\mathcal{O},\mathcal{E}]$$

$$+ \frac{i}{6m^3c^6}\beta\mathcal{O}^3 - \frac{i}{8m^3c^6}\beta[[\mathcal{O},\mathcal{E}],\mathcal{E}] + \frac{i}{16m^3c^6}\beta[\mathcal{O}^2,\mathcal{E}]. \tag{35}$$

The operator $\mathfrak{S}$ differs from S_{FW} due to the even last term. Therefore, the original method of the FW transformation [1] does not lead to the FW representation. This paradoxical fact was first mentioned by Eriksen and Korlsrud [42] (see also Refs. [9,43,45,46]). The original method [1] can be corrected due to an additional transformation [43]. This correction allows one to reach the FW representation.

Any representation which block diagonalizes the Hamiltonian but differs from the FW representation can be successfully used for a calculation of energy spectrum of particles in stationary states. However, an application of such a representation for other purposes is restricted. In particular, the representation which differs from the FW one is, at least, inconvenient for description of spin processes (see, for example, Refs. [4,18,52]).

Thus, we have derived the exact exponential FW transformation operator which is applicable for a particle with an arbitrary spin. This result provides an opportunity to verify any FW transformation method based on the exponential operator. Moreover, the validity of any other FW transformation method can also be checked. For this purpose, one has to use Eq. (29) in order to calculate the FW Hamiltonian and to compare it with the corresponding Hamiltonian found by the checked method. The latter possibility may need a greater computational effort.

ACKNOWLEDGMENTS

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