Question of Unitarity of Foldy-Wouthuysen Transformations and Volkov States in Two-Component Forms

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The Foldy-Wouthuysen transformations are not always unitary within the space of solutions of the Dirac equation with boundary conditions. Therefore, imprecise nonrelativistic limits can be obtained for particular interactions if these transformations are always used. This assertion is confirmed by considering the case of plane electromagnetic waves and by comparing with the result given by an exact (closed-form) unitary transformation.

In a well-known paper, Foldy and Wouthuysen[1] (FW) derived the nonrelativistic approximation (to order $1/m^2$) of the external-electromagnetic-field Dirac equation by means of a sequence of canonical transformations. It is the generalized Pauli equation (GPE) $[i\partial/\partial t - H^{(2)}]\chi^{(2)} = 0$, where, with $e > 0$,

$$H^{(2)} = \gamma^0[m + (1/2m)(-i\nabla + e\vec{A})^2] - eA^0 + (e/2m)\gamma^0\vec{\sigma}\cdot\vec{H} + (e/8m^2)\nabla\cdot\vec{E} + (e/4m^2)\vec{\sigma}\cdot[\vec{E}\times(-i\nabla + e\vec{A})] + i(e/8m^2)\vec{\sigma}\cdot(\nabla\times\vec{E}). \quad (1)$$

Their method was developed on the model of the field-free case where the unitary transformation can be found in closed form. They showed its physical meaning which is to transform a free-electron state φ_p (of given four-momentum p) into a two-component spin state.

Their idea was generalized later to higher-spin equations (Duffin-Kemmer-Petiau[2] and Bhabha[3] equations). As the space of solutions of these equations is an indefinite-metric space, the generalized FW transformations[2,3] are then not unitary but metric unitary.

The FW procedure is not free of difficulties, however. In an external-field problem, a time-dependent unitary transformation may not conserve energy. The time-dependent FW transformation is known to yield energy ambiguities.[4] The difficulty which is in question here concerns the very problem of unitarity of the FW procedure. My contention is as follows.

While a transformation U (assumed to be invertible) can always be used to transform the equation

$$(i\partial/\partial t - H)\psi = 0 \quad \text{(I)}$$

into

$$(i\partial/\partial t - H')\psi' = 0, \quad \text{(II)}$$

where $\psi' = U\psi$ and

$$H' = UHU^{-1} - U[i\partial/\partial t, U^{-1}],$$

it is only when U is unitary that (I) and (II) are said to be equivalent. If $U = e^{iS}$, ψ and ψ' are unitarily equivalent if and only if S is self-adjoint[5] (not only Hermitian). Thus, the generator $S = -(i/2m)\vec{\gamma}\cdot(i\nabla + e\vec{A})$ of the first FW transformation has to be self-adjoint within the space of all the solutions ψ of (I) (which satisfy appropriate boundary conditions) for the GPE and the Dirac equation to be unitarily equivalent. Now, it is tacitly assumed that introducing an electromagnetic interaction by minimal-coupling prescription ($i\partial^\mu \to i\partial^\mu + eA^\mu$) yields an Hermitian Hamiltonian. While this should be true for the *total* interaction Hamiltonian, this assumption may fail for one part of it (the external-field problem).

In fact, let $D(0)$ be the space within which the three-momentum operator $-i\nabla$ is defined and is self-adjoint. Introducing an external-field interaction involves defining a new domain $D(A_{\text{ext}})$ within which the operator $-i\nabla + e\vec{A}_{\text{ext}}$ will operate. The solutions ψ of (I) belong necessarily to $D(A_{\text{ext}})$. Now, it can occur[6,7] that for particular interactions and boundary conditions $-i\nabla$ is not self-adjoint within $D(A_{\text{ext}})$. In such a case $\psi' = e^{iS}\psi$ is not unitarily equivalent to ψ, in which case $(\psi', \psi') \neq (\psi, \psi)$. In summary, self-adjointness of the three-momentum operator can be lost because of the interaction with an external field and the imposition of boundary conditions, and the FW transformations are not always unitary.

I shall here prove this fact by considering Volkov's exact solution[7] of the Dirac equation for an electron in the classical external field of a plane electromagnetic wave (of arbitrary shape). As is well known, Volkov states play an essential part in the calculation of scattering processes that occur in an intense laser beam.

The case of plane waves is known as a pathological case.[7] The momentum operator and Hamiltonian are not Hermitian[7] within the space of Volkov states with asymptotic conditions (necessary to recover a free-particle state). Therefore, the generator $S = -(i/2m)\vec{\gamma}\cdot(-i\nabla + e\vec{A})$ of the first FW transformation is not self-adjoint within the space of those solutions. In other words, the solution $\chi_p^{(2)}$ of the GPE (for plane waves) and the Volkov solution ψ_p, which both reduce to free-particle states of given momentum p when $A\to 0$ (that is when $\tau\to\pm\infty$), are not unitarily equivalent.

To see this more explicitly, let us consider the Volkov state[7,8]

$$\psi_p = T_p \exp[-i(e/n\cdot p)\Lambda_p]\varphi_p,$$

where

$$T_p = 1 + (e/2n\cdot p)\gamma\cdot n\vec{\gamma}\cdot\vec{A},$$

and where

$$\Lambda_p = \int_{-\infty}^{\tau}(\vec{A}\cdot\vec{p} + \tfrac{1}{2}e\vec{A}^2)\,d\tau'.$$

The electron motion described by a Volkov state is quasiclassical (that is, is solution of the Lorentz force equation). Furthermore, this state describes a spin motion given by the classical Thomas-Bargmann-Michel-Telegdi (TBMT) equation.[9]

Let us consider the operator[9]

$$M^\mu{}_\nu = \delta^\mu{}_\nu - (e/n\cdot p)(n^\mu A_\nu - A^\mu n_\nu) - \tfrac{1}{2}(e/n\cdot p)^2 A^2 n^\mu n_\nu, \tag{2}$$

which is such that $p'^\mu = M^\mu{}_\nu p^\nu$ is the classical four-momentum of the electron in the wave. As M is a Lorentz-type matrix (hence $p'^2 = p^2 m^2$), we can transform the algebraic equation satisfied by the free state φ_p into an algebraic equation satisfied by the Volkov state ψ_p:

$$(\gamma\cdot p - m)\varphi_p = (\gamma_\nu M_\mu{}^\nu p'^\mu - m)\varphi_p = 0,$$

that is,

$$(T_p^{-1}\gamma\cdot p' T_p - m)\varphi_p = 0, \tag{3}$$

where T_p is just the spinor image[9] of the Lorentz-type operator M ($M^\mu{}_\nu\gamma^\nu = T_p^{-1}\gamma^\mu T_p$). Equation (3) shows that ψ_p satisfies the simple algebriac equation

$$p'^0\psi_p = (\gamma^0\vec{\gamma}\cdot\vec{p}' + \gamma^0 m)\psi_p, \tag{4}$$

which differs from the algebraic equation satisfied by φ_p only by the replacements $p^0\to p'^0$; $\vec{p}\to\vec{p}'$. Therefore, the Volkov state ψ_p can be cast in a two-component form by means of the FW-like unitary transformation ($F_{p'}^\dagger = F_{p'}^{-1}$) $\psi_p' = F_{p'}\psi_p$, where $F_{p'} = \exp[\vec{\gamma}\cdot\vec{p}'\theta']$ with $\theta' = (2|\vec{p}'|)^{-1}\tan^{-1}(|\vec{p}'|/m)$. We easily obtain

$$\psi_p' = [2p'^0/(p'^0+m)]^{1/2}\tfrac{1}{2}[(\vec{\gamma}\cdot\vec{p}' + m)/p'^0 + 1]\psi_p = [2p'^0/(p'^0+m)]^{1/2}\tfrac{1}{2}(1+\gamma^0)\psi_p;$$

that is,

$$\psi_p' = (p'^0/p^0)^{1/2}\exp[-ip\cdot r - i(e/n\cdot p)\Lambda_p]\begin{pmatrix} S_p W \\ 0 \end{pmatrix}, \tag{5}$$

where W is a constant spinor which can be assumed such that $\vec{\sigma}\cdot\vec{\rho}_0 W = \pm W$, where $\vec{\rho}_0$ is the initial spin vector. S_p is the unitary operator

$$S_p = [(p^0+m)(p'^0+m)]^{-1/2}\{(p^0+m)[1 + i(e/2n\cdot p)\vec{\sigma}\cdot\vec{n}\times\vec{A}] + (e/2n\cdot p)\vec{\sigma}\cdot\vec{A}\vec{\sigma}\cdot\vec{p})\}. \tag{6}$$

Obviously, when the field is switched off, ψ'_p becomes identical to the state φ'_p obtained from the free state φ'_p obtained from the free state φ_p by using the closed-form field-free FW unitary transformation.[1]

The physical meaning of the unitary transformation $F_{p'}$ will appear by seeking a unit vector $\vec{\rho}$ such that $\vec{\sigma}\cdot\vec{\rho}\psi_p' = \pm\psi_p'$. This relation will be satisfied if

$$\vec{\sigma}\cdot\vec{\rho} = S_p\vec{\sigma}\cdot\vec{\rho}_0 S_p^{-1}. \tag{7}$$

Differentiating Eq. (7), we have

$$\vec{\sigma}\cdot\frac{d\vec{p}}{dt}=\left(\frac{d}{dt}S_p\right)S_p^{-1}\vec{\sigma}\cdot\vec{p}+\vec{\sigma}\cdot\vec{p}S_p\left(\frac{d}{dt}S_p^{-1}\right), \tag{8}$$

whence it follows that

$$d\vec{p}/dt=-(e/n\cdot p)(p'^0+m)^{-1}[(n\cdot p+m)\vec{p}\times\vec{H}+(\vec{p}'\cdot\vec{H})\vec{p}\times\vec{n}] \tag{9}$$

which is recognized as the TBMT equation[9] in which the fields are those of a plane electromagnetic wave. Now, the TBMT equation is known as rigorously valid in the plane-wave case.[9] Hence, ψ_p' simply describes a spin state and exhibits the expected properties of a two-component wave function obtained by a closed-form FW transformation. Therefore, the correct nonrelativistic limits of the Volkov state ψ_p can simply be obtained by expanding ψ_p' to the desired order in $1/m$. To order $1/m^2$ we readily get

$$\psi_p'^{(2)}=[1+(e/2m^2)d\Lambda_p/d\tau]\exp[-i(e/m)(1+\vec{n}\cdot\vec{p}/m)\Lambda_p]\exp[-i(m+\vec{p}^2/2m)t+i\vec{p}\cdot\vec{r}]S_p^{(2)}W,$$

where

$$S_p^{(2)}=1-(e^2\vec{A}^2/8m^2)+i(e/4m^2)\vec{\sigma}\cdot\vec{A}\times\vec{p}+i(e/2m)(1+\vec{n}\cdot\vec{p}/m)\vec{\sigma}\cdot\vec{n}\times\vec{A}. \tag{10}$$

As expected from the above discussion, we find that $\psi_p'^{(2)}$ is not a solution of the GPE. It could eventually be the solution of another equation transformed from the GPE by an (even) unitary transformation, however. Now, if we seek the solution $\chi_p^{(2)}$ of the GPE which reduces to $\varphi_p'^{(2)}$ for $A\to 0$, we can get it in the form

$$\chi_p^{(2)}=\exp[(e/8m^2)\vec{\sigma}\cdot\vec{H}]\psi_p'^{(2)},$$

thus exhibiting the *unitary inequivalence* of these two solutions. As $\psi_p'^{(2)}$ is unitarily equivalent to order $1/m^2$ with ψ_p, we can therefore conclude that $\chi_p^{(2)}$ is not the nonrelativistic limit of the Volkov state ψ_p. Instead, $\psi_p'^{(2)}$ is the correct limit. It describes to order $1/m^2$ the correct electron-spin motion [given in quaternionic form by Eqs. (7) and (10)], which $\chi_p^{(2)}$ does not.

Let us remark that the difficulties of the FW procedure here are due to the time dependence of the fields. The operator $\exp[(e/8m^2)\vec{\sigma}\cdot\vec{H}]$ commutes (to order $1/m^2$) with the Hamiltonian (1) but not with $i\partial/\partial t$. In the special (limit) case of a constant and uniform field where $\vec{E}$ and $\vec{H}$ are perpendicular and equal in magnitude (crossed fields), $\psi_p'^{(2)}$ is effectively the solution of the GPE.

On the other hand, the unitary inequivalence of the GPE and Dirac equations for plane waves can be significant in the high-frequency domain, which has recently received a lot of attention.[10]

In conclusion, using a space-time-dependent case where the Dirac equation is solvable exactly, I have shown that FW transformations are not always unitary. Unitarity (or metric unitarity) and Hermiticity of the external-field interaction Hamiltonian can depend on the form of the external interaction, on its time dependence, and on the boundary conditions. This discussion touches on the problem of a proper interpretation of the non-Hermitian operators that occur because of the external-field approximation.

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[5]See, for example, P. Roman, *Some Modern Mathematics for Physicists and Other Outsiders* (Pergamon, New York, 1975), Vol. 2, p. 660.

[6]Problems of self-adjointness of Dirac operators can principally occur in the time-independent case for strongly singular potentials (e.g., hydrogen-like potentials with $Z>138$): H. Kalf, U. W. Schmincke, J. Walter, and R. Wüst, in *Lecture Notes in Mathematics: Spectral Theory and Differential Equations*, edited by W. N. Everitt (Springer, Berlin, 1975), Vol. 448, with numerous references therein. The time-dependent case is more difficult in that self-adjointness must be verified for all time.

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[8]Units are $\hbar = c = 1$. The metric is (+−−−). The four-vector n is null: $n=(1,\vec{n})$, with $\vec{n}^2=1$. The four-potential of the plane wave is $A(\tau)=(0,\vec{A})$, where $\vec{n}\cdot\vec{A}=0$ and $\tau = n\cdot r = t-\vec{n}\cdot\vec{r}$. $\vec{E}(\tau)$ and $\vec{H}(\tau)=\vec{n}\times\vec{E}$ are the electric and magnetic fields of the plane wave. The γ matrices are chosen in the standard representation.

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Evidence for the Υ″ and a Search for New Narrow Resonances

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The production of the Υ family in proton-nucleus collisions is clarified by a sixfold increase in statistics. Constraining Υ,Υ′ masses to those observed at DORIS we find the statistical significance of the Υ″ to be 11 standard deviations. The dependence of Υ production on p_t, y, and s is presented. Limits for other resonance production in the mass range 4–18 GeV are determined.

We report on further details of upsilon[1,2] production in proton-nucleus collisions at Fermilab. In addition to data published previously,[1-4] we present here results from data taken in 1978. Our entire data sample can be divided into four subsets: (I) published data with 400-GeV incident proton energy and 1200 Υ (or Υ′) events, mass resolution ($\Delta M/M$) of 2.2% (rms)[1,2]; (II) 200/300 GeV, 500 Υ's, $\Delta M/M = 2.2\%$; (III) 400 GeV, 7000 Υ's, $\Delta M/M = 2.2\%$; (IV) 400 GeV, 500 Υ's, $\Delta M/M = 1.7\%$. Except where noted all results hereafter are from the 400-GeV data. The resolution improvement in data set IV was achieved by lowering the intensity of protons so that a multiwire proportional chamber could be installed and operated halfway between the target and the analysis magnet.

All the data from sets I, III, and IV between masses of 7.3 and 12.9 GeV were fitted simultaneously. Cross sections per Pt nucleus were converted to cross section per nucleon by dividing by $A_{\rm Pt}=195$. An isotropic decay-angle distribution was assumed for resonances while $1+\cos^2\theta$ (Gottfried-Jackson frame) was assumed for the continuum. A linear exponential form was assumed for the continuum. This form fits the continuum well in this mass range.

The continuum shape, resonance mass separations, and relative cross sections were the same for all data sets but mass resolution,[5] acceptance, normalization,[5] and mass scale were particular to each set. Assuming three resonances and letting all parameters vary we obtain the first column in Table I.[6] This fit yields the spacing $m_{\Upsilon'} - m_{\Upsilon} = 0.57 \pm 0.03$ GeV. If we constrain $m_{\Upsilon'} - m_{\Upsilon}$ to the value of 0.555 ± 0.011 GeV measured at DORIS[7] we obtain the result in the second column of Table I. In this case assuming two resonances instead of three increases χ^2 by 125 indicating a statistical significance of 11 standard deviations for the Υ″. We consider this convincing evidence for a third resonance. Data set III with continuum subtracted is plotted in Fig. 1 and compared with the fit constrained by the DORIS measurements.

These results combined with the observation of Υ and Υ′ at DORIS[7,8] strongly support the interpretation that the Υ, Υ′, and Υ″ are the $n^3S_1Q\bar{Q}$ states ($n=1,2,3$) of a new heavy quark with charge $\frac{1}{3}$ ("bottom"). Successful fitting of both J/ψ and Υ families with a common potential,[9,10] successful prediction of ⩾ 3 states,[11] $m_{\Upsilon''} - m_{\Upsilon}$,[9,10] Γ_{ee} (Υ and Υ′),[7,8,11] and $B(\Upsilon\to\mu\mu)$,[12] all reinforce this interpretation.

In Fig. 2 we show the energy dependence of Υ

