Foldy-Wouthuysen transformations in an indefinite-metric space. I. Necessary and sufficient conditions for existence †

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We prove that the necessary and sufficient conditions that a pseudounitary (Foldy-Wouthuysen) transformation exists which will diagonalize a nondiagonal pseudo-Hermitian matrix $\mathcal{O}$ on a (nonsingular) indefinite-metric space are that all the eigenvalues of $\mathcal{O}$ be real and all the eigenvectors of $\mathcal{O}$ have nonzero norm. Physical applications are discussed. For example, the 2×2 case is discussed in general and for the Sakata-Taketani spin-0 field and the Lee model. This theorem also allows one to show that one can transform all the Bhabha Poincaré generators to a form which decouples the different mass (and normed) states.

I. INTRODUCTION

In certain quantum-mechanical field theories, it can occur that states have negative as well as positive norms. This is a field theory with an "indefinite metric." The most familiar examples are the antiparticle states of a charged Klein-Gordon spin-0 field and the Gupta-Bleuler indefinite metric of QED. In general an indefinite metric will cause problems for a probabilistic interpretation, although in the above first-mentioned case one can avoid the problem by using the Pauli-Weisskopf[1] ansatz of interpreting the states as charge probability amplitudes.

If one has an indefinite-metric field theory, the norm of a state will be given by

$$||\psi_i||^2=\int d\tau\, \psi_i^\dagger M\psi_i\,, \tag{1.1}$$

where M is the metric operator, and usually the states are normalized to

$$||\psi_i||^2=\pm 1. \tag{1.2}$$

In addition, the matrix elements of an operator (say the Hamiltonian H) are

$$\langle\mathcal{O}\rangle_{ij}=\int d\tau\, \psi_i^\dagger M\mathcal{O}\psi_j\,. \tag{1.3}$$

The condition for

$$\langle\mathcal{O}\rangle^\dagger=\langle\mathcal{O}\rangle \tag{1.4}$$

is that

$$(M\mathcal{O})=(M\mathcal{O})^\dagger, \tag{1.5}$$

which, if M is nonsingular and, for convenience, taken along the diagonal and real, means

$$M\mathcal{O}=\mathcal{O}^\dagger M^\dagger=\mathcal{O}^\dagger M. \tag{1.6}$$

The diagonal elements of M could be taken to be ±1 so that

$$M\rightarrow\hat{M}=\hat{M}^{-1}. \tag{1.7}$$

However, in general the diagonal elements of M can be given by $\pm$(real numbers), so we will use that description in this paper.

An operator $\mathcal{O}$ which satisfies Eq. (1.5) is said to be *pseudo-Hermitian*. A transformation U on the state ψ is called *pseudounitary* if it leaves the norm unchanged:

$$\pm 1=\int d\tau\, \psi_i^\dagger M\psi_i=\int d\tau\, \psi_i^\dagger U^\dagger MU\psi_i\,. \tag{1.8}$$

(We will introduce[2] and prefer the more descriptive terminology "metric-Hermitian" and "metric-unitary" but use the common "pseudo" in this paper.) Thus, the condition that a matrix transformation be pseudounitary is that

$$U^\dagger MU=M. \tag{1.9}$$

Note that the definitions of pseudo-Hermitian and pseudounitary reduce to the standard definitions of Hermitian and unitary on a Hilbert space when $M=I$.

From Eq. (1.3) the condition that a pseudounitary transformation *not* change the matrix elements of an operator is that

$$\langle\mathcal{O}\rangle_{ij}=\int d\tau\, \psi_i^\dagger M\mathcal{O}\psi_j=\int d\tau\, \psi_i^\dagger U^\dagger M\mathcal{O}'U\psi_j\,, \tag{1.10}$$

or, with Eq. (1.8),

$$\mathcal{O}'=U\mathcal{O}U^{-1}. \tag{1.11}$$

In particular, if $\mathcal{O}'$ is a diagonal matrix D with the diagonal elements being the eigenvalues of the matrix $\mathcal{O}$, then in quantum-mechanical parlance one has performed a Foldy-Wouthuysen[3] transformation.[4] For a Hermitian matrix in Hilbert space one can always find a unique (up to a phase) unitary transformation which will diagonalize the matrix. For an indefinite metric this is no longer true in general (see below). Thus, it is of quantum-theoretic interest to ask: "Under what conditions on Θ can one find a pseudounitary transformation U which will diagonalize Θ to its eigenvalues (perform a generalized Foldy-Wouthuysen transformation)?" The answer is given in the theorem of the next section. Section III discusses physical applications. The following article[2] gives theorems dealing with explicit calculations of FW transformations in an indefinite-metric space.

Before proceeding, however, we wish to point out what is perhaps an intuitively clear result:

Result. The pseudounitary transformation of a pseudo-Hermitian matrix is also pseudo-Hermitian.

This result follows simply from (1.5) and (1.11):

$$(M\Theta')^\dagger = (MU\Theta U^{-1})^\dagger = (U^{-1})^\dagger \Theta^\dagger U^\dagger M = M[M^{-1}(U^{-1})^\dagger M][M^{-1}\Theta^\dagger M][M^{-1}U^\dagger M] = MU\Theta U^{-1} = M\Theta'. \qquad (1.12)$$

II. NECESSARY AND SUFFICIENT CONDITIONS

Theorem. A nondiagonal pseudo-Hermitian matrix Θ in an indefinite-metric space with a nonsingular metric M (M^{-1} exists) can be transformed by a pseudounitary matrix U to a diagonal matrix D whose elements are the complete set of eigenvalues of Θ if and only if all the eigenvalues of Θ are real and all the eigenvectors of Θ have nonzero norm.

The results of a number of persons (see, for example, Refs. 5–10), which have been summarized by Nagy,[10] can be used to prove this theorem.[11] Always taking the metric to be nonsingular, one has that[7,10] a pseudo-Hermitian matrix can in general have three classes of eigenvalue-eigenvectors:

(A) Eigenvalues x_i real with eigenvectors u_i of nonzero norm. The k eigenvectors u_i can all be made metric-orthonormal,

$$u_i^\dagger M u_j = m_i \delta_{ij}, \quad m_i \equiv M_{ii}|M_{ii}^{-1}| = \pm 1. \qquad (2.1)$$

The u_i will also span k dimensions of the space.

(B) Eigenvalues y_i real with eigenvectors v_i of zero norm.

(C) Eigenvalues z_i complex with eigenvectors r_i of zero norm.

The zero-norm eigenvectors are not in general orthogonal, and they also do not complete the space partially spanned by the u_i. However, having found all the u_i, v_i, and r_i, it is possible to find a set of states s_i which, combined with the u_i, will span the space. Now we can proceed with the proof.

Proof of sufficiency. The proof of sufficiency proceeds exactly as is the case for ordinary Hilbert space. Let U^{-1} be given by the columns of the n class (A) renormalized eigenvectors $\hat{u}_i$:

$$U^{-1} = [\hat{u}_1, \hat{u}_2, \ldots, \hat{u}_n], \; \hat{u}_i \equiv u_i |M_{ii}|^{1/2}. \qquad (2.2)$$

Then we can take U as

$$U = M^{-1}(U^{-1})^\dagger M, \qquad (2.3)$$

since from Eqs. (2.1) and (2.2)

$$UU^{-1} = M^{-1}(U^{-1})^\dagger M U^{-1} = M^{-1}M = 1, \qquad (2.4)$$

and also

$$U^{-1}U = U^{-1}M^{-1}(U^{-1})^\dagger M = M^{-1}M = 1. \qquad (2.5)$$

Further, since by definition U^{-1} is pseudounitary, taking the inverse adjoint of the pseudounitary defining equation for U^{-1} shows that U is pseudounitary. Now sufficiency follows immediately, since

$$\Theta U^{-1} = [\lambda_1\hat{u}_1, \lambda_2\hat{u}_2, \ldots, \lambda_n\hat{u}_n], \qquad (2.6)$$

so that

$$U\Theta U^{-1} = \text{diagonal}\,(\lambda_1, \lambda_2, \ldots, \lambda_n) = D. \qquad (2.7)$$

Proof of necessity. It is informative to separately rule out class (C) eigenvalue-eigenvectors. This can be done by appealing to the "result" (1.12), or explicitly calculating

$$D^\dagger = D^\dagger M^{-1}M = M^{-1}D^\dagger M = M^{-1}(U^{-1})^\dagger \Theta^\dagger U^\dagger M = [M^{-1}(U^{-1})^\dagger M]\Theta(M^{-1}U^\dagger M) = U\Theta U^{-1} = D. \qquad (2.8)$$

Both class (B) and class (C) solutions can be ruled out by noting that Eq. (2.7) must satisfy

$$\Theta U_{BC}^{-1} = U_{BC}^{-1}D = [\lambda_1\hat{t}_1, \lambda_2\hat{t}_2, \ldots, \lambda_n\hat{t}_n], \qquad (2.9)$$

where the $\hat{t}_n$ are the columns of U_{BC}^{-1}. But Eq. (2.9) is just the eigenvalue equation, so U_{BC}^{-1} must be

$$U_{BC}^{-1} = [\hat{u}_1, \hat{u}_2, \ldots, \hat{u}_k, \hat{v}_1, \hat{v}_2, \ldots, \hat{v}_c, \hat{r}_1, \ldots, \hat{r}_d], \qquad (2.10)$$

$$k + c + d = n.$$

Thus, we have found the matrix which diagonalizes Θ, but it is not pseudounitary for $k < n$, since then from the properties of class (B) and class (C) solutions,

$$U_{BC}U_{BC}^{-1} \neq 1, \quad (U_{BC}^{-1})^{\dagger} M (U_{BC}^{-1}) \neq M. \qquad (2.11)$$

III. PHYSICAL APPLICATIONS

A. General 2 × 2 case

The 2×2 space with metric

$$M = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad (3.1)$$

affords physical insight into our result. With the M of Eq. (3.1), a general psuedo-Hermitian matrix must have the form

$$\Theta = \begin{pmatrix} x & z \\ -z^* & y \end{pmatrix}, \qquad (3.2)$$

with x and y real and z complex. Except for the trivial $z=0$ case, the two solutions are

$$\lambda_{\pm} = \tfrac{1}{2}(x+y) \pm \tfrac{1}{2}A^{1/2}, \qquad (3.3)$$

$$A^{1/2} \equiv (x-y)B^{1/2}, \quad B \equiv 1 - 4|z|^2/(x-y)^2, \quad \mathrm{Re}(B^{1/2}) \geq 0, \quad \mathrm{Im}(B^{1/2}) \geq 0, \qquad (3.4)$$

$$u_{\pm} = N_{\pm} \begin{bmatrix} (x-y) \pm A^{1/2} \\ -2z^* \end{bmatrix}. \qquad (3.5)$$

The condition for the type of solutions is seen to be

$$\begin{pmatrix} \text{class (A)} \\ \text{class (B)} \\ \text{class (C)} \end{pmatrix} \Rightarrow \begin{pmatrix} B > 0 \\ B = 0 \\ B < 0 \end{pmatrix}. \qquad (3.6)$$

Metric orthonormalization would yield

$$u_{\pm}^{\dagger} M u_{\pm} = \pm |N_{\pm}|^2 (x-y)^2 R, \qquad (3.7)$$

$$R \equiv [B^{1/2} + (B^{1/2})^* \pm (B + |B|)] \geq 0. \qquad (3.8)$$

Thus, for class (A) solutions Eq. (3.7) can be normalized to ±1. For class (B) solutions the eigenstates are zero-normed, and for class (C) solutions the eigenstates are zero-normed, but are not orthogonal. We now discuss two well-known examples of such a metric.

B. Two-component spin-0 equation

The first example is the two-component spin-0 equation[12] of Sakata and Taketani[13-15] obtained from the Duffin-Kemmer-Petiau (DKP)[16-18] equation by projecting out the subsidiary components. (The same equation was also obtained from the Klein-Gordon equation by Tamm[19] and Feshbach and Villars[20] by combining ϕ and $\partial\phi/\partial t$ states.) The free Hamiltonian is

$$H = m\tau_z + (\tau_z + i\tau_y)\frac{p^2}{2m} = \begin{pmatrix} m + \frac{p^2}{2m} & \frac{p^2}{2m} \\ -\frac{p^2}{2m} & -\left(m + \frac{p^2}{2m}\right) \end{pmatrix}. \qquad (3.9)$$

Substituting the values of the H matrix of Eq. (3.9) into Eqs. (3.2)–(3.7) one will find that the solutions are class (A) with $\lambda_{\pm}$ and $u_{\pm}$ being the well-known eigenvalues $\pm(p^2+m^2)^{1/2}$ and the particle and antiparticle solutions u and v.

It is to be observed that discussions[21,22] of the Foldy-Wouthuysen transformation for this system have used the two-component form, not the five-component DKP form. We can see that this was not just a possible choice, but the proper choice. In the five-component form, where the built-in subsidiary components have not been removed, the metric is singular.

C. Lee model

A second example of the 2×2 metric of Sec. III A is the Lee model.[22-25] There, depending on the strength of the coupling constant, one can get all three classes of solutions. The static Lee model, describing the processes $V \rightleftarrows N + \theta$, is given by the second-quantized Hamiltonian

$$H = -mV^{\dagger}V + \mu N^{\dagger}N + \omega\theta^{\dagger}\theta - g(V^{\dagger}N\theta - \theta^{\dagger}N^{\dagger}V), \quad M = (-1)^{V^{\dagger}V}, \qquad (3.10)$$

with the coupling constant g being real. If one takes the states in the $N+\theta$ sector

$$|1\rangle = |N\rangle|\theta\rangle, \quad |2\rangle = |V\rangle, \qquad (3.11)$$

then Eqs. (3.10) and (3.11) can be put in our indefinite-metric matrix form as

$$M = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad H = \begin{pmatrix} (\mu+\omega) & g \\ -g & -m \end{pmatrix}. \qquad (3.12)$$

Thus, although for g small the solutions are class (A), for large enough positive or negative g, class (B) and class (C) solutions will emerge. Specifically, the eigenvalues are

$$\lambda_{\pm} = \tfrac{1}{2}(\mu + \omega - m) \pm \tfrac{1}{2}|(\mu+\omega+m)^2 - 4g^2|, \qquad (3.13)$$

so that one has

class (A) $\mathcal{E}^2 \equiv (\mu+\omega+m)^2 > 4g^2$,

class (B) $\mathcal{E}^2 = 4g^2$, what Heisenberg calls a dipole ghost,[25]

class (C) $\mathcal{E}^2 < 4g^2$, what Heisenberg calls a complex ghost.[25]

D. Free-field theories

From the above discussion, we observe that one will be able to diagonalize the Hamiltonians of well-behaved free-field theories with an indefinite metric. The eigenvalues will be the real energies, that is, the Lorentz-transformed masses of the rest system. Thus, the solutions will be class (A), not class (C) and not close to class (B), which one now realizes is a border case between (A) and (C). To obtain class (B) or class (C) solutions one must introduce a coupling which either binds the particles below their rest masses or else, by its very nature, introduces class (B) or class (C) eigenvalues.

Further, one may then be able to show that the same transformation which diagonalizes the Hamiltonian of a multimass field theory will transform all the Poincaré generators to a form which decouples the different mass states and hence also decouples the different normed states.

E. Bhabha fields

A particular example of the above is the Bhabha system which we have been working on elsewhere.[26] There[27] the U which diagonalizes the Hamiltonian H will also leave $\vec{P}$ diagonal and leave $\vec{J}$ in a form which does not couple different mass states. One can then show, since $i\vec{P}=[\vec{K},H]$ still holds for the FW transformed generators, that this transformation will change the boost generators $\vec{K}$ to a form which no longer couples the different mass states. That is, a complete Foldy-Wouthuysen transformation is possible.

This observation is well known for the separation of the particle and antiparticle mass states of the Dirac and Duffin-Kemmer-Petiau (DKP) fields, these fields being special cases of the general Bhabha fields. Observe that for both general integer-spin as well as the particular DKP case, one must first remove the zero-normed subsidiary components and work with the nonzero-normed particle components fields and generators, as we mentioned in discussing Refs. 21 and 22.

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