Diagonal forms of the Dirac Hamiltonian

R. E. Moss and A. Okniński*

Chemistry Department, The University, Southampton, S09 5NH, England

(Received 29 March 1976; revised manuscript received 10 May 1976)

A method is described for obtaining a class of unitary transformations that bring the Dirac Hamiltonian for the free electron into diagonal form which may be decoupled with respect to the positive and negative states of an appropriate Hermitian operator; the class includes those described recently by Weaver. The Dirac equation for an electron with an anomalous magnetic moment in a constant magnetic field is also diagonalized. The use of the even/odd concept to indicate the suitability of a Hamiltonian form for nonrelativistic/ultrarelativistic problems is questioned.

I. INTRODUCTION

Recently, various unitary transformations of the Dirac equation for a spin-$\frac{1}{2}$ particle,[1]

$$p_0\psi=(\vec{\alpha}\cdot\vec{p}+\beta m)\psi=H\psi,\quad H^\dagger=H \tag{1}$$

have been discussed by several authors.[2,3] A large class of diagonal Hamiltonians, including the familiar Foldy-Wouthuysen[4-6] (FW) and Cini-Touschek[7,8] (CT) Hamiltonians, has been obtained.[2] Nondiagonal forms of H have also been constructed,[2,3] but in most cases they can be reduced to diagonal form as in the case of the CT Hamiltonian.[2,7,8]

It appears that diagonal forms of H are especially important in the theory of spin-s particles.[2,9] For example, diagonal forms of the Hamiltonian permit the decoupling of a bispinor equation by means of suitable projection operators to give two equations involving two-component spinors only. Furthermore, this corresponds to separation of positive and negative states of some Hermitian operator, which provides a physical interpretation. FW and CT transformations, for example, permit the decoupling of positive and negative states of energy and helicity operators, respectively.[2,4-6,8]

Accordingly, we limit our considerations to unitary transformations of the Dirac Hamiltonian (1) leading to diagonal equations. The method described in the next section is then used to obtain all the diagonal Hamiltonians discussed in Ref. 2, and generalizations are also given. We then discuss connections between even/odd Hamiltonians (notions introduced by Foldy and Wouthuysen[6]) and nonrelativistic/ultrarelativistic limits of the Dirac equation.

II. DESCRIPTION OF THE METHOD

We start with a corollary of the theorem stated by Cohen[10] and by Johnson and Chang[11]: Given two Hermitian, anticommuting, normalized operators A and B,

$$A^\dagger=A,\quad B^\dagger=B,\quad [A,B]_+=2\delta_{AB}, \tag{2}$$

the unitary transformation

$$U=(A+B)/\sqrt{2}=U^\dagger \tag{3}$$

applied to linear combinations of A and B exchanges A and B:

$$U(c_AA+c_BB)U^\dagger=c_AB+c_BA. \tag{4}$$

It will prove useful to have, in the Hamiltonian formalism, an analog of the γ_5 matrix[12] in the covariant form of the Dirac equation. It is readily seen that, if $\vec{\alpha}$ and β anticommute and are normalized and Hermitian, the matrix

$$\delta=\alpha_1\alpha_2\alpha_3\beta \tag{5}$$

has the properties

$$[\alpha_k,\delta]_+=[\beta,\delta]_+=0\quad(k=1,2,3),\qquad \delta^2=1,\quad \delta^\dagger=\delta. \tag{6}$$

If we cast the Dirac equation (1) in the form

$$p_0\psi=[(\vec{\alpha}\cdot\vec{p}+\beta m)/E]E\psi,\quad E=+(m^2+\vec{p}\cdot\vec{p})^{1/2} \tag{7}$$

then the unitary transformation

$$U=\frac{\delta+(\vec{\alpha}\cdot\vec{p}+\beta m)/E}{\sqrt{2}} \tag{8}$$

fulfills the conditions (2)–(4) of the corollary and, since it commutes with E and p_0, brings Eq. (7) into the form

$$p_0\psi_U=\delta E\psi_U,\quad \psi_U=U\psi. \tag{9}$$

Equation (9) is representation-independent and is the basic equation of our formalism.

If we choose the standard representation for the Dirac matrices $\vec{\alpha},\beta$ or the spinor representation[12] $\vec{\alpha}',\beta'$,

$$\vec{\alpha}=\begin{pmatrix}0&\vec{\sigma}\\ \vec{\sigma}&0\end{pmatrix},\quad \beta=\begin{pmatrix}1&0\\0&-1\end{pmatrix},$$

$$\vec{\alpha}'=\begin{pmatrix}\vec{\sigma}&0\\0&-\vec{\sigma}\end{pmatrix},\quad \beta'=\begin{pmatrix}0&1\\1&0\end{pmatrix}, \tag{10}$$

$$\alpha_1\alpha_2\alpha_3\beta=-\alpha_1'\alpha_2'\alpha_3'\beta'=\delta=\begin{pmatrix}0&-i\\i&0\end{pmatrix},$$

then we realize that the matrix δ anticommutes with both standard $\vec{\alpha}, \beta$ and spinor $\vec{\alpha}', \beta'$ Dirac matrices. It is obvious that the set $\mathfrak{D}$ of Hermitian, normalized operators

$$\mathfrak{D} = \{\beta, \vec{\alpha}', (\vec{\alpha}' \cdot \vec{F})/(\vec{F} \cdot \vec{F})^{1/2}\}, \tag{11}$$

where $\vec{F}$ contains no Dirac matrices and commutes with E and p_0, contains only diagonal operators which anticommute with δ.

We see that by applying any unitary transformation

$$U_A = (\delta + A)/\sqrt{2}, \quad A \in \mathfrak{D} \tag{12}$$

to Eq. (9) we convert it into the diagonal form

$$p_0 \psi_{U_A U} = AE\psi_{U_A U}, \quad \psi_{U_A U} = U_A U \psi. \tag{13}$$

We note that it is impossible to get a diagonal form of the Dirac equation (13) with A containing more than three mutually anticommuting matrices (the set of block-diagonal 4×4 anticommuting matrices is isomorphic with the Pauli algebra, which contains only three different anticommuting matrices[13]).

III. DIAGONAL DIRAC HAMILTONIANS

A. Free electron

Let us note that, choosing

$$A = \beta \tag{14a}$$

in Eq. (12), we obtain from Eq. (13)

$$p_0 \psi_{\rm FW} = \beta E \psi_{\rm FW}, \tag{15a}$$

where

$$\psi_{\rm FW} = \tfrac{1}{2}(\delta + \beta)[\delta + (\vec{\alpha} \cdot \vec{p} + \beta m)/E]\psi, \tag{16a}$$

which is exactly the FW form of the Dirac equation, although the unitary transformation leading to Eq. (15a) is different from the standard one.[4-6]

Furthermore, substituting for A the operators

$$\alpha_k' \quad (k = 1, 2, 3) \tag{14b}$$

$$\vec{\alpha}' \cdot \hat{p} \quad [\hat{p} = \vec{p}/(\vec{p} \cdot \vec{p})^{1/2}], \tag{14c}$$

$$[\alpha_1' p_1 + \alpha_2' p_2 + \alpha_3' (p_3^2 + m^2)^{1/2}]/E, \tag{14d}$$

$$[\vec{\alpha}' \cdot \hat{p}_\perp (p_\perp^2 + m^2)^{1/2} + \alpha_3' p_3]/E, \tag{14e}$$

we get the transformed diagonal equations

$$p_0 \psi_b = \alpha_k' E \psi_b \quad (k = 1, 2, 3) \tag{15b}$$

$$p_0 \psi_{\rm CT} = (\vec{\alpha}' \cdot \hat{p}) E \psi_{\rm CT}, \text{ or } (\vec{\alpha}' \cdot \vec{p}) \psi_{\rm CT} = \epsilon |\vec{p}| \psi_{\rm CT}, \tag{15c}$$

where ϵ is the sign of the energy and

$$\psi_{\rm CT} = \tfrac{1}{2}(\delta + \vec{\alpha}' \cdot \hat{p})[\delta + (\vec{\alpha} \cdot \vec{p} + \beta m)/E]\psi, \tag{16c}$$

$$p_0 \psi_d = [\alpha_1' p_1 + \alpha_2' p_2 + \alpha_3' (p_3^2 + m^2)^{1/2}]\psi_d, \tag{15d}$$

$$p_0 \psi_e = [\vec{\alpha}' \cdot \hat{p}_\perp (p_\perp^2 + m^2)^{1/2} + \alpha_3' p_3]\psi_e. \tag{15e}$$

All the diagonal Hamiltonians discussed by Weaver[2] for spin-$\frac{1}{2}$ particles are represented in Eqs. (15); Eq. (15c) is the Cini-Touschek form of the Dirac equation.[2,7,8]

It is possible, of course, to obtain an infinite number of diagonal Hamiltonian equations using Eqs. (9), (11), and (12). For example, choosing A in Eq. (12) as

$$A = (\vec{\alpha}' \cdot \hat{p}'),$$
$$\hat{p}' = \vec{p}'/(\vec{p}' \cdot \vec{p}')^{1/2}, \tag{14f}$$
$$p_k' = (p_k^2 + \tfrac{1}{3}m^2)^{1/2} \quad (k = 1, 2, 3)$$

we get the diagonal form of the Dirac equation

$$p_0 \psi_f = (\vec{\alpha}' \cdot \hat{p}') E \psi_f, \text{ or } \epsilon |\vec{p}'| \psi_f = (\vec{\alpha}' \cdot \vec{p}')\psi_f. \tag{15f}$$

This equation, which is similar to the Cini-Touschek form Eq. (15c), is the four-component form of the neutrino equation with $\vec{p}$ replaced by $\vec{p}'$.

B. Electron in constant magnetic field

The method described above can also be applied to an electron (charge $-e$) with an anomalous magnetic moment κ in a constant homogeneous magnetic field $\vec{B}$. In this case the Dirac equation is

$$p_0 \psi = [\vec{\alpha} \cdot \vec{\pi} + \beta m + (\kappa e/2m)\beta \vec{\Sigma} \cdot \vec{B}]\psi, \tag{17}$$

where $\vec{\pi} = \vec{p} + e\vec{A}$, $\vec{B} = \vec{\nabla} \times \vec{A}$, $\vec{A}$ is a time-independent vector potential, and

$$\vec{\Sigma} = \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & \vec{\sigma} \end{pmatrix}. \tag{18}$$

Since we wish to work with the standard representation matrices, it is convenient to first perform the unitary transformation

$$U' = \delta(\delta + \beta)/\sqrt{2}. \tag{19}$$

This changes β into δ but leaves $\vec{\Sigma}$ and $\vec{\alpha}$ unchanged; the additional δ factor preserves the sign of $\vec{\alpha}$. The Dirac equation is now $p_0 \psi' = H'\psi'$, where

$$H' = \vec{\alpha} \cdot \vec{\pi} + \delta m + (\kappa e/2m)\delta \vec{\Sigma} \cdot \vec{B}, \tag{20}$$

and can be rewritten in a form analogous to Eq. (7) as

$$p_0 \psi' = [H'/(H'^2)^{1/2}](H'^2)^{1/2}\psi', \tag{21}$$

with

$$H'^2 = m^2 + \vec{\pi} \cdot \vec{\pi} + e(1 + \kappa)\vec{\Sigma} \cdot \vec{B} + (\kappa e/2m)^2(\vec{\Sigma} \cdot \vec{B})^2 + (i\kappa e/m)\delta\vec{\alpha} \cdot \vec{B} \times \vec{\pi}. \tag{22}$$

Note that, since $\delta\vec{\alpha} = -i\beta\vec{\Sigma}$, H'^2 and hence $(H'^2)^{1/2}$ are diagonal. In addition, β commutes with H'^2 and hence $(H'^2)^{1/2}$ but anticommutes with H', so that the unitary transformation

$$U'' = \frac{\beta + H'/(H'^2)^{1/2}}{\sqrt{2}} \tag{23}$$

brings the Dirac equation into the diagonal form

$$p_0\psi'' = \beta(H'^2)^{1/2}\psi'' , \tag{24}$$

where H'^2 is given by Eq. (22).

This result is to be compared with the results of Tsai[14] and Weaver.[15] If $\vec{A}$ and $\vec{B}$ vanish the free-electron case Eq. (15a) is recovered, while setting $\kappa = 0$ gives the Case form of the Dirac equation for an electron without an anomalous magnetic moment.[16]

Equation (17) may be diagonalized in a different way by first rearranging it as

$$[p_0 - m\beta - (e\kappa/2m)\beta\vec{\Sigma}\cdot\vec{B}]\psi = \vec{\alpha}\cdot\vec{\pi}\psi \tag{25}$$

and then operating on it from the left with $-\gamma_5$, where[12]

$$\gamma_5 = -i\gamma_0\gamma_1\gamma_2\gamma_3 = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} . \tag{26}$$

Since $-\gamma_5\vec{\alpha} = \vec{\Sigma}$, this gives

$$G\psi = \vec{\Sigma}\cdot\vec{\pi}\psi , \tag{27}$$

where

$$G = -\gamma_5 p_0 + \gamma_5\beta[m + (e\kappa/2m)\vec{\Sigma}\cdot\vec{B}] , \tag{28}$$

and this may be rewritten as

$$[G/(G^2)^{1/2}](G^2)^{1/2}\psi = \vec{\Sigma}\cdot\vec{\pi}\psi \tag{29}$$

with

$$G^2 = p_0{}^2 - [m + (e\kappa/2m)\vec{\Sigma}\cdot\vec{B}]^2 . \tag{30}$$

The operator

$$S = \frac{\beta + G/(G^2)^{1/2}}{\sqrt{2}} = S^{-1} \tag{31}$$

is similar to that in Eq. (3). It commutes with $\vec{\Sigma}\cdot\vec{\pi}$ and when used in a similarity transformation puts Eq. (29) in the final (diagonal) form

$$\beta(G^2)^{1/2}(S\psi) = \vec{\Sigma}\cdot\vec{\pi}(S\psi) \tag{32}$$

with G^2 given by Eq. (30). This equation is readily reduced to the Cini-Touschek form Eq. (15c) for the case of a free electron.

The transformation using S in Eq. (31) may be interpreted as unitary if we restrict it to the space of the eigenstates ψ of Eq. (17) because in this case the operator on the left-hand side of Eq. (29) acts on ψ as the Hermitian operator $\vec{\Sigma}\cdot\vec{\pi}$. Hence, S acts on ψ as a unitary operator.

Johnson and Chang[11] have given a similar definition for a transformation defined only on the eigenstates ψ of the Dirac equation $\gamma\cdot P\psi = m\psi$. They diagonalized the covariant form of the Dirac equation for an electron in any arbitrary electromagnetic field using a unitary transformation defined in the above sense. Their covariant approach brings the Dirac equation into m-linear form and is different from our Hamiltonian method, which leads to p_0-linear diagonal equations.[17]

IV. EVEN (ODD) HAMILTONIANS AND NONRELATIVISTIC (ULTRARELATIVISTIC) LIMITS OF THE DIRAC EQUATION

It is often assumed that even or odd Hamiltonians represent nonrelativistic or ultrarelativistic limits of the Dirac equation, respectively.[18] Accordingly, even or odd forms of the Dirac Hamiltonian have been constructed.[3] It appears, however, that such a classification is not always suitable.

Let us first consider the unitary transformation Eq. (19) applied to Eq. (1) using the standard representation. We get the transformed equation

$$p_0\psi' = H'\psi' , \quad \psi' = U'\psi \tag{33}$$

where

$$H' = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}\cdot\vec{p} + \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} m \tag{34}$$

is an odd Hamiltonian. Because of the presence of four Dirac matrices in H', Eq. (33) cannot be decoupled into two spinor equations by any projection operator (only multiples of the unit matrix commute with a Hamiltonian containing four anticommuting 4×4 matrices[13]). The Hamiltonian H', apart from being odd, does not resemble the ultrarelativistic Hamiltonian of Cini and Touschek[2,7,8] and does not appear suitable for the analysis of the high-momentum limit of the Dirac equation. Thus, odd Hamiltonians do not necessarily imply the ultrarelativistic limit of the Dirac equation. On the other hand, even forms of the Hamiltonian do not necessarily correspond to the nonrelativistic limit of the Dirac Hamiltonian.

The ultrarelativistic form of Cini and Touschek,[2,7,8] for example, may be cast into either antidiagonal (odd)[7,8] or diagonal (even)[2] form.[19] In these cases we can use the projection operators $\frac{1}{2}(1\pm\gamma_5)$ or $\frac{1}{2}(1\pm\gamma_5')$, respectively, to decouple the CT form.[2,8] The resulting uncoupled equations are identical and correspond to the separation of positive- and negative-helicity states[2,8] irrespective of the odd or even structure of the transformed Hamiltonian.

Thus, we realize that care is required in classifying transformed Hamiltonians as nonrelativistic/ultrarelativistic using even/off notions (see the discussion of the transformed Hamiltonians in Ref. 2).

V. DISCUSSION

We have obtained in a uniform way a class of diagonal Hamiltonians that are unitarily equivalent to the Dirac Hamiltonian (1). We note, however, that the Hamiltonians of Foldy and Wouthuysen [Eq. (15a)] and Cini and Touschek [Eq. (15c)] have been obtained by applying unitary transformations different from the original ones.[2,4-8] The nonuniqueness of the unitary transformation leading to transformed Dirac equations was discussed by Pursey.[20] The relations between different unitary operators leading to the same transformed Hamiltonian were analyzed by de Vries[18]; a unitary operator can always be found that explicitly relates the different unitary transformations.

We realize that for the free electron the diagonal Hamiltonians (15) with the operator A from the set $\mathfrak{D}$ of Eq. (11) have the form

$$p_0\psi = AE\psi, \quad AE = \begin{pmatrix} a & 0 \\ 0 & -a \end{pmatrix}, \quad a^\dagger = a. \tag{35}$$

Thus, by applying projection operators $P_\pm = \frac{1}{2}(1 \pm \beta)$ to Eq. (35) we can decouple it with respect to positive and negative states of the Hermitian operator AE. For the FW and CT cases [Eqs. (15a), (15c)] the operators corresponding to AE are energy and helicity operators, respectively.[4-6,8] Similar remarks apply to the Hamiltonian (24) for an electron with an anomalous magnetic moment in a constant magnetic field.

Finally, we point out that even (odd) Hamiltonians do not have a one-to-one correspondence to nonrelativistic (ultrarelativistic) Hamiltonians and that perhaps some other criteria should be formulated.

ACKNOWLEDGMENTS

We thank J. D. Morrison for many useful discussions and the Science Research Council for support for one of us (A.O.).

*On leave from the Institute of Organic Chemistry and Technology, Technical University (Politechnika), Warsaw, Poland.

[1] We follow the notation of Ref. 2.

[2] D. L. Weaver, Phys. Rev. D 12, 2325 (1975).

[3] J. -F. Roux and Phan Van Loc, Nuovo Cimento 29B, 225 (1975).

[4] M. H. L. Pryce, Proc. R. Soc. London A195, 62 (1948).

[5] S. Tani, Prog. Theor. Phys. 6, 267 (1951).

[6] L. L. Foldy and S. A. Wouthuysen, Phys. Rev. 78, 29 (1950).

[7] H. Mendlowitz, Phys. Rev. 102, 527 (1956).

[8] M. Cini and B. Touschek, Nuovo Cimento 7, 422 (1958).

[9] L. L. Foldy, Phys. Rev. 102, 568 (1956).

[10] H. A. Cohen, Am. J. Phys. 39, 409 (1971).

[11] J. E. Johnson and K. K. Chang, Phys. Rev. D 10, 2421 (1974).

[12] J. D. Bjorken and S. D. Drell, *Relativistic Quantum Mechanics* (McGraw-Hill, New York, 1964).

[13] R. H. Good, Jr., Rev. Mod. Phys. 27, 187 (1955).

[14] W. -y. Tsai, Phys. Rev. D 7, 1945 (1973).

[15] D. L. Weaver, Phys. Rev. D 12, 4001 (1975).

[16] K. M. Case, Phys. Rev. 95, 1323 (1954).

[17] For the p_μ-linear and m-linear classification see A. J. Bracken and H. A. Cohen, Prog. Theor. Phys. 41, 816 (1969).

[18] E. de Vries, Fortschr. Phys. 18, 149 (1970).

[19] Compare Eq. (3) of Ref. 8 and Eq. (2b) of Ref. 2 [or Eq. (15c) of this work].

[20] D. L. Pursey, Nucl. Phys. 8, 595 (1958).