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All you need to know about the Dirac equation

P. Weinberger*

Center for Computational Nanoscience, Seilerstätte 10/22, A-1010 Vienna, Austria

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A very brief introduction is given to all that is needed to appreciate the formal structure of the Dirac equation and why – without destroying this structure – it cannot be reduced to a Pauli-Schrödinger type equation.

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1. Introduction

For about 30 years I have run around in Europe and in the USA and told everybody in the field that if relativistic effects are important for a certain physical phenomenon, then one has to use the Dirac equation rather than the Pauli-Schrödinger equation. For nearly as long as this I have been confronted with the canonical question, but how big are the relativistic effects? Usually whenever this question was posed in the past it was accompanied by a pitiful smile which clearly was intended to indicate that I was obviously addressing something completely irrelevant. The perhaps less sarcastic reply consisted frequently in a friendly statement that I should not worry since all that is needed is to throw in some spin-orbit interaction. My standard reply, namely the counter-question of why should I completely neglect Einstein and his special theory of relativity, was usually brushed aside with the comment that we are in solid state physics and not astrophysics. This kind of attitude was (is) perhaps best expressed by Richard Feynman in his *Six Not-So-Easy Pieces* [1], quoted below:

Newton's Second Law, which we have expressed by the equation

$$F = \mathrm{d}(mv)/\mathrm{d}t,$$

was stated with the tacit assumption that m is a constant, but we now know that this is not true, and that the mass of a body increases with velocity. In Einstein's corrected formula m has the value

$$m = \frac{m_0}{\sqrt{1 - v^2/c^2}},$$

where the 'rest mass' m_0 represents the mass of a body that is not moving and c is the speed of light, which is about 3.10^5 km.sec^{-1} or about 186 000 mi.sec^{-1}.

*Email: weinberger@computational-nanoscience.de

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For those who want to learn just enough about it so they can solve problems, that is all there is to the theory of relativity – it just changes Newton's laws by introducing a correction factor to the mass. From the formula itself it is easy to see that this mass increase is very small in ordinary circumstances . . .

Fortunately for me it turned out that solid state physics nowadays is ruled by nanoscience. And we all know that without relativity there would not be magnetic anisotropies, and there would be no perpendicular magnetism. Without relativistic effects the development in information technology would have been minute. Without relativistic effects none of the beautiful GMR devices we have in nearly all everyday-life devices would make sense. It seems that lately there are only a few colleagues left who intentionally ignore relativistic effects because of not being familiar with a proper treatment of such effects.

In this contribution a very short summary of 'relativity essentials' will be given. In particular it will be pointed out why a so-called 'four-component' theory cannot be reduced to a 'two-component' scheme without destroying the inherent algebraic structure that follows from the general postulates of quantum mechanics and Einstein's (special) theory of relativity. The arguments given are based on two completely different points of view, namely (a) application of group theory and (b) making use of the condition of relativistic covariance. The basics of these arguments are not new; however, I hope it perhaps helps to repeat them yet another time.

2. Minkowski space

Suppose the set of space-time vectors is given by

$$M = \{x^\mu\}, \tag{1}$$

$$x^\mu \equiv \left(x^0, x^1, x^2, x^3\right) = \left(x^0, x^k\right) = (ct, \mathbf{r}), \tag{2}$$

$$\mu = 0, 1, 2, 3, \quad k = 1, 2, 3,$$

where $x^0 = ct$ is the time component and $\mathbf{r} = (x^1, x^2, x^3)$ the space component of an arbitrary space-time vector x^μ. For any arbitrary pair of elements $x, y \in M$ the scalar product in M is defined as follows

$$(x, y) \equiv \sum_{\mu=0}^{3} x_\mu y^\mu = x_0 y^0 - \sum_{k=1}^{3} x_k y^k, \tag{3}$$

and in particular therefore the norm as

$$\|x\| = (x, x) = x_0 x^0 - (\mathbf{r}, \mathbf{r}). \tag{4}$$

The metric in M is said to be **pseudo-Euclidean**, since the **metric tensor** $g_{\mu\nu}$ is of the following form

$$g_{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -\underline{1}_3 \end{pmatrix} = g^{\mu\nu}. \tag{5}$$

The set M is sometimes also called **Minkowski space**.

In M a vector a is called **contravariant** (usually denoted by e.g. a^{μ}) if it 'transforms like a space-time vector' x^{μ} and **covariant** (usually denoted by, e.g. a_{μ}) if it transforms like $\partial/\partial x^{\mu}$. The transformation of a contravariant vector by means of the metric tensor $g_{\mu\nu}$ yields a covariant vector:

$$a_{\mu} = \sum_{\nu=0}^{3} g_{\mu\nu} a^{\nu} \equiv g_{\mu\nu} a^{\nu}, \tag{6}$$

while by the opposite procedure a contravariant vector is obtained:

$$a^{\mu} = \sum_{\nu=0}^{3} g^{\mu\nu} a_{\nu} \equiv g^{\mu\nu} a_{\nu}. \tag{7}$$

It should be noted that in either case $a_0 = a^0$. The implicit summation over repeated indices as indicated in the last two equations is usually called the **Einstein sum convention**. The product of the metric tensor with itself

$$\sum_{\rho=0}^{3} g_{\mu\rho} g^{\rho\nu} \equiv g_{\mu\rho} g^{\rho\nu} = \delta_{\mu}^{\nu}, \quad \delta_{\mu}^{\nu} = \begin{cases} 1, & \nu = \mu \\ 0, & \nu \neq \mu, \end{cases} \tag{8}$$

is a unit matrix. A vector a^{μ} is called a **space-like vector** if its norm $a_{\mu} a^{\mu} < 0$ and oppositely a **time-like vector** if the norm is positive.

Defined in M, the **gradient** can be written as a covariant vector ∂_{μ},

$$\partial_{\mu} \equiv \frac{\partial}{\partial x^{\mu}} = \left(\frac{\partial}{\partial x^0}, \frac{\partial}{\partial x^1}, \frac{\partial}{\partial x^2}, \frac{\partial}{\partial x^3} \right) = \left(\frac{\partial}{\partial ct}, \nabla \right), \tag{9}$$

or, as a contravariant vector ∂^{μ},

$$\partial^{\mu} = \left(\frac{\partial}{\partial ct}, -\nabla \right), \tag{10}$$

whereby

$$\partial_{\mu} \partial^{\mu} \equiv \Box = \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla \cdot \nabla = \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \Delta \tag{11}$$

is usually called the **D'Alembert operator**.

If $\mathbf{A} = \mathbf{A}(\mathbf{r}, t)$ denotes the vector potential and $\phi = \phi(\mathbf{r}, t)$ the scalar potential then the electromagnetic field can be written as the following contravariant vector A^{μ},

$$A^{\mu} = (\phi, \mathbf{A}), \tag{12}$$

such that the electric and magnetic field, **E** and **H**, respectively, are given by

$$\mathbf{E} = (E_x, E_y, E_z) = -\nabla\phi - \frac{\partial A}{\partial x^0}, \tag{13}$$

$$\mathbf{H} = (H_x, H_y, H_z) = \operatorname{rot} \mathbf{A}. \tag{14}$$

The so-called electromagnetic field tensor $F_{\mu\nu}$, formally written as

$$F_{\mu\nu} = \frac{\partial A_\nu}{\partial x^\mu} - \frac{\partial A_\mu}{\partial x^\nu}, \tag{15}$$

is an antisymmetric tensor in M, whose elements are given by the components of **E** and **H**,

$$F_{\mu\nu} = \begin{pmatrix} 0 & E_x & E_y & E_z \\ -E_x & 0 & -H_z & H_y \\ -E_y & H_z & 0 & -H_x \\ -E_z & -H_y & H_x & 0 \end{pmatrix}. \tag{16}$$

The gradient and the electromagnetic field vectors finally can be combined to yield the following four-component vector D_μ

$$D_\mu = \delta_\mu + ieA_\mu = \left(\frac{\partial}{\partial x^0} + ie\phi,\ -\nabla + ie\mathbf{A}\right). \tag{17}$$

3. Poincaré and Lorentz transformations

Poincaré transformations are inhomogeneous linear transformations that preserve the quadratic form $x_\mu x^\mu$, i.e. the norm in M. Such a transformation is defined by

$$(x^\mu)' = \Omega^\mu_\nu x^\upsilon + a^\mu, \tag{18}$$

where $(x^\mu)'$ is the transformed vector, Ω^μ_ν a space-time point operation Ω, which keeps the origin invariant, and a^μ a translation. If $(\Omega|a)$ denotes the operator that maps x^μ on $(x^\mu)'$,

$$(\Omega|a)x^\mu = \Omega^\mu_\nu x^\upsilon + a^\mu = (x^\mu)', \tag{19}$$

then the matrix Ω^μ_ν is the representation of the corresponding space-time point operation, whereby matrices like $\Omega_{\mu\nu}$ and $\Omega^{\mu\nu}$ can be obtained by using the metric tensor $g_{\mu\nu}$ as follows

$$\Omega^{\mu\nu} = g^\rho_\nu \Omega^\mu_\rho.$$

From the condition that the norm has to be left invariant and that the transformations are real, the properties of the matrices Ω^ν_μ can be deduced, namely

$$\Omega^*_{\mu\upsilon} = \Omega_{\mu\upsilon}, \tag{20}$$

$$\Omega_{\mu\upsilon}\Omega^{\mu\lambda} = \Omega_{\nu\mu}\Omega^{\lambda\mu} = \delta^\lambda_\nu, \tag{21}$$

$$\det|\Omega^\mu_\nu| = \pm 1. \tag{22}$$

The set of operators (Ω/a) forms a group, the so-called **Poincaré group**,

$$P = \left\{(\Omega|a)|(\Omega|a)(\Omega'|a') = (\Omega\Omega'|\Omega a' + a)\right\}, \tag{23}$$

in which the identity element $(\epsilon|0)$ has the following representation for the pure space-time point operation ϵ

$$D(\epsilon) = \begin{pmatrix} 1 & 0 \\ 0 & \underline{1}_3 \end{pmatrix}. \tag{24}$$

Similarly, the pure time-inversion operator $(T|0)$ and pure space inversion operator $(J|0)$ are defined by the representations of their corresponding space-time point operations

$$D(T) = \begin{pmatrix} -1 & 0 \\ 0 & \underline{1}_3 \end{pmatrix}, \quad D(J) = \begin{pmatrix} 1 & 0 \\ 0 & -\underline{1}_3 \end{pmatrix}. \tag{25}$$

The set of operators $(\Omega|a)$ for which $\Omega^{00} > 0$, i.e. which preserve the direction of time, forms a subgroup $\overline{P} \subset P$ of index two:

$$\overline{P} = \left\{ (\overline{\Omega}|a) \middle| \overline{\Omega}^{00} \geq 0 \right\}, \tag{26}$$

since the complement $(P - \overline{P})$ is defined by

$$(P - \overline{P}) = \left\{ (\Omega|a) \middle| (\Omega|a) = (\overline{\Omega}|a)(T|0) \right\}. \tag{27}$$

$\overline{P}$ is called the **orthochronous Poincaré group**, which in turn has a subgroup of index two, namely the so-called **proper orthochronous Poincaré group**, $\overline{P}_+$, which is the set of time conserving transformations for which $\det|\Omega^\mu_\nu| = 1$:

$$\overline{P}_+ = \left\{ (\overline{\Omega}|a) \middle| \overline{\Omega}^{00} \geq 0, \det|\Omega^\mu_\nu| = 1 \right\}. \tag{28}$$

In terms of left cosets, the Poincaré group $P \supset \overline{P} \supset \overline{P}_+$ can therefore be written as

$$P = \left\{ \overline{P}, (T|0)\overline{P} \right\}, \tag{29}$$

$$\overline{P} = \left\{ \overline{P}_+, (J|0)\overline{P}_+ \right\}. \tag{30}$$

These three Poincaré groups contain as corresponding subgroups all those operations for which the translational part is zero, i.e. $a = 0$:

$$L = \left\{ (\Omega|a) \right\} = \left\{ \overline{L}, (T|0)\overline{L} \right\}, \tag{31}$$

$$\overline{L} = \left\{ \overline{L}_+, (J|0)\overline{L}_+ \right\}. \tag{32}$$

L is called the **Lorentz group**, $\overline{L}$ the **orthochronous Lorentz group** and $\overline{L}_+$ the **proper orthochronous Lorentz group**.

The subset of operators of the Poincaré group that corresponds to pure space translations only also forms a subgroup, the so-called **Euclidean group**:

$$P \supset E = \left\{ (\Omega|a) \middle| \forall a^0 = 0 \right\}. \tag{33}$$

The corresponding subgroup of the Lorentz group is the familiar **rotation-inversion group** in R_3. It should be appreciated that the above very brief characterization in terms of the left coset representatives $(T|0)$ and $(J|0)$ most likely is the most compact way of viewing the general structure of these groups. Specific aspects of group theory, namely in particular representation theory, will also be used in the following sections in order to pin-point the relation between Paul spin matrices and Dirac matrices. For historical reasons it has to be mentioned that of course Dirac in his 1928 paper [2,3] carefully 'checked' the Lorentz invariance of his newly found equation in an extensive separate section.

4. The Dirac equation

For a single particle of charge e and mass m the relativistic Hamilton function is given by[1], $c=1$,

$$H = e\phi + \sqrt{(\mathbf{p} - e\mathbf{A})^2 + m^2}, \tag{34}$$

where ϕ is the scalar potential, $\mathbf{A}$ the vector potential and $\mathbf{p}$ the momentum. Assuming now in accordance with the postulates of quantum mechanics that the probability density $\rho = \psi^*\psi$ is positive definite then it follows immediately that the corresponding Hamilton operator, $\hat{H}$, has to be Hermitian, since:

$$\int \underbrace{\frac{\partial \rho}{\partial t}}_{\text{linear}} d^3x = -\frac{i}{\hbar} \int \left(\psi^* \hat{H} \psi - \left(\hat{H} \psi \right)^* \psi \right) d^3x = 0. \tag{35}$$

For the sake of simplicity in the following discussion only the Hamilton function in the absence of a field shall be considered:

$$H = \sqrt{\mathbf{p}^2 + m^2}. \tag{36}$$

Since the *left-hand side* of (35) is linear in $\partial/\partial t \equiv \partial/\partial x^0$, see in particular Equation (9), this implies that also $\hat{H}$ on the *right-hand side* of (35) has to be linear with respect to $\partial/\partial x^k$, $k = 1, 3$, i.e. with respect to components of the momentum operator $\hat{\mathbf{p}}$. This condition is usually called the **condition of relativistic covariance**.

If one replaces according to the **correspondence principle** $E \rightarrow i\partial/\partial t$ and $\mathbf{p} \rightarrow -i\nabla$, i.e.

$$\hat{H}\psi = \underbrace{\frac{i\partial}{\partial t}}_{\text{linear}} \psi = \underbrace{\left(\sqrt{\hat{\mathbf{p}}^2 + m^2} \right)}_{\text{has to be linear}} \psi, \tag{37}$$

one can immediately see that the condition of linearity cannot be fulfilled in a straightforward manner, since the square root is not a linear operator. As is perhaps less known the Dirac problem [2–4], but also the problem of Pauli's spin theory [5], can be viewed in terms of a special polynomial algebra [14].

4.1. *Polynomial algebras*

Let $P_2(x)$ be a second order polynomial of the following form

$$P_2(x) = a_{21} \sum_{i \neq j} x_i x_j + a_{22} \sum_j x_j^2, \quad i,j = 1, 2, \ldots, m, \tag{38}$$

where the a_{ij} are elements of a symmetric matrix. Consider further that the linear form

$$L(x) = \sum_{j=1}^{m} \alpha_j x_j \tag{39}$$

satisfies the condition

$$P_2(x) + L^2(x) = 0. \tag{40}$$

Then the set of coefficients $\{\alpha_j\}$ has to satisfy the following properties [14]:

$$i = j: \quad [\alpha_i, \alpha_j]_+ = -2a_{22}I, \tag{41}$$

$$i \neq j: \quad [\alpha_i, \alpha_j]_+ = -a_{21}I, \tag{42}$$

where I denotes the identity element in $\{\alpha_j\}$ and $[,]_+$ anticommutators. The set of coefficients $\{\alpha_j\}$ is called an associative algebra. Two special cases carry famous names, namely

$$a_{21} = a_{22} = 0 \rightarrow [\alpha_i, \alpha_j]_+ = 0, \tag{43}$$

the so-called **Grassmann algebra**[2] and

$$a_{21} = 0, \; a_{22} = -1 \rightarrow [\alpha_i, \alpha_j]_+ = 2\delta_{ij}, \tag{44}$$

the so-called **Clifford algebra**. Comparing now Equation (37) with Equation (36) one can see that exactly the case of the Clifford algebra is needed in tackling the problem of the linearization of the square root:

$$\underbrace{\sqrt{\left(\sum_{j=1}^{m} p_j^2\right)}}_{P_2(p)} = \underbrace{\sum_{j=1}^{m} \alpha_j p_j}_{L(p)}. \tag{45}$$

In the following first the case for $m=2$ and 3 (Pauli spin theory) is discussed by considering the smallest groups with Clifford algebraic structure, and only then is the Dirac problem ($m=4$) addressed in a similar way.

4.2. *The Pauli groups*

4.2.1. *The Pauli group for $m=2$*

For $m=2$ the smallest set of elements α_i that shows group closure [11–13] is given by

$$G_P^{(m=2)} = \{\pm I, \pm\alpha_1, \pm\alpha_2, \pm\alpha_1\alpha_2\}. \tag{46}$$

This group is of order 8 and has five classes (C_i), as can easily be found by using Equation (44), see Table 1.

There are therefore five irreducible representations ($\Gamma_i^{(m=2)}, i = 1,5$) of dimensions n_i such that

$$\sum_{i=1}^{5} n_i^2 = 8. \tag{47}$$

Table 1. Class structure of $G_P^{(m=2)}$.

C_1: $\{I\}$
C_2: $\{-I\}$
C_3: $\{\pm\alpha_1\}$
C_4: $\{\pm\alpha_2\}$
C_5: $\{\pm\alpha_1\alpha_2\}$

This implies that four irreducible representations ($\Gamma_i^{(m=2)}, i = 1, \ldots, 4$) have to be one-dimensional and one two-dimensional. Since one-dimensional representations are commutative, i.e. do not satisfy the conditions of a Clifford algebra, only the two-dimensional representation ($\Gamma_5^{(m=2)}$) is of help. The matrices for this irreducible representation are listed below:

$$\Gamma_5^{(m=2)}(\pm I) = \pm\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \Gamma_5^{(m=2)}(\pm\alpha_1) = \pm\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$
$$\Gamma_5^{(m=2)}(\pm\alpha_2) = \pm\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \Gamma_5^{(m=2)}(\pm\alpha_1\alpha_2) = \pm\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}. \tag{48}$$

Using this set of matrices it is easy to show that it indeed forms a representation of $G_P^{(m=2)}$ and that these matrices are Clifford algebraic. For the case of $m = 2$ the problem of the linearization of the square root is therefore solved:

$$\sqrt{\hat{p}_1^2 + \hat{p}_2^2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \hat{p}_1\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \hat{p}_2\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \tag{49}$$

4.2.2. *The Pauli group for $m = 3$*

For $m = 3$ the smallest set of elements d_i forming a group is given by

$$G_P^{(m=3)} = \{\pm I, \pm\alpha_1, \pm\alpha_2, \pm\alpha_3, \pm\alpha_1\alpha_2, \pm\alpha_1\alpha_3, \pm\alpha_2\alpha_3, \pm\alpha_1\alpha_2\alpha_3\}. \tag{50}$$

The order of this group is 16. It has 10 classes (see Table 2), and therefore 10 irreducible representations,

$$\sum_{i=1}^{10} n_i^2 = 16, \tag{51}$$

of which eight ($\alpha_i^{(m=3)}, i = 1, \ldots, 8$) are one-dimensional and two ($\alpha_i^{(m=3)}, i = 9, 10$) are two-dimensional. Again only the two-dimensional irreducible representations are Clifford algebraic.

For α_1 and α_2 one can use the same matrix representatives as in the $m = 2$ case,

$$\Gamma_9^{(m=3)}(\alpha_1) = \Gamma_5^{(m=2)}(\alpha_1), \quad \Gamma_9^{(m=3)}(\alpha_2) = \Gamma_5^{(m=2)}(\alpha_2), \tag{52}$$

provided that the corresponding matrix for α_3 is defined by

$$\Gamma_9^{(m=3)}(\alpha_3) = -i\Gamma_9^{(m=3)}(\alpha_1)\Gamma_9^{(m=3)}(\alpha_2). \tag{53}$$

Table 2. Class structure of $G_P^{(m=3)}$.

$C_1: \{I\}$	$C_6: \{\pm\alpha_1\alpha_2\}$
$C_2: \{-I\}$	$C_7: \{\pm\alpha_1\alpha_3\}$
$C_3: \{\pm\alpha_1\}$	$C_8: \{\pm\alpha_2\alpha_3\}$
$C_4: \{\pm\alpha_2\}$	$C_9: \{\alpha_1\alpha_2\alpha_3\}$
$C_5: \{\pm\alpha_3\}$	$C_{10}: \{-\alpha_1\alpha_2\alpha_3\}$

The second two-dimensional irreducible representation ($\Gamma_{10}^{(m=3)}$) is by the way the complex conjugate representation of $\Gamma_9^{(m=3)}$. It is rather easy to prove that these two irreducible representations are indeed non-equivalent.

For the $m=3$ case the problem of the linearization of the square root reduces therefore to the following matrix equation:

$$\sqrt{\hat{p}_1^2+\hat{p}_2^2+\hat{p}_3^2}\,\Gamma_9^{(m=3)}(I) = \hat{p}_1\Gamma_9^{(m=3)}(\alpha_1)+\hat{p}_2\Gamma_9^{(m=3)}(\alpha_2)+\hat{p}_3\Gamma_9^{(m=3)}(\alpha_3). \tag{54}$$

The matrices

$$\Gamma_9^{(m=3)}(\alpha_1)\equiv\sigma_1=\begin{pmatrix}0&1\\1&0\end{pmatrix},\quad \Gamma_9^{(m=3)}(\alpha_2)\equiv\sigma_2=\begin{pmatrix}0&-i\\i&0\end{pmatrix},$$
$$\Gamma_9^{(m=3)}(\alpha_3)\equiv\sigma_3=\begin{pmatrix}1&0\\0&-1\end{pmatrix}, \tag{55}$$

are nothing but the famous **Pauli spin matrices**, usually – as indicated in the last equation – denoted simply by σ_1, σ_2 and σ_3. For $m=2$, 3 the corresponding groups, $G_P^{(m=2)}$ and $G_P^{(m=3)}$, are called **Pauli groups** (as indicated by the index P).

4.3. *The Dirac group*

For $m=4$ the following subset of the Clifford algebra forms the smallest group

$$G_D^{(m=4)}=\left\{\pm I, \pm\alpha_i\ (i\le 4), \pm\alpha_i\alpha_j\ (i<j), \pm\alpha_i\alpha_j\alpha_k\ (i<j<k), \pm\alpha_1\alpha_2\alpha_3\alpha_4\equiv\pm\alpha_5\right\}, \tag{56}$$

where 'traditionally' the elements α_i are usually denoted in the literature also by γ_μ. The order of this group is 32. It has 17 classes, and therefore 17 irreducible representations.

As can easily be checked in analogy to Equation (47) 16 of these irreducible representations ($\Gamma_i^{(m=4)}, i=1,\ldots,16$) are one-dimensional and one is four-dimensional ($\Gamma_{17}^{(m=4)}$). Again only the matrices of the four-dimensional irreducible representation satisfy the conditions of the Clifford algebra.

The following matrices

$$\Gamma_{17}^{(m=4)}(\alpha_i)\equiv\alpha_i\equiv\gamma_i=\begin{pmatrix}0&\sigma_i\\\sigma_i&0\end{pmatrix},\quad i=1,2,3, \tag{57}$$

$$\Gamma_{17}^{(m=4)}(\alpha_4)\equiv\beta\equiv\gamma_4=\begin{pmatrix}\underline{I}_2&0\\0&-\underline{I}_2\end{pmatrix}, \tag{58}$$

where the σ_i are the Pauli spin matrices and $\underline{I}_2$ is a two-dimensional unit matrix, are then **irreducible representatives** of the elements $\alpha_i \in G_D^{(m=4)}$. These particular representatives, usually as indicated above simply by α_i and β, are the famous **Dirac matrices**; $G_D^{(m=4)}$ is called the **Dirac group**.

4.4. *Relations between the Dirac group and the Pauli groups*

4.4.1. *The subgroup structure*

The Dirac group $G_D^{(m=4)}$ contains the Pauli groups as subgroups,

$$G_P^{(m=2)} \subset G_P^{(m=3)} \subset G_D^{(m=4)}, \tag{59}$$

whereby $G_P^{(m=2)}$ is a normal subgroup in $G_P^{(m=3)}$ and $G_D^{(m=4)}$. This implies that in a coset decomposition of $G_D^{(m=4)}$ in terms of $G_P^{(m=2)}$,

$$G_D^{(m=4)} = \left\{ IG_P^{(m=2)},\, \alpha_3 G_P^{(m=2)},\, \alpha_4 G_P^{(m=2)},\, \alpha_3\alpha_4 G_P^{(m=2)} \right\}, \tag{60}$$

left and right cosets are identical,

$$\begin{aligned} \alpha_3 G_P^{(m=2)} &= \{\pm\alpha_3, \pm\alpha_3\alpha_1, \pm\,\alpha_3\alpha_2, \pm\alpha_3\alpha_1\alpha_2\} \\ &= \{\pm\alpha_3, \pm\alpha_1\alpha_3, \pm\alpha_2\alpha_3, \pm\alpha_1\alpha_2\alpha_3\} = G_P^{(m=2)}\alpha_3, \end{aligned} \tag{61}$$

and that $G_P^{(m=2)}$ consists of complete classes of $G_D^{(m=4)}$, see Table 3, denoted for the moment as $C_i(G_D^{(m=4)})$,

$$G_P^{(m=2)} = \left\{ C_1\left(G_D^{(m=4)}\right), C_2\left(G_D^{(m=4)}\right), C_3\left(G_D^{(m=4)}\right), C_4\left(G_D^{(m=4)}\right), C_5\left(G_D^{(m=4)}\right) \right\}. \tag{62}$$

It should be noted that $G_P^{(m=3)}$ is not a normal subgroup in $G_D^{(m=4)}$, since

$$C_{17}\left(G_D^{(m=4)}\right) = C_9\left(G_D^{(m=3)}\right) \cup C_{10}\left(G_D^{(m=3)}\right). \tag{63}$$

4.4.2. *Subduced representations*

The set of matrices,

$$\Gamma_{17}^{(m=4)}\left(G_P^{(m=2)}\right) \equiv \left\{ \Gamma_{17}^{(m=4)}(\alpha), \forall\alpha \in G_P^{(m=2)} \right\},$$

and

$$\Gamma_{17}^{(m=4)}\left(G_P^{(m=3)}\right) \equiv \left\{ \Gamma_{17}^{(m=4)}(\alpha), \forall\alpha \in G_P^{(m=3)} \right\},$$

Table 3. Class structure of $G_D^{(m=4)}$.

C_1:	$\{I\}$
C_2:	$\{-I\}$
C_{3-6}:	$\{\pm\alpha_i \mid i \le 4\}$
C_{7-12}:	$\{\pm\alpha_i\alpha_j \mid i<j \le 4\}$
C_{13-16}:	$\{\pm\alpha_i\alpha_j\alpha_k \mid i<j<k \le 4\}$
C_{17}:	$\{\pm\alpha_1\alpha_2\alpha_3\alpha_4\}$

of course also forms a representation for $G_P^{(m=2)}$ and $G_P^{(m=3)}$, respectively, which, however, is reducible. Such representations are called **subduced representations**. Reducing these two representations (for example by means of the orthogonality relation for characters), one finds the following decompositions into irreducible representations:

$$\Gamma_{17}^{(m=4)}\left(G_P^{(m=2)}\right) = 2\Gamma_5^{(m=2)}\left(G_P^{(m=2)}\right), \tag{64}$$

and

$$\begin{aligned}\Gamma_{17}^{(m=4)}\left(G_P^{(m=3)}\right) &= \Gamma_9^{(m=3)}\left(G_P^{(m=3)}\right) + \Gamma_{10}^{(m=3)}\left(G_P^{(m=3)}\right) \\ &= \Gamma_9^{(m=3)}\left(G_P^{(m=3)}\right) + \left(\Gamma_9^{(m=3)}\left(G_P^{(m=3)}\right)\right)^*.\end{aligned} \tag{65}$$

Since the irreducible representation $\Gamma_{17}^{(m=4)}$ of $G_D^{(m=4)}$ always subduces only the group of the Pauli spin matrices (and their complex conjugates), there is no way to linearize properly the square root $\sqrt{\mathbf{p}^2 + m^2}$ for a four-component momentum in terms of 2×2 matrices only! In other words: there is no other 'truly' relativistic description but the one using the Dirac matrices:

$$\underline{I}_4\left(\underbrace{\hat{p}_1^2 + \hat{p}_2^2 + \hat{p}_3^2}_{\hat{\mathbf{p}}^2} + \underbrace{\hat{p}_4^2}_{m^2}\right)^{1/2} = \alpha_1\hat{p}_1 + \alpha_2\hat{p}_2 + \alpha_3\hat{p}_3 + \beta\hat{p}_4 \tag{66}$$

Equation (66) is nothing but a consequence of the condition of relativistic covariance!

It is interesting to note that conversely by inducing representations of $G_P^{(m=4)}$ from the irreducible representations of the normal subgroup $G_P^{(m=2)} \subset G_P^{(m=4)}$ (not shown here) one indeed obtains a four-dimensional irreducible representation, namely $\Gamma_{17}^{(m=4)}$.

One can summarize the properties of these three groups $G_P^{(m=2,3)}$ and $G_P^{(m=4)}$ very compactly in Table 4.

4.4.3. *Fundamental theorem of Dirac matrices*

The so-called **fundamental theorem of Dirac matrices**, namely that a necessary and sufficient condition for a set of four matrices γ_i' to be Dirac matrices, i.e. to be irreducible and Clifford algebraic, is that they have to be obtained via a similarity transformation W from the matrices in (57), (58):

$$\gamma_i' = W^{-1}\gamma_i W, \quad i = 1, 4, \tag{67}$$

Table 4. Summary of group properties for $m \leq 4$.

m	Group-order	# of classes	# of one-dim. irreps	# of two-dim. irreps	# of four-dim. irreps
	2^{m+1}	m^2+1	2^m		
2	8	5	4	1	0
3	16	10	8	2	0
4	32	17	16	0	1

is, in the context of the Dirac group, nothing but Schur's lemma for irreducible representations.

5. Dirac's original derivation

Of course Dirac in his famous paper [2,3] did not use group theory, nor did he realize that his matrices were Clifford algebraic. He found 'his' matrices by trial and error, knowing very well, however, that if quantum mechanics and Einstein's special theory of relativity were to be compatible at all, then they can be found only on the condition that the postulates of quantum mechanics had to be fulfilled rigorously.

In an appendix of his first paper he also introduced the so-called elimination method in order to arrive at expressions that at his time were very much *en vogue*, namely the *Darwin term*, the *mass-velocity term* and the *spin-orbit term*, the last of which causing so much confusion in the following decades. For matters of completeness his derivation of these terms is reformulated in the following section [7].

6. The Pauli-Schrödinger equation

Consider for simplicity a Dirac-type Hamiltonian for a non-magnetic system, in atomic units ($\hbar = m = 1$),

$$\mathcal{H} = c\boldsymbol{\alpha} \cdot \mathbf{p} + (\beta - I_4)c^2 + VI_4, \tag{68}$$

where c is the speed of light. In making use of the bi-spinor property of the wavefunction,[3]

$$|\psi\rangle = \begin{pmatrix} |\phi\rangle \\ |\chi\rangle \end{pmatrix},$$

the corresponding eigenvalue equation,

$$\mathcal{H}|\psi\rangle = \epsilon|\psi\rangle, \tag{69}$$

can be split into two equations, namely

$$\begin{aligned} c\boldsymbol{\sigma} \cdot \mathbf{p}|\chi\rangle - V|\phi\rangle &= \epsilon|\phi\rangle, \\ c\boldsymbol{\sigma} \cdot \mathbf{p}|\phi\rangle + \left(V - 2c^2\right)|\chi\rangle &= \epsilon|\chi\rangle. \end{aligned} \tag{70}$$

Clearly, the spinor $|\chi\rangle$ can now be expressed in terms of $|\phi\rangle$:

$$|\chi\rangle = (1/2c)B^{-1}\boldsymbol{\sigma} \cdot \mathbf{p}|\phi\rangle, \tag{71}$$

$$B = 1 + \left(1/2c^2\right)(\epsilon - V), \tag{72}$$

thus leading to only one equation for $|\phi\rangle$:

$$\mathcal{D}|\phi\rangle = \varepsilon|\phi\rangle, \tag{73}$$

$$\mathcal{D} = (1/2)\boldsymbol{\sigma} \cdot \mathbf{p}B^{-1}\boldsymbol{\sigma} \cdot \mathbf{p} + V. \tag{74}$$

6.1. *The central field formulation*

For a *central field*, $V(\mathbf{r}) = V(|\mathbf{r}|)$, the operator $\mathcal{D}$ in Equation (74) has the same constants of motion [8–10] as the corresponding Dirac Hamiltonian, namely the angular momentum operators $\mathbf{J}^2$, J_z, and $K = \beta(1 + \boldsymbol{\sigma} \cdot \mathbf{L})$:

$$
\begin{aligned}
\mathbf{J}^2|\phi\rangle &= j(j+1)|\phi\rangle, \quad \mathbf{J}^2|\chi\rangle = j(j+1)|\chi\rangle,\\
J_z|\phi\rangle &= \mu|\phi\rangle, \quad J_z|\chi\rangle = \mu|\chi\rangle,\\
(1+\boldsymbol{\sigma}\cdot\mathbf{L})|\phi\rangle &= \kappa|\phi\rangle, \quad (1+\boldsymbol{\sigma}\cdot\mathbf{L})|\chi\rangle = -\kappa|\chi\rangle,\\
j &= \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots,\\
-j &\le \mu \le j,\\
\kappa &= \begin{cases} -\ell - 1; & j = \ell + 1/2\\ \ell; & j = \ell - 1/2. \end{cases}
\end{aligned}
$$

Their simultaneous eigenfunctions are the so-called spin spherical harmonics [8],

$$
\begin{aligned}
|\kappa\mu\rangle \equiv |Q\rangle &= \sum_{s=\pm 1/2} c\left(\ell\frac{1}{2};\mu - s, s\right)\,|\ell, \mu - s\rangle\Phi(s),\\
\langle\hat{\mathbf{r}}|\ell, \mu - s\rangle &= Y_{\ell,\mu-s}(\hat{\mathbf{r}}),\\
\Phi\left(\frac{1}{2}\right) = \begin{pmatrix}1\\0\end{pmatrix}&, \quad \Phi\left(-\frac{1}{2}\right) = \begin{pmatrix}0\\1\end{pmatrix},\\
c\left(\ell\frac{1}{2};\mu - s, s\right) &= \frac{(-1)^{\ell+\mu-1/2}}{(2j+1)^{1/2}}\begin{pmatrix}\ell & 1/2 & j\\ m & s & \mu\end{pmatrix},
\end{aligned}
$$

where the $Y_{\ell m}(\hat{\mathbf{r}})$ are (complex) spherical harmonics, $\Phi(\pm\frac{1}{2})$ the so-called spin eigenfunctions [5] and the $c(\ell\frac{1}{2};\mu - s, s)$ the famous Clebsch-Gordan coefficients [6], which in turn are related to the Wigner 3*j*-coefficients [6]. It is important to note that $|\ell, \mu - s\rangle\ \Phi(s)$ is a tensorial product of functions belonging to different spaces.

Because of the constants of motion $\mathbf{J}^2$, J_z, and $K = \beta(1 + \boldsymbol{\sigma}\cdot\mathbf{L})$ Equation (73) is separable with respect to the radial and angular variables, i.e. an eigenfunction of $\mathcal{D}$ belonging to a particular eigenspace of these constants of motions is then of the form

$$
\langle\mathbf{r}|\phi_Q\rangle = \frac{R_\kappa(r)}{r}\langle\hat{\mathbf{r}}|Q\rangle, \tag{75}
$$

where the radial amplitudes $R_\kappa(r)$ are solutions of the following differential equation [2,3,7]

$$
\begin{aligned}
&\left[\frac{1}{2}\left(-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{\ell(\ell+1)}{r^2}\right) + V(r) - \epsilon\right]R_\kappa(r)\\
&\quad = \frac{1}{4c^2}B^{-2}(r)\frac{\mathrm{d}V(r)}{\mathrm{d}r}\frac{\kappa}{r}R_\kappa(r) + \frac{1}{4c^2}\left[(\epsilon - V(r))B^{-1}(r)\left(-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{\ell(\ell+1)}{r^2}\right)\right]R_\kappa(r)\\
&\qquad + \frac{1}{4c^2}\left[B^{-2}(r)\frac{\mathrm{d}V(r)}{\mathrm{d}r}\frac{\mathrm{d}}{\mathrm{d}r}\right]R_\kappa(r).
\end{aligned} \tag{76}
$$

Equation (76) shows a remarkably 'physical structure', namely

(1) For $c=\infty$ (non-relativistic limit) this equation is reduced to the well-known *radial Schrödinger equation*.
(2) By approximating the elimination operator B in Equation (72) by unity ($B=1$) the so-called (radial) *Pauli-Schrödinger equation* is obtained. The terms on the right-hand side of Equation (76) are then in turn the *spin-orbit coupling*, the *mass velocity term*, and the *Darwin shift*.
(3) For $B\neq 1$ relativistic corrections in order higher than c^{-4}, enter, e.g. via the normalization of the wavefunction.
(4) It should be noted that although all three terms on the right-hand side of Equation (76) have a prefactor $1/4c^2$, i.e. are of relativistic origin, the only one, however, which explicitly depends on a (relativistic) quantum number, namely κ, is *spin-orbit coupling*.
(5) It should be noted in particular that $\mathrm{d}V/\mathrm{d}r$ has the unpleasant property of being singular for $r\to 0$.

7. Comparison to the 'radial Dirac equation'

Clearly in the case of a central field also Equation (69) can be separated using polar coordinates, i.e. using the constants of motion $\mathbf{J}^2$, J_z, and $K=\beta(1+\boldsymbol{\sigma}\cdot\mathbf{L})$,

$$\langle\mathbf{r}|\psi_{\kappa\mu}\rangle=\begin{pmatrix} g_\kappa(r)\langle\hat{\mathbf{r}}|\kappa\mu\rangle \\ if_\kappa(r)\langle\hat{\mathbf{r}}|-\kappa\mu\rangle\end{pmatrix}, \tag{77}$$

$$g_\kappa(r)=\frac{P_\kappa(r)}{r},\quad f_\kappa(r)=\frac{Q_\kappa(r)}{cr}, \tag{78}$$

where the radial amplitudes $P_\kappa(r)$ and $Q_\kappa(r)$ are solution of the following differential equation (in atomic Rydberg units)

$$\frac{\mathrm{d}Q_\kappa(r)}{\mathrm{d}r}=\kappa\frac{Q_\kappa(r)}{r}-(\epsilon-V(r))P_\kappa(r), \tag{79}$$

$$\frac{\mathrm{d}P_\kappa(r)}{\mathrm{d}r}=-\kappa\frac{P_\kappa(r)}{r}+\left(\frac{\epsilon-V(r)}{c^2}+1\right)Q_\kappa(r). \tag{80}$$

This radial differential equation has now to be compared to the one corresponding to the Pauli-Schrödinger equation ($B(r)=1$, $\forall r$)

$$\begin{aligned}&\left[\left(-\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{\ell(\ell+1)}{r^2}\right)+V(r)-\epsilon\right]R_\kappa(r)\\ &\quad=\frac{1}{4c^2}\frac{\mathrm{d}(V(r))}{\mathrm{d}r}\frac{\kappa}{r}R_\kappa(r)+\frac{1}{4c^2}\left[(\epsilon-V(r))\left(-\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{\ell(\ell+1)}{r^2}\right)\right]R_\kappa(r)\\ &\quad+\frac{1}{4c^2}\left[\frac{\mathrm{d}(V(r))}{\mathrm{d}r}\frac{\mathrm{d}}{\mathrm{d}r}\right]R_\kappa(r).\end{aligned} \tag{81}$$

As can easily be seen, Equation (81) is a second-order differential equation, while Equations (79)–(80) form a system of coupled first-order differential equations.

Remembering now that the key requirement for a proper inclusion of relativity into quantum mechanics is the **condition of relativistic covariance**, see in particular Equations (9)–(10), namely the condition of linearity for a relativistic Hamiltonian, see Equation (37), when using the correspondence principle (one of the postulates of quantum mechanics), then one has to arrive immediately at the conclusion that the Pauli-Schrödinger equation **does not meet this requirement**. This equation only partially satisfies the postulates of (relativistic) quantum mechanics! It has, however, the big advantage that one can immediately prove that in the non-relativistic limit ($c \to \infty$) the Schrödinger equation is recovered, a fact which is less easy to see by inspecting the Dirac equation.

It is utterly important not to confuse the 'large component' $g_\kappa(r)$ in Equation (77) or for that matter $\langle \mathbf{r} | \phi_Q \rangle$ in Equation (75) with a corresponding solution of the Schrödinger equation: only in the limit of $c \to \infty$ can such a relationship be established.

8. A last remark

We all know that nowadays nearly all calculations in solid state physics are performed using Density Functional Theory (DFT), in particular local DFT. For a magnetic system the Kohn-Sham-Dirac Hamiltonian is given by

$$\mathcal{H}(\mathbf{r}) = c\boldsymbol{\alpha} \cdot \mathbf{p} + (\beta - I_4)c^2 + V^{\mathrm{eff}}(\mathbf{r}) I_4 + \beta \Sigma_z B_z^{\mathrm{eff}}(\mathbf{r}), \tag{82}$$

where $V^{\mathrm{eff}}(\mathbf{r})$ is the effective potential, $B_z^{\mathrm{eff}}(\mathbf{r})$ the effective exchange field and

$$\Sigma_z = \begin{pmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{pmatrix}. \tag{83}$$

Because LDFT provides $B_z^{\mathrm{eff}}(\mathbf{r})$ only with respect to a fictitious z-axis, in order to evaluate anisotropy energies for example, it is necessary to 'rotate' $\mathcal{H}$

$$S(R)\mathcal{H}(R^{-1}\mathbf{r})S^{-1}(R) = \mathcal{H}'(\mathbf{r}), \tag{84}$$

where $S(R)$ is a 4×4 matrix transforming the Dirac matrices α_i, β, and Σ_i. Since β is a real matrix, it can be shown [10] that $S(R)$ is of block-diagonal form,

$$S(R) = \begin{pmatrix} U(R) & 0 \\ 0 & \det[\pm] U(R) \end{pmatrix}, \tag{85}$$

where $U(R)$ is a (unimodular) 2×2 matrix and $\det[\pm] = \det[D^{(3)}(R)]$ is the determinant of $D^{(3)}(R)$, the latter one being the representation of R in R_3. Clearly enough by such a transformation not only $\beta \Sigma_z B_z^{\mathrm{eff}}(\mathbf{r})$ is transformed but also $c\boldsymbol{\alpha} \cdot \mathbf{p}$.

On the other hand considering a two-component formulation

$$\mathcal{H}(\mathbf{r}) = -\nabla^2 I_2 + \Xi + V^{\mathrm{eff}}(\mathbf{r}) I_2 + \sigma_z B_z^{\mathrm{eff}}(\mathbf{r}), \tag{86}$$

where for matters of simplicity Ξ contains all relativistic correction terms, one easily can see that of course ∇^2 is unaffected by any rotation in spin space. This implies that by using a Kohn-Sham-Dirac operator the kinetic energy part is properly transformed (a special case of Lorentz group invariance), while in a two-component formulation it is not. Of course the Pauli-Schrödinger and the Dirac Hamiltonian do have different spectra.

9. Summary

The formal deficiencies of the Pauli-Schrödinger equation discussed above were in the past always my main arguments for insisting on using directly the Dirac equation and not some alternative two-component descriptions. Clearly, many more things can be said about the Dirac equation, see for example [6,10].

Nowadays – it seems – things have changed for very practical reasons as it is much easier to use the Dirac equation in actual calculations than fiddling around with the spin–orbit term in the Pauli-Schrödinger equation. The theoretical description of anisotropic magnetic properties of magnetic nanostructures, even of domain walls, would not have been possible without this numerical advantage!

To my great satisfaction the use of the time-dependent Dirac equation in the presence of an external electromagnetic field and of the concept of the so-called polarization operator led very recently [15] to a quantum mechanically correct identification of spin currents, spin-transfer, and spin-Hall effects, which in turn will hopefully lead to a completely new stage in spintronics!

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Notes

1. For a discussion of classical relativistic dynamics see, e.g. the book by Messiah [6].
2. This is exactly the algebra of creation and annihilation operators for fermions.
3. Because of the block-diagonal form of the Dirac matrix β.

References

[1] R.P. Feynman, *Six-Not-So-Easy Pieces*, Perseus Books, Cambridge, Massachusetts, 1997.
[2] P.A.M. Dirac, Proc. Roy. Soc. A117 (1928) p.610.
[3] P.A.M. Dirac, Proc. Roy. Soc. A126 (1930) p.360.
[4] P.A.M. Dirac, *The Principles of Quantum Mechanics*, Oxford University Press, Oxford, first edition 1930, paperback 1981.
[5] W. Pauli, *Die allgemeinen Prinzipien der Wellenmechanik*, Handbuch der Physik, Springer-Verlag, Berlin, 1933.
[6] A. Messiah, *Quantum Mechanics*, North Holland Publishing Company, Amsterdam, 1969.
[7] F. Rosicky, P. Weinberger and F.J. Mark, Phys.: Molec. Phys. 9 (1976) p.2971.
[8] E.M. Rose, *Relativistic Electron Theory*, John Wiley, New York, 1961.
[9] J.D. Bjorken and S.D. Drell, *Relativistic Quantum Mechanics*, McGraw Hill, New York, 1964.

[10] L.D. Landau and E.M. Lifschitz, *Lehrbuch der Theoretischen Physik,* Band IV, *Relativistische Quantentheorie*, Akademie Verlag, Berlin, 1980.
[11] L. Jansen and M. Boon, *Theory of Finite Groups. Applications to Physics*, North Holland Publishing Company, Amsterdam, 1967.
[12] S.L. Altmann, *Induced Representations in Crystals and Molecules*, Academic Press, New York, 1977.
[13] S.L. Altmann, *Rotation, Quaternions and Double Groups*, Oxford University Press, Oxford, 1986.
[14] I.V.V. Raghavaryulua and N.B.J. Menon, Math. Phys. 11 (1970) p.3055.
[15] A. Vernes, B.L. Gyorffy and P. Weinberger, Phys. Rev. B 76 (2007) p.012408.