On the linear forms of the Schrödinger equation

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Abstract

Generalizing the linearisation procedure used by Dirac and later by Lévy-Leblond, we derive the first-order non-relativistic wave equations for particles of spin 1 and spin 3/2 starting from the Schrödinger equation.

By the introduction in the momentum of a correction linear in coordinates, we establish the wave equation of the radial harmonic oscillator with spin-orbit coupling.

1 Introduction

The standard procedure to derive the Dirac’s free particle equation \(^1\) is based on the search of linear relation between momentum and energy starting from Klein-Gordon equation. Making use of the Dirac idea, Lévy-Leblond \(^2\) performed such linearization procedure for the Schrödinger equation and established a linear equation in both momentum and energy which leads to the Pauli equation with the correct value of the Landé \(g\) factor. A generalisation of such equation was realised for higher spin particles using the Bargmann-Wigner method in Galilean Relativity and the Galilei-invariant wave equation \(^3\), \(^4\) and \(^5\). In \(^5\) Hurley has proposed, in a rigorous and sophisticated manner, a Galilean higher spin wave equation. Using the Galilei group and from general invariance assumptions, the author has established a first-order wave equation with \((6s + 1)\) components for spin-s particles which admits a consistent quantum-mechanical interpretation.

In this work, we are interested by the question of why the Dirac and Lévy-Leblond linearization algebraic procedure leads only to spin 1/2 wave equation. Is it possible to generalise this method to obtain wave equations for particles of spin greater than 1/2.

On the other hand, we focus on the non-relativistic harmonic oscillator. The Schrödinger’s equation for this system involves a quadratic potential in coordinates and it’s seems natural in the context of first-order equations to search a linear potential describing this system. Such problem has been studied in relativistic quantum mechanics. The Dirac oscillator system \(^6\)-\(^9\) leads to the standard harmonic oscillator in the non-relativistic limit, the Duffin-Kemmer-Petiau oscillator \(^10\)-\(^17\) is a generalisation to spin zero and one particles. This task has been realised in the framework of the five dimensional Galilean covariance in \(^18\) and \(^19\).
Our purpose in this work is of double interest: the first is the generalisation of the Dirac and Lévy-Leblond procedure to spin 1 and spin 3/2 particles. The obtained equations are not new but coincide with those established by Hurley. In the present paper, the derivation of the wave equation is achieved without referring to Galilean invariance and group theoretical techniques and it’s based on the linearization concept. The second goal is to introduce in these wave equations a linear potential in coordinate which leads to the standard non-relativistic harmonic oscillator plus the spin-orbit coupling for spin 1/2, 1 and 3/2 particles.

2 Linearisation

In the Schrödinger equation, the presence of the energy operator $E$ is linear while the momentum $p$ appears quadratically in the Hamiltonian. To eliminate this asymmetry between the time ($\partial/\partial t$) and spaces variables ($\partial/\partial x$), we require that the wave equation must be of first order in all derivatives. This leads to put the wave equation in the form

$$(AE + B \cdot p + C) \psi = 0 \quad (1)$$

here $A$, $B$ ($B_1, B_2, B_3$) et $C$ is a set of five operators with no dependence on $E$ and $p$ and which have to be determined. If we act on the left of (1) with the operator

$$A' E - B \cdot p + C'$$

where $A'$ and $C'$ are a two new numerical matrices, we find

$$(A'AE^2 + (A'B_i - B_i A)p_i E + (A'C + C'A) E - B_j B_i p_j p_i + (B_i C - C'B_i) p_i + C'C) \psi = 0 \quad (3)$$

the repeated indices are summed over $i, j = 1, 2, 3$. If we now impose on (3) to be identical to Schrödinger’s equation

$$(2mE - p^2) \psi = 0 \quad (4)$$

the following relations must be satisfied

$$A' A = C'C = 0, \quad A'B_i - B_i A = 0, \quad (5)$$
$$A'C + C'A = 2m, \quad C'B_i - B_i C = 0, \quad (6)$$
$$B_j B_i p_j p_i = p^2. \quad (7)$$

Let us note that there is 7 unknown operators to be found $A$, $B_i$, $C$, $A'$ and $C'$ unlike ten operators in the case of Lévy-Leblond procedure. We will see in the next sections that the expressions and dimensions of these numerical matrices are related to the spin of the particle.

3 Particle of spin 1/2

We start by solving the last set of algebraic equation in the spin 1/2 case and we will reproduce the Lévy-Leblond equation by a way which could be generalised to spin greater than one-half. The $\sigma_i$ Pauli matrices obey the identity

$$\sigma_i \sigma_j p_i p_j = (p_i)^2 1_{2 \times 2}. \quad (8)$$
where $1_{2 \times 2}$ is a $2 \times 2$ unit matrix. Comparing (7) and (8), it is straightforward to show that $B_j \neq \sigma_j$, because otherwise the second equation in (8) would lead to $A' = A$ which contradicts the first conditions in (5). We look for operators $B_i$ depending on $\sigma_i$ solutions of (7). Since in (8) there is a product of two $\sigma_i$ matrices with different indices $i$ and $j$, we choose the form

$$B_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix},$$

which leads to (7). The determination of $B_i$ makes the task easier for the rest of the operators. Indeed, using (5) and (6), one obtains

$$\left( A' + \frac{C'}{2m} \right) B_i = B_i \left( A + \frac{C}{2m} \right), \quad i = 1, 2, 3$$

(10)

$$\left( A' + \frac{C'}{2m} \right) \left( A + \frac{C}{2m} \right) = 1,$$

(11)

here 1 is the unit matrix. Taking into account (9), we see that is sufficient to put $A + \frac{C}{2m}$ equal to 1. Combined to the first equation in (5), this leads in one hand to $A' + A = C'/2m + C/2m = 1$ and on the other hand to $A = \frac{C'}{2m}$ and $A' = \frac{C}{2m}$. The following solutions are then obtained

$$A = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, C = 2m \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$  

(12)

The wave function $\psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix}$ is now a four components object where $\varphi$ and $\chi$ are two-component spinors. Finally, the first order wave equation is written as

$$\left[ \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} E + \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix} \cdot \pmb{p} + 2m \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \right] \psi = 0,$$

(13)

which is nothing else but the Lévy-Leblond equation reproduced here in a different way. The Clifford algebra doesn’t appear as in the original paper of this author. However, we will see in the next sections devoted to the spin 1 and 3/2 particles that this method can be easily generalized.

Now, we will introduce in (13) the harmonic oscillator potential. We seek some expression that should be linear in $\pmb{r}$ and leading to the three-dimensional harmonic oscillator. We choose the substitution

$$\pmb{p} \rightarrow \pmb{p} - im\omega \eta \pmb{r},$$

(14)

where $\omega$ denote the frequency of the oscillator, $\pmb{r}$ the position vector ($\pmb{r} \equiv x_i$) and $\eta$ is a matrix equal to $2A^2 - 1$. The motion equation for this system becomes

$$(A E + \eta \cdot (\pmb{p} - im\omega \eta \pmb{r}) + C) \psi = 0,$$

(15)

which turns into a coupled system of equations for the components $\varphi$ and $\chi$

$$2m \chi = -\sigma \cdot (\pmb{p} - im\omega \pmb{r}) \varphi$$

(16)

$$E\varphi = -\sigma \cdot (\pmb{p} + im\omega \pmb{r}) \chi,$$

(17)
multiplying (16) by $\sigma (p + im\omega r)$ and using (17) and the identity

$$\sigma_i \sigma_j = \delta_{ij} + i\varepsilon_{ijk}\sigma_k$$

we obtain the wave equation for the $\varphi$ component

$$E\varphi = \left[ \frac{p^2}{2m} + \frac{1}{2}m\omega^2 r^2 - \frac{3}{2}\frac{\hbar}{\hbar} (L.s) \right] \varphi,$$

(18)

where

$$s = \frac{\hbar}{2}\sigma, \quad L = r \times p.$$

Equation (18) corresponds to the standard harmonic oscillator with the addition of the spin-orbit coupling. This result is in agreement with that obtained by the non relativistic limit of the Dirac oscillator [6].

4 Particle of Spin 1

The problem is to construct the five unknown operators $A$, $B_i$ and $C$ obeying conditions (5) to (7) for a such particle. Following an approach similar to the one used above for spin 1/2, we start by solving (7). The $B_i$ operators in this case, should contain the 3×3 spin one matrices which are given in the standard representation by

$$(s_i)_{jk} = -i\hbar\varepsilon_{ijk}$$

(20)

$\varepsilon_{ijk}$ being the totally antisymmetric Levi-Cevita symbol. Inserting the identity $-i\hbar^{-1}(s.p)u = p \times u$ where $u = (u_1, u_2, u_3)$ is a vector field, into the well-known vector identity $\nabla (\nabla \cdot u) - \nabla \times (\nabla \times u) = \Delta u$ leads to a relation between the square of the momentum and the three components of the spin operator, i.e.

$$\hbar^{-2} (N_j N_i^T + s_j s_i) p_j p_i = p^2 1_{3 \times 3}$$

(21)

where $N_i^T$ denote the transposed matrix of $N_i$ which is a 3×3 matrix defined by

$$N_i = \hbar \left( \begin{array}{ccc} e_i^T & 0_{3 \times 1} & 0_{3 \times 1} \\ 0_{3 \times 1} & 0_{3 \times 1} & 0_{3 \times 1} \end{array} \right)$$

(22)

with

$$e_1 = (1 \ 0 \ 0), \quad e_2 = (0 \ 1 \ 0), \quad e = (0 \ 0 \ 1).$$

(23)

In the same way as in the spin 1/2 case, one may write for the $B_i$ matrices

$$B_i = \hbar^{-1} \left( \begin{array}{ccc} 0 & N_i & s_i \\ N_i^T & 0 & 0 \\ s_i & 0 & 0 \end{array} \right),$$

(24)

Thus, from (24) one obtains

$$B_j B_i p_j p_i = \hbar^{-2} \left( \begin{array}{ccc} N_j N_i^T + s_j s_i & 0 & 0 \\ 0 & N_j^T N_i & 0 \\ 0 & s_j s_i & s_j s_i \end{array} \right) p_j p_i.$$

(25)
The non diagonal terms are zero

\[(N^T_j p_j) (s_i p_i) = (s_j p_j) (N_i p_i) = 0\]  \hspace{1cm} (26)

but the diagonal elements are different from zero and consequently equation (7) is not satisfied. This is due to the presence in (21) of an additional term contrary to equation (8) for the spin 1/2 case. Imposing in the identification procedure that the spinor \(\psi\) must be included, the condition (7) becomes after acting on \(\psi\) as

\[B_j B_i p_j p_i \psi = p^2 \psi.\]  \hspace{1cm} (27)

In the present case, the wave function \(\psi\) is a three components object given by

\[\psi = \begin{pmatrix} u \\ v \\ w \end{pmatrix} \text{ with } u = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix}, v = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} \text{ and } w = \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix}.\]  \hspace{1cm} (28)

It is straightforward to show that (27) is satisfied when

\[p \cdot w = 0\]  \hspace{1cm} (29)

\[v \equiv v(v_1, v_2 = 0, v_3 = 0).\]  \hspace{1cm} (30)

This equations means that the third component of \(\psi\) has a zero divergence and that the second must be a scalar. We will see that these conditions will be automatically fulfilled when the remaining operators \(A\) and \(C\) will be determined. Using (24) and in an analogous way as in the spin one half, one can easily obtain the numerical expressions of these matrices. Thus, the first-order free wave equation for spin one particle takes the form

\[
\begin{pmatrix}
1 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{pmatrix}
E - i \begin{pmatrix}
0 & N & s \\
N^T & 0 & 0 \\
s & 0 & 0
\end{pmatrix}
\nabla + 2m \begin{pmatrix}
0 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{pmatrix}
\psi = 0,
\]  \hspace{1cm} (31)

where \(N = (N_1, N_2, N_3)\). Separating the components, one immediately verifies the relations (29) and (30). Since the matrices \(N^T\) have two rows composed entirely of zeros, (31) can be reduced to an equation with \(6s + 1 = 7\) components and then coincides with the wave equation established by Hurley [5] using a different approach centered on the Galilean invariance.

We now examine the harmonic oscillator problem. We introduce this potential via the following substitution

\[p \to p - im\omega r,\]  \hspace{1cm} (32)

where the matrix \(\eta\) is given now by

\[\eta = 2A^2 - 1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.\]  \hspace{1cm} (33)

Equation (31) can be decomposed into a set of the coupled equations

\[
\begin{align*}
Eu &= -\hbar^{-1}[N(p + im\omega r)v + s(p + im\omega r)w] \\
2mv &= -\hbar^{-1}N^+(p - im\omega r)u \\
2mw &= -\hbar^{-1}s(p - im\omega r)u,
\end{align*}
\]  \hspace{1cm} (34)

where

\[N = (N_1, N_2, N_3).\]
thus the wave equation for the field $u$ is given by

$$2mE u = \hbar^{-2} \left[ (N, p^+) (N^+ p^-) + (s, p^+) (s, p^-) \right] u \quad (35)$$

where $p^\pm = p \pm i m \omega r$. From the definitions (20) and (22), one readily shows that $N_i$ and $s_i$ verify

$$N_i N^+_j + s_is_j = i \hbar \varepsilon_{ijk} s_k + \frac{\hbar^2}{2} \delta_{ij}. \quad (36)$$

With the help of the above relation, the evaluation of (35) yields

$$E u = \left[ \frac{p^2}{2m} + \frac{1}{2} m \omega^2 r^2 - \frac{3}{2} \hbar \omega - \frac{\omega}{\hbar} (L, s) \right] u \quad (37)$$

which describes the usual isotropic harmonic oscillator plus the spin-orbit interaction with the strength $(-\omega/\hbar)$. Let us note that this strength is one half that obtained for spin 1/2 case and it’s coincides with the non relativistic limit of the DKP oscillator [10] and that obtained in the framework of the five dimensional Galilean covariance [19].

### 5 Spin 3/2 particle

For such particle, we will adopt the following matrix representation for the components of spin operator $s$

$$s_1 = \hbar \begin{pmatrix} 0 & \frac{1}{2} \sqrt{3} & 0 & 0 \\ \frac{1}{2} \sqrt{3} & 0 & 1 & 0 \\ 0 & 1 & 0 & \frac{1}{2} \sqrt{3} \\ 0 & 0 & \frac{1}{2} \sqrt{3} & 0 \end{pmatrix}, s_2 = \hbar \begin{pmatrix} 0 & -i \frac{1}{2} \sqrt{3} & 0 & 0 \\ i \frac{1}{2} \sqrt{3} & 0 & -i & 0 \\ 0 & i & 0 & -i \frac{1}{2} \sqrt{3} \\ 0 & 0 & i \frac{1}{2} \sqrt{3} & 0 \end{pmatrix}, s_3 = \hbar \begin{pmatrix} \frac{3}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{3}{2} \end{pmatrix}. \quad (38)$$

We seek the $B_i$ solutions of (7) containing the hermitian matrices $s_i$. We introduce the $4 \times 2$-matrices $K_i$ and their $2 \times 4$ hermitian conjugates $K_i^+$ defined by [20]

$$K_i^+ = \hbar \begin{pmatrix} -\sqrt{\frac{2}{3}} & 0 & \sqrt{\frac{1}{2}} & 0 \\ 0 & -\sqrt{\frac{2}{3}} & 0 & \sqrt{\frac{1}{2}} \\ \sqrt{\frac{2}{3}} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, K_2^+ = \hbar \begin{pmatrix} -i \sqrt{\frac{2}{3}} & 0 & -i \sqrt{\frac{1}{2}} & 0 \\ 0 & -i \sqrt{\frac{2}{3}} & 0 & -i \sqrt{\frac{1}{2}} \\ i \sqrt{\frac{2}{3}} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, K_3^+ = \hbar \begin{pmatrix} 0 & \sqrt{\frac{2}{3}} & 0 & 0 \\ \sqrt{\frac{2}{3}} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \quad (39)$$

The $K_i$ and $s_i$ matrices and the components of the the momentum $p$ obey the relation

$$(4/9) \hbar^{-2} (K_j K_i^+ + s_j s_i) p_j p_i = p^2 1_{4 \times 4}. \quad (40)$$
Since the previous equation is similar to (21), one can take the form given by (24) where \( N_i \) and \( \hbar \) are replaced by \( K_i \) and \( 3\hbar/2 \). As in the spin one case, we find that the \((6s + 1) \times (6s + 1)\) following matrix

\[
B_j B_p p_i = (4/9) \hbar^{-2} \begin{pmatrix} K_j K_i^+ + s_i s_i & 0 & 0 \\ 0 & K_i^+ K_i & K_j^+ s_i \\ 0 & s_j K_i & s_j s_i \end{pmatrix} \ p_j p_i, \tag{41}
\]

is not equal to \( p^2 \) and therefore (4) is not satisfied. Again, the requirement that the wave function must be taken into account leads to (27), where now \( \psi \) is a ten-component object

\[
\psi = \begin{pmatrix} \varphi \\ \Omega \\ \chi \end{pmatrix}, \tag{42}
\]

here \( \varphi \) and \( \chi \) are four-component and \( \Omega \) is a two-component functions. Equation (27) yields for the spin 3/2 particle

\[
(4/9) \hbar^{-2} \left[ (K_j p_j) \left( K_i^+ p_i \right) + (s_j p_j) (s_i p_i) \right] \varphi = p^2 \varphi, \tag{43}
\]

\[
(4/9) \hbar^{-2} \left( K_j^+ p_j \right) \left( K_i p_i \right) \Omega + (s_j p_i) \chi = p^2 \Omega, \tag{44}
\]

\[
(4/9) \hbar^{-2} (s_j p_j) \left( K_i p_i \right) \Omega + (s_i p_i) \chi = p^2 \chi. \tag{45}
\]

The first equation is obvious and the last two equations leads to conditions on the components of the wave function

\[
\Omega = - (2\alpha/3) \left( K_i^+ p_i \right) \varphi \tag{46}
\]

\[
\chi = - (2\alpha/3) (s_i p_i) \varphi, \tag{47}
\]

where \( \alpha \) is a constant to be determined. The last step is to construct the \( A \) and \( C \) matrices consistent with the two previous equations. We proceed with a method different to the one used in the previous cases and without using (5) to (7) deduced from the linearization procedure. Taking into account the expression of \( B_i \) and (32), the resolution of equation

\[
B_i p_i \psi = -(AE + C) \psi, \tag{48}
\]

subject to the constraints (16), (17) and (1), we find that \( A \) and \( C \) are given by expressions similar to that of spin one case with the appropriates dimensions and the \( \alpha \) constant is given by \( \alpha = (2m\hbar)^{-1} \). Finally, the \((6s + 1)\) components first-order wave equation for this particle is given by

\[
\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} E + (3\hbar/2)^{-1} \begin{pmatrix} 0 & K & s \\ K^+ & 0 & 0 \\ s & 0 & 0 \end{pmatrix} p + 2m \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \psi = 0. \tag{49}
\]

This result coincides with the Hurley’s equation [5] for spin 3/2 particle.

For the harmonic oscillator problem, again we perform the substitution \( p \rightarrow p - i\omega \eta r \) with \( \eta = 2A^2 - 1 \). The decomposition of the wave equation into its components and the elimination of \( \Omega \) and \( \chi \) in favour of \( \varphi \) gives

\[
2mE \varphi = (4/9) \hbar^{-2} \left[ (K^+ p_+) \left( K_+ p_- \right) + (s p_+) \left( s p_- \right) \right] \varphi \tag{50}
\]
with the help of the property [20]

\[ K_i K_j^+ + s_i s_j = i (3\hbar/2) \varepsilon_{ijk} s_k + (9\hbar/4) \delta_{ij} \]  

(51)

obtained using the definitions (38) and (39), the evaluation of the right-hand side of (50) yields

\[ E\phi = \left[ \frac{p^2}{2m} + \frac{1}{2} m\omega^2 r^2 - \frac{3}{2} \hbar \omega - \frac{2\omega}{3\hbar} (L.s) \right] \phi, \]  

(52)

which corresponds to the isotropic harmonic oscillator plus the spin-orbit coupling whose strength is one third to the one obtained for spin 1/2 case.

6 Conclusion

A new method is presented based on the linearization of the wave equation which allow us to deduce the first order equations for non-relativistic particles of spin 1/2, 1 and 3/2. Requiring that the wave function \( \psi \) must be taken into account in the set of relations (5) to (7), we were able to construct the operators \( A, B_i, C \) for particles of spin 1 and spin 3/2. This requirement is no longer necessary for a particle of spin 1/2 and the resolution of the previous set of equations leads then to the particular solution established by Lévy-Leblond.

In addition, we considered the problem of the harmonic oscillator in the framework of linear wave equations and we were able to find the standard wave equations plus the terms giving the spin-orbit coupling in each case.

The method presented in this paper can be generalized to the case of a non-relativistic (and relativistic) particle of arbitrary spin as well as that of a spinless particle (works in progress).

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