An introduction to Relativistic Quantum Mechanics: a round trip between Schrödinger and Dirac equations

Patricio Robles

Abstract— **This paper presents an introduction to Dirac's theory addressed to students who are beginning a postgraduate program in physics and which have acquired a suitable grounding in quantum physics and special relativity theory at the level of standard text books related with these topics. The aim of this article is to bring the concepts of relativistic quantum mechanics closer to these students as an introduction and motivation for research in current and future applications, such as those related with spintronics, positron emission devices and quantum information technology.**

Index Terms— **Electron, Hamiltonian, Lorentz transformations, relativistic energy, wave function.**

I. Introduction

In undergraduate levels of physics careers students acquire basic groundings in special relativity theory and non-relativistic quantum physics. Concerning with relativity theory they mainly learn the basic principles, Lorentz transformations, relativistic dynamics and equivalence between mass and energy [1]-[3]. In relation with non-relativistic quantum physics the main topics they learn are the wave-particle duality of light and particles like electrons, the Schrödinger's equation and its applications for some typical situations which can be studied in one dimension (for example the quantization of the energy in an infinite potential box and the corresponding wave functions). The model of the atom is described by means of the solutions of Schrödinger's equation in spherical coordinates and explaining how they lead to the quantum numbers associated with energy, angular momentum magnitude and its projection in the *z* direction [4]. The concept of spin is briefly introduced in the context of Stern-Gerlach experiment and its orientation is related with a fourth quantum number for the quantum description of the atom [5]-[6]. A rough description of the spin is given by an analogy with an intrinsic angular momentum of a particle. Due to restrictions in the duration of these careers it is not possible to include topics related with relativistic quantum mechanics, so that a knowledge about Dirac's theory and some of its issues like antiparticles and a formal justification of the spin property, are out of the scope of students of these careers unless they become incorporated to a postgraduate program which includes at least a course on Quantum Mechanics and its applications. Nevertheless the current technological developments in electronic systems imply an increasing requirement that future physics researchers related with this area acquire the basic tools for getting a deeper knowledge of issues like positrons and the spin of a particle like an electron, which require at least of a basic understanding of Dirac theory. This will allow them to get a better understanding of effects like magnetic nuclear resonance [7]-[8] and positron emission tomography devices [9]-[10] widely applied in nuclear medicine, among some actual technological applications, and also analyze technological innovation process like that associated to spintronics [11]-[12] and quantum information science [13]-[14]. The main objective of the present article is to give a conceptual introduction to Dirac's theory using mathematical tools at an undergraduate level and emphasizing in the physical aspects involved. Even though the material here presented may be found in several textbooks and publications online accessible by internet, it is difficult and time consuming for the students to get an introduction as that given in this article. For reaching this goal the article is organized as follows. Section II presents a pedagogical link between Schrödinger and Dirac equations. In fact, arguments are given for incorporating in Schrödinger's equation a term associated with spin so that the non-relativistic Pauli's equation is obtained. Then a simplified derivation of Dirac's equation is presented for the one dimensional case of a free particle moving in only one direction. In section III Dirac's equation is analyzed discussing the negative energy solutions and how the spin property is included. In particular the non-relativistic limit of this equation is studied verifying that it corresponds to Pauli's equation, so that a round trip between these equations is presented for helping students to integrate their learning of Quantum Mechanics and Relativity Theory. Section IV contains a brief discussion of the Zitterbewegung effect ("trembling motion") which Schrödinger predicted when he analyzed the time dependence of the expectation value of the position of a free particle according to Dirac's theory. In section V some numerical examples are presented. One of them shows the Zitterbewegung effect due to the interference between two wave packets representing a pair particle-antiparticle. The second example shows a comparison between bound sates energies obtained from Dirac and Schrödinger equations, discussing the differences.

Patricio Robles, Electric Engineering Department, Pontifical Catholic University of Valparaíso, Chile, phone 56-32-2273696, Mobile No. 993380555

II. GOING FROM SCHRÖDINGER TO DIRAC'S EQUATION

A. Incorporating a term associated to spin in Schrödinger's equation

Introduction of spin in non-relativistic quantum mechanics looks as an ad hoc procedure, but here is done in this form as an approach for facilitating a better physical understanding of Dirac's theory. It must be taken into account that the correct meaning of spin requires the use of relativistic quantum field theory, what certainly is out of the scope of the present article.

Considering this context, this section presents a conceptual insight about the connection between Schrödinger and Dirac equations. First of all the relativistic expression for the energy of a particle without spin moving in an electromagnetic field is discussed, determining its non-relativistic limit. Then arguments are given for adding a term to Schrödinger's equation for including the interaction between the spin and a magnetic field, leading to an interpretation of Pauli's equation which can be seen as a link between Schrödinger and Dirac equations. In fact this link is illustrated in section III analyzing the non- relativistic limit of Dirac's equation.

The spin is an intrinsic property of particles that could be understood as an angular momentum and was postulated in 1925 by Uhlenbeck and Goudsmit [15]. The name spin for this property was given by Pauli and it is generally seen as a non- orbital intrinsic angular momentum of a particle like an electron which can be associated to a magnetic moment $\vec{\mu}_s$ according to the relation [16]-[17]

$$\vec{\mu} = g\frac{q}{2m}\vec{S} \tag{1}$$

In the above equation q and m are the electric charge and mass of the particle, respectively, $\vec{S}$ is the spin vector and g is the gyromagnetic ratio which for an electron has a value approximately equal to 2. Though this factor cannot be explained classically, in introductory courses to quantum physics an intuitive interpretation is sometimes given using a rough model which considers the above particle as an sphere with uniform distribution of charge and rotating with respect to an axes trough its center. Dividing the sphere in infinitesimal disks and integrating their contribution to the total magnetic moment, a value of approximately 2.2 is obtained. Nevertheless, attempts to consider the electron not as a point particle lead to contradictory results such as tangential velocity greater than the speed of light [18]. Therefore it is not pedagogic to induce such interpretation.

In presence of a magnetic field $\vec{B}$ the interaction energy between the spin magnetic moment and the magnetic field is

$$E_s = -\vec{\mu}_s \cdot \vec{B} = -\frac{q}{mc}\vec{S}\cdot\vec{B} \tag{2}$$

First, we consider a spinless relativistic particle subjected to an electromagnetic field described by a cuadrivector A_μ with time-like and space-like components ϕ and $\vec{A}$, respectively. According to [19] section 12.1 the total energy E is given by

$$E = \sqrt{\left(c\vec{P} - q\vec{A}\right)^2 + \left(mc^2\right)^2} + q\phi \tag{3}$$

where $\vec{P}$ is the conjugate momentum defined as in [20]

$$\vec{P} = \vec{p} + \frac{q}{c}\vec{A} \tag{4}$$

Equations (3) and (4) consider that due to the interaction with an electromagnetic field, the dynamics of a particle with charge q is described using the time derivative of the conjugate momentum $\vec{P}$ instead of the usual mechanical momentum $\vec{p} = m\vec{\upsilon}$. The components of the momentum are correctly defined as the derivatives of the Lagrangian with respect to the components of the velocity. With a magnetic field this results in Eq. (4) and use of Hamilton's equations with the Hamiltonian corresponding to the energy given by (3), leads to the Lorentz force equation $d\vec{p}/dt = q\left(\vec{E} + \vec{\upsilon}\times\vec{B}\right)$ for a particle of charge q moving with velocity $\vec{\upsilon}$ in an electromagnetic field with electric and magnetic field components $\vec{E}$ and $\vec{B}$, respectively. This is not possible if one uses the mechanical momentum $\vec{p}$ instead of the conjugate momentum $\vec{P}$.

In the non-relativistic limit $\left|c\vec{P} - q\vec{A}\right| = \left|c\vec{p}\right| << mc^2$ so that

$$E - q\phi = mc^2\left\{\frac{\left(c\vec{P} - q\vec{A}\right)^2}{m^2c^4} + 1\right\}^{1/2} \approx mc^2\left\{1 + \frac{1}{2}\frac{\left(c\vec{P} - q\vec{A}\right)^2}{m^2c^4}\right\}$$

$$= \frac{1}{2m}\left(\vec{P} - q\frac{\vec{A}}{c}\right)^2 + mc^2 \tag{5}$$

The first term of this last equation may be interpreted as the kinetic energy including the interaction with an external electromagnetic field. Since the kinetic energy must include the contributions of the translational motion (associated to the linear momentum $\vec{p}$) and in general, of an angular momentum $\vec{L} = \vec{r}\times\vec{P}$ with respect to some specific point, it is necessary to identify these contributions in (5). For that purpose let us consider a particle of charge q moving on a weak homogeneous magnetic field with a corresponding vector potential given by

$$\vec{A} = \frac{1}{2}\vec{B}\times\vec{r} \tag{6}$$

For a weak magnetic field the first term of (5) can be approached as

$$\frac{1}{2m}\left(\vec{P} - \frac{e}{c}\vec{A}\right)^2 \approx \frac{1}{2m}\left(\vec{P}^2 - \frac{e}{c}\vec{B}\times\vec{r}\cdot\vec{P}\right) = \frac{1}{2m}\left(\vec{P}^2 - \frac{e}{c}\vec{B}\cdot\vec{L}\right) \tag{7}$$

where $\vec{L} = \vec{r}\times\vec{P} \approx \vec{r}\times\vec{p}$ and $\vec{P}^2 \approx \vec{p}^2$. Therefore under this approach we recognize $\vec{L} = \vec{r}\times\vec{P}$ as the orbital angular momentum and (5) becomes

$$E = \frac{\vec{p}^2}{2m} - \frac{q}{2mc}\vec{L}\cdot\vec{B} + mc^2 + q\phi \tag{8}$$

Now, the expression for the energy of a particle in an external electromagnetic field looks more familiar since the first and third term of (8) represent the kinetic energy associated to the momentum $\vec{p}$ and the rest energy of the mass m, respectively. The second term represents the interaction energy of the angular momentum with the external magnetic field and the fourth corresponds to the interaction of the charge with the external electric field.

For including the spin property and its interaction with the considered electromagnetic field, the energy given by (2) is added to (8) resulting in the following expression for the energy measured with respect to the rest energy

$$E - mc^2 = \frac{\vec{p}^2}{2m} - \frac{q}{2mc}\left(\vec{L} + 2\vec{S}\right)\cdot\vec{B} + q\phi \tag{9}$$

The above expression may be associated with the Hamiltonian of the Pauli's equation [21]

$$i\hbar\frac{\partial\psi}{\partial t}=\left\{\frac{\hat{p}^2}{2m}-\frac{q}{2mc}\left(\hat{L}+2\hat{S}\right)\cdot\vec{B}+q\phi\right\}\psi \qquad (10)$$

In this last equation $\hat{p}$, $\hat{L}$ and $\hat{S}$ are the linear momentum, angular momentum and spin operators, respectively. As shown in [22] - [24] Pauli's equation is the nonrelativistic limit of Dirac's equation and in next subsection a simplified derivation of this equation is presented.

B. *A simplified derivation of Dirac's equation*

In this section a conceptual derivation of Dirac's equation is presented, beginning from the known relation between energy and momentum for a free relativistic particle of mass m propagating in the z direction with momentum of magnitude p

$$E^2=c^2p^2+\left(mc^2\right)^2 \qquad (11)$$

Dirac tried to obtain an equation linear with the first time derivative of the wave function ψ and compatible with (11) of the form [22]

$$i\hbar\frac{\partial\psi}{\partial t}=\hat{H}\psi \qquad (12)$$

with $\hat{H}$ being the hamiltonian operator.

For a free particle the operator $\hat{H}$ is constant, so that the temporal evolution of ψ is given by a factor $\exp[-i(E/\hbar)t]$. Therefore (12) becomes

$$E\psi=\hat{H}\psi \qquad (13)$$

Since the eigenvalues of $\hat{H}$ are the energy values and they are real, this operator must satisfy $\hat{H}^+=\hat{H}$ where $\hat{H}^+$ is the hermitean conjugate of $\hat{H}$ (the matrix resulting from transposing $\hat{H}$ and taking the conjugate complex of its elements). Therefore from (13) we have

$$\hat{H}^+\hat{H}\psi=E^2\psi \qquad (14)$$

Since (12) is linear in the time derivative, it appears natural to construct a hamiltonian operator also linear in the spatial derivatives, so that to consider time and space coordinates in a form more symmetric as compared with Schrödinger's equation. This is compatible with the relativistic expression for the energy given by (11) and allows to get its form invariant under Lorentz transformations. Therefore, following an approach similar to that used by Dirac the hamiltonian $\hat{H}$ is written in the form

$$\hat{H}=\alpha c\hat{p}+\beta mc^2 \qquad (15)$$

where $\hat{p}$ is the momentum operator given in this case by $\hat{p}=-i\hbar\partial/\partial z$, and α , β are elements such that a combination of (11), (14) and (15) leads to the conclusion that they must be matrices of dimension $n\times n$ and not ordinary numbers. In fact, after a little algebra one obtains that α and β must satisfy the following relations

$$\alpha^2+\beta^2=I$$
$$\alpha\beta+\beta\alpha=0 \qquad (16)$$

where I is the identity matrix. A dimensional analysis of (13) shows that the wave function ψ must be a column matrix of dimension $n\times 1$ called spinor. Since the eigenvalues of $\hat{H}$ are real, the first relation of (16) tells us that the eigenvalues of α and β must be real taking only values ± 1 . The dimensions of α and β can be determined as follows:

The second relation of (16) allows to write α as $\alpha=-\beta\alpha\beta^{-1}$. Considering that the trace of a matrix is the sum of its diagonal elements (corresponding to its eigenvalues for a matrix diagonalized using its eigenvectors) and considering that for any two matrices A and B, $Tr[AB]=Tr[BA]$, one obtains

$$Tr[\alpha]=-Tr\left[\beta\alpha\beta^{-1}\right]=-Tr[\alpha] \qquad (17)$$

This last equation implies that $Tr[\alpha]=0$. In a similar form it can be obtained that $Tr[\beta]=0$. Therefore from this result it can be deduced that each of these matrices must have as many positive and negative eigenvalues requiring that the dimension n be even.

For $n=2$ the only matrices $\alpha\neq\beta$ satisfying the first relation of (16) are the identity matrix and one of the Pauli matrices. Since it is considered that the particle is moving along the z direction, this last matrix should be σ_3 given by

$$\sigma_3=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} \qquad (18)$$

Nevertheless in this case it is not possible to satisfy the second relation of (16). Therefore matrices α and β must have dimensions 4×4 and according to the representation introduced by Dirac they are given by

$$\alpha=\alpha_3=\begin{pmatrix}0 & \sigma_3\\ \sigma_3 & 0\end{pmatrix} \qquad (19)$$

$$\beta=\begin{pmatrix}I_{2\times 2} & 0\\ 0 & -I_{2\times 2}\end{pmatrix} \qquad (20)$$

From this analysis the relativistic Dirac's equation in one dimension for a free particle moving in the z direction can be written as

$$i\hbar\frac{\partial\psi}{\partial t}=\left(c\alpha_3\hat{p}+mc^2\beta\right)\psi \qquad (21)$$

This equation can be generalized to three dimensions and including an electromagnetic field described by the cuadrivector A_μ , it can be written as follows

$$i\hbar\frac{\partial\psi}{\partial t}=\left(c\hat{\alpha}\cdot\left(\hat{p}+\frac{q}{c}\vec{A}\right)+q\phi+mc^2\beta\right)\psi \qquad (22)$$

In this last equation $\hat{p}$ is the operator $\hat{p}=-i\hbar\nabla$ and $\hat{\alpha}$ is a three-dimensional vector whose elements are matrices α_i with i=1,2,3. These numbers are associated to directions x, y and z, respectively, so that

$$\hat{\alpha} \cdot \hat{p} = \alpha_1 \hat{p}_x + \alpha_2 \hat{p}_y + \alpha_3 \hat{p}_z \tag{23}$$

Matrices α_1, α_2 and α_3 have dimensions 4×4 and are given in terms of Pauli matrices α_i by

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \tag{24}$$

III. ANALYSIS OF DIRAC'S EQUATION AND ITS SOLUTIONS

This section contains an analysis of Dirac's equation, starting by the solutions corresponding to a free particle and discussing how the negative values obtained for the energy can be associated to antiparticles. Next, it is discussed how the spin property can be explicitly seen from this equation if the particle is subjected to an electromagnetic field. For this purpose an analysis of the non-relativistic limit of Dirac's equation is presented verifying that this leads to Pauli's equation, where as shown by (10) a term related with spin becomes explicit.

A. *Solutions of Dirac's equation and Negative Energies*

The solutions of Dirac's equation for a free particle at rest are given by the eigenvalues and eigenvectors of the Hamiltonian operator given by (15) with $\hat{p} = 0$. From (15) and (20) it can be seen that there are two solutions with positive energy E_k equal to $+mc^2$, where $k = 1,2$; the other two solutions have negative energies denoted as E_{k+2} with a value equal to $-mc^2$. The corresponding eigenvectors of the Hamiltonian for $E > 0$ may be expressed as column matrices with elements $+\delta_{i,k}$ with $i = 1,2,3,4$ identifying the corresponding row. Similarly, for $E < 0$ the corresponding eigenvectors are expressed as column matrices with elements $-\delta_{i,k+2}$. For a free particle moving in the z-direction with momentum of magnitude p the eigenvalues of the Hamiltonian given by (21) correspond to solutions with positive and negative energies $E = \pm\sqrt{(cp)^2 + (mc^2)^2}$ and the solution of (21) is of the form

$$\psi = u(p) e^{-i(pz - Et)/\hbar} \tag{25}$$

Eqs. (19-21) lead to the following system of coupled equations

$$\sigma_3 c\hat{p} u_B = (E - mc^2) u_A \tag{26}$$

$$\sigma_3 c\hat{p} u_A = (E + mc^2) u_B \tag{27}$$

where u_A and u_B are columnn vectors of dimension 2×1 resulting from dividing the spinor $u(p)$ into two 2-component spinors. For the two solutions with $E > 0$ let us define $u_A = \eta^{(j)}$ where $j = 1,2$ is a superscript for labeling the two-component column matrices (called bispinors) associated to the orientation of spin, whose elements are given by $\delta_{i,j}$, so that $j = 1 (j = 2)$ corresponds to spin oriented in the $+z$ $(-z)$ direction and $i = 1,2$ identifies the corresponding rows.

From (27) one obtains

$$u_B = \frac{c\sigma_3 \hat{p}}{E + mc^2} \eta^{(j)} \tag{28}$$

Therefore, for the solutions with positive energy the spinors *u(p)* are given by

$$u^{(j)}(p) = N \begin{pmatrix} \eta^{(j)} \\ f(p)\eta^{(j)} \end{pmatrix} \tag{29}$$

In this last equation the function *f (p)* is defined as $f(p) = c\sigma_3 \hat{p} / (E + mc^2)$ and N is a normalization factor. For a reference frame where the particle is at rest, from (15) and (20) it can be seen that the two resulting spinors *u(p)* correspond to the solutions with positive energy $E = +mc^2$. Similarly, for the solutions with negative energy the spinors *u(p)* are given by

$$u^{(j)}(p) = N \begin{pmatrix} g(p)\eta^{(j)} \\ \eta^{(j)} \end{pmatrix} \tag{30}$$

where *g (p)* is defined as $g(p) = -c\sigma_3 \hat{p} / (|E| + mc^2)$.

Let us discuss the solutions given by (30) corresponding to negative energy values and considering the case of an electron. First of all it is very important to understand that negative energy solutions arise mathematically from Dirac's equation as has been discussed in the previous sections of this article, requiring a basis of four vectors for specifying the possible states of a particle like an electron (two states with positive energy and the other two with negative energy, each one with two possible orientations of the spin). In a paper of 1929, H. Weyl studied the relation of Dirac's theory with the General Relativity Theory, showing that there must be a mathematical link between an electron and a particle with the same mass but with opposite charge [25]. A few years later, C. Anderson analyzed the results of an experiment of photographing cosmic-rays tracks produced in a Wilson chamber, concluding that these tracks could be associated to particles with positive charge and with a mass of the order of magnitude of that corresponding to the electron. He gave to this kind of positive electron the name of positron [26]. One usually accepted interpretation of a negative energy solution is that it describes a particle which propagates backward in time or, equivalently, a positive energy antiparticle propagating forward in time [27]. Relativistic Quantum Mechanics predicts that every particle has a corresponding antiparticle with the same mass and spin but, for charged particles, with a charge (and other properties described by quantum numbers) with opposite sign. The antiparticle of the electron is called the positron. According to Dirac it is not possible to assert that the negative energy solutions represent positrons, as this would make the dynamical relations wrong [28]-[29]. For removing the possibility of a transition of a positive energy electron into an unphysical state of negative energy, Dirac defined a new concept of physical vacuum (known as Dirac sea), so that all the states with negative energies are completely filled. It should be possible to lift an electron out of the Dirac sea via a high energy gamma particle.

Then there would be a " hole " in the Dirac sea. If the original electron in the sea had momentum $\vec{p}$, energy $E=-\sqrt{c^2\vec{p}^2+(mc^2)^2}$ and charge $q=-|e|$, the hole would have momentum $-\vec{p}$, energy $E=+\sqrt{c^2\vec{p}^2+(mc^2)^2}$ and charge $q=+|e|$. The "hole" represents the antiparticle of the electron, with mass m_e and charge $+|e|$, and is called positron.

It is worthy to note that after redefining the concept of vacuum, Dirac made no attempt to find the positron wave function. In a relatively recent publication [30], Truebanbacher proposes a re-definition of the relativistic 4-momentum operator which allows to describe the positron by negative energy plane waves.

B. *Going from Dirac to Pauli's equation*

In the general expression for Dirac's equation given by (22) a term associated to spin is not explicitly shown. For students that are taking a first course in Relativistic Quantum Mechanics this could imply a difficulty for obtaining a suitable initial understanding of this theory. Nevertheless, Dirac's equation predicts the spin as an intrinsic property of a particle whose existence becomes observable by the coupling with an electromagnetic field through the charge of the particle [21- 22]. One way for making clearer the spin in Dirac's equation is the analysis of its non-relativistic limit as presented in this subsection, verifying that this leads to Pauli's equation, where a term related with spin is clearly specified as shown by (10). As discussed in previous subsection, Dirac's equation has solutions with positive and negative energy. Since in this case the particle is subjected to an electromagnetic field, the momentum is not constant as occurs for a free particle. Therefore, the elements of the spinor $u(\vec{p})$ are functions of the position and of the time, so that the solutions of (22) may be expressed as

$$\psi=\begin{pmatrix}\eta(\vec{r},t)\\ \rho(\vec{r},t)\end{pmatrix}\exp[-iEt/\hbar] \tag{31}$$

where $\eta(\vec{r},t)$ and $\rho(\vec{r},t)$ are column matrices (called bispinors) of dimension 2×1 associated with positive and negative energy solutions of Dirac's equation. Inserting this last equation in (22) leads to the following system of equations

$$E\eta+i\hbar\frac{\partial\eta}{\partial t}=c\vec{\sigma}\cdot\hat{P}\rho+q\phi\eta+mc^2\eta \tag{32}$$

$$E\rho+i\hbar\frac{\partial\rho}{\partial t}=c\vec{\sigma}\cdot\hat{P}\eta+q\phi\rho-mc^2\rho \tag{33}$$

In (32) and (33) $\hat{P}$ is the operator defined according to relation in Eq.(4) as $\hat{p}+\frac{q}{c}\vec{A}$.

In the non-relativistic limit the energy E is approximately equal to $+mc^2$ and the positive energy solutions predominate over the negative solutions, so that in this limit the term $i\hbar\frac{\partial\rho}{\partial t}$ may be neglected and for $q\phi << mc^2$ the following relation is obtained from (33)

$$\rho=\frac{\vec{\sigma}\cdot\hat{P}}{2mc}\eta \tag{34}$$

From (32) and (34) and using the identity $(\vec{\sigma}\cdot\vec{a})(\vec{\sigma}\cdot\vec{b})=\vec{a}\cdot\vec{b}+i\vec{\sigma}\cdot(\vec{a}\times\vec{b})$ valid for any two vectors $\vec{a}$ and $\vec{b}$, one obtains [23]

$$i\hbar\frac{\partial\eta}{\partial t}=\left(\frac{1}{2m}\hat{P}^2-\frac{\hbar q}{2mc}\vec{\sigma}\cdot\vec{B}\right)\eta \tag{35}$$

It must be noted that for obtaining (35) from the above vector identity, it has been considered that in this case $\vec{a}=\vec{b}=\hat{P}$ and since $\hat{P}$ contains the operator $\hat{p}$, the vector product $\vec{a}\times\vec{b}$ does not vanish as would be expected for two equal ordinary vectors. With $\hat{P}$ given by (4) the second term of (35) is obtained after some vector algebra, using the identity $\nabla\times(\eta\vec{A})=\eta\nabla\times(\vec{A})+\nabla\eta\times\vec{A}$ and considering that $\vec{B}=\nabla\times\vec{A}$.

With the usual definition of the spin operator as $\vec{S}=\hbar\vec{\sigma}/2$, (35) becomes

$$i\hbar\frac{\partial\eta}{\partial t}=\left(\frac{1}{2m}\hat{P}^2-\frac{q}{mc}\vec{\sigma}\cdot\vec{B}\right)\eta \tag{36}$$

A similar approach as that used for obtaining (8) from (5) allows to rewrite (36) as

$$i\hbar\frac{\partial\eta}{\partial t}=\left(\frac{1}{2m}\hat{p}^2-\frac{q}{2mc}(\hat{L}+2\hat{S})\cdot\vec{B}\right)\eta \tag{37}$$

The above equation is the Pauli's equation given by (10) for the case of electric potential $\phi=0$. Therefore this section has provided a conceptual way for incorporating spin and obtaining Pauli's equation, verifying that it corresponds to the non-relativistic limit of Dirac's equation. It is worthy to note that the solutions of Pauli and Dirac equations correspond to vectors with two and four components, respectively, instead of only scalar functions as is the case of Schrödinger's equation.

IV. CONSIDERATIONS ABOVE THE VELOCITY OF AN ELECTRON ACCORDING TO DIRAC'S EQUATION AND ZITTERBEWEGUNG

Dirac's equation successfully combines quantum mechanics with special relativity, providing the theoretical foundation of antiparticles and spin. Nevertheless this equation leads to some peculiar effects, such as Klein's paradox [31]-[32] and Zitterbewegung [33]-[36]. In this section a brief discussion about this last effect is presented and in section V a numerical example is shown. As known, in non-relativistic quantum mechanics the velocity operator is proportional to the momentum operator by means of the mass of the particle.
However in Dirac's theory the velocity is represented by an operator whose components have only eigenvalues $\pm c$ [37].

Schrödinger examined the time dependence of the position operator associated with Dirac's equation for a free particle and discovered a highly oscillatory microscopic motion which he called Zitterbewegung [38]. He noted that if a superposition of positive and negative energies states evolves in time according to the single particle Dirac's equation, then the time-dependent expectation value of the position operator shows oscillatory motion with velocity varying between $+c$ and $-c$, frequency $2mc^2/h \sim 10^{20}\ \mathrm{s}^{-1}$ and amplitude corresponding to the reduced Compton wavelength of the electron ($\sim 10^{-13}$ m) . These values still are practically impossible to direct observation with current technological capabilities. According to K. Huang [34] this effect may be described as a circular motion about the direction of the electron spin with a radius equal to the reduced Compton wavelength for the electron and its intrinsic spin may be considered as due to the orbital angular momentum of this motion. During last years some evidence of the Zitterbewegung effect has been obtained by experiments of electron channeling in crystals where the transmission probability shows a peak at the atomic row direction, result that is interpreted as an interaction with the Zitterbewegung frequency [35]. According to [39] and [40] manifestations of Zitterbewegung in crystalline solids have been observed with amplitudes of the order of $\hbar/m^*u$, where m^* is the effective mass at the band edge, $u=\sqrt{E_g/2m^*}$ and E_g being the energy gap. However as far as the author of the present paper knows, the origin of this effect is not yet clear and it is understood as due to the interference between the positive and energy solutions of Dirac's equation [41]. In [42] S.T. Park has derived an analytical solutions of Dirac wave packets to first order for a small momentum spread. He shows that the single-particle wave packet for a free electron does not exhibit any oscillatory motion, while for a superposition state corresponding for example to and electron and positron this motion is manifested.

V. NUMERICAL RESULTS

A. *Zitterwebegung due to interference of two wave packets*

In Figure 1 an illustration of the Zitterwebegung effect is shown by means of the expectation value of the position along the *z* axis of a mixed wave function corresponding to a pair particle-antiparticle according to (50) of [42] here reproduced as

$$\psi(z,t)=A_+\psi_+(z,t)+A_-\psi_-(z,t) \tag{38}$$

where ψ_+ and ψ_- are the wave functions of the particle and antiparticle with amplitudes A_+ and A_- respectively. For this case values $A_+=A_-=1/\sqrt{2}$ have been chosen. The oscillatory component of $\langle z(t)\rangle$ is shown for the superposition state of two wave packets with a value $p_0=0.97mc$ for the momentum at the center of each wave packet and considering three values of the momentum spread.

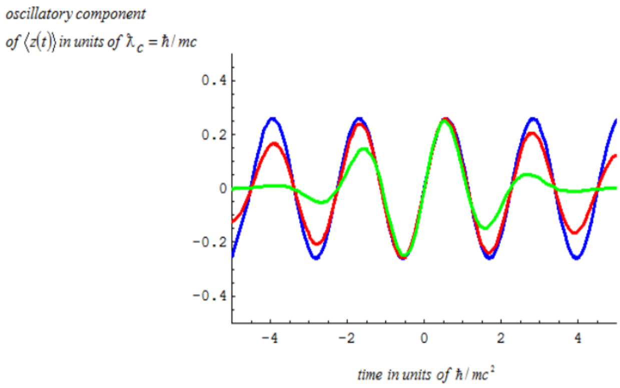

Fig. 1. Expectation value of the position along the z axis for a mixed wave function corresponding to a pair particle-antiparticle for three values of momentum spread: $\sigma_p=0.35mc$ (green curve), $\sigma_p=0.125mc$ (red curve), $\sigma_p=0.001mc$ (blue curve). The momentum at the center of each wave packet is $p_0=0.97mc$.

It can be seen that as σ_p decreases the longer is the duration of the oscillatory behavior. This can be explained as follows: from the Uncertainty Principle of Heisenberg the lower is the momentum spread the higher is the spatial extension of each wave packet. Since they travel in opposite directions, the duration of the interference effect increases.

B. *Transmission of a charged particle through a potential well and bound states*

As a second example, the behavior of a charged particle under the influence of a rectangular potential well of depth V_o and width a is studied, comparing results obtained using both the solutions of Dirac and Schrödinger equations. A one dimensional analysis is made considering the spatial variation along the x axis, so that this potential well is described as follows: $V(x)=0$ for x < *-a/2* and x > *+a/2* ; and $V(x)=V_o$ for *–a/2* < x < *+a/2* with $V_o<0$. The solutions using Dirac's equation are obtained imposing the requirement of continuity of the wave functions at the edges of the potential well, while in the nonrelativistic approach the requirement of continuity of the first derivative with respect to x must be added.

The solution of Dirac's equation leads to bound states for values of energy such as $mc^2-|V_o|<E<-mc^2$ [21]. These energies can also be numerically obtained using analytical expressions as those indicated in [43]. Similarly, the solution of Schrödinger's equation leads to bound states for $-|V_o|<E<0$. In this last case it is possible to identify even and odd solutions for the wave functions corresponding to bound states [44]. For even solutions $\psi(-x)=\psi(x)$ while for odd solutions $\psi(-x)=-\psi(x)$.

Figure 2 shows some of the energies corresponding to bound sates for a potential well of width $a=10\lambda_c/2\pi$ for different values of V_o. Values obtained using solutions of Dirac's equations are shown with red points. Black and blue points correspond to even and odd solutions of Schrödinger's equation, respectively.

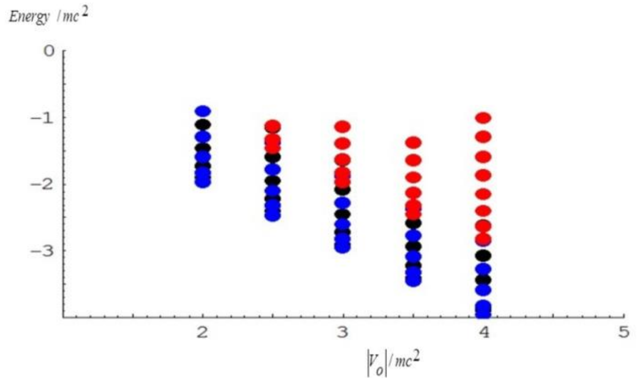

Fig. 2. Energies of the bound states of a rectangular potential well of width $a = 10\hbar / mc$ varying V_o . Values obtained using solutions of Dirac's equation are shown with red points. Black and blue points correspond to even and odd solutions of Schrödinger equation, respectively.

It can be observed that the non-relativistic approach gives bound states with energies more negative than those obtained from Dirac's equation, result compatible with the corresponding ranges for bound states.

As a complementary discussion, it is worthy to consider that the analysis presented in this subsection can be related with Klein paradox, whose physical essence lies in the prediction that according to the solutions of Dirac equation fermions can pass through large repulsive potentials without exponential damping. This is called Klein tunneling. As shown in [45] a Dirac particle of mass m and arbitrarily small momentum can tunnel without reflection through a potential barrier of height $+|V_o|$ if the potential well of depth $-|V_o|$ supports a bound state of energy $E = -mc^2$. This is called a supercritical potential well. In fact, this reference shows that Klein tunneling is a general feature of the Dirac equation: any potential well strong enough to support a supercritical state when inverted becomes a potential barrier which a fermion of arbitrarily low momentum can tunnel through without reflection. Since the relativistic Dirac's theory covers particle as well as antiparticle scattering, this implies that there are two distinct results considering that the zero momentum limit corresponds both to particles with energy $E = +mc^2$ and antiparticle states with $E = -mc^2$. The result that antiparticles can have transmission resonances when they scatter off potential well is equivalent to particles having transmission resonances when scattering off potential barriers.

VI. Conclusion

A pedagogical insight about Dirac's theory has been presented using a mathematical formalism at an undergraduate level with emphasis on the physical concepts involved and including some illustrative examples. A simplified way for obtaining Pauli's equation has been presented using a classical approach for the concept of spin. Then a conceptual derivation of Dirac's equation has been presented discussing how its non-relativistic limit leads to Pauli's equation. The solutions of Dirac's equation have been studied discussing how the concepts of spin, antiparticle and Zitterbewegung effect arises. These last two concepts are related since as discussed, up to now this last effect is usually interpreted as due to an interference between states of positive and negative energies, what is still a subject of research.

A comparison between the behavior of a particle in a potential well predicted from Dirac's equation, shows important differences in the values of energies for total transmission and bound sates, with respect to those obtained from Schrödinger's equation. Therefore conditions for using the non-relativistic approach must be carefully considered.

In addition to the pedagogical objective of this article, it aims at motivating future researchers to study in more detail effects here presented like Zitterbewegung obtaining the corresponding theoretical framework for a suitable explanation. Furthermore this author thinks that it is necessary an extension of a formalism as that of Dirac to the case of photons and bosons in general, obtaining an adequate wave function for describing their dynamics. In the case of photons several articles have been published on this topic but still is a matter that deserves further research.

Acknowledgment

The author thanks to Escuela de Ingeniería Eléctrica, Pontificia Universidad Católica de Valparaíso, for its support during the elaboration of this paper. I would like also to thank Dr. Roberto Rojas, Professor of Physical Department of Santa María University, for useful discussion and suggestions.

References

[1] H.D.Young, R. A. Freedman and L. Ford, "University Physics" Volumen 2, Pearson Addison-Wesley, 2007.
[2] P.A.Tipler and G. Mosca "Physics for Scientists and Engineers: Extended Version", W. H. Freeman, 2003.
[3] J. Dunningham, "Introductory Quantum Physics and Relativity", Imperial College Press, London, 2011.
[4] L.I.Shiff,_ "Quantum Mechanics", Mc Graw- Hill Book Company, N. York, St. Louis, San Francisco, London, Mexico, Sydney, Toronto, 1968.
[5] J.J.Sakurai, "Modern Quantum Mechanics", Addison-Wesley, N.York, 1980.
[6] B. Friedrich and D. Herschbach, "Stern and Gerlach: How a bad cigar helped reorient Atomic Physics", Physics Today Volume 53, 497 (2003).
[7] I.I. Rabi, J.R.Zacharias, S. Millman and P. Kush, "A new Method of Measuring Nuclear Magnetic Moment", Physical Review Volume 53, 318 (1938).
[8] J.A. Koutcher and C.T. Burst, "Principles of Nuclear Magnetic Resonance", Journal Nuclear Medicine. Volume 25, 101 (1984).
[9] A.K. Shuckla and U. Kumar, "Positron emission tomography: An overview", Journal Medical Physics Volume 31, 13 (2006).
[10] S. I. Ziegler, "Positron Emission Tomography Principles, Technology and Recent Developments", Nuclear Physics A Volume 752, 679 (2005).
[11] I. Zutic, J. Fabian and S. Das Sarma, "Spintronics: Fundamental and applications", Review Modern Physics Volumen 76, 323 (2004).
[12] S.A. Wolf, D.D. Awschalom, R.A. Burhman, J.M. Daughton, S.von Moln_ar, M.L. Roukes, A.Y. Chtchelkanova and D.M. Treger, "Spintronics: A Spin-based Electronics Vision for the Future", Science Volume 294, 1488 (2001).
[13] M.A.Nielsen and I.L.Chuang, "Quantum Computation and Quantum Information", ninth printing, Cambrigge University Press, Cambridge, 2007.
[14] Ch. H. Bennett, G. Brassard, C. Crpeau, R.Jozsa, A. Peres and W.K. Wootters, "Teleporting an unknown quantum state via dual classical and Einstein-Podolsky-Rosen channels", Physical Review Letters Volume 70, 1895 (1993).
[15] G.E. Uhlenbeck and S. Goudsmit, "Spinning Electrons and the Structure of Spectra" Nature Volume 117, 264 (1926).
[16] David J. Griffiths, "Introduction to Electrodynamics", first edition, Prentice-Hall Inc., Englewood Cliffs, New Jersey, 1981.

[17] J. Binney and D. Skinner, "The Physics of Quantum Mechanics", first edition, Oxford University Press, Oxford, 2014.
[18] L. J. Curtis, "Atomic Structure and Lifetime: A Conceptual Approach", first edition, Cambridge University Press, Cambridge, 2003.
[19] J.D. Jackson, "Classical Electrodynamics", third edition, John Wiley and Sons, New York 1998.
[20] Leonard Susskind "Quantum Mechanics, the theoretical mínimum", first edition, Basic Books, New York, 2014.
[21] W. Greiner, "Relativistic quantum mechanics - Wave Equations", third edition, Springer- Verlag Berlin, Heidelberg, New York, 2000.
[22] B. Thaller, "The Dirac Equation", first edition, Springer-Verlag Berlin, Heidelberg, New York, 1992.
[23] E. G. Harris, "A pedestrian approach to quantum field theory", first edition, Dover Publications, Inc., Mineola, New York, 2014.
[24] R.P. Feynman, "Quantum Electrodynamics", second edition, Addison-Wesley Publishing Company, Inc., Redwood, California, 1962.
[25] H. Weyl, "Gravitation and the Electron", Proceedings of the National Academy of Sciences of USA Volume 15, 323 (1929).
[26] C. D. Anderson, "The Positive Electron", Physical Review Volume 43, 491 (1933).
[27] R. P. Feynman, "The Theory of Positrons", Physical Review Volume 76, 749 (1949).
[28] P. A. M. Dirac, "A Theory of Electrons and Protons", Proc. Roy. Soc. A Volume 126, 360 (1930) .
[29] P. A. M. Dirac, "The principles of Quantum Mechanics", Oxford at the Clarendon Press, fourth edition, Oxford, 1962.
[30] E. Truebanbacher, "Dirac equation: the positron wave function and the relativistic energy momentum operators", American Journal of Modern Physics Volume 2, 38 (2013).
[31] S. D. Bosanac, "Solution of Dirac equation for a step potential and the Klein Paradox", Journal of Physics A : Mathematical Theory Volume 40, 84991 (2007).
[32] A. Hansen and R. Finn, "Klein's Paradox and its Resolution", Physica Scripta Volume 23, 1036 (1981).
[33] D. Hestenes, "Zitterbewegung in Quantum Mechanics", Found. Phys Volume 40, 1 (2010).
[34] K.Huang, "On the Zitterbewegung of the Dirac electron", American Journal of Physics Volume 20, 479 (1952).
[35] P.Catillon, M.J.Gaillard, R.Genre, M.Gouanre, R.G.Kirsch, J-C.Poizat, J.Remillieux, L.Roussel and M.Spighel, "A Searh for the de Broglie Particle Internal Clock by means of Electron Channeling", Found. Phys. Volume 38, 659 (2008).
[36] B.G. Sidharth, "Revisiting Zitterbewegung", Int. J. Theor. Physics Volume 48, 497 (2009).
[37] A.O. Barut and J. Bracken, "Zitterbewegung and the internal geometry of the electron", Physical Review D Volume 23, 2454 (1981).
[38] E. Schrödinger, "Sitzungsber" Press. Akad. Wiss. Phys. Math. K1 Volume 24, 418 (1930).
[39] W.Zawadzki and T.M.Rusin, "Zitterbewegung (trembling motion) of electrons in semiconductors: a Review", Physical Review A Volume 63, 053806 (2011).
[40] W.Zawadzki, "Electron Dynamics in Crystalline Semiconductors", Acta Physica Polonica A Volume 123, 132 (2013).
[41] R. Gerritsma, G. Kirchmair, F. Zhringer, E. Solano, R. Blatt and C.F. Roos, "Quantum simulation of the Dirac equation", Nature 463, Volume 68 (2010).
[42] S.T. Park, "Propagation of a relativistic wave packet in the Dirac equation", Physical Review A Volume 86, 062105-1 (2012).
[43] A.D. Alhaidari, "Dirac particle in a square well and in a box", arXiv:0908.2205 [quant-ph], AIP Conf. Proc. 1370, 21 (2011).
[44] D.J. Griffiths, "Introduction to Quantum Mechanics", second edition, Pearson Prentice Hall, Upper Saddle River, 2005.
[45] N. Dombey, P. Kennedy and A. Cologeracos, "Supercriticality and transmission resonances in the Dirac equation", Physical Review Letters Volume 9, 1787 (2000).

Patricio Robles is professor and researcher of the Electrical Engineering Department of Pontifical Catholic University of Valparaíso, Chile. He has a degree of Master in Physics obtained in 1999 at Santa María University, Chile. He has been main author and coauthor of papers published in reviews as Physical Review B, International Journal of Modern Physics B and European Journal of Physics, related with optical response of arrays of particles to an external electromagnetic field, massive photons and superluminal transmission of electromagnetic waves, among others.