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A pedagogical approach to relativity effects in quantum mechanics

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Abstract
A simple but precise approach to relativistic quantum mechanics is presented. The approach is based on the use of a Schrödinger-like, little-known but well-studied quantum mechanics wave equation. Such formal similitude allows undergraduate students to quantitatively explore how the results corresponding to a typical non-relativistic quantum problem change when the particle is moving at relativistic speeds. No additional mathematical skills are required. We argue in favor of the academic use of this approach for including the implications of the special theory of relativity in introductory quantum mechanics courses.

Keywords: quantum mechanics, relativistic wave equations, philosophy of science

1. Introduction

Undergraduate students in most introductory courses of special theory of relativity learn that the total energy (E) of a classical free particle of mass (m), which is moving with speed (v) and linear momentum (p), is given by the simple formula [1, 2]:

$$E = \gamma mc^2, \quad \text{with}\gamma = \frac{1}{\sqrt{1-\frac{v^2}{c^2}}} = \sqrt{1+\frac{p^2}{m^2c^2}}. \tag{1}$$

In equation (1), c is the speed of the light in the vacuum, and γ is the Lorentz factor. The most emblematic equation in introductory quantum mechanics courses is the Schrödinger equation

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for a quantum particle moving in a scalar potential (V) [3, 4]:

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi. \tag{2}$$

In equation (2) $\hbar$ is the Plank constant divided by 2π, and the Laplace operator includes partial derivatives of the second order in the spatial variables [3, 4]. The Schrödinger equation associates a wavefunction (ψ) to any spin-0 particle with mass (m) [3, 4]. However, most introductory quantum mechanics courses focus on the electron, not a spin-0 but a spin-1/2 quantum particle [3, 4]. Consequently, often undergraduate students are taught later in the course that electrons are quantum particles with a spin 1/2, and they are introduced to the concept of spin, and to some version of Pauli's equation [3, 4]:

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\psi_\mathrm{P} = \frac{\left[\hat{\boldsymbol{p}} - \frac{e}{c}\boldsymbol{A}\right]^2}{2m}\psi_\mathrm{P} - \mu_\mathrm{B}H_\mathrm{ext}\sigma_z\psi_\mathrm{P}. \tag{3}$$

This version of Pauli's equation corresponds to the simple case of an electron moving in the same direction of a constant external magnetic field (H_ext) pointing in the z-direction. Equation (3) contains the operator linear momentum, the vectorial potential ($\boldsymbol{A}$) associated to H [4, 5], and the so-called Bohr's magneton, $\mu_\mathrm{B} = e\hbar/(2mc)$, where ($e$) is the absolute value of the electron charge. The stationary solutions of equation (3) are the spinors (ψ_P), i.e. two-component wavefunctions [4]. ψ_P and the z-component of the Pauli's matrix (σ_z) [3, 4], are:

$$\psi_\mathrm{P}(\boldsymbol{r}, t) = \varphi(\boldsymbol{r})\,\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Et}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{4}$$

In contrast with equation (1), equations (2)–(3) do not explicitly include the speed of the quantum particle. Often undergraduate students are taught not to worry about this feature of equations (2) and (3). Moreover, we often teach this feature as an advantage of these wave equations because quantum particles are odd in that they do not have trajectories, at least in the orthodox interpretation of quantum mechanics, which is the interpretation most often taught in introductory quantum mechanics courses [3, 4]. In addition, we teach that both Schrödinger's and Pauli's equations are only valid when $v \ll c$. Physics, Chemistry, and Engineering undergraduate students expend a lot of time mastering the skills needed for solving Schrödinger's and Pauli's equations; however, the study of how the speed of the particle affects the non-relativistic results are often postponed for graduated studies [6, 7]. This is because considerable effort must be dedicated to mastering the skills needed for handling first, the Dirac equation, and then the relativistic field theories [6–8].

Let us consider a hypothetical pedagogical dream. Consider how simple things would be if a combination of equations (1)–(3) were sufficient for, at least, the start of the study of relativistic quantum mechanics. For instance, let us imagine how lucky we would be if the effects of the speed of the particle on the wave equations could be 'packaged' in the following equations:

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{(\gamma+1)\,m}\nabla^2\psi + V\psi. \tag{5}$$

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\psi_\mathrm{P} = \frac{\left[\hat{\boldsymbol{p}} - \frac{e}{c}\boldsymbol{A}\right]^2}{(\gamma+1)\,m}\psi_\mathrm{P} - \frac{2\hbar e}{(\gamma+1)\,m}H_\mathrm{ext}\sigma_z\psi_\mathrm{P}. \tag{6}$$

Clearly, $\gamma \approx 1$ when $v \ll c$; thus, equations (5) and (6) beautifully convert to equations (2) and (3), respectively. Formally, equations (2) and (5), and equations (3) and (6) could be rewritten with the following similar format:

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2\mu}\nabla^2\psi + V\psi, \quad \text{with } \mu = \frac{\gamma+1}{2}m. \tag{7}$$

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\psi_{\mathrm{P}} = \frac{\left[\hat{\boldsymbol{p}} - \frac{e}{c}\boldsymbol{A}\right]^2}{2\mu}\psi_{\mathrm{P}} - \frac{\hbar e}{\mu m}H_{\mathrm{ext}}\sigma_z\psi_{\mathrm{P}}. \tag{8}$$

Clearly, equations (7) and (8) are Schrödinger-like and Pauli-like equations, respectively. This means solving equations (7) and (8) requires the same skills as solving equations (2) and (3) requires. We would then be simultaneously teaching non-relativistic and relativistic quantum mechanics.

However, dreams are not reality but dreams, we could cautiously say.

Nevertheless, this work shows some beautiful dreams can be real. For instance, for free quantum particles with spin 0 and 1/2, solving equations (7) and (8) exactly give the solutions with positive kinetic energy of the Klein–Gordon and Dirac equations, respectively [6, 7].

One could comment that these are trivial examples.

However, equation (7) with $\gamma > 1$ has already been solved for many problems of high pedagogical interest. This was done following the same mathematical procedures required for solving the corresponding non-relativistic problems. These problems include, but are not limited to, a spin-0 particle with mass m in a box [9, 10], in a Coulomb potential [11, 12], moving through a piecewise constant potential [13], and the relativistic quantum harmonic oscillator [14]. Moreover, it has been shown that solving equation (7) in the ultrarelativistic limit can be used for illustrating how the inclusion of special relativity modifies quantum mechanics. For instance, this approach gave a relatively simple explanation to the gravitational collapse of white dwarf stars when their mass equals the Chandrasekhar mass limit [15].

Interesting… but before getting too excited, it could be argued quantum particles are odd in that they do not have trajectories; therefore, equations (7) and (8) may be ill-defined because they implicitly include the speed of the particle.

The rest of this work is dedicated to exploring the validity of equations (7) and (8), their heuristic values, and the pedagogical challenges associated with using them for including a meaningful and useful discussion of relativistic quantum mechanics in introductory quantum mechanics courses.

2. Validity of the Schrödinger-like equation

It is not difficult to precisely obtain equation (7) from basic special relativity and quantum mechanics concepts [9, 10, 14]. A summary about this is included in the appendix A. In this section, we will only present the principal ideas behind this equation. We could start by a formal first-quantization substitution in equation (1) [3, 4, 9, 10]:

$$E \to \hat{H} = \mathrm{i}\hbar\frac{\partial}{\partial t}, \qquad \boldsymbol{p} \to \hat{\boldsymbol{p}} = -\mathrm{i}\hbar\nabla. \tag{9}$$

This procedure results in an evidently Lorentz-covariant wave equation for a free spin-0 quantum particle with mass (m) [10, 16]:

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\psi = mc^2\hat{\gamma}\psi, \quad \text{with } \hat{\gamma} = \sqrt{1 + \frac{\hat{p}^2}{m^2c^2}}. \tag{10}$$

High energy physicists may recognize equation (10) as a particular case of the spinless Salpeter equation [17, 18]. By realizing that the kinetic energy of a classical relativistic free particle can be written in the following two equivalent ways [5, 19]:

$$K = \gamma mc^2 - mc^2 = \frac{p^2}{(\gamma + 1)\, m}. \tag{11}$$

The Lorentz-covariant Poirier–Grave de Peralta equation for a spin-0 particle moving in a scalar potential can be obtained [10]:

$$\mathrm{i}\hbar \frac{\partial}{\partial t}\psi = \frac{\hat{p}^2}{(\hat{\gamma} + 1)\, m}\psi + V\psi. \tag{12}$$

As it is shown in the appendix A, the wavefunctions (ψ) in equations (10) and (12) are not identical but only different by the phase factor $\exp[-(\mathrm{i}mc^2/\hbar)t]$ [10]. The Lorentz factor in equation (1) and the operator γ in equations (10) and (12) look alike; however, in the coordinate representation, the operator γ is the square root of a differential operator. Nevertheless, our pedagogical proposal is based on the formal similitude between equations (2), (7) and (12). This approach is based on the possibility of substituting the operator γ in (12) with a parameter γ, real and positive, such that the solutions of equation (7), the parametrized equation, are identical to the solutions of equation (12). The details of obtaining adequate parametrizations—and how to solve equation (7) in cases of high pedagogical interest- can be found in previous publications [9–14, 19].

3. Validity of the Pauli-like equation

The Lorentz-covariant wave equation for a spin-0 particle with mass (m) is the Dirac equation [4, 6, 7, 16]. The stationary solutions of Dirac's equation are bispinors of the form [4]:

$$\psi_{\mathrm{D}}\left(\boldsymbol{r}, t\right) = \begin{bmatrix} \varphi\left(\boldsymbol{r}\right) \\ \chi\left(\boldsymbol{r}\right) \end{bmatrix} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Et}. \tag{13}$$

How equation (8) can be obtained from Dirac's equation is discussed in more detail in the appendix B. In short, it is well-known that the stationary Dirac's equation, for a particle interacting with an external electromagnetic field, is equivalent to the following system of two coupled spinor equations [4]:

$$c\left\{\hat{\boldsymbol{\sigma}}.\left[\hat{\boldsymbol{p}} - \frac{e}{c}\boldsymbol{A}\right]\right\}\chi = \left(E - mc^2 - eA_{\mathrm{o}}\right)\varphi, \tag{14}$$

$$c\left\{\hat{\boldsymbol{\sigma}}.\left[\hat{\boldsymbol{p}} - \frac{e}{c}\boldsymbol{A}\right]\right\}\varphi = \left(E + mc^2 - eA_{\mathrm{o}}\right)\chi. \tag{15}$$

In equations (14) and (15), $\boldsymbol{A}$ and A_{o} are the vectorial and scalar potentials associated with the external electromagnetic field [4, 5], and each component of the vectorial Pauli's matrix is a 2×2 matrix [4, 7, 16]:

$$\hat{\boldsymbol{\sigma}} = \left(\sigma_x, \sigma_y, \sigma_z\right). \tag{16}$$

For an electron that is only interacting with a magnetic field, equation (15) can be rewritten as:

$$\frac{c\left\{\hat{\boldsymbol{\sigma}}.\left[\hat{\boldsymbol{p}} - \frac{e}{c}\boldsymbol{A}\right]\right\}}{(\gamma + 1)mc^2}\varphi = \chi. \tag{17}$$

Substituting equation (17) in equation (14), we obtain:

$$\frac{\left\{\hat{\boldsymbol{\sigma}}.\left[\hat{\boldsymbol{p}}-\frac{e}{c}\boldsymbol{A}\right]\right\}^2}{(\gamma+1)m}\varphi = E'\varphi, \quad E' = E - mc^2. \tag{18}$$

Notably, for a free particle in the ultrarelativistic limit ($\gamma \gg 1$), equation (18) coincides with the stationary Weyl equation [7, 20]. Finally, using the identity [4, 16]:

$$\left\{\hat{\boldsymbol{\sigma}}.\left[\hat{\boldsymbol{p}}-\frac{e}{c}\boldsymbol{A}\right]\right\}^2 = \left[\hat{\boldsymbol{p}}-\frac{e}{c}\boldsymbol{A}\right]^2 - \frac{\hbar e}{c}\left[\hat{\boldsymbol{\sigma}}.\vec{H}\right]. \tag{19}$$

And assuming a constant external magnetic field (H_{ext}) in the direction z, we obtain the stationary equation corresponding to equation (8). Therefore, in this case, we obtain the exact spinor component (φ) of Dirac's wavefunction by solving equation (8). The spinor (φ) corresponds to positive values of the electron's kinetic energy [4]. This example is of pedagogical interest because the Stern–Gerlach experiments are often used in introductory quantum mechanics courses for justifying the existence of the spin [3]. The details of the general relation between the Dirac equation and equation (8) will be published elsewhere [21]. Disregarding the contribution of $\boldsymbol{A}^2$ to equation (8) allows for a simpler and more pedagogical form of equation (8) [22]:

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\psi_{\mathrm{P}} = -\frac{\hbar^2}{(\gamma+1)\,m}\nabla^2\psi_{\mathrm{P}} - \frac{2\mu_{\mathrm{B}}}{(\gamma+1)}H_{\mathrm{ext}}\sigma_z\psi_{\mathrm{P}}. \tag{20}$$

In contrast with equation (3), now it is evident the energy difference between the electron's spin up and spin down quantum states depends on the speed of the electron [22]:

$$\Delta E = 2\frac{2\mu_{\mathrm{B}}}{(\gamma+1)}H_{\mathrm{ext}}. \tag{21}$$

4. Pedagogical challenges

It is not difficult to get around the arguments about equations (7) and (8) being ill-defined because they implicitly include the speed of the particle. This also occurs in the Schrödinger equation because such implicit dependence could be formally obtained from the formula of kinetic energy of a classical particle [10, 11]:

$$K = \frac{p^2}{2m} = \frac{1}{2}mv^2. \tag{22}$$

Consequently:

$$\hat{K} = \frac{\hat{p}^2}{2m} = \frac{1}{2}m\hat{v}^2. \tag{23}$$

It should be noted, as this is done in equation (10), equation (1) allows for a definition of γ, making explicit reference not to the speed of the particle but instead to its linear momentum.

The best-known relativistic quantum wave equations for particles with spin 0 and 1/2 are the Klein–Gordon and Dirac equations, respectively [4, 6, 7, 16]. Both have solutions where the particle has positive and negative kinetic energy values; however, equations (7) and (8) only have positive kinetic energy value solutions. In addition, equations (7) and (8) describe processes where the number of particles is conserved. Therefore, when teaching relativistic quantum mechanics using equations (7) and (8), the instructor should ensure the students are aware of these differences and the corresponding implications.

The superposition principle is a cornerstone of quantum mechanics. This requires the linearity of the wave equations [3, 4, 16]; however, equations (7) and (8) are not linear because, in general, γ depends on the energy of the quantum state [10, 11, 19]. This challenging pedagogical problem can be avoided by focusing the attention on the non-relativistic ($\gamma \approx 1$) and ultra-relativistic ($\gamma \gg 1$) limits. Equations (7) and (8) are linear in those limits.

The perturbation theory is used in most introductory quantum mechanics courses for discussing the hydrogen atom [3, 4]. The time-independent perturbed Schrödinger equation to be solved in this case is [3, 4]:

$$\mathrm{i}\hbar \frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\nabla^2\psi + V_{\mathrm{C}}\psi + \hat{W}\psi. \tag{24}$$

In equation (24), (V_{C}) is the Coulomb potential [1, 5]. The perturbation operator is [3, 4]:

$$\hat{W} \approx \hat{W}_{\mathrm{K}} + \frac{1}{2m^2c^2}\left(\hat{W}_{\mathrm{so}} + \hat{W}_{\mathrm{D}}\right). \tag{25}$$

The operators (W_{K}), (W_{so}), and (W_{D}) correspond to the kinetic energy, spin–orbit, and Darwin relativistic corrections to the non-relativistic energies, respectively [3, 4]:

$$\hat{W}_{\mathrm{so}} = \frac{Ze^2}{r^3}\left(\hat{\boldsymbol{s}}.\hat{\boldsymbol{L}}\right), \quad \hat{W}_{\mathrm{D}} = \pi Z e^2 \hbar^2 \delta(r). \tag{26}$$

The W_{so} and W_{D} operators include the spin ($\boldsymbol{s}$) and linear momentum ($\boldsymbol{L}$) operators and the Dirac's delta function (δ), respectively [3, 4]. Interestingly, as it is discussed in the appendix B, the quasi-relativistic version of equation (24) for a spin-1/2 particle is the following Pauli-like equation [21, 22]:

$$\mathrm{i}\hbar \frac{\partial}{\partial t}\psi_{\mathrm{P}} = \left[-\frac{\hbar^2}{2\mu}\nabla^2 + U_{\mathrm{C}}(r) + \hat{W}\right]\psi_{\mathrm{P}}. \tag{27}$$

With:

$$\hat{W} \approx \frac{1}{2\mu^2c^2}\left(\hat{W}_{\mathrm{so}} + \hat{W}_{\mathrm{D}}\right). \tag{28}$$

As expected, the operator W_{K} is not present in equation (28) because the substitution of m by μ in equation (24) introduces in equation (27) the relativistic correction to the kinetic energy. A comparison between equations (5) and (27) clearly shows how different the interactions with a Coulomb potential of charged particles with spin 0 and 1/2 are.

The authors of this work have been in the two extremes of teaching and receiving an introductory quantum mechanics course using the approach discussed here for the first time. This is a two-semester course using reference [3] as a textbook. First, the students traditionally learn how to solve the Schrödinger and Pauli equations; then, they apply the learned techniques for solving equations (7) and (8). Students that demonstrate the ability of solving the quasi-relativistic versions of non-relativistic problems received extra credits toward the final course grade. Students learning simultaneously non-relativistic and relativistic quantum mechanics allows teaching how to obtain quantum mechanics wave equations from classical non-relativistic and relativistic formulas, using the first quantization procedure. It is worth noting that Dirac's equation cannot be obtained in this way because the quantum spin is not a property of classical particles. Nevertheless, Pauli's equation can be conveniently justified from well-known experiments. Finally, the students were motivated by the unexpected possibility to celebrate the first centenary of quantum mechanics while exploring amazingly new quantum mechanics wave equations.

5. Conclusions

We presented a simple, pedagogical, precise approach for including, in introductory quantum mechanics courses, a thoughtful discussion about the consequences, for quantum mechanics, of the basic concepts and ideas commonly taught in introductory special theory of relativity courses. The approach is based on the use of equations (7) and (8). These equations are formally like Schrödinger's and Pauli's equations. This similitude allows undergraduate students to quantitatively explore how the results, corresponding to a typical non-relativistic quantum problem, change when the particle is moving at relativistic speeds. We also presented a discussion about the validity of equations (7) and (8), their heuristic values, and the pedagogical challenges associated with using them. Nevertheless, the authors hope that these ideas might be empirically evaluated, analyzed, and improved in the future, after their broad dissemination and implementation occurs.

Appendix A

An illuminating discussion about equation (7) can be found in references [9, 10]. Starting from the Lorentz-covariant equation (1), which is then followed by the formal first-quantization substitution given by equation (9), we obtain equation (10). Alternatively, we could start from the following equation, which is equivalent to equation (1) [10]:

$$E = \frac{p^2}{(\gamma + 1)m} + mc^2, \quad \text{with } \gamma = \sqrt{1 + \frac{p^2}{m^2c^2}} \tag{A.1}$$

and then we can use equation (9) for obtaining [10]:

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\Omega = -\frac{\hbar^2}{(\hat{\gamma} + 1)\,m}\nabla^2\Omega + mc^2\Omega. \tag{A.2}$$

Now, it is well known in quantum mechanics that applying a constant energy shift to the Hamiltonian gives way to an immaterial time-evolving phase factor in the solution wavefunction. Therefore, equation (12) can be obtained from equation (A.2), which is equivalent to equation (10), after adding a time independent 'scalar' potential V and replacing Ω as follows:

$$\Omega(x, t) = \Psi(x, t)\mathrm{e}^{-\mathrm{i}\frac{mc^2}{\hbar}t}. \tag{A.3}$$

Note that under Lorentz transform, V becomes the time-like component of a full electromagnetic four-potential vector. In equation (12), γ is the operator given by equation (10). Nevertheless, it can be shown that the operator γ in (12) can be substituted with a parameter γ, which is real and positive, such that the solutions of equation (7), the parametrized equation, are identical to or approximately equal to the solutions of equation (12).

For instance, there are many pedagogical problems in which a spin-0 particle moving through piecewise constant potentials has stationary solutions. In these cases, the particle has piecewise constant kinetic energy when it is in a stationary quantum state, resulting in piecewise constant values of p^2 and the Lorentz factor [3, 4]. In these problems the exact solution of equation (12) can be obtained by solving equation (7) as the corresponding Schrödinger equation is solved [10, 13]. Consequently, in these problems the kinetic energy of the stationary states found by solving equation (7) depends on the value of the parameter γ, thus:

$$E' = K(\gamma) + V. \tag{A.4}$$

Finally, the value of γ should be taken as exactly equal to the classical Lorentz factor value, thus:

$$K(\gamma) = (\gamma - 1)\, mc^2. \tag{A.5}$$

Solving the system of equations (A.4) and (A.5) allows for simultaneously finding the values of E' and γ [12, 13].

There are several pedagogical problems involving a time-independent scalar potential that is not piecewise constant. The harmonic oscillator and the hydrogen atom are two of the more emblematic of them. The solution of the relativistic harmonic oscillator following the approach discussed in this work was recently reported [14]. We encourage the readers to look there for clever methods for choosing the parameter γ such that the solutions of equation (7) give an excellent approximation to the solutions of equation (12). We can communicate here that the solutions of equation (7) for a Coulomb potential, when γ is taken as exactly equal to the classical Lorentz factor, are identical to the solutions of the corresponding Klein–Gordon equation with positive kinetic energies. A detailed study of this case will be published elsewhere.

Appendix B

The system of the two coupled spinor equations (14) and (15) is equivalent to Dirac's equation [4]. The kinetic energy of a spin-1/2 particle in the quantum states corresponding to the spinors φ and χ has positive and negative values, respectively [4, 7]. Therefore, we could obtain a quasi-relativistic extension of the time-independent Pauli equation by obtaining the spinor equation satisfied by φ. Equation (15) can be rewritten in the following way [21]:

$$\frac{c\left[\hat{\boldsymbol{\sigma}}.\left(\hat{\boldsymbol{p}} - \frac{e}{c}\boldsymbol{A}\right)\right]}{\left(E + mc^2 - eA_o\right)}\varphi = \chi. \tag{B.1}$$

Substituting equation (B.1) in equation (14), we obtain [21]:

$$\left[\hat{\boldsymbol{\sigma}}.\left(\hat{\boldsymbol{p}} - \frac{e}{c}\boldsymbol{A}\right)\right]\left[\frac{c^2}{\left(E + mc^2 - eA_o\right)}\right]\left[\hat{\boldsymbol{\sigma}}.\left(\hat{\boldsymbol{p}} - \frac{e}{c}\boldsymbol{A}\right)\right]\varphi$$
$$= \left(E - mc^2 - eA_o\right)\varphi\chi. \tag{B.2}$$

Making $E' = E - mc^2$, and conveniently introducing a parameter γ such that $E' + 2mc^2 = (\gamma + 1)mc^2 = 2\mu c^2$, where μ is given by equation (1), we finally obtain the desired equation [21]:

$$\left[\hat{\boldsymbol{\sigma}}.\left(\hat{\boldsymbol{p}} - \frac{e}{c}\boldsymbol{A}\right)\right]\left[\frac{c^2}{2\mu c^2 - eA_o}\right]\left[\hat{\boldsymbol{\sigma}}.\left(\hat{\boldsymbol{p}} - \frac{e}{c}\boldsymbol{A}\right)\right]\varphi = +eA_o\varphi = E'\varphi. \tag{B.3}$$

As expected, equation (B.3) reduces to equation (18) when $A_{\mathrm{o}} \equiv 0$. The quantum states of the electron with $K > 0$ in heavy hydrogen-like atoms can be obtained by solving equation (B.3) when $\boldsymbol{A} \equiv 0$ and eA_{o} equal to the Coulomb potential (U_{C}) [21]:

$$\left\{(\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{p}})\left[\frac{c^2}{2\mu c^2 - U_{\mathrm{C}}(r)}\right](\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{p}})\right\}\varphi + U_{\mathrm{C}}(r)\,\varphi = E'\varphi. \tag{B.4}$$

In contrast to a spin-0 particle, as it is shown below, the energy of an electron moving in a Coulomb potential is not $E' = K + U_{\mathrm{C}}$; however, if hypothetically $E' = K + U_{\mathrm{C}}$, then $2\mu c^2 - U_{\mathrm{C}} = K + 2mc^2 = (\gamma + 1)mc^2$, with γ equal to the Lorentz factor given by equation (1). Therefore, it would be possible to rewrite equation (B.4) as [21]:

$$-\frac{\hbar^2}{2\mu}\nabla^2\varphi + U_{\mathrm{C}}(r)\,\varphi = E'\varphi. \tag{B.5}$$

In the non-relativistic limit, $\gamma \approx 1$, thus $\mu = m$. Therefore, each component of the time-dependent Pauli-like wave equation corresponding to equation (B.5) satisfies equation (2) with $V = V_{\mathrm{C}}$, i.e. the Schrödinger equation for a spin-0 particle with the mass and charge of an electron which is moving in a Coulomb potential. Consequently, the energies E' calculated solving the time-independent spinor equation given by equation (B.5) include the relativistic correction to the kinetic energy but include neither the Darwin nor the spin–orbit corrections [11, 12, 22].

However, as it is shown below, the energy of a spin-1/2 particle in a Coulomb potential is not $E' = K + U_{\mathrm{C}}$ but $E' = K + U_{\mathrm{C}} + W$, where W is a potential energy related to the spin of the particle. Nevertheless, if $W \ll K + U_{\mathrm{C}}$, equation (B.5) could be used as a good zero-order approximation for solving equation (B.4) using the perturbation theory [3, 4]. A non-relativistic version of equation (B.4), with μ substituted by m, was previously solved using a perturbative approach. This approach produces equations (24) to (26) [4]. Similarly, we can obtain a useful approximation of equation (B.4) by approximating the function between brackets in equation (B.4) in the following way [22]:

$$\frac{c^2}{2\mu c^2 - U_{\mathrm{C}}(r)} \approx \frac{1}{2\mu}\left[1 + \frac{U_{\mathrm{C}}(r)}{2\mu c^2}\right]. \tag{B.6}$$

Substituting equation (B.6) in equation (B.4), we obtain [21]:

$$-\frac{\hbar^2}{2\mu}\nabla^2\varphi + U_{\mathrm{C}}(r)\,\varphi + \hat{W}\varphi = E'\varphi, \quad \hat{W} = (\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{p}})\left[\frac{U_{\mathrm{C}}(r)}{4\mu^2c^2}\right](\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{p}}). \tag{B.7}$$

A comparison of equations (B.5) and (B.7) reveals that, in contrast with a spin-0 particle, there is an additional potential energy in equation (B.7) related to the spin of the particle. The operator W in equation (B.7) can be treated as a small perturbation of equation (B.5). Equation (B.7) is the time-independent equation corresponding to the natural extension to quasi-relativistic speeds of the Pauli equation for an electron moving in a Coulomb potential [21]:

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\psi_{\mathrm{P}} = \left[-\frac{\hbar^2}{2\mu}\nabla^2 + U_{\mathrm{C}}(r) + \hat{W}\right]\psi_{\mathrm{P}}. \tag{B.8}$$

Previously, equation (B.8) was solved using the perturbation theory [22]. In the zero-order approximation, the energy values, and the spatial part of each component of the spinor ψ_{P} are obtained by solving equation (B.5) [11, 12]. Thus, it already includes the relativistic correction to the kinetic energy of the electron [12]. More importantly, in the first-order approximation of the perturbation theory, it was found that there is an excellent agreement between the calculated energies and the energy values obtained by solving Dirac's equation [22]. As it is done in the non-relativistic limit [4], the Darwin and the spin–orbit energy contributions can be obtained after somewhat involved mathematical manipulations; this results in the approximation of the operator W in equations (B.7) and (B.8) by the operator W in equations (27) and (28) [21, 22]. It is worth noting that both the Darwin and the spin–orbit corrections decrease when the electron moves at relativistic speeds [12].

The readers should realize that it might not be a good pedagogical idea to include, in an introductory course of quantum mechanics, the deduction of equations (B.7), (B.8) and (27) from Dirac's equation. Indeed, often equations (24) to (26) are not deducted from the non-relativistic limit of Dirac's equation like in reference [4] rather they are introduced in alternative ways [3]. Similarly, equations (27) and (28) could be introduced in some heterodox way. What really has an important pedagogical value is the comparison of the wave equations for charged particles of different natures moving in a Coulomb potential. For a slow-moving particle with spin-0, the corresponding wave equation is the Schrödinger equation given by equation (2) with V equal to the Coulomb potential. However, the Pauli-like equation (27) is the correct wave equation for a fast-moving particle with spin-1/2. When the spin-1/2 particle moves relatively slow, the energy values calculated by solving equation (24) are an excellent approximation for the energies corresponding to equation (27) [22].

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