A notable quasi-relativistic wave equation and its relation to the Schrödinger, Klein-Gordon, and Dirac equations.

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An intriguing quasi-relativistic wave equation, which is useful in between the range of applications of the Schrödinger and the Klein-Gordon equations, is discussed. This equation allows for a quantum description of a constant number of spin-0 particles moving at quasi-relativistic energies. It is shown how to obtain a Pauli-like version of this equation from the Dirac equation. This Pauli-like quasi-relativistic wave equation allows for a quantum description of a constant number of spin-1/2 particles moving at quasi-relativistic energies and interacting with an external electromagnetic field. In addition, it was found an excellent agreement between the energies of the electron in heavy Hydrogen-like atoms obtained using the Dirac equation, and the energies calculated using a perturbation approach based on the quasi-relativistic wave equation. Finally, it is argued that the notable quasi-relativistic wave equation discussed in this work provides interesting pedagogical opportunities for a fresh approach to the introduction to relativistic effects in introductory quantum mechanics courses.

Introduction

Most Physics bachelors are familiar with the Schrödinger equation, which describes the movement of a spin-0 particle with mass (m) moving at speeds much smaller than the speed of light (c) [1-5]. The one-dimensional Schrödinger equation corresponding to a free particle is given by the following expression [1-5]:

$$i\hbar\frac{\partial}{\partial t}\psi_{Sch}(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_{Sch}(x,t). \qquad (1)$$

In Eq. (1), $\hbar$ is the Plank constant (h) divided by 2π and ψ_{Sch} is the (scalar) wavefunction. Most Physics Ph. D. graduated know about the Klein-Gordon equation, which describes the movement of a spin-0 particle with mass moving at relativistic speeds [6-7]. The one-dimensional Klein-Gordon equation corresponding to a free particle is given by the following expression [6-7]:

$$\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\psi_{KG}(x,t) = \frac{\partial^2}{\partial x^2}\psi_{KG}(x,t) - \frac{m^2c^2}{\hbar^2}\psi_{KG}(x,t). \qquad (2)$$

In Eq. (2), ψ_{KG} is also a scalar wavefunction. Eq. (2) is not a Schrödinger-like equation because in contrast to the Schrödinger equation, Eq. (2) includes a second order temporal derivative. Introductory Quantum Mechanics courses often cover the Schrödinger equation [1-5]. More advance Quantum Mechanics courses often cover the Klein Gordon equation [6-7]. This is done for introducing the readers to the consequences for quantum mechanics of taking seriously the concepts and ideas of Special Theory of Relativity [8-9]. Historically, while looking in 1926 for the right quantum equation, Erwin Schrödinger first explored, but did not publish, the equation that we today call the Klein-Gordon equation, which was also published in 1926 by Oskar Klein and Walter Gordon. Schrödinger was well-aware of the Einstein's Special Theory of Relativity; thus, he was looking for a Lorentz invariant wave equation [6-10]. The Schrödinger equation is not Lorentz invariant but Galilean invariant [10-11]; therefore, a relativistic quantum mechanics cannot be based on the Schrödinger equation. A fully relativistic quantum theory requires to be funded on equations like the Klein-Gordon equation, which is valid for any two observers moving respect to each other at constant velocity [6-7]. However, judging by its popularity between present physicists, Schrödinger took the correct decision. The solutions of the Klein-Gordon equation are plagued with several unwanted properties that made Eq. (2) less easy to work with than using Eq. (1) [6-7]. Eq. (1)

describes a particle with mass (m), and linear momentum (p) and kinetic energy (K) related by the classical relation $K = p^2/2m$, which is not valid at relativistic speeds [6-7, 11]. Fortunately for Schrödinger, he was able to reproduce the results previously obtained by Bohr for the energies of the bounded states of the electron in the Hydrogen atom [1-5]. This was possible because the electron in the Hydrogen atom has non-relativistic energies [1-5]. However, electrons are not spin-0 particles but spin-1/2 particles. Electrons moving at low velocities respect to c, can be approximately described by a two-component vector wavefunction (spinor) [2, 6-7]. The spinor nature of the electron wavefunction produces experimentally detectable results when the electron interacts with an external electromagnetic field [4, 6-7]. The Pauli equation, which was discovered by Wolfgang Ernst Pauli in 1927, is a Schrödinger-like equation; therefore, it is not a Lorentz-invariant. The Pauli equation describing the interaction of a free electron with a constant magnetic field, with magnitude B_{ext} pointing in the z direction, can be written in the following way [4]:

$$i\hbar\frac{\partial}{\partial t}\psi_P(\vec{r},t) = -\frac{\hbar^2}{2m}\nabla^2\psi_P(\vec{r},t) - \mu_B\, B_{ext}\,\sigma_z\,\psi_P(\vec{r},t). \quad (3)$$

In Eq. (3), ∇^2 is the Laplace operator [1-5], $\mu_B = e\hbar/(2mc)$ is the Bohr magneton [4], e is the electron charge, and σ_z is the 2 × 2 Pauli matrix [2]:

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (4)$$

ψ_P is not a scalar wavefunction but the two-components spinor wavefunction:

$$\psi_P(\vec{r},t) = \begin{pmatrix} \psi_{P+}(\vec{r},t) \\ \psi_{P-}(\vec{r},t) \end{pmatrix}. \quad (5)$$

Consequently, Eq. (3) is equivalent to a system of two independent Schrödinger equations for ψ_{P+} and ψ_{P-} that are only different in the sign of the last term in the right side of the equations. When $B_{ext} = 0$, both equations are equal to the three-dimensional version of Eq. (1) [1-5]. The exact description of electrons moving at relativistic velocities requires a four-components (biespinor) wavefunction, and the solution of the Lorentz invariant Dirac equation [6-7]. The Dirac equation of a free electron is given by the following equation [2, 6-7, 14]:

$$i\hbar\frac{\partial}{\partial t}\psi_D(\vec{r},t) = c\left[\overrightarrow{(\hat{\alpha})}\cdot\overrightarrow{(\hat{p})}\right]\psi_D(\vec{r},t) + mc^2\,\hat{\beta}. \quad (6)$$

In Eq. (6), each of the three components of the vector $\overrightarrow{(\hat{\alpha})}$ and $\hat{\beta}$ are 4 × 4 Dirac's matrices [2, 6-7, 14]. Each of the tree components of the vector $\overrightarrow{(\hat{p})}$ is the differential operator [2, 6-7, 14]:

$$\hat{p_i} = -i\hbar\frac{\partial}{\partial i}, \quad i = x, y, z. \quad (7)$$

Consequently, the Dirac equation is not a Schrödinger-like equation because only includes spatial derivatives of first order, while Eqs. (1) and (3) include spatial derivatives of second order. The bispinor ψ_D has four components; therefore, it can be represented using two spinors in the following way [2, 14]:

$$\psi_D(\vec{r},t) = \begin{pmatrix} \varphi(\vec{r},t) \\ \chi(\vec{r},t) \end{pmatrix}. \quad (8)$$

Clearly, a price in mathematical complexity is paid for improving the relativistic description of quantum particles. Consequently, from a purely pedagogical point of view, it would be convenient to be able to have a Schrödinger-like equation capable to describe quantum-particles at relativistic energies. Unfortunately, this is not in general possible [6-7]. Nevertheless, it was recently found a Schrödinger-like equation capable to describe quantum-particles at quasi-relativistic energies [11-13, 15-16]. Rigorously, the number of particles may not be constant in a fully relativistic quantum theory [6-7]. This is because when the sum of the kinetic and the potential (U) energy of a particle with mass m doubles the energy associate to the mass of the particle, i.e., $E' = K + U = 2mc^2$, then a pair particle-antiparticle could be created from E' [2, 6-7]. Consequently, the number of particles is constant at quasi-relativistic energies, i. e., when $E' = K + U < 2mc^2$. At quasi-relativistic energies close to mc^2, the Schrödinger equation does not provide a good description of the states of the quantum particle because it assumes that $K = p^2/2m$, while at relativistic speeds the correct relation between K, p, and the square of the velocity of the particle (V^2) is given by the following equation [8-9, 11-13, 15-16]:

$$K = \frac{p^2}{(\gamma_V + 1)m}, \quad \gamma_V = \frac{1}{\sqrt{1 - \frac{V^2}{c^2}}} \quad (9)$$

The quasi-relativistic wave equation for a free spin-0 particle is given by the following equation [11-13, 15-16]:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{(\gamma_V+1)m}\frac{\partial^2}{\partial x^2}\psi(x,t). \qquad (10)$$

Clearly, Eq. (10) is a Schrödinger-like equation. Like in Eq. (1), ψ is a scalar wavefunction. Moreover, Eq. (10) coincides with Eq. (1) at low velocities when $\gamma_V \sim 1$. However, Eq. (10) describes a particle at quasi-relativistic energies because it implies the relation between *K*, *p*, and V^2 given by Eq. (9) [11-13, 15-16]. Consequently, from a purely pedagogical point of view, the quasi-relativistic wave equation (Eq. (10)) is very interesting. Moreover, the quasi-relativistic wave equation can be solved following the same mathematical steps required for solving the Schrödinger equation in most of the problems often included in Introductory Quantum Mechanics courses. This includes a free particle [11], confinement of a quantum particle in box [11, 13, 15], reflexion by a sharp quantum potential [15], tunnel effect [15], and the quasi-relativistic description of Hydrogen-like atoms [12, 15-16]. Therefore Eq. (10) allows for a smooth introduction of special relativity concepts and ideas in Introductory Quantum Mechanics courses.

The quasi-relativistic wave equation also enriches the accumulated physics knowledge, and open new ways to tackle quantum problems involving particles at quasi-relativistic energies. Because Eq. (10) is a Schrödinger-like equation, it permits to calculate probabilities like it is done for Eq. (1) [11]. Moreover, Eq. (10) allows for a quasi-relativistic description of multi-particle systems where the number of particles is constant [17]. This includes all problems in Chemistry where the number of electrons is constant and $E' < 2mc^2$. The energy of the most energetic electrons in heavy elements is quasi-relativistic. Therefore, often their description either involve a perturbative theory based on the Schrödinger equation [2, 4-5], or a more precise but much more complicate quantum electrodynamic description [18]. The quasi-relativistic wave equation potentially represent a novel non-perturbative approach for tackling such problems without having to paid a heavy price in mathematical complexity, thus helping to grasp the essence of the consequences of introducing the ideas and concepts of spatial theory of relativity in quantum mechanics. In this work, first, for completeness, the connection between Eq. (10) and the Klein-Gordon equation will be summarized. Then, for the first time, a quasi-relativistic version of Eq. (3) will be directly obtained from the Dirac equation. Finally, also for the first time, an equation giving the quasi-relativistic energies of the bound states of the electron in Hydrogen-like atoms will be obtained using a perturbative approach based on the quasi-relativistic wave equation. The quasi-relativistic energies calculated in this way have a much better correspondence, with the energies calculated using the Dirac equation, than the energies calculated using a perturbative theory based on the Schrödinger equation.

Relationship between the Klein-Gordon and the quasi-relativistic wave equations

From the following well-known relativistic equations [8-9, 15]:

$$E^2 - m^2c^4 = p^2c^2 \Leftrightarrow (E + mc^2)\,(E - mc^2) = p^2c^2. \qquad (11)$$

And:

$$E = \gamma_V mc^2,\ p = \gamma_V mV,\ E = K + mc^2. \qquad (12)$$

One can formally obtain Eq. (2) by substituting *E* and *p* in Eq. (11) by the following energy and momentum quantum operators [1-4, 6-7]:

$$\hat{E} = i\hbar\frac{\partial}{\partial t},\ \hat{p} = -i\hbar\frac{\partial}{\partial x}. \qquad (13)$$

The factor ($E + mc^2$) in Eq. (11) is always different than zero for $E > 0$; consequently, Eq. (11) and the following algebraic equation are equivalents for $E > 0$:

$$K = (E - mc^2) = \frac{p^2}{(\gamma_V+1)m} \qquad (14)$$

Then from Eqs. (13) and (14) results the following differential equation [12-13, 15]:

$$i\hbar\frac{\partial}{\partial t}\psi_{KG+}(x,t) = -\frac{\hbar^2}{(\gamma_V+1)m}\frac{\partial^2}{\partial x^2}\psi_{KG+}(x,t) + mc^2\psi_{KG+}(x,t)\,. \qquad (15)$$

A simple substitution in Eqs. (2) and (15) shows that the following plane wave is a solution of both equations for $E > 0$:

$$\psi_{KG+}(x,t) = e^{\frac{i}{\hbar}(px-Et)}, \qquad (16)$$

Moreover, the following wavefunction is a solution of Eq. (10) [11, 13, 15]:

$$\psi(x,t) = \psi_{KG+}e^{iw_m t},\ w_m = \frac{mc^2}{\hbar}. \qquad (17)$$

Therefore, Eq. (17) allows finding a solution of Eq. (2) with E > 0 from a solution of Eq. (10). This is the relationship between the free-particle Klein-Gordon and quasi-relativistic wave equations. This relationship is also valid when the particle is moving through a potential U [11-13, 14-15]. For instance, the quasi-relativistic wave equation for a particle moving at quasi-relativistic energies through piecewise constant potentials is given by the following equation [15]:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{(\gamma_V+1)m}\frac{\partial^2}{\partial x^2}\psi(x,t) + U(x)\psi(x,t). \quad (18)$$

Looking for a solution of the form:

$$\psi(x,t) = X(x)\, e^{-\frac{i}{\hbar}Kt},\ K = E' - U \quad (19)$$

Results the time-independent quasi-relativistic wave equation [15]:

$$\frac{d^2}{dx^2}X(x) + \kappa^2 X(x) = 0,\ \kappa = \frac{p}{\hbar} = \frac{1}{\hbar}\sqrt{(\gamma_V+1)mK} = \frac{1}{\hbar}\sqrt{(\gamma_V+1)m(\text{E}'-U)}\,. \quad (20)$$

At low velocities, when $\gamma_V \sim 1$, Eq. (1) coincides with the time-independent Schrödinger equation for the same problem [1-4]. The allowed values of κ are determined by the boundary conditions of the problem. From Eqs. (12) and (14) follows that [15, 17]:

$${\gamma_V}^2 = 1 + \left(\frac{\hbar k}{mc}\right)^2 \ \Rightarrow\ K = \frac{\hbar^2\kappa^2}{\left[1+\sqrt{1+\frac{\hbar}{mc}k}\right]m}. \quad (21)$$

At low velocities, when $\gamma_V \sim 1$ and $\hbar\kappa << mc$, Eq. (21) gives $K = \hbar^2\kappa^2/2m$, which is the non-relativistic relation between K and κ [1-4]. It is worth noting that Eqs. (10) and (18) are not linear equations [11-13, 15]. This may rise some objections due to the importance of the superposition principle in quantum mechanics [1-7, 11-13, 15]. However, it should be noted if X_1 and X_2 are two solutions of the time-independent quasi-relativistic wave equation (Eq. (20)), respectively corresponding to different kinetic energies K_1 and K_2, then the following wavefunction is a solution of the Klein-Gordon equation:

$$\psi_{KG+}(x,t) = X_1(x)e^{-\frac{i}{\hbar}(K_1+mc^2)t} + X_2(x)e^{-\frac{i}{\hbar}(K_2+mc^2)t}\,. \quad (22)$$

From this point of view, the time-independent relativistic wave equation should not be considered a fundamental equation, but a useful auxiliar equation for finding solutions of a fundamental Lorentz invariant wave equation satisfying the superposition principle [13].

The quasi-relativistic wave equation of a free electron

The wavefunction in Eqs. (1), (2), (10), and (18) are scalars, thus describe the state of a spin-0 particle with mass. However, electrons are not spin-0 particles but spin-1/2 particles. Eq. (6) gives the correct relativistic correction of a free electron. However, as it is shown below, a spinor quasi-relativistic wave equation can be obtained when $E > 0$. Proposing a solution of Eq. (6) of the following form [2]:

$$\psi_D(\vec{r},t) = \begin{pmatrix}\varphi(\vec{r})\\ \chi(\vec{r})\end{pmatrix} e^{-\frac{i}{\hbar}Et}, \quad (23)$$

Substituting Eq. (23) in Eq. (6), and considering that for a free electron $E = K + mc^2$, allows for rewriting Eq. (6) as the following system of two time-independent spinor equations [2]:

$$c\left[\overrightarrow{(\hat{\sigma})}.\overrightarrow{(\hat{p})}\right]\chi = (E - mc^2)\varphi = K\varphi,$$
$$c\left[\overrightarrow{(\hat{\sigma})}.\overrightarrow{(\hat{p})}\right]\varphi = (E + mc^2)\chi. \quad (24)$$

In Eq. (24), each of the three components of the vector $\overrightarrow{(\sigma)}$ is a 2 × 2 Pauli's matrix [2, 6-7, 14]. $E + mc^2 > 0$ when $E > 0$, thus when $E > 0$, the bottom equation of Eq. (24) can be rewritten in the following way:

$$\chi = \frac{c\left[\overrightarrow{(\hat{\sigma})}.\overrightarrow{(\hat{p})}\right]}{(E+mc^2)}\varphi = \frac{\left[\overrightarrow{(\hat{\sigma})}.\overrightarrow{(\hat{p})}\right]}{(\gamma_V+1)mc}\varphi\ . \quad (25)$$

Substituting Eq. (25) in in the top equation of Eq. (24) results in the following equation:

$$\frac{\left[\overrightarrow{(\hat{\sigma})}.\overrightarrow{(\hat{p})}\right]^2}{(\gamma_V+1)m}\varphi = -\frac{\hbar^2}{(\gamma_V+1)m}\nabla^2\varphi = K\varphi. \quad (26)$$

Therefore, when $E > 0$, each one of the two components of φ exactly satisfices the same time-independent quasi-relativistic wave equation, which corresponds to a free spin-0 particle with kinetic energy K. Consequently, when $E > 0$, the three-dimensional version of Eq. (10) is the time-dependent quasi-relativist wave equation corresponding to each component of φ in Eq. (26).

The Pauli-like quasi-relativistic wave equation

The Schrödinger-like Pauli equation given by Eq. (3) can be obtained from the Dirac equation for an electron interacting with an external electromagnetic field [2]. Following the same procedure, a quasi-relativistic version of Eq. (3) can be obtained. When an external electromagnetic field interact with the electron, Eq. (24) should be modified in the following way [2]:

$$c\left[\overrightarrow{(\hat{\sigma})}.\overrightarrow{(\hat{p})}-\frac{e}{c}\vec{A}\right]\chi = (E-mc^2-eA_o)\varphi,$$
$$c\left[\overrightarrow{(\hat{\sigma})}.\overrightarrow{(\hat{p})}-\frac{e}{c}\vec{A}\right]\varphi = (E+mc^2-eA_o)\chi. \quad (27)$$

In Eq. (27), $-eA_o$ is the electron electrostatic energy and $\vec{A}$ is the vector potential associated to an external magnetic field [2, 8]. When $(E + mc^2 - eA_o) > 0$, the bottom equation of Eq. (27) can be rewritten in the following way:

$$\chi = \frac{c\left[\overrightarrow{(\hat{\sigma})}.\overrightarrow{(\hat{p})}-\frac{e}{c}\vec{A}\right]}{(E+mc^2-eA_o)}\varphi. \quad (28)$$

The Schrödinger-like Pauli equation can be obtained doing $E = E' + mc^2$ and assuming $|E' - eA_o| << mc^2$. Therefore, the fraction $c/(E' - eA_o + 2mc^2)$ in Eq. (1) can be developed in powers of $(E' - eA_o)$ and Eq. (28) can be approximated by the following expression (2):

$$\chi \approx \frac{1}{2mc}\left[\overrightarrow{(\hat{\sigma})}.\overrightarrow{(\hat{p})}-\frac{e}{c}\vec{A}\right]\varphi. \quad (29)$$

Substituting Eq. (29) in the top equation of Eq. (27) allows obtaining the Schrödinger-like time-independent Pauli equation [2]:

$$\left\{\frac{\left[\overrightarrow{(\hat{p})}-\frac{e}{c}\vec{A}\right]^2}{2m}+eA_o-\mu_B\left(\overrightarrow{(\hat{\sigma})}.\vec{B}\right)\right\}\varphi = E'\varphi. \quad (30)$$

For a free electron moving through a constant magnetic field, with magnitude B_{ext} pointing in the z direction, Eq. (30) can be approximated as:

$$-\frac{\hbar^2}{2m}\nabla^2\varphi(\vec{r}) - \mu_B B_{ext}\,\sigma_z\varphi(\vec{r}) = E'\varphi. \quad (31)$$

Which is the time-independent Pauli-equation corresponding to Eq. (3). However, if one assumed that $|-eA_o| << \mathrm{E} + \mathrm{mc}^2$, then the fraction $c/(-eA_o + E'+2mc^2)$ in Eq. (1) can be developed in powers of $-eA_o$ and Eq. (28) can be approximated by the following expression (2):

$$\chi \approx \frac{1}{(\gamma_V+1)mc}\left[\overrightarrow{(\hat{\sigma})}.\overrightarrow{(\hat{p})}-\frac{e}{c}\vec{A}\right]\varphi. \quad (32)$$

Substituting Eq. (32) in the top equation of Eq. (27) allows obtaining the following time-independent Pauli-like quasi-relativistic wave equation:

$$\left\{\frac{\left[\overrightarrow{(\hat{p})}-\frac{e}{c}\vec{A}\right]^2}{(\gamma_V+1)m}+eA_o-\frac{2\mu_B}{(\gamma_V+1)}\left(\overrightarrow{(\hat{\sigma})}.\vec{B}\right)\right\}\varphi = E'\varphi. \quad (33)$$

For a free electron moving through a constant magnetic field, with magnitude B_{ext} pointing in the z direction, Eq. (33) can be approximated as:

$$-\frac{\hbar^2}{(\gamma_V+1)m}\nabla^2\varphi(\vec{r}) - \frac{2\mu_B}{(\gamma_V+1)} B_{ext}\,\sigma_z\varphi(\vec{r}) = E'\varphi. \quad (34)$$

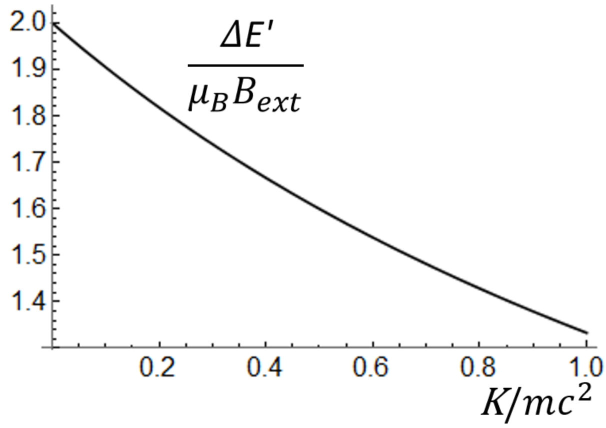

FIG. 1: Plot of twice $2/(\gamma_V+1)$ as a function of K in mc^2 units.

Equation (34) is the quasi-relativistic version of Eq. (31). When the electron moves slowly, $\gamma_V \sim 1$, thus Eq. (34) coincides with Eq. (31). Eq. (34) includes two corrections to Eq. (3). First, includes the correct relativistic relation between K and p. Second, as shown in Fig. (1), the energy difference corresponding to the two components of φ is not independent of K, as suggested by Eq. (31), but decreases by a factor of twice $2/(\gamma_V+1)$ at quasi-relativistic energies. This relevant result could be easily tested experimentally.

Relativistic corrections to the energies of the bound states in Hydrogen-like atoms

For Hydrogen-like atoms, the vector potential in Eq. (27) is null and:

$$eA_o = U_C(r) = -\frac{e^2}{4\pi\varepsilon_o}\frac{Z}{r}. \quad (35)$$

In Eq. (35), U_C is the Coulombic electrostatic energy, Z is the atomic number, and ε_o is the electric permittivity of vacuum [2, 4, 12, 15]. The exact Dirac's energies of the bound states of the electron in Hydrogen-like atoms are given by the following equation [2]:

$$E' = \mu c^2 \left[1 + \left(\frac{Z\alpha}{n - \left(j + \frac{1}{2}\right) + \sqrt{\left(j + \frac{1}{2}\right) - Z^2\alpha^2}} \right)^2 \right]^{-\frac{1}{2}} - \mu c^2. \quad (36)$$

In Eq. (36), $n = 1, 2, \ldots, l = 0, 1, \ldots (n-1), j = l \pm ½$, $\alpha = (1/4\pi\varepsilon_o)\times(e^2/\hbar c) \approx 1/137$ is the fine structure constant, $\mu = (m_e m_n)/(m_e+m_n)$ is the reduced mass of the electron in a Hydrogen-like atom with a nucleus of mass m_n, and m_e is the electron mass [2]. Often the following approximation to Eq. (36), which is valid when $E' << mc^2$, is obtained using a perturbative approach based in the Schrödinger equation [2, 14]:

$$E' = E_{Sch}\left(1 + \Delta E_{K,Sch} + \Delta E_{D,Sch} + \Delta E_{SO,Sch}\right). \quad (37)$$

In Eq. (37), E_{Sch} gives the values, of the bounded energies of the electron in Hydrogen-like atoms, obtained using the Schrödinger equation [1-5, 12]:

$$E_{Sch} = -\left[\frac{\mu}{2\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_o}\right)^2\right]\frac{Z^2}{n^2} = -\frac{\mu c^2}{4}\frac{\alpha^2 Z^2}{n^2} \quad (38)$$

$\Delta E_{K,Sch}$ is the relativistic correction to the kinetic energy, which is given by the following expression [2, 11-14]:

$$\Delta E_{K,Sch} = -E_{Sch}\,\frac{\alpha^2 Z^2}{n^2}\left(\frac{3}{4} - \frac{n}{l+\frac{1}{2}}\right) \quad (39)$$

$\Delta E_{D,Sch}$ is the so-called the Darwin correction, which is only not null when $l = 0$ [2, 14]:

$$\Delta E_{D,Sch} = -E_{Sch}\,\frac{\alpha^2 Z^2}{n} \quad (40)$$

Finally, $\Delta E_{SO,Sch}$ is the so-called spin-orbit correction, which is only not null when $l \neq 0$ [2, 14]:

$$\Delta E_{D,Sch} = -E_{Sch}\,\frac{\alpha^2 Z^2}{2n}\frac{j(j+1) - l(l+1) + 3/4}{l\left(l+\frac{1}{2}\right)(l+1)} \quad (41)$$

From Eqs. (38) to (41) follows the relativistic corrections are much smaller that E_{Sch} when $(\alpha Z/n)^2 << 1$. One should expect the energies calculated using Eq. (37) sensibly differs from the exact Dirac's energies for the lowest energy states (smallest n-values) of heavy Hydrogen-like atoms. At this point, however, no one should be surprised because following a similar procedure than the used for obtaining Eq. (37), but using a perturbative approach based in the quasi-relativistic wave equation (details shown in the Appendix), one can find a much better approximation to Eq. (36), which is valid until quasi-relativistic energies:

$$E' = E_{QR}\left(1 + \Delta E_{D,QR} + \Delta E_{SO,QR}\right). \quad (42)$$

In Eq. (42), E_{QR} gives the bound energies obtained using the quasi-relativistic wave equation for Hydrogen-like atoms [15]:

$$E_{QR} = -\frac{\mu c^2}{\Xi}\left[\Xi - (2n + \Delta)\sqrt{\Xi}\right]. \quad (43)$$

In Eq. (43), $\Delta = \Delta(l, Z)$ and Ξ are given by the following equations [15]:

$$\Xi = 4n^2 + 4\alpha^2 Z^2 + 4n\Delta + \Delta^2. \quad (44)$$

$$\Delta(l, Z) = \left[\left(1 + \sqrt{(1+2l)^2 - 4\alpha^2 Z^2}\right) - 2(l + 1)\right], \quad \sqrt{(1+2l)^2 - 4\alpha^2 Z^2} \approx (1+2l) - \frac{2\alpha^2 Z^2}{(1+2l)} - \frac{2\alpha^4 Z^4}{(1+2l)^3}. \quad (45)$$

In some cases, for heavy Hydrogen-like atoms with Z >> 1, the term inside the square root in Eq. (45) could be negative; in these cases, the approximation to the square root included in Eq. (45) should be used. As should be expected, $E_{QR} = E_{Sch}(1 + \Delta E_{K,Sch})$ when $E' << mc^2$ [15]. $\Delta E_{D,QR}$ is the new Darwin correction, which also is only not null when $l = 0$:

$$\Delta E_{D,QR} = -k_D E_{QR}\,\frac{\alpha^2 Z^2}{n}, \; k_D = \left(\gamma_V + 1\right)^{\frac{n}{n+1}}. \quad (46)$$

$\Delta E_{SO,QD}$ is the new spin-orbit correction, which also is only not null when $l \neq 0$:

$$\Delta E_{D,Sch} = -k_{SO} E_{QR}\,\frac{\alpha^2 Z^2}{2n}\frac{j(j+1) - l(l+1) + \frac{3}{4}}{l\left(l+\frac{1}{2}\right)(l+1)}, \; k_{SO} = \left(\frac{\gamma_V + 1}{2}\right)^{-(n-l+1)^{5/2}} \quad (47)$$

The energies of the ground state ($n = 1$, $l = 0$, $j = ½$) of the Hydrogen atom (Z = 1) calculated using Eqs. (36), (37), (38), (42), and (43) are E' = -13.6022, -13.6022, -13.6020, -13.6019, and -13.6029 eV, respectively. All these values are within a 0.005 % error respect to the exact Dirac's energy. This is because $E' << mc^2$ when $Z = 1$. A comparison between the calculated values of the energy difference between two emission lines (ΔE_L) of the Hydrogen atom are shown in Table 1.

ΔE_L (meV)	α-Lyman	α-Balmer	Other
Eq. (36)	0.0452718	0.0134139	0.00447118
Eq. (37)	0.0452703	0.0134134	0.00447114
Eq. (42)	0.0452715	0.0134138	0.00447119

TABLE 1: Hydrogen atom calculated values of ΔE_L (in meV) obtained using Eqs. (36), (37), and (42) for (a) α-Lyman doublet, (b) α-Balmer doublet, and (c) corresponding to the energy difference between two others emission lines.

ΔE_L was calculated using the following equation:

$$\Delta E_L = \left[E'\left(n_2,\ l_2,\ j_2 = l_2 + \tfrac{1}{2}\right) - E'\left(n_1,\ l_1,\ j_1 = l_1 + \tfrac{1}{2}\right)\right] - \left[E'\left(n_2,\ l_2,\ j_2 = l_2 - \tfrac{1}{2}\right) - E'\left(n_1,\ l_1,\ j_1 = l_1 + \tfrac{1}{2}\right)\right] \quad (39)$$

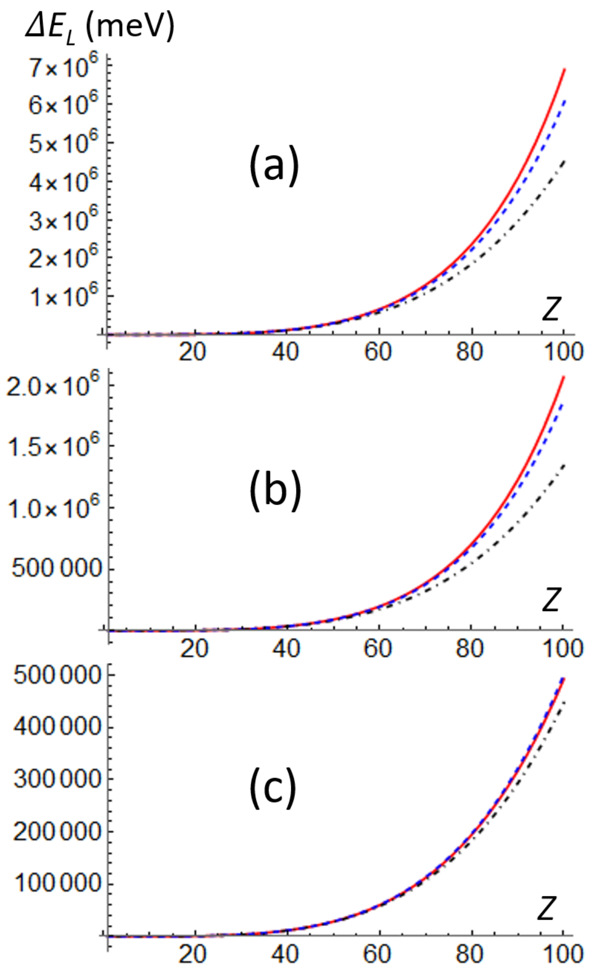

FIG. 2: Dependence on Z of ΔE_L (in meV) calculated using (red, continuous) Eq. (36), (black, dot-dashed,) Eq. (37), and (blue, dashed) Eq. (42) for (a) α-Lyman doublet, (b) α-Balmer doublet, (c) another example corresponding to the last column of Table 1.

E' was evaluated using Eqs. (36), (37), and (42). For the α-Lyman doublet: $n_2 = 2$, $l_2 = 1$ and $n_1 = 1$, $l_1 = 0$ [2, 14]. For the α-Balmer doublet, $n_2 = 3$, $l_2 = 1$ and $n_1 = 2$, $l_1 = 0$ [2, 14]. The last column of Table 1 corresponds to $n_2 = 3$, $l_2 = 2$ and $n_1 = 2$, $l_1 = 1$. It was chosen as an instance where both l_2 and l_1 are not zero. In all instances in Table 1, there is an excellent correspondence between the calculated values. Again, this is because $E' << mc^2$ when $Z = 1$. Nevertheless, Eq. (42) provides a better approximation than Eq. (37) to the values of ΔE_L calculated using Eq. (36). This is confirmed by the plots shown in Fig. 1 showing the dependence on Z of ΔE_L. Clearly, as expected, at quasi-relativistic energies ($Z >> 1$), Eq. (42) provides a much better approximation than Eq. (37) to the values of ΔE_L calculated using the exact Dirac's energies.

Conclusions.

It was shown that the time dependent Eqs. (1) and (18), and the time-independent Eq. (20) are very useful equations which are directly related to the Klein-Gordon equation, thus allowing a quantum description of a constant number of spin-0 particles moving at quasi-relativistic energies. It was presented and discussed, for the first time, a Pauli-like quasi-relativistic wave equation which is directly related to the Dirac equation, thus allowing for a quantum description of a constant number of spin-1/2 particles moving at quasi-relativistic energies and interacting with an external electromagnetic field. Finally, using a perturbative approach based on the quasi-relativistic wave equations discussed in this work, it was found and validated, also for the first time, an equation giving the energies of the bound states in Hydrogen-like atoms. The author hopes he has been able to motivate the curiosity of the readers. Undoubtedly, the equations and methods discussed here enrich the accumulated physics knowledge, open new ways to tackle quantum problems involving a constant number of particles at quasi-relativistic energies, and provides interesting pedagogical opportunities for a fresh approach to the introduction of relativistic effect in introductory quantum mechanics courses.

Appendix

Equations (37) and (42) can both be obtained from Eqs. (27) with $\vec{A} = 0$ and eA_o given by Eq. (35). For obtaining Eq. (37), Eq. (28) should be approximated in the following way [2]:

$$\chi \approx \frac{1}{2mc}\left(1 - \frac{E' - U_C}{2mc^2}\right)\left[\overrightarrow{(\hat{\sigma})} \cdot \overrightarrow{(\hat{p})}\right]\varphi . \quad (A1)$$

Then, substituting Eq. (A1) in the top equation of Eq. (27) results [2]:

$$\frac{1}{2m}\left[\overrightarrow{(\hat{\sigma})}.\overrightarrow{(\hat{p})}\right]\left(1-\frac{E'-U_C}{2mc^2}\right)\left[\overrightarrow{(\hat{\sigma})}.\overrightarrow{(\hat{p})}\right]\varphi = \left[E' - U_C(r)\right]\varphi. \quad (A2)$$

Or:

$$\left[-\frac{\hbar^2}{2m}\nabla^2\varphi + U_C(r)\right]\varphi - \left\{\frac{1}{2m}\left[\overrightarrow{(\hat{\sigma})}.\overrightarrow{(\hat{p})}\right]\left[\frac{E'-U_C(r)}{2mc^2}\right]\left[\overrightarrow{(\hat{\sigma})}.\overrightarrow{(\hat{p})}\right]\right\}\varphi = E'\varphi \quad (A3)$$

The time-independent Schrödinger equation for Hydrogen-like atoms is equal to Eq. (A3) after excluding the term between curls in the left size of Eq. (A3) [1-5]; therefore, the relativistic corrections to the energies calculated using the Schrödinger equation are contained in this term [2]. However, if Eq. (28) is approximated in the following way:

$$\chi \approx \frac{1}{(\gamma_V+1)mc}\left(1+\frac{U_C}{(\gamma_V+1)mc^2}\right)\left[\overrightarrow{(\hat{\sigma})}.\overrightarrow{(\hat{p})}\right]\varphi . \quad (A4)$$

Then, substituting Eq. (A4) in the top equation of Eq. (27) results:

$$\frac{1}{(\gamma_V+1)m}\left[\overrightarrow{(\hat{\sigma})}.\overrightarrow{(\hat{p})}\right]\left(1+\frac{U_C}{(\gamma_V+1)mc^2}\right)\left[\overrightarrow{(\hat{\sigma})}.\overrightarrow{(\hat{p})}\right]\varphi = \left[E' - U_C(r)\right]\varphi. \quad (A5)$$

Or:

$$\left[-\frac{\hbar^2}{(\gamma_V+1)m}\nabla^2\varphi + U_C(r)\right]\varphi + \left\{\frac{1}{2m}\left[\overrightarrow{(\hat{\sigma})}.\overrightarrow{(\hat{p})}\right]\left[\frac{U_C(r)}{(\gamma_V+1)mc^2}\right]\left[\overrightarrow{(\hat{\sigma})}.\overrightarrow{(\hat{p})}\right]\right\}\varphi = E'\varphi \quad (A6)$$

The time-independent quasi-relativistic wave equation for Hydrogen-like atoms is equal to Eq. (A6) after excluding the term between curls in the left size of Eq. (A6) [12]; therefore, the relativistic corrections to the energies calculated using the quasi-relativistic wave equation are contained in this term. In Eq. (A3), the term between curls produces three relativistic corrections to the energy, which are given by Eqs. (39) to (41) [2]. It can be shown, following the same procedure [2], but using the wavefunctions satisfying the quasi-relativistic wave equation for Hydrogen-like atoms [12, 16], that the term between curls in Eq. (A6) produces two relativistic corrections to the energy, which are given by Eqs. (46) and (47).

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