Did Schrödinger have other options?

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Wave mechanics triumphed when Schrödinger published his now famous equation and showed how to describe Hydrogen-like atoms using it. However, while looking for the right equation, Schrödinger first explored, but did not publish, the equation that we today call the Klein-Gordon equation. An alternative possible choice is explored in this work. It is shown a quasi-relativistic wave equation which solutions match the Schrödinger's results at electron energies much smaller than the energy associated to the electron's mass, but include the relativistic Thomas correction at higher energies. A discussion is presented about several consequences that would follow from using this quasi-relativistic wave equation as a quantum mechanics foundational equation.

Introduction

The Schrödinger equation is the most famous equation in Quantum Mechanics [1-5]. In 1926, Erwin Schrödinger published his now famous equation and showed how to describe Hydrogen-like atoms using it [6]. However, it is now known that while looking for the right equation, Schrödinger first explored, but did not publish, the equation that we today call the Klein-Gordon equation, which was first published also in 1926 by Oskar Klein and Walter Gordon [7-8]. Schrödinger was well-aware of the Einstein's Special Theory of Relativity; thus, he was looking for a Lorentz invariant wave equation [7-9]. 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 [7-9]. In contrast, the Galilean invariance of the Schrödinger equation means that two such observers will only agree in the adequacy of the Schrödinger equation, for describing the movement of a quantum particle, when the relative speeds between the observers is much smaller that the speed of the light in the vacuum (c). In practice, this is not a terrible limitation of the Schrödinger equation because up to today humans have been only able to travel at speeds much smaller than c. This is one of the principal reasons why the Schrödinger equation is still relevant almost 100 years after its discovery. Moreover, there is another important limitation of the Schrödinger equation: it describes a particle with mass (m), which linear momentum (p) and kinetic energy (K) are related by the classical relation $K = p^2/(2m)$, which is not valid at relativistic speeds [7-9]. Nevertheless, wave mechanics triumphed when Schrödinger, using the equation chosen by him, was able to reproduce the results previously obtained by Bohr for the energies of the bound 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]. Rigorously, the number of particles may not be constant in a fully relativistic quantum theory [7-8]. This is because when the sum of the kinetic and the potential (U) energy of a particle with mass m equals the energy associate to the mass of the particle, i.e., *Ȩ* $= K + U = mc^2$, then a second particle with the same mass could be created from Ȩ. Consequently, the number of particles is constant when *Ȩ* $= K + U < mc^2$. This is what happens in atoms and molecules; thus, this explains why the results obtained using the Schrödinger equation are a good first approximation in chemistry applications [5].

In between the Galilean invariant Schrödinger equation and the fully relativistic quantum mechanics, there is a quasi-relativistic energy region where *Ȩ* $+ U < mc^2$ but *Ȩ* is so large that it is necessary to use an equation that describes a particle having a relativistic relation between p and K. It is then argued in this work that there is an intermediate option between the one chosen by Schrödinger (the equation named after him) and the one discarded by him (the Klein-Gordon equation). This third option, which is valid in the quasi-relativistic energy region, is the following wave equation [11-13]:

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

In Eq. (1), $\hbar$ is the Plank constant (h) divided by 2π, and γ_V a relativistic parameter depending on the square of the particle speed (V^2) [9]:

$$\gamma_V = \frac{1}{\sqrt{1-\frac{V^2}{c^2}}}. \quad (2)$$

There is a striking similitude between the quasi-relativistic wave equation explored here (Eq. (1)) and the Schrödinger equation [1-5]. In fact, $\gamma_V \sim 1$ when $V << c$; therefore, Eq. (1) coincides with the Schrödinger equation at low particle speeds. While Eq. (1) is Galilean invariant for observers traveling at low speeds ($V_o << c$) respect to each other [11], Eq. (1) describes a particle with mass which linear momentum and kinetic energy are related by the correct relativistic relation [11-13]. Consequently, while wondering about what would have done Schrödinger if he would have encountered this equation, the author of this work embarked in the exciting task of recreating the foundational times of wave mechanics. Facilitated by the similitude between the quasi-relativistic wave equation (Eq. (1)) and the Schrödinger equation, several interesting things have been found. First, a positive probability density can be defined for the solutions of quasi-relativistic wave equation [11]. Second, it has been possible to solve Eq. (1) in the context of several problems often included in introductory courses of quantum mechanics [11-13]; moreover, this has been done with no more difficulties than the ones encountered when solving the Schrödinger equation in the same context [1-5]. Third, a repetition of the Schrödinger success was achieved when using Eq. (1) for describing Hydrogen-like atoms [13]. It was found that the exact solutions of this equation include the relativistic Thomas correction to the energies found using the Schrödinger equation [13]. This suggests that the quasi-relativistic wave equation explored here could have been the foundational equation of quantum mechanics. Moreover, this equation could be used today for finding quasi-relativistic solutions of several practical problems, and for introducing the students to the intricacies of relativistic quantum mechanics without a notable complication of the involved mathematical techniques. In what follows, first, a brief summary of previous results is presented, then some of their consequences are discussed. Finally, the conclusions of this work are given in the last Section.

The Grave de Peralta equation

Formally, the one-dimensional (1D) Schrödinger equation for a free quantum particle with mass m can be obtained from the classical relation between K and p for a free particle when its speed (V) is much smaller than the c [1-5]:

$$K = \frac{p^2}{2m}, \;\; p = mV. \quad (3)$$

Then, substituting K and p by the following energy and momentum quantum operators [1-4]:

$$\hat{E} = \hat{K} = i\hbar\frac{\partial}{\partial t}, \;\; \hat{p} = -i\hbar\frac{\partial}{\partial x}. \quad (4)$$

Results the 1D Schrödinger equation for a free quantum particle with mass m [1-5]:

$$i\hbar\frac{\partial}{\partial t}\psi_{Sch}(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_{Sch}(x,t). \quad (5)$$

However, Eq. (3) does not give the correct relation between K and p when the particle moves at faster speeds. Correspondingly, the Schrödinger equation (Eq. (5)) is not Lorentz invariant but Galileo invariant [10-11]; thus, only should be used for slowly moving particles. At larger particle's speed, one should use the following well-known relativistic relations [9]:

$$E^2 - m^2c^4 = p^2c^2 \;\Leftrightarrow (E+mc^2)\,(E-mc^2) = p^2c^2. \quad (6)$$

And:

$$E = \gamma_V mc^2, \; p = \gamma_V mV, \;\; E = K + mc^2. \quad (7)$$

One can then formally proceed as it is done for obtaining the 1D Schrödinger equation, and use Eq. (4) for assigning the temporal partial derivative operator to E in the first expression of Eq. (6) [7-8, 11]. In this way, one can formally obtain the 1D Klein-Gordon equation [7-8]:

$$\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\psi_{KG}(x,t) = \frac{\partial^2}{\partial x^2}\psi_{KG}(x,t) - \frac{m^2c^2}{\hbar^2}\psi_{KG}(x,t). \quad (8)$$

The Klein-Gordon equation is Lorentz invariant and describes a free quantum particle with mass m and spin-0 [7-8]. In contrast to the Schrödinger equation, a second-order temporal derivative is present in Eq. (8). This determines that Eq. (8) has solutions with positive and negative energy values while Eq. (5) has only solutions with positive energies, which is in correspondence with K having only positive values in Eq. (3) but E having positive and negative values in Eq. (6). The factor $(E + mc^2)$ is always different than zero for $E > 0$; consequently, Eq. (6) and the following algebraic equation are equivalents for $E > 0$:

$$(E - mc^2) = \frac{p^2}{(\gamma_V + 1)m} \quad (9)$$

Each member of Eq. (9) is just a different expression of the relativistic kinetic energy of the particle [11]. Assigning the temporal partial derivative operator in Eq. (4) to E in Eq. (9) results in the following differential equation [12]:

$$i\hbar\frac{\partial}{\partial t}\psi_{KG+}(x,t) = -\frac{\hbar^2}{(\gamma_V+1)m}\frac{\partial^2}{\partial x^2}\psi_{KG+}(x,t) + mc^2\psi_{KG+}(x,t)\,. \quad (10)$$

A simple substitution in Eqs. (8) and (10) shows that the following plane wave is a solution of both equations for $E > 0$:

$$\psi_{KG+}(x,t) = e^{\frac{i}{\hbar}(px-Et)}, \quad (11)$$

The plane wave ψ_{KG+} has an unphysical phase velocity equal to $c^2/V > c$ [11-12]. However, one can look for a solution of Eq. (10) of the following form:

$$\psi(x,t) = \psi_{KG+}e^{iw_m t}, \; w_m = \frac{mc^2}{\hbar}. \quad (12)$$

Such that ψ has a phase velocity smaller than c [11-12]; thus:

$$\psi(x,t) = e^{\frac{i}{\hbar}(px-Kt)}. \quad (13)$$

Substituting ψ given by Eq. (12) in Eq. (10) results in the 1D Grave de Peralta equation for a free quantum particle with mass m and spin-0 [11-13]:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{(\gamma_V+1)m}\frac{\partial^2}{\partial x^2}\psi(x,t). \quad (14)$$

At low particle's speeds, Eq. (14) clearly coincides with the 1D Schrödinger equation for a free particle with mass m. Moreover, a positive probability density can be defined for the solutions of Eq. (14) by analogy of how it is defined for the solutions of the Schrödinger equation and, like the Schrödinger equation, Eq. (14) is Galilean invariant for observers traveling at low speeds respect to each other [11]. Despite this, Eq. (14) can be used for obtaining precise solutions of very interesting quantum problems at quasi-relativistic energies [11-12], where a particle moves at so large speeds that it is necessary to use the correct relativistic relation between p and K, but where the particle should not be moving too fast so that the number of particles remains constant. When the particle moves through a 1D piecewise constant potential $U(x)$, Eq. (14) should be generalized in the following way [12-13]:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{[\gamma_V(x)+1]m}\frac{\partial^2}{\partial x^2}\psi(x,t) + U(x)\psi(x,t). \quad (15)$$

Often, one looks for solutions of Eq. (15) corresponding to a constant value of the energy $Ȩ = K + U = E + U - mc^2$. At quasi-relativistic energies, the number of particles is constant; therefore, $Ȩ$ is constant whenever $E + U$ is constant. For a 1D piecewise constant potential $Ȩ$, K, γ_V, and V^2 are constants in each x-region where U is constant. In contrast to $Ȩ$, however, K, γ_V and V^2 have a discontinuity wherever $U(x)$ has one. Consequently, γ_V is a function of x in Eq. (15) because, in general, the square of the particle's speed (V^2) depends on the position [12]. Nevertheless, for 1D piecewise constant potentials, one can look for a solution of Eq. (15) with the following form in each of the regions where K, γ_V, and V^2 are constants [1-4, 12-13]:

$$\psi(x,t) = X_K(x)e^{-\frac{i}{\hbar}Ȩt}, \; Ȩ = K + U \quad (16)$$

In Eq. (16), X_K is a solution of the following equation [1-4, 12-13]:

$$\frac{d^2}{dx^2}X_K(x) + \kappa^2 X_K(x) = 0, \; \kappa = \frac{p}{\hbar}. \quad (17)$$

And [12-13]:

$$\kappa = \frac{p}{\hbar} = \frac{1}{\hbar}\sqrt{(\gamma_V + 1)mK} = \frac{1}{\hbar}\sqrt{(\gamma_V + 1)m(Ȩ - U)}\;. \quad (18)$$

Consequently, κ and X_K are not determined by the values of $Ȩ$ but by the values of $K = Ȩ - U$. Once the allowed values of κ are determined from Eq. (17) and the boundary conditions, the allowed values of the relativistic kinetic energy of the particle $K = Ȩ - U$ are given by:

$$K = \frac{\hbar^2 \kappa^2}{(\gamma_V + 1)m}. \quad (19)$$

As expected, when $\gamma_V \sim 1$, Eq. (19) gives the non-relativistic values of the particle's energies at low speeds, $K \sim \hbar^2\kappa^2/(2m)$ [1-4]. Moreover, from Eq. (19) and the relativistic equation, $K = (\gamma_V - 1)\, mc^2$, follows that [12-13]:

$$\gamma_V{}^2 = 1 + \left(\frac{\lambda_C}{\lambda}\right)^2, \ \lambda_C = \frac{h}{mc}, \ \lambda = \frac{2\pi}{\kappa}. \quad (20)$$

In Eq. (20), λ_C is the Compton wavelength associate to the mass of the particle [7, 9], and λ is the De Broglie wavelength associated to p [1-4]. Substituting Eq. (20) in Eq. (19) allows obtaining an analytical expression of the precise quasi-relativistic kinetic energy of the particle [13]:

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

As expected, Eq. (21) match the non-relativistic expression of the particle's kinetic energy when $p = h/\lambda$ is very small because $\lambda >> \lambda_C$. However, in each region where the value of U is constant, the values of K and then $E = K + U$ calculated using Eq. (21) are smaller than the ones calculated using the Schrödinger equation. Several 1D problems have been solved using Eq. (15) including the 1D infinite rectangular well [11], the quantum rotor [11], reflection in a potential step [12], tunneling through a barrier [12], and bound states in a rectangular well [12]. The tridimensional Eq. (1) has been solved for a central potential including the infinite spherical well and the Coulomb potential in Hydrogen like atoms [13]. The last case is particularly important because permits a detailed comparison between the theoretical results and the experimental data. [13]. In all these cases, the solutions of the Grave de Peralta equation were found following the same procedures than the ones used for solving the Schrödinger equation in those cases. This could permit the easy introduction in introductory quantum mechanics courses of non-perturbative relativistic corrections to the Schrödinger equation.

Some consequences of the quasi-relativistic wave equation

When solving both the Grave de Peralta and the Schrödinger equation, for the 1D rectangular and the spherical infinite wells, the obtained values of κ are given by the following equation [4, 11, 13]:

$$\kappa_n = \frac{n\pi}{\mathcal{L}}, n = 1,2, \ldots \quad (22)$$

In Eq. (22), $\mathcal{L}$ is the length of the 1D well or the diameter of the spherical one. Consequently:

$$K_n = \frac{n^2}{\left[1 + \sqrt{1 + \left(\frac{n\lambda_C}{\mathcal{L}}\right)^2}\right]} \left(\frac{\lambda_C}{\beta\mathcal{L}}\right)^2 mc^2. \quad (23)$$

For the spherical well, the parameter $\beta = 1$ but $\beta = 1/2$ for the 1D well. As expected, the term between brackets in Eq. (23) is ~ 2 when $n = 1$ and $\mathcal{L} >> \lambda_C$; thus, $K_1 << mc^2$ and K_1 given by Eq. (23) coincides with the energies of the infinite wells calculated using the Schrödinger equation [4]. In contrast, when the dimension of the well is close to λ_C, the minimum particle energy is quasi-relativistic; therefore, Eq. (23) must be used. From Eq. (23) follows a fundamental connection between quantum mechanics and especial theory of relativity: no single particle with mass can be confined in a volume much smaller than $\lambda_C{}^3$ because when this occurs, $K > mc^2$ and the number of particles may not be constant anymore; therefore, a single point-particle with mass cannot exist. Point-particles with mass can only exist in fully relativistic quantum field theories where the number of particles is not constant [11-13]. This is a fundamental and general statement in relativistic quantum mechanics [7-8]. Introducing the quasi-relativistic equation then provides a simple but precise way to present this concept in introductory quantum mechanics courses. Moreover, due to the fact that this statement just refers to the confinement of a particle with mass, one could adventure the following far reaching consequences: it is impossible to confine a single particle with mass in a point, this should be true for an electron, a quark, and probably may also be true for a black hole and the whole universe at the beginning of the Big Bang.

Solving Eq. (1) for the Coulomb potential in Hydrogen like atoms allows for checking the validity of the quasi-relativistic wave equation. Moreover, this also permits to find out what is included and what is not in the quasi-relativistic approximation. Due to its importance, a summary of the solution of the Grave de Peralta equation for Hydrogen-like atoms is given in the Annex A. The values of E for the bound states calculated by solving Eq. (1) are approximately given by the following equation [13]:

$$E_{n,l} \sim E_{n,Sch} Z^2 \left(1 + \frac{2\alpha^2}{n(2l+1)}\right) . \quad (24)$$

In Eq. (24), Z is the atomic number, l is an integer in the interval from 0 to (n-1), α is the fine-structure constant [7-8]:

$$\alpha = \frac{1}{4\pi\varepsilon_o} \frac{e^2}{\hbar c} \sim 1/137 . \quad (25)$$

And $E_{n,Sch}$ corresponds to the bounded energies values of the electron in the Hydrogen atom calculated using the Schrödinger equation [2-4]:

$$E_{n,Sch} = -\left[\frac{\mu}{2\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_o}\right)^2\right]\frac{1}{n^2} , \quad n = 1, 2, 3, ... \quad (26)$$

In Eq. (26), $\mu=(m_e m_n)/(m_e+m_n)$ is the reduced mass of the electron in a hydrogen-like atom with a nucleus of mass m_n; m_e and e are the electron mass and charge, respectively; and ε_o is the electric permittivity of vacuum. The exact values of $E_{n,l}$, which are calculated by exactly solving Eq. (1) as described in Annex A, can be validated by comparing them to the electron energies calculated by adding, as a first perturbative correction, the relativistic Thomas correction to Eq. (26); i.e., comparing to the values obtained using the following expression [14]:

$$E_{n,l,Th} \sim E_{n,Sch} Z^2 \left\{1 - \frac{\alpha^2}{n^2}\left[\frac{3}{4} - \frac{n}{l+\frac{1}{2}}\right]\right\} . \quad (27)$$

(n,l)	Eq. (1) - Eq(26)	Eq. (27) - Eq(26)
(1,0)	-0.905260	-0.905159
(2,0)	-0.147102	-0.147088
(2,1)	-0.026401	-0.026400
(3,0)	-0.046938	-0.046934
(3,1)	-0.011175	-0.011174
(3,2)	-0.004023	-0.004022

Table 1: Values of E_{nl} - $E_{n,Sch}$ (second column) and $E_{nl,Th}$ - $E_{n,Sch}$ (third column) in meV.

Table 1 shows energy differences values in meV corresponding to the Hydrogen's (Z=1) electron states with n = 1, 2, and 3. The values in the second column corresponds to the difference between the exact values of E_{nl} calculated by solving the Eq. (A16) as described in Annex A, and the values of $E_{n,Sch}$ given by Eq. (26). The energy difference values in the second column corresponds to the difference between the values of $E_{nl,Th}$ given by Eq. (27) and the values of $E_{n,Sch}$. By comparing the values reported in both columns, as should be expected because the relativistic Thomas correction includes the difference between the correct relativistic and the non-relativistic expression of K [14], one can conclude that the electron energies calculated using the quasi-relativistic wave equation (Eq. (1)) includes the relativistic Thomas correction. This also permits to realize the limitations of Eq. (1). It is well-know that the Dirac equation is the correct relativistic equation for describing the bounded states of the electron in a Hydrogen-like atom [7-8]. Besides the relativistic Thomas correction, two other corrections to Eq. (26) should be included for describing the fine structure of the Hydrogen spectrum [14]. Neither the Darwin nor the spin-orbit corrections are included in the quasi-relativistic wave equation [13-14]. Nevertheless, it is good to emphasize that Eq. (1) exactly includes the correct relativistic relation between p and K. The Grave de Peralta equation for Hydrogen-like atoms can be exactly solved [13], while the relativistic Thomas correction is just an approximate result.

The superposition principle is one of the pillars of quantum mechanics [1-4]. The Schrödinger, the Klein-Gordon, and the Dirac equations are all linear equations. This means, for instance, that if $\psi_1$and ψ_2 are two solutions of any of these equations for a particle in an infinite well corresponding to different values of K, then the wavefunction $\psi = a\psi_1 + b\psi_2$, where a and b are complex numbers such that $|a|^2 + |b|^2 = 1$, is also a solution of the linear equation. The wavefunction ψ represents a legitime possible state of a particle in the infinite well. The superposition state represented by ψ is often interpreted as an state where the particle is neither in the state ψ_1 where the kinetic energy is K_1 nor in the state ψ_2 where the kinetic energy is K_2, but somehow the particle is simultaneously in both states. The existence of superposition states like ψ is then a fundamental consequence, with no classical counterpart, of the linearity of the foundational equation. This exemplifies the weirdness of quantum mechanics [10, 15]. However, neither the Grave de Peralta equation nor Eq. (10) are linear. If $\psi_1$and ψ_2 are two solutions of Eq. (1) for a particle in an infinite well corresponding to different values of V^2, then strictly speaking, they are not solutions of the same Eq. (1) but of slightly different Eqs. (1) with different values of γ_V. Moreover, $\psi = a\psi_1 + b\psi_2$ is not a solution of any Eq. (1). Consequently, if the Grave de Peralta equation could be a foundational equation, then the validity of the superposition principle in quantum mechanics should be questioned or revised [11]. May be this is why Schrödinger settled for the equation named after him instead of using a non-linear quasi-relativistic wave equation, which can be solved with no more difficulties than the ones present when solving the Schrödinger equation, but gives more precise results than the equation that he chose. Nevertheless, the existence of such non-linear equation rises the intriguing possibility of a quantum mechanics based on a non-linear wave equation. This is currently important because it is often assumed that the superposition state ψ represent a qubit, concept that is at the heart of current attempts for demonstrating a practical quantum computer [15-16]. Would the eventual demonstration of a quantum computer exclude the possible existence of a quantum mechanics without a superposition principle? Could exist an alternative explanation of the eventual demonstration of a quantum computer that was based in a foundational non-linear wave equation? These are fascinating questions of current interest that are motivated by a third option that may be Schrödinger did not consider.

Alternatively, the non-linearity of the Grave de Peralta equation could indicate that it is not a foundational wave equation but a kind of eigenvalue equation like, for instance, Eqs. (17) and (A9) (shown in Annex A). This can be made evident by using Eq. (7) for eliminating γ_V from Eq. (1), thus rewriting Eq. (1) as the following eigenvalue equation where ψ and $Ȩ$ should be found simultaneously:

$$i\hbar\frac{\partial}{\partial t}\psi = -\frac{c^2\hbar^2}{[Ȩ-U]+2\mu c^2}\nabla^2\psi + U\psi. \qquad (28)$$

While both forms of the same equation are equivalent, Eq. (1) is more suggestive due its striking similarity to the Schrödinger equation. The foundational equation corresponding to Eqs. (1) and (28) would then be the Klein-Gordon equation, which is linear and Lorentz invariant. For instance, let be $\psi_1$and ψ_2 two solutions of the non-linear 1D Grave de Peralta equation (Eq. (14)), for a particle in an infinite well, and corresponding to different values of $Ȩ = K$; therefore, the wavefunction $\psi = a\psi_1 + b\psi_2$ is not a solution of Eq. (14). However, due to Eq. (12), a solution of Eqs. (8) and (10) can be found from a solution of Eq. (14) in the following way:

$$\psi_{KG+}(x,t) = \psi(x,t)e^{-iw_m t},\ w_m = \frac{mc^2}{\hbar}. \qquad (29)$$

Therefore, if $\psi_{KG+,1}$ and $\psi_{KG+,2}$ are respectively related to ψ_1 and ψ_2 through Eq. (29); then, the wavefunction $\psi_{KG+,1,2} = a\psi_{KG+,1} + b\psi_{KG+,2}$ is not a solution of the non-linear Eq. (10) but, due to the linearity of Eq. (8), $\psi_{KG+,1,2}$ is a solution of the 1D Klein-Gordon equation. From this point of view, Eq. (1) provides a useful way to find exact solution of the Klein-Gordon equation with positives energies when $Ȩ = K + U < mc^2$. The Schrödinger equation then appears as a limit case of the Grave de Peralta equation when $Ȩ << mc^2$. Luckily, the Schrödinger equation recovers the linearity required by the superposition principle. This allowed Schrödinger to construct a non-relativistic quantum mechanics based on the equation named after his genius.

Conclusions

Several properties of the solutions of the Grave de Peralta equation were summarized and discussed. It was shown that this quasi-relativistic equation can be solved following the same procedures and mathematical techniques needed for solving the Schrödinger equation; however, the results obtained are valid for particles energies where the correct relativistic relation between p and K must be used. This suggest the academic use of the Grave de Peralta equation for introducing the students to the implications of the special theory of relativity in introductory quantum mechanics courses. In addition, several consequences that would follow from using this quasi-relativistic wave equation as a quantum mechanics foundational equation were discussed. It was argued that no single particle with mass can be confined in a point, and it was suggested that this statement may be extrapolated to black holes and the whole universe at the beginning of the Big Bang. It was also suggested that the current febrile competition for demonstrating a practical quantum computer obligates us to think about the possibility or not of the existence of a quantum mechanics theory based on a non-linear foundational wave equation. Finally, it was clarified the existing relationship between the Klein-Gordon, the Grave de Peralta, and the Klein-Gordon equation.

Annex A:

The Grave de Peralta equation for Hydrogen-like atoms is given by the following expression [13]:

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) = -\frac{\hbar^2}{[\gamma_V(r)+1]\mu}\nabla^2\psi(\vec{r},t) + U_C(r)\psi(\vec{r},t). \quad \text{(A1)}$$

The Coulomb potential is given by:

$$U_C(r) = -\frac{e^2}{4\pi\varepsilon_o}\frac{Z}{r}\ . \quad \text{(A2)}$$

Equation (A1) can be solved looking for a solution of the form [1, 13]:

$$\psi(r,\theta,\varphi,t) = R(r)\Omega(\theta,\varphi)e^{\frac{i}{\hbar}Ɇt}. \quad \text{(A3)}$$

Substitution of Eq. (A3) in Eq. (1) then results in [1, 13]:

$$\frac{1}{r}\frac{d^2}{dr^2}(rR) + \frac{[\gamma_V(r)+1]\mu r^2}{\hbar^2}[Ɇ - U(r)]R = -l(l+1)\frac{R}{r^2}. \quad \text{(A4)}$$

And:

$$\Omega_{l,m}(\theta,\varphi) = Y_l^{(m)}(\theta,\varphi),\ \ l = 0,1,2\ldots;\ \ m = -l,-l+1,\ldots 0,1,\ldots,l\ . \quad \text{(A5)}$$

In Eq. (A5), $Y_l^{(m)}$ are the spherical harmonic functions [1-5]. Eq. (A4) can be solved making $R(r) = \chi(r)/r$, then resulting the following equation [4, 13]:

$$\frac{d^2}{dr^2}\chi(r) + \frac{[\gamma_V(r)+1]\mu}{\hbar^2}[Ɇ - W_C(r)]\chi(r) = 0\ . \quad \text{(A6)}$$

With:

$$W_C(r) = \left[U_C(r) + \frac{\hbar^2}{[\gamma_V(r)+1]\mu}\frac{l(l+1)}{r^2}\right]. \quad \text{(A7)}$$

As expected, when $V << c$ then $\gamma_V \sim 1$; therefore, Eq. (A7) reduces to the radial equation of a hydrogen-like atom obtained using the Schrödinger equation [4]. Using Eq. (7), it is possible to eliminate γ_V from Eqs. (A6) and (A7) by making:

$$\frac{[\gamma_V(r)+1]\mu}{\hbar^2} = \frac{K+2\mu c^2}{c^2\hbar^2} = \frac{[Ɇ-U_C(r)]+2\mu c^2}{c^2\hbar^2}. \quad \text{(A8)}$$

Using Eq. (A8) then allows for rewriting Eq. (A6) in the following way [13]:

$$\left\{-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}\chi(r) - [Ɇ - U_C(r)]\chi(r) + \frac{\hbar^2}{2\mu}\frac{l(l+1)}{r^2}\chi(r)\right\} - \frac{1}{2\mu c^2}[Ɇ - U_C(r)]^2\chi(r) = 0\ . \quad \text{(A9)}$$

The term between braces in Eq. (A9) coincides with the radial equation that should be solved when using the Schrödinger equation [4]. The last term of Eq. (A9) can be disregarded when $K << \mu c^2$; therefore, the last term is a quasi-relativistic correction to the non-relativistic radial equation. Proceeding like it is done when solving the non-relativistic radial equation, one can introduce [4, 13]:

$$\zeta = \frac{1}{\hbar}\sqrt{-2\mu Ɇ}\ . \quad \text{(A10)}$$

For bound states, $Ɇ < 0$; therefore, ζ is real. Using Eq. (A10) allows for rewriting Eq. (A9) in the following way [4, 13]:

$$\frac{d^2}{d\rho^2}\chi(\rho) = \left[\rho_1 - \frac{\rho_o}{\rho} + \frac{l(l+1) - \alpha^2 Z^2}{\rho^2}\right]\chi(\rho). \quad \text{(A11)}$$

With:

$$\rho \equiv \zeta r,\quad \rho_o \equiv \left(\frac{\mu e^2}{2\pi\varepsilon_o\hbar^2\zeta} - \alpha\frac{\hbar\zeta}{\mu c}\right)Z\ ,\quad \rho_1 \equiv \left[1 - \left(\frac{\hbar\zeta}{2\mu c}\right)^2\right]. \quad \text{(A12)}$$

Formally, when $\hbar\zeta << \mu c$ and if α was null, then Eqs. (A11) and (A10) would reduce to the corresponding equations obtained when solving the Schrödinger equation [4]; therefore, there is a relativistic correction in each term inside the brackets in Eq. (A11). Looking for a solution of Eq. (A11) of the following form [13]:

$$\chi(\rho) \equiv \tau(\rho)\ \rho^{\frac{1}{2}\left[1+\sqrt{(1+2l)^2-4\alpha^2Z^2}\right]}e^{-\sqrt{\rho_1}\,\rho}\ . \quad \text{(A13)}$$

Results [13]:

$$\rho\frac{d^2}{d\rho^2}\tau(\rho) + \left[1 - \left(2\sqrt{\rho_1}\right)\rho + \sqrt{(1+2l)^2 - 4\alpha^2Z^2}\right]\frac{d}{d\rho}\tau(\rho) + \left[\rho_o - \sqrt{\rho_1}\left(1 + \sqrt{(1+2l)^2 - 4\alpha^2Z^2}\right)\right]\tau(\rho) = 0. \quad \text{(A14)}$$

Again, as expected, if the quasi-relativistic corrections are very small, then Eq. (A14) reduces to the one obtained when using the Schrödinger equation [4, 13]. Finally, assuming that $\tau(\rho)$ can expressed as a finite power series in ρ [4, 13]:

$$\tau(\rho) = \sum_{j=0}^{j_{max}} a_j\,\rho^j. \quad \text{(A15)}$$

And substituting Eq. (A15) in Eq. (A14) results [13]:

$$\rho_o = [2n + \Delta(l,Z)]\sqrt{\rho_1}\,. \qquad \text{(A16)}$$

With:

$$\Delta(l,Z) = \left[\left(1 + \sqrt{(1+2l)^2 - 4\alpha^2 Z^2}\right) - 2(l+1)\right]. \qquad \text{(A17)}$$

Formally, when $\hbar\zeta << \mu c$ and if α was null, then Eq. (A16) would reduce to $\rho_o = 2n$, with $n = j + l + 1$, which is the resulting equation when solving the Schrödinger equation [4]. Substituting ρ_o and ρ_1 given by Eq. (A12) in Eq. (A16), solving the resulting equation for ζ, and using Eq. (A10) allows for obtaining an exact analytical expression for $\mathcal{E}$, which now depends not only on the principal quantum number n, but also on the angular quantum number l, and Z. For instance, assuming that the quasi-relativistic corrections included in ρ_o and ρ_1 do not need to be accounting for because they are too small, the effect of the quasi-relativistic correction included in the centrifugal term in Eq. (A11) is quantified by the following equation [13]:

$$\mathcal{E}_{n,l} = -\left[\frac{\mu}{2\hbar^2}\left(\frac{e^2}{2\pi\varepsilon_o}\right)^2\right]\frac{Z^2}{[2n+\Delta(l,Z)]^2}\,. \qquad \text{(A18)}$$

As expected, if α was null and $Z = 1$, Eq. (A18) would be identical to $\mathcal{E}_{n,Sch}$ given by Eq. (26). However, $\Delta(l, Z) < 0$ and $|\Delta(l, Z)|$ increases when Z increases. Therefore, for $n > 1$ and $l > 0$, the degeneration of $\mathcal{E}_{n,Sch}$ is broken by the quasi-relativistic correction $\Delta(l, Z)$. This effect is more pronounced for heavy elements. In addition, $|\Delta(l, Z)|$ decreases when l increases; therefore, $\mathcal{E}_{n,l} \rightarrow \mathcal{E}_{n,Sch}$ when l is large. Eq. (A18) can be rewritten as:

$$\mathcal{E}_{n,l} = -\mu c^2\alpha^2 Z^2\frac{1}{[2n+\Delta(l,Z)]^2}\,. \qquad \text{(A19)}$$

Then Eq. (24) can be obtained from Eq. (A19) using the following approximated relations:

$$\frac{1}{[2n+\Delta(l,Z)]^2} \sim \frac{1}{(2n)^2}\left[1 - \frac{\Delta(l,Z)}{n}\right]. \qquad \text{(A20)}$$

$$\Delta(l,Z) \sim -\frac{2\alpha^2}{2l+1}. \qquad \text{(A21)}$$

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