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Making relativistic quantum mechanics simple

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Abstract

The fundamentals of a quasi-relativistic wave equation, whose solutions match the Schrödinger results for slow-moving particles but are also valid when the particle moves at relativistic speeds, are discussed. This quasi-relativistic wave equation is then used for examining some interesting quantum problems where the introduction of relativistic considerations may produce remarkable consequences. We argue in favor of the academic use of this equation, for introducing students to the implications of the special theory of relativity in introductory quantum mechanics courses.

Keywords: quantum mechanics, relativity, relativistic quantum mechanics, foundations of physics

(Some figures may appear in colour only in the online journal)

1. Introduction

Quantum mechanics and the special theory of relativity are both taught to most undergraduate physics students [1–3]. However, due to the mathematical complexities of relativistic quantum mechanics and field theories [4, 5], the study of the consequences for quantum mechanics, of the basic concepts of the special theory of relativity, are often postponed for graduate studies.

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In this work, we argue that a recently explored quasi-relativistic wave equation may be used for introducing undergraduate students to relativistic quantum mechanics. The following equation [6–10]:

$$i\hbar\frac{\partial}{\partial t}\Psi = -\frac{\hbar^2}{(\gamma+1)\,m}\nabla^2\Psi + V\Psi, \quad \text{with} \quad \gamma = \frac{1}{\sqrt{1-\frac{v^2}{c^2}}}. \tag{1}$$

Equation (1) is so similar to the Schrödinger equation that once one learns to solve the latter, then the former should be easy to solve as well. We discuss practical strategies for doing so in section 2. Note that spin does not appear explicitly in the 'Hamiltonian' (right side) of equation (1). We can either take this equation to describe a spin-zero boson particle, or a particle with any spin for which the spin degree of freedom may be ignored. Either way, the solution Ψ is presumed to be a *spatial* wavefunction only.

In equation (1) above, m is the mass of the particle, $\hbar$ is the Plank constant (h) divided by 2π, V is a (scalar) potential energy function, and γ is the well-known Lorentz parameter [1, 2], which appears in numerous formulas in the special theory of relativity and depends on the ratio v^2/c^2, where v^2 and c^2 are the squares of the speeds of the particle, and of light in vacuum, respectively. Clearly, $\gamma \sim 1$ when $v^2 \ll c^2$; therefore, equation (1) reduces to the Schrödinger equation in the limit of low particle speeds. However, as is discussed below, when $\gamma > 1$, equation (1) exactly accounts for the quantum mechanical consequences of relativity, in Lorentz-invariant fashion.

Specifically, the relation between the kinetic energy (K) and the linear momentum (p) of a fast-moving particle is not $K_{\text{Sch}} = p^2/2m$ (as in the Schrödinger equation), but $K = p^2/(\gamma + 1)m$—which is given here in a very specific form that has proven to be *exceptionally* useful for quantum mechanics [1, 2, 6, 7]. Moreover, equation (1) can be straightforwardly applied to various practical quantum mechanics problems, in order to smoothly generalize known non-relativistic solutions into the relativistic domain.

In what follows, first, a summary of the fundamentals of equation (1) is presented in section 2. Then in section 3, a simple pedagogical problem is solved using this equation. Other examples may be found in the cited literature [6–10]. Next, it is shown in section 4, how the prediction of quantum mechanics about the size of hydrogen-like atoms is affected—in the $Z \to \infty$ limit, very dramatically—by the inclusion of special relativity in the calculations. Then, in section 5, a bold relativity-related hypothesis is discussed. Specifically, we discuss, using arguments based exclusively on quantum mechanics and special relativity concepts, the possible existence of a critical mass separating the quantum and classical worlds. Finally, the conclusions of this work are given in section 6.

2. Fundamentals

In the special theory of relativity, the relevant Lorentz-invariant quantity is the four-component momentum vector given by the following equation [4, 11]:

$$P^\mu = \left(\frac{E}{c}, p_x, p_y, p_z\right). \tag{2}$$

The magnitude of this 'mechanical momentum' four-vector is the Lorentz-invariant scalar quantity, mc. Therefore, a relativistic quantum theory for a free particle of mass m can be formally obtained from first quantization of the Lorentz-invariant relation between the particle's energy (E) and the three-component momentum vector [4]:

$$\sqrt{\frac{E^2}{c^2} - \vec{p}^2} = mc, \quad \text{with} \quad \vec{p}^2 = p_x^2 + p_y^2 + p_z^2. \tag{3}$$

For instance, we can square equation (3) and obtain:

$$E^2 = m^2c^4 + \vec{p}^2c^2. \tag{4}$$

Then, by making in equation (4) the following formal first-quantization procedure substitutions [4],

$$E \to \widehat{H} = i\hbar\frac{\partial}{\partial t}, \quad \text{and} \quad \vec{p} \to \hat{p} = -i\hbar\nabla, \tag{5}$$

we obtain the well-known Lorentz-invariant Klein–Gordon equation for a free spin-0 particle of mass m [4]:

$$\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\Omega_{\mathrm{KG}} = \nabla^2\Omega_{\mathrm{KG}} - \frac{m^2c^2}{\hbar^2}\Omega_{\mathrm{KG}}. \tag{6}$$

Alternatively, we can start by rewriting equation (3) in the following way [12, 13]:

$$E = mc^2\sqrt{1 + \frac{\vec{p}^2}{m^2c^2}} = \gamma mc^2, \quad \text{with} \quad \gamma = \sqrt{1 + \frac{\vec{p}^2}{m^2c^2}}. \tag{7}$$

Equation (7) (apart from a factor of c) represents the time-like component of the mechanical momentum four-vector—i.e. the relativistic 'mechanical energy', which includes the rest energy mc^2, as well as the kinetic energy associated with particle motion. Thus, by subtracting mc^2 from each term of equation (7), we obtain the following expressions for K, the relativistic kinetic energy of the particle [1, 2, 6, 7]:

$$E - mc^2 = (\gamma - 1)\,mc^2 = K, \quad \text{or} \quad K = \frac{\vec{p}^2}{(\gamma + 1)m}. \tag{8}$$

Note that the second equation above, which is the desired form (as discussed in section 1), may be obtained by multiplying both sides of the first equation by $(\gamma + 1)\,m$, and then substituting in the square of the second part of equation (7). As discussed, $K \to K_{\mathrm{Sch}}$ in the non-relativistic limit, but more generally, $K < K_{\mathrm{Sch}}$. It is *as if* the effective mass in equation (8) increases with increasing v^2 (e.g. the so-called 'relativistic mass'), although strictly speaking, the true or 'rest' mass m is always a Lorentz-invariant scalar.

Although ultimately we will remove the rest energy from consideration, for the moment we retain it. We thus replace equation (7) with the following Lorentz-covariant form [12, 13]:

$$E = \frac{\vec{p}^2}{(\gamma + 1)m} + mc^2, \quad \text{with} \quad \gamma = \sqrt{1 + \frac{\vec{p}^2}{m^2c^2}}. \tag{9}$$

The final step, which turns the above into a quantum mechanical result, is to apply the formal operator substitutions given by equation (5), to (9). This results in the following Lorentz-covariant wave equation:

$$i\hbar\frac{\partial}{\partial t}\Omega = -\frac{\hbar^2}{(\widehat{\gamma} + 1)\,m}\nabla^2\Omega + mc^2\Omega, \quad \text{with} \quad \widehat{\gamma} = \sqrt{1 + \frac{\hat{p}^2}{m^2c^2}}. \tag{10}$$

Now, it is well known in quantum mechanics that applying a constant energy shift to the Hamiltonian gives rise to an immaterial time-evolving phase factor in the solution wavefunction. Therefore, in order to obtain a more Schrödinger-like result, we can remove the rest-energy contribution from equation (10) above, by replacing Ω as follows:

$$\Omega(x,t) = \Psi(x,t)\mathrm{e}^{-\mathrm{i}\frac{mc^2}{\hbar}t}. \tag{11}$$

Adding, in addition, a scalar potential contribution $V\left(\vec{r}\right)$,the final result is the Poirier-Grave de Peralta (PGP) *equation* [13]:

$$i\hbar\frac{\partial}{\partial t}\Psi = \left[\widehat{K}_P + V\left(\vec{r}\right)\right]\Psi, \quad \text{with} \quad \widehat{K}_P = \frac{\hat{p}^2}{(\widehat{\gamma}+1)m}. \tag{12}$$

The PGP equation above is fully Lorentz-covariant [13]. Note that under Lorentz transform, the 'scalar' potential $V\left(\vec{r}\right)$ becomes the time-like component of a full electromagnetic four-potential vector. The PGP equation could have been presented in such manifestly covariant fashion, but for pedagogical purposes (e.g. to highlight the connection with the Schrödinger equation), the form of equation (12) is preferred here. A detailed analysis of the PGP equation will be published elsewhere, but a brief further discussion may be found here in the appendix.

As a logistical matter, the PGP equation may be solved directly using straightforward basis-set representations, which are not too much more difficult to apply in practice than in the Schrödinger case. For pedagogical purposes, however, it is useful to consider approximations, which in any event also result in simpler calculations.

The first such approximation we will consider is based on the Poveda parametrization formalism. This consists of approximating the *operator* γ by a *parameter*:

$$\widehat{\gamma} \to \gamma = \sqrt{1 + \frac{\langle\Psi\,|\hat{p}^2|\,\Psi\rangle}{m^2c^2}}. \tag{13}$$

More specifically, equation (13) defines the parameter γ in terms of the average value, on the state Ψ, of the square of the well-defined momentum operator. Substituting equation (13) into (12) then literally leads to the Schrödinger equation with a rescaled effective mass, which can be solved in exactly the same manner as the Schrödinger equation itself.

Note that in practice, one has to know the exact numerical value of γ, which from equation (13), in turn requires knowledge of the exact solution Ψ. There are various standard ways to resolve this 'chicken-and-egg' dilemma. To begin with, we first modify the problem slightly, by replacing Ψ in equation (13) with the approximate solution itself. We call this the *Grave de Peralta-Poveda-Poiri*er (GPPP) approximation, Ψ_{GPPP}, which, according to the above description, must satisfy the following equation:

$$i\hbar\frac{\partial}{\partial t}\Psi_{\mathrm{GPPP}} = -\frac{\hbar^2}{(\gamma+1)\,m}\nabla^2\Psi_{\mathrm{GPPP}} + V\left(\vec{r}\right)\Psi_{\mathrm{GPPP}},$$

$$\text{with} \quad \gamma = \sqrt{1 + \frac{\langle\Psi_{\mathrm{GPPP}}\,|\hat{p}^2|\,\Psi_{\mathrm{GPPP}}\rangle}{m^2c^2}}. \tag{14}$$

Equation (14) above is a non-linear Schrödinger equation, in terms of which Ψ_{GPPP} becomes a self-consistent 'mean-field' solution. The simplest and most pedagogical way to compute Ψ_{GPPP} is via an iterative approach—of the type used routinely, e.g. in Hartree–Fock calculations. More specifically, one constructs a sequence of approximate, n'th order solutions to equation (14), wherein the expectation value that is used to determine the value of γ for the n'th order calculation, is itself computed using the solution obtained from the $(n-1)$'th order calculation. Convergence to the fully self-consistent GPPP solution, Ψ_{GPPP}, can be shown to be quite fast, at least for relatively slow-moving particles.

Of course, for pedagogical applications, it is not always necessary to fully converge the GPPP sequence. In the very first, $n = 0$ iteration, for example, the expectation value contribution to γ is simply ignored altogether, resulting in $\gamma = 1$. If one were to stop there, this would lead to a zeroth-order approximate solution that is just the usual Schrödinger equation wavefunction itself, i.e. Ψ_{Sch}: [2, 3]

$$i\hbar\frac{\partial}{\partial t}\Psi_{\mathrm{Sch}} = -\frac{\hbar^2}{2m}\nabla^2\Psi_{\mathrm{Sch}} + V\left(\vec{r}\right)\Psi_{\mathrm{Sch}}[\text{zeroth order}]. \tag{15}$$

Of course, this zeroth-order result contains no relativistic effects whatsoever.

The first nontrivial relativistic result—what we call the *Grave de Peralta* (GP) approximation, Ψ_{GP}—is therefore not obtained until first order. To obtain the first-order GP solution, one first inserts the zeroth-order Ψ_{Sch} solution of equation (15) into the second part of equation (14), in order to obtain a more accurate, first-order γ value. Substitution of this value for γ into the first part of equation (14) then leads to the first-order approximate solution for Ψ_{GPPP}(i.e. Ψ_{GP}) satisfying the following equation:

$$\begin{aligned} & i\hbar\frac{\partial}{\partial t}\Psi_{\mathrm{GP}} = -\frac{\hbar^2}{(\gamma+1)\,m}\nabla^2\Psi_{\mathrm{GP}} + V\left(\vec{r}\right)\Psi_{\mathrm{GP}}, \\ & \text{with}\quad \gamma = \sqrt{1+\frac{2}{mc^2}K_{\mathrm{Sch}}}\ [\text{first order}] \\ & \text{and}\quad K_{\mathrm{Sch}} = \left\langle \psi_{\mathrm{Sch}} \left| \frac{\hat{p}^2}{2m} \right| \psi_{\mathrm{Sch}} \right\rangle. \end{aligned} \tag{16}$$

This formalizes the approach initially followed by Grave de Peralta, for avoiding the use of the square root operator γ in equation (12) [6–10, 12, 13].

Now, it should be clear that all of the solutions above—i.e. Ψ, Ψ_{GPPP}, Ψ_{GP}, and Ψ_{Sch}—all approach each other, in the non-relativistic limit where

$$\left\langle \Psi \left| \hat{p}^2 \right| \Psi \right\rangle \ll m^2c^2. \tag{17}$$

Moreover, there is at least one important case for which one finds that $\Psi = \Psi_{\mathrm{GPPP}} = \Psi_{\mathrm{GP}} = \Psi_{\mathrm{Sch}}$, even when one is *not* in the non-relativistic limit [7, 9]. This occurs for the free particle system, i.e. when there is no potential energy so that $V\left(\vec{r}\right) = 0$. In this case, the three relativistic energies will be equal to each other, but will differ from the non-relativistic Schrödinger energy, because

$$\left\langle \Psi \left| \hat{p}^2 \right| \Psi \right\rangle = \left\langle \Psi_{\mathrm{GPPP}} \left| \hat{p}^2 \right| \Psi_{\mathrm{GPPP}} \right\rangle = \left\langle \Psi_{\mathrm{GP}} \left| \hat{p}^2 \right| \Psi_{\mathrm{GP}} \right\rangle = \left\langle \Psi_{\mathrm{Sch}} \left| \hat{p}^2 \right| \Psi_{\mathrm{Sch}} \right\rangle. \tag{18}$$

For the free particle case, the three relativistic solutions are thus identical in every respect. We therefore may as well use the simplest approach, i.e. the GP approach. In particular, the exact value of γ may be obtained from equation (16)—i.e. directly from the corresponding *non*-relativistic Schrödinger solution (equation (15)). Once γ is calculated, the GP equation can be solved following an essentially identical procedure, but with appropriately rescaled effective mass. The wavefunction solutions are the same, but the eigenenergies become altered via

$$E = \gamma mc^2 = \sqrt{m^2c^4 + \vec{p}^2c^2}, \tag{19}$$

which manifest the correct relativistic relation between the free particle's energy and linear momentum.

3. A simple pedagogical example

The problem of a quantum particle completely confined in a finite spatial region is of considerable interest as a crude model of numerous quantum systems where bound energy levels exist (e.g. quantum dots). This explains why in most introductory quantum mechanics courses, students learn to solve the Schrödinger equation for a particle confined in a one-dimensional (1D) infinite well (i.e. the 'particle in a box'), before being introduced to more realistic problems like the hydrogen atom [3].

When looking for stationary solutions for the 1D infinite well of width L, we note that there is no potential within the well region of interest. Accordingly, we must have $\Psi = \Psi_{\mathrm{GPPP}} = \Psi_{\mathrm{GP}} = \Psi_{\mathrm{Sch}}$. These are all solutions of the following eigenvalue equation [3, 7, 9]:

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi(x) + k^2\psi(x) = 0 \text{ with boundary conditions,} \quad \psi(x = 0, L) = 0. \tag{20}$$

Consequently:

$$\psi(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right), \quad k = \frac{n\pi}{L}, \quad n = 1, 2, \ldots. \tag{21}$$

Using the Schrödinger equation, it is found that [3]:

$$E_{\mathrm{Sch}} = \frac{n^2\pi^2\hbar^2}{2mL^2} = \frac{n^2\pi^2}{2}\left(\frac{\lambda\!\!\!^{-}_{\mathrm{C}}}{L}\right)^2 mc^2, \quad \text{with} \quad \lambda\!\!\!^{-}_{\mathrm{C}} = \frac{\hbar}{mc}. \tag{22}$$

This result is only valid in the non-relativistic limit, when $E_{\mathrm{Sch}} \ll mc^2$. For the ground state ($n = 1$), this implies that L is much larger than the reduced Compton wavelength ($\lambda\!\!\!^{-}_{\mathrm{C}}$) associated with the particle [2]. For particle energies close to or larger than mc^2, one of the relativistic equations should be used. Since these all result in the same relativistic eigenenergies in this case, we choose the simplest relativistic equation, i.e. the GP equation of equation (16) [7, 9]:

$$E_{\mathrm{GP}} = \frac{n^2\pi^2\hbar^2}{(\gamma+1)\,mL^2}, \quad \text{with} \quad \gamma = \sqrt{1 + \frac{2}{mc^2}E_{\mathrm{Sch}}}. \tag{23}$$

Using equations (22) and (23), we obtain:

$$E_{\mathrm{GP}} = E_{\mathrm{Sch}}\frac{2}{1 + \sqrt{1 + n^2\pi^2\left(\frac{\lambda\!\!\!^{-}_{\mathrm{C}}}{L}\right)^2}}. \tag{24}$$

Alternatively, E_{GP} can be calculated using the following equivalent equation:

$$E_{\mathrm{GP}} = (\gamma - 1)mc^2, \quad \gamma = \sqrt{1 + n^2\pi^2\left(\frac{\lambda\!\!\!^{-}_{\mathrm{C}}}{L}\right)^2}. \tag{25}$$

Note that since E_{GP} can be directly compared with E_{Sch}, it does *not* include the rest mass contribution, e.g. as in equation (19).

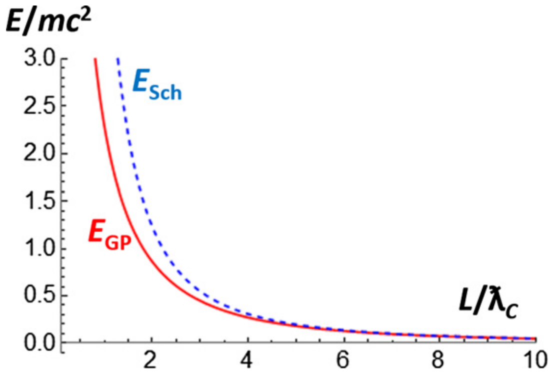

Figure 1. Ground state energy calculated using (discontinuous curve) equation (22) and (continuous curve) equation (24).

Clearly, as shown in figure 1, when $n = 1$ and $L \gg ƛ_{\mathrm{C}}$, $E_{\mathrm{GP}} \approx E_{\mathrm{Sch}}$. However, $E_{\mathrm{GP}} < E_{\mathrm{Sch}}$ appreciably when $L \approx ƛ_{\mathrm{C}}$. It is worth noting that the plotted values of E_{GP} have an excellent correspondence with the kinetic energies of the particle calculated using the Dirac equation [12]. Generation of particle-antiparticle pairs is possible when the kinetic energy of the particle trapped in the infinite well is $E_{\mathrm{GP}} \geqslant 2mc^2$. This is a relativistic phenomenon that is not described by the GP equation, which only describes the states of a single particle.

4. The size of hydrogen-like atoms

The size of the hydrogen atom can be qualitatively obtained by realizing that, in the hydrogen atom, the electron is approximately trapped in a localized spherical region of radius r. Therefore, the Bohr radius (a_0 [2, 3]) can be easily obtained as the value of r that minimizes the sum of the particle-in-a-box energy, plus the potential energy of the slow-moving electron:

$$E_{\mathrm{Sch}} \approx \frac{\hbar^2}{2m_{\mathrm{e}}r^2} - \frac{e^2}{4\pi\varepsilon_0 r}. \tag{26}$$

The first term in equation (26) corresponds to the *non*-relativistic kinetic energy of the ground state of a trapped slow-moving particle with the electron mass ($m = m_{\mathrm{e}}$). The second term corresponds to the potential energy associated with the Coulombic attraction between a particle, with a charge equal to the electron charge ($-e$), and a positive charge $+e$ placed at $r = 0$ [1, 11]. Equation (26) has a minimum when

$$r = a_0 = \frac{4\pi\varepsilon_0\hbar^2}{m_{\mathrm{e}}e^2} = \frac{1}{\alpha}\frac{\hbar}{m_{\mathrm{e}}c}, \quad \text{with} \quad \alpha = \frac{e^2}{4\pi\varepsilon_0\hbar c} \approx \frac{1}{137}. \tag{27}$$

Therefore, the size of the hydrogen atom is approximately 137 times the electron's reduced Compton wavelength, which confirms the initial slow-moving assumption.

On the other hand, however, the ground-state electron moves at relativistic speeds in hydrogen-like atoms for which the nuclear charge $Z \gg 1$. Therefore, to obtain a better qualitative estimate of the size of hydrogen-like atoms, we should modify equation (26) in the

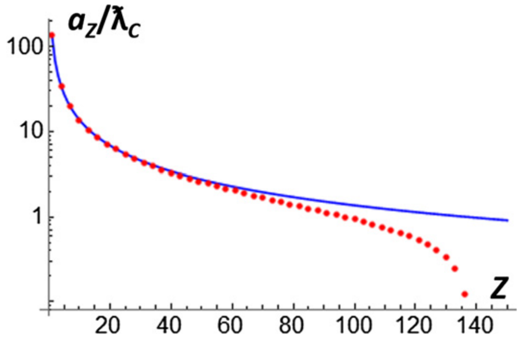

Figure 2. Calculated sizes of hydrogen-like atoms in $\lambda\!\!\!^{-}_{\mathrm{C}}$ units as a function of Z using (continuous curve) equation (26) and (points) equation (28).

following way:

$$E_{\mathrm{GP}} \approx \frac{\hbar^2}{(\gamma+1)\,m_{\mathrm{e}}r^2} - \frac{Ze^2}{4\pi\varepsilon_0 r}, \quad \text{with} \quad \gamma = \sqrt{1+\left(\frac{\lambda\!\!\!^{-}_{\mathrm{C}}}{r}\right)^2}. \tag{28}$$

Equation (28) has a minimum when:

$$r = a_Z = a\sqrt{1-\left(\frac{\lambda\!\!\!^{-}_{\mathrm{C}}}{a}\right)^2}, \quad \text{with} \quad a = \frac{a_o}{Z}. \tag{29}$$

In equation (29), $a = a_0/Z$ is the Bohr radius for a hydrogen-like atom with $Z \ll 1/\alpha \approx 137$. This value can be obtained by substituting e^2 with Ze^2 in equation (26); therefore, it assumes a slow-moving electron. However, when $Z \gg 1$, the electron moves at relativistic speeds; this results in the square root factor in equation (29) becoming significant.

As shown in figure 2, the relativistic correction to the size of the ground state of hydrogen-like atoms becomes significant when $a \approx \lambda\!\!\!^{-}_{\mathrm{C}}$. Moreover, the size of the hydrogen-like atom becomes undefined when $Z > 1/\alpha \approx 137$. This could be interpreted as a prediction about the impossibility of the natural existence of elements with Z >137. However, it must be borne in mind that the above represents a very crude approximation, even to the simplest, GP theory presented in this paper; a more accurate assessment, based on exact calculation using equation (12), is currently underway.

In any event, this prediction, which is based in semi-quantitative arguments, coincides with earlier predictions based on the energy of the ground state of hydrogen-like atoms calculated using the Dirac equation [14]. While no element with $Z > 118$ have ever been found, the current opinion of the superheavy elements experts is that elements with $Z \leqslant 172$ may be possible [15]. However, these assessments are based on stability arguments pertaining to the atomic *nuclei*, rather than the electronic structure arguments presented here.

5. Quantum mechanics and the natural boundary with the classical world

There are several interpretations of what quantum mechanics is [16–18]. While initially the so-called ‘Copenhagen interpretation’ was the favorite of instructors and textbooks [3], the current push for the realization of quantum sensors and computers [19, 20], together with recent experiments in Bose–Einstein condensation [21], large-scale quantum interference [22] and quantum entanglement [23] (among other factors), have served to bring 'quantum weirdness' to the forefront of discussion. All of this implies a demand that budding young physicists be exposed to broader ways of thinking about the foundations and possible interpretations of quantum mechanics [24].

For instance, a very fundamental question posed by the above considerations is the following: at what scale does wavefunction 'collapse' occur? Evidently, based on recent experiments, quantum interference can extend up to large biological molecules with over 800 atoms—a proposition which may well have 'shocked' the founders of quantum theory a century ago. But what does this imply about even larger systems, such as cats, and even human beings? Is there any limit at all on the size of a coherent quantum wave? Is 'collapse' of the wavefunction in reality just a myth? If collapse is not a myth, then what sort of new physics is needed to bring it about (e.g. along the lines of the 'objective collapse' theories of Ghirardi, Rimini, and Weber [25], or those of Diósi and Penrose [26, 27]).

Remarkably, the relativistic quantum approach presented here may have something interesting to say on this subject—which will, in any event, prove to be of educational interest. Consider that the probabilistic interpretation of the wavefunction (i.e. the Born rule) states that $\rho = \psi^*\psi$ is the probability density function associated with a quantum particle. On the other hand, $m\rho$ is the *mass density* of a quantum fluid in quantum hydrodynamics [17, 28, 29]. The chosen interpretation has consequences. Any extended body of mass m should gravitationally interact with itself if the quantum hydrodynamic point of view is adopted. Black holes exist due to the gravitational interaction between the different parts of its originally spatially-distributed mass. The enormous pressure existing inside planets has the same origin.

An important, fundamental question, then, is the following: is an elemental quantum particle a 'point particle' with no intrinsic size, or does its mass spread out like the mass density of a quantum fluid? The answer to this basic question has consequences. Assuming the quantum hydrodynamic point of view, the energy of a slow-moving free particle, with mass spread out over a finite spatial region, would be given by the following modification of equation (26) [12, 26]:

$$E_{\rm Sch} \approx \frac{\hbar^2}{2mr^2} - \frac{Gm^2}{r}. \tag{30}$$

In equation (30), the gravitational interaction of the particle with itself substitutes the Coulomb interaction included in equation (26). It is worth noting that equation (30) has a good pedigree, and it is at the core of the proposal of Diósi and Penrose for explaining the boundary with the classical, macroscopic, everyday world that seems to surround us [26, 27]. Several experiments are currently being conducted for proving or disproving this hypothesis [30, 31]. The gravitational term in equation (30) would have to be removed, if the particle could not interact with itself, due to its null size. In this case, the kinetic energy term of equation (30) would not have a local minimum, resulting in an infinitely spatially extended plane wave as the wavefunction for a free particle.

In contrast, equation (30) has a minimum when [12, 26]:

$$r = a_D = \frac{\hbar^2}{Gm^3} = l_{\rm P}\left(\frac{m_{\rm P}}{m}\right)^3,$$

$$\text{with} \quad l_{\rm P} = \sqrt{\frac{\hbar G}{c^3}} \quad \text{and} \quad m_{\rm P} = \sqrt{\frac{\hbar c}{G}}. \tag{31}$$

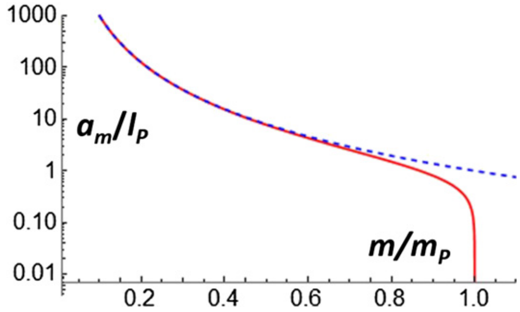

Figure 3. Calculated values of a_m as a function of m in Plank units using (discontinuous curve) equation (31) and (continuous curve) equation (33).

In equation (31), l_P and m_P are the Plank's length and mass, respectively. Equation (31) was first obtained by Diósi as the minimum size of a soliton-like solution of the so-called 'Newton–Schrödinger wave equation' [26]. Equations (30) and (31) are only valid for slow-moving particles. At relativistic speeds, equation (30) should be substituted by [12]:

$$E_{\mathrm{GP}} \approx \frac{\hbar^2}{(\gamma+1)\,mr^2} - \frac{Gm^2}{r}, \quad \text{with} \quad \gamma = \sqrt{1+\left(\frac{\lambda\!\!\!^{-}_{\mathrm{C}}}{r}\right)^2}. \tag{32}$$

This has a minimum when [12]

$$r = a_m = a_D\sqrt{1-\left(\frac{\lambda_{\mathrm{C}}}{a_D}\right)^2} = l_{\mathrm{P}}\left(\frac{m_{\mathrm{P}}}{m}\right)^3\sqrt{1-\left(\frac{m}{m_{\mathrm{P}}}\right)^4}. \tag{33}$$

Therefore, as shown in figure 3, a notable consequence of the quantum hydrodynamic interpretation of quantum mechanics, combined with the special theory of relativity, is the existence of a critical mass, $m_c = m_P$, above which the size of the particle becomes undefined. As in section 4, however, this intriguing prediction is based on a very crude analysis, and so it is perhaps more appropriate to conclude simply that 'something very interesting happens' near $m = m_P$.

This critical mass could be interpreted as the frontier between the quantum and the classical world. It should be noted that this critical mass value ($m_P \approx 22\ \mu$g) is quite small for having to consider the full complexity of quantum mechanics in the daily life, but quite large when compared with molecular masses, and the quantum experiments that have been done to date. Interestingly, biological cells, including human neurons, could still be quantum objects [32].

In any event, the experimental confirmation or rejection of this hypothesis would have fundamental consequences for quantum mechanics and cosmology. In particular, the confirmation of the existence of m_c could mean that there is not a universal wavefunction [18]—i.e. that the Schrödinger cat does not exist [3], and that the world that surrounds us is as classical as it seems to be. At the least, experimental validation of objective collapse theories along these lines would also impose serious limitations on the universal wavefunction or 'many-worlds' interpretation of quantum mechanics.

6. Conclusions

We have shown that the PGP equation of equation (12), together with two sensible approximations—i.e. GPPP (equation (14)) and GP (equation (16))—rest on a solid Lorentz-invariant theoretical foundation, conforming to the correct relativistic relation between the energy and linear momentum (even for fast-moving particles). We then discussed, exclusively using concepts of quantum mechanics and the special theory of relativity (as are often taught to undergraduate physics majors), three interesting problems with increasing level of complexity.

It is the authors' hope that we have provided a convenient and intuitive academic approach, for introducing students in introductory quantum mechanics courses, to the implications for quantum mechanics of the special theory of relativity. In particular, our approach complements, but does not replace, the more traditional Klein–Gordon theory. In comparing the two, it appears that our approach bears a much closer resemblance to the familiar non-relativistic Schrödinger equation, although for its part, the Klein–Gordon equation presents a more manifestly covariant form. Note that neither approach encompasses QED or pair creation/annihilation effects.

In future, we plan to extend the theory to multiple particles—which could be of interest, e.g. in the instruction of quantum chemistry, and perhaps also even condensed matter physics.

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Appendix.

From equation (8), it can be shown that the relativistic kinetic energy K satisfies the following equation [13]:

$$K = \frac{\vec{p}^2 c^2}{2mc^2 + K}. \tag{A1}$$

When $K \ll 2mc^2$, as it should be expected, equation (A1) approaches the non-relativistic kinetic energy $K = p^2/2m$. Inspired by the recursive form of equation (A1), Poirier proposed the following continued fraction definition of the relativistic kinetic energy operator [13]:

$$\widehat{K}_P = \frac{\hat{p}^2 c^2}{2mc^2 + \widehat{K}_P} = \frac{\hat{p}^2 c^2}{2mc^2 + \left\{ \frac{\hat{p}^2 c^2}{2mc^2 + \left[\frac{\hat{p}^2 c^2}{2mc^2 + \left(\frac{\hat{p}^2 c^2}{2mc^2 + \cdots} \right)} \right]} \right\}}. \tag{A2}$$

Note that unlike the usual operator-square-root form, for which there are in principle two solutions, equation (A2) has no such 'root ambiguity'. As a consequence, there are only positive-energy solutions for the free-particle problem defined by equation (12) (with equation (A2) used for $\widehat{K}_P$).

The continued fraction form of equation (A2) also suggests a natural sequence of successively more accurate approximations $\widehat{K}_P$, obtained by truncating the continued fraction at successive orders. More specifically, equation (A2) can be understood as the limit of the following sequence of operators:

$$\widehat{K}_{P,0} = \frac{\hat{p}^2 c^2}{2mc^2} = \frac{\hat{p}^2}{2m} = \widehat{K}_{\text{Sch}}. \tag{A3}$$

$$\widehat{K}_{P,1} = \frac{\hat{p}^2 c^2}{2mc^2 + \widehat{K}_{P,0}} = \widehat{K}_{\text{Sch}} \left[\frac{1}{1 + \frac{1}{2}\frac{\widehat{K}_{P,0}}{mc^2}}\right]. \tag{A4}$$

$$\widehat{K}_{P,2} = \frac{\hat{p}^2 c^2}{2mc^2 + \widehat{K}_{P,1}} = \widehat{K}_{\text{Sch}} \left[\frac{1}{1 + \frac{1}{2}\frac{\widehat{K}_{P,1}}{mc^2}}\right]. \tag{A5}$$

Of course, each of the $\widehat{K}_{P,N}$ operators above has the same plane-wave eigenstate wavefunctions; they differ only with respect to the corresponding eigenenergies, which present a convergent sequence. Thus, for the plane-wave solution with momentum $\vec{p}$, the corresponding $\widehat{K}_{P,N}$ eigenenergies are as follows:

$$\widehat{K}_{P,0} \rightarrow \frac{p^2}{2m} \tag{A6}$$

$$\widehat{K}_{P,1} \rightarrow \frac{p^2}{2m}\left[\frac{1}{1 + \frac{1}{4}\left(\frac{p}{mc}\right)^2}\right] \tag{A7}$$

$$\widehat{K}_{P,2} \rightarrow \frac{p^2}{2m}\left\{\frac{1}{1 + \frac{1}{4}\left(\frac{p}{mc}\right)^2\left[\frac{1}{1+\frac{1}{4}\left(\frac{p}{mc}\right)^2}\right]}\right\}. \tag{A8}$$

As a specific example, for a free particle moving at relativistic speeds such that $p = mc$, we obtain:

$$\widehat{K}_{P,0} \rightarrow \frac{1}{2}mc^2 \tag{A9}$$

$$\widehat{K}_{P,1} \rightarrow \frac{1}{2}\left[\frac{1}{1 + \frac{1}{4}}\right]mc^2 = \frac{2}{5}mc^2 \tag{A10}$$

$$\widehat{K}_{P,2} \rightarrow \frac{1}{2}\left[\frac{1}{1 + \frac{1}{4}\left(\frac{1}{1+\frac{1}{4}}\right)}\right]mc^2 = \frac{12}{29}mc^2. \tag{A11}$$

Despite the highly relativistic speed, this sequence rapidly converges to the exact result,

$$\widehat{K}_P \rightarrow \left(\sqrt{2} - 1\right)mc^2 \approx 0.4142mc^2, \tag{A12}$$

which is exactly the classical kinetic energy for a free particle with momentum magnitude $p = mc$, as given by equation (8). Interestingly, the above continued fraction sequence convergence is quite different than—and generally more rapidly convergent than—the standard Taylor series expansion of equation (7).

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