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Quasi-relativistic description of a quantum particle moving through one-dimensional piecewise constant potentials

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ABSTRACT

Using a novel quasi-relativistic wave equation, which can give precise results up to energies $\sim mc^2$, exact quantum mechanical solutions are found which corresponds to a particle with mass moving through one-dimensional piecewise constant potentials. As expected, at low particle's speeds, the found solutions coincide with the solutions of the same problems calculated using the Schrödinger equation; however, as it should be, both solutions have a significative difference at quasi-relativistic speeds. Then, it is argued that the quasi-relativistic wave equation provides a simpler description than a fully relativistic theory or the perturbation approach for a quantum particle moving at quasi-relativistic energies through piecewise constant potentials.

Introduction

Recently, the properties of an intriguing but previously unexplored wave equation describing a free quantum particle with mass m moving at quasi-relativistic speeds, were reported [1]. The so-named quasi-relativistic wave equation [1]:

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

Is very similar to the well-known Schrödinger equation [2–7]:

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

In Eqs. (1) and (2), $\hbar$ is the Plank constant (h) divided by 2π. Formally, Eq. (1) can be obtained from Eq. (2) by substituting the factor 2 which multiples m in the Schrödinger equation by the relativistic factor $(\gamma_V + 1)$ in Eq. (1), where [8,9]:

$$\gamma_V = \frac{1}{\sqrt{1-\frac{V^2}{c^2}}} \tag{3}$$

And V and c are the speeds of the particle and the speed of the light in vacuum, respectively. The term "quasi-relativistic" is used in this work as meaning a particle moving at so large speeds that it is necessary to use the correct relativistic relation between the linear momentum of the particle, p, and its kinetic energy, K, i.e. [1,8,9]:

$$K = \frac{p^2}{(\gamma_V+1)m}, \quad p = \gamma_V mV \tag{4}$$

Nevertheless, the speed of the quasi-relativistic particle should not be too much large so that the number of particles remains constant. A fully relativistic quantum theory where the number of particles is constant already exists [10]. Strictly speaking, the method described in this work is specifically designed for particles acting under the influence of an external, time-independent scalar potential. This implies the existence of a preferred reference frame associated to a static potential. In this context, the constancy of the number of particles requires that $K < mc^2$ for a free particle because a new particle could be generated from the kinetic energy of the particle when $K > mc^2$ [1,11–14]. However, when a particle is moving through the one-dimensional (1D) piecewise constant potentials ($U(x)$) studied in this work, the number of particles is constant when $K + |\Delta U| < mc^2$. This is because particles can also be generated from a potential that is maintained constant by an external source of energy [15,16]. Limiting the scope of this work to quasi-relativistic energies excludes the study of relativistic effects like the Klein paradox that occurs for very large potentials ($|\Delta U| > 2\,mc^2$) [9,11]. Nevertheless, this does not diminish the relevance of problems where a quantum particle moves at quasi-relativistic speeds. These problems include all chemistry and all problems where the number of particles is constant. For instance, for electrons $m_ec^2 \sim 0.5$ MeV; thus, electrons moving at quasi-relativistic speeds were commonly used in large color TV displays based on the now obsolete cathode-ray tube technology, where electron beams with kinetic energies $\sim 0.1\,mc^2$ were

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produced by electron guns with voltages of up to tens of kV. The most internal electrons in heavy elements have energies of the same order, while the ionization energy of atoms and the energy per molecular chemical bond are of the order of 1 to10 eV ($\sim 10^{-5}\, mc^2$). This explains why the results obtained using the Schrödinger equation are a good first approximation in chemistry applications [5]. In excellent correspondence with this, Eq. (1) clearly coincides with the Schrödinger equation at low particle's speeds. Moreover, a positive probability density can be defined for the solutions of Eq. (1) by analogy of how it is defined for the solutions of the Schrödinger equation and, like the Schrödinger equation, Eq. (1) is Galilean invariant for observers traveling at low speeds respect to each other [1]. Despite this, Eq. (1) can be used for obtaining precise solutions of very interesting quantum problems at quasi-relativistic energies [1]. Qualitatively, the capability of Eq. (1) for describing particles, which move respect to the preferred reference frame at quasi-relativistic speeds, can be understood by realizing that Eq. (1) implies the correct relativistic relation between K and p. Eq. (1) is not Lorentz invariant, but this is not a terrible impediment for describing particles moving at quasi-relativistic speeds because, for all practical porpoises, two observers moving slowly respect to the static potential will observe the particle moving at the same quasi-relativistic speed. It has also been shown that a plane wave (ψ), which is solution of Eq. (1), is given by [1]:

$$\psi(x,t) = \psi_{KG}(x,t)e^{iw_m t}$$

$$w_m = \frac{mc^2}{\hbar}, \quad \psi_{KG}(x,t) = e^{\frac{i}{\hbar}(px-Et)} \tag{5}$$

In Eq. (5), $E = K + \mathrm{mc}^2$ and ψ_{KG} is a plane wave which is a solution with positive energy of the relativistic Klein–Gordon equation [1,11–14]:

$$\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\psi_{KG}(x,t) = \frac{\partial^2}{\partial x^2}\psi_{KG}(x,t) - \frac{m^2c^2}{\hbar^2}\psi_{KG}(x,t) \tag{6}$$

Therefore [1]:

$$\psi(x,t) = e^{\frac{i}{\hbar}(px-Kt)} \tag{7}$$

The quasi-relativistic wave equation has been used for obtaining precise quasi-relativistic solutions of the well-known infinite rectangular well and quantum rotor problems [1,2]. The formal similitude between Eqs. (1) and (2) permitted finding exact analytical solutions of Eq. (1) for these problems with no more mathematical difficulty than are present when Eq. (2) is used. This is in contrast with the difficulties and complexities associated with finding solutions of similar relativistic quantum problems [11–18], or with the common theory of perturbations approach for including relativistic corrections to the energy values obtained from the Schrödinger equation [4]. In this work, it is shown that an extension of Eq. (1) can also be used for finding precise solutions of a whole class of interesting problems where a quantum particle with mass m move at quasi-relativistic speeds through a 1D piecewise constant potential. These problems have real applications and illustrate many important quantum-mechanics effects, such as penetration of a potential barrier, reflection of matter waves by a sharp change in potential, and the energy quantization in bounded states. Due to their importance and simplicity, these problems are often solved using the Schrödinger equation in quantum mechanics textbooks; however, the solutions found are only valid for particle's speeds much smaller than c. Therefore, the solution of the same problems using Eq. (1) allows extending our knowledge about these quantum-mechanics effects to the quasi-relativistic domain without a significant increment in the complexity of the theory. In Section 2 are presented general considerations about the movement of a quantum particle at quasi-relativistic speeds through 1D piecewise constant potentials, while in Sections 3–5 the reflection of a quantum particle by a sharp quantum step potential, the transmission through a potential barrier, and the bonds states in a rectangular quantum well are discussed, respectively. Finally, the conclusions of this work are given in Section 6. In addition, for completeness, a summary discussion about the quasi-relativistic wave equation for a free quantum particle is presented in the Appendix, where also is discussed the existing relationship between the Klein–-Gordon, the quasi-relativistic wave, and the Schrödinger equation.

1D piecewise constant potentials

The wavefunction of a quantum particle slowly traveling through a 1D piecewise constant potential $U(x)$ can be found solving the following Schrödinger equation [2–7]:

$$i\hbar\frac{\partial}{\partial t}\psi_{Sch}(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_{Sch}(x,t) + U(x)\psi_{Sch}(x,t) \tag{8}$$

However, by analogy with the free particle case [1], when the particle is moving at quasi-relativistic speeds, it is necessary to solve the following quasi-relativistic wave equation:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{(\gamma_V+1)m}\frac{\partial^2}{\partial x^2}\psi(x,t) + U(x)\psi(x,t). \tag{9}$$

Due to the formal similarity between Eqs. (8) and (9), one can expect to solve Eq. (9) following similar procedures as those used to solve Eq. (8) [2–7]. Looking for solutions of Eq. (9) corresponding to a constant value of the energy $E' = K + U = E + U - mc^2$. At quasi-relativistic energies, the number of particles is constant; therefore, E' is constant whenever $E + U$ is constant. For a 1D piecewise constant potential, E' and K and then V^2 are constants in each x-region where U is constant; therefore, one can look in each of the regions for a solution of Eq. (9) with the following form [2–7]:

$$\psi(x,t) = X_K(x)e^{-\frac{i}{\hbar}E't}, \quad E' = K + U \tag{10}$$

In Eq. (10), X_K is a solution of the following equation [2–7]:

$$\frac{d^2}{dx^2}X_K(x) + \kappa^2 X_K(x) = 0, \quad \kappa = \frac{p}{\hbar} \tag{11}$$

Eq. (11) and the relation between κ and p are identical to the ones obtained when solving Eq. (8) [2–7]. In addition, the possible values of κ are determined by the boundary conditions [1–7], which for a given problem are the same when resolving Eqs. (8) and (9); therefore, for a given problem, the spatial part of the solution of Eqs. (8) and (9) are equal. Using Eqs. (4) and (10) allows for rewritten κ in the following way:

$$\kappa = \frac{p}{\hbar} = \frac{1}{\hbar}\sqrt{(\gamma_V+1)mK} = \frac{1}{\hbar}\sqrt{(\gamma_V+1)m(E'-U)} \tag{12}$$

Consequently, κ and X_K are not determined by the values of E' but by the values of $K = E' - U$. Once the allowed values of κ are determined from Eq. (11) and the boundary conditions, the allowed values of $K = E' - U$ are given by:

$$K = \frac{\hbar^2\kappa^2}{(\gamma_V+1)m} \tag{13}$$

Eq. (13) corresponds to the relativistic kinetic energy of the particle, which is different than the non-relativistic kinetic energy that is obtained when solved Eq. (8). Therefore, for a given value of U, the values of $E' = K + U$ obtained solving Eq. (9) are different than the energy values corresponding to Eq. (8). Nevertheless, as expected, Eq. (13) gives the non-relativistic values of the particle's energies at low speeds when $\gamma_V \sim 1$ [2–7]. Moreover, from Eq. (13) and the relativistic equation, $K = (\gamma_V - 1)\, mc^2$, follows that:

$$\gamma_V{}^2 = 1 + \left(\frac{\lambda_C}{\lambda}\right)^2, \quad \lambda_C = \frac{h}{mc}, \quad \lambda = \frac{2\pi}{\kappa} \tag{14}$$

In Eq. (14), λ_C is the Compton wavelength associate to the mass of the particle [11], and λ is the De Broglie wavelength of the wavefunction given by Eqs. (7) and (11) [2–7]. As expected $\gamma_V{}^2 \sim 1$ when

$p = h/\lambda$ is very small because $\lambda \gg \lambda_C$; then $K \sim \hbar^2\kappa^2/(2m)$, which is the non-relativistic expression of the particle's kinetic energy [2–7]. Substituting Eq. (14) in Eq. (13) allows obtaining an analytical expression of the precise quasi-relativistic kinetic energy of the particle:

$$K = \frac{\hbar^2\kappa^2}{\left[1 + \sqrt{1 + \left(\frac{\lambda_C}{\lambda}\right)^2}\right]m} = \frac{\hbar^2\kappa^2}{\left[1 + \sqrt{1 + \left(\frac{\hbar k}{mc}\right)^2}\right]m} \tag{15}$$

As expected, Eq. (15) match the non-relativistic expression of the particle's kinetic energy when $p = h/\lambda$ is very small because $\lambda \gg \lambda_C$. However, in each region where the value of U is constant, the values of K and then $E' = K + U$ calculated using Eq. (15) are smaller than those calculated using the Schrödinger equation. It is worth noting that the wavefunction given by Eq. (10) corresponds to quantum states with well determined values of $E' = K + U$. Thus, E' is the same everywhere. However, there are different values of U in different regions of the piecewise constant potential; therefore, the values of $K = E' - U$ are well determined and constant in each region but different in different regions. In addition, due Eq. (11), the values of p are also well determined and constant in each region but different in different regions. Consequently, due Eqs. (4) and (13), the values of $(\gamma_V + 1)$ must be well determined and constant in each region but different in different regions. Also, due the relativistic relation $K = (\gamma_V - 1)\,mc^2$, this must happen for $(\gamma_V - 1)$ too. Consequently, the same must happen for $\gamma_V{}^2 = (\gamma_V + 1)(\gamma_V - 1) + 1$ and thus also for γ_V and V^2. This means that strictly speaking a different Eq. (9) with a different value of V^2 should be solved in each region where the potential is constant, or alternatively, the equation that should be solved is the following one:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{[\gamma_V(x) + 1]m}\frac{\partial^2}{\partial x^2}\psi(x,t) + U(x)\psi(x,t) \tag{16}$$

In Eq. (16) γ_V is a function of x because, in general, the square of the particle's speed (V^2) depends on the position. The boundary conditions of Eq. (11), at the points in between two regions with constant but different values of $U(x)$, correspond to the continuity of the wavefunction and its first spatial derivative [2–7]. In what follows the general ideas discussed in this Section will be applied to some representative cases of 1D piecewise constant potentials.

Reflection of a quantum particle by a sharp potential step

The simplest example of a pure quantum mechanical effect is the existence of a probability of reflection when a quantum particle with $E' > U(x)$ pass by a region where there is a sharp change in the potential, $|\Delta U| = U_o$, such that $E' = K + U_o < mc^2$. The one-dimensional piecewise constant potential corresponding to this situation is a potential that undergoes only one sharp discontinuous change and is given by the following expression:

$$U(x) = \begin{cases} 0, & \infty < x < 0 \\ U_o > 0, & 0 \leqslant x < +\infty \end{cases} \tag{17}$$

Due to the formal similitude between Eqs. (8) and (9), one can proceed to solve Eq. (9) as it is done for Eq. (8). The task here is to calculate the reflectivity (R) associated with the sharp potential variation at $\times = 0$ [2–5]. When $E' > U_o$, one can look for a solution as given by Eq. (10) with $X(x)$ given by [2]:

$$X(x) = \begin{matrix} Be^{\frac{i}{\hbar}p_1x} + Ce^{-\frac{i}{\hbar}p_1x}, & x \leqslant 0 \\ Ae^{\frac{i}{\hbar}p_2x}, & x \geqslant 0 \end{matrix} \tag{18}$$

This solution describes a steady flow of particles with mass m and kinetic energy $K_1 = E' < mc^2$, which are traveling with speed V_1 from left to right and then are partially reflected and partially transmitted at $x = 0$. Due to Eqs. (4) and (12), in Eq. (18):

$$p_1 = \gamma_{V_1}mV_1 = \sqrt{(\gamma_{V_1} + 1)mE'},\quad p_2 = \gamma_{V_2}mV_2 = \sqrt{(\gamma_{V_2} + 1)m(E' - U_o)} \tag{19}$$

This is in contrast with the following expressions for p_1 and p_2 when the Schrödinger equation is solved [2]:

$$p_1 = mV_1 = \sqrt{2mE'},\quad p_2 = mV_2 = \sqrt{2m(E' - U_o)} \tag{20}$$

The movement of the particles is not confined to a finite region; therefore, in Eqs. (19) and (20) the values of p_1, p_2 and E' are not quantized. Both Eqs. (19) and (20) determine the values of V^2 everywhere. From Eq. (20) follows that:

$$V_1^2 = \frac{2E'}{m},\quad V_2^2 = \frac{2(E' - U_o)}{m} \tag{21}$$

While from Eq. (19) follows that:

$$V_1^2 = \frac{E'(E' + 2mc^2)}{(E' + mc^2)^2}c^2,$$

$$V_2^2 = \frac{(E' - U_o)[(E' - U_o) + 2mc^2]}{[(E' - U_o) + mc^2]^2}c^2 \tag{22}$$

For instance, when $K_1 = E' \sim mc^2$, then $V_1{}^2 \sim \frac{3}{4}c^2$, $\gamma_V{}^2 \sim 4$, and $V_1 \sim \pm 0.87c$. The constant A, B, C must now be determined from the boundary conditions requiring that the wave function and its first derivative are continuous at $x = 0$. From this, one can determine that R is given by the following expressions, which are identical to the ones obtained when solving the Schrödinger equation [2]:

$$R = \frac{(p_1 - p_2)^2}{(p_1 + p_2)^2} \tag{23}$$

$R(E')$ for particles moving at quasi-relativistic speeds can be obtained from Eqs. (23), (19) and (22), while for particles moving at very low speeds one should use Eqs. (23) and (20). Fig. 1 shows a comparison of $R(E')$ calculated using the Schrödinger and the quasi-relativistic wave equations. In both cases, the reflection coefficient becomes large only when U_o is comparable in size with E' (not shown). As expected, both reflection coefficients coincide when $E' \ll mc^2$ (not shown); however, as shown in Fig. 1 for $m = m_e$ and $U_o = 0.3\,m_ec^2$, at quasi-relativistic energies $R(E)$ calculated using the quasi-relativistic wave equation is slightly larger than $R(E)$ calculated using the Schrödinger equation.

Tunneling through a barrier

Another example of a pure quantum mechanical effect is the tunneling of a quantum particle through a potential barrier of high $|\Delta U| = U_o < mc^2$ when $E' < U_o$. The one-dimensional piecewise constant potential corresponding to this situation is given by the following expression [2]:

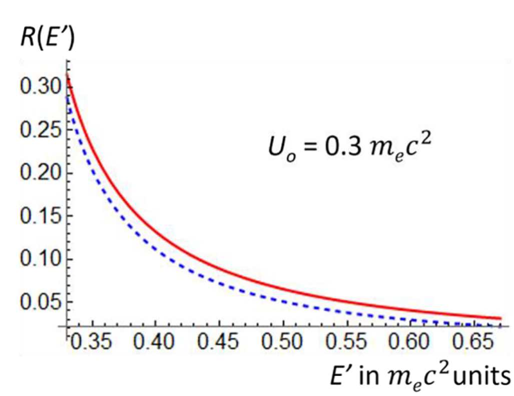

Fig. 1. $R(E')$ calculated for $m = m_e$ and $U_o = 0.3\,m_ec^2$ using (continuous) quasi-relativistic wave and (dashed) Schrödinger equations.

$$U(x) = \begin{cases} 0\,, & x\,\langle 0,\ x\rangle\, L \\ U_o > 0, & 0 \leqslant x \leqslant L \end{cases} \tag{24}$$

Due to the formal similitude between Eqs. (8) and (9), one can proceed to solve Eq. (9) as it is done for Eq. (8). Assuming incident particles from the region $x < 0$ with linear momentum p_1 and quasi-relativistic energy $E' = K_1 < U_o$ such that $K_1 + U_o < mc^2$, and assuming that the width of the barrier (L) is large enough; i.e., $p_2 L/\hbar \gg 1$, where p_2 is the particle momentum inside of the barrier; one can look for a solution as given by Eq. (10) with $X(x)$ given by [2]:

$$X(x) = \begin{cases} Ae^{\frac{i}{\hbar}p_1 x}\,, & x < 0 \\ Be^{\frac{p_2}{\hbar}x} + Ce^{-\frac{p_2}{\hbar}x}, & 0 \leqslant x \leqslant L \\ De^{\frac{i}{\hbar}p_1 x}\,, & x > L \end{cases} \tag{25}$$

Formally, looking for a solution as Eq. (25) means that inside of the barrier the particle has an effective kinetic energy $K_2 = U_o - E'$. Solving the Schrödinger equation for the ratio of the intensity of the wave transmitted to the region $x > L$ to that of the incident wave, allows then obtaining [2]:

$$T = \frac{16e^{-2p_2 L/\hbar}}{\left[1+\left(\frac{p_2}{p_1}\right)^2\right]\left[1+\left(\frac{p_1}{p_2}\right)^2\right]},\ p_2 = \sqrt{2m(U_o - E')} \tag{26}$$

In Eq. (25), p_1 is given by Eq. (20). Eq. (26) can also be obtained using the quasi-relativistic wave equation and thus is also valid for quasi-relativistic energies but then p_1 and V_1 are given by Eqs. (19) and (22), respectively, and p_2 and V_2 are given by:

$$p_2 = \gamma_{V_2} m V_2 = \sqrt{(\gamma_{V_2}+1)mK_2} \Rightarrow V_2^2 = \frac{K_2[K_2 + 2mc^2]}{[K_2 + mc^2]^2}c^2,\ K_2 = U_o - E' \tag{27}$$

Fig. 2 shows a comparison of $T(E')$ calculated using the Schrödinger and the quasi-relativistic wave equations. As it is well known, there is a small probability that a particle can penetrate a potential barrier which it could not even enter according to classical theory. This probability decreases rapidly as the barrier get thicker and as it gets higher (not shown). As expected, both transmission coefficients coincide when $E' \ll mc^2$ (not shown); however, as shown in Fig. 2 for $m = m_e$, $U_o = 0.5\ m_e c^2$, and $L = \lambda_C$, at quasi-relativistic energies $T(E')$ calculated using the quasi-relativistic wave equation is slightly smaller than $T(E')$ calculated using the Schrödinger equation.

Bound states in the rectangular well

Quantization of the energy of a quantum particle trapped in a potential well is one of the must emblematic quantum effects. The one-dimensional piecewise constant potential corresponding to this situation is given by the following expression [2]:

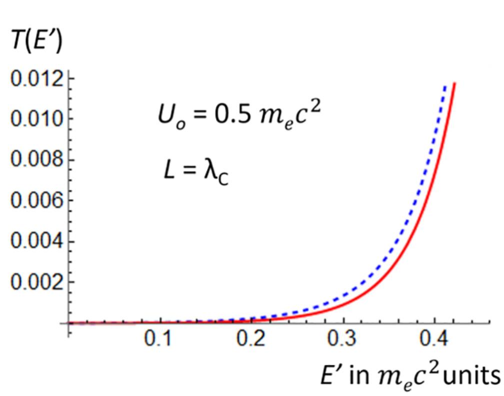

Fig. 2. $T(E')$ for $m = m_e$, $U_o = 0.5\ m_e c^2$, and $L = \lambda_C$ calculated using (continuous) quasi-relativistic wave and (dashed) Schrödinger equations.

$$U(x) = \begin{cases} 0\,, & x\left\langle -\frac{L}{2},\ x\right\rangle + \frac{L}{2} \\ -U_o < 0, & -\frac{L}{2} \leqslant x \leqslant +\frac{L}{2} \end{cases} \tag{28}$$

Here again, due to the formal similitude between Eqs. (8) and (9), one can proceed to solve Eq. (9) as it is done for Eq. (8). Consequently, assuming $E' < 0$, it can be obtained in both cases the following transcendental equation [2]:

$$\frac{p_1}{p_2} = \tan\left(\frac{p_2 L}{2\hbar} + \frac{n\pi}{2}\right) = \begin{cases} \tan\ \frac{p_2 L}{2\hbar},\ n\ even \\ -\cot\ \frac{p_2 L}{2\hbar},\ n\ odd \end{cases} \tag{29}$$

where n is an integer, and p_1 and p_2 are the particle's linear momenta outside and inside of the well, respectively. The allowed values of E' can be obtained from Eq. (29) by expressing p_1 and p_2 in terms of E' and U_o. Consequently, a different transcendental equation is obtained when solving Eq. (8) than when solving Eq. (9). For the Schrödinger equation can be obtained the following transcendental equation [2]:

$$\sqrt{\frac{|E'|}{U_o - |E'|}} = \begin{cases} \tan\left[\frac{L}{2\hbar}\sqrt{2m(U_o - |E'|)}\right],\ n\ even \\ -\cot\left[\frac{L}{2\hbar}\sqrt{2m(U_o - |E'|)}\right],\ n\ odd \end{cases} \tag{30}$$

While the following transcendental equation can be obtained when solving the quasi-relativistic wave equation:

$$\sqrt{\frac{(\gamma_{V_1}+1)|E'|}{(\gamma_{V_2}+1)(U_o - |E'|)}} = \begin{cases} \tan\left[\frac{L}{2\hbar}\sqrt{(\gamma_{V_2}+1)m(U_o - |E'|)}\right],\ n\ even \\ -\cot\left[\frac{L}{2\hbar}\sqrt{(\gamma_{V_2}+1)m(U_o - |E'|)}\right],\ n\ odd \end{cases}. \tag{31}$$

In Eq. (31):

$$V_1^2 = \frac{|E'|\,(|E'| + 2mc^2)}{(|E'| + mc^2)^2}c^2,\ V_2^2 = \frac{(U_o - |E'|)[(U_o - |E'|) + 2mc^2]}{[(U_o - |E'|) + mc^2]^2}c^2 \tag{32}$$

As expected, Eq. (31) coincides with Eq. (30) at very low particle's speeds. Using Eq. (32) allows for numerical evaluation of both sizes of Eq. (31). Wherever both sizes match, there is a possible energy level. In contrast, it is well known that one can obtain exact solutions of the Schrödinger equation for the infinite rectangular well problem, which corresponds to the following potential [2–5]:

$$U(x) = \begin{cases} U_o \to +\infty, x < 0,\ x > L \\ 0, \qquad 0 \leqslant x \leqslant L \end{cases} \tag{33}$$

Therefore, finding the bound states of the infinite rectangular well problem can be considered as a limit case of the finite problem when $U_o \longrightarrow +\infty$ [2]. This case has a high scholastic value and describes a quantum particle absolutely trapped in a finite region of length L [2–5]. For the infinite well, the solution of Eq. (11), which gives the spatial dependence of the wave function inside of the infinite well for Eq. (8), is given by the following expression [4]:

$$X_n(x) = \sqrt{\frac{2}{L}}\,Sin\left(\frac{n\pi}{L}x\right), \quad \kappa_n = \frac{n\pi}{L}, \quad n = 1, 2, \tag{34}$$

Consequently, for the Schrödinger equation, the allowed energies in the infinite rectangular well are given by [2–5]:

$$K_n = n^2\frac{\pi^2\hbar^2}{2mL^2} \tag{35}$$

Strictly speaking, the problem corresponding to the potential defined by Eq. (33) is a relativistic problem because $|\Delta U| = U_o \gg mc^2$ and thus the number of particles may not be constant [11–18]. Nevertheless, the non-relativistic and quasi-relativistic infinite well problems could be considered approximations to the problem of a quantum particle absolutely trapped in a finite region. This is because for obtaining Eqs. (34) and (35) the infinitude of the potential is only used for

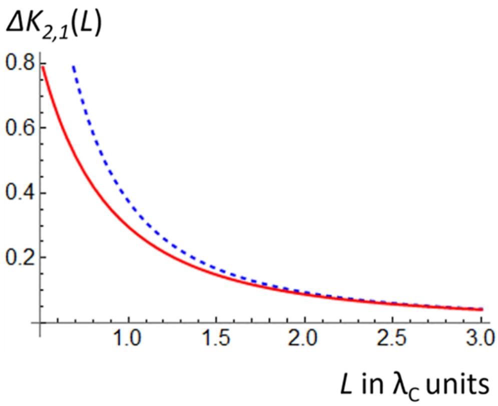

Fig. 3. $\Delta K_{2,1}$ calculated for $m = m_e$ using (continuous) quasi-relativistic wave and (dashed) Schrödinger equations.

arguing that $X(x)$ should be null everywhere except inside of the well [2–5], thus assigning null boundary conditions to Eq. (11). In this sense, one could resolve Eq. (9) for the infinite rectangular well as it is done for Eq. (8). Proceeding in this way [16], one can demonstrate that Eq. (34) is also valid at quasi-relativistic energies ($E' = K < mc^2$) [1,17,18]. However, the energies of the bound states for the quasi-relativistic wave equation are given by Eqs. (13), (14) and (15) evaluated for κ_n given by Eq. (34), this resulting in [1]:

$$K_n = n^2 \frac{\pi^2\hbar^2}{\left[1 + \sqrt{1 + n^2\left(\frac{\lambda_C}{2L}\right)^2}\,\right] mL^2}, \quad \gamma_{V_n}{}^2 = 1 + n^2\left(\frac{\lambda_C}{2L}\right)^2, \quad \lambda_n = \frac{2L}{n}. \tag{36}$$

As expected, Eq. (36) coincides with Eq. (35) when the linear momentum of the particle in the infinite well is very small because $\lambda = h/p \gg 1$. This happens for small values of n when $L \gg \lambda_C$. In contrast, when the width of the well is close to $\lambda_C/2$, the minimum particle energy is quasi-relativistic; therefore, Eq. (36) should be used instead of Eq. (35). For instance, $\gamma_V{}^2 = 2$, $V \sim 0.7c$, and $K \sim 0.4\ mc^2$ when Eq (36) is evaluated for $n = 1$ and $L = \lambda_C/2$. However, $\gamma_V{}^2 = 5$ and $K \sim 1.2\ mc^2$ when $n = 1$ and $L = \lambda_C/4$. The number of particles may not be constant at these energies. This result for a 1D infinite rectangular well can easily be extended to the 3D infinite rectangular well as it is done for the Schrödinger equation [5]. Consequently, Eq. (9) establishes 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 $\frac{1}{8}\lambda_C{}^3$ 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. This is 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. This is consistent, for instance, with the confinement of an electron in the Hydrogen atom because for an electron $\lambda_C \sim 2.4 \times 10^{-3}$ nm, which is ~ 20 times smaller than the Bohr radius of the Hydrogen atom, $r_B \sim 5.3 \times 10^{-2}$ nm [1–5]. Fig. 3 shows a comparison of the calculated energies of a particle in an infinite rectangular well using the Schrödinger and the quasi-relativistic wave equations. The values of K_n calculated using Eq. (36) are smaller than those calculated using Eq. (35) (not shown). This is in good qualitative agreement with more involved numerical results obtained solving the Dirac equation for the 1D infinite rectangular well [18]. Moreover, as shown in Fig. 3 for $m = m_e$, the values of $\Delta K_{2,1} = K_2 - K_1$ calculated using Eq. (36) are significatively smaller than those calculated using Eq. (35) when $L \sim \lambda_C$. This is important because it is the energy difference between two energy levels what can be experimentally measured. As expected, the difference between the values of $\Delta K_{2,1}$ calculated using both approaches coincide at low particle's velocities, i.e., when $L \gg \lambda_C$ (not shown) but are significatively different at quasi-relativistic velocities, i.e., when $L \sim \lambda_C$.

Conclusions

It has been shown how to solve the quasi-relativistic wave equation for a quantum particle with mass moving at quasi-relativistic energies through one-dimensional piecewise constant potentials. The solutions were found following the same procedures and with no more difficulty than the corresponding to solving the same problems using the Schrödinger equation. As expected, at low particle's speeds, the solutions found coincide with the solutions of the same problems calculated using the Schrödinger equation; however, as it should be, both solutions have a significative difference at quasi-relativistic energies. This demonstrates the practical scholastic utility of the quasi-relativistic wave equation, which may impact how relativistic corrections are introduced in future textbooks of Quantum Mechanic. Nevertheless, for reliable comparison with experiments, problems with more realistic potentials should be solved. The author is currently involved in this task.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix. The one-dimensional quasi-relativistic wave equation for a free quantum particle

Formally, the Schrödinger equation for a free quantum particle can be obtained from the classical relation between K and p for a free particle when $V \ll c$ [1–7]:

$$K = \frac{p^2}{2m}, \quad p = mV \tag{A1}$$

Then, Eq. (2) is obtained by substituting K and p by the following energy and momentum quantum operators [1–4]:

$$\hat{E} = \hat{K} = i\hbar\frac{\partial}{\partial t}, \quad \hat{p} = -i\hbar\frac{\partial}{\partial x} \tag{A2}$$

By analogy, Eq. (1) can be simply obtained combining Eqs. (4) and A(2) [1]. Eq. (4) can be easily obtained from the following well-known relativistic equations [8,9,11]:

$$\begin{aligned} &E^2 - m^2c^4 = p^2c^2 \Leftrightarrow \\ &(E + mc^2)(E - mc^2) = p^2c^2 \end{aligned} \tag{A3}$$

And:

$$K = E - mc^2, \quad E = \gamma_V mc^2 \tag{A4}$$

The Klein–Gordon equation (Eq. (6)) can formally be obtained from Eq. (A2) and the first expression of Eq. (A3) by assigning the temporal partial derivative operator to E, which is the sum of particle's kinetic energy plus the energy associated to the mass of the particle [8,9,11]. However, if one chooses to assign this operator to K, as it is done when obtaining the Schrödinger equation, then from Eqs. (4) and (A2) follows Eq. (1) [1]. Alternatively, one can use Eq. (A4) and the second expression of Eq. (A3) for obtaining the following algebraic equation:

$$(E - mc^2) = \frac{p^2}{(\gamma_V + 1)m} \tag{A5}$$

The factor $(E + mc^2)$ is always different than 0 for $E > 0$; therefore Eq. (A5) is equivalent to Eq. Eq. (A3) for positive energies of E. Assigning the temporal partial derivative operator in Eq. (A2) to E in Eq. (A5) results the following differential equation:

$$i\hbar\frac{\partial}{\partial t}\psi_{KG+}(x, t) = -\frac{\hbar^2}{(\gamma_V + 1)m}\frac{\partial^2}{\partial x^2}\psi_{KG+}(x, t) + mc^2\psi_{KG+}(x, t) \tag{A6}$$

In Eq. (A6), ψ_{KG+} is a solution of the Klein–Gordon equation given by Eq. (5) for $E > 0$. Thus, the quasi-relativistic wave equation can be obtained by using Eq. (5) and looking for a solution of Eq. (A6) of the form $\psi_{KG+} = \psi e^{-iw_m t}$. Eqs. (5) and (7) suggest that the time-independent equations corresponding to Eqs. (1) and (6) are equal. In fact, looking for solutions of the form $X(x)T(t)$ of Eqs. (1), (2), and (6), where $T(t) = e^{-\frac{i}{\hbar}Kt}$for Eqs. (1) and (2) but $T(t) = e^{-\frac{i}{\hbar}Et}$ for Eq. (6), produces the same time-independent equation in the three cases:

$$\frac{d^2}{dx^2}X(x) + \kappa^2 X(x) = 0, \quad \kappa = \frac{p}{\hbar} \tag{A7}$$

Often $X(x)$ and κ are determined solving Eq. (A7) under adequate boundary conditions [1–5]; then the possible values of p are determinate from the possible values of κ. However, the relation between K and p are different for non-relativistic and quasi-relativistic speeds; therefore, the solutions of Eqs. (1) and (2) have equal spatial dependences but different values of K. Also, the relation between E or K and p are different for quasi-relativistic speeds; therefore, the solutions of Eqs. (1) and (6) have equal spatial dependences but different values of K and E. Eqs. (4) and (A3) can be obtained from each other using Eq. (A4); however, Eq. (A3) admits solutions with positive and negative energies but K only can be positive in Eq. (A4). This is in correspondence to the presence of a second-order temporal partial derivative in Eq. (6), which determines that Eq. (6) has solutions with positive and negative energies [11–14]. In contrast, there is a first-order temporal partial derivative in Eqs. (1) and (2). This determines that Eqs. (1) and (2) only have solutions with positive energies. Eq. (5) gives a simple recipe from obtaining a plane wave solution of Eq. (1) from a plane wave solution of Eq. (6) with positive energy and vice versa. The wavefunction of a free particle with mass m moving at quasi-relativistic speeds, which is given by Eq. (7), have well determined values of K, $E = K + mc^2$, p, and thus of γ_V and V^2. Consequently, Eq. (1) is well determinate and the same everywhere. Finally, it is worth noting that Eq. (1) is non-linear in the sense that if ψ_1 and ψ_2 are two solutions of Eq. (1) corresponding to two different values of V^2, then strictly 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) [1]. However, Eq. (6) is linear and the wavefunction $\psi_{KG+} = (\mathbf{a}\psi_1 + \mathbf{a}\psi_2)e^{-iw_m t}$ is indeed a solution of Eq. (6). In this sense, Eqs. (1) and (9) are like Eqs. (11) and (A8) in that solving them requires simultaneously finding eigenvalue-eigenfunction pairs. This can be made evident by using Eq. (A4) for eliminating γ_V from Eq. (9), thus rewriting Eq. (9) as the following eigenvalue equation where ψ and E' should be found simultaneously:

$$i\hbar\frac{\partial}{\partial t}\psi(x, t) = -\frac{c^2\hbar^2}{[E' - U] + 2mc^2}\frac{\partial^2}{\partial x^2}\psi(x, t) + U(x)\psi(x, t) \tag{A8}$$

While both forms of the same equation are equivalent, Eq. (9) is more suggestive due its striking similarity to the Schrödinger equation. From this point of view, the quasi-relativistic wave equation provides a useful way to find exact solutions of the Klein–Gordon equation with positives energies when $E' = K + U < mc^2$. The Schrödinger equation then appears as a limit case of the quasi-relativistic wave equation when $E' \ll mc^2$. It should be noted that in all the problems discussed in this work, and in others of great interest [19,20], the temporal part of ψ is the time-dependent exponential given in Eqs. (7) and (10); therefore, only time-independent equations were really solved. However, in problems involving the propagation of a wave-packet wavefunction the nonlinearity of Eq. (1) may be in issue [20].

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