Relativistic particle in a box

P Alberto†, C Fiolhais† and V M S Gil‡

†Departamento de Física da Universidade de Coimbra, P-3000 Coimbra, Portugal
‡Departamento de Química da Universidade de Coimbra, P-3000 Coimbra, Portugal

Received 3 August 1995

Abstract. The problem of a relativistic spin 1/2 particle confined to a one-dimensional box is solved in a way that resembles closely the solution of the well known quantum-mechanical textbook problem of a non-relativistic particle in a box. The energy levels and probability density are computed and compared with the non-relativistic case.

Resumo. O problema de uma partícula de spin 1/2 confinada por uma caixa a uma dimensão é resolvido de uma maneira muito semelhante à da resolução do problema de uma partícula no-relativista numa caixa referido em muitos livros introdutórios de Mecânica Quntâica. Os níveis de energia e a densidade de probabilidade são calculados e comparados com os valores não-relativistas.

1. Introduction

Energy quantization in atoms and molecules plays an essential role in the physical sciences.

From which theoretical arguments does the quantization of energy comes from? The axioms of quantum theory were built to explain that phenomenon. A simple example of application of these rules, which has great pedagogical value, is the study of a particle in a one-dimensional box, i.e., an infinite one-dimensional square well. Indeed, in many introductory courses of physics or chemistry the study of electronic wavefunctions in atoms and molecules is made by analogy with a particle in a box, without having to solve the more involved Schrödinger equation for systems ruled by the Coulomb potential. In this way one is able to introduce the concepts of energy quantization and orbitals for atoms and molecules without being lost in the mathematical details of solving the Schrödinger equation for a central potential.

We note that for obtaining quantization it is not so much the type of differential equation which must be solved but the boundary condition which must be obeyed by the solution: a particle confined to a finite region of space does have discrete energy levels. In order to solve the time-independent Schrödinger equation for a free non-relativistic particle of mass m inside a one-dimensional box of length L in the z-axis,

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}z^2} = E\psi \tag{1}$$

which is the stationary wave ($0 \ll z \ll L$)

$$\psi(z) = C\sin(kz) \tag{2}$$

one has to impose the boundary conditions $\psi(0) = \psi(L) = 0$. These same conditions give rise to the quantization rule for the wavenumber, $k = n\pi/L$, $n = 1, 2, \ldots$. Outside the box the wavefunction vanishes which means that the derivative of the wavefunction is discontinuous at the well walls ($z = 0$ and $z = L$). This is related to the fact that the potential has a infinite jump at the well walls. It is worth stressing this point as we move later to the relativistic case. The energy levels of equation (1) are given by

$$E_n = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2mL^2} \tag{3}$$

where $p = \hbar k = n\pi/L$ is the quantized momentum.

In a similar fashion, we propose to solve the Dirac equation for a particle in a box, emphasizing the role of the boundary conditions in the solution of the wave equation in this paper ourselves. At the same time, we will get the solutions in a way which closely resembles the non-relativistic approach. The method we shall use set ourselves apart from either the one-dimensional Dirac equation approach [3, 4] and the calculations of Greiner [5] both using a finite square well. By using the three-dimensional Dirac with a one-dimensional potential well in the z-axis, we are able to include spin in the wavefunction without increasing much the mathematical burden. The crucial points are the use of a Lorentz scalar potential, which avoids the Klein paradox problem, and boundary conditions which assure the continuity of the probability current rather than that of wavefunction itself. In this way we are able to avoid the problems referred in [3–5] when the depth of the potential goes to infinity.

In the next section we solve the Dirac equation in an one-dimensional infinite square well, leaving the mathematical details for an appendix. In the conclusions we present some comment on our solution and compare it with other approaches found in the literature.

0143-0807/96/010019+06$19.50

2. Solution of the Dirac equation in an one-dimensional infinite square well

Let us consider the time-independent relativistic equation for the wavefunction of a free electron of mass m moving along the z direction. This Dirac equation can be written as

$$\hat{H}\psi = (\alpha_z \hat{p}_z c + \beta m c^2)\psi = E\psi \tag{4}$$

where $\hat{H} = \alpha_z \hat{p}_z c + \beta m c^2$ is the Dirac energy operator (Hamiltonian), $\hat{p}_z = -\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}z}$ is the z component of the momentum operator and α_z and β the matrices

$$\alpha_z = \begin{pmatrix} 0 & \sigma_z \\ \sigma_z & 0 \end{pmatrix} \qquad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \, . \tag{5}$$

Here, σ_z is a 2×2 Pauli matrix and I is the 2×2 unit matrix.

We wish now to consider the solutions of (4) for a free particle moving in the direction of the positive z-axis with momentum $\hbar k$. These can be taken from a relativistic quantum mechanics textbook (for example, [1]), giving the following normalized† wavefunction

$$\psi_k(z) = \frac{1}{2\pi}\sqrt{\frac{E + mc^2}{2mc^2}}\, \mathrm{e}^{\mathrm{i}kz} \begin{pmatrix} \chi \\ \frac{\sigma_z \hbar k c}{E + mc^2}\chi \end{pmatrix} \tag{6}$$

where $E = \sqrt{(\hbar k c)^2 + m^2 c^4}$ is the energy of the particle and χ an arbitrary two-component normalized spinor, i.e., $\chi^\dagger \chi = 1$ ($\chi = \binom{1}{0}$ for spin 'up', $\chi = \binom{0}{1}$ for spin 'down', or any linear combination of these two). Equation (4) admits also negative energy solutions with energy $-\sqrt{(\hbar k c)^2 + m^2 c^4}$. We will come back to this point. We notice that for non-relativistic momenta, i.e., $\hbar k \ll mc$, the lower two-component spinor in (6) vanishes and we get a wavefunction which is a plane-wave solution of the Schrödinger equation for a free particle with spin $1/2$

$$\psi_k(z) \propto \mathrm{e}^{\mathrm{i}kz} \begin{pmatrix} \chi \\ 0 \end{pmatrix} \, . \tag{7}$$

One can show that the wavefunction (6) is an eigenstate of the square of spin operator $\sum_{j=1}^{3} \hat{S}_j^2$ with eigenvalue $\frac{3}{4}\hbar^2$. Actually, this wavefunction is also an eigenstate of $\hat{S}_z$, given by

$$S_z = \frac{\hbar}{2}\begin{pmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{pmatrix} \tag{8}$$

if χ has the spin up or spin down form, but this is an artifact of having restricted the motion only to the z-axis. This means that each state is be twice degenerate. Note, however, that it is *not* an eigenstate of the square of the *total* angular momentum operator $\sum_{j=1}^{3}(\hat{S}_j + \hat{L}_j)^2$.

We are now interested in finding solutions describing a relativistic particle in a infinitely deep one-dimensional well. By analogy with the non-relativistic case, we could proceed by adding to the Dirac Hamiltonian in (4) a potential $V(z)$ such that

$$V(z) = \begin{cases} V_0 & z \ll 0 \\ 0 & 0 < z < L \\ V_0 & z \gg L \end{cases} \tag{9}$$

and then letting V_0 go to infinity. As said in the introduction, the solution for the time-independent Schrödinger equation with this potential, with $V_0 \to \infty$, is a standing wavefunction in the region $0 < z < L$

$$\psi_{k_n}(z) \propto \sin(k_n z) \tag{10}$$

with $k_n = (n\pi)/L$, $n = 1, 2, \ldots$, the energy eigenvalues being given by (3), and a null function for $z \ll 0$ and $z \gg L$.

This procedure, however, leads to the so-called 'Klein paradox': the flux of the reflected plane wave in the walls of the potential is larger than the flux of the incident wave [6]. This happens because the wavefunction starts to pick up components from the negative energy states once $|V_0 - E| > m$. As V_0 continues to increase, more and more negative energy states contribute as these are unbounded from below.

A way out of this problem is to assume that the mass of the particle is itself a function of z. This is equivalent of using a Lorentz scalar potential instead of a vector potential. The infinite well is then introduced replacing the mass in (4) by the function $m(z)$ defined by

$$m(z) = \begin{cases} M & z \ll 0 \\ m & 0 < z < L \\ M & z \gg L \end{cases} \tag{11}$$

where M is a constant which we will let go to infinity later. The function $m(z)$ is represented in figure 1.

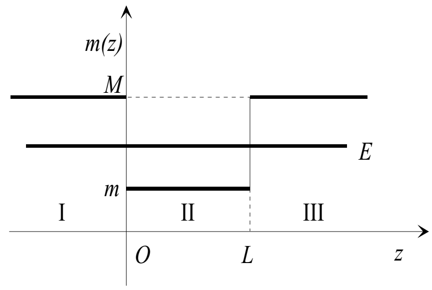

Figure 1. Plot of the mass as function of position $m(z)$ showing the three different zones I, II, III in which the solution of the Dirac is evaluated. Eventually we take the limit $M \to \infty$.

This method was used in the MIT bag model of hadrons [2], in which an infinite spherical well (bag) confines the otherwise free constituent quarks inside the bag. The solutions of the Dirac equation with $m(z)$ given by (11) can be considered separately in regions I, II and III, corresponding to $z < 0$, $0 \ll z \ll L$ and $z > L$, respectively. In each of these regions the

† In the sense that for wavefunctions with wavevectors k and k', denoted by $\psi_k(z)$ and $\psi_{k'}(z)$ respectively, one has $\int_{-\infty}^{\infty} \mathrm{d}z\, \psi_k^\dagger(z)\psi_{k'}(z) = \delta(k - k')$, where $\delta(k - k')$ is the Dirac delta function.

solution of the Dirac equation is of the form of (6) since the function $m(z)$ is constant in each of them. We consider that inside the well we have two plane waves travelling in opposite directions (an incident and a reflected wave on the walls of the well). Outside the well, we just consider one wave travelling outwards, anticipating the condition $\lim_{z\to\pm\infty}\psi(z) = 0$ for a bound solution. Thus, we may write for the three regions:

$$\begin{aligned}
\psi_{\rm I}(z) &= A\ {\rm e}^{-{\rm i}k'z}\begin{pmatrix}\chi\\ \frac{-\sigma_z\hbar k'c}{E+Mc^2}\chi\end{pmatrix}\\
\psi_{\rm II}(z) &= B\ {\rm e}^{{\rm i}kz}\begin{pmatrix}\chi\\ \frac{\sigma_z\hbar kc}{E+mc^2}\chi\end{pmatrix} + C\ e^{-ikz}\begin{pmatrix}\chi\\ \frac{-\sigma_z\hbar kc}{E+mc^2}\chi\end{pmatrix} \qquad (12)\\
\psi_{\rm III}(z) &= D\ e^{ik'z}\begin{pmatrix}\chi\\ \frac{\sigma_z\hbar k'c}{E+Mc^2}\chi\end{pmatrix}
\end{aligned}$$

where $k' = \sqrt{E^2/c^2 - M^2c^2}/\hbar$, and A, B, C and D are constants.

In the appendix we compute the solutions in the case $M\to\infty$ with suitable boundary conditions (the outward flux of probability at walls is zero). The result is that $\psi_{\rm I}(z)$ and $\psi_{\rm III}(z)$ vanish identically, and $\psi_{\rm II}(z)$ is given by

$$\psi_{\rm II}(z) = B\ {\rm e}^{{\rm i}\delta/2}\begin{pmatrix}2\cos\left(kz-\frac{\delta}{2}\right)\chi\\ 2{\rm i}P\sin\left(kz-\frac{\delta}{2}\right)\sigma_z\chi\end{pmatrix} \qquad (13)$$

where

$$\delta = \arctan\left(\frac{2P}{P^2-1}\right) \quad P = \frac{\hbar kc}{E+mc^2}\ . \qquad (14)$$

The need for a special boundary condition instead of simply requiring that the wavefunction be continuous at the walls is explained in the appendix. Actually, the wavefunction turns out to be discontinuous at the boundaries of the box, as can be seen from (13) This is not surprising if one realizes that the Dirac equation is a *first* order differential equation with a infinite jump in the potential in this case. In the non-relativistic particle in a box, we have a second-order differential equation, leading to a discontinuity in the first derivative of the wavefunction.

For non-relativistic momenta, $\hbar k \ll mc$ and $P\sim 0$ so that

$$\delta \sim \arctan\left(\frac{0}{-1}\right) = \pi\ . \qquad (15)$$

Setting $\delta=\pi$ and $P=0$ in (13) we get

$$\begin{aligned}
\psi_{\rm II}(z) &= B\ {\rm e}^{{\rm i}\pi/2}\begin{pmatrix}2\cos\left(kz-\frac{\pi}{2}\right)\chi\\ 0\end{pmatrix} \qquad (16)\\
&= B\ {\rm e}^{{\rm i}\pi/2}\begin{pmatrix}2\sin(kz)\chi\\ 0\end{pmatrix}
\end{aligned}$$

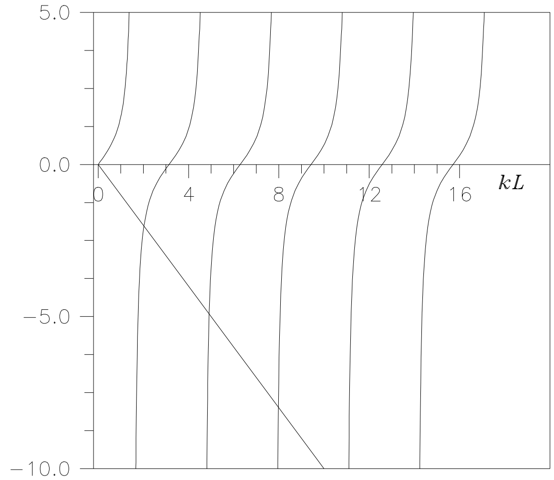

Figure 2. Graphical solution of (16) when $L=\hbar/(mc)$. The functions $\tan(kL)$ and $-kL$ are plotted. The values of kL for which the two curves intersect are the solutions of the equation $\tan(kL) = -kL$.

which is exactly the non-relativistic result (10) apart from a normalization factor and the spinor χ.

In the appendix we show that the wavenumber k is provided by the transcendental equation

$$\tan(kL) = \frac{2P}{P^2-1} = -\frac{\hbar k}{mc}\ . \qquad (17)$$

From the discrete set of values of k that satisfy (17) equation we get the discrete energy eigenvalues $E = \sqrt{\hbar^2c^2k^2+m^2c^4}$. We can check that for non-relativistic momenta $\tan(kL)\sim 0$ and $kL\sim n\pi$, $n=1,2,\ldots$, recovering the non-relativistic result. The size L of the box provides a criterion to decide whether a particle inside a well is relativistic or not, at least for the first energy eigenvalues. The distance scale is set by the length $L_0 = \hbar/(mc)$, which is the Compton wavelength of the particle divided by 2π. For $L\sim L_0$ or smaller the particle is relativistic and we must apply the relation (17). This length is about 0.004 Å for an electron. Figure 2 shows the graphic solution of (17) when $L=L_0$. If L is much bigger than L_0, the slope of the line approaches zero, in which case the two curves cross at $kL = \pi,\ 2\pi,\ 3\pi,\ ,\ldots$, corresponding to the non-relativistic behaviour. Figure 3 shows the values of kL/π for boxes with $L=L_0$, $L=10L_0$ and $L=100L_0$, in comparison with the non-relativistic case. One sees that a particle inside a box with $L=100L_0$ is already non-relativistic, at least for the lower spectrum. It is clear from Figure 4 that the relativistic levels are lower than the corresponding non-relativistic ones.

It is interesting to note that the relativistic probability density constructed from the wavefunction (13) has no

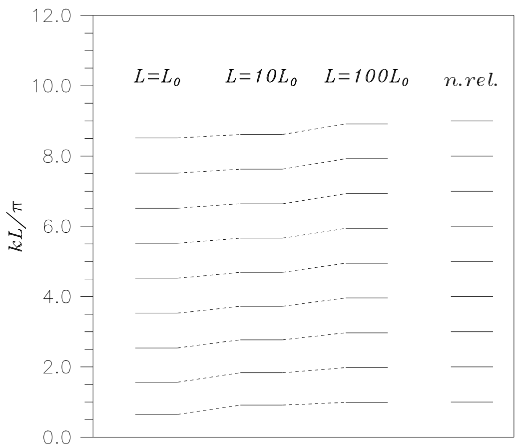

Figure 3. Solutions of (16) for boxes of sizes $L = L_0$, $L = 10L_0$ and $L = 100L_0$, together with the non-relativistic case (for which $kL = n\pi$).

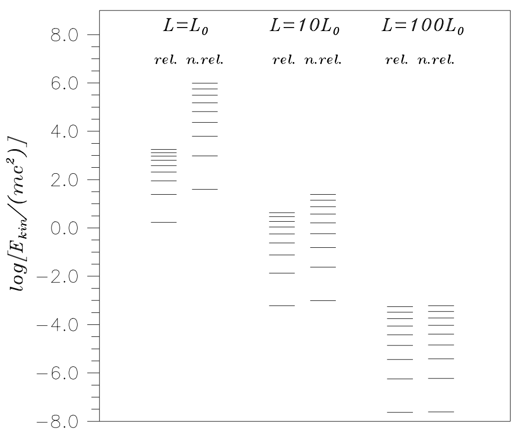

Figure 4. Relativistic spectrum of kinetic energies for the same box sizes of figure 3 ($E_{kin} = \sqrt{(\hbar kc)^2 + m^2c^4} - mc^2$) in comparison with the non-relativistic spectrum ($E_{kin} = (n\hbar\pi)^2/(2mL^2)$). The values shown are the logarithm of the kinetic energy in units of mc^2 for the lowest nine levels.

zeros. Indeed, if we compute $\psi_{\rm II}(z)^\dagger\psi_{\rm II}(z)$ we obtain

$$\psi_{\rm II}(z)^\dagger\psi_{\rm II}(z) = 4|B|^2\left[\cos^2\left(kz - \frac{\delta}{2}\right) + P^2\sin^2\left(kz - \frac{\delta}{2}\right)\right] = 4|B|^2\left[1 + (P^2-1)\sin^2\left(kz - \frac{\delta}{2}\right)\right]. \tag{18}$$

This quantity is never zero for $k \neq 0$ (if $k = 0$ the wavefunction is zero inside the well) because $0 < P < 1$. This could only happen if $P \to 0$, i.e., in the non-relativistic limit. Figure 5 shows the densities corresponding to the first three levels of a particle in a box with sizes L_0, $10L_0$ and $100L_0$. The latter case is non-relativistic and can be taken as a reference, showing the characteristic nodes of a stationary wave in a closed box.

3. Conclusions

We have analysed the relativistic particle in a one-dimensional box and compared it with the non-relativistic case. The quantized momentum values and corresponding energies emerge as solutions of a simple transcendental equation, in contrast with the more involved case of the relativistic particle in the three dimensional Coulomb problem. We have checked that both the spectrum and the wavefunctions go to their non-relativistic values as the size of the box grows. The basic scale is set by the length L_0 which is related to the Compton wavelength for the particle in the box. The probability density shows no nodes in a relativistic regime ($L \sim L_0$) but its minima approach zero as the box becomes larger.

Finally, let us compare the boundary conditions we have used with other approaches. For instance, (17) similar in form to the one obtained by Greiner [5]. However, one cannot make a correspondence between the two equations because of the way the potential well is defined in [5] and the problems that the approach used has when the depth of the well is allowed to go to infinity. In that work the wavefunction is required to be continuous at the walls of the well. One should also mention a textbook treatment of the same problem [7] in which two components of the wavefunction were required to be continuous at the box walls, while the other two were not. We think that there is no reason to treat the components of the wavefunction differently, especially when one is far from the non-relativistic regime. However, if one would demand that all components be continuous and also to be zero outside the box, the wavefunction would be identically zero everywhere. This means that the treatment of [7] is in fact *restricted* to the non-relativistic regime. On the other hand, the continuity of the wavefunction, which was crucial for solving the Schrödinger equation (a second order equation), does not need to be imposed for solving the Dirac equation (a first order equation), with a mass going to infinity outside a certain region. This allows one to impose a boundary condition in which the flux of probability is continuous at the box walls but the wavefunction is not. By doing that, one is still able to guarantee the fulfillment of the continuity equation for the probability density.

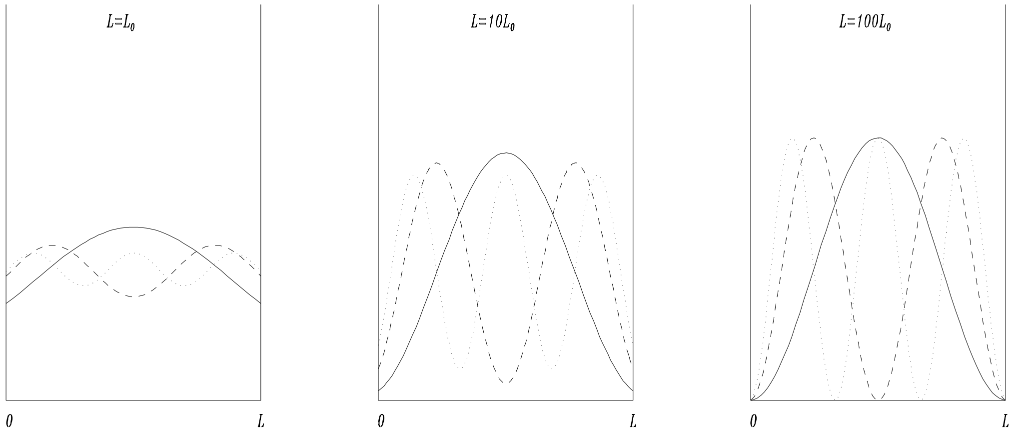

Figure 5. Plot of the probability density $\psi^\dagger(z)\psi(z)$ normalized to unity for the first three levels of a relativistic particle in boxes of sizes $L = L_0$, $L = 10L_0$ and $L = 100L_0$. The latter case is almost identical with the non-relativistic limit, as it is apparent from Figs. 4 and 5. Note that the density is discontinuous at the walls in the relativistic regime.

Appendix

In this appendix we present the mathematical formalism leading to (17).

Let us start by considering the solutions of the Dirac equation given by (12). Since we are going to let $M \to \infty$, we have $E < Mc^2$, so that the quantity

$$k' = \frac{1}{\hbar}\sqrt{\frac{E^2}{c^2} - M^2c^2} = \frac{\mathrm{i}}{\hbar}\sqrt{M^2c^2 - \frac{E^2}{c^2}} \qquad (19)$$

is an imaginary number, and thus the exponentials in k' are real decreasing exponentials, making $\psi_{\mathrm{I}}(z) \to 0$ and $\psi_{\mathrm{III}}(z) \to 0$ as $M \to \infty$. We have absorbed the normalization constants into the arbitrary complex constants A, B, C and D and set the same spinor χ for all plane waves for simplicity.

To find the relationship between the constants B and C and to get the energy eigenvalues we need to impose boundary conditions at $z = 0$ and $z = L$. We might be tempted to set the usual boundary conditions of the non-relativistic case, i.e., set the wavefunction to zero at those points. However, this implies that the wavefunction inside the well is zero. One alternative is to demand that the outward flux of probability at the walls of the well be zero, as was done in the MIT bag model [2]. The boundary condition is

$$\pm(-\mathrm{i})\beta\alpha_z\psi = \psi \qquad (20)$$

where the minus sign corresponds to $z = 0$ and the plus sign to $z = L$. We can check that the flux is zero by multiplying (20) at the left by $\bar\psi = \psi^\dagger\beta$. We obtain

$$\pm(-\mathrm{i})\bar\psi\beta\alpha_z\psi = \bar\psi\psi\ . \qquad (21)$$

Since $(-\mathrm{i})\bar\psi\beta\vec\alpha.\vec k/|\vec k|\psi$ represents the probability current density for a Dirac spinor in the direction of the wave vector $\vec k = \vec p/\hbar$, this condition just states that the probability current density at $z = 0$ and $z = L$ is equal to the value of $\bar\psi\psi$ at those points. Applying now (20) to $\psi_{\mathrm{II}}(z)$ at $z = 0$ gives the condition

$$C = B\frac{\mathrm{i}P - 1}{\mathrm{i}P + 1} \qquad (22)$$

with

$$P = \frac{\hbar kc}{E + mc^2}\ . \qquad (23)$$

On the other hand, $\bar\psi_{\mathrm{II}}\psi_{\mathrm{II}}$ at $z = 0$ is given by

$$\bar\psi_{\mathrm{II}}\psi_{\mathrm{II}}\big|_{z=0} = |B + C|^2 - |B - C|^2P^2 = 0 \qquad (24)$$

taking (22) into account. This means that, according to (21), there is no outward flow of probability at $z = 0$. The same result is obtained if we apply the boundary condition at $z = L$.

Let us look at the resulting wavefunction. Noticing that $(\mathrm{i}P - 1)/(\mathrm{i}P + 1)$ has unit modulus, we can write

$$\frac{\mathrm{i}P - 1}{\mathrm{i}P + 1} = \mathrm{e}^{\mathrm{i}\delta} \qquad \delta = \arctan\left(\frac{2P}{P^2 - 1}\right)\ . \qquad (25)$$

Replacing condition (22) in the wavefunction $\psi_{\mathrm{II}}(z)$ in the expressions (12) we obtain

$$\begin{aligned}\psi_{\mathrm{II}}(z) &= B\begin{pmatrix}\left(\mathrm{e}^{\mathrm{i}kz} + \mathrm{e}^{-\mathrm{i}kz}\mathrm{e}^{\mathrm{i}\delta}\right)\chi \\ P\left(\mathrm{e}^{\mathrm{i}kz} - \mathrm{e}^{-\mathrm{i}kz}\mathrm{e}^{\mathrm{i}\delta}\right)\sigma_z\chi\end{pmatrix} \\ &= B\,\mathrm{e}^{\mathrm{i}\delta/2}\begin{pmatrix}2\cos\left(kz - \frac{\delta}{2}\right)\chi \\ 2\mathrm{i}P\sin\left(kz - \frac{\delta}{2}\right)\sigma_z\chi\end{pmatrix}\ .\end{aligned} \qquad (26)$$

To calculate the eigenvalues for the energy we have to consider the boundary condition (20) at $z = L$. This results in the condition

$$-\mathrm{i}(B\,\mathrm{e}^{\mathrm{i}kL} - C\,\mathrm{e}^{-\mathrm{i}kL})P = B\,\mathrm{e}^{\mathrm{i}kL} + C\,\mathrm{e}^{-\mathrm{i}kL} \tag{27}$$

which, after collecting terms and using (22) yields

$$\mathrm{e}^{\mathrm{i}kL}(\mathrm{i}P+1)^2 = \mathrm{e}^{-\mathrm{i}kL}(\mathrm{i}P-1)^2$$
$$\frac{\mathrm{e}^{\mathrm{i}kL} - \mathrm{e}^{-\mathrm{i}kL}}{\mathrm{e}^{\mathrm{i}kL} + \mathrm{e}^{-\mathrm{i}kL}} = \frac{2\mathrm{i}P}{P^2-1}. \tag{28}$$

Using (23), we write finally

$$\tan(kL) = \frac{2P}{P^2-1} = -\frac{\hbar k}{mc}. \tag{29}$$

References

[1] Bjorken J D and Drell S D 1964 *Relativistic Quantum Mechanics* (New York: McGraw-Hill)
[2] Chodos A *et al* 1974 *Phys. Rev.* D **9** 3471
Chodos A *et al* 1974 *Phys. Rev.* D **10** 2599;
Thomas A W 1984 *Adv. Nucl. Phys.* **13** 1
[3] Coulter B L and Adler C G 1971 *Am. J. Phys.* **39** 305
[4] Coutinho F A B *et al* 1988 *Am. J. Phys.* **56** 904
[5] Greiner W 1990 *Relativistic Quantum Mechanics* (Berlin: Springer)
[6] Itzykson C and Zuber J 1980 *Quantum Field Theory* (New York: McGraw-Hill)
[7] Sherwin C W 1959 *Introduction to Quantum Mechanics* (New York: Henry Holt)