Relativistic spin-0 particle in a box: Bound states, wave packets, and the disappearance of the Klein paradox

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ADVANCED TOPICS SECTION

Relativistic spin-0 particle in a box: Bound states, wave packets, and the disappearance of the Klein paradox

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The "particle-in-a-box" problem is investigated for a relativistic particle obeying the Klein–Gordon equation. To find the bound states, the standard methods known from elementary non-relativistic quantum mechanics can only be employed for "shallow" wells. For deeper wells, when the confining potentials become supercritical, we show that a method based on a scattering expansion accounts for Klein tunneling (undamped propagation outside the well) and the Klein paradox (charge density increase inside the well). We will see that in the infinite well limit, the wave function outside the well vanishes, and Klein tunneling is suppressed: Quantization is, thus, recovered, similar to the non-relativistic particle in a box. In addition, we show how wave packets can be constructed semi-analytically from the scattering expansion, accounting for the dynamics of Klein tunneling in a physically intuitive way. © *2022 Published under an exclusive license by American Association of Physics Teachers.*
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I. INTRODUCTION

In non-relativistic quantum mechanics, the "particle in a box," i.e., when the square well potential is extended to infinite depth, is the simplest problem considered in textbooks, usually in order to introduce the quantization of energy levels. In contrast, in the first quantized relativistic quantum mechanics (RQM), the situation is not so simple, and the problem is understandably hardly treated in RQM textbooks. The reason is that when the potential reaches a sufficiently high value, the energy gap $2mc^2$ separating the positive energy solutions from the negative energy ones is crossed (m is the rest mass of the particle). For such potentials, known as "supercritical potentials," the wave function does not vanish outside the well but propagates undamped in the high potential region, a phenomenon known as Klein tunneling.[1,2] Indeed, RQM—although remaining a single-particle formalism—intrinsically describes a generic quantum state as a superposition of positive energy solutions (related to particles) and negative energy solutions (related to antiparticles).

Therefore, for relativistic particles, the particle-in-a-box problem is not suited to introductory courses. For this reason, only finite, non-supercritical rectangular potential wells are usually presented in RQM classes (see, for example, Sec. 9.1 of Ref. 3 for the Dirac equation describing fermions in a square well or Sec. 1.11 of the textbook[4] for the Klein–Gordon equation, spin-0 bosons, in a radial square well). For a Dirac particle in an infinite well, a "bag" model was developed by not introducing an external potential, but assuming a variable mass taken to be constant and finite in a box, but infinite outside;[5,6] in this way, Klein tunneling is suppressed, and solutions similar to those known in the non-relativistic case can be obtained. This method was recently extended to the Klein–Gordon equation.[7]

In this work, we show that for the Klein–Gordon equation in a one-dimensional box, it is not necessary to change the mass to infinity outside the well in order to confine the particle. To do so, we shall consider multiple scattering expansions inside the well. Such expansions were recently employed to investigate relativistic dynamics across supercritical barriers.[8] We will see below that Klein tunneling, which is prominent for a supercritical potential well sufficiently higher than the particle energy placed inside, disappears as the well's depth V is increased. In the infinite-well limit, Klein tunneling is suppressed, and the walls of the well become perfectly reflective, as in the non-relativistic case.

The relativistic bosonic particle in a box is an interesting problem because it yields a simple understanding, in the first quantized framework, of the charge creation property that is built into the Klein–Gordon equation, extending tools (scattering solutions to simple potentials) usually encountered in introductory non-relativistic classes. Moreover, as we will show in this paper, time-dependent wave packets can be easily built from the scattering solutions. This is important because wave packets allow us to follow in an intuitive way the dynamics of charge creation in a relativistic setting. The physics of charge creation in the presence of supercritical potentials is much more transparent for the Klein–Gordon equation than for the Dirac equation, which needs to rely in the first quantized formulation on hole theory (see Ref. 9 for a Dirac wave packet approach for scattering on a supercritical step).

The paper is organized as follows. We first recall in Sec. II the Klein–Gordon equation and address the finite square well problem, obtaining the bound-state solutions. In Sec. III, we introduce the method of the multiple scattering expansion (MSE) in order to calculate the wave function inside and outside a square well. We will then see (Sec. IV)

that the wave function outside the well vanishes as the well depth tends to infinity. The fixed energy solutions are similar to the well-known Schrödinger ones. Finally, we show (Sec. V) how the MSE can be used to construct simple wave packets in a semi-analytical form. We will give illustrations showing the time evolution of a Gaussian initially inside square wells of different depths.

II. KLEIN–GORDON SOLUTIONS FOR A PARTICLE IN A SQUARE WELL

A. The Klein–Gordon equation

The wave function $\Psi(t,x)$ describing relativistic spin-0 particles is well-known to be described by the Klein–Gordon (KG) equation.[3,4] In one spatial dimension and in the presence of an electrostatic potential energy $V(x)$, the KG equation is expressed in the canonical form and in the minimal coupling scheme as

$$[i\hbar\partial_t - V(x)]^2\Psi(t,x) = (c^2\hat{p}^2 + m^2c^4)\Psi(t,x), \qquad (1)$$

where c is the speed of light in vacuum, $\hat{p} = -i\hbar\partial_x$ is the momentum operator, and $\hbar$ is the reduced Planck constant. The charge density $\rho(t,x)$, which can take positive or negative values associated with particles and anti-particles, is given by (see, e.g., Refs. 3 and 4)

$$\rho(t,x) = (i\hbar/2mc^2)[\Psi^*(t,x)\partial_t\Psi(t,x) - \Psi(t,x)\partial_t\Psi^*(t,x)]$$
$$- (V(x)/mc^2)\Psi^*(t,x)\Psi(t,x). \qquad (2)$$

A generic state may contain both particle and anti-particle contributions, corresponding to positive and negative energies, respectively [see Eq. (6) below]. The scalar product of two wave functions $\Psi_I(t,x)$ and $\Psi_{II}(t,x)$ is defined as

$$\langle\Psi_I(t,x)|\Psi_{II}(t,x)\rangle$$
$$= \int dx\Big\{(i\hbar/2mc^2)$$
$$\times [\Psi_I^*(t,x)\partial_t\Psi_{II}(t,x) - \partial_t\Psi_I^*(t,x)\Psi_{II}(t,x)]$$
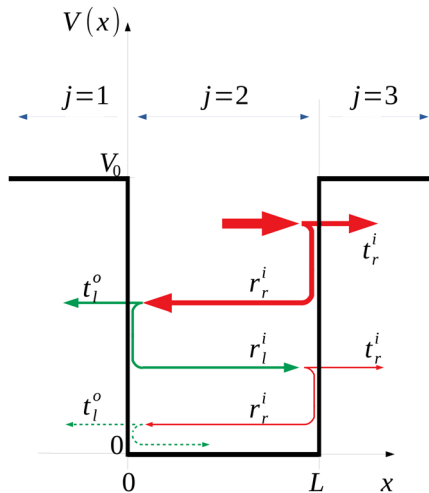$$- (V(x)/mc^2)[\Psi_I^*(t,x)\Psi_{II}(t,x)]\Big\}. \qquad (3)$$

Fig. 1. A square well with the three regions j considered in the text. The arrows depict the multiple scattering expansion for a wave initially traveling toward the right edge of the well (see Sec. III for details).

B. The finite square well

1. Plane-wave solutions

Before getting to the problem of a particle in an infinite well, let us address first a particle inside a square well of finite depth. A square well in one dimension can be described by the potential,

$$V(x) = V_0\theta(-x)\theta(x-L), \qquad (4)$$

where $\theta(x)$ is the Heaviside step function, V_0 is the depth of the well, and L is its width. As illustrated in Fig. 1, we consider the three regions indicated by $j = 1, 2$, and 3. In each of the three regions, the KG equation (1) accepts plane wave solutions of the form:

$$\Psi_j(t,x) = (A_je^{ip_jx/\hbar} + B_je^{-ip_jx/\hbar})e^{-iEt/\hbar}, \qquad (5)$$

where we set E to be the energy inside the well (region 2). By inserting those solutions in Eq. (1), one obtains E in terms of the momentum inside the well,

$$E(p) = \pm\sqrt{c^2p^2 + m^2c^4}, \qquad (6)$$

where, for convenience, we put $p = p_2$. These are the plane wave solutions in free space known from RQM textbooks.[3,4] A plane wave with $E(p) > 0$ represents a particle, whereas a solution with $E(p) < 0$ represents an antiparticle. We will be considering situations in which a particle is placed inside the well, so we will take positive plane-wave solutions in region 2. Outside the well (in regions 1 and 3), it is straightforward to see that $\Psi_j(t,x)$ is a solution provided $p_{1,3} = q(p)$, where

$$q(p) = \pm\sqrt{(E(p) - V_0)^2 - m^2c^4}/c. \qquad (7)$$

Note that in the limit of an infinite well ($V_0 \gg mc^2$), $q(p)$ is always real, so that typical solutions $\Psi_j(t,x)$ in regions $j = 1$ and 3 are oscillating. Note also that a classical particle with energy E would have inside the well a velocity $v = pc^2/E$ (so p and v have the same sign). Hence, for the region 2 solutions $\Psi_2(t,x)$, when p is positive, $e^{ipx/\hbar}$ corresponds to a particle moving to the right (and $e^{-ipx/\hbar}$ to the left). However, outside the well, we have

$$v' = qc^2/(E - V_0), \qquad (8)$$

so that for large V_0, the velocity and the momentum of a classical particle have opposite signs.[10,11] So a plane wave $e^{iqx/\hbar}$ with $q > 0$ now corresponds to a particle moving to the left. This can also be seen by rewriting the plane waves in terms of the energy outside the well, say $\exp i(p_1x - \bar{E}t)/\hbar$. This is tantamount to taking the potential to be 0 in region 1 and $\bar{V} = -V_0$ in region 2 (with $V_0 > 0$). Since we require $\bar{E} - \bar{V}$ to be positive and smaller than V_0 (in order to represent a particle inside the well), we must have $\bar{E} < 0$. In this case, a given point x described by the plane wave $\exp i(p_1x - \bar{E}t)/\hbar$ travels to the right if p_1 is negative. For instance, the position of an antinode changes by $\Delta x = \Delta t\bar{E}/p_1$ in the time interval Δt, so if $\bar{E} < 0$, the sign of Δx will be opposite to the sign of p_1.[26]

2. Bound states

Bound states are obtained when the solutions outside the well are exponentially decaying. This happens when $q(p)$ has imaginary values, that is for potentials satisfying

$E - mc^2 < V_0 < E + mc^2$. Note that for a particle at rest in the well frame, $E \approx mc^2$, and the condition for the existence of bound states becomes $V_0 < 2mc^2$.

In order to find the bound state solutions, we employ the same method used in elementary quantum mechanics for the Schrödinger equation square well. We first set the boundary conditions on the wave functions (5) accounting for no particles incident from the left in region 1 nor from the right in region 3, yielding

$$A_1 = B_3 = 0. \tag{9}$$

We then require the continuity of the wave functions $\Psi_j(t, x)$ of Eq. (5) and their spatial derivatives at the potential discontinuity points $x = 0$ and $x = L$:

$$\Psi_1(t, 0) = \Psi_2(t, 0), \quad \Psi_2(t, L) = \Psi_3(t, L),$$
$$\Psi_1'(t, 0) = \Psi_2'(t, 0), \quad \Psi_2'(t, L) = \Psi_3'(t, L). \tag{10}$$

This gives

$$B_1 = A_2 + B_2, \quad A_2 e^{ipL} + B_2 e^{-ipL} = A_3 e^{iqL},$$
$$-qB_1 = p(A_2 - B_2), \quad p(A_2 e^{ipL} - B_2 e^{-ipL}) = qA_3 e^{iqL}. \tag{11}$$

By eliminating A_3 and B_1, we obtain a system of two equations in A_2 and B_2,

$$(q + p)A_2 + (q - p)B_2 = 0,$$
$$(q - p)A_2 e^{ipL} + (q + p)B_2 e^{-ipL} = 0, \tag{12}$$

where q is given by Eq. (7). This system admits nontrivial solutions when the determinant of the system (12) vanishes,

$$(q + p)^2 e^{-ipL} - (q - p)^2 e^{ipL} = 0. \tag{13}$$

Nontrivial solutions exist only if q is an imaginary number $q = iq_r$, where $q_r \in \mathbb{R}$. Solving Eq. (13) for q gives the two solutions:

$$q_{ra} = p \tan(pL/2),$$
$$q_{rb} = -p \cot(pL/2). \tag{14}$$

As is familiar for the Schrödinger square well,[12] the bound state energies are obtained from the intersections of the curves $q_{ra,b}(p)$ with the curve $q_r(p) = \sqrt{m^2 c^4 - (E(p) - V)^2}/c$. For simplicity, we use the dimensionless variables
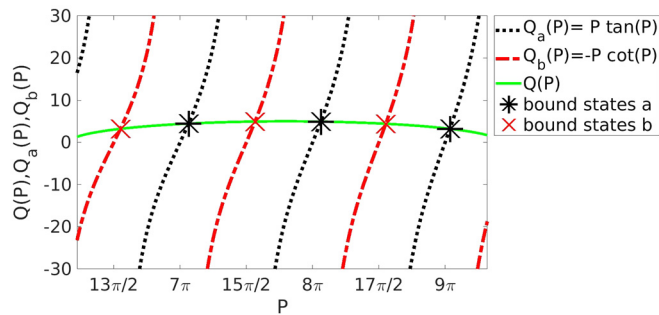

Fig. 2. The bound state energies of a particle of mass $m = 1$ ($L = 10$, natural units are used, see text) are found from the values of $P = pL/(2\hbar)$ at the intersections of the curves defined in Eq. (15).

$$Q = qL/(2\hbar),$$
$$Q_{a,b} = q_{r,a,b}L/(2\hbar),$$
$$P = pL/(2\hbar). \tag{15}$$

Figure 2 gives an illustration for a particle confined in a well of width $L = 10$ (we employ natural units $c = \hbar = \varepsilon_0 = 1$ as well as $m = 1$; the conversion to SI units depends on the particle's mass, e.g., for a pion meson π^+, the mass is 139.57 MeV/c^2). The energies are inferred from the values of P at the intersection points.

III. MULTIPLE SCATTERING EXPANSION FOR SUPERCRITICAL WELLS

A. Principle

We have just seen that the method depending on matching conditions jointly at $x = 0$ and $x = L$ as per Eq. (10) only works if $q(p)$ is imaginary, since, otherwise, Eq. (13) has no solutions. However, as is seen directly from Eq. (7), for sufficiently large V_0, $q(p)$ is real. For this case, we use a different method in which the wave function is seen as resulting from a multiple scattering process on the well's edges. The well is actually considered as being made out of two potential steps, and the matching conditions apply separately at each step.

More precisely, consider the following step potentials: a left step, $V_l(x) = V_0 \theta(-x)$, and a right step, $V_r(x) = V_0 \theta(x - L)$. Let us focus on the wave function inside the well, whose general form is given by $\Psi_2(t, x)$ [Eq. (5)]; the boundary conditions are those given by Eq. (9), meaning no waves are incoming toward the well. Let us first consider a plane wave $\alpha e^{ipx/\hbar}$ with amplitude α propagating inside the well toward the right ($p > 0$; see Fig. 1). On hitting the right step, this wave will be partly reflected and partly transmitted to region 3. The part reflected inside the well will now travel toward the left, until it hits the left step, at which point, it suffers another reflection and transmission. This multiple scattering process continues as the reflected wave inside the well travels toward the right edge. Similarly, we can consider a plane wave $\beta e^{-ipx/\hbar}$ of amplitude β initially inside the well but propagating to the left. This wave hits the left step first and then scatters multiple times off the two edges similarly. Multiple scattering expansions, generally employed when several scatterers are involved, are also often used in potential scattering problems in order to gain insight in the buildup of solutions involving many reflections (see Ref. 13 for an application to plane-wave scattering on a rectangular barrier).

B. Determination of the amplitudes

The coefficients giving the scattering amplitudes due to reflection and transmission at the two steps will be denoted as $r_{l,r}$ and $t_{l,r}$, respectively, where l and r indicate the left and right steps, respectively. In order to calculate those coefficients, one has to solve the step problem separately for each of the two steps.

The continuity of the plane wave $e^{ipx/\hbar}$ and its first spatial derivative at the right step ($x = L$) yield the following two equations:

$$e^{ipL/\hbar} + r_r e^{-ipL/\hbar} = t_r e^{iqL/\hbar},$$
$$e^{ipL/\hbar} - r_r e^{-ipL/\hbar} = (q/p) t_r e^{iqL/\hbar} \tag{16}$$

giving

$$t_r = 2p/(p+q)e^{i(p-q)L/\hbar},$$
$$r_r = (p-q)/(p+q)e^{i2pL/\hbar}. \tag{17}$$

Similarly, in order to calculate the coefficients of reflection and transmission suffered by a plane wave propagating inside the well toward the left step, one uses the continuity of the plane wave and its space derivative at $x = 0$ to obtain:

$$t_l = 2p/(p+q), \quad r_l = (p-q)/(p+q). \tag{18}$$

After the plane wave reflects for the first time either on the right or left steps, it will undergo a certain number of reflections before being finally transmitted outside the well. Let $\alpha e^{ipx/\hbar}$ be the initial wave inside the well moving to the right (recall $B_3 = 0$). After the first cycle of reflections from both steps, the amplitude of the same plane wave becomes $\alpha r_r r_l$, and $\alpha(r_r r_l)^n$ after n cycles of successive reflections. This process is illustrated in Fig. 1. In addition, an initial plane wave moving to the left (recall $A_1 = 0$), $\beta e^{-ipx/\hbar}$, contributes, after reflecting on the left step, to the wave moving to the right, first with amplitude βr_l and then multiplied by $(r_r r_l)$ after each cycle of reflections. The amplitude of the plane wave $e^{ipx/\hbar}$ in region 2 is the sum of these contributions, namely, $(\alpha + \beta r_l) \sum_n (r_r r_l)^n$. We can identify this term with the amplitude A_2 in region 2, Eq. (5) (recall we have set $p \equiv p_2$).

Along the same lines, we identify B_2 in Eq. (5) with the amplitude of the term $e^{-ipx/\hbar}$ inside the well resulting from multiple scattering as well as B_1 in region 1 and A_3 in region 3. The result is

$$B_1 = t_l(\alpha r_r + \beta) \sum_{n=0}^{\infty} (r_r r_l)^n,$$

$$A_2 = (\alpha + \beta r_l) \sum_{n=0}^{\infty} (r_r r_l)^n,$$

$$B_2 = (\alpha r_r + \beta) \sum_{n=0}^{\infty} (r_r r_l)^n,$$

$$A_3 = t_r(\alpha + \beta r_l) \sum_{n=0}^{\infty} (r_r r_l)^n,$$

$$A_1 = B_3 = 0. \tag{19}$$

The behavior of the series $\sum_{n \geq 0} (r_l r_r)^n$ is interesting as it is related to charge creation. The term

$$|r_l r_r| = |(p-q)/(p+q)|^2 \tag{20}$$

can, indeed, be greater or smaller than 1, corresponding, respectively, to a divergent or convergent series. As follows from Eq. (8), for a supercritical potential $(E - V_0) < 0$, so the direction of the motion is opposite to the direction of the momentum. Hence, given the boundary conditions $A_1 = B_3 = 0$, we see that we must set $q < 0$ in order to represent outgoing waves in regions 1 and 3 (moving in the negative and positive directions, respectively). We conclude that for supercritical wells, $|r_l r_r| > 1$ and the amplitudes (19) diverge. The physical meaning of a diverging series is best understood in a time-dependent picture, as we will see in Sec. V. The nth term of the series will be seen to correspond to the nth time the wave packet hits one of the edges, each hit increasing the wave packet's amplitude.

Note that for $q < 0$, both $|r_l| > 1$ and $|r_r| > 1$. This is an illustration of bosonic superradiance at a supercritical potential

step: For a given plane-wave incoming on the potential step (here the left or right steps), the reflected current is higher than the incoming one.[14,15] This phenomenon, that at first sight appears surprising, became known as the "Klein paradox."

IV. THE INFINITE WELL

As we have just seen, one of the signatures of the Klein–Gordon supercritical well—a feature unknown in non-relativistic wells—is that the amplitudes outside the well, B_1 and A_3, are not only non-zero, but grow with time. Each time that a particle hits an edge of the well, the reflected wave has a higher amplitude, but since the total charge is conserved, antiparticles are transmitted in zones 1 and 3.

However, it can be seen that as the depth of the supercritical well increases, the amplitudes of the wave function transmitted outside the well decrease. Indeed, the step transmission coefficients t_r and t_l given by Eqs. (17) and (18) are proportional to $1/V_0$. Hence, in the limit of infinite potentials, $V_0 \to \infty$, the transmission vanishes. We also see from Eqs. (17) and (18) that $r_l \to -1, r_r \to -e^{2ipL/\hbar}$, and $\sum_n (r_r r_l)^n$ is bounded and oscillates. Hence, from Eq. (19), in this limit, $A_3 \to 0$ and $B_1 \to 0$. This implies $\psi(x = 0) = \psi(x = L) = 0$, and these conditions can only be obeyed provided

$$p = k\pi\hbar/L, \tag{21}$$

where k is an integer; we also then have $B_2 = -A_2$. The unnormalized wave function inside the well takes the form:

$$\Psi_2(t, x) = 2iA_2 \sin\left(\frac{k\pi}{L} x\right) e^{-i(E_k t/\hbar)}, \tag{22}$$

while the amplitudes outside the well obey $B_1 \to 0$ and $A_3 \to 0$ (although for $p = k\pi\hbar/L$, $\sum_n (r_r r_l)^n$ diverges). This can be seen by remarking that when Eq. (21) holds, $r_r r_l = 1$, and B_1 can be parsed as

$$B_1 = t_l(\alpha r_r + \beta) + t_l(\alpha r_r + \beta) + \cdots. \tag{23}$$

Since $t_l \to 0$ as $V_0 \to \infty$, the wave function in region 1 vanishes in this limit. A similar argument holds for A_3.

Note, however, that A_2 (and B_2) become formally infinite, given that the series $\sum_n^{n_{max}} e^{2inpL/\hbar} = n_{max} + 1$ is unbounded when Eq. (21) holds as $n_{max} \to \infty$. Since the total charge must be conserved (and cannot change each time n_{max} increases), the wave function inside the well should be renormalized to the total charge. Unit charge normalization corresponds to

$$\Psi_2^k(t, x) = \sqrt{\frac{2}{L}} \sin\left(\frac{k\pi}{L} x\right) e^{-i(E_k t/\hbar)} \tag{24}$$

with [Eqs. (6) and (21)]

$$E_k = \sqrt{(k\pi\hbar/L)^2 c^2 + m^2 c^4}. \tag{25}$$

In the non-relativistic limit, the kinetic energy is small relative to the rest mass, yielding

$$E \approx E_k^{NR} = mc^2 + k^2\pi^2\hbar^2/2mL^2 \tag{26}$$

recovering the non-relativistic particle in a box energy (up to the rest mass energy term). Equation (25) is the same result obtained recently by Alberto et al.,[7] who employed a

bag-model (taking the mass to be infinite mass in regions 1 and 3) in order to ensure the suppression of Klein tunneling.

In a real situation, neither V_0 nor the number of reflections (corresponding to the time spent inside the well) can be infinite. Given a finite value of V_0, a particle placed inside the well is represented by a wave packet that will start leaking after a certain number of internal reflections, as we discuss in Sec. V. This shows that although quantization for infinitely deep wells looks similar to the corresponding non-relativistic well, the mechanism is very different, as in the latter case, we have exponentially decreasing solutions that vanish immediately outside the well, whereas in the present case, we have oscillating solutions that are suppressed.

Note that although quantization only appears in the limit $V_0 \to \infty$, for high but finite values of V_0, resonant Klein tunneling (e.g., Ref. 16) takes place: The amplitudes (19) peak for energy values around E_k given by Eq. (25). This can be seen by plotting the amplitudes as a function of E or p. An illustration is given in Fig. 3, showing $B_1(p)$ and $A_2(p)$ for different values of V_0. It can be seen that the amplitudes are peaked around the quantized p values [Eq. (21)] while concomitantly decreasing as the well depth increases.

For completeness, let us mention that the square well bound states of Sec. II B 2 can also be recovered employing the MSE. Indeed, for bound states, the wave function must be a standing wave. Given the symmetry of the problem, the wave function is either symmetric or anti-symmetric with respect to the center of the well, $x = L/2$. In the symmetric case, the standing wave is, thus, given by $C \cos[p(x - L/2)/\hbar]$. Matching this form to $\Psi_2(x) = A_2 e^{ipx/\hbar} + B_2 e^{-ipx/\hbar}$ leads to

$$A_2/B_2 = e^{-ipL/\hbar}. \tag{27}$$

The anti-symmetric standing wave is of the form $C \sin[p(x - L/2)/\hbar]$, which is equated to $\Psi_2(x)$ to obtain $A_2/B_2 = -e^{-ipL/\hbar}$. Replacing A_2 and B_2 by their respective MSE expansion given by Eqs. (19), therefore, leads to

$$(\alpha + \beta r_l)/(\alpha r_r + \beta) = \pm e^{-ipL/\hbar}. \tag{28}$$

Using $r_r = r_l e^{2ipL/\hbar}$ from Eqs. (17) and (18) and keeping in mind that α and β are arbitrary complex numbers, Eq. (28) becomes

$$r_l = \pm e^{-ipL}. \tag{29}$$

Now, using $r_l = (p - q)/(p + q)$ from Eq. (18) and squaring both sides of this equation lead to Eq. (13) and, hence, to the quantization conditions obtained above in Sec. II B 2.

Note that these bound states are obtained when the solutions outside the well are exponentially decaying. In this case, the series $\sum_n (r_r r_l)^n$ is bounded and oscillates, whereas in the supercritical regime, this series was seen to be exponentially divergent. When the MSE diverges, applying joint matching conditions of the type given by Eq. (10) is incorrect and leads to unphysical results (for instance, in the scattering of Klein–Gordon particles on a barrier, doing so leads to acausal wave packets and superluminal barrier traversal times[17,18]).

V. WAVE PACKET DYNAMICS

A. Wave packet construction

Since the solutions $\Psi_j(t, x)$ of Eq. (5), with the amplitudes given by Eq. (19), obey the Klein Gordon equation inside and outside the well, we can build a wave packet by superposing plane waves of different momenta p. We will follow the evolution of an initial Gaussian-like wave function localized at the center of the box and launched toward the right edge (that is with a mean momentum $p_0 > 0$). We will consider two instances of supercritical wells: one with a "moderate" depth displaying Klein tunneling and the other with a larger depth in which Klein tunneling is suppressed.

Let us consider an initial wave packet

$$G(0, x) = \int dp \, g(p)(A_2(p)e^{ipx/\hbar} + B_2(p)e^{-ipx/\hbar}) \tag{30}$$

with

$$g(p) = e^{-(p-p_0)^2/4\sigma_p^2} e^{-ipx_0}. \tag{31}$$

We will choose x_0 to be the center of the well and take p_0 as well as all the momenta in the integration range in Eq. (30) positive. We, therefore, set $\beta = 0$ in the amplitudes (19) and choose α in accordance with unit normalization for the wave packet. σ_p^2 fixes the width of the wave packet in momentum space (ideally narrow, though its spread in position space should remain small relative to L). Finally, the sum $\sum (r_r r_l)^n$ is taken from $n = 0$ to n_{max}, where the choice of n_{max} depends on the values of t for which the wave packet dynamics will be computed. Indeed, each term $(r_r r_l)^n$ translates the wave packet by a distance $2nL$, so this term will only come into play at times of the order of $t \sim 2nL/v$, where $v \sim p_0 c/\sqrt{c^2 m^2 + p_0^2}$ is the wave packet mean velocity.
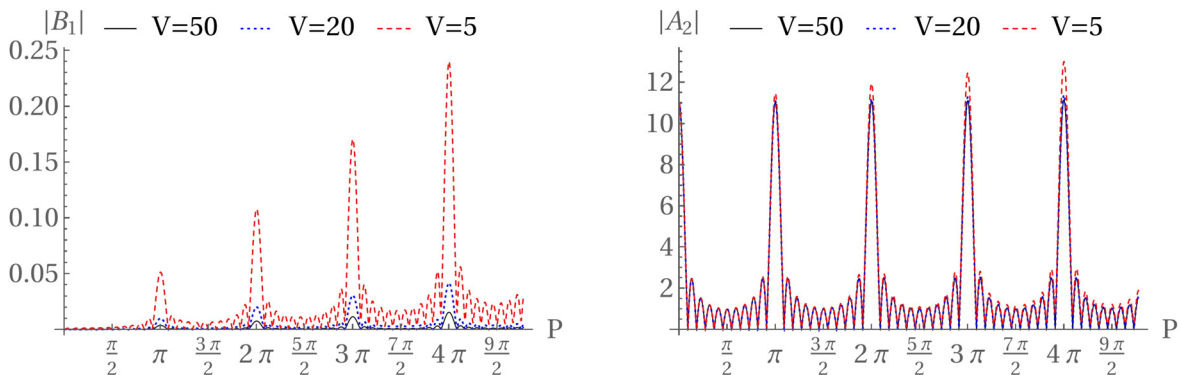

Fig. 3. The amplitudes $|B_1|$ and $|A_2|$ calculated using the MSE relations Eq. (19) with $n_{max} = 10$, $\alpha = 1$, and $\beta = 0$ are shown for different values of the supercritical well depth $V_0 = 5, 20$, and 50 (p is given in units of $1/L$ and $c = \hbar = 1$). Inside the well, the resonant structure of $|A_2|$ is not much affected as V_0 changes (the curves nearly superpose), but the amplitude $|B_1|$ outside the well, indicative of Klein tunneling, is seen to decrease as V_0 increases.

Note that in position space, $G(0, x)$ is essentially a Gaussian proportional to $e^{-(x-x_0)^2/4\sigma_x^2}e^{ip_0x}$.[27]

Following Eq. (5), the wave packet in each region is given by

$$G_j(t,x) = \int dp\, g(p)\Psi_j(t,p) \qquad (32)$$

where the amplitudes $A_j(p)$ and $B_j(p)$ are obtained from the MSE. For supercritical potential wells, we have to take $q < 0$ in the MSE amplitudes. The charge $\rho(t,x)$ associated with the wave packet in each region is computed from $G_j(t,x)$ by means of Eq. (2).

B. Illustrations

We show in Figs. 4 and 6 the time evolution of the charge corresponding to the initial wave packet (30) in supercritical wells. The only difference between both figures is the well depth, $V_0 = 5\,mc^2$ in Fig. 4 and $V_0 = 50\,mc^2$ in Fig. 6. The calculations are semi-analytical in the sense that the integration in Eq. (32) must be done numerically for each space-time point (t, x).

For $V_0 = 5\,mc^2$, Klein tunneling is prominent: The positive charged wave packet moves toward the right, and upon reaching the right edge, the supercritical potential produces negative charge outside the well (corresponding to antiparticles) and

positive charge inside. The reflected charge is higher than the incoming charge—this is a time-dependent version of Klein's paradox—but the total charge is conserved. The reflected wave packet then reaches the left edge of the well, resulting in a transmitted negatively charged wave packet and a reflected wave packet with a higher positive charge, now moving to the right inside the well. We have also displayed (Fig. 5) results obtained from solving numerically the KGE equation through a finite difference scheme. The numerical method employed is described elsewhere[8]—here its use is aimed at showing the accuracy of our MSE based wave packet approach.

For a higher confining potential (Fig. 6), transmission outside the well is considerably reduced: The wave packet is essentially reflected inside the well. This is due to the fact, noted above, that the plane-wave transmission amplitudes from which the wave packet is built are proportional to $1/V_0$. Hence in the limit $V_0 \to \infty$, Klein tunneling becomes negligible. We recover a behavior similar to the one familiar for the non-relativistic infinite well wave packets.[19]

VI. DISCUSSION AND CONCLUSION

In this work, we studied a Klein–Gordon particle in a deep (supercritical) square well. We have seen that the method based on connecting the wave function at both potential discontinuities, employed for non-relativistic square wells, only
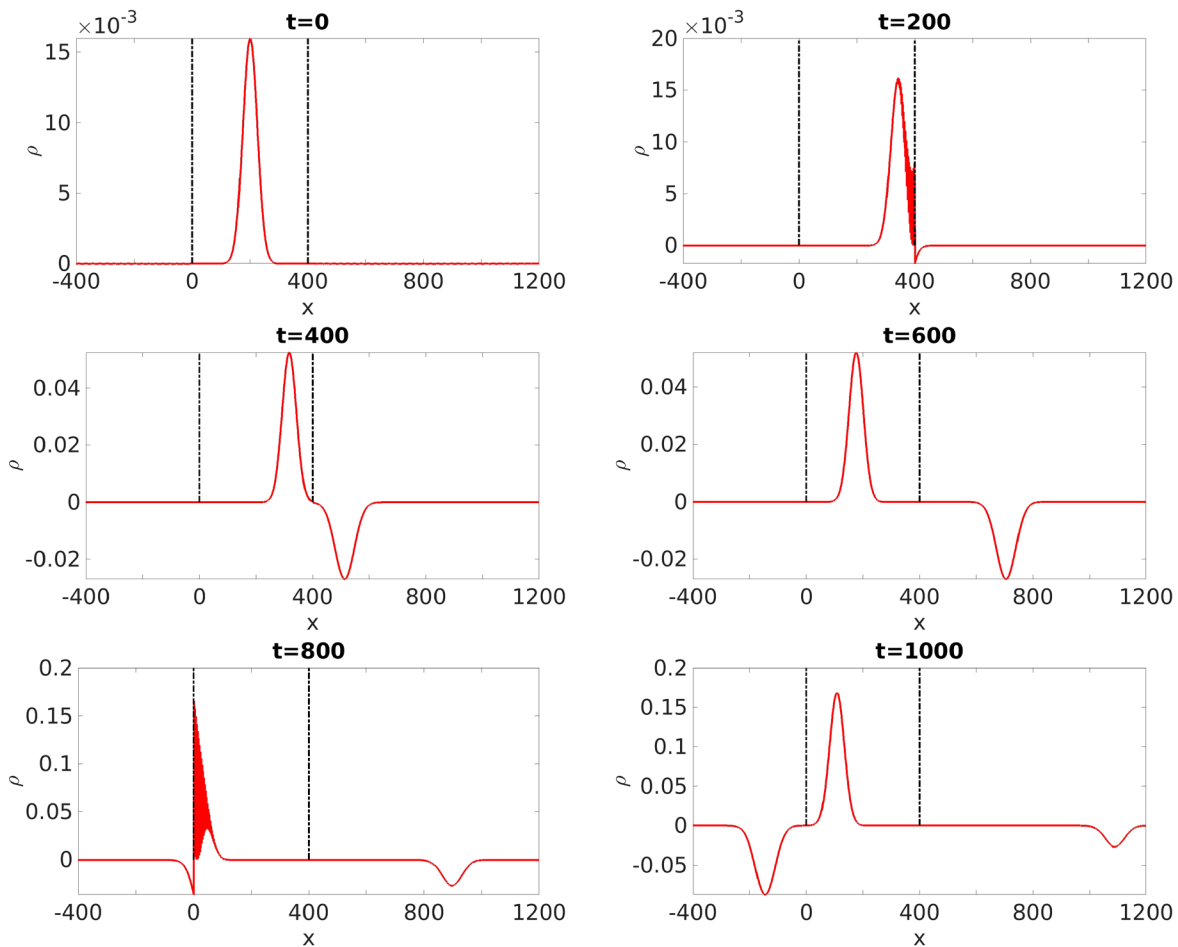

Fig. 4. The charge $\rho(t,x)$ associated with the wave packet given by Eq. (32) for a particle of unit mass is shown for different times as indicated within each panel. The parameters are the following: $L = 400$ and $V_0 = 5\,mc^2$ for the well, $x_0 = 200$, $p_0 = 1$, and $\sigma_p = 0.02$ for the initial state, $\alpha = 1$, $\beta = 0$, and $n_{max} = 10$ for the MSE series (natural units $c = \hbar = 1$ are used). The change in the vertical scale is due to charge creation (no adjustment or renormalization has been made).
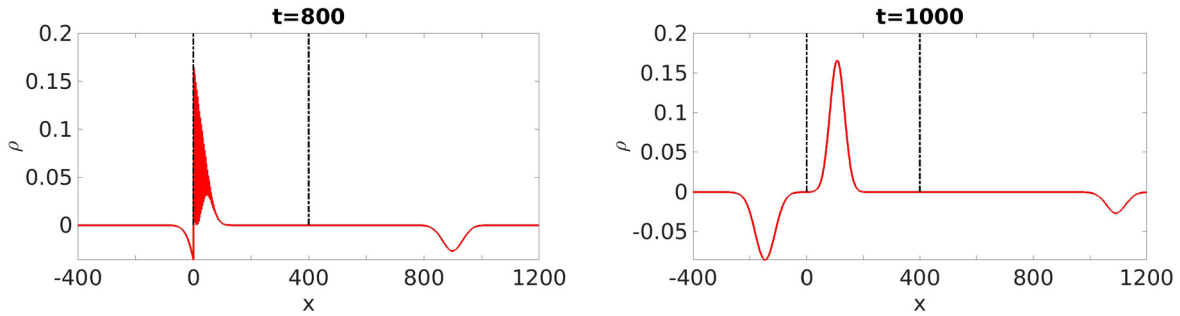
Fig. 5. The charge density for the system shown in Fig. 4 as given by numerical computations from a finite difference scheme (only the results at $t = 800$ and $t = 1000$ are shown).

works for non-supercritical wells. For supercritical wells, a divergent multiple scattering expansion was introduced to obtain the solutions. This expansion accounts for Klein tunneling and for the Klein paradox. In the limit of an infinitely deep well, the amplitudes obtained from the expansion show that Klein tunneling is suppressed. The quantized particle in a box similar to the non-relativistic one is then recovered, although contrary to the non-relativistic case, this happens by oscillating Klein tunneling solutions becoming negligible (rather than through exponentially decaying wave functions becoming negligible outside the well). We have also seen how these amplitudes can be used to build time-dependent wave packets.

The methods employed here to study the square well for a relativistic spin-0 particle can be understood readily from the knowledge of non-relativistic quantum mechanics. These methods have allowed us to introduce in a simple way specific relativistic trait, such as charge creation (that in the Klein–Gordon case already appears at the first quantized level) or Klein tunneling and the Klein paradox. In particular, the wave packet dynamics give an intuitive understanding of these phenomena that are not very well tackled in a stationary approach.

The framework employed in this paper—that of relativistic quantum mechanics (RQM)—lies halfway between standard quantum mechanics and the relativistic quantum field
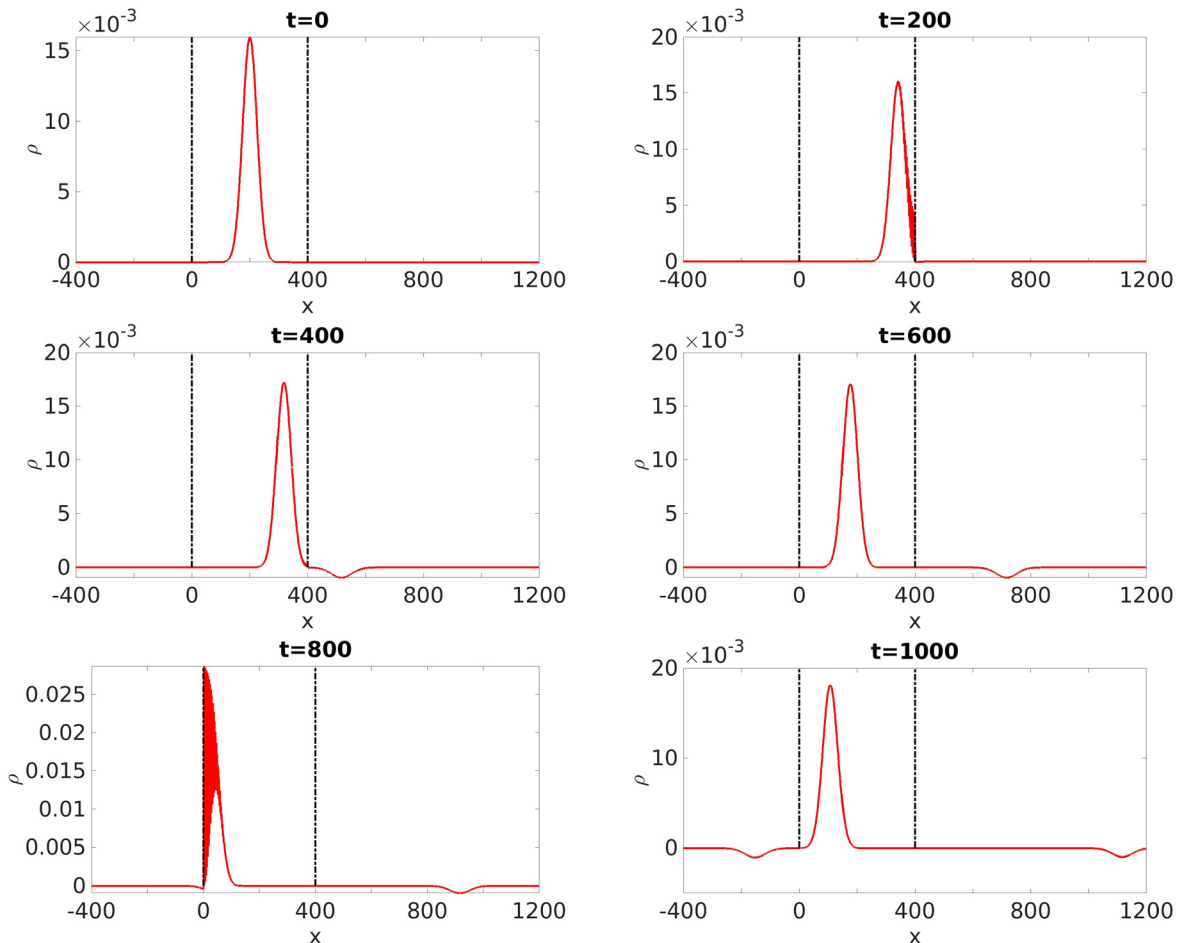

Fig. 6. Same as Fig. 4 but for a well of depth $V_0 = 50 \, mc^2$. Klein tunneling is suppressed relative to Fig. 4.

theory (QFT). Indeed, RQM describes formally a single particle wave function with a spacetime varying charge, while the physically correct account afforded by QFT involves creation and annihilation of particles and their respective antiparticles. The correspondence between the RQM and QFT descriptions for a boson in the presence of a background supercritical potential has been worked out in detail[20] for the case of the step potential discussed in Sec. III A. According to QFT, the potential spontaneously produces particle/antiparticle pairs, a feature that is absent from the RQM description. For a Klein–Gordon particle, the RQM wave function correctly represents the incoming boson as well as the QFT enhancement to the pair production process; the enhancement results from the interaction between the incoming boson and the supercritical potential (this is the charge increase visible in Fig. 4). This correspondence can be established in a time-independent approach,[14,21] or more conclusively by employing space-time resolved QFT calculations.[15] From an experimental viewpoint, direct pair production from a supercritical background field has remained elusive up until now, though the current development of strong laser facilities could lead to an experimental observation (for the fermionic electron–positron pair production) in a foreseeable future.[22] The bosonic supercritical well and the conditions under which quantized energy levels could be observed are not at present experimentally on the table.

Note finally that the disappearance of Klein tunneling in the infinite well limit should be of interest to recent works that have studied the Klein–Gordon equation in a box with moving walls[23–25] (the special boundary conditions chosen in these works were, indeed, not justified). The method employed here for spin-0 particles obeying the Klein–Gordon equation is also suited to treat a spin-1/2 particle in a square well obeying the Dirac equation. The scattering amplitudes in the Dirac case will, however, be different, and the results obtained here for spin-0 particles regarding the suppression of Klein tunneling in infinite wells will not hold.

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[1] N. Dombey and A. Calogeracos, Phys. Rep. **315**, 41–58 (1999).

[2] A. Wachter, *Relativistic Quantum Mechanics* (Springer, Dordrecht, 2011), Sec. 1.3.4.

[3] P. Strange, *Relativistic Quantum Mechancis* (Cambridge U. P., Cambridge, 1998).

[4] W. Greiner, *Relativistic Quantum Mechanics*, 3rd ed. (Springer, Berlin, 2000).

[5] P. Alberto, C. Fiolhais, and V. M. S. Gil, Eur. J. Phys. **17**, 19–24 (1996).

[6] V. Alonso, S. De Vincenzo, and L. Mondino, Eur. J. Phys. **18**, 315–320 (1997).

[7] P. Alberto, S. Das, and E. C. Vagenas, Eur. J. Phys. **39**, 025401 (2018).

[8] M. Alkhateeb, X. Gutierrez de la Cal, M. Pons, D. Sokolovski, and A. Matzkin, Phys. Rev. A **103**, 042203 (2021).

[9] H. Nitta, T. Kudo, and H. Minowa, Am. J. Phys. **67**, 966–971 (1999).

[10] A. O. Barut, *Electrodynamics and Classical Theory of Fields and Particles* (Dover, New York, 1980), Sec. 3 of Chap. II.

[11] J. P. Costella, B. H. J. McKellar, and A. A. Rawlinson, Am. J. Phys. **65**, 835–841 (1997).

[12] F. M. S. Lima, Am. J. Phys. **88**, 1019–1022 (2020).

[13] J. E. Beam, Am. J. Phys. **38**, 1395–1401 (1970).

[14] C. A. Manogue, Ann. Phys. **181**, 261–283 (1988).

[15] T. Cheng, M. R. Ware, Q. Su, and R. Grobe, Phys. Rev. A **80**, 062105 (2009).

[16] M. Barbier, F. M. Peeters, P. Vasilopoulos, and JMilton Pereira, Jr., Phys. Rev. B **77**, 115446 (2008).

[17] X. Gutierrez de la Cal, M. Alkhateeb, M. Pons, A. Matzkin, and D. Sokolovski, Sci. Rep. **10**, 19225 (2020).

[18] D. Xu, T. Wang, and X. Xue, Found. Phys. **43**, 1257–1274 (2013).

[19] R. W. Robinett, Am. J. Phys **68**, 410–420 (2000).

[20] S. P. Gavrilov and D. M. Gitman, Phys. Rev. D **93**, 045002 (2016).

[21] B. R. Holstein, Am. J. Phys. **66**, 507–512 (1998).

[22] H. Hu, Contemp. Phys. **61**, 12–25 (2020).

[23] M. Koehn, Europhys. Lett. **100**, 60008 (2012).

[24] O. Hamidi and H. Dehghan, Rep. Math. Phys. **73**, 11–16 (2014).

[25] S. Colin and A. Matzkin, Europhys. Lett. **130**, 50003 (2020).

[26] We thank an anonymous referee for suggesting this argument.

[27] Strictly speaking, a Gaussian in position space would have negative energy contributions not included in $G(0, x)$ given by Eq. (30). Such contributions are negligible in the non-relativistic regime and become dominant in the ultra-relativistic regime. For more details in the context of barrier scattering, see Ref. 18.